



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:44 PM UTC

PDB ID : 3K19 / pdb_00003k19
Title : OmpF porin
Authors : Kefala, G.; Ahn, C.; Krupa, M.; Maslennikov, I.; Kwiatkowski, W.; Choe, S.;
Center for Structures of Membrane Proteins (CSMP)
Deposited on : 2009-09-26
Resolution : 3.79 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

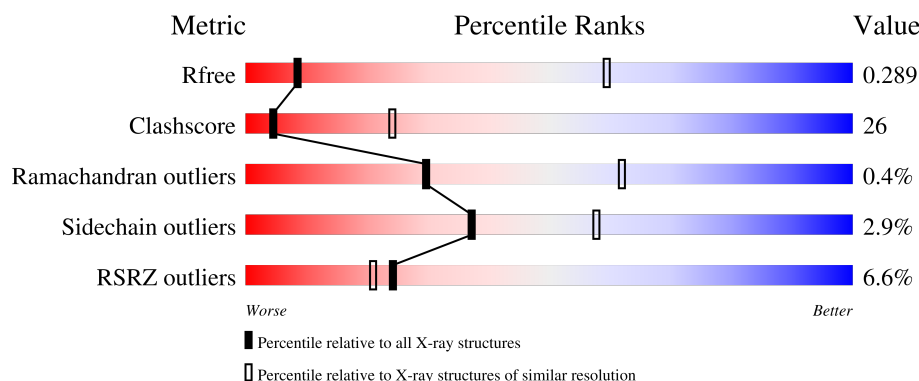
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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.



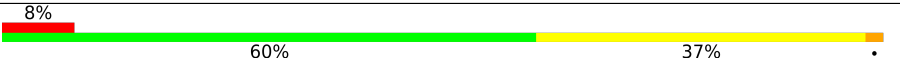
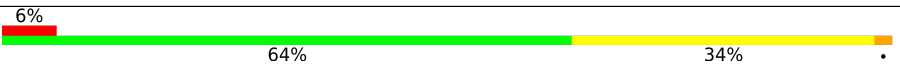
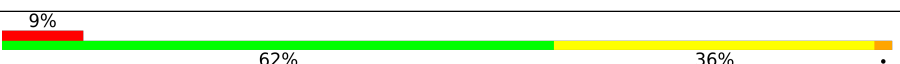
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	340	6% 63% 34% .
1	B	340	7% 62% 35% .
1	C	340	6% 64% 34% .
1	D	340	9% 64% 34% .
1	E	340	4% 63% 34% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	340	
1	G	340	
1	H	340	
1	I	340	
1	J	340	
1	K	340	
1	L	340	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31524 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.

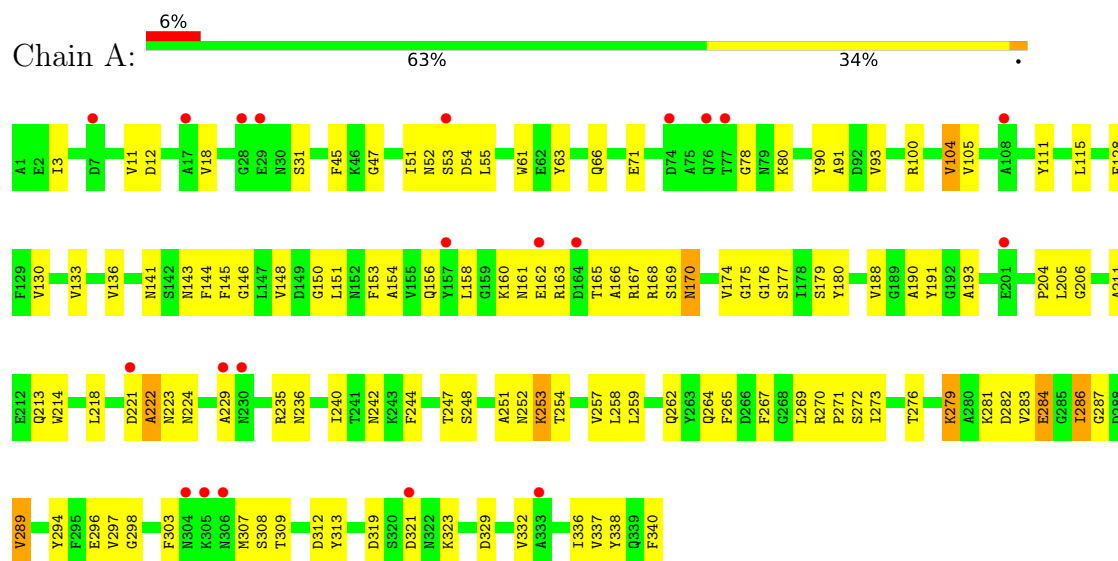
- Molecule 1 is a protein called Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	8	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	8	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	F	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	G	340	Total	C	N	O	S	8	0	0
			2627	1654	438	532	3			
1	H	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	I	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	J	340	Total	C	N	O	S	8	0	0
			2627	1654	438	532	3			
1	K	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	L	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

