



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 PM UTC

PDB ID : 4X8F / pdb_00004x8f
Title : Vibrio cholerae O395 Ribokinase in apo form
Authors : Paul, R.; Patra, M.D.; Sen, U.
Deposited on : 2014-12-10
Resolution : 3.40 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

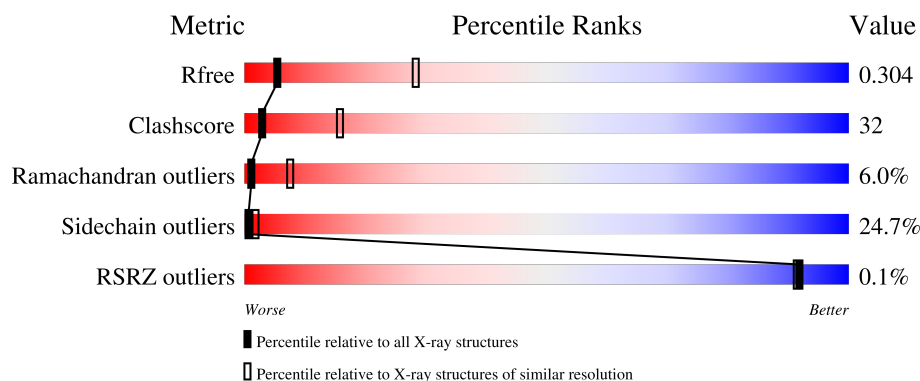
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



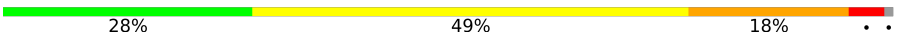
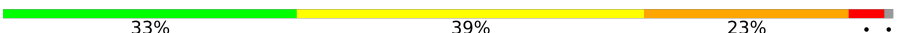
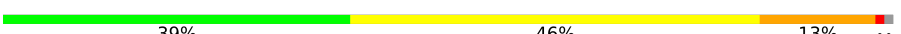
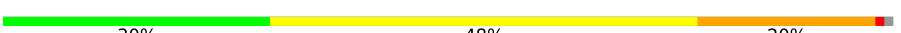
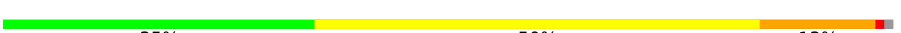
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	309	 33% 49% 16% ..
1	G	309	 28% 49% 18% . .
1	H	309	 33% 39% 23% . .
1	I	309	 39% 45% 14% ..
1	J	309	 39% 46% 13% ..
1	K	309	 30% 48% 20% ..
1	L	309	 35% 50% 13% ..
1	M	309	 43% 42% 13% ..
1	N	309	 38% 45% 16% ..
1	O	309	 37% 43% 19% .
1	P	309	 39% 45% 13% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 36000 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 Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	B	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	C	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	D	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	E	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	F	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	G	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	H	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	I	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	J	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	K	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	L	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	M	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	N	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	O	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			
1	P	306	Total	C	N	O	S	0	0	0
			2250	1408	391	441	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A5F1B7
A	-1	SER	-	expression tag	UNP A5F1B7
A	0	HIS	-	expression tag	UNP A5F1B7
B	-2	GLY	-	expression tag	UNP A5F1B7
B	-1	SER	-	expression tag	UNP A5F1B7
B	0	HIS	-	expression tag	UNP A5F1B7
C	-2	GLY	-	expression tag	UNP A5F1B7
C	-1	SER	-	expression tag	UNP A5F1B7
C	0	HIS	-	expression tag	UNP A5F1B7
D	-2	GLY	-	expression tag	UNP A5F1B7
D	-1	SER	-	expression tag	UNP A5F1B7
D	0	HIS	-	expression tag	UNP A5F1B7
E	-2	GLY	-	expression tag	UNP A5F1B7
E	-1	SER	-	expression tag	UNP A5F1B7
E	0	HIS	-	expression tag	UNP A5F1B7
F	-2	GLY	-	expression tag	UNP A5F1B7
F	-1	SER	-	expression tag	UNP A5F1B7
F	0	HIS	-	expression tag	UNP A5F1B7
G	-2	GLY	-	expression tag	UNP A5F1B7
G	-1	SER	-	expression tag	UNP A5F1B7
G	0	HIS	-	expression tag	UNP A5F1B7
H	-2	GLY	-	expression tag	UNP A5F1B7
H	-1	SER	-	expression tag	UNP A5F1B7
H	0	HIS	-	expression tag	UNP A5F1B7
I	-2	GLY	-	expression tag	UNP A5F1B7
I	-1	SER	-	expression tag	UNP A5F1B7
I	0	HIS	-	expression tag	UNP A5F1B7
J	-2	GLY	-	expression tag	UNP A5F1B7
J	-1	SER	-	expression tag	UNP A5F1B7
J	0	HIS	-	expression tag	UNP A5F1B7
K	-2	GLY	-	expression tag	UNP A5F1B7
K	-1	SER	-	expression tag	UNP A5F1B7
K	0	HIS	-	expression tag	UNP A5F1B7
L	-2	GLY	-	expression tag	UNP A5F1B7
L	-1	SER	-	expression tag	UNP A5F1B7
L	0	HIS	-	expression tag	UNP A5F1B7
M	-2	GLY	-	expression tag	UNP A5F1B7
M	-1	SER	-	expression tag	UNP A5F1B7
M	0	HIS	-	expression tag	UNP A5F1B7
N	-2	GLY	-	expression tag	UNP A5F1B7
N	-1	SER	-	expression tag	UNP A5F1B7
N	0	HIS	-	expression tag	UNP A5F1B7

Continued on next page...

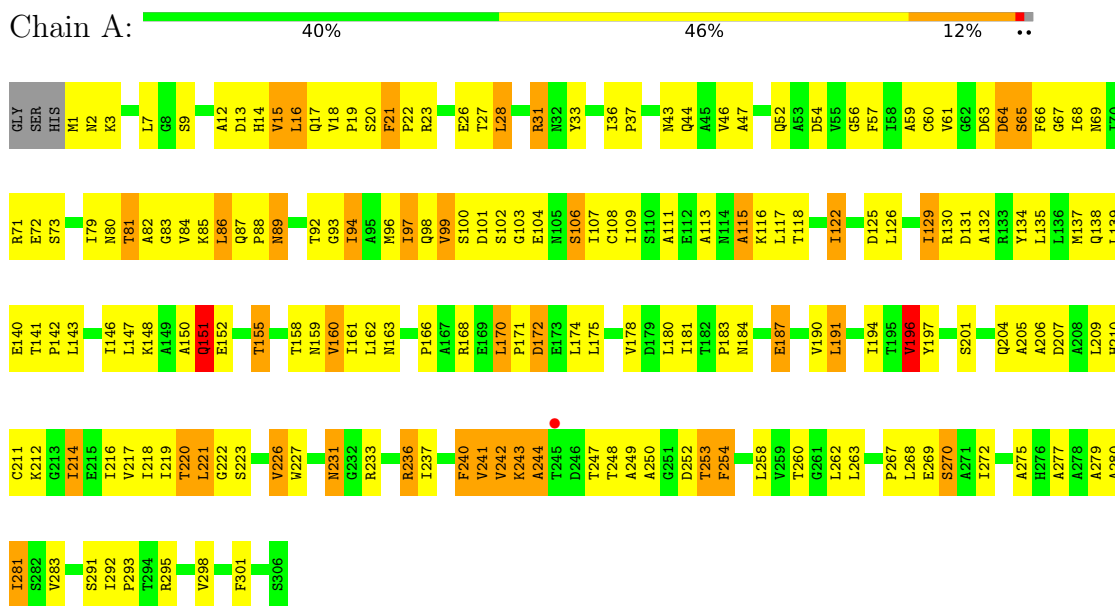
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP A5F1B7
O	-1	SER	-	expression tag	UNP A5F1B7
O	0	HIS	-	expression tag	UNP A5F1B7
P	-2	GLY	-	expression tag	UNP A5F1B7
P	-1	SER	-	expression tag	UNP A5F1B7
P	0	HIS	-	expression tag	UNP A5F1B7

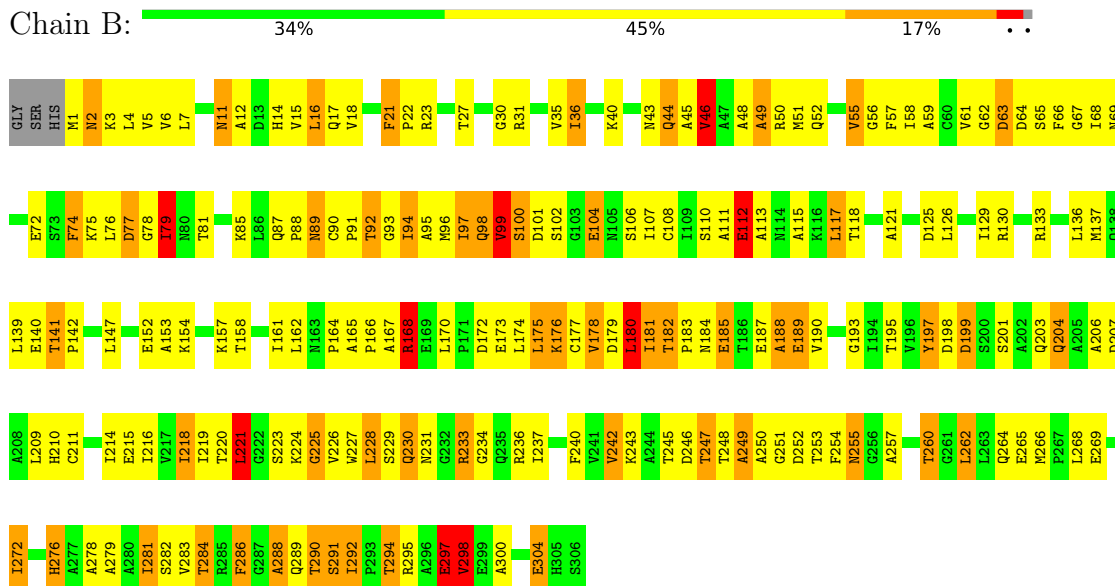
3 Residue-property plots

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.

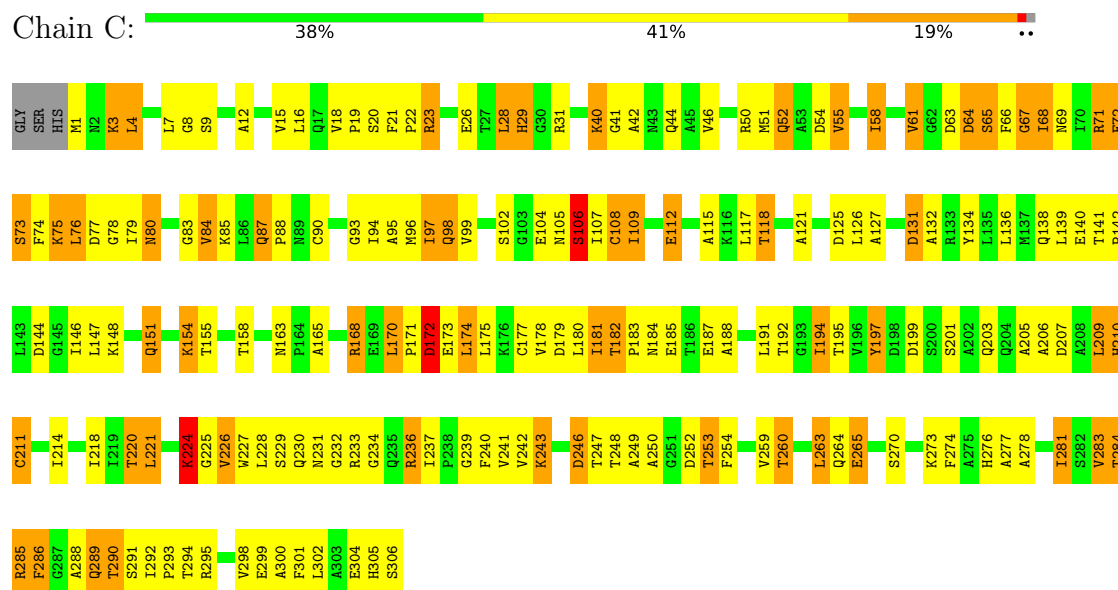
• Molecule 1: Ribokinase



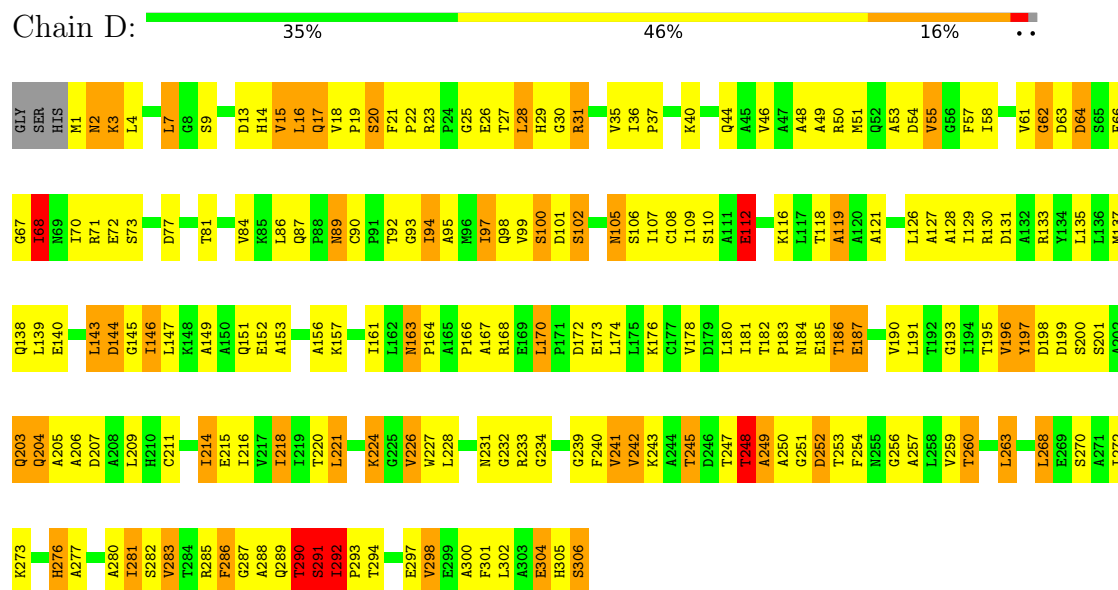
• Molecule 1: Ribokinase



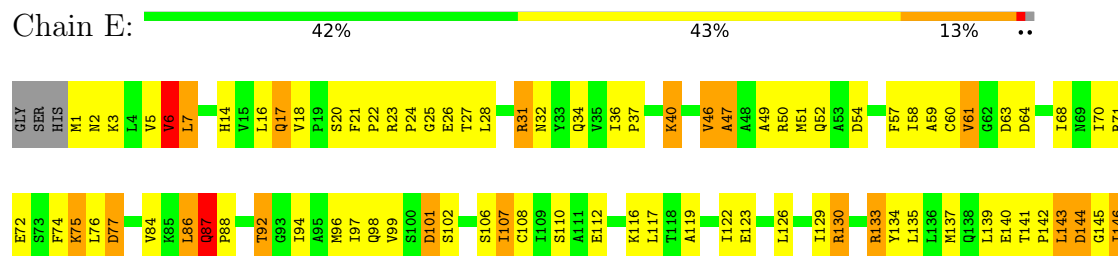
• Molecule 1: Ribokinase

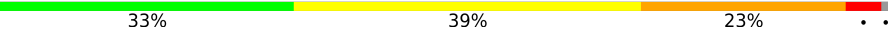


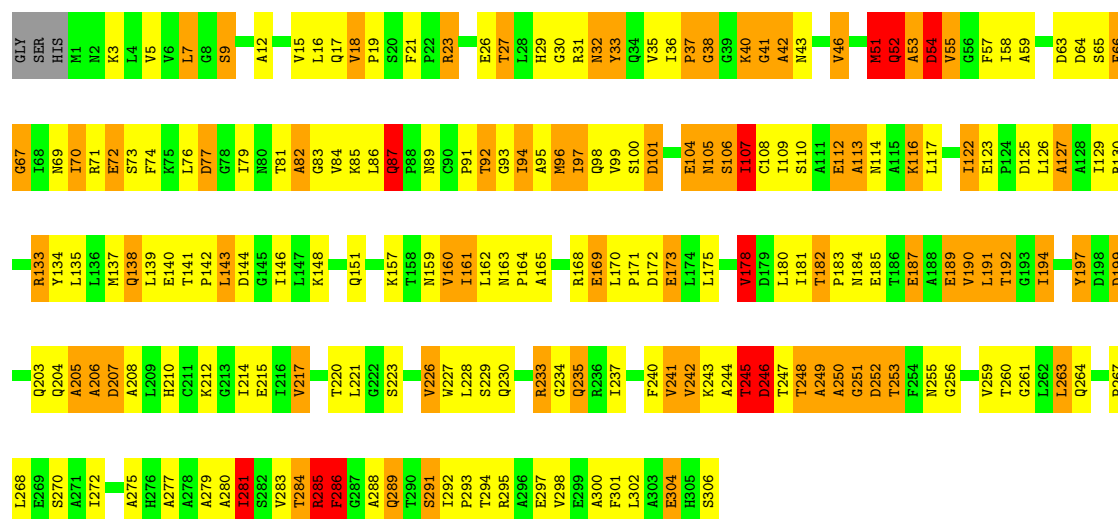
• Molecule 1: Ribokinase



• Molecule 1: Ribokinase

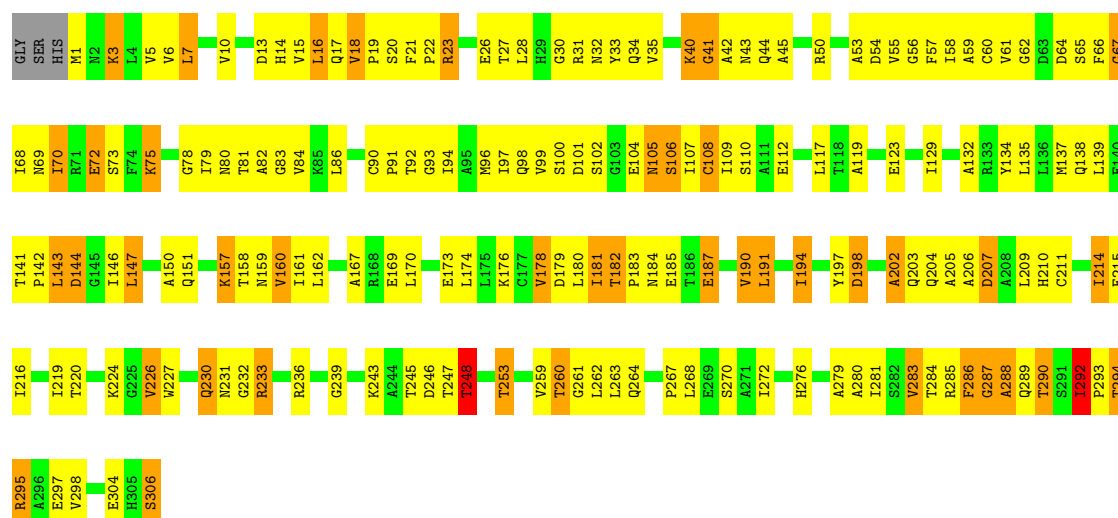


Chain H:  33% 39% 23% ..

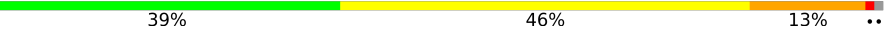


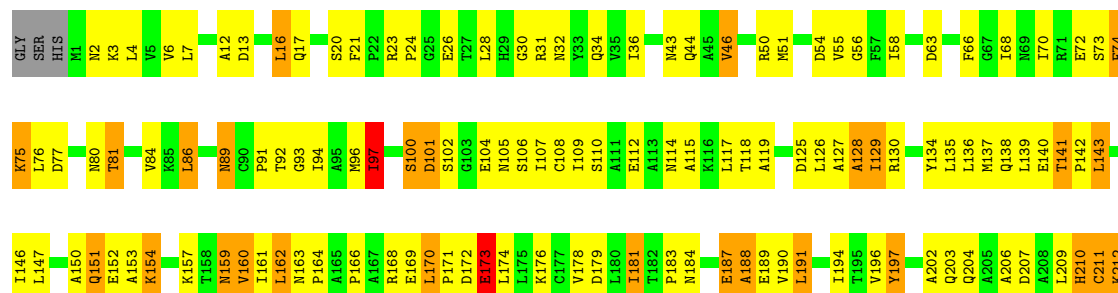
• Molecule 1: Ribokinase

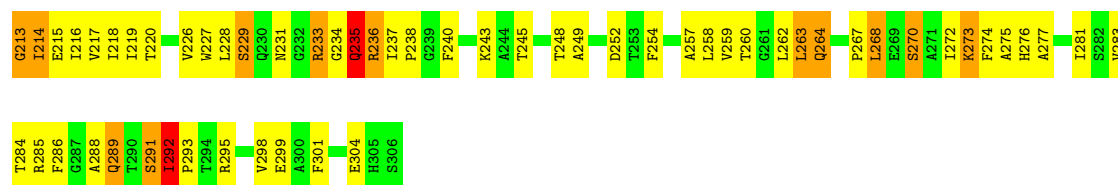
Chain I:  39% 45% 14% ..



• Molecule 1: Ribokinase

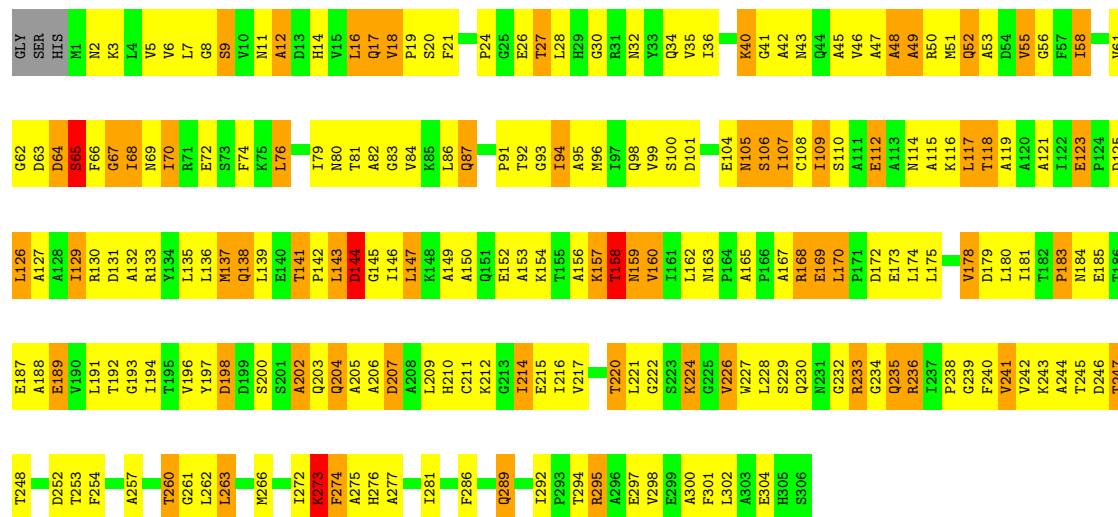
Chain J:  39% 46% 13% ..





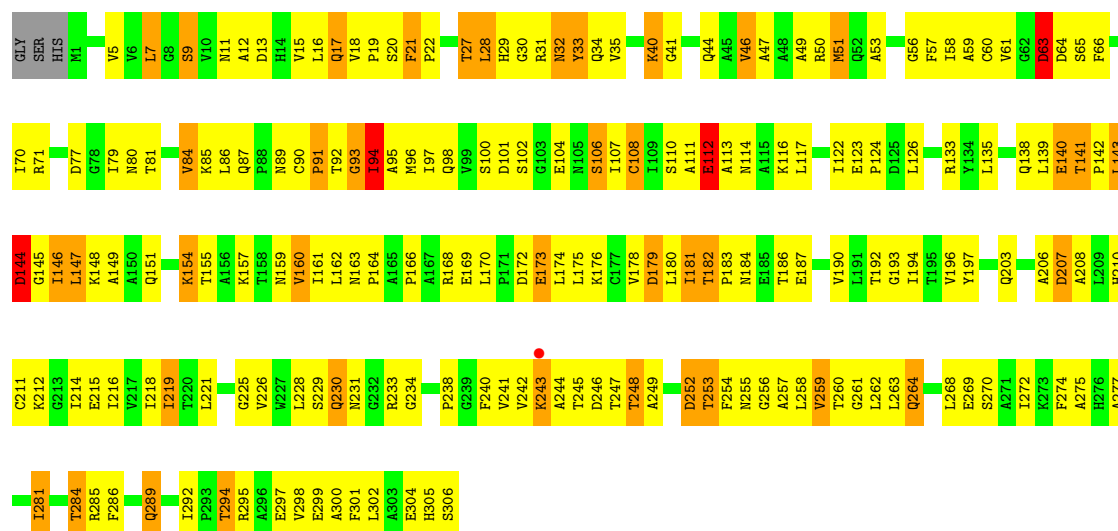
• Molecule 1: Ribokinase

Chain K: 30% 48% 20% ..



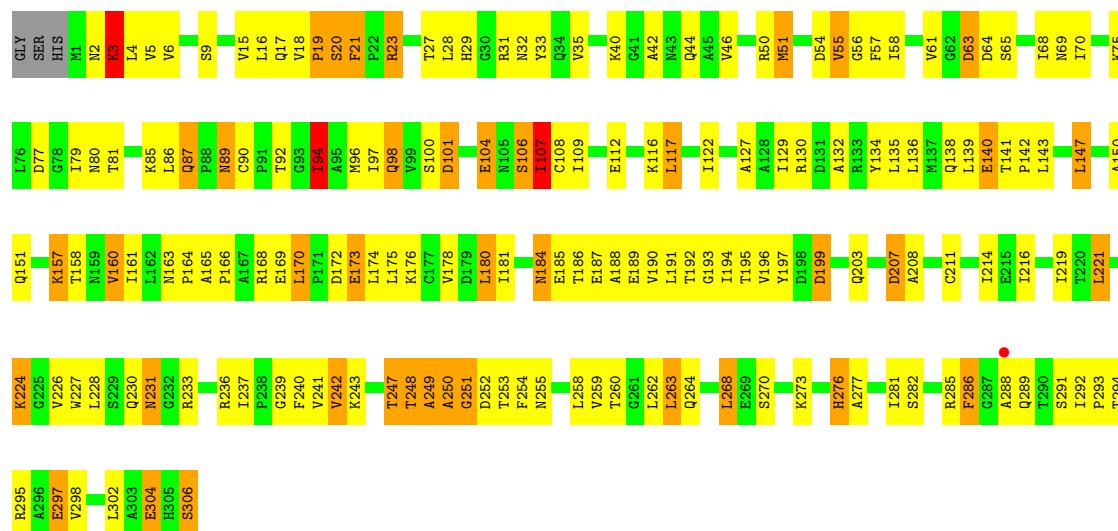
• Molecule 1: Ribokinase

Chain L: 35% 50% 13% ..



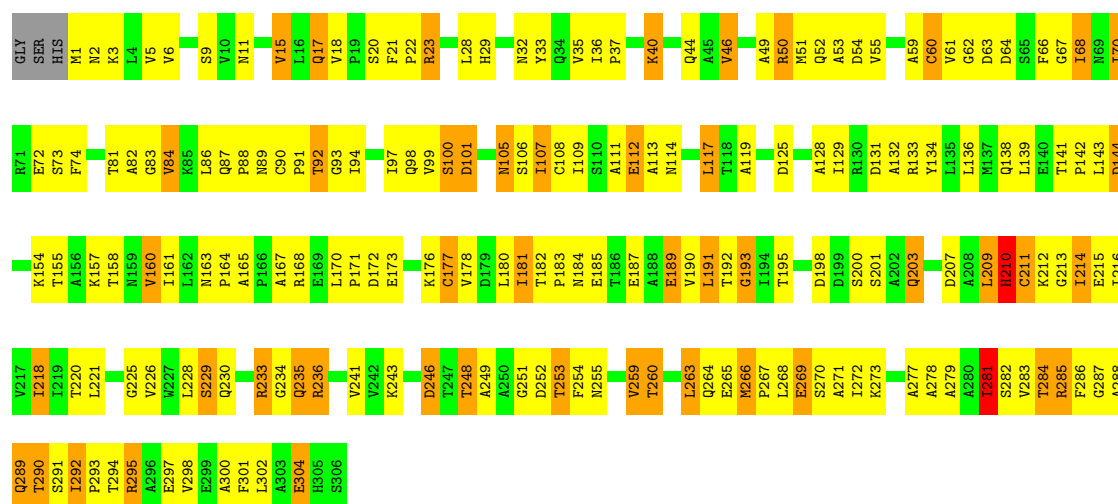
• Molecule 1: Ribokinase

Chain M: 43% 42% 13% ..



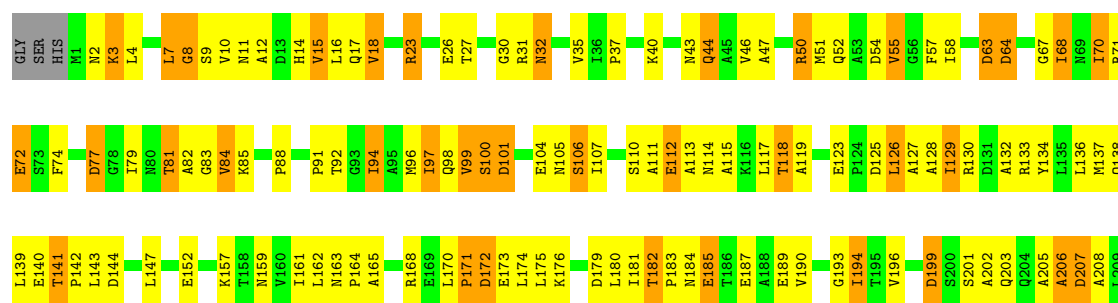
● Molecule 1: Ribokinase

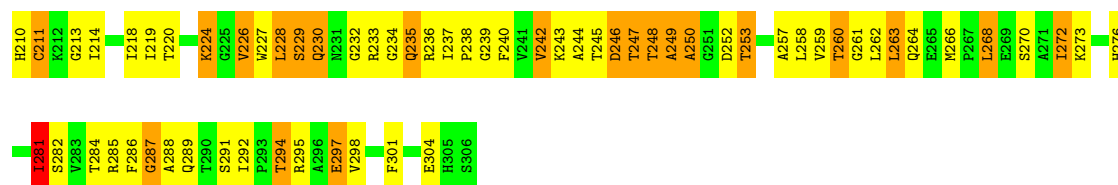
Chain N: 38% 45% 16% ..



● Molecule 1: Ribokinase

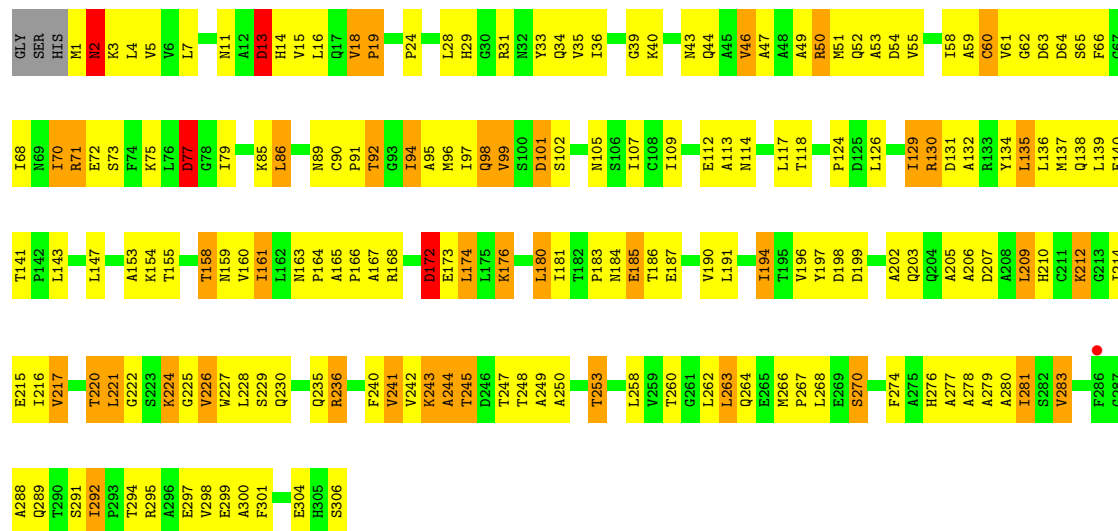
Chain O: 37% 43% 19% .