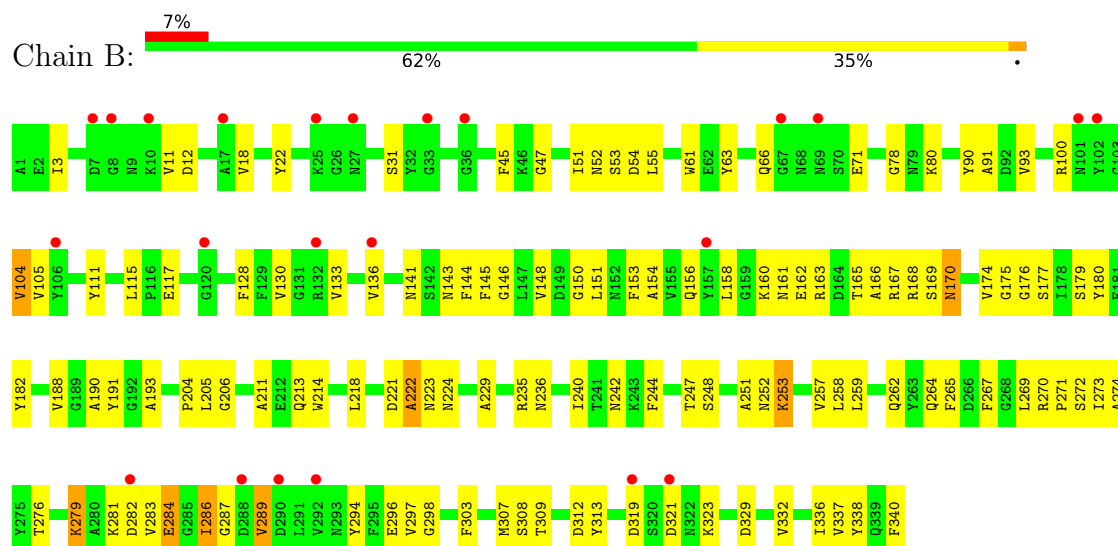
3 Residue-property plots

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: Outer membrane protein F

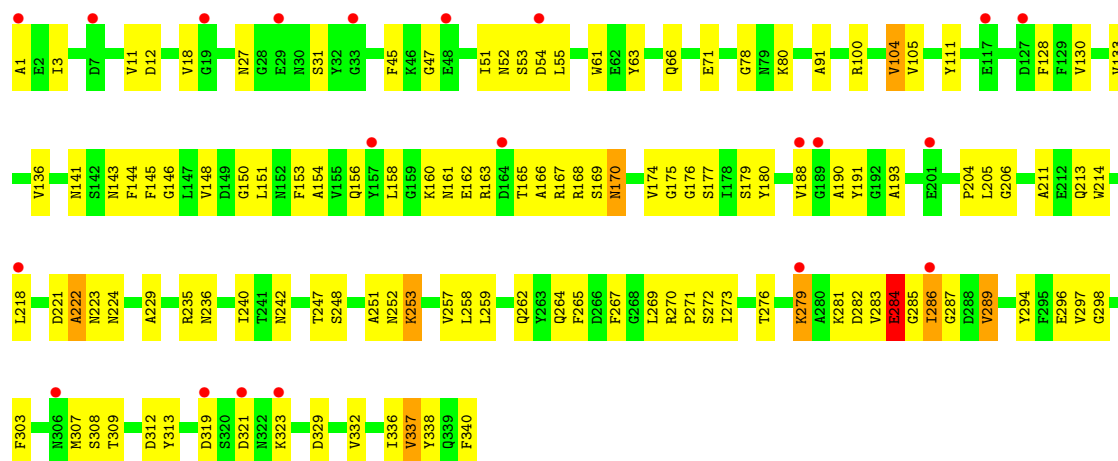


• Molecule 1: Outer membrane protein F

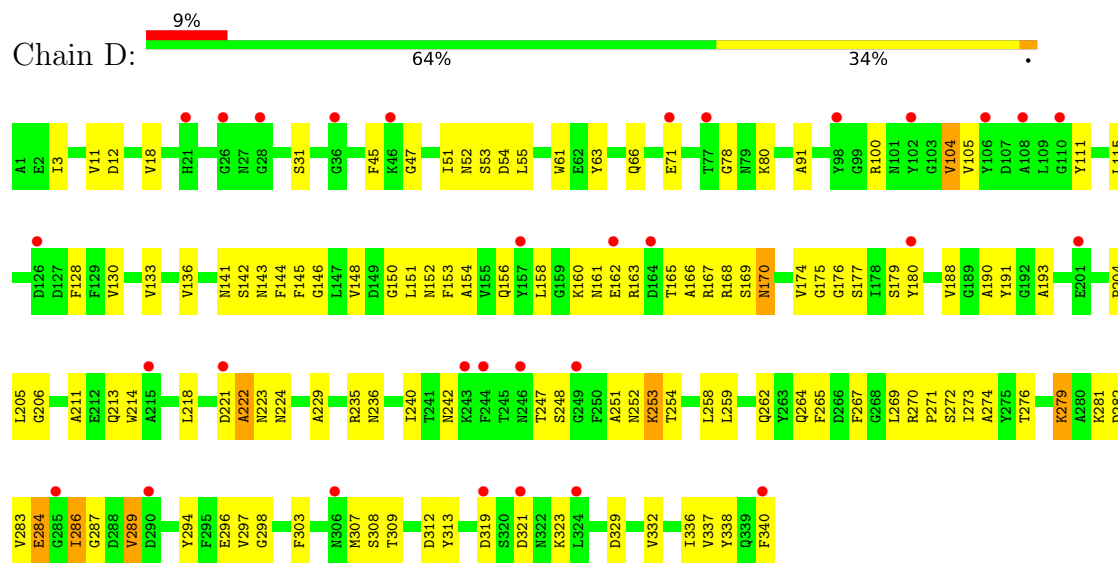


• Molecule 1: Outer membrane protein F

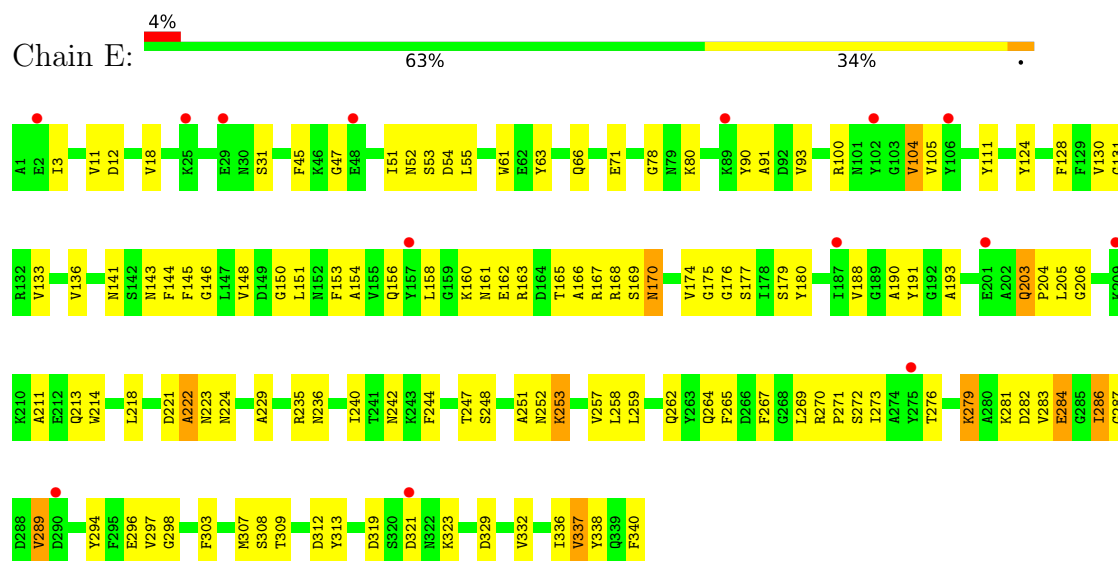




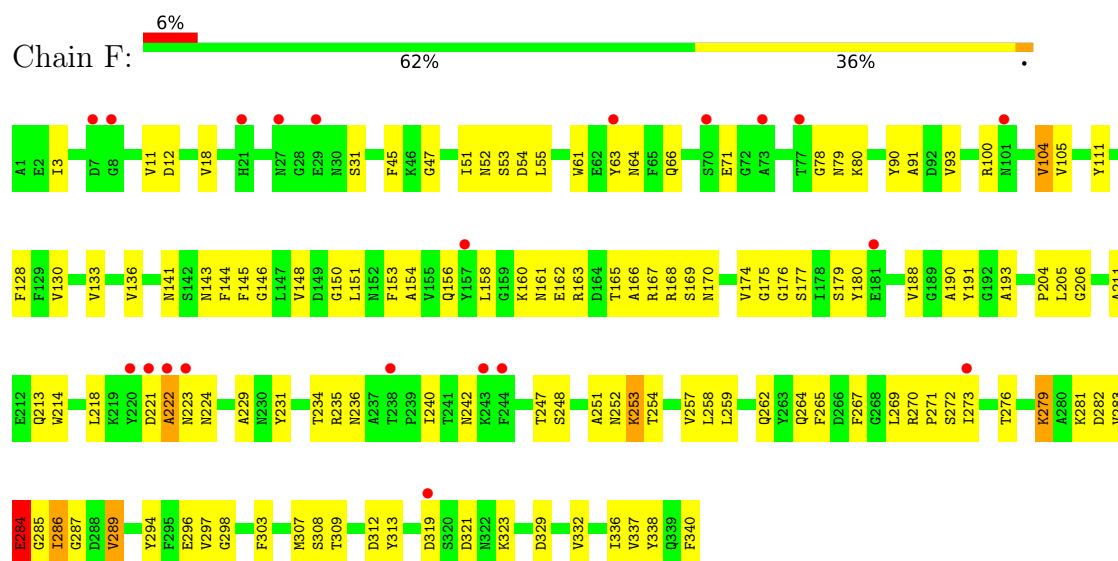
• Molecule 1: Outer membrane protein F



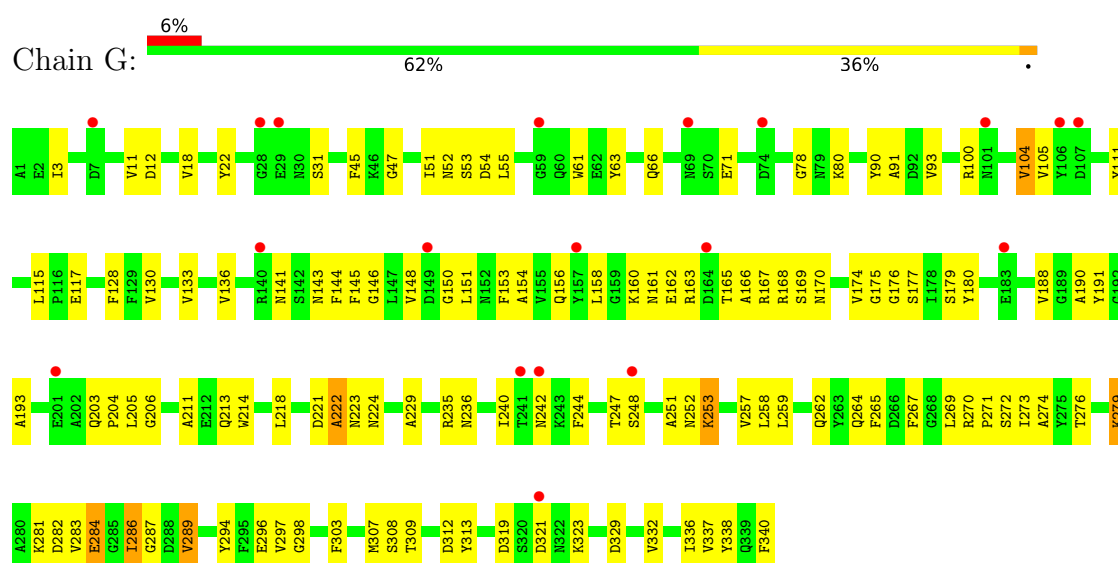
• Molecule 1: Outer membrane protein F



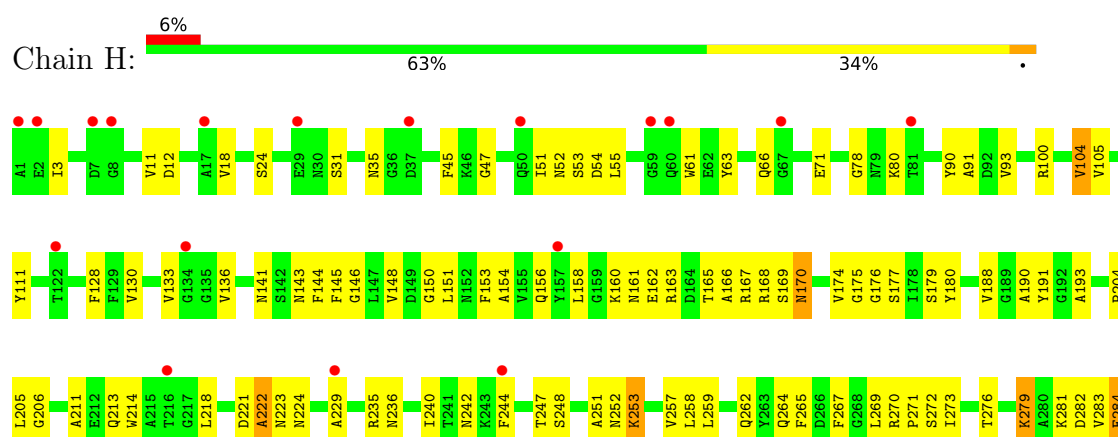
• Molecule 1: Outer membrane protein F

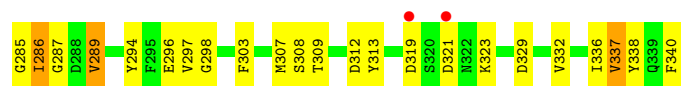


• Molecule 1: Outer membrane protein F

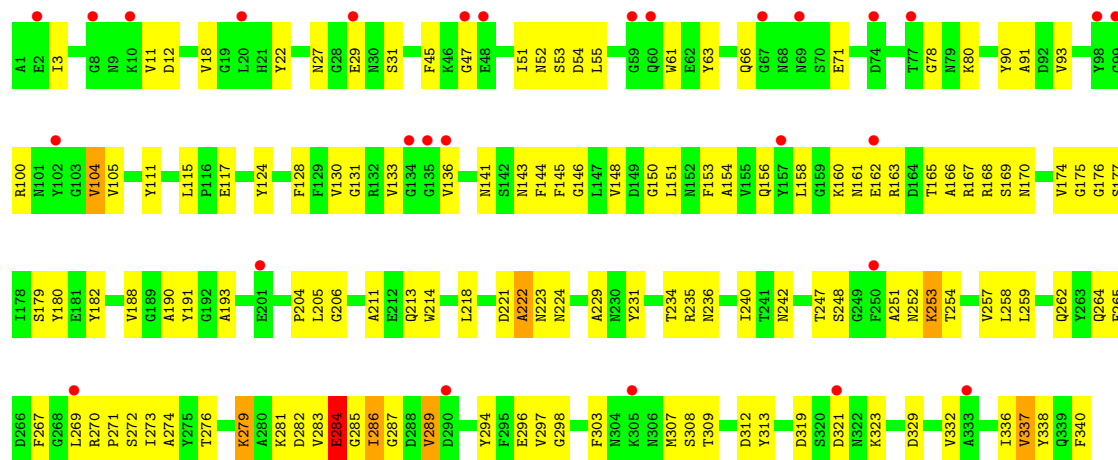


• Molecule 1: Outer membrane protein F

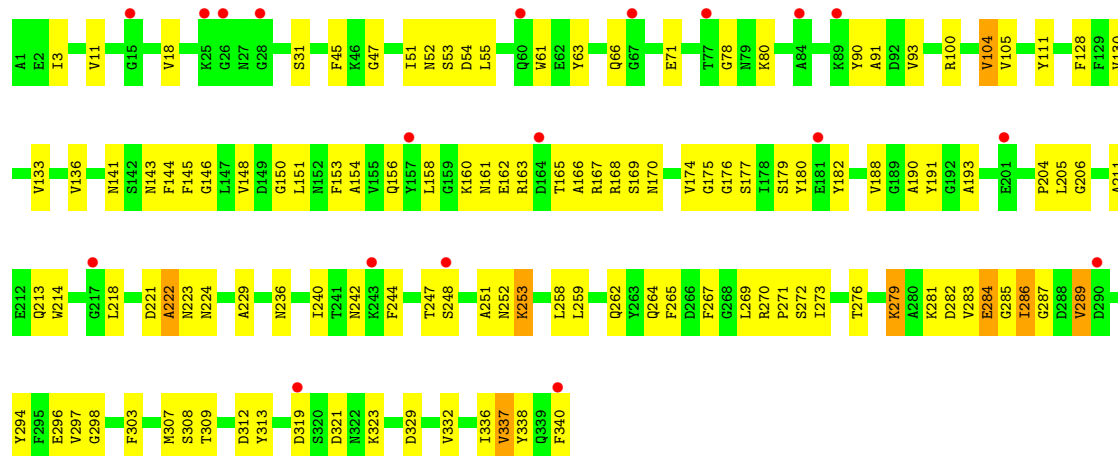




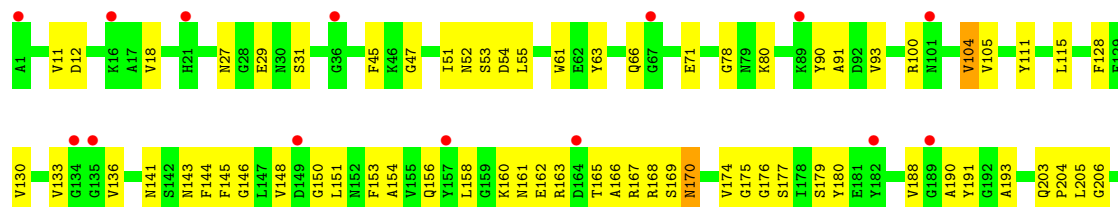
• Molecule 1: Outer membrane protein F

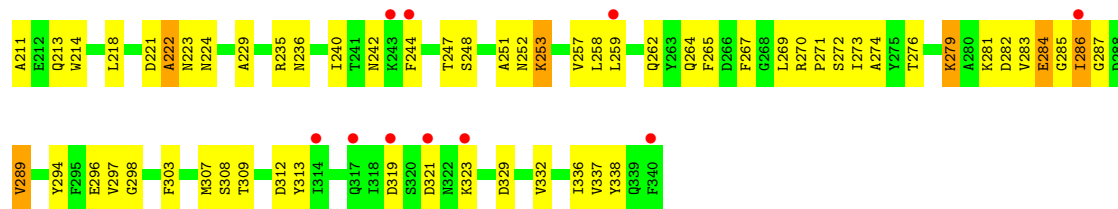


• Molecule 1: Outer membrane protein F

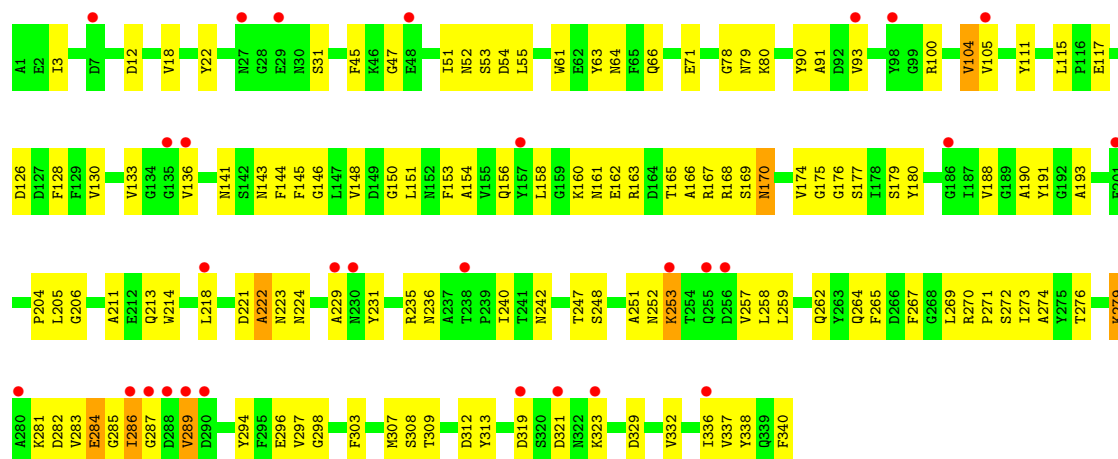


• Molecule 1: Outer membrane protein F





● Molecule 1: Outer membrane protein F



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.71Å 210.52Å 137.04Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	49.57 – 3.79 49.57 – 3.79	Depositor EDS
% Data completeness (in resolution range)	49.6 (49.57-3.79) 99.1 (49.57-3.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.280 , 0.288 0.280 , 0.289	Depositor DCC