• Molecule 1: Ribokinase

Chain P: 39% 45% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	129.22Å 130.85Å 145.69Å 110.52° 90.00° 119.59°	Depositor
Resolution (Å)	43.57 – 3.40 43.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (43.57-3.40) 92.9 (43.57-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.239 , 0.308 0.237 , 0.304	Depositor DCC
R_{free} test set	4832 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.277 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	36000	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.67	0/2283	1.17	7/3105 (0.2%)
1	B	0.67	0/2283	1.20	13/3105 (0.4%)
1	C	0.74	0/2283	1.26	17/3105 (0.5%)
1	D	0.79	0/2283	1.34	24/3105 (0.8%)
1	E	0.85	0/2283	1.32	18/3105 (0.6%)
1	F	0.80	1/2283 (0.0%)	1.22	12/3105 (0.4%)
1	G	0.89	2/2283 (0.1%)	1.39	33/3105 (1.1%)
1	H	0.88	0/2283	1.33	19/3105 (0.6%)
1	I	0.79	0/2283	1.24	16/3105 (0.5%)
1	J	0.77	0/2283	1.23	9/3105 (0.3%)
1	K	0.82	1/2283 (0.0%)	1.32	19/3105 (0.6%)
1	L	0.86	0/2283	1.24	14/3105 (0.5%)
1	M	0.80	0/2283	1.24	12/3105 (0.4%)
1	N	0.71	0/2283	1.21	14/3105 (0.5%)
1	O	0.66	0/2283	1.19	15/3105 (0.5%)
1	P	0.62	0/2283	1.20	15/3105 (0.5%)
All	All	0.77	4/36528 (0.0%)	1.26	257/49680 (0.5%)

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	D	0	1
1	G	0	1
1	J	0	1
1	K	0	2
1	N	0	1
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	110	SER	CA-C	-6.12	1.47	1.53
1	G	165	ALA	CA-CB	-5.31	1.46	1.53
1	F	12	ALA	CA-CB	-5.20	1.44	1.53
1	K	91	PRO	CA-C	5.17	1.58	1.53

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	ARG	N-CA-C	-11.44	96.58	110.31
1	G	75	LYS	N-CA-C	-10.91	102.18	114.62
1	D	23	ARG	N-CA-C	-10.31	97.93	110.31
1	F	232	GLY	N-CA-C	-10.14	101.59	114.37
1	G	163	ASN	CA-C-N	-10.08	107.24	119.84
1	G	163	ASN	C-N-CA	-10.08	107.24	119.84
1	C	291	SER	N-CA-C	-9.93	99.48	111.69
1	D	90	CYS	CA-C-N	-9.83	110.23	120.85
1	D	90	CYS	C-N-CA	-9.83	110.23	120.85
1	H	245	THR	N-CA-C	-9.66	94.26	107.88
1	C	174	LEU	N-CA-C	-9.60	99.92	112.68
1	C	23	ARG	CA-C-N	-9.20	108.34	119.84
1	C	23	ARG	C-N-CA	-9.20	108.34	119.84
1	L	208	ALA	N-CA-C	-9.10	101.06	110.97
1	P	77	ASP	N-CA-C	-8.95	101.80	112.89
1	G	290	THR	N-CA-C	-8.69	101.43	114.64
1	K	9	SER	N-CA-C	8.68	122.82	110.23
1	B	99	VAL	N-CA-C	8.68	120.77	108.36
1	K	11	ASN	N-CA-C	8.63	120.59	110.41
1	B	284	THR	N-CA-C	-8.54	102.62	113.72
1	G	259	VAL	N-CA-C	-8.53	105.60	113.71
1	L	252	ASP	N-CA-C	-8.37	100.81	112.45
1	H	55	VAL	N-CA-C	8.25	121.43	108.89
1	B	147	LEU	N-CA-C	8.12	119.91	111.14
1	D	292	ILE	CA-C-N	-8.09	112.39	120.31
1	D	292	ILE	C-N-CA	-8.09	112.39	120.31
1	G	266	MET	CA-C-N	-8.05	111.61	120.14
1	G	266	MET	C-N-CA	-8.05	111.61	120.14
1	E	252	ASP	N-CA-C	-8.04	101.28	112.45
1	A	93	GLY	N-CA-C	-8.01	94.21	113.18
1	N	290	THR	N-CA-C	-7.99	103.74	113.97
1	G	87	GLN	N-CA-C	-7.96	99.78	109.72
1	K	49	ALA	N-CA-C	-7.95	105.56	114.62
1	K	130	ARG	N-CA-C	-7.89	98.13	109.96
1	E	237	ILE	CA-C-N	-7.88	111.89	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	237	ILE	C-N-CA	-7.88	111.89	119.85
1	P	90	CYS	CA-C-N	-7.84	112.75	120.52
1	P	90	CYS	C-N-CA	-7.84	112.75	120.52
1	C	224	LYS	N-CA-C	-7.82	102.07	111.69
1	H	298	VAL	CB-CA-C	-7.71	101.92	112.02
1	C	73	SER	N-CA-C	-7.69	102.90	111.28
1	G	173	GLU	N-CA-C	-7.65	105.12	114.75
1	H	190	VAL	N-CA-C	7.57	120.56	111.09
1	F	3	LYS	N-CA-C	-7.53	103.01	111.14
1	G	218	ILE	N-CA-C	7.47	117.06	106.53
1	M	94	ILE	N-CA-C	7.41	118.82	108.23
1	E	123	GLU	CA-C-N	-7.40	112.17	119.87
1	E	123	GLU	C-N-CA	-7.40	112.17	119.87
1	H	53	ALA	N-CA-C	7.34	119.59	109.54
1	M	193	GLY	N-CA-C	-7.28	105.45	114.92
1	O	224	LYS	N-CA-C	-7.28	103.86	112.89
1	F	71	ARG	N-CA-C	-7.21	104.35	113.72
1	P	283	VAL	N-CA-C	7.19	117.95	110.62
1	M	90	CYS	CA-C-N	-7.15	113.12	120.85
1	M	90	CYS	C-N-CA	-7.15	113.12	120.85
1	G	225	GLY	N-CA-C	7.11	118.60	111.21
1	H	123	GLU	CA-C-N	-7.11	112.48	119.87
1	H	123	GLU	C-N-CA	-7.11	112.48	119.87
1	H	42	ALA	N-CA-C	-7.05	103.53	111.14
1	G	68	ILE	N-CA-C	-6.98	103.39	111.00
1	G	156	ALA	N-CA-C	6.97	119.33	110.61
1	P	172	ASP	N-CA-C	6.93	118.91	111.36
1	P	129	ILE	N-CA-C	6.91	118.49	110.62
1	C	253	THR	N-CA-C	-6.84	103.90	111.36
1	J	23	ARG	N-CA-C	-6.82	101.46	110.40
1	C	61	VAL	N-CA-C	-6.82	100.05	109.46
1	G	76	LEU	N-CA-C	-6.79	104.99	113.20
1	H	277	ALA	N-CA-C	-6.78	103.51	111.03
1	G	259	VAL	CB-CA-C	6.76	116.99	110.63
1	D	27	THR	N-CA-C	6.74	120.87	110.42
1	I	23	ARG	N-CA-C	-6.73	101.58	110.40
1	N	72	GLU	N-CA-C	-6.70	104.93	113.23
1	O	23	ARG	N-CA-C	-6.69	100.36	110.39
1	K	266	MET	N-CA-C	6.69	118.13	109.64
1	K	64	ASP	N-CA-C	-6.64	101.72	110.43
1	L	21	PHE	N-CA-C	-6.64	101.69	109.93
1	G	174	LEU	N-CA-C	-6.61	102.64	111.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	VAL	N-CA-C	6.59	118.08	108.53
1	O	8	GLY	N-CA-C	6.56	121.70	111.08
1	I	83	GLY	N-CA-C	-6.56	104.39	115.34
1	D	196	VAL	N-CA-C	6.52	116.00	106.55
1	N	2	ASN	N-CA-C	6.52	120.15	109.72
1	O	3	LYS	N-CA-C	-6.49	104.28	111.36
1	G	23	ARG	N-CA-C	-6.47	100.62	110.07
1	N	253	THR	N-CA-C	-6.47	104.31	111.36
1	N	23	ARG	N-CA-C	-6.46	102.55	110.31
1	L	193	GLY	N-CA-C	-6.46	106.16	115.27
1	J	211	CYS	N-CA-C	-6.41	104.21	111.07
1	E	77	ASP	N-CA-C	-6.39	104.64	112.88
1	I	123	GLU	CA-C-N	-6.38	113.15	120.04
1	I	123	GLU	C-N-CA	-6.38	113.15	120.04
1	I	283	VAL	N-CA-C	6.36	119.00	111.05
1	N	23	ARG	CA-C-N	-6.36	111.89	119.84
1	N	23	ARG	C-N-CA	-6.36	111.89	119.84
1	D	68	ILE	N-CA-C	-6.26	104.23	110.62
1	J	77	ASP	N-CA-C	-6.22	104.86	112.88
1	I	292	ILE	CA-C-N	6.21	127.56	120.85
1	I	292	ILE	C-N-CA	6.21	127.56	120.85
1	D	249	ALA	CA-C-N	6.20	132.85	121.70
1	D	249	ALA	C-N-CA	6.20	132.85	121.70
1	B	87	GLN	CA-C-N	-6.19	113.30	119.99
1	B	87	GLN	C-N-CA	-6.19	113.30	119.99
1	H	107	ILE	N-CA-C	6.15	116.78	108.17
1	E	36	ILE	CA-C-N	6.13	126.08	119.76
1	E	36	ILE	C-N-CA	6.13	126.08	119.76
1	O	81	THR	N-CA-C	6.13	117.65	110.97
1	N	218	ILE	N-CA-C	6.11	115.14	106.53
1	F	247	THR	N-CA-C	6.10	117.59	111.07
1	M	23	ARG	N-CA-C	-6.08	101.15	108.14
1	I	159	ASN	N-CA-C	6.04	118.57	110.35
1	A	129	ILE	N-CA-C	6.04	116.78	110.62
1	O	129	ILE	N-CA-C	-6.04	105.18	111.58
1	A	79	ILE	N-CA-C	6.04	117.42	109.21
1	M	237	ILE	CA-C-N	-6.03	114.06	120.03
1	M	237	ILE	C-N-CA	-6.03	114.06	120.03
1	F	21	PHE	N-CA-C	-5.98	102.52	109.93
1	O	182	THR	CA-C-N	-5.97	114.48	120.21
1	O	182	THR	C-N-CA	-5.97	114.48	120.21
1	C	250	ALA	N-CA-C	-5.97	105.83	112.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	193	GLY	N-CA-C	-5.97	106.41	115.00
1	O	270	SER	N-CA-C	-5.96	104.36	111.69
1	G	141	THR	CA-C-N	-5.95	113.63	119.76
1	G	141	THR	C-N-CA	-5.95	113.63	119.76
1	K	260	THR	N-CA-C	-5.95	104.92	111.82
1	D	218	ILE	N-CA-C	5.95	114.91	106.53
1	K	205	ALA	N-CA-C	-5.93	104.72	111.07
1	K	198	ASP	N-CA-C	5.92	116.10	108.34
1	M	23	ARG	CA-C-N	-5.91	112.45	119.84
1	M	23	ARG	C-N-CA	-5.91	112.45	119.84
1	G	281	ILE	CB-CA-C	-5.91	104.32	112.24
1	F	252	ASP	N-CA-C	-5.89	105.18	112.90
1	P	224	LYS	N-CA-C	5.89	118.02	109.71
1	A	146	ILE	CB-CA-C	-5.88	104.45	111.97
1	G	133	ARG	N-CA-C	-5.86	104.48	111.69
1	E	229	SER	N-CA-C	5.86	116.98	107.32
1	I	90	CYS	N-CA-C	-5.85	99.25	109.48
1	E	178	VAL	N-CA-C	5.83	117.40	108.71
1	D	187	GLU	N-CA-C	-5.83	105.06	111.82
1	E	6	VAL	N-CA-C	5.82	116.97	108.53
1	L	112	GLU	N-CA-C	5.82	123.19	110.80
1	G	51	MET	N-CA-C	-5.80	104.83	112.72
1	H	51	MET	N-CA-C	-5.80	106.82	112.97
1	N	281	ILE	N-CA-C	-5.79	107.48	113.10
1	I	202	ALA	N-CA-C	-5.79	105.11	111.82
1	B	176	LYS	N-CA-C	-5.79	105.05	111.36
1	C	151	GLN	N-CA-C	5.78	117.58	111.28
1	L	63	ASP	N-CA-C	-5.76	106.23	113.20
1	J	218	ILE	N-CA-C	5.74	114.63	106.53
1	K	196	VAL	N-CA-C	5.73	116.67	107.73
1	D	170	LEU	CA-C-N	-5.73	113.29	120.51
1	D	170	LEU	C-N-CA	-5.73	113.29	120.51
1	L	31	ARG	N-CA-C	5.73	116.64	108.74
1	I	253	THR	N-CA-C	-5.72	105.12	111.36
1	L	159	ASN	N-CA-C	5.71	118.52	110.23
1	P	292	ILE	CA-C-N	5.70	127.00	120.85
1	P	292	ILE	C-N-CA	5.70	127.00	120.85
1	K	65	SER	N-CA-C	-5.68	105.18	111.71
1	E	75	LYS	N-CA-C	5.67	117.14	111.07
1	C	52	GLN	N-CA-C	5.65	118.99	111.30
1	J	258	LEU	N-CA-C	5.65	118.98	111.75
1	E	146	ILE	N-CA-C	-5.64	104.36	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	199	ASP	N-CA-C	5.64	118.19	111.71
1	H	252	ASP	N-CA-C	-5.63	104.63	112.45
1	E	290	THR	N-CA-C	-5.60	106.58	113.41
1	E	87	GLN	N-CA-C	-5.60	102.73	109.72
1	F	246	ASP	N-CA-C	-5.59	103.52	111.24
1	D	105	ASN	N-CA-C	5.59	118.35	110.14
1	J	26	GLU	N-CA-C	5.58	118.09	110.55
1	D	131	ASP	N-CA-C	-5.57	105.79	112.59
1	F	55	VAL	N-CA-C	5.54	115.56	107.37
1	K	286	PHE	N-CA-C	5.54	118.05	110.24
1	B	225	GLY	N-CA-C	5.53	119.62	110.55
1	O	246	ASP	N-CA-C	5.53	122.57	110.80
1	M	151	GLN	N-CA-C	-5.52	106.59	113.55
1	A	72	GLU	N-CA-C	-5.51	105.68	112.90
1	P	245	THR	N-CA-C	-5.51	106.33	113.16
1	I	284	THR	N-CA-C	-5.49	106.54	113.18
1	C	68	ILE	CB-CA-C	-5.49	104.86	112.04
1	M	107	ILE	N-CA-C	5.47	115.76	108.27
1	L	289	GLN	N-CA-C	-5.47	105.97	113.30
1	C	260	THR	N-CA-C	-5.46	105.48	111.82
1	L	94	ILE	N-CA-C	5.46	116.56	108.65
1	E	159	ASN	N-CA-C	5.45	117.77	110.35
1	E	207	ASP	N-CA-C	5.45	117.65	111.11
1	D	163	ASN	CA-C-N	-5.44	113.04	119.84
1	D	163	ASN	C-N-CA	-5.44	113.04	119.84
1	B	234	GLY	N-CA-C	-5.44	105.32	112.82
1	G	105	ASN	N-CA-C	5.44	118.13	110.14
1	C	72	GLU	N-CA-C	-5.43	107.31	114.31
1	B	161	ILE	N-CA-C	5.43	116.40	108.53
1	C	58	ILE	CB-CA-C	-5.41	103.96	110.99
1	H	199	ASP	N-CA-C	5.41	118.09	111.82
1	O	126	LEU	N-CA-C	5.41	117.60	111.11
1	N	74	PHE	N-CA-C	-5.40	104.26	112.04
1	K	123	GLU	CA-C-N	-5.40	114.21	120.04
1	K	123	GLU	C-N-CA	-5.40	114.21	120.04
1	G	36	ILE	CB-CA-C	-5.40	104.97	111.18
1	P	225	GLY	N-CA-C	5.39	120.75	111.47
1	I	219	ILE	CB-CA-C	-5.38	106.10	111.80
1	G	171	PRO	N-CA-C	5.37	122.27	111.69
1	H	217	VAL	CB-CA-C	-5.37	104.34	110.73
1	E	47	ALA	N-CA-C	-5.37	105.12	110.97
1	I	295	ARG	N-CA-C	-5.37	105.33	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	146	ILE	CB-CA-C	-5.36	105.11	111.81
1	G	143	LEU	CA-CB-CG	5.36	135.05	116.30
1	L	207	ASP	N-CA-C	5.35	119.06	112.54
1	N	260	THR	N-CA-C	-5.35	105.56	111.71
1	F	83	GLY	N-CA-C	-5.34	106.42	115.34
1	F	79	ILE	N-CA-C	5.33	115.93	108.89
1	D	193	GLY	N-CA-C	-5.33	107.76	115.27
1	B	221	LEU	N-CA-C	-5.33	106.01	112.88
1	K	159	ASN	N-CA-C	5.30	122.10	110.80
1	D	287	GLY	N-CA-C	-5.28	100.67	113.18
1	G	6	VAL	N-CA-C	5.27	116.17	108.53
1	D	93	GLY	N-CA-C	-5.27	106.54	112.33
1	P	2	ASN	N-CA-C	5.27	122.02	110.80
1	O	287	GLY	N-CA-C	5.27	117.86	110.38
1	N	141	THR	CA-C-N	-5.26	114.36	119.78
1	N	141	THR	C-N-CA	-5.26	114.36	119.78
1	G	201	SER	N-CA-C	-5.24	106.15	112.54
1	K	252	ASP	N-CA-C	-5.22	105.19	112.45
1	H	87	GLN	N-CA-C	-5.21	101.99	109.24
1	A	151	GLN	N-CA-C	5.21	116.64	111.07
1	G	82	ALA	N-CA-C	-5.20	106.26	113.18
1	P	160	VAL	CB-CA-C	-5.19	104.24	110.99
1	F	133	ARG	N-CA-C	-5.18	105.70	112.23
1	F	148	LYS	N-CA-C	-5.18	105.72	111.36
1	K	179	ASP	N-CA-C	-5.17	107.14	113.50
1	L	219	ILE	CB-CA-C	-5.17	106.32	111.80
1	I	198	ASP	N-CA-C	5.17	114.96	108.45
1	I	182	THR	N-CA-C	5.16	118.73	110.73
1	G	111	ALA	N-CA-C	-5.16	104.78	111.74
1	B	79	ILE	N-CA-C	5.15	120.06	109.34
1	L	9	SER	N-CA-C	5.15	117.14	108.96
1	H	27	THR	N-CA-C	-5.14	102.46	110.42
1	D	205	ALA	N-CA-C	-5.13	104.95	111.11
1	M	247	THR	N-CA-C	5.12	121.70	110.80
1	J	213	GLY	N-CA-C	5.11	125.30	113.18
1	J	229	SER	N-CA-C	5.11	115.75	107.32
1	G	256	GLY	N-CA-C	-5.10	106.61	112.73
1	P	159	ASN	N-CA-C	5.09	117.28	110.35
1	K	27	THR	N-CA-C	-5.09	101.98	110.17
1	H	72	GLU	N-CA-C	-5.08	106.86	113.16
1	D	268	LEU	N-CA-C	5.07	117.21	111.02
1	G	218	ILE	CB-CA-C	-5.06	105.72	111.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLN	N-CA-C	5.04	116.85	111.36
1	O	23	ARG	CA-C-N	-5.03	113.55	119.84
1	O	23	ARG	C-N-CA	-5.03	113.55	119.84
1	J	97	ILE	N-CA-C	5.03	114.81	107.37
1	D	62	GLY	N-CA-C	-5.03	103.92	112.51
1	G	146	ILE	CB-CA-C	-5.03	105.27	111.70
1	H	178	VAL	CB-CA-C	-5.02	104.20	111.68
1	N	133	ARG	N-CA-C	-5.02	105.47	112.45
1	K	55	VAL	N-CA-C	5.02	116.52	108.89
1	B	46	VAL	N-CA-C	-5.01	104.72	111.44
1	B	249	ALA	N-CA-C	-5.00	105.74	111.14
1	H	207	ASP	CB-CA-C	-5.00	100.47	110.42

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	290	THR	Peptide
1	G	100	SER	Peptide
1	J	100	SER	Peptide
1	K	156	ALA	Peptide
1	K	157	LYS	Peptide
1	N	100	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2250	0	2273	151	0
1	B	2250	0	2273	189	0
1	C	2250	0	2273	130	0
1	D	2250	0	2273	168	0
1	E	2250	0	2273	140	0
1	F	2250	0	2273	150	0
1	G	2250	0	2273	169	0
1	H	2250	0	2273	208	0
1	I	2250	0	2273	127	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2250	0	2273	129	0
1	K	2250	0	2273	174	0
1	L	2250	0	2273	169	0
1	M	2250	0	2273	125	0
1	N	2250	0	2273	136	0
1	O	2250	0	2273	143	0
1	P	2250	0	2273	139	0
All	All	36000	0	36368	2335	0

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 32.

All (2335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ARG:NH2	1:H:101:ASP:OD1	1.89	1.06
1:K:94:ILE:HD12	1:K:95:ALA:H	1.18	1.04
1:L:51:MET:HB2	1:L:260:THR:HG21	1.43	1.00
1:H:243:LYS:HG3	1:K:101:ASP:HA	1.42	1.00
1:E:87:GLN:HG2	1:E:116:LYS:HG3	1.45	0.99
1:D:250:ALA:H	1:D:252:ASP:HB2	1.23	0.98
1:A:21:PHE:HD2	1:A:22:PRO:HD2	1.28	0.98
1:H:204:GLN:HE22	1:O:234:GLY:H	1.11	0.97
1:E:94:ILE:HG22	1:E:110:SER:H	1.29	0.97
1:G:209:LEU:HB3	1:G:214:ILE:HD11	1.46	0.97
1:M:224:LYS:HB2	1:M:236:ARG:HH12	1.28	0.96
1:H:285:ARG:NH2	1:H:297:GLU:OE2	1.99	0.95
1:E:130:ARG:NH1	1:E:152:GLU:OE1	2.00	0.94
1:E:50:ARG:HD2	1:E:292:ILE:HG22	1.50	0.94
1:H:264:GLN:OE1	1:H:295:ARG:NH1	2.03	0.92
1:B:181:ILE:HG23	1:B:183:PRO:HD3	1.52	0.91
1:G:181:ILE:HG23	1:G:183:PRO:HD3	1.53	0.90
1:N:212:LYS:O	1:N:214:ILE:N	2.04	0.90
1:C:3:LYS:HB2	1:C:54:ASP:HB3	1.52	0.90
1:G:285:ARG:HG2	1:G:291:SER:HA	1.51	0.90
1:P:14:HIS:ND1	1:P:33:TYR:OH	2.00	0.90
1:O:224:LYS:O	1:O:236:ARG:NH1	2.05	0.89
1:F:181:ILE:HG23	1:F:183:PRO:HD3	1.52	0.89
1:G:207:ASP:OD1	1:G:207:ASP:N	1.99	0.89
1:L:181:ILE:HG23	1:L:183:PRO:HD3	1.51	0.88
1:J:31:ARG:HH21	1:J:101:ASP:HB3	1.38	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:ILE:HG22	1:H:107:ILE:HA	1.52	0.87
1:H:51:MET:HB2	1:H:260:THR:HG21	1.57	0.87
1:B:154:LYS:NZ	1:B:177:CYS:O	2.08	0.86
1:G:251:GLY:O	1:G:255:ASN:ND2	2.08	0.86
1:L:97:ILE:HG12	1:L:107:ILE:HG23	1.56	0.86
1:O:285:ARG:HB2	1:O:291:SER:HB2	1.59	0.85
1:K:126:LEU:HA	1:K:129:ILE:HG13	1.60	0.84
1:C:209:LEU:O	1:C:211:CYS:N	2.09	0.84
1:M:249:ALA:O	1:M:251:GLY:N	2.11	0.84
1:A:138:GLN:HG3	1:A:163:ASN:HB3	1.58	0.83
1:E:60:CYS:SG	1:E:87:GLN:NE2	2.51	0.83
1:G:163:ASN:ND2	1:G:255:ASN:OD1	2.11	0.83
1:C:125:ASP:O	1:C:127:ALA:N	2.11	0.83
1:B:230:GLN:HG3	1:B:233:ARG:HG3	1.61	0.83
1:F:143:LEU:HG	1:F:168:ARG:HH12	1.41	0.83
1:J:128:ALA:O	1:J:130:ARG:N	2.11	0.82
1:D:3:LYS:HG2	1:D:54:ASP:HB2	1.60	0.82
1:K:12:ALA:O	1:K:94:ILE:HD13	1.77	0.82
1:D:126:LEU:O	1:D:128:ALA:N	2.13	0.82
1:K:52:GLN:HG3	1:K:295:ARG:HG3	1.61	0.82
1:C:74:PHE:HA	1:C:79:ILE:HD12	1.62	0.82
1:F:81:THR:O	1:F:83:GLY:N	2.12	0.81
1:L:207:ASP:OD1	1:M:233:ARG:N	2.13	0.81
1:H:38:GLY:HA2	1:H:289:GLN:HG3	1.62	0.81
1:L:143:LEU:O	1:L:146:ILE:N	2.14	0.81
1:E:285:ARG:HG3	1:E:291:SER:HA	1.61	0.81
1:O:81:THR:O	1:O:83:GLY:N	2.13	0.81
1:E:143:LEU:O	1:E:145:GLY:N	2.14	0.81
1:P:19:PRO:HD2	1:P:28:LEU:HD11	1.61	0.81
1:C:243:LYS:HD2	1:C:284:THR:HA	1.62	0.81
1:D:249:ALA:HB3	1:D:250:ALA:HB3	1.63	0.81
1:L:143:LEU:O	1:L:145:GLY:N	2.14	0.80
1:C:154:LYS:HD2	1:C:177:CYS:SG	2.20	0.80
1:D:143:LEU:O	1:D:145:GLY:N	2.14	0.80
1:E:116:LYS:NZ	1:I:304:GLU:OE2	2.14	0.80
1:I:15:VAL:HG22	1:I:97:ILE:HB	1.62	0.80
1:K:95:ALA:HB2	1:K:109:ILE:HG23	1.61	0.80
1:K:143:LEU:HD12	1:K:168:ARG:HH21	1.46	0.80
1:G:286:PHE:O	1:G:290:THR:OG1	1.99	0.80
1:D:13:ASP:HA	1:D:95:ALA:HB3	1.62	0.80
1:L:53:ALA:HB2	1:L:260:THR:HG23	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:PHE:HD1	1:H:301:PHE:HE2	1.29	0.79
1:K:273:LYS:O	1:K:276:HIS:N	2.15	0.79
1:I:43:ASN:OD1	1:I:289:GLN:NE2	2.16	0.79
1:K:96:MET:HE3	1:L:96:MET:HE3	1.63	0.79
1:N:281:ILE:O	1:N:284:THR:OG1	2.00	0.79
1:E:168:ARG:NH1	1:I:306:SER:O	2.16	0.78
1:O:110:SER:OG	1:O:112:GLU:OE2	2.01	0.78
1:O:8:GLY:HA2	1:O:141:THR:HG21	1.65	0.78
1:O:15:VAL:HG13	1:O:97:ILE:HB	1.65	0.78
1:A:21:PHE:CD2	1:A:22:PRO:HD2	2.18	0.78
1:B:140:GLU:HG3	1:B:166:PRO:HD3	1.64	0.78
1:D:87:GLN:HG2	1:D:116:LYS:HG3	1.65	0.78
1:K:167:ALA:HB2	1:K:187:GLU:HG2	1.65	0.78
1:A:2:ASN:ND2	1:A:54:ASP:OD1	2.17	0.78
1:D:22:PRO:HD3	1:D:28:LEU:HD21	1.66	0.78
1:L:240:PHE:HD1	1:L:301:PHE:HE2	1.33	0.77
1:H:294:THR:N	1:H:297:GLU:OE1	2.17	0.77
1:K:94:ILE:HD12	1:K:95:ALA:N	1.98	0.77
1:N:62:GLY:H	1:N:92:THR:HG23	1.49	0.77
1:H:306:SER:OG	1:L:143:LEU:N	2.17	0.77
1:L:248:THR:OG1	1:L:249:ALA:N	2.14	0.77
1:O:4:LEU:HB2	1:O:263:LEU:HD11	1.67	0.77
1:G:267:PRO:HD2	1:G:270:SER:HB2	1.66	0.77
1:K:198:ASP:OD1	1:K:200:SER:OG	2.03	0.77
1:A:249:ALA:O	1:A:253:THR:OG1	2.04	0.76
1:D:256:GLY:O	1:D:260:THR:OG1	2.02	0.76
1:L:97:ILE:HG23	1:L:107:ILE:HG12	1.67	0.76
1:P:14:HIS:HD1	1:P:33:TYR:HH	0.76	0.76
1:N:51:MET:HB2	1:N:260:THR:HG21	1.66	0.76
1:D:7:LEU:HD13	1:D:58:ILE:HG22	1.68	0.76
1:K:7:LEU:HB3	1:K:137:MET:HG2	1.67	0.76
1:B:4:LEU:HD23	1:B:55:VAL:HB	1.68	0.76
1:B:100:SER:OG	1:B:104:GLU:O	2.02	0.76
1:E:143:LEU:H	1:I:306:SER:HB2	1.51	0.76
1:P:132:ALA:O	1:P:158:THR:OG1	2.04	0.76
1:B:74:PHE:HB3	1:B:79:ILE:HD11	1.66	0.76
1:H:182:THR:O	1:H:182:THR:OG1	2.00	0.76
1:K:143:LEU:O	1:K:145:GLY:N	2.17	0.76
1:N:228:LEU:HD11	1:N:268:LEU:HD23	1.66	0.76
1:G:21:PHE:CE2	1:G:106:SER:HB3	2.20	0.76
1:C:230:GLN:O	1:C:232:GLY:N	2.19	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:248:THR:O	1:M:250:ALA:N	2.18	0.76
1:B:15:VAL:HG22	1:B:97:ILE:HD11	1.68	0.75
1:F:95:ALA:HB2	1:F:109:ILE:HD12	1.66	0.75
1:A:43:ASN:ND2	1:A:252:ASP:OD1	2.18	0.75
1:B:64:ASP:O	1:B:66:PHE:N	2.19	0.75
1:D:2:ASN:OD1	1:D:2:ASN:N	2.18	0.75
1:D:245:THR:OG1	1:D:283:VAL:O	2.04	0.75
1:I:91:PRO:HG2	1:I:112:GLU:HG3	1.67	0.75
1:G:65:SER:O	1:G:69:ASN:ND2	2.19	0.75
1:I:97:ILE:HG12	1:I:107:ILE:HG23	1.69	0.75
1:B:182:THR:OG1	1:B:255:ASN:OD1	2.04	0.75
1:D:281:ILE:HB	1:D:293:PRO:HG3	1.69	0.75
1:P:60:CYS:HB2	1:P:117:LEU:HD13	1.68	0.75
1:P:51:MET:HE1	1:P:298:VAL:HG21	1.67	0.75
1:P:15:VAL:HG22	1:P:97:ILE:HB	1.68	0.75
1:C:283:VAL:HG23	1:C:284:THR:H	1.52	0.75
1:F:101:ASP:OD1	1:I:243:LYS:NZ	2.18	0.75
1:N:11:ASN:OD1	1:N:114:ASN:ND2	2.20	0.74
1:A:65:SER:O	1:A:69:ASN:ND2	2.16	0.74
1:K:147:LEU:HD22	1:K:174:LEU:HB2	1.68	0.74
1:G:226:VAL:HG12	1:G:227:TRP:H	1.52	0.74
1:J:207:ASP:HB3	1:K:232:GLY:HA3	1.70	0.74
1:K:94:ILE:CD1	1:K:95:ALA:H	2.00	0.74
1:K:203:GLN:HE22	1:K:232:GLY:HA2	1.53	0.74
1:P:36:ILE:HG21	1:P:288:ALA:HB3	1.69	0.74
1:C:44:GLN:NE2	1:C:252:ASP:OD1	2.17	0.74
1:H:122:ILE:HG22	1:H:125:ASP:HB2	1.70	0.73
1:D:239:GLY:HA2	1:D:276:HIS:CD2	2.22	0.73
1:H:15:VAL:HG22	1:H:97:ILE:HD11	1.70	0.73
1:J:81:THR:HG22	1:J:84:VAL:HB	1.70	0.73
1:K:239:GLY:HA2	1:K:276:HIS:CD2	2.23	0.73
1:A:181:ILE:HB	1:A:214:ILE:HG21	1.69	0.73
1:G:295:ARG:C	1:G:295:ARG:HD3	2.14	0.73
1:N:181:ILE:HG22	1:N:183:PRO:HD3	1.69	0.73
1:E:251:GLY:HA2	1:E:254:PHE:HB3	1.70	0.73
1:H:161:ILE:HG23	1:H:180:LEU:HB3	1.71	0.73
1:K:133:ARG:HE	1:K:158:THR:HG21	1.54	0.73
1:G:111:ALA:HA	1:G:114:ASN:HD22	1.53	0.73
1:H:285:ARG:HB3	1:H:291:SER:HB2	1.69	0.73
1:J:211:CYS:HA	1:K:233:ARG:HD3	1.71	0.73
1:M:249:ALA:C	1:M:251:GLY:H	1.96	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:64:ASP:OD2	1:N:92:THR:N	2.21	0.73
1:K:119:ALA:N	1:K:144:ASP:OD2	2.20	0.72
1:D:62:GLY:H	1:D:92:THR:HG22	1.53	0.72
1:L:294:THR:N	1:L:297:GLU:OE1	2.22	0.72
1:H:126:LEU:O	1:H:130:ARG:HG3	1.90	0.72
1:K:47:ALA:O	1:K:49:ALA:N	2.21	0.72
1:A:12:ALA:HB3	1:A:94:ILE:HG13	1.70	0.72
1:E:240:PHE:CD1	1:E:301:PHE:HE2	2.08	0.72
1:F:143:LEU:CG	1:F:168:ARG:HH12	2.02	0.72
1:F:267:PRO:HD2	1:F:270:SER:HB2	1.71	0.72
1:K:6:VAL:HG12	1:K:136:LEU:HB3	1.69	0.72
1:A:98:GLN:OE1	1:A:106:SER:OG	2.05	0.72
1:D:110:SER:OG	1:D:112:GLU:OE2	2.07	0.72
1:D:250:ALA:HA	1:D:252:ASP:N	2.05	0.72
1:L:246:ASP:O	1:L:248:THR:N	2.23	0.72
1:A:99:VAL:HG12	1:A:100:SER:H	1.55	0.72
1:D:130:ARG:NH1	1:D:152:GLU:OE1	2.22	0.72
1:B:18:VAL:H	1:B:99:VAL:HG12	1.55	0.71
1:A:244:ALA:HA	1:A:283:VAL:HB	1.72	0.71
1:I:17:GLN:OE1	1:I:32:ASN:ND2	2.22	0.71
1:J:63:ASP:OD2	1:J:89:ASN:N	2.21	0.71
1:J:140:GLU:HG3	1:J:166:PRO:HD3	1.71	0.71
1:N:134:TYR:HD1	1:N:161:ILE:HD11	1.55	0.71
1:B:85:LYS:NZ	1:B:121:ALA:O	2.16	0.71
1:I:50:ARG:HD2	1:I:292:ILE:HG22	1.73	0.71
1:O:206:ALA:O	1:O:208:ALA:N	2.23	0.71
1:L:169:GLU:HG2	1:L:190:VAL:HG12	1.71	0.71
1:A:19:PRO:HA	1:A:101:ASP:HB2	1.73	0.71
1:G:143:LEU:HD12	1:G:168:ARG:HH12	1.56	0.71
1:J:126:LEU:HD23	1:J:129:ILE:HD13	1.72	0.71
1:M:19:PRO:O	1:M:21:PHE:N	2.22	0.71
1:A:44:GLN:OE1	1:A:138:GLN:NE2	2.24	0.71
1:H:40:LYS:O	1:H:43:ASN:N	2.23	0.71
1:M:101:ASP:HA	1:P:243:LYS:HD3	1.72	0.71
1:H:184:ASN:H	1:H:187:GLU:HB2	1.56	0.71
1:A:97:ILE:HD12	1:A:107:ILE:HG13	1.71	0.71
1:E:97:ILE:HG12	1:E:107:ILE:HD13	1.73	0.71
1:K:43:ASN:OD1	1:K:289:GLN:HG3	1.91	0.71
1:G:207:ASP:O	1:G:211:CYS:N	2.22	0.70
1:A:13:ASP:HB2	1:A:36:ILE:HG22	1.73	0.70
1:B:7:LEU:HB3	1:B:137:MET:HG2	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:VAL:HG23	1:D:86:LEU:HD23	1.74	0.70
1:E:184:ASN:ND2	1:E:187:GLU:H	1.89	0.70
1:H:181:ILE:HG12	1:H:183:PRO:HD3	1.72	0.70
1:A:220:THR:HA	1:A:226:VAL:HG23	1.74	0.70
1:K:143:LEU:HD12	1:K:168:ARG:NH2	2.06	0.70
1:L:182:THR:OG1	1:L:182:THR:O	2.08	0.70
1:G:147:LEU:HD11	1:G:151:GLN:HE21	1.57	0.70
1:J:187:GLU:O	1:J:189:GLU:N	2.24	0.70
1:B:61:VAL:HA	1:B:92:THR:HG23	1.73	0.70
1:G:174:LEU:O	1:G:176:LYS:N	2.25	0.70
1:O:183:PRO:HG2	1:O:219:ILE:HG12	1.74	0.70
1:A:126:LEU:HD13	1:A:152:GLU:HG2	1.74	0.70
1:C:221:LEU:HD11	1:C:227:TRP:HB2	1.73	0.70
1:F:232:GLY:C	1:G:207:ASP:HB3	2.17	0.70
1:I:147:LEU:HD12	1:I:151:GLN:HB3	1.74	0.70
1:E:224:LYS:O	1:E:236:ARG:NH1	2.24	0.69
1:H:70:ILE:O	1:H:73:SER:HB2	1.92	0.69
1:O:9:SER:OG	1:O:140:GLU:OE1	2.10	0.69
1:M:294:THR:OG1	1:M:297:GLU:OE2	2.09	0.69
1:P:181:ILE:HG23	1:P:183:PRO:HD3	1.74	0.69
1:B:207:ASP:OD1	1:I:203:GLN:NE2	2.25	0.69
1:H:245:THR:CG2	1:H:284:THR:HA	2.22	0.69
1:P:136:LEU:HD13	1:P:161:ILE:HG22	1.75	0.69
1:P:97:ILE:HG23	1:P:107:ILE:HG12	1.73	0.69
1:G:53:ALA:HB2	1:G:260:THR:HG23	1.75	0.69
1:H:245:THR:HG21	1:H:284:THR:HA	1.75	0.69
1:J:281:ILE:HB	1:J:293:PRO:HG3	1.72	0.69
1:B:51:MET:HA	1:B:295:ARG:HG3	1.75	0.69
1:H:40:LYS:O	1:H:42:ALA:N	2.24	0.69
1:I:110:SER:OG	1:I:112:GLU:OE2	2.09	0.69
1:L:41:GLY:HA2	1:L:138:GLN:HE22	1.57	0.69
1:A:61:VAL:O	1:A:87:GLN:HB2	1.93	0.69
1:K:300:ALA:O	1:K:304:GLU:HG3	1.92	0.69
1:N:209:LEU:O	1:N:211:CYS:N	2.20	0.69
1:B:184:ASN:N	1:B:187:GLU:OE2	2.26	0.69
1:I:224:LYS:O	1:I:236:ARG:NH1	2.25	0.69
1:K:126:LEU:HB2	1:K:152:GLU:HG2	1.74	0.69
1:N:181:ILE:HG13	1:N:214:ILE:HG21	1.72	0.69
1:O:126:LEU:HA	1:O:129:ILE:HD12	1.75	0.69
1:A:181:ILE:HG22	1:A:217:VAL:HA	1.74	0.69
1:C:134:TYR:HD2	1:C:263:LEU:HD23	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ILE:HG13	1:D:214:ILE:HG21	1.75	0.69
1:P:300:ALA:O	1:P:304:GLU:HG3	1.94	0.69
1:B:91:PRO:HD2	1:B:112:GLU:HG2	1.75	0.68
1:F:194:ILE:HD13	1:F:204:GLN:HB3	1.76	0.68
1:H:306:SER:HB3	1:L:143:LEU:HG	1.74	0.68
1:K:18:VAL:HG21	1:K:98:GLN:HB3	1.75	0.68
1:L:172:ASP:O	1:L:174:LEU:N	2.26	0.68
1:M:100:SER:OG	1:M:104:GLU:O	2.09	0.68
1:M:170:LEU:HD23	1:M:174:LEU:HD23	1.76	0.68
1:I:96:MET:HE3	1:J:96:MET:HE3	1.74	0.68
1:N:264:GLN:OE1	1:N:295:ARG:NH2	2.27	0.68
1:B:231:ASN:HD22	1:I:232:GLY:HA3	1.55	0.68
1:H:81:THR:O	1:H:83:GLY:N	2.27	0.68
1:B:180:LEU:HG	1:B:216:ILE:HB	1.75	0.68
1:B:228:LEU:HD12	1:B:229:SER:N	2.09	0.68
1:P:44:GLN:OE1	1:P:138:GLN:NE2	2.24	0.68
1:H:279:ALA:O	1:H:283:VAL:N	2.25	0.68
1:K:6:VAL:HG21	1:K:45:ALA:HB2	1.76	0.68
1:L:40:LYS:NZ	1:L:252:ASP:OD1	2.26	0.68
1:A:117:LEU:O	1:A:142:PRO:HG2	1.93	0.68
1:C:72:GLU:HA	1:C:75:LYS:HG3	1.75	0.68
1:F:233:ARG:HD3	1:G:211:CYS:HB2	1.75	0.68
1:L:63:ASP:OD2	1:L:89:ASN:N	2.25	0.68
1:M:135:LEU:HD23	1:M:160:VAL:HG13	1.76	0.68
1:D:291:SER:OG	1:D:292:ILE:N	2.24	0.68
1:F:26:GLU:HG3	1:F:27:THR:N	2.09	0.68
1:J:249:ALA:HB2	1:J:288:ALA:HB1	1.76	0.68
1:M:251:GLY:O	1:M:255:ASN:ND2	2.26	0.68
1:P:228:LEU:HD11	1:P:268:LEU:HD21	1.76	0.68
1:C:182:THR:O	1:C:182:THR:OG1	2.10	0.68
1:E:184:ASN:C	1:E:184:ASN:HD22	2.01	0.68
1:F:241:VAL:HG13	1:I:19:PRO:HB3	1.75	0.68
1:H:230:GLN:O	1:H:233:ARG:HG3	1.94	0.68
1:H:250:ALA:HB1	1:H:283:VAL:HG12	1.74	0.68
1:K:14:HIS:H	1:K:94:ILE:HD11	1.59	0.68
1:P:77:ASP:HB3	1:P:79:ILE:HG13	1.76	0.68
1:G:51:MET:HB2	1:G:260:THR:HG21	1.77	0.67
1:A:140:GLU:HG3	1:A:166:PRO:HD3	1.76	0.67
1:B:245:THR:HG21	1:B:286:PHE:HD2	1.59	0.67
1:H:87:GLN:HG3	1:H:116:LYS:HG3	1.77	0.67
1:J:56:GLY:HA2	1:J:80:ASN:HB3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:91:PRO:HG2	1:J:112:GLU:HG3	1.77	0.67
1:L:183:PRO:HG2	1:L:219:ILE:HG12	1.75	0.67
1:F:184:ASN:ND2	1:F:186:THR:H	1.93	0.67
1:C:147:LEU:O	1:C:151:GLN:HG3	1.94	0.67
1:C:171:PRO:O	1:C:173:GLU:N	2.28	0.67
1:F:83:GLY:O	1:F:85:LYS:NZ	2.27	0.67
1:I:230:GLN:O	1:I:233:ARG:HG3	1.94	0.67
1:B:110:SER:OG	1:B:112:GLU:OE2	2.09	0.67
1:F:228:LEU:HD21	1:F:268:LEU:HD21	1.76	0.67
1:M:51:MET:HE1	1:M:298:VAL:HG21	1.75	0.67
1:M:187:GLU:O	1:M:191:LEU:HB2	1.94	0.67
1:D:143:LEU:HD21	1:D:168:ARG:NH1	2.09	0.67
1:H:110:SER:OG	1:H:112:GLU:OE2	2.12	0.67
1:L:163:ASN:HA	1:L:182:THR:HG23	1.77	0.67
1:H:74:PHE:HB3	1:H:79:ILE:HB	1.76	0.67
1:M:175:LEU:HD22	1:M:214:ILE:HD11	1.76	0.67
1:F:66:PHE:O	1:F:68:ILE:N	2.28	0.67
1:K:138:GLN:N	1:K:138:GLN:HE21	1.92	0.67
1:N:139:LEU:HD11	1:N:170:LEU:HD11	1.76	0.67
1:P:138:GLN:HG3	1:P:163:ASN:HB3	1.77	0.67
1:A:134:TYR:CD1	1:A:159:ASN:HB2	2.30	0.67
1:J:234:GLY:N	1:K:207:ASP:OD2	2.28	0.67
1:H:280:ALA:HA	1:H:283:VAL:HG22	1.77	0.66
1:J:86:LEU:H	1:J:86:LEU:HD12	1.59	0.66
1:K:133:ARG:NE	1:K:158:THR:HG21	2.10	0.66
1:M:216:ILE:HD13	1:M:268:LEU:HD21	1.77	0.66
1:D:20:SER:OG	1:D:21:PHE:N	2.22	0.66
1:B:286:PHE:O	1:B:290:THR:OG1	2.13	0.66
1:H:221:LEU:HD12	1:H:227:TRP:H	1.58	0.66
1:K:3:LYS:HB3	1:K:263:LEU:HD21	1.76	0.66
1:L:207:ASP:HB3	1:M:233:ARG:HB3	1.76	0.66
1:A:27:THR:HG22	1:B:107:ILE:HB	1.75	0.66
1:F:229:SER:HA	1:F:234:GLY:HA2	1.77	0.66
1:G:189:GLU:O	1:G:193:GLY:N	2.28	0.66
1:H:294:THR:H	1:H:297:GLU:CD	2.03	0.66
1:L:225:GLY:HA3	1:L:238:PRO:HA	1.77	0.66
1:E:181:ILE:HG23	1:E:183:PRO:HD3	1.78	0.66
1:H:294:THR:OG1	1:H:297:GLU:HG3	1.95	0.66
1:L:50:ARG:HD2	1:L:292:ILE:HG22	1.77	0.66
1:L:253:THR:HG23	1:L:292:ILE:HG12	1.76	0.66
1:N:192:THR:OG1	1:N:193:GLY:N	2.20	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ILE:HG22	1:E:110:SER:N	2.07	0.66
1:E:246:ASP:HB2	1:E:283:VAL:HG23	1.77	0.66
1:C:15:VAL:HG22	1:C:97:ILE:HD12	1.78	0.66
1:E:135:LEU:HD21	1:E:137:MET:HE2	1.77	0.66
1:H:279:ALA:O	1:H:283:VAL:HG13	1.95	0.66
1:J:21:PHE:HE2	1:J:106:SER:HB3	1.59	0.66
1:J:234:GLY:O	1:J:235:GLN:HB3	1.95	0.66
1:B:66:PHE:O	1:B:69:ASN:N	2.29	0.65
1:G:234:GLY:O	1:G:235:GLN:HB2	1.95	0.65
1:L:138:GLN:OE1	1:L:138:GLN:N	2.28	0.65
1:O:16:LEU:HD21	1:O:30:GLY:HA3	1.77	0.65
1:B:249:ALA:O	1:B:252:ASP:N	2.27	0.65
1:I:203:GLN:OE1	1:I:227:TRP:NE1	2.28	0.65
1:N:216:ILE:HG12	1:N:268:LEU:HD21	1.78	0.65
1:F:47:ALA:HB3	1:F:256:GLY:HA3	1.78	0.65
1:G:56:GLY:HA2	1:G:80:ASN:HB3	1.78	0.65
1:H:175:LEU:HB3	1:H:214:ILE:HD11	1.77	0.65
1:I:137:MET:HE1	1:I:150:ALA:HB2	1.78	0.65
1:O:181:ILE:HG23	1:O:183:PRO:HD3	1.77	0.65
1:O:202:ALA:HB3	1:O:227:TRP:CZ3	2.32	0.65
1:A:66:PHE:O	1:A:68:ILE:N	2.29	0.65
1:C:104:GLU:HB2	1:D:25:GLY:H	1.60	0.65
1:F:91:PRO:HG2	1:F:112:GLU:HG2	1.78	0.65
1:F:101:ASP:OD1	1:I:243:LYS:HG3	1.97	0.65
1:G:110:SER:OG	1:G:112:GLU:HG2	1.96	0.65
1:H:281:ILE:O	1:H:285:ARG:HG3	1.96	0.65
1:D:139:LEU:C	1:D:166:PRO:HD2	2.21	0.65
1:J:207:ASP:O	1:J:210:HIS:HB2	1.97	0.65
1:M:189:GLU:HG2	1:M:195:THR:HA	1.77	0.65
1:N:249:ALA:O	1:N:252:ASP:N	2.27	0.65
1:A:15:VAL:HG13	1:A:97:ILE:HG12	1.78	0.65
1:K:209:LEU:HB3	1:K:214:ILE:HD11	1.79	0.65
1:L:91:PRO:HG2	1:L:112:GLU:HB3	1.78	0.65
1:D:248:THR:HG23	1:D:249:ALA:HA	1.79	0.65
1:H:42:ALA:O	1:H:46:VAL:HG22	1.96	0.65
1:I:117:LEU:O	1:I:142:PRO:HG2	1.97	0.65
1:B:139:LEU:HD13	1:B:168:ARG:HD2	1.79	0.65
1:I:167:ALA:HB1	1:I:190:VAL:HG21	1.78	0.65
1:D:249:ALA:H	1:D:250:ALA:C	2.04	0.65
1:J:171:PRO:HB2	1:J:173:GLU:HG3	1.79	0.65
1:L:47:ALA:HB3	1:L:256:GLY:HA3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:ASN:H	1:L:187:GLU:HB2	1.61	0.65
1:A:181:ILE:HG21	1:A:209:LEU:HD13	1.78	0.64
1:G:261:GLY:O	1:G:263:LEU:N	2.29	0.64
1:L:15:VAL:O	1:L:34:GLN:N	2.28	0.64
1:C:246:ASP:CG	1:C:286:PHE:HB2	2.22	0.64
1:D:126:LEU:O	1:D:129:ILE:N	2.30	0.64
1:E:64:ASP:OD1	1:E:92:THR:OG1	2.13	0.64
1:F:5:VAL:O	1:F:135:LEU:HD22	1.97	0.64
1:F:143:LEU:HG	1:F:168:ARG:NH1	2.11	0.64
1:H:243:LYS:CG	1:K:101:ASP:HA	2.22	0.64
1:H:250:ALA:O	1:H:253:THR:N	2.30	0.64
1:I:3:LYS:HB2	1:I:54:ASP:HB3	1.79	0.64
1:C:117:LEU:O	1:C:142:PRO:HG2	1.97	0.64
1:D:97:ILE:HG22	1:D:107:ILE:HD12	1.79	0.64
1:F:31:ARG:NH2	1:F:101:ASP:OD1	2.29	0.64
1:H:19:PRO:HB3	1:K:241:VAL:HG13	1.79	0.64
1:I:181:ILE:HG12	1:I:183:PRO:HD3	1.79	0.64
1:M:259:VAL:O	1:M:263:LEU:HB2	1.97	0.64
1:D:62:GLY:H	1:D:92:THR:CG2	2.10	0.64
1:K:180:LEU:HD12	1:K:216:ILE:HB	1.79	0.64
1:C:139:LEU:HD11	1:C:170:LEU:HD11	1.78	0.64
1:H:18:VAL:O	1:H:101:ASP:HB2	1.97	0.64
1:C:151:GLN:HA	1:C:154:LYS:HD3	1.78	0.64
1:G:134:TYR:HD1	1:G:161:ILE:HD11	1.62	0.64
1:G:216:ILE:HG21	1:G:268:LEU:HD21	1.79	0.64
1:C:281:ILE:HG23	1:C:293:PRO:HG3	1.78	0.64
1:O:57:PHE:HB2	1:O:79:ILE:HG21	1.78	0.64
1:A:183:PRO:HB3	1:A:187:GLU:HB3	1.80	0.64
1:M:127:ALA:HA	1:M:130:ARG:HH21	1.61	0.64
1:O:7:LEU:HD12	1:O:58:ILE:HG21	1.79	0.64
1:B:187:GLU:O	1:B:190:VAL:HG22	1.96	0.64
1:D:232:GLY:O	1:D:234:GLY:N	2.31	0.64
1:E:225:GLY:HA3	1:E:238:PRO:HA	1.80	0.64
1:L:240:PHE:CD1	1:L:301:PHE:HE2	2.15	0.64
1:A:172:ASP:C	1:A:174:LEU:H	2.06	0.63
1:D:100:SER:HA	1:D:101:ASP:HB3	1.81	0.63
1:C:194:ILE:HG13	1:C:205:ALA:HA	1.81	0.63
1:K:65:SER:O	1:K:69:ASN:ND2	2.31	0.63
1:B:126:LEU:HB3	1:B:152:GLU:HG2	1.80	0.63
1:C:230:GLN:O	1:C:233:ARG:N	2.18	0.63
1:N:172:ASP:O	1:N:176:LYS:HG3	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:MET:HE2	1:L:98:GLN:HE21	1.62	0.63
1:N:295:ARG:HG2	1:N:295:ARG:HH11	1.63	0.63
1:B:88:PRO:O	1:B:89:ASN:ND2	2.31	0.63
1:E:218:ILE:HG12	1:E:228:LEU:HD13	1.80	0.63
1:F:300:ALA:O	1:F:304:GLU:HG2	1.98	0.63
1:G:162:LEU:HD11	1:G:174:LEU:HD21	1.80	0.63
1:K:99:VAL:HA	1:K:105:ASN:HB3	1.80	0.63
1:K:204:GLN:HA	1:K:207:ASP:HB2	1.80	0.63
1:A:56:GLY:HA2	1:A:80:ASN:HB3	1.79	0.63
1:A:98:GLN:HG2	1:B:96:MET:HE1	1.81	0.63
1:F:58:ILE:HD11	1:F:122:ILE:HG22	1.80	0.63
1:I:53:ALA:HB2	1:I:260:THR:HG23	1.79	0.63
1:O:171:PRO:HG2	1:O:174:LEU:HB3	1.81	0.63
1:A:151:GLN:O	1:A:155:THR:OG1	2.17	0.63
1:B:99:VAL:HG13	1:B:101:ASP:HB2	1.80	0.63
1:H:112:GLU:O	1:H:114:ASN:N	2.32	0.63
1:K:47:ALA:C	1:K:49:ALA:H	2.07	0.63
1:P:63:ASP:OD2	1:P:89:ASN:N	2.29	0.63
1:P:294:THR:HG22	1:P:297:GLU:OE2	1.99	0.63
1:D:300:ALA:O	1:D:304:GLU:HG2	1.99	0.63
1:H:261:GLY:O	1:H:264:GLN:N	2.29	0.63
1:K:294:THR:O	1:K:298:VAL:HG23	1.99	0.63
1:C:64:ASP:N	1:C:64:ASP:OD2	2.32	0.63
1:J:240:PHE:CD2	1:J:301:PHE:HE2	2.16	0.63
1:M:248:THR:OG1	1:M:249:ALA:N	2.32	0.63
1:J:240:PHE:HE1	1:J:273:LYS:HE3	1.64	0.62
1:N:210:HIS:C	1:N:212:LYS:H	2.07	0.62
1:O:3:LYS:HD2	1:O:133:ARG:NH1	2.14	0.62
1:B:187:GLU:O	1:B:189:GLU:N	2.33	0.62
1:P:134:TYR:CD2	1:P:263:LEU:HD23	2.34	0.62
1:C:139:LEU:HD13	1:C:168:ARG:HG2	1.81	0.62
1:D:197:TYR:HD1	1:D:197:TYR:H	1.45	0.62
1:M:239:GLY:HA2	1:M:276:HIS:CD2	2.34	0.62
1:H:3:LYS:HB2	1:H:54:ASP:HB2	1.81	0.62
1:H:184:ASN:N	1:H:187:GLU:OE2	2.33	0.62
1:K:5:VAL:O	1:K:135:LEU:HA	1.99	0.62
1:B:182:THR:OG1	1:B:182:THR:O	2.18	0.62
1:D:294:THR:HG22	1:D:297:GLU:HG3	1.81	0.62
1:F:170:LEU:HD13	1:F:171:PRO:HD2	1.81	0.62
1:F:264:GLN:O	1:F:265:GLU:HB2	1.99	0.62
1:L:142:PRO:O	1:L:146:ILE:HG12	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100:SER:OG	1:O:105:ASN:OD1	2.13	0.62
1:D:68:ILE:HG23	1:D:86:LEU:HD11	1.82	0.62
1:C:4:LEU:HD21	1:C:55:VAL:HG23	1.80	0.62
1:C:224:LYS:HE3	1:C:236:ARG:NH2	2.15	0.62
1:F:126:LEU:HD21	1:F:148:LYS:HG3	1.82	0.62
1:G:98:GLN:NE2	1:G:106:SER:OG	2.33	0.62
1:N:53:ALA:HB2	1:N:260:THR:HG23	1.82	0.62
1:A:92:THR:O	1:A:113:ALA:N	2.33	0.62
1:A:126:LEU:O	1:A:130:ARG:HG3	2.00	0.62
1:D:61:VAL:CG2	1:D:86:LEU:HD23	2.29	0.62
1:E:148:LYS:HA	1:E:151:GLN:HG3	1.82	0.62
1:M:188:ALA:O	1:M:192:THR:N	2.29	0.62
1:N:44:GLN:NE2	1:N:252:ASP:OD1	2.30	0.62
1:B:221:LEU:HD21	1:B:227:TRP:HB2	1.82	0.62
1:H:243:LYS:HG3	1:K:101:ASP:CA	2.25	0.62
1:P:134:TYR:HD2	1:P:263:LEU:HD23	1.63	0.62
1:O:27:THR:HG22	1:P:107:ILE:HB	1.81	0.61
1:P:53:ALA:HB2	1:P:260:THR:HG23	1.80	0.61
1:G:119:ALA:HB1	1:G:148:LYS:HE2	1.82	0.61
1:H:139:LEU:HD11	1:H:170:LEU:HD11	1.81	0.61
1:M:97:ILE:HG23	1:M:107:ILE:HG23	1.83	0.61
1:N:198:ASP:OD1	1:N:201:SER:OG	2.13	0.61
1:B:300:ALA:O	1:B:304:GLU:HG2	2.01	0.61
1:F:37:PRO:O	1:F:289:GLN:HB2	2.00	0.61
1:G:3:LYS:HD3	1:G:133:ARG:HG3	1.82	0.61
1:N:171:PRO:HB2	1:N:173:GLU:OE1	2.00	0.61
1:E:14:HIS:CD2	1:E:94:ILE:HD11	2.35	0.61
1:H:117:LEU:O	1:H:142:PRO:HG2	1.99	0.61
1:L:95:ALA:HA	1:L:108:CYS:O	2.00	0.61
1:D:101:ASP:O	1:D:102:SER:OG	2.16	0.61
1:O:97:ILE:HD13	1:O:107:ILE:HG23	1.81	0.61
1:A:18:VAL:O	1:A:101:ASP:HB2	2.01	0.61
1:A:64:ASP:C	1:A:66:PHE:H	2.09	0.61
1:J:161:ILE:HD12	1:J:259:VAL:HG23	1.83	0.61
1:N:176:LYS:HG2	1:N:212:LYS:HB3	1.82	0.61
1:F:14:HIS:CE1	1:F:33:TYR:HH	2.17	0.61
1:N:198:ASP:OD2	1:N:200:SER:OG	2.18	0.61
1:O:37:PRO:O	1:O:289:GLN:NE2	2.33	0.61
1:B:74:PHE:HB3	1:B:79:ILE:CD1	2.30	0.61
1:C:16:LEU:HD11	1:D:110:SER:HB2	1.83	0.61
1:F:162:LEU:O	1:F:164:PRO:HD3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:PRO:HB2	1:G:173:GLU:HG3	1.83	0.61
1:I:207:ASP:N	1:I:207:ASP:OD1	2.26	0.61
1:J:92:THR:HG22	1:J:93:GLY:H	1.66	0.61
1:O:264:GLN:OE1	1:O:295:ARG:NH2	2.34	0.61
1:B:175:LEU:HA	1:B:178:VAL:HG23	1.83	0.61
1:C:134:TYR:CD2	1:C:263:LEU:HD23	2.35	0.61
1:G:295:ARG:HD3	1:G:295:ARG:O	2.01	0.61
1:N:81:THR:O	1:N:83:GLY:N	2.34	0.61
1:N:259:VAL:O	1:N:263:LEU:HD23	2.00	0.61
1:E:230:GLN:O	1:E:233:ARG:HG3	2.01	0.60
1:G:137:MET:HE3	1:G:146:ILE:HG23	1.83	0.60
1:L:16:LEU:HD12	1:L:33:TYR:HB2	1.81	0.60
1:A:216:ILE:HG21	1:A:268:LEU:HD11	1.83	0.60
1:G:50:ARG:O	1:G:295:ARG:HB2	2.00	0.60
1:N:154:LYS:HE2	1:N:177:CYS:HA	1.83	0.60
1:B:17:GLN:HA	1:B:99:VAL:CG1	2.31	0.60
1:F:64:ASP:OD1	1:F:64:ASP:N	2.34	0.60
1:G:43:ASN:ND2	1:G:252:ASP:OD2	2.27	0.60
1:I:43:ASN:HA	1:I:289:GLN:HE21	1.65	0.60
1:P:28:LEU:HD22	1:P:29:HIS:H	1.66	0.60
1:B:170:LEU:HD23	1:B:174:LEU:HD23	1.82	0.60
1:G:94:ILE:CG1	1:G:110:SER:HB2	2.32	0.60
1:K:228:LEU:HD22	1:K:272:ILE:HD12	1.84	0.60
1:O:227:TRP:HE1	1:O:234:GLY:HA3	1.66	0.60
1:B:43:ASN:HB3	1:B:252:ASP:HB3	1.83	0.60
1:H:249:ALA:O	1:H:251:GLY:N	2.33	0.60
1:B:253:THR:O	1:B:257:ALA:N	2.31	0.60
1:H:191:LEU:H	1:H:191:LEU:HD12	1.65	0.60
1:K:100:SER:HA	1:K:101:ASP:HB2	1.84	0.60
1:L:111:ALA:O	1:L:113:ALA:N	2.34	0.60
1:L:135:LEU:HD21	1:L:149:ALA:HB1	1.84	0.60
1:D:64:ASP:OD1	1:D:64:ASP:N	2.33	0.60
1:D:139:LEU:O	1:D:166:PRO:HD2	2.02	0.60
1:P:266:MET:HE1	1:P:274:PHE:HB2	1.81	0.60
1:A:253:THR:HG23	1:A:292:ILE:HG12	1.84	0.60
1:D:241:VAL:O	1:D:242:VAL:HG22	2.01	0.60
1:E:50:ARG:HH11	1:E:50:ARG:HG3	1.67	0.60
1:E:175:LEU:HB3	1:E:214:ILE:HD11	1.82	0.60
1:M:147:LEU:HA	1:M:174:LEU:HD13	1.84	0.60
1:A:170:LEU:HD11	1:A:191:LEU:HD22	1.84	0.60
1:N:134:TYR:CD1	1:N:161:ILE:HD11	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:298:VAL:O	1:P:301:PHE:HB3	2.02	0.60
1:C:184:ASN:H	1:C:187:GLU:HB2	1.67	0.59
1:G:189:GLU:OE1	1:G:190:VAL:HG23	2.02	0.59
1:C:249:ALA:HB1	1:C:288:ALA:HB2	1.83	0.59
1:G:255:ASN:ND2	1:G:255:ASN:H	1.99	0.59
1:K:110:SER:HB3	1:L:16:LEU:HD11	1.83	0.59
1:A:98:GLN:HE22	1:B:98:GLN:HE22	1.50	0.59
1:D:53:ALA:HB2	1:D:260:THR:HG22	1.83	0.59
1:F:131:ASP:N	1:F:131:ASP:OD1	2.33	0.59
1:K:229:SER:HA	1:K:234:GLY:HA2	1.83	0.59
1:C:181:ILE:HG23	1:C:183:PRO:HD3	1.83	0.59
1:C:264:GLN:O	1:C:265:GLU:HG2	2.02	0.59
1:E:7:LEU:HD12	1:E:58:ILE:HG21	1.85	0.59
1:M:207:ASP:OD2	1:M:208:ALA:N	2.35	0.59
1:C:264:GLN:C	1:C:265:GLU:HG2	2.27	0.59
1:D:13:ASP:HB3	1:D:97:ILE:HD11	1.83	0.59
1:E:50:ARG:HD2	1:E:292:ILE:CG2	2.29	0.59
1:F:134:TYR:HB2	1:F:263:LEU:HD21	1.84	0.59
1:I:14:HIS:ND1	1:I:35:VAL:HG22	2.16	0.59
1:N:269:GLU:O	1:N:273:LYS:HG2	2.02	0.59
1:O:207:ASP:HA	1:O:210:HIS:HB2	1.84	0.59
1:P:203:GLN:O	1:P:207:ASP:HB2	2.03	0.59
1:B:180:LEU:HD23	1:B:181:ILE:H	1.67	0.59
1:C:246:ASP:OD2	1:C:286:PHE:HB2	2.02	0.59
1:F:232:GLY:O	1:G:207:ASP:HB3	2.03	0.59
1:K:56:GLY:HA2	1:K:80:ASN:HB3	1.85	0.59
1:A:63:ASP:OD1	1:A:89:ASN:N	2.35	0.59
1:G:226:VAL:HG23	1:G:237:ILE:O	2.02	0.59
1:K:62:GLY:O	1:K:64:ASP:N	2.31	0.59
1:L:300:ALA:O	1:L:304:GLU:HG3	2.02	0.59
1:A:106:SER:OG	1:A:106:SER:O	2.19	0.59
1:A:295:ARG:HA	1:A:298:VAL:HG12	1.85	0.59
1:B:249:ALA:O	1:B:251:GLY:N	2.35	0.59
1:H:43:ASN:OD1	1:H:289:GLN:HG2	2.03	0.59
1:M:186:THR:O	1:M:190:VAL:HG23	2.02	0.59
1:C:12:ALA:HB2	1:C:66:PHE:CE2	2.37	0.59
1:C:95:ALA:HB2	1:C:109:ILE:HG23	1.83	0.59
1:N:279:ALA:HA	1:N:282:SER:OG	2.02	0.59
1:O:63:ASP:OD2	1:O:88:PRO:HA	2.02	0.59
1:B:203:GLN:HE22	1:I:204:GLN:HG3	1.68	0.59
1:F:4:LEU:HD23	1:F:55:VAL:HG12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:PRO:HD2	1:G:270:SER:CB	2.32	0.59
1:H:37:PRO:O	1:H:289:GLN:NE2	2.35	0.59
1:I:220:THR:HA	1:I:226:VAL:HG23	1.84	0.59
1:K:230:GLN:O	1:K:233:ARG:HG3	2.02	0.59
1:D:68:ILE:HA	1:D:86:LEU:HD21	1.84	0.58
1:G:295:ARG:O	1:G:298:VAL:HG12	2.03	0.58
1:F:87:GLN:OE1	1:F:116:LYS:HB3	2.03	0.58
1:G:81:THR:HG22	1:G:84:VAL:HG21	1.85	0.58
1:J:196:VAL:HG13	1:J:202:ALA:HB2	1.84	0.58
1:K:64:ASP:O	1:K:68:ILE:HG12	2.03	0.58
1:L:210:HIS:CE1	1:L:231:ASN:H	2.21	0.58
1:C:136:LEU:HD22	1:C:259:VAL:HG11	1.84	0.58
1:H:279:ALA:C	1:H:283:VAL:HG13	2.28	0.58
1:K:145:GLY:O	1:K:149:ALA:N	2.33	0.58
1:L:240:PHE:HD1	1:L:301:PHE:CE2	2.17	0.58
1:P:85:LYS:HZ1	1:P:124:PRO:HG2	1.68	0.58
1:A:226:VAL:HG12	1:A:237:ILE:HB	1.84	0.58
1:F:147:LEU:HD12	1:F:151:GLN:OE1	2.04	0.58
1:G:12:ALA:HB2	1:G:66:PHE:CE2	2.38	0.58
1:J:240:PHE:HD2	1:J:301:PHE:HE2	1.50	0.58
1:L:139:LEU:O	1:L:166:PRO:HD2	2.04	0.58
1:J:207:ASP:CB	1:K:232:GLY:HA3	2.33	0.58
1:L:162:LEU:O	1:L:164:PRO:HD3	2.03	0.58
1:B:17:GLN:HA	1:B:99:VAL:HG12	1.86	0.58
1:B:180:LEU:HA	1:B:216:ILE:O	2.04	0.58
1:G:53:ALA:HB2	1:G:260:THR:CG2	2.33	0.58
1:H:171:PRO:HB2	1:H:173:GLU:HG2	1.86	0.58
1:E:247:THR:C	1:E:249:ALA:H	2.11	0.58
1:M:306:SER:O	1:O:168:ARG:NH2	2.27	0.58
1:N:278:ALA:O	1:N:282:SER:N	2.36	0.58
1:P:224:LYS:O	1:P:236:ARG:NH1	2.36	0.58
1:G:3:LYS:H	1:G:54:ASP:HB3	1.67	0.58
1:G:117:LEU:O	1:G:142:PRO:HG2	2.04	0.58
1:J:58:ILE:HD11	1:J:125:ASP:HB3	1.86	0.58
1:N:267:PRO:HD2	1:N:270:SER:HB3	1.86	0.58
1:B:99:VAL:HG13	1:B:101:ASP:CB	2.34	0.58
1:B:229:SER:HA	1:B:233:ARG:O	2.03	0.58
1:B:297:GLU:O	1:B:300:ALA:N	2.37	0.58
1:H:281:ILE:HD11	1:H:301:PHE:HB2	1.86	0.58
1:N:68:ILE:HG23	1:N:86:LEU:HD11	1.86	0.58
1:A:31:ARG:HE	1:D:241:VAL:HG23	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLN:O	1:C:146:ILE:HD11	2.04	0.58
1:C:184:ASN:OD1	1:C:187:GLU:N	2.36	0.58
1:F:285:ARG:HB3	1:F:291:SER:HB3	1.86	0.58
1:F:304:GLU:HB2	1:J:115:ALA:HB1	1.85	0.58
1:G:67:GLY:HA2	1:G:70:ILE:HG22	1.85	0.58
1:I:43:ASN:HA	1:I:289:GLN:NE2	2.19	0.58
1:K:30:GLY:O	1:L:110:SER:OG	2.19	0.58
1:L:15:VAL:O	1:L:33:TYR:HA	2.03	0.58
1:C:65:SER:O	1:C:69:ASN:ND2	2.32	0.57
1:E:139:LEU:HD11	1:E:170:LEU:HD11	1.84	0.57
1:E:170:LEU:HD13	1:E:174:LEU:HD23	1.85	0.57
1:J:162:LEU:HD23	1:J:178:VAL:HG21	1.86	0.57
1:K:95:ALA:HA	1:K:108:CYS:O	2.04	0.57
1:L:12:ALA:HB2	1:L:66:PHE:CZ	2.39	0.57
1:M:51:MET:HB3	1:M:260:THR:HG21	1.83	0.57
1:P:184:ASN:ND2	1:P:187:GLU:OE2	2.37	0.57
1:A:14:HIS:ND1	1:A:33:TYR:OH	2.37	0.57
1:A:143:LEU:HD21	1:A:168:ARG:NH1	2.19	0.57
1:C:46:VAL:HG21	1:C:289:GLN:HG2	1.86	0.57
1:E:181:ILE:C	1:E:183:PRO:HD3	2.29	0.57
1:H:204:GLN:HE22	1:O:234:GLY:N	1.92	0.57
1:J:154:LYS:O	1:J:154:LYS:NZ	2.30	0.57
1:J:203:GLN:NE2	1:K:207:ASP:OD1	2.37	0.57
1:L:281:ILE:HD11	1:L:301:PHE:HB2	1.85	0.57
1:B:198:ASP:OD1	1:B:201:SER:OG	2.21	0.57
1:C:108:CYS:SG	1:D:28:LEU:HD13	2.45	0.57
1:E:47:ALA:HB3	1:E:256:GLY:HA3	1.86	0.57
1:J:226:VAL:HG11	1:J:254:PHE:HE2	1.68	0.57
1:L:41:GLY:HA2	1:L:138:GLN:NE2	2.19	0.57
1:N:44:GLN:OE1	1:N:138:GLN:NE2	2.36	0.57
1:N:63:ASP:OD2	1:N:89:ASN:N	2.37	0.57
1:B:21:PHE:CZ	1:B:106:SER:HB3	2.39	0.57
1:D:170:LEU:HD12	1:D:191:LEU:HD21	1.85	0.57
1:G:162:LEU:O	1:G:164:PRO:HD3	2.05	0.57
1:M:251:GLY:HA2	1:M:254:PHE:HB3	1.86	0.57
1:A:227:TRP:CE3	1:A:236:ARG:HG3	2.39	0.57
1:E:220:THR:HA	1:E:226:VAL:HG23	1.86	0.57
1:K:183:PRO:O	1:K:220:THR:HG23	2.03	0.57
1:L:21:PHE:CD2	1:L:22:PRO:HD2	2.39	0.57
1:O:194:ILE:HD13	1:O:205:ALA:HA	1.85	0.57
1:P:2:ASN:ND2	1:P:4:LEU:H	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ILE:O	1:D:285:ARG:HG2	2.05	0.57
1:E:3:LYS:HE2	1:E:263:LEU:HD11	1.86	0.57
1:E:71:ARG:O	1:E:75:LYS:HG3	2.04	0.57
1:G:135:LEU:HD21	1:G:137:MET:SD	2.44	0.57
1:I:294:THR:HB	1:I:297:GLU:H	1.68	0.57
1:J:216:ILE:HD13	1:J:268:LEU:HD21	1.86	0.57
1:O:248:THR:O	1:O:250:ALA:N	2.37	0.57
1:A:66:PHE:C	1:A:68:ILE:H	2.12	0.57
1:E:242:VAL:HG21	1:E:280:ALA:HA	1.87	0.57
1:G:72:GLU:O	1:G:75:LYS:HG3	2.05	0.57
1:G:208:ALA:O	1:G:212:LYS:HG3	2.04	0.57
1:N:81:THR:C	1:N:83:GLY:H	2.13	0.57
1:O:31:ARG:HG2	1:O:32:ASN:N	2.19	0.57
1:P:249:ALA:O	1:P:253:THR:OG1	2.21	0.57
1:B:31:ARG:NH2	1:B:101:ASP:OD2	2.37	0.57
1:B:183:PRO:HB2	1:B:188:ALA:HB2	1.86	0.57
1:D:9:SER:OG	1:D:140:GLU:OE1	2.17	0.57
1:D:234:GLY:O	1:E:204:GLN:NE2	2.38	0.57
1:D:240:PHE:CD1	1:D:301:PHE:CE2	2.93	0.57
1:N:15:VAL:HG23	1:N:97:ILE:HB	1.86	0.57
1:N:291:SER:O	1:N:292:ILE:HG13	2.05	0.57
1:B:153:ALA:HB1	1:B:158:THR:HB	1.86	0.57
1:D:181:ILE:HG22	1:D:183:PRO:HD3	1.86	0.57
1:D:184:ASN:H	1:D:187:GLU:HB2	1.69	0.57
1:H:38:GLY:CA	1:H:289:GLN:HG3	2.35	0.57
1:I:44:GLN:OE1	1:I:138:GLN:NE2	2.36	0.57
1:J:73:SER:OG	1:J:74:PHE:N	2.38	0.57
1:N:97:ILE:HG12	1:N:107:ILE:HG22	1.85	0.57
1:B:117:LEU:HD23	1:B:141:THR:OG1	2.05	0.56
1:D:203:GLN:O	1:D:206:ALA:HB3	2.05	0.56
1:D:280:ALA:O	1:D:283:VAL:HG22	2.05	0.56
1:F:52:GLN:HB2	1:F:295:ARG:HH21	1.69	0.56
1:I:184:ASN:OD1	1:I:187:GLU:HG3	2.04	0.56
1:J:147:LEU:HD11	1:J:151:GLN:HE21	1.70	0.56
1:N:185:GLU:CD	1:N:221:LEU:HA	2.30	0.56
1:P:62:GLY:H	1:P:92:THR:HG23	1.70	0.56
1:C:22:PRO:HG3	1:C:98:GLN:NE2	2.21	0.56
1:D:61:VAL:HG23	1:D:86:LEU:HA	1.86	0.56
1:E:57:PHE:CE1	1:E:59:ALA:HB2	2.40	0.56
1:L:151:GLN:O	1:L:155:THR:HG23	2.06	0.56
1:M:285:ARG:HB2	1:M:291:SER:CB	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:9:SER:HB2	1:N:114:ASN:ND2	2.19	0.56
1:B:183:PRO:HG2	1:B:219:ILE:HG12	1.87	0.56
1:D:4:LEU:HB2	1:D:263:LEU:HD11	1.85	0.56
1:D:44:GLN:HG2	1:D:252:ASP:O	2.05	0.56
1:E:7:LEU:HD22	1:E:137:MET:SD	2.45	0.56
1:F:240:PHE:CD1	1:F:301:PHE:HE2	2.22	0.56
1:I:31:ARG:NH2	1:I:101:ASP:OD2	2.38	0.56
1:J:172:ASP:O	1:J:174:LEU:N	2.39	0.56
1:K:95:ALA:HA	1:K:109:ILE:HA	1.86	0.56
1:K:115:ALA:HA	1:K:142:PRO:HD3	1.85	0.56
1:K:215:GLU:HB3	1:K:216:ILE:HG13	1.87	0.56
1:L:207:ASP:HA	1:L:210:HIS:CD2	2.40	0.56
1:L:230:GLN:O	1:L:233:ARG:HG3	2.05	0.56
1:N:251:GLY:O	1:N:255:ASN:HB2	2.05	0.56
1:P:278:ALA:HA	1:P:281:ILE:HD12	1.86	0.56
1:A:218:ILE:HG22	1:A:226:VAL:HG21	1.88	0.56
1:F:66:PHE:CE1	1:F:70:ILE:HG21	2.41	0.56
1:F:279:ALA:O	1:F:283:VAL:HG13	2.05	0.56
1:J:184:ASN:ND2	1:J:187:GLU:HG3	2.20	0.56
1:L:181:ILE:HD12	1:L:214:ILE:HD13	1.86	0.56
1:L:242:VAL:O	1:L:243:LYS:HB2	2.04	0.56
1:P:2:ASN:ND2	1:P:54:ASP:O	2.36	0.56
1:B:206:ALA:O	1:B:210:HIS:N	2.31	0.56
1:B:281:ILE:O	1:B:284:THR:HG22	2.05	0.56
1:E:5:VAL:O	1:E:135:LEU:HD12	2.06	0.56
1:F:174:LEU:O	1:F:177:CYS:N	2.29	0.56
1:I:139:LEU:HD11	1:I:170:LEU:HD11	1.88	0.56
1:M:224:LYS:O	1:M:236:ARG:NH1	2.39	0.56
1:P:4:LEU:HD23	1:P:55:VAL:HB	1.85	0.56
1:C:106:SER:O	1:C:106:SER:OG	2.12	0.56
1:D:126:LEU:C	1:D:128:ALA:H	2.08	0.56
1:H:51:MET:C	1:H:52:GLN:HG2	2.30	0.56
1:M:2:ASN:HD21	1:M:80:ASN:HD22	1.54	0.56
1:N:3:LYS:HG2	1:N:263:LEU:HD12	1.86	0.56
1:O:218:ILE:HD13	1:O:272:ILE:HD11	1.88	0.56
1:B:199:ASP:OD2	1:B:199:ASP:N	2.38	0.56
1:B:207:ASP:OD2	1:I:203:GLN:HG3	2.05	0.56
1:D:163:ASN:HD22	1:D:164:PRO:N	2.04	0.56
1:F:207:ASP:O	1:F:210:HIS:HB2	2.06	0.56
1:F:233:ARG:HA	1:G:207:ASP:HB2	1.88	0.56
1:G:230:GLN:O	1:G:233:ARG:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:GLU:O	1:K:76:LEU:HD22	2.06	0.56
1:A:178:VAL:HG23	1:A:214:ILE:HG23	1.86	0.56
1:B:14:HIS:CD2	1:B:94:ILE:HG23	2.41	0.56
1:B:246:ASP:OD1	1:B:247:THR:N	2.39	0.56
1:E:161:ILE:HD12	1:E:180:LEU:HD23	1.86	0.56
1:H:51:MET:HA	1:H:295:ARG:HB2	1.88	0.56
1:I:264:GLN:OE1	1:I:295:ARG:NH2	2.39	0.56
1:K:117:LEU:O	1:K:142:PRO:HG2	2.05	0.56
1:O:285:ARG:O	1:O:287:GLY:N	2.39	0.56
1:P:154:LYS:HG3	1:P:155:THR:N	2.19	0.56
1:D:161:ILE:HG23	1:D:180:LEU:HD22	1.86	0.56
1:E:228:LEU:HD11	1:E:268:LEU:HD21	1.86	0.56
1:F:21:PHE:CE2	1:F:106:SER:HB2	2.41	0.56
1:G:56:GLY:CA	1:G:80:ASN:HB3	2.36	0.56
1:H:57:PHE:HB2	1:H:79:ILE:HG21	1.86	0.56
1:J:138:GLN:O	1:J:146:ILE:HD11	2.06	0.56
1:N:136:LEU:HD22	1:N:259:VAL:HG11	1.88	0.56
1:B:257:ALA:O	1:B:260:THR:N	2.39	0.56
1:H:31:ARG:HH22	1:H:101:ASP:CG	2.09	0.56
1:H:94:ILE:HG12	1:H:95:ALA:N	2.21	0.56
1:K:192:THR:HG21	1:K:209:LEU:HD22	1.88	0.56
1:N:283:VAL:O	1:N:285:ARG:N	2.39	0.56
1:P:85:LYS:NZ	1:P:124:PRO:HG2	2.20	0.56
1:B:46:VAL:HG21	1:B:289:GLN:HE22	1.71	0.55
1:C:172:ASP:OD2	1:C:172:ASP:N	2.37	0.55
1:D:195:THR:O	1:D:201:SER:OG	2.17	0.55
1:A:220:THR:CA	1:A:226:VAL:HG23	2.36	0.55
1:D:184:ASN:OD1	1:D:187:GLU:HG3	2.05	0.55
1:D:259:VAL:O	1:D:263:LEU:HB2	2.05	0.55
1:K:12:ALA:HB2	1:K:66:PHE:CE1	2.41	0.55
1:L:139:LEU:HD11	1:L:170:LEU:HD11	1.86	0.55
1:A:249:ALA:HA	1:A:252:ASP:HB2	1.89	0.55
1:B:14:HIS:HD2	1:B:94:ILE:HG23	1.71	0.55
1:B:57:PHE:HD1	1:B:58:ILE:H	1.54	0.55
1:K:273:LYS:O	1:K:274:PHE:C	2.49	0.55
1:M:31:ARG:HH22	1:P:243:LYS:HG3	1.72	0.55
1:M:50:ARG:NE	1:M:77:ASP:OD1	2.35	0.55
1:C:224:LYS:HE3	1:C:236:ARG:HH21	1.71	0.55
1:D:99:VAL:O	1:D:101:ASP:HB3	2.06	0.55
1:G:61:VAL:HA	1:G:92:THR:HG23	1.88	0.55
1:L:56:GLY:HA2	1:L:80:ASN:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:111:ALA:O	1:N:114:ASN:N	2.39	0.55
1:O:44:GLN:HE21	1:O:44:GLN:N	2.04	0.55
1:O:234:GLY:C	1:O:235:GLN:HG2	2.31	0.55
1:O:236:ARG:HH12	1:O:238:PRO:HA	1.70	0.55
1:E:63:ASP:HB3	1:E:86:LEU:HD23	1.89	0.55
1:G:163:ASN:ND2	1:G:182:THR:OG1	2.38	0.55
1:G:257:ALA:O	1:G:259:VAL:N	2.39	0.55
1:J:267:PRO:HD2	1:J:270:SER:HB2	1.87	0.55
1:I:5:VAL:O	1:I:135:LEU:HD12	2.07	0.55
1:L:91:PRO:O	1:L:113:ALA:HB2	2.06	0.55
1:A:97:ILE:HD12	1:A:107:ILE:CG1	2.35	0.55
1:E:97:ILE:HG12	1:E:107:ILE:HG23	1.88	0.55
1:I:72:GLU:HG3	1:I:75:LYS:HE2	1.87	0.55
1:N:284:THR:HG22	1:N:285:ARG:HG2	1.89	0.55
1:C:71:ARG:HB2	1:C:84:VAL:HG11	1.88	0.55
1:P:5:VAL:O	1:P:135:LEU:HA	2.06	0.55