R_{free} test set	3787 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 0.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	31524	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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	0.34	0/2683	0.69	0/3628
1	B	0.32	0/2683	0.69	0/3628
1	C	0.33	0/2683	0.69	1/3628 (0.0%)
1	D	0.34	0/2683	0.69	0/3628
1	E	0.33	0/2683	0.69	3/3628 (0.1%)
1	F	0.34	0/2683	0.69	0/3628
1	G	0.32	0/2683	0.68	0/3628
1	H	0.31	0/2683	0.68	1/3628 (0.0%)
1	I	0.30	0/2683	0.69	1/3628 (0.0%)
1	J	0.32	0/2683	0.68	1/3628 (0.0%)
1	K	0.31	0/2683	0.69	2/3628 (0.1%)
1	L	0.30	0/2683	0.69	0/3628
All	All	0.32	0/32196	0.69	9/43536 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	337	VAL	N-CA-C	5.17	115.29	107.80
1	E	337	VAL	N-CA-C	5.16	115.28	107.75
1	I	337	VAL	N-CA-C	5.15	115.27	107.80
1	E	203	GLN	CA-C-N	5.08	124.39	118.85
1	E	203	GLN	C-N-CA	5.08	124.39	118.85
1	J	337	VAL	N-CA-C	5.08	115.17	107.75
1	K	203	GLN	CA-C-N	5.04	124.34	118.85
1	K	203	GLN	C-N-CA	5.04	124.34	118.85
1	C	337	VAL	N-CA-C	5.03	115.09	107.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2444	147	0
1	B	2627	0	2444	154	0
1	C	2627	0	2444	148	0
1	D	2627	0	2444	151	0
1	E	2627	0	2444	149	0
1	F	2627	0	2444	153	0
1	G	2627	0	2444	157	0
1	H	2627	0	2444	149	0
1	I	2627	0	2444	157	0
1	J	2627	0	2444	146	0
1	K	2627	0	2444	152	0
1	L	2627	0	2444	153	0
All	All	31524	0	29328	1589	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 26.