1:P:247:THR:HA	1:P:250:ALA:HB3	1.88	0.55
1:E:303:ALA:O	1:E:306:SER:OG	2.24	0.55
1:F:267:PRO:O	1:F:269:GLU:N	2.40	0.55
1:B:76:LEU:O	1:B:78:GLY:N	2.35	0.55
1:F:170:LEU:CD1	1:F:174:LEU:HD23	2.38	0.55
1:H:12:ALA:HB2	1:H:66:PHE:CE1	2.41	0.55
1:M:3:LYS:HG3	1:M:54:ASP:HB3	1.89	0.55
1:N:17:GLN:HG3	1:N:99:VAL:HG23	1.89	0.55
1:O:199:ASP:O	1:O:202:ALA:N	2.39	0.55
1:A:101:ASP:N	1:A:102:SER:HA	2.22	0.54
1:B:44:GLN:HB3	1:B:136:LEU:HD21	1.90	0.54
1:J:211:CYS:HA	1:K:233:ARG:HH11	1.72	0.54
1:N:300:ALA:O	1:N:304:GLU:HG2	2.06	0.54
1:P:147:LEU:HD13	1:P:174:LEU:HB2	1.89	0.54
1:P:180:LEU:HD11	1:P:216:ILE:HD12	1.89	0.54
1:A:61:VAL:HA	1:A:92:THR:HG23	1.89	0.54
1:B:228:LEU:HD12	1:B:229:SER:H	1.73	0.54
1:B:230:GLN:O	1:B:233:ARG:NE	2.39	0.54
1:E:46:VAL:HG12	1:E:292:ILE:HG12	1.89	0.54
1:E:189:GLU:HG2	1:E:194:ILE:O	2.07	0.54
1:G:261:GLY:C	1:G:263:LEU:H	2.15	0.54
1:H:226:VAL:HG12	1:H:237:ILE:O	2.06	0.54
1:J:210:HIS:CD2	1:J:231:ASN:HA	2.43	0.54
1:J:233:ARG:HD3	1:K:211:CYS:HA	1.90	0.54
1:L:64:ASP:OD1	1:L:92:THR:OG1	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:THR:HG22	1:G:93:GLY:H	1.72	0.54
1:L:170:LEU:HB2	1:L:175:LEU:HD11	1.89	0.54
1:P:221:LEU:HD11	1:P:227:TRP:HB2	1.89	0.54
1:H:113:ALA:O	1:H:116:LYS:HB2	2.07	0.54
1:L:57:PHE:HD1	1:L:58:ILE:H	1.55	0.54
1:C:58:ILE:HD12	1:C:125:ASP:OD1	2.08	0.54
1:H:38:GLY:HA2	1:H:289:GLN:CG	2.35	0.54
1:H:182:THR:HG21	1:H:255:ASN:OD1	2.07	0.54
1:H:243:LYS:HE2	1:K:101:ASP:HA	1.89	0.54
1:I:61:VAL:HG23	1:I:86:LEU:HD23	1.90	0.54
1:J:3:LYS:HB3	1:J:263:LEU:HD21	1.90	0.54
1:A:242:VAL:HG11	1:A:280:ALA:HB1	1.88	0.54
1:D:285:ARG:HB3	1:D:291:SER:CB	2.36	0.54
1:F:206:ALA:HA	1:F:217:VAL:HG11	1.89	0.54
1:F:225:GLY:HA3	1:F:238:PRO:HA	1.90	0.54
1:H:134:TYR:HB2	1:H:263:LEU:HD11	1.90	0.54
1:I:147:LEU:HD22	1:I:174:LEU:HB2	1.89	0.54
1:J:295:ARG:NH1	1:J:299:GLU:OE2	2.41	0.54
1:K:107:ILE:HB	1:L:27:THR:OG1	2.08	0.54
1:L:93:GLY:HA2	1:L:112:GLU:HB2	1.88	0.54
1:P:277:ALA:O	1:P:281:ILE:HG13	2.07	0.54
1:A:89:ASN:N	1:A:89:ASN:OD1	2.41	0.54
1:D:129:ILE:HD12	1:D:135:LEU:HD22	1.88	0.54
1:L:139:LEU:HD13	1:L:170:LEU:HD21	1.89	0.54
1:M:87:GLN:HG3	1:M:116:LYS:HG3	1.88	0.54
1:M:172:ASP:O	1:M:174:LEU:N	2.41	0.54
1:M:277:ALA:HB2	1:M:302:LEU:HD21	1.89	0.54
1:P:97:ILE:HG22	1:P:99:VAL:HG13	1.88	0.54
1:P:253:THR:HG23	1:P:292:ILE:HG12	1.90	0.54
1:A:183:PRO:O	1:A:219:ILE:HA	2.08	0.54
1:B:57:PHE:HD1	1:B:58:ILE:N	2.04	0.54
1:B:281:ILE:HD11	1:B:298:VAL:HG13	1.90	0.54
1:B:172:ASP:HA	1:B:175:LEU:HD12	1.89	0.54
1:B:249:ALA:HB1	1:B:252:ASP:HB2	1.89	0.54
1:C:206:ALA:O	1:C:209:LEU:HB2	2.08	0.54
1:D:240:PHE:CD1	1:D:301:PHE:HE2	2.25	0.54
1:H:228:LEU:HD11	1:H:268:LEU:HD21	1.90	0.54
1:J:202:ALA:O	1:J:206:ALA:N	2.30	0.54
1:J:245:THR:HB	1:J:283:VAL:O	2.07	0.54
1:O:4:LEU:O	1:O:55:VAL:HA	2.08	0.54
1:O:4:LEU:HD23	1:O:55:VAL:HB	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:60:CYS:HB3	1:P:113:ALA:O	2.07	0.54
1:C:274:PHE:HA	1:C:302:LEU:HD11	1.89	0.54
1:E:59:ALA:HB3	1:E:84:VAL:HG22	1.90	0.54
1:J:97:ILE:HG13	1:J:107:ILE:HG23	1.90	0.54
1:N:98:GLN:HE21	1:N:106:SER:HB3	1.73	0.54
1:P:19:PRO:HG2	1:P:28:LEU:HD21	1.89	0.54
1:P:40:LYS:HE3	1:P:165:ALA:HB1	1.88	0.54
1:B:281:ILE:HD11	1:B:298:VAL:CG1	2.38	0.53
1:D:139:LEU:HD11	1:D:170:LEU:HD11	1.89	0.53
1:G:184:ASN:H	1:G:187:GLU:HB2	1.73	0.53
1:H:7:LEU:HD22	1:H:137:MET:SD	2.48	0.53
1:H:64:ASP:OD1	1:H:92:THR:OG1	2.25	0.53
1:L:21:PHE:HE2	1:L:106:SER:HB2	1.73	0.53
1:M:264:GLN:OE1	1:M:295:ARG:NH2	2.42	0.53
1:B:278:ALA:HA	1:B:281:ILE:HG13	1.90	0.53
1:M:18:VAL:HG21	1:M:98:GLN:HB3	1.90	0.53
1:F:207:ASP:HA	1:F:210:HIS:CD2	2.43	0.53
1:G:21:PHE:HE2	1:G:106:SER:HB3	1.72	0.53
1:G:58:ILE:CD1	1:G:125:ASP:HB3	2.38	0.53
1:N:295:ARG:HG2	1:N:295:ARG:NH1	2.23	0.53
1:A:267:PRO:HB2	1:A:269:GLU:OE1	2.09	0.53
1:I:21:PHE:CG	1:I:22:PRO:HD2	2.42	0.53
1:I:132:ALA:O	1:I:158:THR:OG1	2.19	0.53
1:N:168:ARG:HH22	1:P:306:SER:C	2.16	0.53
1:O:3:LYS:HE2	1:O:54:ASP:HB2	1.89	0.53
1:P:206:ALA:O	1:P:209:LEU:HB2	2.07	0.53
1:C:240:PHE:O	1:C:242:VAL:HG13	2.09	0.53
1:H:226:VAL:O	1:H:226:VAL:HG13	2.08	0.53
1:K:12:ALA:HB2	1:K:66:PHE:CZ	2.43	0.53
1:N:220:THR:HA	1:N:226:VAL:HA	1.89	0.53
1:A:181:ILE:HG21	1:A:209:LEU:CD1	2.37	0.53
1:B:189:GLU:O	1:B:193:GLY:N	2.40	0.53
1:B:257:ALA:O	1:B:260:THR:HG22	2.09	0.53
1:C:139:LEU:N	1:C:165:ALA:O	2.29	0.53
1:E:3:LYS:HB3	1:E:263:LEU:HD21	1.91	0.53
1:H:81:THR:HB	1:H:84:VAL:HG12	1.89	0.53
1:H:250:ALA:C	1:H:252:ASP:H	2.17	0.53
1:A:194:ILE:HG22	1:A:196:VAL:H	1.73	0.53
1:B:264:GLN:CD	1:B:295:ARG:HH22	2.16	0.53
1:J:92:THR:HG22	1:J:93:GLY:N	2.23	0.53
1:N:17:GLN:NE2	1:N:32:ASN:OD1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:37:PRO:HB2	1:O:289:GLN:HE22	1.74	0.53
1:B:288:ALA:O	1:B:291:SER:OG	2.23	0.53
1:G:49:ALA:HB1	1:G:77:ASP:O	2.09	0.53
1:H:243:LYS:NZ	1:H:244:ALA:HB3	2.24	0.53
1:I:44:GLN:HE22	1:I:138:GLN:HG2	1.74	0.53
1:K:53:ALA:HB2	1:K:260:THR:HG23	1.90	0.53
1:L:180:LEU:HD21	1:L:218:ILE:HD12	1.91	0.53
1:L:244:ALA:O	1:L:246:ASP:N	2.41	0.53
1:O:175:LEU:HB3	1:O:214:ILE:HD11	1.90	0.53
1:G:21:PHE:O	1:G:23:ARG:N	2.42	0.53
1:N:3:LYS:HE3	1:N:263:LEU:HD12	1.91	0.53
1:P:243:LYS:HE2	1:P:244:ALA:H	1.73	0.53
1:A:19:PRO:HA	1:A:101:ASP:CB	2.39	0.53
1:D:9:SER:HB3	1:D:140:GLU:HB3	1.90	0.53
1:D:197:TYR:CD1	1:D:197:TYR:N	2.77	0.53
1:H:180:LEU:HD23	1:H:181:ILE:N	2.24	0.53
1:G:139:LEU:HD13	1:G:168:ARG:HG2	1.91	0.52
1:G:294:THR:HB	1:G:297:GLU:HB2	1.90	0.52
1:J:188:ALA:HA	1:J:191:LEU:HG	1.89	0.52
1:J:209:LEU:HB3	1:J:214:ILE:HD12	1.90	0.52
1:M:18:VAL:CG2	1:M:98:GLN:HB3	2.39	0.52
1:N:51:MET:HE1	1:N:298:VAL:HG21	1.89	0.52
1:N:139:LEU:N	1:N:165:ALA:O	2.37	0.52
1:N:233:ARG:O	1:N:235:GLN:N	2.41	0.52
1:B:2:ASN:O	1:B:3:LYS:HD3	2.09	0.52
1:J:73:SER:O	1:J:76:LEU:N	2.25	0.52
1:D:138:GLN:HA	1:D:163:ASN:HB3	1.91	0.52
1:I:280:ALA:HA	1:I:283:VAL:HG22	1.90	0.52
1:J:16:LEU:HD11	1:J:30:GLY:HA3	1.91	0.52
1:K:16:LEU:HD11	1:L:110:SER:HB2	1.90	0.52
1:K:188:ALA:O	1:K:192:THR:OG1	2.21	0.52
1:N:266:MET:HB3	1:N:271:ALA:HB2	1.90	0.52
1:O:203:GLN:HB2	1:O:227:TRP:CZ2	2.44	0.52
1:B:15:VAL:HG21	1:B:36:ILE:HD11	1.92	0.52
1:B:184:ASN:HB3	1:B:187:GLU:CD	2.33	0.52
1:H:70:ILE:HD13	1:H:74:PHE:CZ	2.45	0.52
1:J:226:VAL:HG11	1:J:254:PHE:CE2	2.44	0.52
1:L:51:MET:N	1:L:51:MET:SD	2.83	0.52
1:L:111:ALA:O	1:L:114:ASN:N	2.39	0.52
1:M:285:ARG:HB2	1:M:291:SER:HB3	1.90	0.52
1:D:14:HIS:HB2	1:D:95:ALA:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:SER:OG	1:F:112:GLU:OE2	2.23	0.52
1:G:86:LEU:HD23	1:G:86:LEU:N	2.24	0.52
1:I:215:GLU:HG2	1:I:216:ILE:HG13	1.92	0.52
1:B:225:GLY:HA2	1:B:237:ILE:O	2.10	0.52
1:B:245:THR:N	1:B:283:VAL:O	2.42	0.52
1:E:31:ARG:HG3	1:E:32:ASN:H	1.73	0.52
1:E:126:LEU:HB3	1:E:152:GLU:HG2	1.90	0.52
1:G:111:ALA:HA	1:G:114:ASN:ND2	2.24	0.52
1:G:192:THR:HG23	1:G:194:ILE:HG13	1.90	0.52
1:H:64:ASP:OD2	1:H:64:ASP:N	2.41	0.52
1:H:248:THR:OG1	1:H:249:ALA:N	2.42	0.52
1:P:131:ASP:OD2	1:P:132:ALA:N	2.43	0.52
1:P:139:LEU:N	1:P:165:ALA:O	2.33	0.52
1:B:91:PRO:HD2	1:B:112:GLU:CG	2.39	0.52
1:B:117:LEU:O	1:B:142:PRO:HG2	2.09	0.52
1:D:163:ASN:HD22	1:D:164:PRO:CD	2.23	0.52
1:E:147:LEU:O	1:E:151:GLN:HG2	2.09	0.52
1:E:173:GLU:O	1:E:176:LYS:HE3	2.10	0.52
1:F:58:ILE:HD11	1:F:122:ILE:CG2	2.39	0.52
1:N:184:ASN:H	1:N:187:GLU:HB2	1.75	0.52
1:P:14:HIS:CD2	1:P:94:ILE:HD11	2.44	0.52
1:B:221:LEU:HD12	1:B:225:GLY:C	2.34	0.52
1:C:203:GLN:O	1:C:207:ASP:HB2	2.09	0.52
1:E:63:ASP:OD2	1:E:88:PRO:HA	2.09	0.52
1:G:15:VAL:HG12	1:G:34:GLN:O	2.10	0.52
1:G:282:SER:O	1:G:285:ARG:HB2	2.10	0.52
1:H:294:THR:HG23	1:H:297:GLU:OE1	2.10	0.52
1:D:196:VAL:HA	1:D:201:SER:OG	2.10	0.52
1:E:130:ARG:O	1:E:130:ARG:HG2	2.10	0.52
1:G:23:ARG:HB2	1:G:24:PRO:HD2	1.91	0.52
1:H:15:VAL:O	1:H:33:TYR:HA	2.09	0.52
1:H:242:VAL:HG21	1:H:283:VAL:HG21	1.91	0.52
1:K:175:LEU:HD11	1:K:191:LEU:HD21	1.91	0.52
1:L:98:GLN:HB2	1:L:106:SER:HB3	1.92	0.52
1:N:40:LYS:HB3	1:N:138:GLN:HG2	1.91	0.52
1:A:172:ASP:O	1:A:174:LEU:N	2.36	0.51
1:B:74:PHE:O	1:B:76:LEU:N	2.42	0.51
1:B:218:ILE:HD13	1:B:272:ILE:HD11	1.92	0.51
1:C:154:LYS:HG2	1:C:155:THR:HG23	1.92	0.51
1:C:283:VAL:O	1:C:285:ARG:N	2.43	0.51
1:D:240:PHE:HD1	1:D:301:PHE:CE2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:LYS:HB2	1:E:54:ASP:HB3	1.91	0.51
1:G:248:THR:C	1:G:250:ALA:H	2.17	0.51
1:H:16:LEU:HD11	1:H:30:GLY:HA3	1.92	0.51
1:H:92:THR:HG22	1:H:93:GLY:H	1.75	0.51
1:J:159:ASN:HA	1:J:179:ASP:OD2	2.10	0.51
1:A:15:VAL:HG22	1:A:97:ILE:CG2	2.41	0.51
1:C:183:PRO:O	1:C:220:THR:HG23	2.10	0.51
1:D:172:ASP:O	1:D:174:LEU:N	2.43	0.51
1:H:245:THR:HG23	1:H:283:VAL:O	2.10	0.51
1:I:215:GLU:HG3	1:I:231:ASN:OD1	2.10	0.51
1:M:46:VAL:HG13	1:M:292:ILE:HD13	1.92	0.51
1:M:56:GLY:HA2	1:M:80:ASN:HB3	1.92	0.51
1:B:17:GLN:HB2	1:B:31:ARG:HG2	1.92	0.51
1:F:4:LEU:HD23	1:F:55:VAL:CG1	2.41	0.51
1:H:91:PRO:HG2	1:H:112:GLU:HG3	1.92	0.51
1:J:21:PHE:CE2	1:J:106:SER:HB3	2.42	0.51
1:J:46:VAL:HG12	1:J:292:ILE:HD13	1.91	0.51
1:K:48:ALA:O	1:K:53:ALA:HB3	2.10	0.51
1:K:110:SER:OG	1:K:112:GLU:OE2	2.27	0.51
1:L:9:SER:CB	1:L:140:GLU:HG2	2.40	0.51
1:A:21:PHE:CE1	1:A:104:GLU:HB2	2.46	0.51
1:C:42:ALA:O	1:C:46:VAL:HG22	2.10	0.51
1:D:49:ALA:HB1	1:D:77:ASP:O	2.09	0.51
1:E:228:LEU:HD22	1:E:272:ILE:CD1	2.41	0.51
1:F:126:LEU:HA	1:F:129:ILE:HD12	1.92	0.51
1:G:86:LEU:HD23	1:G:86:LEU:H	1.76	0.51
1:G:94:ILE:HG12	1:G:110:SER:HB2	1.92	0.51
1:G:115:ALA:HA	1:G:142:PRO:HD3	1.92	0.51
1:G:249:ALA:HA	1:G:252:ASP:HB2	1.93	0.51
1:I:57:PHE:HD1	1:I:58:ILE:H	1.58	0.51
1:J:72:GLU:O	1:J:75:LYS:HG3	2.11	0.51
1:K:87:GLN:HG3	1:K:116:LYS:HG3	1.91	0.51
1:P:172:ASP:O	1:P:174:LEU:N	2.43	0.51
1:C:46:VAL:HG21	1:C:289:GLN:CG	2.41	0.51
1:G:172:ASP:CG	1:G:212:LYS:HD3	2.35	0.51
1:H:141:THR:HB	1:H:142:PRO:HD2	1.91	0.51
1:A:16:LEU:HD11	1:B:110:SER:HB2	1.92	0.51
1:I:281:ILE:HB	1:I:293:PRO:HG3	1.92	0.51
1:B:11:ASN:O	1:B:11:ASN:ND2	2.43	0.51
1:C:151:GLN:HA	1:C:154:LYS:HB3	1.93	0.51
1:E:210:HIS:CE1	1:E:215:GLU:O	2.64	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:GLU:HG3	1:F:27:THR:H	1.74	0.51
1:F:141:THR:HB	1:F:142:PRO:HD2	1.93	0.51
1:I:3:LYS:HE2	1:I:263:LEU:HG	1.92	0.51
1:L:252:ASP:O	1:L:256:GLY:N	2.43	0.51
1:N:132:ALA:O	1:N:158:THR:OG1	2.17	0.51
1:A:194:ILE:HG13	1:A:205:ALA:HA	1.93	0.51
1:C:28:LEU:HD22	1:C:29:HIS:N	2.26	0.51
1:E:57:PHE:HD1	1:E:58:ILE:H	1.58	0.51
1:E:110:SER:OG	1:E:112:GLU:OE2	2.29	0.51
1:E:135:LEU:CD2	1:E:137:MET:HE2	2.38	0.51
1:H:138:GLN:H	1:H:138:GLN:CD	2.19	0.51
1:H:143:LEU:HG	1:H:168:ARG:NH1	2.26	0.51
1:L:20:SER:OG	1:L:21:PHE:N	2.42	0.51
1:L:294:THR:O	1:L:298:VAL:HG23	2.11	0.51
1:P:220:THR:HA	1:P:226:VAL:HG22	1.91	0.51
1:A:60:CYS:SG	1:A:116:LYS:HB2	2.50	0.51
1:D:221:LEU:O	1:D:224:LYS:HD3	2.11	0.51
1:D:285:ARG:HB3	1:D:291:SER:CA	2.41	0.51
1:F:235:GLN:HG2	1:F:235:GLN:O	2.10	0.51
1:H:142:PRO:O	1:H:146:ILE:HG13	2.11	0.51
1:H:162:LEU:O	1:H:164:PRO:HD3	2.11	0.51
1:H:207:ASP:O	1:H:210:HIS:HB2	2.11	0.51
1:I:57:PHE:CE1	1:I:59:ALA:HB2	2.46	0.51
1:N:119:ALA:N	1:N:144:ASP:OD1	2.29	0.51
1:A:96:MET:O	1:A:108:CYS:N	2.44	0.51
1:L:59:ALA:HB3	1:L:84:VAL:HG13	1.92	0.51
1:L:100:SER:O	1:L:102:SER:N	2.44	0.51
1:E:284:THR:HG23	1:E:285:ARG:HE	1.75	0.50
1:H:185:GLU:CD	1:H:221:LEU:HD23	2.35	0.50
1:I:173:GLU:HA	1:I:176:LYS:HD3	1.93	0.50
1:J:66:PHE:CZ	1:J:70:ILE:HD12	2.46	0.50
1:J:135:LEU:HD22	1:J:160:VAL:HG22	1.93	0.50
1:L:46:VAL:HG12	1:L:292:ILE:HD13	1.92	0.50
1:L:161:ILE:HD13	1:L:259:VAL:HG12	1.92	0.50
1:N:64:ASP:OD1	1:N:67:GLY:N	2.25	0.50
1:O:64:ASP:OD1	1:O:64:ASP:N	2.36	0.50
1:P:71:ARG:HH11	1:P:71:ARG:HB2	1.76	0.50
1:A:69:ASN:O	1:A:73:SER:HB2	2.11	0.50
1:G:4:LEU:O	1:G:55:VAL:HA	2.10	0.50
1:I:60:CYS:SG	1:I:117:LEU:HD13	2.51	0.50
1:P:53:ALA:HB2	1:P:260:THR:CG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:PHE:HA	1:C:304:GLU:HG3	1.92	0.50
1:F:81:THR:HG22	1:F:84:VAL:HG11	1.93	0.50
1:H:250:ALA:C	1:H:252:ASP:N	2.69	0.50
1:I:187:GLU:O	1:I:191:LEU:HD11	2.10	0.50
1:I:239:GLY:HA2	1:I:276:HIS:ND1	2.26	0.50
1:K:139:LEU:HD13	1:K:170:LEU:HD21	1.94	0.50
1:L:7:LEU:HD12	1:L:58:ILE:HG21	1.93	0.50
1:O:77:ASP:OD2	1:O:77:ASP:N	2.43	0.50
1:O:162:LEU:O	1:O:164:PRO:HD3	2.12	0.50
1:P:279:ALA:O	1:P:283:VAL:HG13	2.12	0.50
1:D:178:VAL:HG12	1:D:180:LEU:H	1.77	0.50
1:D:277:ALA:HB1	1:D:301:PHE:HD2	1.76	0.50
1:E:183:PRO:HA	1:E:187:GLU:OE1	2.11	0.50
1:F:62:GLY:HA3	1:F:91:PRO:C	2.36	0.50
1:F:240:PHE:HD1	1:F:301:PHE:HE2	1.59	0.50
1:O:72:GLU:C	1:O:74:PHE:H	2.19	0.50
1:P:66:PHE:CE1	1:P:70:ILE:HD12	2.46	0.50
1:A:16:LEU:CD1	1:B:110:SER:HB2	2.41	0.50
1:A:254:PHE:HA	1:A:275:ALA:HB1	1.94	0.50
1:B:180:LEU:HD21	1:B:218:ILE:HD11	1.94	0.50
1:B:215:GLU:HB3	1:B:216:ILE:HG13	1.93	0.50
1:C:61:VAL:HB	1:C:67:GLY:HA2	1.93	0.50
1:O:237:ILE:HG22	1:O:239:GLY:H	1.75	0.50
1:A:143:LEU:H	1:A:143:LEU:HD12	1.77	0.50
1:B:245:THR:HG21	1:B:286:PHE:CD2	2.43	0.50
1:D:94:ILE:O	1:D:109:ILE:HG13	2.11	0.50
1:D:99:VAL:HA	1:D:105:ASN:CG	2.37	0.50
1:D:282:SER:HA	1:D:285:ARG:HB2	1.94	0.50
1:F:139:LEU:HD13	1:F:168:ARG:HD2	1.92	0.50
1:H:240:PHE:HD1	1:H:301:PHE:CE2	2.18	0.50
1:H:243:LYS:HE2	1:K:101:ASP:H	1.77	0.50
1:N:97:ILE:HG23	1:N:107:ILE:HG23	1.93	0.50
1:O:127:ALA:HA	1:O:130:ARG:NH1	2.27	0.50
1:E:21:PHE:CD2	1:E:22:PRO:HD2	2.47	0.50
1:G:60:CYS:SG	1:G:117:LEU:HD13	2.52	0.50
1:H:133:ARG:O	1:H:159:ASN:N	2.42	0.50
1:H:267:PRO:HD2	1:H:270:SER:HB3	1.94	0.50
1:H:280:ALA:O	1:H:284:THR:HG22	2.12	0.50
1:K:50:ARG:NH1	1:K:292:ILE:HB	2.27	0.50
1:K:137:MET:C	1:K:138:GLN:HE21	2.20	0.50
1:L:228:LEU:HD22	1:L:272:ILE:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:SER:HA	1:O:233:ARG:O	2.11	0.50
1:B:125:ASP:O	1:B:129:ILE:HG12	2.12	0.50
1:B:182:THR:HG21	1:B:255:ASN:HD21	1.77	0.50
1:G:63:ASP:O	1:G:68:ILE:HD11	2.12	0.50
1:J:207:ASP:CG	1:K:232:GLY:HA3	2.36	0.50
1:K:226:VAL:HG11	1:K:272:ILE:HD13	1.93	0.50
1:L:218:ILE:CG2	1:L:226:VAL:HG21	2.41	0.50
1:A:162:LEU:HD23	1:A:181:ILE:HD11	1.94	0.50
1:E:240:PHE:O	1:E:242:VAL:HG12	2.12	0.50
1:H:53:ALA:O	1:H:55:VAL:N	2.45	0.50
1:K:81:THR:O	1:K:84:VAL:HG12	2.12	0.50
1:L:122:ILE:C	1:L:124:PRO:HD2	2.37	0.50
1:L:160:VAL:HG12	1:L:178:VAL:HA	1.94	0.50
1:O:57:PHE:HB2	1:O:79:ILE:CG2	2.41	0.50
1:B:12:ALA:HB2	1:B:66:PHE:CE1	2.47	0.49
1:E:181:ILE:HG21	1:E:209:LEU:HD13	1.94	0.49
1:F:189:GLU:HA	1:F:194:ILE:O	2.12	0.49
1:F:224:LYS:O	1:F:236:ARG:NH1	2.43	0.49
1:G:13:ASP:O	1:G:35:VAL:HA	2.11	0.49
1:H:164:PRO:HG3	1:H:181:ILE:HD11	1.93	0.49
1:H:246:ASP:OD1	1:H:286:PHE:HA	2.11	0.49
1:K:109:ILE:O	1:L:29:HIS:HA	2.12	0.49
1:L:141:THR:HB	1:L:142:PRO:HD2	1.92	0.49
1:M:40:LYS:NZ	1:M:165:ALA:HB3	2.26	0.49
1:O:18:VAL:H	1:O:99:VAL:HG12	1.77	0.49
1:B:167:ALA:HB2	1:B:187:GLU:HB3	1.94	0.49
1:E:184:ASN:HD22	1:E:187:GLU:H	1.57	0.49
1:J:170:LEU:HD12	1:J:174:LEU:HD23	1.94	0.49
1:K:257:ALA:O	1:K:260:THR:N	2.45	0.49
1:L:57:PHE:HD1	1:L:58:ILE:N	2.10	0.49
1:L:91:PRO:HG2	1:L:112:GLU:CB	2.41	0.49
1:L:243:LYS:HB3	1:L:244:ALA:HB2	1.95	0.49
1:M:108:CYS:C	1:M:109:ILE:HD12	2.36	0.49
1:O:40:LYS:HG3	1:O:140:GLU:OE2	2.12	0.49
1:A:247:THR:HA	1:A:250:ALA:HB2	1.93	0.49
1:B:117:LEU:HB3	1:B:141:THR:HG23	1.94	0.49
1:B:264:GLN:O	1:B:266:MET:N	2.45	0.49
1:F:110:SER:OG	1:F:111:ALA:N	2.44	0.49
1:H:26:GLU:HG3	1:H:27:THR:H	1.77	0.49
1:I:248:THR:HG21	1:I:288:ALA:HB1	1.95	0.49
1:L:113:ALA:O	1:L:116:LYS:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:SER:C	1:M:107:ILE:HG13	2.36	0.49
1:N:63:ASP:OD2	1:N:88:PRO:HA	2.12	0.49
1:O:30:GLY:N	1:P:109:ILE:O	2.33	0.49
1:O:176:LYS:HA	1:O:213:GLY:HA3	1.93	0.49
1:P:164:PRO:HG2	1:P:183:PRO:HA	1.93	0.49
1:B:91:PRO:HG2	1:B:112:GLU:HG2	1.93	0.49
1:B:201:SER:HA	1:B:204:GLN:OE1	2.11	0.49
1:E:46:VAL:HG21	1:E:289:GLN:OE1	2.12	0.49
1:F:243:LYS:CD	1:F:244:ALA:H	2.26	0.49
1:H:138:GLN:H	1:H:138:GLN:NE2	2.10	0.49
1:J:46:VAL:O	1:J:50:ARG:HG2	2.13	0.49
1:K:230:GLN:OE1	1:K:233:ARG:NH2	2.43	0.49
1:L:57:PHE:HB2	1:L:79:ILE:HG21	1.92	0.49
1:N:167:ALA:HB1	1:N:190:VAL:HG21	1.94	0.49
1:A:143:LEU:HD21	1:A:168:ARG:HH11	1.77	0.49
1:B:6:VAL:HG11	1:B:45:ALA:HB2	1.95	0.49
1:B:294:THR:OG1	1:B:297:GLU:OE1	2.27	0.49
1:C:29:HIS:HA	1:D:109:ILE:O	2.12	0.49
1:C:51:MET:HG3	1:C:260:THR:HG21	1.94	0.49
1:C:118:THR:H	1:C:121:ALA:HB3	1.77	0.49
1:C:221:LEU:N	1:C:225:GLY:O	2.42	0.49
1:E:6:VAL:O	1:E:58:ILE:N	2.41	0.49
1:E:143:LEU:H	1:I:306:SER:CB	2.24	0.49
1:F:56:GLY:HA2	1:F:80:ASN:HB3	1.93	0.49
1:H:197:TYR:N	1:H:197:TYR:CD1	2.80	0.49
1:H:252:ASP:O	1:H:256:GLY:N	2.41	0.49
1:P:99:VAL:HG12	1:P:105:ASN:CG	2.38	0.49
1:P:184:ASN:H	1:P:187:GLU:HB2	1.78	0.49
1:A:148:LYS:HE3	1:A:152:GLU:HB2	1.94	0.49
1:B:126:LEU:O	1:B:130:ARG:HG3	2.12	0.49
1:B:201:SER:HA	1:B:204:GLN:HG3	1.94	0.49
1:D:147:LEU:O	1:D:151:GLN:HG3	2.12	0.49
1:E:240:PHE:HD1	1:E:301:PHE:HE2	1.58	0.49
1:F:223:SER:HA	1:F:243:LYS:HB3	1.93	0.49
1:H:221:LEU:CD1	1:H:227:TRP:H	2.25	0.49
1:H:306:SER:CB	1:L:143:LEU:H	2.24	0.49
1:I:16:LEU:HD21	1:I:30:GLY:HA3	1.94	0.49
1:I:161:ILE:HG23	1:I:180:LEU:HD22	1.94	0.49
1:I:210:HIS:CE1	1:I:215:GLU:O	2.65	0.49
1:N:253:THR:HB	1:N:282:SER:OG	2.13	0.49
1:O:81:THR:O	1:O:84:VAL:N	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:268:LEU:HD12	1:O:272:ILE:HG13	1.94	0.49
1:P:172:ASP:OD2	1:P:172:ASP:N	2.28	0.49
1:A:138:GLN:HA	1:A:163:ASN:O	2.11	0.49
1:A:231:ASN:OD1	1:A:231:ASN:N	2.44	0.49
1:D:7:LEU:HD13	1:D:58:ILE:CG2	2.40	0.49
1:D:89:ASN:O	1:D:89:ASN:ND2	2.46	0.49
1:E:134:TYR:CD1	1:E:159:ASN:HB2	2.47	0.49
1:J:229:SER:HA	1:J:233:ARG:O	2.11	0.49
1:K:135:LEU:HD21	1:K:137:MET:SD	2.52	0.49
1:K:169:GLU:H	1:K:169:GLU:CD	2.21	0.49
1:M:40:LYS:HZ2	1:M:165:ALA:HB3	1.77	0.49
1:N:99:VAL:HG12	1:N:105:ASN:CG	2.38	0.49
1:O:207:ASP:O	1:O:211:CYS:HB2	2.13	0.49
1:A:97:ILE:HA	1:A:107:ILE:HA	1.94	0.49
1:A:139:LEU:HD13	1:A:168:ARG:HG2	1.95	0.49
1:D:161:ILE:HD13	1:D:259:VAL:HG22	1.94	0.49
1:H:40:LYS:HE3	1:H:165:ALA:C	2.37	0.49
1:H:284:THR:HG23	1:H:285:ARG:H	1.77	0.49
1:J:101:ASP:N	1:J:102:SER:HA	2.28	0.49
1:M:6:VAL:HG13	1:M:136:LEU:HB3	1.94	0.49
1:N:18:VAL:O	1:N:101:ASP:HB2	2.13	0.49
1:O:232:GLY:O	1:O:234:GLY:N	2.46	0.49
1:A:267:PRO:HD2	1:A:270:SER:HB2	1.95	0.49
1:G:33:TYR:CD1	1:H:94:ILE:HD12	2.47	0.49
1:H:7:LEU:HD12	1:H:58:ILE:HG21	1.94	0.49
1:K:93:GLY:HA2	1:K:112:GLU:H	1.76	0.49
1:M:219:ILE:HB	1:M:227:TRP:HB3	1.94	0.49
1:M:243:LYS:HB2	1:P:31:ARG:NE	2.27	0.49
1:N:129:ILE:H	1:N:129:ILE:HD12	1.77	0.49
1:P:47:ALA:HA	1:P:292:ILE:HG21	1.94	0.49
1:A:61:VAL:HG23	1:A:86:LEU:HD23	1.94	0.49
1:A:196:VAL:HG12	1:A:201:SER:O	2.13	0.49
1:E:300:ALA:O	1:E:304:GLU:HG3	2.13	0.49
1:G:187:GLU:O	1:G:191:LEU:HB2	2.13	0.49
1:G:240:PHE:CD1	1:G:301:PHE:HE2	2.30	0.49
1:H:17:GLN:OE1	1:H:32:ASN:ND2	2.46	0.49
1:J:50:ARG:C	1:J:51:MET:HE2	2.38	0.49
1:J:181:ILE:HG23	1:J:183:PRO:HD3	1.94	0.49
1:A:68:ILE:HG13	1:A:69:ASN:N	2.27	0.48
1:A:243:LYS:HB2	1:D:31:ARG:HH12	1.77	0.48
1:A:279:ALA:O	1:A:283:VAL:HG13	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:TRP:CH2	1:C:234:GLY:HA3	2.47	0.48
1:F:230:GLN:HB2	1:F:233:ARG:HG3	1.95	0.48
1:M:17:GLN:HB2	1:M:31:ARG:HG2	1.95	0.48
1:N:62:GLY:H	1:N:92:THR:CG2	2.23	0.48
1:A:99:VAL:HG12	1:A:100:SER:N	2.25	0.48
1:F:230:GLN:NE2	1:F:235:GLN:HE22	2.12	0.48
1:G:50:ARG:C	1:G:52:GLN:H	2.19	0.48
1:G:140:GLU:HG3	1:G:166:PRO:HD3	1.93	0.48
1:G:282:SER:O	1:G:291:SER:OG	2.31	0.48
1:K:126:LEU:CB	1:K:152:GLU:HG2	2.43	0.48
1:L:13:ASP:O	1:L:35:VAL:HA	2.13	0.48
1:M:100:SER:HA	1:M:101:ASP:HB2	1.94	0.48
1:N:37:PRO:O	1:N:289:GLN:HB2	2.12	0.48
1:P:207:ASP:HA	1:P:210:HIS:HD2	1.78	0.48
1:G:8:GLY:C	1:G:41:GLY:HA3	2.38	0.48
1:H:37:PRO:O	1:H:289:GLN:HG3	2.13	0.48
1:H:59:ALA:HB3	1:H:84:VAL:HG23	1.94	0.48
1:H:250:ALA:O	1:H:252:ASP:N	2.46	0.48
1:J:257:ALA:O	1:J:260:THR:HB	2.12	0.48
1:O:104:GLU:HB2	1:P:24:PRO:HB2	1.95	0.48
1:O:133:ARG:O	1:O:134:TYR:HD1	1.96	0.48
1:B:91:PRO:CD	1:B:112:GLU:HG2	2.44	0.48
1:E:215:GLU:HG3	1:E:231:ASN:ND2	2.29	0.48
1:H:70:ILE:HD13	1:H:74:PHE:CE1	2.48	0.48
1:M:63:ASP:OD1	1:M:63:ASP:N	2.39	0.48
1:N:235:GLN:HG3	1:N:236:ARG:N	2.28	0.48
1:P:59:ALA:HA	1:P:117:LEU:HD21	1.94	0.48
1:A:258:LEU:O	1:A:262:LEU:HG	2.14	0.48
1:B:218:ILE:HA	1:B:227:TRP:O	2.14	0.48
1:C:104:GLU:CB	1:D:25:GLY:H	2.27	0.48
1:C:109:ILE:HD12	1:D:29:HIS:HE1	1.77	0.48
1:D:94:ILE:HG22	1:D:110:SER:H	1.77	0.48
1:D:100:SER:CA	1:D:101:ASP:HB3	2.43	0.48
1:E:172:ASP:OD1	1:E:172:ASP:N	2.46	0.48
1:F:12:ALA:HB2	1:F:66:PHE:CZ	2.48	0.48
1:G:138:GLN:HA	1:G:163:ASN:O	2.14	0.48
1:H:26:GLU:HG3	1:H:27:THR:N	2.28	0.48
1:H:127:ALA:HA	1:H:130:ARG:NH2	2.28	0.48
1:I:279:ALA:O	1:I:283:VAL:HG13	2.12	0.48
1:J:43:ASN:OD1	1:J:289:GLN:HG3	2.14	0.48
1:K:41:GLY:N	1:K:138:GLN:OE1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:LEU:O	1:K:146:ILE:N	2.45	0.48
1:K:254:PHE:C	1:K:254:PHE:CD2	2.91	0.48
1:L:49:ALA:HB1	1:L:77:ASP:O	2.14	0.48
1:L:257:ALA:O	1:L:260:THR:N	2.47	0.48
1:M:40:LYS:HZ3	1:M:138:GLN:HB3	1.77	0.48
1:P:11:ASN:HB2	1:P:39:GLY:N	2.28	0.48
1:A:254:PHE:C	1:A:254:PHE:CD2	2.92	0.48
1:B:94:ILE:HG22	1:B:95:ALA:N	2.28	0.48
1:B:172:ASP:O	1:B:174:LEU:N	2.46	0.48
1:C:22:PRO:HG3	1:C:98:GLN:HE22	1.78	0.48
1:D:17:GLN:HG3	1:D:31:ARG:HG2	1.95	0.48
1:G:258:LEU:HB2	1:G:275:ALA:HB2	1.96	0.48
1:H:163:ASN:C	1:H:163:ASN:HD22	2.20	0.48
1:H:245:THR:OG1	1:H:284:THR:O	2.31	0.48
1:I:157:LYS:O	1:I:158:THR:OG1	2.30	0.48
1:I:262:LEU:HD21	1:I:268:LEU:HD12	1.95	0.48
1:I:287:GLY:O	1:I:290:THR:N	2.44	0.48
1:M:166:PRO:O	1:M:168:ARG:HG2	2.14	0.48
1:P:194:ILE:HD12	1:P:205:ALA:HA	1.96	0.48
1:B:197:TYR:CD1	1:B:197:TYR:N	2.80	0.48
1:D:280:ALA:HA	1:D:283:VAL:HG22	1.95	0.48
1:F:101:ASP:CG	1:I:243:LYS:HG3	2.39	0.48
1:F:304:GLU:HB3	1:J:115:ALA:O	2.14	0.48
1:I:57:PHE:HD1	1:I:58:ILE:N	2.12	0.48
1:L:100:SER:O	1:L:100:SER:OG	2.25	0.48
1:M:117:LEU:O	1:M:142:PRO:HG2	2.14	0.48
1:P:13:ASP:HB3	1:P:97:ILE:HD11	1.94	0.48
1:P:240:PHE:O	1:P:242:VAL:N	2.43	0.48
1:G:171:PRO:C	1:G:173:GLU:H	2.22	0.48
1:I:198:ASP:O	1:I:202:ALA:N	2.46	0.48
1:K:106:SER:C	1:K:107:ILE:HG13	2.39	0.48
1:M:61:VAL:HA	1:M:92:THR:HG23	1.96	0.48
1:N:294:THR:H	1:N:297:GLU:HG2	1.77	0.48
1:P:52:GLN:HG3	1:P:295:ARG:HB2	1.95	0.48
1:C:51:MET:HB2	1:C:295:ARG:HD3	1.94	0.48
1:C:270:SER:O	1:C:273:LYS:N	2.39	0.48
1:G:27:THR:HA	1:H:107:ILE:O	2.14	0.48
1:G:147:LEU:HD11	1:G:151:GLN:NE2	2.28	0.48
1:K:99:VAL:HG23	1:K:105:ASN:ND2	2.29	0.48
1:P:209:LEU:HA	1:P:212:LYS:HD3	1.94	0.48
1:D:184:ASN:OD1	1:D:187:GLU:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:VAL:HG22	1:F:97:ILE:HB	1.95	0.48
1:G:58:ILE:HD13	1:G:125:ASP:HB3	1.95	0.48
1:I:6:VAL:HG21	1:I:45:ALA:HB2	1.95	0.48
1:I:14:HIS:ND1	1:I:33:TYR:OH	2.47	0.48
1:I:141:THR:HB	1:I:142:PRO:HD2	1.96	0.48
1:J:285:ARG:HB2	1:J:291:SER:HB3	1.96	0.48
1:L:81:THR:HA	1:L:84:VAL:HG23	1.95	0.48
1:L:284:THR:HG23	1:L:285:ARG:HG3	1.95	0.48
1:M:180:LEU:HG	1:M:216:ILE:HB	1.96	0.48
1:N:20:SER:HB3	1:N:28:LEU:HD21	1.95	0.48
1:N:160:VAL:HB	1:N:178:VAL:HA	1.96	0.48
1:C:71:ARG:O	1:C:75:LYS:HG3	2.14	0.47
1:E:98:GLN:HB2	1:E:106:SER:HB3	1.96	0.47
1:E:197:TYR:N	1:E:197:TYR:CD1	2.82	0.47
1:G:199:ASP:HB3	1:G:227:TRP:HZ3	1.78	0.47
1:I:101:ASP:HA	1:I:102:SER:HA	1.47	0.47
1:J:31:ARG:NH2	1:J:101:ASP:O	2.47	0.47
1:J:228:LEU:HD13	1:J:272:ILE:HD11	1.96	0.47
1:L:91:PRO:HG2	1:L:112:GLU:CG	2.44	0.47
1:L:258:LEU:O	1:L:262:LEU:HG	2.14	0.47
1:M:101:ASP:N	1:M:101:ASP:OD1	2.47	0.47
1:M:109:ILE:O	1:N:29:HIS:HA	2.14	0.47
1:E:183:PRO:O	1:E:220:THR:N	2.41	0.47
1:G:47:ALA:HA	1:G:292:ILE:HG23	1.95	0.47
1:G:261:GLY:C	1:G:263:LEU:N	2.73	0.47
1:M:44:GLN:HG2	1:M:252:ASP:O	2.14	0.47
1:O:58:ILE:HD11	1:O:125:ASP:HB3	1.96	0.47
1:P:28:LEU:HD22	1:P:29:HIS:N	2.29	0.47
1:P:39:GLY:O	1:P:43:ASN:ND2	2.38	0.47
1:A:207:ASP:O	1:A:211:CYS:N	2.39	0.47
1:B:141:THR:HG23	1:B:142:PRO:HD2	1.96	0.47
1:E:17:GLN:H	1:E:17:GLN:HG2	1.48	0.47
1:E:68:ILE:H	1:E:68:ILE:HD12	1.79	0.47
1:E:70:ILE:HG13	1:E:74:PHE:CE1	2.49	0.47
1:E:210:HIS:NE2	1:E:229:SER:O	2.47	0.47
1:F:117:LEU:O	1:F:142:PRO:HG2	2.13	0.47
1:H:41:GLY:N	1:H:138:GLN:OE1	2.40	0.47
1:H:81:THR:HB	1:H:84:VAL:CG1	2.44	0.47
1:H:228:LEU:HD12	1:H:229:SER:H	1.79	0.47
1:J:172:ASP:C	1:J:174:LEU:H	2.22	0.47
1:K:40:LYS:NZ	1:K:165:ALA:HB1	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:ALA:HB1	1:K:227:TRP:CD1	2.48	0.47
1:K:254:PHE:C	1:K:254:PHE:HD2	2.22	0.47
1:O:196:VAL:HG13	1:O:202:ALA:CB	2.44	0.47
1:C:79:ILE:O	1:C:80:ASN:C	2.57	0.47
1:C:170:LEU:HD12	1:C:174:LEU:HD23	1.97	0.47
1:F:294:THR:OG1	1:F:297:GLU:HG3	2.14	0.47
1:H:280:ALA:O	1:H:283:VAL:HG22	2.14	0.47
1:J:2:ASN:HB3	1:J:54:ASP:O	2.13	0.47
1:L:184:ASN:OD1	1:L:187:GLU:N	2.37	0.47
1:L:192:THR:HB	1:L:194:ILE:HD13	1.96	0.47
1:N:212:LYS:O	1:N:214:ILE:HG13	2.14	0.47
1:O:7:LEU:HA	1:O:58:ILE:HB	1.95	0.47
1:O:14:HIS:HD2	1:O:94:ILE:HG23	1.79	0.47
1:A:135:LEU:HD23	1:A:160:VAL:HB	1.95	0.47
1:D:228:LEU:HD22	1:D:272:ILE:HD12	1.96	0.47
1:G:129:ILE:HG23	1:G:135:LEU:HD13	1.97	0.47
1:H:169:GLU:C	1:H:170:LEU:HD23	2.39	0.47
1:H:204:GLN:O	1:H:207:ASP:HB2	2.14	0.47
1:H:302:LEU:HD23	1:H:302:LEU:HA	1.66	0.47
1:I:64:ASP:OD2	1:I:92:THR:OG1	2.33	0.47
1:J:4:LEU:O	1:J:55:VAL:HA	2.15	0.47
1:M:226:VAL:HG12	1:M:227:TRP:N	2.28	0.47
1:O:184:ASN:H	1:O:187:GLU:HB3	1.79	0.47
1:O:257:ALA:O	1:O:261:GLY:N	2.41	0.47
1:F:59:ALA:HA	1:F:117:LEU:CD1	2.45	0.47
1:N:60:CYS:HB2	1:N:117:LEU:HD23	1.95	0.47
1:A:33:TYR:CZ	1:B:94:ILE:HD12	2.50	0.47
1:A:181:ILE:HG23	1:A:183:PRO:CD	2.45	0.47
1:B:4:LEU:O	1:B:56:GLY:N	2.43	0.47
1:B:62:GLY:HA3	1:B:90:CYS:O	2.15	0.47
1:B:110:SER:OG	1:B:111:ALA:N	2.47	0.47
1:D:14:HIS:HD2	1:D:94:ILE:HG13	1.80	0.47
1:D:37:PRO:HB3	1:D:70:ILE:HD11	1.97	0.47
1:D:40:LYS:HB2	1:D:140:GLU:OE1	2.15	0.47
1:D:247:THR:HG22	1:D:248:THR:H	1.79	0.47
1:D:290:THR:HB	1:D:291:SER:H	1.63	0.47
1:F:15:VAL:HG22	1:F:97:ILE:HD12	1.97	0.47
1:F:229:SER:O	1:F:231:ASN:N	2.47	0.47
1:G:75:LYS:C	1:G:78:GLY:H	2.23	0.47
1:H:205:ALA:O	1:H:206:ALA:C	2.57	0.47
1:H:228:LEU:HD22	1:H:272:ILE:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:GLU:CD	1:I:27:THR:H	2.22	0.47
1:I:206:ALA:O	1:I:209:LEU:HB2	2.15	0.47
1:K:5:VAL:HG12	1:K:135:LEU:HD12	1.97	0.47
1:K:150:ALA:O	1:K:153:ALA:HB3	2.14	0.47
1:L:9:SER:OG	1:L:140:GLU:HG2	2.15	0.47
1:L:264:GLN:H	1:L:264:GLN:HG2	1.55	0.47
1:M:240:PHE:O	1:M:242:VAL:N	2.48	0.47
1:P:196:VAL:HG12	1:P:202:ALA:HA	1.96	0.47
1:P:249:ALA:HB1	1:P:292:ILE:HD11	1.96	0.47
1:C:185:GLU:HG2	1:C:221:LEU:HD23	1.97	0.47
1:F:72:GLU:OE1	1:F:75:LYS:HD2	2.15	0.47
1:J:3:LYS:H	1:J:54:ASP:HB3	1.80	0.47
1:J:126:LEU:O	1:J:130:ARG:HG3	2.15	0.47
1:L:57:PHE:HB2	1:L:79:ILE:CG2	2.44	0.47
1:L:61:VAL:HG23	1:L:86:LEU:HD23	1.96	0.47
1:L:147:LEU:HD21	1:L:174:LEU:HB2	1.96	0.47
1:L:207:ASP:HA	1:L:210:HIS:HD2	1.79	0.47
1:O:27:THR:CG2	1:P:107:ILE:HB	2.45	0.47
1:P:167:ALA:HA	1:P:187:GLU:HG2	1.96	0.47
1:D:145:GLY:O	1:D:149:ALA:N	2.39	0.47
1:D:228:LEU:HD22	1:D:272:ILE:CD1	2.44	0.47
1:G:192:THR:O	1:G:194:ILE:HG12	2.14	0.47
1:J:12:ALA:HB2	1:J:66:PHE:CZ	2.50	0.47
1:K:61:VAL:O	1:K:86:LEU:HA	2.15	0.47
1:M:89:ASN:N	1:M:89:ASN:OD1	2.48	0.47
1:N:61:VAL:HG23	1:N:86:LEU:HD23	1.97	0.47
1:O:281:ILE:HA	1:O:284:THR:HG22	1.96	0.47
1:A:116:LYS:O	1:A:118:THR:N	2.48	0.47
1:A:161:ILE:HG23	1:A:180:LEU:HD22	1.97	0.47
1:F:175:LEU:HD22	1:F:214:ILE:HD11	1.96	0.47
1:F:198:ASP:OD2	1:F:201:SER:OG	2.23	0.47
1:F:267:PRO:O	1:F:270:SER:N	2.31	0.47
1:H:241:VAL:HG22	1:K:19:PRO:HG2	1.97	0.47
1:J:190:VAL:HB	1:J:191:LEU:HD23	1.96	0.47
1:K:19:PRO:HA	1:K:101:ASP:HB3	1.96	0.47
1:K:58:ILE:HA	1:K:83:GLY:O	2.15	0.47
1:M:134:TYR:HD1	1:M:161:ILE:HD11	1.80	0.47
1:O:138:GLN:HA	1:O:163:ASN:O	2.15	0.47
1:O:249:ALA:HB2	1:O:288:ALA:HB1	1.96	0.47
1:P:7:LEU:HA	1:P:58:ILE:O	2.15	0.47
1:P:140:GLU:HB2	1:P:166:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PHE:C	1:B:254:PHE:CD2	2.93	0.46
1:D:250:ALA:HA	1:D:252:ASP:H	1.76	0.46
1:E:51:MET:HB2	1:E:260:THR:HG21	1.97	0.46
1:H:228:LEU:HD12	1:H:229:SER:N	2.30	0.46
1:L:19:PRO:HD2	1:L:28:LEU:HD13	1.98	0.46
1:L:182:THR:HG21	1:L:255:ASN:OD1	2.15	0.46
1:N:228:LEU:O	1:N:229:SER:HB2	2.15	0.46
1:P:129:ILE:O	1:P:158:THR:HG21	2.15	0.46
1:A:103:GLY:O	1:A:104:GLU:HG2	2.15	0.46
1:D:2:ASN:HD22	1:D:55:VAL:C	2.22	0.46
1:D:61:VAL:O	1:D:87:GLN:N	2.37	0.46
1:D:204:GLN:O	1:D:207:ASP:HB3	2.15	0.46
1:E:7:LEU:O	1:E:7:LEU:HD23	2.14	0.46
1:E:241:VAL:O	1:E:241:VAL:HG12	2.16	0.46
1:F:287:GLY:HA3	1:F:290:THR:OG1	2.14	0.46
1:G:151:GLN:C	1:G:153:ALA:H	2.23	0.46
1:I:57:PHE:HB2	1:I:79:ILE:CG2	2.45	0.46
1:J:274:PHE:CE1	1:J:298:VAL:HG11	2.50	0.46
1:K:274:PHE:HZ	1:K:295:ARG:HE	1.61	0.46
1:O:17:GLN:O	1:O:31:ARG:N	2.46	0.46
1:O:207:ASP:O	1:O:211:CYS:N	2.45	0.46
1:A:130:ARG:O	1:A:158:THR:OG1	2.32	0.46
1:A:243:LYS:HE2	1:D:31:ARG:HH22	1.80	0.46
1:A:269:GLU:CD	1:A:269:GLU:H	2.23	0.46
1:F:59:ALA:HB3	1:F:84:VAL:HG23	1.97	0.46
1:F:157:LYS:O	1:F:158:THR:OG1	2.32	0.46
1:I:134:TYR:HD1	1:I:161:ILE:HD11	1.80	0.46
1:L:18:VAL:HB	1:L:28:LEU:HD12	1.98	0.46
1:O:244:ALA:HA	1:O:284:THR:HA	1.96	0.46
1:A:171:PRO:O	1:A:175:LEU:HD13	2.15	0.46
1:B:175:LEU:HB3	1:B:214:ILE:HD11	1.97	0.46
1:C:99:VAL:HG23	1:C:105:ASN:OD1	2.16	0.46
1:F:147:LEU:HD21	1:F:174:LEU:HB2	1.96	0.46
1:F:163:ASN:C	1:F:165:ALA:H	2.24	0.46
1:G:72:GLU:C	1:G:74:PHE:H	2.23	0.46
1:H:65:SER:O	1:H:69:ASN:ND2	2.47	0.46
1:H:74:PHE:N	1:H:74:PHE:CD1	2.80	0.46
1:I:7:LEU:HD22	1:I:137:MET:SD	2.55	0.46
1:I:226:VAL:HG11	1:I:272:ILE:HG21	1.97	0.46
1:J:139:LEU:HD13	1:J:168:ARG:HG2	1.98	0.46
1:K:125:ASP:C	1:K:127:ALA:N	2.72	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:ARG:HH22	1:P:243:LYS:HZ2	1.62	0.46
1:C:93:GLY:HA2	1:C:112:GLU:HB2	1.97	0.46
1:C:278:ALA:HA	1:C:281:ILE:HG22	1.97	0.46
1:C:294:THR:O	1:C:298:VAL:HG23	2.16	0.46
1:D:240:PHE:HD1	1:D:301:PHE:HE2	1.62	0.46
1:D:253:THR:O	1:D:257:ALA:N	2.42	0.46
1:E:27:THR:HG23	1:F:107:ILE:O	2.16	0.46
1:G:15:VAL:HG23	1:G:97:ILE:HB	1.98	0.46
1:G:209:LEU:O	1:G:214:ILE:HG12	2.15	0.46
1:N:50:ARG:C	1:N:52:GLN:H	2.22	0.46
1:P:49:ALA:HB2	1:P:55:VAL:HG11	1.96	0.46
1:P:64:ASP:N	1:P:64:ASP:OD1	2.49	0.46
1:C:151:GLN:CA	1:C:154:LYS:HD3	2.43	0.46
1:C:154:LYS:HG2	1:C:155:THR:N	2.29	0.46
1:C:240:PHE:CE2	1:C:301:PHE:HE2	2.32	0.46
1:E:72:GLU:OE1	1:E:75:LYS:HD2	2.14	0.46
1:F:224:LYS:HB3	1:F:236:ARG:HH12	1.80	0.46
1:I:207:ASP:O	1:I:210:HIS:HB2	2.15	0.46
1:K:51:MET:O	1:K:260:THR:HG21	2.16	0.46
1:K:51:MET:HA	1:K:295:ARG:HG2	1.98	0.46
1:N:218:ILE:HD13	1:N:272:ILE:HD11	1.98	0.46
1:N:298:VAL:O	1:N:301:PHE:HB3	2.16	0.46
1:O:68:ILE:C	1:O:70:ILE:H	2.24	0.46
1:P:258:LEU:O	1:P:262:LEU:HG	2.16	0.46
1:A:254:PHE:C	1:A:254:PHE:HD2	2.24	0.46
1:C:220:THR:HA	1:C:226:VAL:HA	1.97	0.46
1:E:142:PRO:O	1:E:146:ILE:HG13	2.16	0.46
1:F:4:LEU:O	1:F:55:VAL:HA	2.15	0.46
1:G:184:ASN:CG	1:G:185:GLU:N	2.74	0.46
1:H:66:PHE:O	1:H:69:ASN:N	2.49	0.46
1:I:81:THR:HG22	1:I:84:VAL:HG21	1.98	0.46
1:I:210:HIS:HE1	1:I:215:GLU:O	1.99	0.46
1:M:185:GLU:O	1:M:189:GLU:HG3	2.16	0.46
1:N:1:MET:HE2	1:N:131:ASP:OD2	2.16	0.46
1:P:7:LEU:HD22	1:P:137:MET:SD	2.55	0.46
1:P:143:LEU:HD21	1:P:168:ARG:NH1	2.30	0.46
1:C:209:LEU:C	1:C:211:CYS:N	2.74	0.46
1:C:299:GLU:O	1:C:300:ALA:C	2.59	0.46
1:D:153:ALA:O	1:D:156:ALA:N	2.36	0.46
1:F:81:THR:HB	1:F:82:ALA:H	1.62	0.46
1:G:47:ALA:HB2	1:G:292:ILE:HG12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:PRO:HB2	1:H:289:GLN:HE21	1.81	0.46
1:H:228:LEU:HD22	1:H:272:ILE:CD1	2.46	0.46
1:J:117:LEU:HD23	1:J:141:THR:HG21	1.97	0.46
1:L:11:ASN:OD1	1:L:12:ALA:N	2.48	0.46
1:M:42:ALA:O	1:M:46:VAL:HG12	2.15	0.46
1:A:216:ILE:CG2	1:A:268:LEU:HD11	2.46	0.46
1:E:206:ALA:HA	1:E:217:VAL:HG11	1.98	0.46
1:E:228:LEU:HD22	1:E:272:ILE:HD12	1.98	0.46
1:G:261:GLY:O	1:G:264:GLN:N	2.49	0.46
1:K:61:VAL:HG23	1:K:86:LEU:CD2	2.46	0.46
1:K:138:GLN:N	1:K:138:GLN:NE2	2.60	0.46
1:M:132:ALA:O	1:M:158:THR:OG1	2.16	0.46
1:H:19:PRO:HA	1:H:101:ASP:CB	2.46	0.46
1:H:97:ILE:H	1:H:97:ILE:HG13	1.59	0.46
1:H:280:ALA:HA	1:H:283:VAL:CG2	2.45	0.46
1:I:22:PRO:HG3	1:I:98:GLN:NE2	2.31	0.46
1:K:184:ASN:ND2	1:K:187:GLU:OE2	2.49	0.46
1:K:236:ARG:NH2	1:K:238:PRO:HA	2.31	0.46
1:L:172:ASP:C	1:L:174:LEU:H	2.24	0.46
1:N:233:ARG:O	1:N:233:ARG:HG2	2.16	0.46
1:B:168:ARG:HH22	1:D:306:SER:C	2.24	0.45
1:D:184:ASN:C	1:D:186:THR:H	2.24	0.45
1:D:286:PHE:HD2	1:D:286:PHE:O	1.99	0.45
1:E:3:LYS:O	1:E:133:ARG:N	2.45	0.45
1:F:51:MET:HE2	1:F:51:MET:HA	1.98	0.45
1:F:277:ALA:O	1:F:280:ALA:N	2.49	0.45
1:G:274:PHE:HE1	1:G:298:VAL:HG11	1.81	0.45
1:I:261:GLY:O	1:I:264:GLN:N	2.49	0.45
1:J:13:ASP:HB3	1:J:97:ILE:HD12	1.98	0.45
1:K:139:LEU:CD1	1:K:170:LEU:HD21	2.46	0.45
1:K:277:ALA:HB2	1:K:302:LEU:HD21	1.98	0.45
1:N:189:GLU:OE1	1:N:195:THR:HG23	2.15	0.45
1:N:203:GLN:HE21	1:N:203:GLN:HB2	1.59	0.45
1:O:3:LYS:H	1:O:54:ASP:HB3	1.80	0.45
1:B:57:PHE:CE1	1:B:59:ALA:HB2	2.51	0.45
1:C:277:ALA:O	1:C:281:ILE:HG22	2.15	0.45
1:E:130:ARG:HB2	1:E:156:ALA:CB	2.47	0.45
1:G:8:GLY:HA3	1:G:41:GLY:HA3	1.99	0.45
1:H:21:PHE:O	1:H:23:ARG:N	2.49	0.45
1:K:61:VAL:HG23	1:K:86:LEU:HD22	1.98	0.45
1:L:179:ASP:N	1:L:179:ASP:OD1	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:SER:O	1:O:229:SER:OG	2.33	0.45
1:O:247:THR:O	1:O:248:THR:HG23	2.17	0.45
1:B:43:ASN:C	1:B:45:ALA:H	2.24	0.45
1:C:4:LEU:CD2	1:C:55:VAL:HG23	2.46	0.45
1:F:122:ILE:O	1:F:126:LEU:N	2.49	0.45
1:G:259:VAL:O	1:G:263:LEU:HB2	2.17	0.45
1:H:300:ALA:O	1:H:304:GLU:HG3	2.16	0.45
1:J:240:PHE:CE1	1:J:273:LYS:HE3	2.49	0.45
1:J:260:THR:O	1:J:264:GLN:HB2	2.17	0.45
1:M:65:SER:O	1:M:69:ASN:ND2	2.47	0.45
1:P:126:LEU:O	1:P:130:ARG:HG2	2.15	0.45
1:P:243:LYS:H	1:P:283:VAL:HG21	1.82	0.45
1:A:1:MET:O	1:A:3:LYS:NZ	2.40	0.45
1:B:66:PHE:HA	1:B:69:ASN:HB2	1.99	0.45
1:D:139:LEU:HD13	1:D:168:ARG:HG2	1.99	0.45
1:E:61:VAL:HG23	1:E:92:THR:HG23	1.97	0.45
1:E:251:GLY:HA2	1:E:254:PHE:CB	2.42	0.45
1:G:234:GLY:O	1:G:235:GLN:CB	2.64	0.45
1:H:163:ASN:O	1:H:165:ALA:N	2.48	0.45
1:C:254:PHE:C	1:C:254:PHE:CD2	2.94	0.45
1:F:267:PRO:HD2	1:F:270:SER:CB	2.43	0.45
1:I:20:SER:OG	1:I:21:PHE:N	2.48	0.45
1:I:40:LYS:O	1:I:42:ALA:N	2.49	0.45
1:J:134:TYR:OH	1:J:262:LEU:HB3	2.16	0.45
1:K:105:ASN:OD1	1:K:105:ASN:N	2.50	0.45
1:O:236:ARG:HH12	1:O:238:PRO:CA	2.29	0.45
1:E:249:ALA:O	1:E:252:ASP:HB2	2.15	0.45
1:E:281:ILE:O	1:E:284:THR:HG22	2.15	0.45
1:H:99:VAL:HG12	1:H:105:ASN:HB3	1.99	0.45
1:H:135:LEU:HD21	1:H:137:MET:SD	2.57	0.45
1:H:197:TYR:N	1:H:197:TYR:HD1	2.14	0.45
1:I:137:MET:O	1:I:162:LEU:HD12	2.17	0.45
1:J:137:MET:HE1	1:J:150:ALA:HB2	1.99	0.45
1:J:212:LYS:O	1:J:214:ILE:HG13	2.15	0.45
1:K:64:ASP:HB3	1:K:67:GLY:H	1.82	0.45
1:K:189:GLU:O	1:K:193:GLY:N	2.42	0.45
1:L:221:LEU:HD12	1:L:226:VAL:HA	1.99	0.45
1:M:31:ARG:HH22	1:P:243:LYS:NZ	2.15	0.45
1:M:249:ALA:O	1:M:252:ASP:N	2.49	0.45
1:N:3:LYS:CB	1:N:54:ASP:HB3	2.47	0.45
1:O:104:GLU:HB2	1:P:24:PRO:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:240:PHE:N	1:P:242:VAL:HG13	2.32	0.45
1:A:184:ASN:H	1:A:187:GLU:HB2	1.81	0.45
1:B:262:LEU:HD21	1:B:268:LEU:HD12	1.97	0.45
1:B:276:HIS:HA	1:B:279:ALA:HB3	1.97	0.45
1:E:87:GLN:HA	1:E:88:PRO:HD3	1.79	0.45
1:F:87:GLN:HA	1:F:88:PRO:HD3	1.74	0.45
1:H:97:ILE:HD12	1:H:97:ILE:O	2.16	0.45
1:I:281:ILE:O	1:I:285:ARG:HB2	2.17	0.45
1:L:154:LYS:HE3	1:L:154:LYS:HB3	1.85	0.45
1:O:273:LYS:HA	1:O:276:HIS:HB2	1.99	0.45
1:P:163:ASN:HD22	1:P:164:PRO:HD2	1.82	0.45
1:P:198:ASP:OD1	1:P:198:ASP:N	2.50	0.45
1:B:172:ASP:HA	1:B:175:LEU:CD1	2.47	0.45
1:C:58:ILE:HA	1:C:83:GLY:O	2.16	0.45
1:G:274:PHE:O	1:G:277:ALA:HB3	2.17	0.45
1:H:18:VAL:HG23	1:H:100:SER:HA	1.98	0.45
1:K:20:SER:OG	1:K:28:LEU:HD21	2.16	0.45
1:M:138:GLN:O	1:M:139:LEU:HD23	2.17	0.45
1:M:294:THR:H	1:M:297:GLU:HG3	1.82	0.45
1:O:7:LEU:HD22	1:O:137:MET:SD	2.57	0.45
1:O:26:GLU:HG3	1:O:27:THR:N	2.32	0.45
1:O:31:ARG:HG2	1:O:32:ASN:HB2	1.99	0.45
1:P:281:ILE:HD12	1:P:298:VAL:HG22	1.98	0.45
1:A:181:ILE:HG23	1:A:183:PRO:HD2	1.98	0.45
1:C:228:LEU:HD12	1:C:229:SER:H	1.82	0.45
1:D:19:PRO:O	1:D:102:SER:OG	2.33	0.45
1:D:172:ASP:C	1:D:174:LEU:N	2.73	0.45
1:D:178:VAL:HG11	1:D:181:ILE:HG12	1.99	0.45
1:E:182:THR:N	1:E:183:PRO:HD3	2.31	0.45
1:G:10:VAL:HG22	1:G:42:ALA:HB2	1.97	0.45
1:H:192:THR:HB	1:H:194:ILE:HG12	1.99	0.45
1:H:235:GLN:NE2	1:H:237:ILE:HD11	2.31	0.45
1:H:245:THR:O	1:H:246:ASP:C	2.59	0.45
1:K:163:ASN:C	1:K:165:ALA:H	2.25	0.45
1:L:60:CYS:SG	1:L:117:LEU:HD13	2.57	0.45
1:L:186:THR:OG1	1:L:187:GLU:N	2.50	0.45
1:M:64:ASP:N	1:M:64:ASP:OD1	2.49	0.45
1:N:66:PHE:CE1	1:N:70:ILE:HD12	2.52	0.45
1:N:216:ILE:CG1	1:N:268:LEU:HD21	2.46	0.45
1:N:255:ASN:O	1:N:259:VAL:HG12	2.17	0.45
1:O:44:GLN:HE21	1:O:44:GLN:H	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASN:C	1:B:11:ASN:HD22	2.25	0.45
1:B:61:VAL:HG12	1:B:92:THR:HG21	1.98	0.45
1:C:289:GLN:O	1:C:290:THR:OG1	2.27	0.45
1:D:197:TYR:HD1	1:D:197:TYR:N	2.12	0.45
1:G:249:ALA:CA	1:G:252:ASP:HB2	2.47	0.45
1:H:40:LYS:C	1:H:42:ALA:N	2.75	0.45
1:I:18:VAL:HG11	1:I:98:GLN:HB3	1.98	0.45
1:J:126:LEU:HD22	1:J:152:GLU:HG2	1.99	0.45
1:J:178:VAL:HG12	1:J:214:ILE:HG23	1.99	0.45
1:M:178:VAL:C	1:M:214:ILE:HG23	2.42	0.45
1:N:21:PHE:CD2	1:N:22:PRO:HD2	2.52	0.45
1:O:47:ALA:HB2	1:O:253:THR:HA	1.99	0.45
1:B:97:ILE:HG23	1:B:107:ILE:HG23	1.99	0.44
1:D:226:VAL:HG12	1:D:276:HIS:NE2	2.32	0.44
1:E:264:GLN:OE1	1:E:295:ARG:NH2	2.50	0.44
1:F:175:LEU:HB3	1:F:214:ILE:HD11	2.00	0.44
1:H:71:ARG:NE	1:H:72:GLU:OE2	2.49	0.44
1:J:191:LEU:HD23	1:J:191:LEU:N	2.33	0.44
1:J:227:TRP:CZ2	1:J:234:GLY:HA3	2.52	0.44
1:L:248:THR:HG1	1:L:249:ALA:H	1.56	0.44
1:O:50:ARG:HG3	1:O:292:ILE:HG22	1.99	0.44
1:O:273:LYS:O	1:O:276:HIS:HB2	2.17	0.44
1:P:217:VAL:HG13	1:P:229:SER:HB3	1.98	0.44
1:P:281:ILE:CD1	1:P:298:VAL:HG22	2.48	0.44
1:A:122:ILE:O	1:A:125:ASP:HB2	2.18	0.44
1:A:132:ALA:O	1:A:158:THR:OG1	2.32	0.44
1:B:79:ILE:HD11	1:B:81:THR:HG22	1.98	0.44
1:B:218:ILE:HG22	1:B:226:VAL:HG12	1.99	0.44
1:D:64:ASP:OD1	1:D:92:THR:HG23	2.17	0.44
1:D:164:PRO:HG2	1:D:183:PRO:HB3	1.99	0.44
1:F:66:PHE:CD1	1:F:67:GLY:N	2.86	0.44
1:I:18:VAL:HG22	1:I:100:SER:HA	1.97	0.44
1:K:184:ASN:OD1	1:K:185:GLU:N	2.49	0.44
1:N:125:ASP:O	1:N:128:ALA:N	2.48	0.44
1:O:111:ALA:O	1:O:112:GLU:C	2.59	0.44
1:P:153:ALA:HA	1:P:158:THR:HG22	1.99	0.44
1:D:16:LEU:O	1:D:98:GLN:HA	2.17	0.44
1:D:281:ILE:HD11	1:D:298:VAL:HA	1.98	0.44
1:E:184:ASN:HD21	1:E:187:GLU:HG3	1.82	0.44
1:F:199:ASP:OD1	1:F:236:ARG:HG3	2.17	0.44
1:G:267:PRO:CD	1:G:270:SER:HB2	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:VAL:O	1:H:135:LEU:HD12	2.17	0.44
1:L:7:LEU:HD12	1:L:58:ILE:CG2	2.47	0.44
1:L:143:LEU:HA	1:L:146:ILE:HB	1.98	0.44
1:M:18:VAL:HB	1:M:28:LEU:HD21	1.98	0.44
1:M:40:LYS:NZ	1:M:138:GLN:HB3	2.33	0.44
1:N:46:VAL:O	1:N:50:ARG:HB2	2.17	0.44
1:N:178:VAL:HG13	1:N:214:ILE:HG23	1.99	0.44
1:P:185:GLU:OE2	1:P:221:LEU:HA	2.18	0.44
1:A:162:LEU:HB3	1:A:181:ILE:HD12	1.99	0.44
1:B:59:ALA:HA	1:B:117:LEU:HD21	2.00	0.44
1:B:264:GLN:OE1	1:B:295:ARG:NH2	2.51	0.44
1:C:305:HIS:O	1:C:306:SER:OG	2.27	0.44
1:D:240:PHE:CE1	1:D:301:PHE:CE2	3.06	0.44
1:F:248:THR:C	1:F:250:ALA:H	2.26	0.44
1:G:139:LEU:O	1:G:166:PRO:HD2	2.18	0.44
1:H:306:SER:O	1:L:168:ARG:NH1	2.50	0.44
1:I:13:ASP:O	1:I:35:VAL:HA	2.17	0.44
1:I:93:GLY:HA2	1:I:112:GLU:HB2	1.99	0.44
1:I:119:ALA:N	1:I:144:ASP:OD1	2.39	0.44
1:I:292:ILE:HA	1:I:293:PRO:HD3	1.67	0.44
1:K:137:MET:HE3	1:K:146:ILE:HG23	1.99	0.44
1:K:240:PHE:O	1:K:242:VAL:N	2.51	0.44
1:M:51:MET:HE1	1:M:298:VAL:CG2	2.46	0.44
1:P:18:VAL:HB	1:P:28:LEU:HD11	1.98	0.44
1:P:172:ASP:C	1:P:174:LEU:H	2.26	0.44
1:P:280:ALA:HA	1:P:283:VAL:HG22	2.00	0.44
1:B:43:ASN:O	1:B:45:ALA:N	2.50	0.44
1:D:3:LYS:HG2	1:D:3:LYS:H	1.55	0.44
1:E:254:PHE:CD1	1:E:275:ALA:HB1	2.53	0.44
1:H:203:GLN:HG2	1:O:207:ASP:OD2	2.17	0.44
1:I:10:VAL:HG11	1:I:70:ILE:HG21	1.99	0.44
1:I:22:PRO:HG3	1:I:98:GLN:HE22	1.83	0.44
1:K:58:ILE:HD11	1:K:125:ASP:HB3	1.98	0.44
1:K:273:LYS:O	1:K:275:ALA:N	2.50	0.44
1:L:229:SER:HA	1:L:234:GLY:HA2	1.98	0.44
1:M:173:GLU:O	1:M:176:LYS:HG2	2.17	0.44
1:M:258:LEU:O	1:M:262:LEU:HG	2.18	0.44
1:A:207:ASP:HA	1:A:210:HIS:HB2	2.00	0.44
1:F:3:LYS:HE3	1:F:54:ASP:HB2	2.00	0.44
1:F:7:LEU:HA	1:F:58:ILE:HG23	2.00	0.44
1:F:15:VAL:CG2	1:F:97:ILE:HD12	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:ASP:N	1:H:77:ASP:OD1	2.51	0.44
1:J:254:PHE:CD1	1:J:275:ALA:HB1	2.51	0.44
1:L:18:VAL:O	1:L:100:SER:HA	2.17	0.44
1:L:21:PHE:HE2	1:L:106:SER:CB	2.31	0.44
1:L:87:GLN:HB3	1:L:90:CYS:CB	2.47	0.44
1:N:117:LEU:O	1:N:142:PRO:HG2	2.17	0.44
1:N:170:LEU:HD12	1:N:191:LEU:HD21	1.98	0.44
1:N:246:ASP:CG	1:N:287:GLY:H	2.23	0.44
1:O:115:ALA:HA	1:O:142:PRO:HD3	1.99	0.44
1:O:258:LEU:O	1:O:262:LEU:HG	2.18	0.44
1:P:5:VAL:HG11	1:P:129:ILE:HD13	1.99	0.44
1:A:31:ARG:HE	1:D:241:VAL:CG2	2.30	0.44
1:A:206:ALA:O	1:A:209:LEU:HB2	2.18	0.44
1:B:164:PRO:HG2	1:B:183:PRO:HB3	1.99	0.44
1:C:63:ASP:OD2	1:C:88:PRO:HA	2.18	0.44
1:C:218:ILE:HG23	1:C:226:VAL:HG13	1.99	0.44
1:E:184:ASN:HA	1:E:220:THR:O	2.18	0.44
1:F:41:GLY:N	1:F:138:GLN:OE1	2.50	0.44
1:F:43:ASN:OD1	1:F:289:GLN:HG2	2.18	0.44
1:F:100:SER:HB3	1:F:104:GLU:O	2.17	0.44
1:F:150:ALA:HB1	1:F:177:CYS:HB2	1.99	0.44
1:F:285:ARG:HH22	1:F:293:PRO:HB3	1.83	0.44
1:G:52:GLN:HG2	1:G:295:ARG:HG2	2.00	0.44
1:I:21:PHE:CZ	1:J:24:PRO:HA	2.53	0.44
1:J:181:ILE:HG22	1:J:217:VAL:HG22	1.99	0.44
1:K:235:GLN:HB3	1:K:236:ARG:H	1.49	0.44
1:L:147:LEU:CD2	1:L:174:LEU:HB2	2.47	0.44
1:N:51:MET:CB	1:N:260:THR:HG21	2.42	0.44
1:N:67:GLY:O	1:N:70:ILE:HG22	2.17	0.44
1:O:117:LEU:O	1:O:142:PRO:HG2	2.18	0.44
1:O:161:ILE:HD12	1:O:259:VAL:HG23	1.99	0.44
1:P:61:VAL:HG23	1:P:86:LEU:HB3	1.98	0.44
1:A:57:PHE:CE1	1:A:59:ALA:HB2	2.53	0.44
1:B:249:ALA:CA	1:B:252:ASP:HB2	2.48	0.44
1:C:46:VAL:O	1:C:50:ARG:HB2	2.18	0.44
1:D:99:VAL:HG13	1:D:105:ASN:HD21	1.83	0.44
1:D:184:ASN:CG	1:D:187:GLU:HG3	2.43	0.44
1:F:138:GLN:HG3	1:F:163:ASN:HB3	1.99	0.44
1:G:134:TYR:CD1	1:G:161:ILE:HD11	2.48	0.44
1:I:66:PHE:O	1:I:69:ASN:N	2.51	0.44
1:I:143:LEU:O	1:I:146:ILE:HB	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:GLY:HA3	1:J:114:ASN:HD21	1.83	0.44
1:K:162:LEU:HB3	1:K:178:VAL:HG11	2.00	0.44
1:K:240:PHE:CE2	1:K:301:PHE:HE2	2.35	0.44
1:L:123:GLU:HA	1:L:126:LEU:HG	1.99	0.44
1:P:209:LEU:HA	1:P:209:LEU:HD22	1.77	0.44
1:A:81:THR:HA	1:A:84:VAL:HG23	2.00	0.44
1:B:40:LYS:HA	1:B:252:ASP:OD1	2.18	0.44
1:B:50:ARG:HD2	1:B:292:ILE:HG22	2.00	0.44
1:C:203:GLN:HA	1:C:203:GLN:OE1	2.18	0.44
1:D:71:ARG:O	1:D:81:THR:HG21	2.18	0.44
1:F:139:LEU:O	1:F:166:PRO:HD2	2.18	0.44
1:H:205:ALA:O	1:H:208:ALA:N	2.51	0.44
1:H:285:ARG:NH2	1:H:293:PRO:HB3	2.33	0.44
1:H:306:SER:HB3	1:L:168:ARG:HH12	1.83	0.44
1:I:104:GLU:HG3	1:I:105:ASN:H	1.82	0.44
1:J:117:LEU:O	1:J:142:PRO:HG2	2.17	0.44
1:J:228:LEU:HD22	1:J:272:ILE:HD12	1.99	0.44
1:K:8:GLY:HA2	1:K:141:THR:HG21	1.99	0.44
1:K:110:SER:O	1:K:112:GLU:N	2.50	0.44
1:K:172:ASP:OD2	1:K:172:ASP:N	2.51	0.44
1:L:170:LEU:HB3	1:L:174:LEU:HD23	2.00	0.44
1:L:216:ILE:HG21	1:L:268:LEU:HD21	2.00	0.44
1:M:15:VAL:O	1:M:33:TYR:HA	2.18	0.44
1:N:254:PHE:CD2	1:N:254:PHE:C	2.96	0.44
1:O:128:ALA:O	1:O:132:ALA:HB2	2.16	0.44
1:O:228:LEU:HD11	1:O:230:GLN:OE1	2.18	0.44
1:B:165:ALA:HB2	1:B:187:GLU:OE1	2.18	0.43
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.77	0.43
1:E:147:LEU:HD12	1:E:151:GLN:HE21	1.83	0.43
1:E:228:LEU:HD12	1:E:229:SER:H	1.83	0.43
1:F:44:GLN:HG2	1:F:252:ASP:O	2.18	0.43
1:F:101:ASP:HA	1:F:102:SER:HA	1.80	0.43
1:G:91:PRO:HD2	1:G:112:GLU:HB3	1.99	0.43
1:K:240:PHE:CD2	1:K:301:PHE:HE2	2.36	0.43
1:M:304:GLU:H	1:M:304:GLU:HG2	1.47	0.43
1:N:112:GLU:OE1	1:N:112:GLU:HA	2.18	0.43
1:O:96:MET:HE3	1:P:96:MET:HB3	2.00	0.43
1:P:138:GLN:HA	1:P:163:ASN:O	2.18	0.43
1:A:56:GLY:CA	1:A:80:ASN:HB3	2.48	0.43
1:A:172:ASP:OD1	1:A:212:LYS:HD3	2.18	0.43
1:B:7:LEU:HD22	1:B:137:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ARG:NE	1:D:77:ASP:OD1	2.51	0.43
1:D:289:GLN:HA	1:D:292:ILE:HD12	2.00	0.43
1:I:40:LYS:O	1:I:43:ASN:N	2.51	0.43
1:J:249:ALA:O	1:J:252:ASP:HB2	2.18	0.43
1:K:129:ILE:HG21	1:K:153:ALA:HB2	1.99	0.43
1:K:261:GLY:O	1:K:262:LEU:C	2.61	0.43
1:L:170:LEU:HD13	1:L:174:LEU:HD23	2.00	0.43
1:L:254:PHE:CD1	1:L:275:ALA:HB1	2.53	0.43
1:M:172:ASP:C	1:M:174:LEU:N	2.76	0.43
1:M:243:LYS:HB2	1:P:31:ARG:CD	2.47	0.43
1:O:199:ASP:HA	1:O:227:TRP:HZ3	1.82	0.43
1:P:216:ILE:HG12	1:P:230:GLN:HA	1.99	0.43
1:A:221:LEU:O	1:A:223:SER:N	2.52	0.43
1:A:240:PHE:CE2	1:A:301:PHE:HE2	2.36	0.43
1:B:100:SER:HA	1:B:101:ASP:C	2.43	0.43
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.76	0.43
1:D:180:LEU:HA	1:D:216:ILE:O	2.18	0.43
1:F:66:PHE:HD1	1:F:67:GLY:N	2.17	0.43
1:F:148:LYS:HD3	1:F:148:LYS:HA	1.77	0.43
1:G:196:VAL:HG13	1:G:202:ALA:HB2	1.99	0.43
1:J:281:ILE:O	1:J:285:ARG:HG3	2.18	0.43
1:K:298:VAL:O	1:K:301:PHE:HB3	2.17	0.43
1:L:5:VAL:O	1:L:135:LEU:HA	2.18	0.43
1:M:33:TYR:HB3	1:N:112:GLU:OE2	2.18	0.43
1:M:282:SER:HB2	1:M:293:PRO:HD3	2.00	0.43
1:N:1:MET:HE3	1:N:128:ALA:HA	2.00	0.43
1:N:111:ALA:O	1:N:113:ALA:N	2.52	0.43
1:B:79:ILE:O	1:B:79:ILE:HG13	2.16	0.43
1:B:216:ILE:HG21	1:B:268:LEU:CD2	2.48	0.43
1:C:21:PHE:CD2	1:C:22:PRO:HD2	2.52	0.43
1:C:210:HIS:HA	1:C:214:ILE:O	2.19	0.43
1:E:184:ASN:ND2	1:E:184:ASN:C	2.74	0.43
1:E:294:THR:H	1:E:297:GLU:CD	2.27	0.43
1:H:163:ASN:C	1:H:163:ASN:ND2	2.75	0.43
1:H:203:GLN:OE1	1:H:227:TRP:NE1	2.45	0.43
1:I:64:ASP:OD2	1:I:64:ASP:N	2.48	0.43
1:J:135:LEU:HD13	1:J:153:ALA:HB2	2.00	0.43
1:J:162:LEU:O	1:J:164:PRO:HD3	2.19	0.43
1:J:197:TYR:CD1	1:J:197:TYR:N	2.86	0.43
1:L:87:GLN:HB3	1:L:90:CYS:HB3	2.01	0.43
1:M:249:ALA:C	1:M:251:GLY:N	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:221:LEU:N	1:N:225:GLY:O	2.38	0.43
1:O:98:GLN:HE21	1:P:96:MET:HE3	1.84	0.43
1:O:139:LEU:HD11	1:O:170:LEU:HD11	1.99	0.43
1:D:15:VAL:HG22	1:D:97:ILE:HG13	1.99	0.43
1:E:206:ALA:CB	1:E:217:VAL:HG11	2.48	0.43
1:F:17:GLN:CD	1:I:243:LYS:HZ2	2.25	0.43
1:F:111:ALA:O	1:F:112:GLU:C	2.61	0.43
1:G:2:ASN:HA	1:G:54:ASP:OD2	2.18	0.43
1:J:172:ASP:C	1:J:174:LEU:N	2.75	0.43
1:L:17:GLN:HG3	1:L:32:ASN:HB2	2.00	0.43
1:L:274:PHE:CZ	1:L:295:ARG:NE	2.87	0.43
1:M:19:PRO:HG3	1:P:241:VAL:HG23	2.01	0.43
1:M:199:ASP:OD1	1:M:199:ASP:N	2.30	0.43
1:M:243:LYS:HB2	1:P:31:ARG:HD2	1.99	0.43
1:O:3:LYS:HE2	1:O:54:ASP:CB	2.48	0.43
1:O:81:THR:O	1:O:84:VAL:HG23	2.18	0.43
1:P:97:ILE:HD12	1:P:97:ILE:N	2.34	0.43
1:A:19:PRO:HD2	1:A:28:LEU:CD2	2.49	0.43
1:A:64:ASP:C	1:A:66:PHE:N	2.70	0.43
1:A:196:VAL:HA	1:A:201:SER:HB2	2.00	0.43
1:B:179:ASP:O	1:B:180:LEU:HB2	2.18	0.43
1:D:57:PHE:HB3	1:D:84:VAL:HG23	2.00	0.43
1:D:304:GLU:HB2	1:D:305:HIS:HD1	1.83	0.43
1:E:170:LEU:HD13	1:E:174:LEU:CD2	2.49	0.43
1:F:254:PHE:CE2	1:F:258:LEU:HD22	2.53	0.43
1:G:272:ILE:O	1:G:276:HIS:HB2	2.19	0.43
1:H:37:PRO:HA	1:H:66:PHE:HZ	1.84	0.43
1:H:191:LEU:HD12	1:H:191:LEU:N	2.33	0.43
1:H:275:ALA:O	1:H:279:ALA:N	2.36	0.43
1:K:212:LYS:N	1:K:212:LYS:HD2	2.33	0.43
1:L:260:THR:O	1:L:264:GLN:HG2	2.18	0.43
1:M:5:VAL:O	1:M:135:LEU:HA	2.18	0.43
1:P:101:ASP:HA	1:P:102:SER:HA	1.56	0.43
1:B:11:ASN:HB2	1:B:93:GLY:C	2.43	0.43
1:B:57:PHE:CD1	1:B:58:ILE:N	2.85	0.43
1:C:28:LEU:O	1:D:108:CYS:HA	2.19	0.43
1:C:180:LEU:HD23	1:C:181:ILE:N	2.33	0.43
1:C:203:GLN:HB2	1:C:227:TRP:CH2	2.54	0.43
1:G:170:LEU:CD1	1:G:174:LEU:HD23	2.48	0.43
1:G:207:ASP:O	1:G:210:HIS:HB2	2.18	0.43
1:G:240:PHE:CE1	1:G:301:PHE:HE2	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ASP:OD2	1:H:89:ASN:N	2.32	0.43
1:H:105:ASN:N	1:H:105:ASN:OD1	2.52	0.43
1:H:126:LEU:HD11	1:H:148:LYS:NZ	2.34	0.43
1:I:181:ILE:HG12	1:I:182:THR:N	2.31	0.43
1:K:243:LYS:HG2	1:K:244:ALA:N	2.34	0.43
1:L:16:LEU:HD21	1:L:30:GLY:HA3	2.00	0.43
1:L:184:ASN:ND2	1:L:187:GLU:OE2	2.52	0.43
1:M:40:LYS:HB3	1:M:40:LYS:HE2	1.58	0.43
1:M:185:GLU:H	1:M:185:GLU:HG3	1.38	0.43
1:P:91:PRO:O	1:P:113:ALA:HB2	2.19	0.43
1:B:15:VAL:HA	1:B:97:ILE:CD1	2.48	0.43
1:B:98:GLN:HE21	1:B:98:GLN:HB2	1.66	0.43
1:C:132:ALA:O	1:C:158:THR:OG1	2.24	0.43
1:D:9:SER:CB	1:D:140:GLU:HB3	2.48	0.43
1:D:22:PRO:CD	1:D:28:LEU:HD21	2.42	0.43
1:D:199:ASP:HB3	1:D:227:TRP:HZ3	1.83	0.43
1:F:3:LYS:NZ	1:F:264:GLN:HE22	2.17	0.43
1:G:61:VAL:CA	1:G:92:THR:HG23	2.48	0.43
1:I:21:PHE:CD1	1:I:22:PRO:HD2	2.54	0.43
1:J:44:GLN:OE1	1:J:136:LEU:HD21	2.18	0.43
1:J:51:MET:CB	1:J:260:THR:HG21	2.48	0.43
1:J:162:LEU:HD12	1:J:163:ASN:C	2.44	0.43
1:K:181:ILE:HG12	1:K:183:PRO:HD3	1.99	0.43
1:L:47:ALA:O	1:L:50:ARG:N	2.51	0.43
1:L:212:LYS:HA	1:L:212:LYS:HD3	1.88	0.43
1:M:143:LEU:HD13	1:M:168:ARG:HH22	1.84	0.43
1:M:170:LEU:CD2	1:M:174:LEU:HD23	2.47	0.43
1:N:209:LEU:C	1:N:211:CYS:H	2.17	0.43
1:B:245:THR:CG2	1:B:286:PHE:HD2	2.28	0.43
1:B:262:LEU:HD23	1:B:262:LEU:H	1.82	0.43
1:E:87:GLN:HG2	1:E:116:LYS:CG	2.32	0.43
1:E:119:ALA:HB2	1:E:144:ASP:O	2.19	0.43
1:F:198:ASP:OD2	1:F:198:ASP:N	2.50	0.43
1:G:22:PRO:HA	1:G:28:LEU:HD11	2.01	0.43
1:G:153:ALA:C	1:G:155:THR:N	2.77	0.43
1:I:56:GLY:HA2	1:I:80:ASN:HB3	2.01	0.43
1:J:13:ASP:HB3	1:J:97:ILE:CD1	2.49	0.43
1:J:215:GLU:HG3	1:J:231:ASN:HB2	2.01	0.43
1:N:59:ALA:HB3	1:N:84:VAL:HG12	2.01	0.43
1:N:98:GLN:HE21	1:N:98:GLN:HB2	1.68	0.43
1:N:277:ALA:O	1:N:281:ILE:HG13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:284:THR:C	1:N:285:ARG:HG2	2.44	0.43
1:O:130:ARG:HD3	1:O:152:GLU:OE1	2.19	0.43
1:O:230:GLN:HE21	1:O:230:GLN:HB3	1.46	0.43
1:A:12:ALA:HB3	1:A:94:ILE:CG1	2.45	0.43
1:A:15:VAL:HG22	1:A:97:ILE:HG21	1.99	0.43
1:A:137:MET:HE1	1:A:150:ALA:HB2	2.01	0.43
1:E:20:SER:OG	1:E:21:PHE:N	2.52	0.43
1:F:115:ALA:HA	1:F:142:PRO:HD3	2.00	0.43
1:G:291:SER:HB3	1:G:292:ILE:H	1.61	0.43
1:H:210:HIS:CE1	1:H:217:VAL:HG23	2.53	0.43
1:H:210:HIS:CE1	1:H:215:GLU:O	2.72	0.43
1:I:142:PRO:O	1:I:146:ILE:HG13	2.19	0.43
1:K:202:ALA:HB1	1:K:227:TRP:CG	2.53	0.43
1:K:224:LYS:HE2	1:K:224:LYS:HB3	1.66	0.43
1:K:239:GLY:HA2	1:K:276:HIS:HD2	1.78	0.43
1:O:43:ASN:CB	1:O:252:ASP:HB3	2.48	0.43
1:O:118:THR:OG1	1:O:119:ALA:N	2.49	0.43
1:B:168:ARG:HD3	1:B:170:LEU:HD12	2.01	0.42
1:B:254:PHE:C	1:B:254:PHE:HD2	2.27	0.42
1:C:95:ALA:HA	1:C:108:CYS:O	2.18	0.42
1:D:137:MET:CE	1:D:146:ILE:HG23	2.48	0.42
1:E:99:VAL:O	1:E:101:ASP:HB2	2.19	0.42
1:F:211:CYS:HA	1:G:233:ARG:HD3	2.01	0.42
1:F:215:GLU:OE1	1:F:216:ILE:HD11	2.18	0.42
1:H:16:LEU:HD21	1:H:30:GLY:HA3	2.01	0.42
1:H:175:LEU:O	1:H:178:VAL:HG23	2.19	0.42
1:I:62:GLY:O	1:I:67:GLY:HA3	2.18	0.42
1:N:81:THR:C	1:N:83:GLY:N	2.73	0.42
1:N:154:LYS:HG3	1:N:177:CYS:SG	2.59	0.42
1:N:286:PHE:O	1:N:291:SER:HB3	2.19	0.42
1:N:294:THR:H	1:N:297:GLU:CD	2.26	0.42
1:O:17:GLN:NE2	1:O:31:ARG:HH21	2.17	0.42
1:P:154:LYS:HE2	1:P:176:LYS:HE3	2.01	0.42
1:A:240:PHE:H	1:A:240:PHE:HD1	1.66	0.42
1:B:17:GLN:O	1:B:31:ARG:N	2.51	0.42
1:B:240:PHE:HB3	1:B:242:VAL:CG2	2.48	0.42
1:C:115:ALA:HA	1:C:142:PRO:HD3	2.01	0.42
1:H:57:PHE:HD1	1:H:58:ILE:H	1.67	0.42
1:H:97:ILE:HG22	1:H:106:SER:O	2.19	0.42
1:I:40:LYS:O	1:I:41:GLY:C	2.62	0.42
1:J:274:PHE:O	1:J:277:ALA:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:ILE:HG23	1:L:95:ALA:N	2.34	0.42
1:L:218:ILE:HG22	1:L:226:VAL:HG21	2.01	0.42
1:M:75:LYS:HE3	1:M:81:THR:OG1	2.19	0.42
1:O:202:ALA:O	1:O:205:ALA:HB3	2.18	0.42
1:O:294:THR:O	1:O:298:VAL:HG22	2.19	0.42
1:E:7:LEU:HA	1:E:58:ILE:O	2.19	0.42
1:E:181:ILE:HG23	1:E:183:PRO:CD	2.47	0.42
1:G:292:ILE:O	1:G:292:ILE:HG22	2.19	0.42
1:K:69:ASN:O	1:K:72:GLU:HB2	2.19	0.42
1:K:206:ALA:HA	1:K:217:VAL:HG11	2.01	0.42
1:L:160:VAL:N	1:L:179:ASP:OD2	2.45	0.42
1:M:19:PRO:HA	1:M:101:ASP:O	2.19	0.42
1:N:66:PHE:HE1	1:N:70:ILE:HD12	1.84	0.42
1:O:17:GLN:HB3	1:O:31:ARG:NH2	2.35	0.42
1:O:285:ARG:HH22	1:O:297:GLU:CD	2.27	0.42
1:P:136:LEU:HA	1:P:161:ILE:O	2.20	0.42
1:A:100:SER:HB3	1:A:104:GLU:O	2.19	0.42
1:B:99:VAL:HG22	1:B:101:ASP:HB2	2.01	0.42
1:B:294:THR:O	1:B:298:VAL:HG22	2.20	0.42
1:C:87:GLN:HB3	1:C:90:CYS:HB3	2.02	0.42
1:D:139:LEU:HD12	1:D:164:PRO:O	2.19	0.42
1:E:194:ILE:HD12	1:E:204:GLN:C	2.44	0.42
1:E:274:PHE:HZ	1:E:295:ARG:HE	1.67	0.42
1:F:14:HIS:ND1	1:F:35:VAL:HG22	2.35	0.42
1:F:184:ASN:O	1:F:188:ALA:N	2.31	0.42
1:H:97:ILE:CG2	1:H:107:ILE:HA	2.38	0.42
1:H:240:PHE:CD1	1:H:301:PHE:HE2	2.21	0.42
1:L:274:PHE:HZ	1:L:295:ARG:NE	2.17	0.42
1:M:18:VAL:O	1:M:101:ASP:HB2	2.19	0.42
1:M:28:LEU:O	1:N:108:CYS:HA	2.19	0.42
1:O:172:ASP:O	1:O:174:LEU:N	2.53	0.42
1:P:14:HIS:N	1:P:95:ALA:O	2.46	0.42
1:A:43:ASN:O	1:A:47:ALA:N	2.45	0.42
1:A:210:HIS:ND1	1:A:214:ILE:O	2.33	0.42
1:B:139:LEU:HD21	1:B:162:LEU:HD11	2.01	0.42
1:B:207:ASP:HA	1:B:210:HIS:HB2	2.01	0.42
1:C:95:ALA:CB	1:C:109:ILE:HG23	2.48	0.42
1:D:119:ALA:H	1:D:144:ASP:CG	2.23	0.42
1:D:119:ALA:HA	1:D:145:GLY:HA2	2.00	0.42
1:D:206:ALA:O	1:D:209:LEU:HB2	2.19	0.42
1:G:171:PRO:O	1:G:173:GLU:N	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:GLU:HA	1:H:194:ILE:O	2.20	0.42
1:I:209:LEU:HB3	1:I:214:ILE:HD12	2.00	0.42
1:J:154:LYS:HZ2	1:J:154:LYS:C	2.19	0.42
1:K:17:GLN:HG3	1:K:99:VAL:HG13	2.01	0.42
1:K:114:ASN:O	1:K:116:LYS:N	2.53	0.42
1:K:123:GLU:HA	1:K:126:LEU:HD21	2.00	0.42
1:L:175:LEU:HD12	1:L:175:LEU:N	2.35	0.42
1:O:63:ASP:O	1:O:68:ILE:HD11	2.19	0.42
1:O:137:MET:O	1:O:162:LEU:HD12	2.19	0.42
1:O:205:ALA:C	1:O:206:ALA:O	2.60	0.42
1:O:240:PHE:CG	1:O:301:PHE:HE2	2.36	0.42
1:B:93:GLY:C	1:B:94:ILE:HG12	2.45	0.42
1:B:221:LEU:HD21	1:B:227:TRP:CB	2.48	0.42
1:C:194:ILE:HG22	1:C:195:THR:H	1.83	0.42
1:E:141:THR:HB	1:E:142:PRO:HD2	2.00	0.42
1:E:283:VAL:O	1:E:283:VAL:HG22	2.20	0.42
1:G:129:ILE:HD13	1:G:135:LEU:HD11	2.00	0.42
1:K:133:ARG:HA	1:K:158:THR:HB	2.01	0.42
1:K:175:LEU:HD23	1:K:175:LEU:HA	1.81	0.42
1:K:191:LEU:O	1:K:191:LEU:HD23	2.19	0.42
1:L:139:LEU:CD1	1:L:170:LEU:HD21	2.48	0.42
1:M:94:ILE:HD12	1:N:33:TYR:CE1	2.54	0.42
1:N:3:LYS:HB2	1:N:54:ASP:HB3	2.00	0.42
1:O:248:THR:HG22	1:O:288:ALA:HB2	2.02	0.42
1:P:294:THR:CG2	1:P:297:GLU:HG2	2.50	0.42
1:A:33:TYR:CD2	1:A:33:TYR:C	2.97	0.42
1:A:116:LYS:O	1:A:118:THR:HG22	2.19	0.42
1:A:162:LEU:HB3	1:A:181:ILE:CD1	2.49	0.42
1:A:227:TRP:CZ3	1:A:236:ARG:HG3	2.54	0.42
1:D:118:THR:HB	1:D:144:ASP:OD1	2.20	0.42
1:E:49:ALA:HB1	1:E:77:ASP:O	2.20	0.42
1:F:127:ALA:O	1:F:130:ARG:HB2	2.19	0.42
1:G:147:LEU:CD1	1:G:151:GLN:HE21	2.29	0.42
1:H:9:SER:OG	1:H:140:GLU:HB3	2.20	0.42
1:H:40:LYS:O	1:H:41:GLY:C	2.63	0.42
1:H:95:ALA:HA	1:H:109:ILE:HA	2.01	0.42
1:I:3:LYS:HD3	1:I:54:ASP:HB3	2.01	0.42
1:K:26:GLU:HG3	1:K:27:THR:H	1.84	0.42
1:M:29:HIS:ND1	1:N:109:ILE:HB	2.35	0.42
1:N:163:ASN:HD22	1:N:164:PRO:HD2	1.85	0.42
1:O:170:LEU:HD23	1:O:170:LEU:HA	1.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:94:ILE:O	1:P:109:ILE:HG23	2.19	0.42
1:A:240:PHE:O	1:A:242:VAL:N	2.52	0.42
1:A:281:ILE:HB	1:A:293:PRO:HG3	2.02	0.42
1:B:233:ARG:CZ	1:I:211:CYS:HB2	2.49	0.42
1:C:197:TYR:HE1	1:C:201:SER:HB3	1.85	0.42
1:C:239:GLY:HA2	1:C:276:HIS:CE1	2.55	0.42
1:D:184:ASN:O	1:D:186:THR:N	2.53	0.42
1:E:46:VAL:HG13	1:E:50:ARG:NH1	2.34	0.42
1:F:138:GLN:CG	1:F:163:ASN:HB3	2.50	0.42
1:F:235:GLN:O	1:F:237:ILE:HG13	2.20	0.42
1:G:7:LEU:HA	1:G:58:ILE:O	2.20	0.42
1:G:12:ALA:HB2	1:G:66:PHE:CZ	2.55	0.42
1:J:73:SER:O	1:J:75:LYS:N	2.52	0.42
1:J:127:ALA:HA	1:J:130:ARG:NH2	2.34	0.42
1:K:26:GLU:HG3	1:K:27:THR:N	2.34	0.42
1:O:236:ARG:HH22	1:O:238:PRO:HB3	1.85	0.42
1:C:230:GLN:C	1:C:232:GLY:H	2.27	0.42
1:C:236:ARG:HG3	1:C:237:ILE:N	2.33	0.42
1:C:301:PHE:CD2	1:C:301:PHE:C	2.98	0.42
1:E:163:ASN:C	1:E:165:ALA:H	2.28	0.42
1:G:279:ALA:O	1:G:283:VAL:HG13	2.20	0.42
1:H:148:LYS:O	1:H:151:GLN:HG2	2.20	0.42
1:I:98:GLN:HG3	1:J:96:MET:HE1	2.02	0.42
1:I:160:VAL:HG12	1:I:178:VAL:HG13	2.01	0.42
1:K:21:PHE:CZ	1:K:106:SER:HB2	2.55	0.42
1:M:9:SER:HB3	1:M:140:GLU:HB3	2.02	0.42
1:M:203:GLN:HB2	1:M:227:TRP:CZ2	2.54	0.42
1:O:43:ASN:HB3	1:O:252:ASP:HB3	2.00	0.42
1:P:86:LEU:H	1:P:86:LEU:HD12	1.85	0.42
1:P:112:GLU:C	1:P:114:ASN:H	2.26	0.42
1:P:240:PHE:C	1:P:242:VAL:N	2.78	0.42
1:A:96:MET:SD	1:B:16:LEU:HD22	2.60	0.42
1:A:131:ASP:N	1:A:131:ASP:OD2	2.53	0.42
1:A:277:ALA:O	1:A:281:ILE:HG13	2.20	0.42
1:B:4:LEU:HD12	1:B:5:VAL:H	1.84	0.42
1:G:199:ASP:HA	1:G:227:TRP:CZ3	2.55	0.42
1:H:163:ASN:C	1:H:165:ALA:H	2.28	0.42
1:I:181:ILE:CD1	1:I:209:LEU:HD13	2.50	0.42
1:K:47:ALA:C	1:K:49:ALA:N	2.73	0.42
1:K:143:LEU:O	1:K:144:ASP:C	2.63	0.42
1:L:57:PHE:CD1	1:L:58:ILE:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:139:LEU:HD23	1:L:139:LEU:HA	1.55	0.42
1:L:218:ILE:HG23	1:L:226:VAL:HG21	2.02	0.42
1:P:46:VAL:O	1:P:50:ARG:HB2	2.20	0.42
1:A:63:ASP:OD2	1:A:88:PRO:HA	2.20	0.41
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.79	0.41
1:C:8:GLY:HA2	1:C:141:THR:HG21	2.02	0.41
1:F:263:LEU:HD13	1:F:263:LEU:HA	1.81	0.41
1:G:68:ILE:H	1:G:68:ILE:HG12	1.67	0.41
1:G:163:ASN:HD21	1:G:255:ASN:CG	2.22	0.41
1:H:81:THR:O	1:H:82:ALA:C	2.63	0.41
1:H:205:ALA:O	1:H:207:ASP:N	2.53	0.41
1:I:41:GLY:HA2	1:I:138:GLN:HE22	1.85	0.41
1:I:57:PHE:CD1	1:I:58:ILE:N	2.88	0.41
1:J:6:VAL:HG13	1:J:136:LEU:HD23	2.01	0.41
1:J:143:LEU:HG	1:J:168:ARG:CZ	2.50	0.41
1:K:143:LEU:HB3	1:K:144:ASP:H	1.73	0.41
1:L:44:GLN:NE2	1:L:163:ASN:OD1	2.48	0.41
1:L:116:LYS:HA	1:L:116:LYS:HD3	1.90	0.41
1:L:299:GLU:HA	1:L:302:LEU:HD12	2.02	0.41
1:M:40:LYS:NZ	1:M:165:ALA:O	2.53	0.41
1:M:129:ILE:HD12	1:M:135:LEU:HD13	2.02	0.41
1:M:174:LEU:O	1:M:178:VAL:HG23	2.20	0.41
1:P:267:PRO:HD2	1:P:270:SER:HB3	2.02	0.41
1:A:109:ILE:O	1:B:30:GLY:N	2.53	0.41
1:A:122:ILE:H	1:A:122:ILE:HG13	1.73	0.41
1:E:197:TYR:N	1:E:197:TYR:HD1	2.18	0.41
1:F:183:PRO:HB2	1:F:184:ASN:H	1.73	0.41
1:F:304:GLU:HG2	1:F:304:GLU:H	1.70	0.41
1:G:16:LEU:HD11	1:H:110:SER:HB2	2.00	0.41
1:G:285:ARG:HB3	1:G:286:PHE:H	1.63	0.41
1:H:96:MET:HB2	1:H:96:MET:HE3	1.73	0.41
1:J:264:GLN:HB2	1:J:264:GLN:HE21	1.51	0.41
1:K:24:PRO:O	1:K:26:GLU:N	2.50	0.41
1:M:19:PRO:HB2	1:M:20:SER:H	1.68	0.41
1:M:57:PHE:HD1	1:M:58:ILE:H	1.68	0.41
1:O:14:HIS:ND1	1:O:35:VAL:HG22	2.35	0.41
1:O:218:ILE:HG23	1:O:226:VAL:HG13	2.03	0.41
1:O:285:ARG:HB2	1:O:291:SER:CB	2.39	0.41
1:P:7:LEU:HB3	1:P:137:MET:HG2	2.02	0.41
1:A:81:THR:HG22	1:A:84:VAL:HG21	2.02	0.41
1:B:115:ALA:O	1:D:304:GLU:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:HG21	1:B:209:LEU:HD13	2.03	0.41
1:D:16:LEU:HD11	1:D:30:GLY:C	2.44	0.41
1:D:51:MET:HB2	1:D:260:THR:HG21	2.01	0.41
1:E:184:ASN:ND2	1:E:187:GLU:HG3	2.34	0.41
1:F:75:LYS:H	1:F:75:LYS:HG3	1.59	0.41
1:G:46:VAL:HG13	1:G:292:ILE:HG21	2.01	0.41
1:G:47:ALA:HB3	1:G:256:GLY:HA3	2.01	0.41
1:G:143:LEU:CD1	1:G:168:ARG:HH12	2.29	0.41
1:G:144:ASP:OD2	1:G:144:ASP:C	2.63	0.41
1:I:75:LYS:HB3	1:I:75:LYS:HE3	1.83	0.41
1:I:108:CYS:SG	1:J:28:LEU:HB2	2.60	0.41
1:K:50:ARG:C	1:K:51:MET:HE2	2.44	0.41
1:L:143:LEU:O	1:L:144:ASP:C	2.63	0.41
1:L:261:GLY:O	1:L:264:GLN:N	2.50	0.41
1:B:74:PHE:O	1:B:77:ASP:N	2.54	0.41
1:C:4:LEU:HD23	1:C:55:VAL:HA	2.01	0.41
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.78	0.41
1:D:71:ARG:HB2	1:D:84:VAL:HG11	2.01	0.41
1:E:51:MET:CB	1:E:260:THR:HG21	2.51	0.41
1:F:228:LEU:HD11	1:F:268:LEU:HD21	2.02	0.41
1:G:97:ILE:HG23	1:G:107:ILE:CD1	2.50	0.41
1:H:7:LEU:O	1:H:7:LEU:HD23	2.21	0.41
1:H:285:ARG:HH21	1:H:293:PRO:HB3	1.84	0.41
1:I:194:ILE:HD13	1:I:205:ALA:HA	2.02	0.41
1:J:183:PRO:HG2	1:J:219:ILE:HD12	2.03	0.41
1:M:4:LEU:HD23	1:M:55:VAL:HB	2.02	0.41
1:M:172:ASP:C	1:M:174:LEU:H	2.28	0.41
1:M:306:SER:C	1:O:143:LEU:HB2	2.45	0.41
1:N:49:ALA:HB2	1:N:55:VAL:HG11	2.02	0.41
1:N:163:ASN:C	1:N:165:ALA:H	2.28	0.41
1:N:294:THR:H	1:N:297:GLU:CG	2.34	0.41
1:O:11:ASN:HB3	1:O:12:ALA:H	1.62	0.41
1:O:91:PRO:O	1:O:113:ALA:HB2	2.20	0.41
1:A:113:ALA:O	1:A:115:ALA:N	2.51	0.41
1:D:172:ASP:C	1:D:174:LEU:H	2.28	0.41
1:E:63:ASP:O	1:E:68:ILE:HD11	2.20	0.41
1:E:247:THR:HA	1:E:250:ALA:HB2	2.02	0.41
1:F:16:LEU:HA	1:F:32:ASN:O	2.20	0.41
1:G:9:SER:N	1:G:41:GLY:HA3	2.35	0.41
1:G:93:GLY:HA3	1:G:114:ASN:HD21	1.86	0.41
1:G:181:ILE:HG22	1:G:217:VAL:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:ARG:O	1:G:237:ILE:HG13	2.20	0.41
1:H:112:GLU:O	1:H:113:ALA:C	2.63	0.41
1:H:117:LEU:HD12	1:H:117:LEU:HA	1.81	0.41
1:I:187:GLU:HG3	1:I:187:GLU:H	1.63	0.41
1:I:267:PRO:O	1:I:270:SER:OG	2.34	0.41
1:K:42:ALA:HB1	1:K:74:PHE:HZ	1.85	0.41
1:O:239:GLY:HA2	1:O:276:HIS:CD2	2.54	0.41
1:P:180:LEU:HG	1:P:216:ILE:HB	2.01	0.41
1:A:36:ILE:HA	1:A:37:PRO:HD3	1.83	0.41
1:B:233:ARG:H	1:B:233:ARG:HG2	1.40	0.41
1:B:245:THR:HB	1:B:283:VAL:O	2.20	0.41
1:C:131:ASP:OD1	1:C:131:ASP:N	2.49	0.41
1:C:163:ASN:C	1:C:165:ALA:H	2.29	0.41
1:C:233:ARG:HG3	1:C:233:ARG:O	2.21	0.41
1:D:48:ALA:O	1:D:260:THR:HG21	2.21	0.41
1:D:199:ASP:HB3	1:D:227:TRP:CZ3	2.55	0.41
1:D:253:THR:O	1:D:254:PHE:C	2.64	0.41
1:D:277:ALA:HB2	1:D:302:LEU:HD21	2.03	0.41
1:E:37:PRO:HB2	1:E:289:GLN:HG3	2.02	0.41
1:E:181:ILE:HG12	1:E:183:PRO:HG3	2.03	0.41
1:G:208:ALA:O	1:G:212:LYS:CG	2.68	0.41
1:H:100:SER:HB3	1:H:104:GLU:O	2.20	0.41
1:J:129:ILE:HG23	1:J:135:LEU:CD1	2.50	0.41
1:K:87:GLN:HE21	1:K:116:LYS:HB3	1.86	0.41
1:N:91:PRO:O	1:N:112:GLU:HB3	2.19	0.41
1:N:302:LEU:HD23	1:N:302:LEU:HA	1.71	0.41
1:O:172:ASP:C	1:O:174:LEU:H	2.28	0.41
1:B:16:LEU:HD21	1:B:98:GLN:HG3	2.02	0.41
1:C:3:LYS:HB3	1:C:263:LEU:HD11	2.02	0.41
1:C:138:GLN:CD	1:C:138:GLN:N	2.79	0.41
1:E:240:PHE:CE1	1:E:301:PHE:HE2	2.39	0.41
1:F:6:VAL:HG22	1:F:136:LEU:HB3	2.03	0.41
1:F:66:PHE:O	1:F:69:ASN:N	2.53	0.41
1:F:154:LYS:C	1:F:156:ALA:H	2.28	0.41
1:G:1:MET:HE3	1:G:1:MET:HB3	1.77	0.41
1:G:7:LEU:HD22	1:G:137:MET:HG2	2.02	0.41
1:G:227:TRP:CD1	1:G:227:TRP:C	2.98	0.41
1:I:161:ILE:HD13	1:I:259:VAL:HG22	2.02	0.41
1:K:42:ALA:O	1:K:46:VAL:HG12	2.21	0.41
1:K:143:LEU:HB2	1:K:168:ARG:HH22	1.85	0.41
1:N:287:GLY:HA2	1:N:291:SER:OG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:159:ASN:HA	1:O:179:ASP:OD2	2.21	0.41
1:O:226:VAL:HG11	1:O:272:ILE:HD13	2.02	0.41
1:P:172:ASP:C	1:P:174:LEU:N	2.78	0.41
1:A:241:VAL:HG13	1:D:19:PRO:HG3	2.01	0.41
1:B:49:ALA:HB2	1:B:55:VAL:HG11	2.02	0.41
1:C:87:GLN:HA	1:C:88:PRO:HD3	1.92	0.41
1:E:26:GLU:OE1	1:E:26:GLU:HA	2.20	0.41
1:E:96:MET:CE	1:F:98:GLN:HE21	2.33	0.41
1:F:137:MET:C	1:F:138:GLN:HE21	2.28	0.41
1:G:13:ASP:HB3	1:G:97:ILE:HD12	2.02	0.41
1:G:199:ASP:HB3	1:G:227:TRP:CZ3	2.55	0.41
1:G:236:ARG:CG	1:G:237:ILE:N	2.83	0.41
1:H:36:ILE:O	1:H:38:GLY:N	2.53	0.41
1:H:210:HIS:HE1	1:H:229:SER:O	2.03	0.41
1:J:197:TYR:HD1	1:J:197:TYR:H	1.68	0.41
1:K:80:ASN:HD21	1:K:82:ALA:HB3	1.85	0.41
1:N:93:GLY:HA2	1:N:112:GLU:HB2	2.02	0.41
1:N:292:ILE:HA	1:N:293:PRO:HD3	1.85	0.41
1:B:63:ASP:OD2	1:B:88:PRO:HA	2.20	0.41
1:D:215:GLU:HG3	1:D:231:ASN:OD1	2.21	0.41
1:D:243:LYS:NZ	1:D:245:THR:HG23	2.36	0.41
1:E:247:THR:C	1:E:249:ALA:N	2.78	0.41
1:F:50:ARG:NH1	1:F:292:ILE:O	2.54	0.41
1:F:185:GLU:HG2	1:F:196:VAL:HB	2.03	0.41
1:G:50:ARG:NE	1:G:77:ASP:OD1	2.51	0.41
1:H:40:LYS:HB3	1:H:138:GLN:HG2	2.03	0.41
1:H:169:GLU:O	1:H:170:LEU:HD23	2.21	0.41
1:H:229:SER:HA	1:H:234:GLY:HA2	2.03	0.41
1:I:97:ILE:HA	1:I:106:SER:O	2.20	0.41
1:I:117:LEU:HA	1:I:117:LEU:HD12	1.73	0.41
1:J:204:GLN:HG3	1:K:203:GLN:HG2	2.03	0.41
1:K:109:ILE:N	1:L:28:LEU:O	2.46	0.41
1:L:32:ASN:O	1:L:33:TYR:O	2.39	0.41
1:L:57:PHE:CE1	1:L:59:ALA:HB2	2.55	0.41
1:L:172:ASP:C	1:L:174:LEU:N	2.78	0.41
1:L:175:LEU:HD12	1:L:175:LEU:H	1.85	0.41
1:L:203:GLN:O	1:L:206:ALA:HB3	2.20	0.41
1:M:139:LEU:CD1	1:M:170:LEU:HD11	2.51	0.41
1:M:141:THR:HB	1:M:142:PRO:HD2	2.03	0.41
1:M:185:GLU:HB3	1:M:196:VAL:HB	2.02	0.41
1:M:221:LEU:O	1:M:224:LYS:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:92:THR:O	1:O:94:ILE:HD12	2.21	0.41
1:O:94:ILE:HD13	1:P:33:TYR:CD2	2.56	0.41
1:O:98:GLN:OE1	1:O:106:SER:OG	2.37	0.41
1:O:99:VAL:HG13	1:O:101:ASP:HB2	2.03	0.41
1:O:163:ASN:C	1:O:165:ALA:H	2.29	0.41
1:O:185:GLU:H	1:O:185:GLU:HG3	1.51	0.41
1:P:13:ASP:HB3	1:P:97:ILE:CD1	2.50	0.41
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.82	0.41
1:B:180:LEU:HD21	1:B:218:ILE:CD1	2.51	0.41
1:B:185:GLU:H	1:B:185:GLU:HG3	1.34	0.41
1:E:204:GLN:HA	1:E:207:ASP:OD2	2.21	0.41
1:G:227:TRP:CD2	1:G:235:GLN:O	2.74	0.41
1:H:267:PRO:O	1:H:270:SER:HB3	2.21	0.41
1:J:236:ARG:HH12	1:J:238:PRO:HB3	1.85	0.41
1:M:163:ASN:HD22	1:M:164:PRO:HD2	1.86	0.41
1:O:51:MET:HG3	1:O:260:THR:HG21	2.03	0.41
1:A:64:ASP:O	1:A:66:PHE:N	2.55	0.40
1:A:172:ASP:C	1:A:174:LEU:N	2.75	0.40
1:B:50:ARG:HH11	1:B:292:ILE:CG2	2.34	0.40
1:D:218:ILE:HG12	1:D:228:LEU:HD13	2.03	0.40
1:F:5:VAL:HG21	1:F:128:ALA:HB1	2.02	0.40
1:F:205:ALA:O	1:F:209:LEU:HD12	2.21	0.40
1:G:207:ASP:HA	1:G:210:HIS:HB2	2.03	0.40
1:H:160:VAL:O	1:H:160:VAL:HG12	2.21	0.40
1:J:168:ARG:HG3	1:J:169:GLU:O	2.21	0.40
1:K:66:PHE:CZ	1:K:70:ILE:HG13	2.56	0.40
1:L:21:PHE:CE2	1:L:106:SER:HB2	2.54	0.40
1:L:274:PHE:O	1:L:277:ALA:HB3	2.21	0.40
1:M:116:LYS:HA	1:M:116:LYS:HD3	1.95	0.40
1:M:161:ILE:N	1:M:161:ILE:HD12	2.36	0.40
1:M:184:ASN:ND2	1:M:186:THR:H	2.18	0.40
1:N:64:ASP:OD1	1:N:66:PHE:HB3	2.21	0.40
1:N:187:GLU:HA	1:N:190:VAL:HG22	2.03	0.40
1:O:40:LYS:N	1:O:140:GLU:OE1	2.54	0.40
1:O:111:ALA:O	1:O:114:ASN:N	2.54	0.40
1:B:216:ILE:HG21	1:B:268:LEU:HD21	2.03	0.40
1:C:3:LYS:HD3	1:C:3:LYS:HA	1.55	0.40
1:C:188:ALA:O	1:C:192:THR:HG23	2.22	0.40
1:C:197:TYR:HD1	1:C:197:TYR:H	1.68	0.40
1:D:304:GLU:HG2	1:D:304:GLU:H	1.52	0.40
1:E:24:PRO:O	1:E:26:GLU:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:GLN:HG2	1:E:151:GLN:H	1.63	0.40
1:F:92:THR:O	1:F:94:ILE:HG23	2.21	0.40
1:G:106:SER:C	1:G:107:ILE:HG12	2.45	0.40
1:G:181:ILE:HG22	1:G:217:VAL:HG22	2.02	0.40
1:H:99:VAL:HG12	1:H:105:ASN:CG	2.46	0.40
1:H:204:GLN:NE2	1:H:207:ASP:OD2	2.55	0.40
1:J:93:GLY:HA3	1:J:114:ASN:ND2	2.37	0.40
1:K:16:LEU:HD21	1:K:30:GLY:HA3	2.03	0.40
1:K:118:THR:H	1:K:121:ALA:HB3	1.86	0.40
1:L:194:ILE:N	1:L:194:ILE:HD12	2.36	0.40
1:N:173:GLU:H	1:N:173:GLU:CD	2.27	0.40
1:P:240:PHE:C	1:P:242:VAL:H	2.27	0.40
1:B:262:LEU:HD23	1:B:262:LEU:N	2.36	0.40
1:C:76:LEU:HD22	1:C:76:LEU:HA	1.78	0.40
1:D:14:HIS:CD2	1:D:94:ILE:HG13	2.57	0.40
1:D:119:ALA:C	1:D:121:ALA:H	2.29	0.40
1:F:11:ASN:HB3	1:F:12:ALA:H	1.59	0.40
1:G:258:LEU:HB2	1:G:275:ALA:CB	2.51	0.40
1:H:19:PRO:HD3	1:H:29:HIS:O	2.22	0.40
1:H:66:PHE:HB3	1:H:67:GLY:H	1.69	0.40
1:L:143:LEU:C	1:L:145:GLY:N	2.79	0.40
1:L:305:HIS:O	1:L:306:SER:OG	2.29	0.40
1:M:178:VAL:O	1:M:214:ILE:HG23	2.21	0.40
1:P:7:LEU:O	1:P:137:MET:HA	2.21	0.40
1:A:18:VAL:HG21	1:A:98:GLN:HB3	2.03	0.40
1:B:3:LYS:HE2	1:B:133:ARG:HG3	2.02	0.40
1:B:11:ASN:ND2	1:B:11:ASN:C	2.80	0.40
1:B:17:GLN:HB3	1:B:31:ARG:CZ	2.51	0.40
1:C:95:ALA:HA	1:C:109:ILE:HA	2.02	0.40
1:E:257:ALA:HB3	1:E:275:ALA:HA	2.04	0.40
1:F:3:LYS:CE	1:F:54:ASP:HB2	2.51	0.40
1:F:231:ASN:HB2	1:F:233:ARG:HE	1.86	0.40
1:G:57:PHE:HD1	1:G:58:ILE:H	1.70	0.40
1:H:184:ASN:O	1:H:185:GLU:C	2.65	0.40
1:J:236:ARG:HG3	1:J:237:ILE:N	2.34	0.40
1:M:100:SER:HA	1:M:101:ASP:CB	2.52	0.40
1:M:178:VAL:HB	1:M:214:ILE:HG12	2.02	0.40
1:N:98:GLN:NE2	1:N:106:SER:HB3	2.35	0.40
1:O:126:LEU:O	1:O:129:ILE:HB	2.21	0.40
1:A:135:LEU:N	1:A:159:ASN:O	2.54	0.40
1:A:206:ALA:O	1:A:209:LEU:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LYS:HD2	1:B:140:GLU:HG3	2.04	0.40
1:B:112:GLU:HB3	1:B:113:ALA:H	1.79	0.40
1:B:187:GLU:O	1:B:190:VAL:N	2.51	0.40
1:E:110:SER:HB2	1:F:16:LEU:HD13	2.03	0.40
1:I:5:VAL:O	1:I:135:LEU:HA	2.22	0.40
1:J:51:MET:HB2	1:J:260:THR:HG21	2.03	0.40
1:J:197:TYR:N	1:J:197:TYR:HD1	2.19	0.40
1:K:114:ASN:C	1:K:116:LYS:H	2.30	0.40
1:K:135:LEU:HD23	1:K:160:VAL:HG22	2.03	0.40
1:L:13:ASP:OD1	1:L:95:ALA:HB3	2.22	0.40
1:O:44:GLN:HB3	1:O:136:LEU:HD21	2.03	0.40
1:O:50:ARG:HG3	1:O:292:ILE:CG2	2.50	0.40
1:P:18:VAL:HG11	1:P:98:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/309 (98%)	242 (80%)	46 (15%)	16 (5%)	1	10
1	B	304/309 (98%)	228 (75%)	50 (16%)	26 (9%)	0	4
1	C	304/309 (98%)	236 (78%)	46 (15%)	22 (7%)	1	5
1	D	304/309 (98%)	251 (83%)	33 (11%)	20 (7%)	1	6
1	E	304/309 (98%)	261 (86%)	34 (11%)	9 (3%)	3	18
1	F	304/309 (98%)	239 (79%)	46 (15%)	19 (6%)	1	7
1	G	304/309 (98%)	236 (78%)	50 (16%)	18 (6%)	1	8
1	H	304/309 (98%)	238 (78%)	38 (12%)	28 (9%)	0	3
1	I	304/309 (98%)	264 (87%)	27 (9%)	13 (4%)	2	13
1	J	304/309 (98%)	244 (80%)	46 (15%)	14 (5%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	304/309 (98%)	238 (78%)	39 (13%)	27 (9%)	0	3
1	L	304/309 (98%)	259 (85%)	30 (10%)	15 (5%)	1	11
1	M	304/309 (98%)	253 (83%)	31 (10%)	20 (7%)	1	6
1	N	304/309 (98%)	262 (86%)	27 (9%)	15 (5%)	1	11
1	O	304/309 (98%)	245 (81%)	40 (13%)	19 (6%)	1	7
1	P	304/309 (98%)	259 (85%)	36 (12%)	9 (3%)	3	18
All	All	4864/4944 (98%)	3955 (81%)	619 (13%)	290 (6%)	1	7