All (1589) 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:E:321:ASP:OD1	1:K:287:GLY:HA2	1.18	1.35
1:E:287:GLY:CA	1:I:321:ASP:OD1	1.76	1.33
1:I:287:GLY:CA	1:K:321:ASP:OD1	1.75	1.32
1:B:287:GLY:CA	1:L:321:ASP:OD1	1.76	1.32
1:C:287:GLY:HA2	1:G:321:ASP:OD1	1.17	1.31
1:H:321:ASP:OD1	1:L:287:GLY:CA	1.78	1.29
1:B:321:ASP:OD1	1:H:287:GLY:HA2	1.22	1.28
1:C:287:GLY:CA	1:G:321:ASP:OD1	1.83	1.27
1:C:321:ASP:OD1	1:D:287:GLY:HA2	1.11	1.27
1:A:321:ASP:OD1	1:J:287:GLY:CA	1.82	1.25
1:D:321:ASP:OD1	1:G:287:GLY:CA	1.83	1.25
1:A:287:GLY:HA2	1:F:321:ASP:OD1	1.10	1.25
1:F:287:GLY:CA	1:J:321:ASP:OD1	1.82	1.25
1:E:321:ASP:OD1	1:K:287:GLY:CA	1.84	1.24
1:F:287:GLY:HA2	1:J:321:ASP:OD1	1.11	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ASP:OD1	1:D:287:GLY:CA	1.85	1.21
1:D:321:ASP:OD1	1:G:287:GLY:HA2	1.06	1.19
1:A:287:GLY:CA	1:F:321:ASP:OD1	1.90	1.18
1:E:287:GLY:HA2	1:I:321:ASP:OD1	1.02	1.17
1:B:287:GLY:HA2	1:L:321:ASP:OD1	1.02	1.17
1:I:287:GLY:HA2	1:K:321:ASP:OD1	1.00	1.15
1:A:321:ASP:OD1	1:J:287:GLY:HA2	0.98	1.15
1:B:321:ASP:OD1	1:H:287:GLY:CA	1.94	1.15
1:H:321:ASP:OD1	1:L:287:GLY:HA2	0.98	1.13
1:G:71:GLU:HB3	1:H:80:LYS:HD2	1.34	1.08
1:D:71:GLU:HB3	1:E:80:LYS:HD2	1.36	1.07
1:L:313:TYR:CD1	1:L:332:VAL:HG22	1.92	1.04
1:A:80:LYS:HD2	1:C:71:GLU:HB3	1.37	1.04
1:I:313:TYR:CD1	1:I:332:VAL:HG22	1.92	1.04
1:K:313:TYR:CD1	1:K:332:VAL:HG22	1.93	1.03
1:C:313:TYR:CD1	1:C:332:VAL:HG22	1.94	1.03
1:J:313:TYR:CD1	1:J:332:VAL:HG22	1.93	1.03
1:H:313:TYR:CD1	1:H:332:VAL:HG22	1.92	1.03
1:A:313:TYR:CD1	1:A:332:VAL:HG22	1.94	1.02
1:G:80:LYS:HD2	1:I:71:GLU:HB3	1.40	1.02
1:F:313:TYR:CD1	1:F:332:VAL:HG22	1.94	1.02
1:G:313:TYR:CD1	1:G:332:VAL:HG22	1.93	1.02
1:J:71:GLU:HB3	1:K:80:LYS:HD2	1.41	1.02
1:B:313:TYR:CD1	1:B:332:VAL:HG22	1.93	1.02
1:H:71:GLU:HB3	1:I:80:LYS:HD2	1.40	1.01
1:D:313:TYR:CD1	1:D:332:VAL:HG22	1.96	1.00
1:E:313:TYR:CD1	1:E:332:VAL:HG22	1.94	1.00
1:K:71:GLU:HB3	1:L:80:LYS:HD2	1.43	1.00
1:D:80:LYS:HD2	1:F:71:GLU:HB3	1.44	1.00
1:A:71:GLU:HB3	1:B:80:LYS:HD2	1.39	1.00
1:B:71:GLU:HB3	1:C:80:LYS:HD2	1.40	0.99
1:J:80:LYS:HD2	1:L:71:GLU:HB3	1.41	0.99
1:E:71:GLU:HB3	1:F:80:LYS:HD2	1.41	0.98
1:E:165:THR:HG22	1:E:167:ARG:H	1.30	0.97
1:D:165:THR:HG22	1:D:167:ARG:H	1.29	0.96
1:C:165:THR:HG22	1:C:167:ARG:H	1.30	0.96
1:A:321:ASP:CG	1:J:287:GLY:HA2	1.91	0.96
1:B:287:GLY:CA	1:L:321:ASP:CG	2.39	0.95
1:B:165:THR:HG22	1:B:167:ARG:H	1.29	0.95
1:J:165:THR:HG22	1:J:167:ARG:H	1.30	0.95
1:F:165:THR:HG22	1:F:167:ARG:H	1.30	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:THR:HG22	1:K:167:ARG:H	1.28	0.94
1:A:165:THR:HG22	1:A:167:ARG:H	1.30	0.94
1:L:165:THR:HG22	1:L:167:ARG:H	1.27	0.94
1:A:321:ASP:CG	1:J:287:GLY:CA	2.41	0.94
1:I:165:THR:HG22	1:I:167:ARG:H	1.29	0.94
1:I:287:GLY:CA	1:K:321:ASP:CG	2.42	0.93
1:G:165:THR:HG22	1:G:167:ARG:H	1.31	0.92
1:H:165:THR:HG22	1:H:167:ARG:H	1.31	0.92
1:E:287:GLY:CA	1:I:321:ASP:CG	2.42	0.91
1:H:321:ASP:CG	1:L:287:GLY:CA	2.44	0.90
1:I:27:ASN:HD22	1:I:29:GLU:HB2	1.36	0.90