All (290) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	67	GLY
1	A	82	ALA
1	A	172	ASP
1	A	196	VAL
1	A	222	GLY
1	A	240	PHE
1	A	244	ALA
1	B	65	SER
1	B	75	LYS
1	B	102	SER
1	B	112	GLU
1	B	157	LYS
1	B	173	GLU
1	B	188	ALA
1	B	250	ALA
1	B	265	GLU
1	B	288	ALA
1	B	297	GLU
1	C	77	ASP
1	C	126	LEU
1	C	172	ASP
1	C	209	LEU
1	C	210	HIS
1	C	231	ASN
1	C	247	THR
1	C	284	THR
1	D	112	GLU
1	D	127	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	LEU
1	D	167	ALA
1	D	173	GLU
1	D	242	VAL
1	E	143	LEU
1	E	144	ASP
1	F	66	PHE
1	F	67	GLY
1	F	82	ALA
1	F	112	GLU
1	F	127	ALA
1	F	132	ALA
1	F	230	GLN
1	F	265	GLU
1	F	268	LEU
1	G	175	LEU
1	G	176	LYS
1	G	235	GLN
1	G	258	LEU
1	H	40	LYS
1	H	41	GLY
1	H	82	ALA
1	H	113	ALA
1	H	206	ALA
1	H	226	VAL
1	H	246	ASP
1	H	248	THR
1	H	285	ARG
1	H	286	PHE
1	H	288	ALA
1	H	291	SER
1	I	288	ALA
1	I	292	ILE
1	J	32	ASN
1	J	74	PHE
1	J	119	ALA
1	J	128	ALA
1	J	173	GLU
1	J	188	ALA
1	J	292	ILE
1	K	2	ASN
1	K	12	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	48	ALA
1	K	63	ASP
1	K	112	GLU
1	K	131	ASP
1	K	132	ALA
1	K	144	ASP
1	K	157	LYS
1	K	235	GLN
1	K	245	THR
1	K	274	PHE
1	L	33	TYR
1	L	93	GLY
1	L	101	ASP
1	L	112	GLU
1	L	144	ASP
1	L	173	GLU
1	L	245	THR
1	L	247	THR
1	L	248	THR
1	M	3	LYS
1	M	19	PRO
1	M	20	SER
1	M	21	PHE
1	M	112	GLU
1	M	249	ALA
1	M	250	ALA
1	N	82	ALA
1	N	112	GLU
1	N	213	GLY
1	N	248	THR
1	N	284	THR
1	N	288	ALA
1	O	82	ALA
1	O	112	GLU
1	O	199	ASP
1	O	206	ALA
1	O	249	ALA
1	O	281	ILE
1	O	286	PHE
1	P	13	ASP
1	P	19	PRO
1	P	173	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	ALA
1	B	52	GLN
1	B	180	LEU
1	B	298	VAL
1	C	80	ASN
1	C	112	GLU
1	C	194	ILE
1	C	283	VAL
1	D	66	PHE
1	D	102	SER
1	D	144	ASP
1	D	185	GLU
1	D	233	ARG
1	D	251	GLY
1	D	252	ASP
1	D	288	ALA
1	D	291	SER
1	E	2	ASN
1	E	25	GLY
1	E	249	ALA
1	F	19	PRO
1	F	156	ALA
1	F	231	ASN
1	G	24	PRO
1	G	32	ASN
1	G	112	GLU
1	G	172	ASP
1	G	234	GLY
1	G	250	ALA
1	G	262	LEU
1	G	288	ALA
1	G	291	SER
1	H	33	TYR
1	H	54	ASP
1	H	205	ALA
1	H	250	ALA
1	H	251	GLY
1	I	82	ALA
1	I	190	VAL
1	I	248	THR
1	I	287	GLY
1	J	101	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	129	ILE
1	J	210	HIS
1	J	213	GLY
1	J	235	GLN
1	K	32	ASN
1	K	143	LEU
1	K	158	THR
1	K	159	ASN
1	K	173	GLU
1	K	222	GLY
1	L	143	LEU
1	L	241	VAL
1	L	286	PHE
1	M	32	ASN
1	M	157	LYS
1	M	173	GLU
1	M	248	THR
1	N	209	LEU
1	N	229	SER
1	N	234	GLY
1	O	2	ASN
1	O	171	PRO
1	O	173	GLU
1	O	247	THR
1	O	250	ALA
1	P	222	GLY
1	P	241	VAL
1	P	248	THR
1	A	65	SER
1	A	83	GLY
1	A	248	THR
1	B	44	GLN
1	B	48	ALA
1	B	49	ALA
1	B	74	PHE
1	B	77	ASP
1	B	223	SER
1	C	20	SER
1	C	26	GLU
1	C	41	GLY
1	D	119	ALA
1	E	40	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	248	THR
1	E	286	PHE
1	F	32	ASN
1	F	63	ASP
1	F	81	THR
1	F	243	LYS
1	G	227	TRP
1	G	248	THR
1	H	32	ASN
1	H	52	GLN
1	H	67	GLY
1	H	138	GLN
1	H	249	ALA
1	I	40	LYS
1	I	157	LYS
1	I	247	THR
1	J	187	GLU
1	K	202	ALA
1	K	210	HIS
1	K	236	ARG
1	K	247	THR
1	K	273	LYS
1	M	150	ALA
1	M	247	THR
1	M	286	PHE
1	M	288	ALA
1	M	289	GLN
1	N	40	LYS
1	N	211	CYS
1	O	242	VAL
1	P	244	ALA
1	A	99	VAL
1	A	115	ALA
1	C	40	LYS
1	C	290	THR
1	D	248	THR
1	D	283	VAL
1	F	157	LYS
1	F	183	PRO
1	H	127	ALA
1	J	291	SER
1	K	183	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	231	ASN
1	M	251	GLY
1	N	157	LYS
1	O	101	ASP
1	O	282	SER
1	P	235	GLN
1	B	67	GLY
1	B	168	ARG
1	C	19	PRO
1	C	106	SER
1	C	131	ASP
1	D	292	ILE
1	E	283	VAL
1	H	66	PHE
1	H	157	LYS
1	K	40	LYS
1	K	67	GLY
1	L	196	VAL
1	N	101	ASP
1	N	193	GLY
1	N	210	HIS
1	O	32	ASN
1	O	100	SER
1	O	157	LYS
1	P	2	ASN
1	B	22	PRO
1	B	224	LYS
1	F	241	VAL
1	G	101	ASP
1	I	286	PHE
1	L	243	LYS
1	C	67	GLY
1	C	78	GLY
1	G	22	PRO
1	K	241	VAL
1	M	242	VAL
1	O	67	GLY
1	H	37	PRO
1	H	281	ILE
1	I	41	GLY
1	A	241	VAL
1	G	226	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	67	GLY
1	I	78	GLY
1	L	91	PRO
1	B	181	ILE
1	A	242	VAL
1	B	292	ILE
1	D	67	GLY
1	H	38	GLY
1	M	241	VAL

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	237/239 (99%)	187 (79%)	50 (21%)	1	3
1	B	237/239 (99%)	170 (72%)	67 (28%)	0	1
1	C	237/239 (99%)	173 (73%)	64 (27%)	0	1
1	D	237/239 (99%)	176 (74%)	61 (26%)	0	1
1	E	237/239 (99%)	187 (79%)	50 (21%)	1	3
1	F	237/239 (99%)	181 (76%)	56 (24%)	1	2
1	G	237/239 (99%)	157 (66%)	80 (34%)	0	0
1	H	237/239 (99%)	169 (71%)	68 (29%)	0	1
1	I	237/239 (99%)	187 (79%)	50 (21%)	1	3
1	J	237/239 (99%)	182 (77%)	55 (23%)	1	2
1	K	237/239 (99%)	177 (75%)	60 (25%)	0	1
1	L	237/239 (99%)	190 (80%)	47 (20%)	1	5
1	M	237/239 (99%)	183 (77%)	54 (23%)	1	3
1	N	237/239 (99%)	180 (76%)	57 (24%)	1	2
1	O	237/239 (99%)	178 (75%)	59 (25%)	0	1
1	P	237/239 (99%)	177 (75%)	60 (25%)	0	1
All	All	3792/3824 (99%)	2854 (75%)	938 (25%)	1	2