1:K:279:LYS:HE3	1:K:281:LYS:HZ2	1.36	0.89
1:L:165:THR:HG22	1:L:167:ARG:N	1.87	0.89
1:C:279:LYS:HE3	1:C:281:LYS:HZ2	1.39	0.88
1:A:165:THR:HG22	1:A:167:ARG:N	1.89	0.88
1:B:287:GLY:HA2	1:L:321:ASP:CG	1.96	0.88
1:F:165:THR:HG22	1:F:167:ARG:N	1.89	0.88
1:K:165:THR:HG22	1:K:167:ARG:N	1.88	0.88
1:B:279:LYS:HE3	1:B:281:LYS:HZ2	1.39	0.87
1:E:165:THR:HG22	1:E:167:ARG:N	1.89	0.87
1:A:309:THR:HG22	1:A:336:ILE:HA	1.57	0.87
1:C:165:THR:HG22	1:C:167:ARG:N	1.89	0.87
1:D:165:THR:HG22	1:D:167:ARG:N	1.89	0.87
1:J:279:LYS:HE3	1:J:281:LYS:HZ2	1.37	0.86
1:C:313:TYR:HD1	1:C:332:VAL:HG22	1.40	0.86
1:J:165:THR:HG22	1:J:167:ARG:N	1.89	0.86
1:A:279:LYS:HE3	1:A:281:LYS:HZ2	1.40	0.86
1:D:321:ASP:CG	1:G:287:GLY:CA	2.48	0.86
1:H:321:ASP:CG	1:L:287:GLY:HA2	1.99	0.86
1:B:165:THR:HG22	1:B:167:ARG:N	1.89	0.86
1:G:165:THR:HG22	1:G:167:ARG:N	1.90	0.86
1:D:279:LYS:HE3	1:D:281:LYS:HZ2	1.38	0.85
1:H:165:THR:HG22	1:H:167:ARG:N	1.90	0.85
1:H:279:LYS:HE3	1:H:281:LYS:HZ2	1.38	0.85
1:I:165:THR:HG22	1:I:167:ARG:N	1.88	0.85
1:J:309:THR:HG22	1:J:336:ILE:HA	1.58	0.85
1:I:287:GLY:HA3	1:K:321:ASP:CG	2.01	0.85
1:I:279:LYS:HE3	1:I:281:LYS:HZ2	1.40	0.85
1:G:313:TYR:HD1	1:G:332:VAL:HG22	1.40	0.85
1:K:313:TYR:HD1	1:K:332:VAL:HG22	1.40	0.85
1:F:309:THR:HG22	1:F:336:ILE:HA	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:THR:HG22	1:C:336:ILE:HA	1.59	0.84
1:D:309:THR:HG22	1:D:336:ILE:HA	1.57	0.84
1:G:279:LYS:HE3	1:G:281:LYS:HZ2	1.42	0.84
1:G:309:THR:HG22	1:G:336:ILE:HA	1.58	0.84
1:K:71:GLU:HG3	1:L:100:ARG:NH2	1.91	0.84
1:L:279:LYS:HE3	1:L:281:LYS:HZ2	1.40	0.84
1:J:313:TYR:HD1	1:J:332:VAL:HG22	1.39	0.84
1:L:286:ILE:HG21	1:L:289:VAL:HG21	1.58	0.84
1:A:313:TYR:HD1	1:A:332:VAL:HG22	1.40	0.84
1:B:309:THR:HG22	1:B:336:ILE:HA	1.58	0.84
1:E:279:LYS:HE3	1:E:281:LYS:HZ2	1.42	0.84
1:E:286:ILE:HG21	1:E:289:VAL:HG21	1.60	0.84
1:F:286:ILE:HG21	1:F:289:VAL:HG21	1.60	0.83
1:E:313:TYR:HD1	1:E:332:VAL:HG22	1.41	0.83
1:F:279:LYS:HE3	1:F:281:LYS:HZ2	1.41	0.83
1:F:313:TYR:HD1	1:F:332:VAL:HG22	1.41	0.83
1:K:309:THR:HG22	1:K:336:ILE:HA	1.60	0.83
1:K:286:ILE:HG21	1:K:289:VAL:HG21	1.59	0.83
1:D:100:ARG:NH2	1:F:71:GLU:HG3	1.94	0.83
1:E:287:GLY:HA3	1:I:321:ASP:CG	2.03	0.83
1:H:309:THR:HG22	1:H:336:ILE:HA	1.60	0.83
1:D:321:ASP:CG	1:G:287:GLY:HA2	2.03	0.82
1:K:31:SER:HA	1:K:329:ASP:HB2	1.61	0.82
1:B:287:GLY:HA3	1:L:321:ASP:CG	2.01	0.82
1:I:313:TYR:HD1	1:I:332:VAL:HG22	1.40	0.82
1:E:309:THR:HG22	1:E:336:ILE:HA	1.59	0.82
1:H:111:TYR:CZ	1:H:188:VAL:CG2	2.63	0.82
1:I:309:THR:HG22	1:I:336:ILE:HA	1.61	0.82
1:C:31:SER:HA	1:C:329:ASP:HB2	1.62	0.82
1:H:313:TYR:HD1	1:H:332:VAL:HG22	1.39	0.82
1:H:321:ASP:CG	1:L:287:GLY:HA3	2.05	0.82
1:L:309:THR:HG22	1:L:336:ILE:HA	1.61	0.82
1:G:31:SER:HA	1:G:329:ASP:HB2	1.62	0.81
1:I:286:ILE:HG21	1:I:289:VAL:HG21	1.59	0.81
1:J:286:ILE:HG21	1:J:289:VAL:HG21	1.61	0.81
1:H:31:SER:HA	1:H:329:ASP:HB2	1.61	0.81
1:E:287:GLY:HA2	1:I:321:ASP:CG	2.00	0.81
1:E:31:SER:HA	1:E:329:ASP:HB2	1.61	0.81
1:B:286:ILE:HG21	1:B:289:VAL:HG21	1.61	0.81