All (938) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	SER
1	A	15	VAL
1	A	16	LEU
1	A	17	GLN
1	A	20	SER
1	A	21	PHE
1	A	23	ARG
1	A	26	GLU
1	A	28	LEU
1	A	31	ARG
1	A	46	VAL
1	A	52	GLN
1	A	71	ARG
1	A	81	THR
1	A	85	LYS
1	A	86	LEU
1	A	89	ASN
1	A	94	ILE
1	A	97	ILE
1	A	106	SER
1	A	122	ILE
1	A	129	ILE
1	A	141	THR
1	A	147	LEU
1	A	151	GLN
1	A	155	THR
1	A	160	VAL
1	A	170	LEU
1	A	187	GLU
1	A	190	VAL
1	A	191	LEU
1	A	196	VAL
1	A	197	TYR
1	A	214	ILE
1	A	220	THR
1	A	221	LEU
1	A	226	VAL
1	A	231	ASN
1	A	233	ARG
1	A	236	ARG
1	A	243	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	253	THR
1	A	254	PHE
1	A	260	THR
1	A	263	LEU
1	A	270	SER
1	A	272	ILE
1	A	281	ILE
1	A	291	SER
1	B	1	MET
1	B	2	ASN
1	B	11	ASN
1	B	16	LEU
1	B	21	PHE
1	B	23	ARG
1	B	27	THR
1	B	35	VAL
1	B	36	ILE
1	B	46	VAL
1	B	55	VAL
1	B	63	ASP
1	B	68	ILE
1	B	72	GLU
1	B	79	ILE
1	B	89	ASN
1	B	92	THR
1	B	94	ILE
1	B	97	ILE
1	B	98	GLN
1	B	99	VAL
1	B	100	SER
1	B	104	GLU
1	B	108	CYS
1	B	112	GLU
1	B	117	LEU
1	B	118	THR
1	B	141	THR
1	B	168	ARG
1	B	175	LEU
1	B	176	LYS
1	B	178	VAL
1	B	180	LEU
1	B	182	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	185	GLU
1	B	189	GLU
1	B	195	THR
1	B	197	TYR
1	B	199	ASP
1	B	204	GLN
1	B	211	CYS
1	B	218	ILE
1	B	220	THR
1	B	221	LEU
1	B	228	LEU
1	B	230	GLN
1	B	233	ARG
1	B	236	ARG
1	B	242	VAL
1	B	243	LYS
1	B	247	THR
1	B	248	THR
1	B	255	ASN
1	B	260	THR
1	B	262	LEU
1	B	269	GLU
1	B	272	ILE
1	B	276	HIS
1	B	281	ILE
1	B	282	SER
1	B	286	PHE
1	B	290	THR
1	B	291	SER
1	B	294	THR
1	B	297	GLU
1	B	298	VAL
1	B	304	GLU
1	C	1	MET
1	C	3	LYS
1	C	4	LEU
1	C	7	LEU
1	C	9	SER
1	C	18	VAL
1	C	23	ARG
1	C	28	LEU
1	C	29	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	31	ARG
1	C	40	LYS
1	C	52	GLN
1	C	64	ASP
1	C	65	SER
1	C	68	ILE
1	C	71	ARG
1	C	73	SER
1	C	75	LYS
1	C	76	LEU
1	C	84	VAL
1	C	85	LYS
1	C	87	GLN
1	C	94	ILE
1	C	96	MET
1	C	97	ILE
1	C	98	GLN
1	C	102	SER
1	C	106	SER
1	C	107	ILE
1	C	108	CYS
1	C	109	ILE
1	C	118	THR
1	C	140	GLU
1	C	144	ASP
1	C	148	LYS
1	C	154	LYS
1	C	168	ARG
1	C	170	LEU
1	C	172	ASP
1	C	178	VAL
1	C	179	ASP
1	C	181	ILE
1	C	182	THR
1	C	191	LEU
1	C	197	TYR
1	C	199	ASP
1	C	211	CYS
1	C	220	THR
1	C	221	LEU
1	C	224	LYS
1	C	226	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	236	ARG
1	C	241	VAL
1	C	243	LYS
1	C	246	ASP
1	C	248	THR
1	C	253	THR
1	C	263	LEU
1	C	265	GLU
1	C	281	ILE
1	C	285	ARG
1	C	286	PHE
1	C	289	GLN
1	C	292	ILE
1	D	1	MET
1	D	2	ASN
1	D	3	LYS
1	D	7	LEU
1	D	15	VAL
1	D	16	LEU
1	D	17	GLN
1	D	18	VAL
1	D	20	SER
1	D	26	GLU
1	D	28	LEU
1	D	31	ARG
1	D	35	VAL
1	D	36	ILE
1	D	46	VAL
1	D	55	VAL
1	D	63	ASP
1	D	64	ASP
1	D	68	ILE
1	D	72	GLU
1	D	73	SER
1	D	89	ASN
1	D	94	ILE
1	D	97	ILE
1	D	100	SER
1	D	106	SER
1	D	112	GLU
1	D	133	ARG
1	D	146	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	157	LYS
1	D	176	LYS
1	D	182	THR
1	D	186	THR
1	D	190	VAL
1	D	197	TYR
1	D	198	ASP
1	D	200	SER
1	D	203	GLN
1	D	204	GLN
1	D	211	CYS
1	D	214	ILE
1	D	220	THR
1	D	221	LEU
1	D	224	LYS
1	D	226	VAL
1	D	241	VAL
1	D	245	THR
1	D	248	THR
1	D	260	THR
1	D	263	LEU
1	D	268	LEU
1	D	270	SER
1	D	273	LYS
1	D	276	HIS
1	D	281	ILE
1	D	286	PHE
1	D	290	THR
1	D	291	SER
1	D	298	VAL
1	D	304	GLU
1	D	306	SER
1	E	1	MET
1	E	6	VAL
1	E	7	LEU
1	E	16	LEU
1	E	17	GLN
1	E	18	VAL
1	E	23	ARG
1	E	28	LEU
1	E	31	ARG
1	E	34	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	40	LYS
1	E	46	VAL
1	E	52	GLN
1	E	61	VAL
1	E	76	LEU
1	E	86	LEU
1	E	87	GLN
1	E	92	THR
1	E	101	ASP
1	E	102	SER
1	E	107	ILE
1	E	108	CYS
1	E	117	LEU
1	E	122	ILE
1	E	129	ILE
1	E	130	ARG
1	E	133	ARG
1	E	140	GLU
1	E	148	LYS
1	E	151	GLN
1	E	169	GLU
1	E	172	ASP
1	E	173	GLU
1	E	184	ASN
1	E	189	GLU
1	E	190	VAL
1	E	194	ILE
1	E	197	TYR
1	E	221	LEU
1	E	226	VAL
1	E	230	GLN
1	E	243	LYS
1	E	270	SER
1	E	281	ILE
1	E	282	SER
1	E	285	ARG
1	E	286	PHE
1	E	291	SER
1	E	295	ARG
1	E	306	SER
1	F	16	LEU
1	F	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	27	THR
1	F	28	LEU
1	F	31	ARG
1	F	36	ILE
1	F	46	VAL
1	F	58	ILE
1	F	64	ASP
1	F	70	ILE
1	F	73	SER
1	F	75	LYS
1	F	81	THR
1	F	86	LEU
1	F	89	ASN
1	F	92	THR
1	F	104	GLU
1	F	105	ASN
1	F	108	CYS
1	F	112	GLU
1	F	117	LEU
1	F	123	GLU
1	F	131	ASP
1	F	138	GLN
1	F	140	GLU
1	F	144	ASP
1	F	147	LEU
1	F	148	LYS
1	F	161	ILE
1	F	162	LEU
1	F	168	ARG
1	F	169	GLU
1	F	170	LEU
1	F	181	ILE
1	F	184	ASN
1	F	191	LEU
1	F	197	TYR
1	F	215	GLU
1	F	236	ARG
1	F	243	LYS
1	F	246	ASP
1	F	247	THR
1	F	248	THR
1	F	253	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	263	LEU
1	F	264	GLN
1	F	268	LEU
1	F	270	SER
1	F	272	ILE
1	F	273	LYS
1	F	276	HIS
1	F	281	ILE
1	F	289	GLN
1	F	291	SER
1	F	298	VAL
1	F	304	GLU
1	G	3	LYS
1	G	5	VAL
1	G	18	VAL
1	G	20	SER
1	G	23	ARG
1	G	31	ARG
1	G	32	ASN
1	G	46	VAL
1	G	65	SER
1	G	68	ILE
1	G	73	SER
1	G	75	LYS
1	G	79	ILE
1	G	85	LYS
1	G	86	LEU
1	G	92	THR
1	G	94	ILE
1	G	96	MET
1	G	99	VAL
1	G	101	ASP
1	G	102	SER
1	G	104	GLU
1	G	107	ILE
1	G	109	ILE
1	G	110	SER
1	G	116	LYS
1	G	118	THR
1	G	129	ILE
1	G	130	ARG
1	G	137	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	138	GLN
1	G	141	THR
1	G	143	LEU
1	G	144	ASP
1	G	148	LYS
1	G	151	GLN
1	G	154	LYS
1	G	159	ASN
1	G	163	ASN
1	G	170	LEU
1	G	173	GLU
1	G	177	CYS
1	G	178	VAL
1	G	181	ILE
1	G	184	ASN
1	G	189	GLU
1	G	191	LEU
1	G	194	ILE
1	G	197	TYR
1	G	199	ASP
1	G	207	ASP
1	G	211	CYS
1	G	218	ILE
1	G	220	THR
1	G	221	LEU
1	G	224	LYS
1	G	226	VAL
1	G	242	VAL
1	G	243	LYS
1	G	245	THR
1	G	246	ASP
1	G	247	THR
1	G	255	ASN
1	G	259	VAL
1	G	260	THR
1	G	263	LEU
1	G	264	GLN
1	G	266	MET
1	G	268	LEU
1	G	270	SER
1	G	273	LYS
1	G	276	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	283	VAL
1	G	286	PHE
1	G	290	THR
1	G	291	SER
1	G	292	ILE
1	G	295	ARG
1	G	299	GLU
1	G	306	SER
1	H	7	LEU
1	H	9	SER
1	H	18	VAL
1	H	23	ARG
1	H	35	VAL
1	H	46	VAL
1	H	51	MET
1	H	52	GLN
1	H	54	ASP
1	H	70	ILE
1	H	76	LEU
1	H	77	ASP
1	H	85	LYS
1	H	86	LEU
1	H	87	GLN
1	H	92	THR
1	H	94	ILE
1	H	96	MET
1	H	97	ILE
1	H	98	GLN
1	H	101	ASP
1	H	104	GLU
1	H	105	ASN
1	H	106	SER
1	H	107	ILE
1	H	108	CYS
1	H	112	GLU
1	H	116	LYS
1	H	122	ILE
1	H	129	ILE
1	H	133	ARG
1	H	143	LEU
1	H	144	ASP
1	H	160	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	161	ILE
1	H	169	GLU
1	H	172	ASP
1	H	173	GLU
1	H	178	VAL
1	H	182	THR
1	H	187	GLU
1	H	189	GLU
1	H	190	VAL
1	H	191	LEU
1	H	192	THR
1	H	194	ILE
1	H	197	TYR
1	H	199	ASP
1	H	212	LYS
1	H	220	THR
1	H	223	SER
1	H	233	ARG
1	H	235	GLN
1	H	241	VAL
1	H	242	VAL
1	H	245	THR
1	H	246	ASP
1	H	247	THR
1	H	253	THR
1	H	259	VAL
1	H	263	LEU
1	H	281	ILE
1	H	284	THR
1	H	285	ARG
1	H	286	PHE
1	H	289	GLN
1	H	292	ILE
1	H	304	GLU
1	I	1	MET
1	I	3	LYS
1	I	7	LEU
1	I	16	LEU
1	I	18	VAL
1	I	23	ARG
1	I	28	LEU
1	I	34	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	55	VAL
1	I	65	SER
1	I	68	ILE
1	I	70	ILE
1	I	72	GLU
1	I	73	SER
1	I	75	LYS
1	I	94	ILE
1	I	99	VAL
1	I	105	ASN
1	I	106	SER
1	I	108	CYS
1	I	109	ILE
1	I	129	ILE
1	I	143	LEU
1	I	144	ASP
1	I	147	LEU
1	I	160	VAL
1	I	169	GLU
1	I	178	VAL
1	I	179	ASP
1	I	181	ILE
1	I	185	GLU
1	I	187	GLU
1	I	191	LEU
1	I	194	ILE
1	I	197	TYR
1	I	207	ASP
1	I	214	ILE
1	I	226	VAL
1	I	230	GLN
1	I	233	ARG
1	I	245	THR
1	I	246	ASP
1	I	248	THR
1	I	253	THR
1	I	260	THR
1	I	286	PHE
1	I	290	THR
1	I	294	THR
1	I	298	VAL
1	I	306	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	7	LEU
1	J	16	LEU
1	J	17	GLN
1	J	20	SER
1	J	34	GLN
1	J	36	ILE
1	J	46	VAL
1	J	68	ILE
1	J	75	LYS
1	J	81	THR
1	J	86	LEU
1	J	89	ASN
1	J	94	ILE
1	J	97	ILE
1	J	100	SER
1	J	104	GLU
1	J	105	ASN
1	J	108	CYS
1	J	109	ILE
1	J	110	SER
1	J	118	THR
1	J	141	THR
1	J	143	LEU
1	J	151	GLN
1	J	154	LYS
1	J	157	LYS
1	J	159	ASN
1	J	160	VAL
1	J	162	LEU
1	J	170	LEU
1	J	173	GLU
1	J	176	LYS
1	J	181	ILE
1	J	191	LEU
1	J	194	ILE
1	J	197	TYR
1	J	212	LYS
1	J	214	ILE
1	J	220	THR
1	J	233	ARG
1	J	235	GLN
1	J	236	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	243	LYS
1	J	248	THR
1	J	263	LEU
1	J	264	GLN
1	J	268	LEU
1	J	270	SER
1	J	273	LYS
1	J	276	HIS
1	J	284	THR
1	J	286	PHE
1	J	289	GLN
1	J	292	ILE
1	J	304	GLU
1	K	9	SER
1	K	16	LEU
1	K	17	GLN
1	K	18	VAL
1	K	34	GLN
1	K	35	VAL
1	K	36	ILE
1	K	52	GLN
1	K	55	VAL
1	K	58	ILE
1	K	65	SER
1	K	68	ILE
1	K	70	ILE
1	K	76	LEU
1	K	79	ILE
1	K	87	GLN
1	K	92	THR
1	K	94	ILE
1	K	104	GLU
1	K	105	ASN
1	K	106	SER
1	K	107	ILE
1	K	109	ILE
1	K	117	LEU
1	K	118	THR
1	K	126	LEU
1	K	129	ILE
1	K	137	MET
1	K	138	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	141	THR
1	K	144	ASP
1	K	147	LEU
1	K	154	LYS
1	K	158	THR
1	K	160	VAL
1	K	168	ARG
1	K	169	GLU
1	K	170	LEU
1	K	178	VAL
1	K	189	GLU
1	K	194	ILE
1	K	197	TYR
1	K	204	GLN
1	K	207	ASP
1	K	214	ILE
1	K	220	THR
1	K	221	LEU
1	K	224	LYS
1	K	226	VAL
1	K	233	ARG
1	K	246	ASP
1	K	247	THR
1	K	248	THR
1	K	253	THR
1	K	263	LEU
1	K	273	LYS
1	K	281	ILE
1	K	289	GLN
1	K	295	ARG
1	K	297	GLU
1	L	7	LEU
1	L	17	GLN
1	L	27	THR
1	L	28	LEU
1	L	32	ASN
1	L	40	LYS
1	L	46	VAL
1	L	51	MET
1	L	63	ASP
1	L	65	SER
1	L	70	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	71	ARG
1	L	84	VAL
1	L	85	LYS
1	L	94	ILE
1	L	104	GLU
1	L	106	SER
1	L	108	CYS
1	L	112	GLU
1	L	133	ARG
1	L	140	GLU
1	L	141	THR
1	L	144	ASP
1	L	147	LEU
1	L	148	LYS
1	L	154	LYS
1	L	157	LYS
1	L	160	VAL
1	L	173	GLU
1	L	176	LYS
1	L	179	ASP
1	L	181	ILE
1	L	182	THR
1	L	197	TYR
1	L	211	CYS
1	L	215	GLU
1	L	230	GLN
1	L	253	THR
1	L	259	VAL
1	L	263	LEU
1	L	264	GLN
1	L	269	GLU
1	L	270	SER
1	L	281	ILE
1	L	284	THR
1	L	289	GLN
1	L	294	THR
1	M	3	LYS
1	M	16	LEU
1	M	23	ARG
1	M	27	THR
1	M	35	VAL
1	M	51	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	55	VAL
1	M	63	ASP
1	M	68	ILE
1	M	70	ILE
1	M	79	ILE
1	M	85	LYS
1	M	86	LEU
1	M	87	GLN
1	M	89	ASN
1	M	94	ILE
1	M	96	MET
1	M	98	GLN
1	M	101	ASP
1	M	104	GLU
1	M	106	SER
1	M	107	ILE
1	M	117	LEU
1	M	122	ILE
1	M	140	GLU
1	M	147	LEU
1	M	157	LYS
1	M	160	VAL
1	M	169	GLU
1	M	170	LEU
1	M	180	LEU
1	M	181	ILE
1	M	184	ASN
1	M	194	ILE
1	M	197	TYR
1	M	199	ASP
1	M	207	ASP
1	M	211	CYS
1	M	221	LEU
1	M	224	LYS
1	M	228	LEU
1	M	230	GLN
1	M	231	ASN
1	M	253	THR
1	M	263	LEU
1	M	268	LEU
1	M	270	SER
1	M	273	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	276	HIS
1	M	281	ILE
1	M	286	PHE
1	M	297	GLU
1	M	304	GLU
1	M	306	SER
1	N	5	VAL
1	N	6	VAL
1	N	15	VAL
1	N	17	GLN
1	N	23	ARG
1	N	35	VAL
1	N	36	ILE
1	N	46	VAL
1	N	50	ARG
1	N	60	CYS
1	N	68	ILE
1	N	70	ILE
1	N	73	SER
1	N	84	VAL
1	N	87	GLN
1	N	90	CYS
1	N	92	THR
1	N	94	ILE
1	N	100	SER
1	N	105	ASN
1	N	107	ILE
1	N	117	LEU
1	N	143	LEU
1	N	144	ASP
1	N	155	THR
1	N	160	VAL
1	N	177	CYS
1	N	180	LEU
1	N	181	ILE
1	N	182	THR
1	N	189	GLU
1	N	191	LEU
1	N	203	GLN
1	N	207	ASP
1	N	210	HIS
1	N	214	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	215	GLU
1	N	230	GLN
1	N	233	ARG
1	N	235	GLN
1	N	236	ARG
1	N	241	VAL
1	N	243	LYS
1	N	246	ASP
1	N	248	THR
1	N	259	VAL
1	N	263	LEU
1	N	265	GLU
1	N	266	MET
1	N	269	GLU
1	N	281	ILE
1	N	285	ARG
1	N	289	GLN
1	N	290	THR
1	N	292	ILE
1	N	295	ARG
1	N	304	GLU
1	O	7	LEU
1	O	10	VAL
1	O	15	VAL
1	O	18	VAL
1	O	23	ARG
1	O	44	GLN
1	O	46	VAL
1	O	50	ARG
1	O	52	GLN
1	O	55	VAL
1	O	63	ASP
1	O	64	ASP
1	O	68	ILE
1	O	70	ILE
1	O	71	ARG
1	O	72	GLU
1	O	77	ASP
1	O	84	VAL
1	O	85	LYS
1	O	94	ILE
1	O	97	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	99	VAL
1	O	106	SER
1	O	118	THR
1	O	123	GLU
1	O	141	THR
1	O	144	ASP
1	O	147	LEU
1	O	172	ASP
1	O	180	LEU
1	O	182	THR
1	O	185	GLU
1	O	189	GLU
1	O	190	VAL
1	O	194	ILE
1	O	201	SER
1	O	207	ASP
1	O	211	CYS
1	O	220	THR
1	O	226	VAL
1	O	228	LEU
1	O	229	SER
1	O	230	GLN
1	O	235	GLN
1	O	242	VAL
1	O	243	LYS
1	O	245	THR
1	O	246	ASP
1	O	248	THR
1	O	253	THR
1	O	260	THR
1	O	263	LEU
1	O	266	MET
1	O	268	LEU
1	O	272	ILE
1	O	281	ILE
1	O	294	THR
1	O	297	GLU
1	O	304	GLU
1	P	1	MET
1	P	3	LYS
1	P	13	ASP
1	P	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	18	VAL
1	P	34	GLN
1	P	35	VAL
1	P	46	VAL
1	P	50	ARG
1	P	60	CYS
1	P	65	SER
1	P	68	ILE
1	P	70	ILE
1	P	71	ARG
1	P	72	GLU
1	P	73	SER
1	P	75	LYS
1	P	77	ASP
1	P	86	LEU
1	P	92	THR
1	P	94	ILE
1	P	98	GLN
1	P	99	VAL
1	P	101	ASP
1	P	118	THR
1	P	130	ARG
1	P	135	LEU
1	P	141	THR
1	P	158	THR
1	P	161	ILE
1	P	172	ASP
1	P	174	LEU
1	P	176	LYS
1	P	180	LEU
1	P	185	GLU
1	P	186	THR
1	P	190	VAL
1	P	191	LEU
1	P	194	ILE
1	P	197	TYR
1	P	209	LEU
1	P	212	LYS
1	P	214	ILE
1	P	215	GLU
1	P	217	VAL
1	P	220	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	221	LEU
1	P	226	VAL
1	P	236	ARG
1	P	243	LYS
1	P	245	THR
1	P	253	THR
1	P	263	LEU
1	P	264	GLN
1	P	270	SER
1	P	276	HIS
1	P	281	ILE
1	P	289	GLN
1	P	291	SER
1	P	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	87	GLN
1	A	98	GLN
1	A	255	ASN
1	B	11	ASN
1	B	17	GLN
1	B	44	GLN
1	B	89	ASN
1	B	163	ASN
1	B	203	GLN
1	B	230	GLN
1	B	231	ASN
1	B	289	GLN
1	C	43	ASN
1	C	80	ASN
1	C	159	ASN
1	C	210	HIS
1	C	276	HIS
1	D	17	GLN
1	D	29	HIS
1	D	44	GLN
1	D	87	GLN
1	D	138	GLN
1	D	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	204	GLN
1	D	235	GLN
1	E	17	GLN
1	E	44	GLN
1	E	87	GLN
1	E	151	GLN
1	E	159	ASN
1	E	184	ASN
1	E	230	GLN
1	E	231	ASN
1	E	276	HIS
1	E	305	HIS
1	F	98	GLN
1	F	184	ASN
1	F	210	HIS
1	F	230	GLN
1	F	231	ASN
1	F	264	GLN
1	G	52	GLN
1	G	69	ASN
1	G	89	ASN
1	G	98	GLN
1	G	114	ASN
1	G	138	GLN
1	G	151	GLN
1	G	163	ASN
1	G	264	GLN
1	G	305	HIS
1	H	17	GLN
1	H	32	ASN
1	H	204	GLN
1	H	210	HIS
1	I	43	ASN
1	I	98	GLN
1	I	151	GLN
1	I	289	GLN
1	J	17	GLN
1	J	32	ASN
1	J	87	GLN
1	J	114	ASN
1	J	151	GLN
1	J	159	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	163	ASN
1	J	230	GLN
1	J	235	GLN
1	J	264	GLN
1	J	276	HIS
1	J	305	HIS
1	K	2	ASN
1	K	69	ASN
1	K	98	GLN
1	K	151	GLN
1	K	203	GLN
1	K	289	GLN
1	L	14	HIS
1	L	43	ASN
1	L	98	GLN
1	L	151	GLN
1	L	210	HIS
1	L	289	GLN
1	M	80	ASN
1	M	163	ASN
1	M	184	ASN
1	M	230	GLN
1	M	276	HIS
1	N	17	GLN
1	N	32	ASN
1	N	163	ASN
1	N	203	GLN
1	N	204	GLN
1	N	235	GLN
1	N	255	ASN
1	O	17	GLN
1	O	44	GLN
1	O	69	ASN
1	O	151	GLN
1	O	163	ASN
1	O	230	GLN
1	O	276	HIS
1	O	289	GLN
1	P	17	GLN
1	P	34	GLN
1	P	69	ASN
1	P	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	210	HIS
1	P	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	306/309 (99%)	-0.70	1 (0%) 90 84	61, 108, 179, 294	0
1	B	306/309 (99%)	-0.78	0 100 100	67, 98, 149, 239	0
1	C	306/309 (99%)	-0.87	0 100 100	42, 83, 141, 201	0
1	D	306/309 (99%)	-0.97	0 100 100	34, 76, 134, 179	0
1	E	306/309 (99%)	-1.02	0 100 100	38, 62, 112, 182	0
1	F	306/309 (99%)	-0.88	0 100 100	46, 81, 140, 173	0
1	G	306/309 (99%)	-0.91	0 100 100	40, 79, 131, 162	0
1	H	306/309 (99%)	-0.97	0 100 100	36, 69, 125, 214	0
1	I	306/309 (99%)	-0.87	0 100 100	43, 76, 125, 199	0
1	J	306/309 (99%)	-0.94	0 100 100	43, 80, 130, 202	0
1	K	306/309 (99%)	-0.88	0 100 100	47, 83, 140, 172	0
1	L	306/309 (99%)	-0.99	1 (0%) 90 84	36, 63, 112, 186	0
1	M	306/309 (99%)	-0.85	1 (0%) 90 84	42, 73, 142, 206	0
1	N	306/309 (99%)	-0.88	0 100 100	44, 82, 146, 189	0
1	O	306/309 (99%)	-0.77	0 100 100	59, 96, 163, 215	0
1	P	306/309 (99%)	-0.69	1 (0%) 90 84	61, 107, 170, 202	0
All	All	4896/4944 (99%)	-0.87	4 (0%) 92 91	34, 82, 146, 294	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	288	ALA	3.8
1	L	243	LYS	3.4
1	A	245	THR	3.2
1	P	286	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.