1:C:286:ILE:HG21	1:C:289:VAL:HG21	1.61	0.81
1:C:321:ASP:CG	1:D:287:GLY:CA	2.53	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:SER:HA	1:J:329:ASP:HB2	1.63	0.81
1:B:313:TYR:HD1	1:B:332:VAL:HG22	1.40	0.81
1:C:287:GLY:HA3	1:G:321:ASP:OD1	1.79	0.81
1:I:27:ASN:ND2	1:I:29:GLU:HB2	1.96	0.81
1:D:31:SER:HA	1:D:329:ASP:HB2	1.63	0.81
1:G:286:ILE:HG21	1:G:289:VAL:HG21	1.63	0.81
1:A:286:ILE:HG21	1:A:289:VAL:HG21	1.63	0.80
1:B:71:GLU:HG3	1:C:100:ARG:NH2	1.96	0.80
1:H:286:ILE:HG21	1:H:289:VAL:HG21	1.61	0.80
1:B:31:SER:HA	1:B:329:ASP:HB2	1.63	0.80
1:G:111:TYR:CZ	1:G:188:VAL:CG2	2.64	0.80
1:L:111:TYR:CZ	1:L:188:VAL:CG2	2.64	0.80
1:I:111:TYR:CZ	1:I:188:VAL:CG2	2.65	0.80
1:J:71:GLU:HG3	1:K:100:ARG:NH2	1.96	0.80
1:F:31:SER:HA	1:F:329:ASP:HB2	1.63	0.80
1:K:111:TYR:CZ	1:K:188:VAL:CG2	2.65	0.80
1:C:111:TYR:CZ	1:C:188:VAL:CG2	2.64	0.80
1:L:31:SER:HA	1:L:329:ASP:HB2	1.62	0.80
1:A:321:ASP:CG	1:J:287:GLY:HA3	2.07	0.79
1:I:287:GLY:HA2	1:K:321:ASP:CG	2.00	0.79
1:A:31:SER:HA	1:A:329:ASP:HB2	1.63	0.79
1:L:313:TYR:HD1	1:L:332:VAL:HG22	1.39	0.79
1:D:286:ILE:HG21	1:D:289:VAL:HG21	1.62	0.79
1:E:111:TYR:CZ	1:E:188:VAL:CG2	2.66	0.79
1:B:111:TYR:CZ	1:B:188:VAL:CG2	2.67	0.78
1:A:111:TYR:CZ	1:A:188:VAL:CG2	2.65	0.78
1:I:31:SER:HA	1:I:329:ASP:HB2	1.63	0.78
1:J:111:TYR:CZ	1:J:188:VAL:CG2	2.66	0.78
1:A:287:GLY:HA2	1:F:321:ASP:CG	2.08	0.78
1:E:321:ASP:OD1	1:K:287:GLY:HA3	1.81	0.78
1:A:287:GLY:CA	1:F:321:ASP:CG	2.56	0.78
1:F:111:TYR:CZ	1:F:188:VAL:CG2	2.66	0.78
1:D:313:TYR:HD1	1:D:332:VAL:HG22	1.44	0.78
1:D:111:TYR:CZ	1:D:188:VAL:CG2	2.68	0.77
1:D:321:ASP:CG	1:G:287:GLY:HA3	2.10	0.76
1:C:321:ASP:CG	1:D:287:GLY:HA2	2.09	0.76
1:G:160:LYS:HD3	1:G:162:GLU:OE2	1.86	0.76
1:H:160:LYS:HD3	1:H:162:GLU:OE2	1.86	0.76
1:H:279:LYS:HE3	1:H:281:LYS:NZ	2.01	0.76
1:H:313:TYR:CD1	1:H:332:VAL:CG2	2.69	0.75
1:I:313:TYR:CD1	1:I:332:VAL:CG2	2.70	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HD3	1:C:162:GLU:OE2	1.86	0.75
1:K:313:TYR:CD1	1:K:332:VAL:CG2	2.70	0.75
1:D:160:LYS:HD3	1:D:162:GLU:OE2	1.86	0.75
1:G:279:LYS:HE3	1:G:281:LYS:NZ	2.02	0.75
1:J:313:TYR:CD1	1:J:332:VAL:CG2	2.70	0.75
1:L:160:LYS:HD3	1:L:162:GLU:OE2	1.86	0.74
1:J:160:LYS:HD3	1:J:162:GLU:OE2	1.87	0.74
1:K:160:LYS:HD3	1:K:162:GLU:OE2	1.87	0.74
1:E:71:GLU:HG3	1:F:100:ARG:NH2	2.03	0.74
1:L:313:TYR:CD1	1:L:332:VAL:CG2	2.69	0.74
1:C:321:ASP:CG	1:D:287:GLY:HA3	2.13	0.74
1:E:160:LYS:HD3	1:E:162:GLU:OE2	1.88	0.74
1:E:313:TYR:CD1	1:E:332:VAL:CG2	2.71	0.74
1:F:287:GLY:CA	1:J:321:ASP:CG	2.61	0.74
1:A:160:LYS:HD3	1:A:162:GLU:OE2	1.87	0.74
1:A:279:LYS:HE3	1:A:281:LYS:NZ	2.02	0.74
1:C:313:TYR:CD1	1:C:332:VAL:CG2	2.70	0.73
1:L:286:ILE:HG21	1:L:289:VAL:CG2	2.18	0.73
1:B:160:LYS:HD3	1:B:162:GLU:OE2	1.87	0.73
1:F:160:LYS:HD3	1:F:162:GLU:OE2	1.88	0.73
1:C:279:LYS:HE3	1:C:281:LYS:NZ	2.03	0.73
1:D:279:LYS:HE3	1:D:281:LYS:NZ	2.04	0.73
1:I:286:ILE:CG2	1:I:289:VAL:CG2	2.67	0.73
1:K:279:LYS:HE3	1:K:281:LYS:NZ	2.03	0.73
1:F:286:ILE:HD12	1:F:286:ILE:N	2.02	0.73
1:I:279:LYS:HE3	1:I:281:LYS:NZ	2.04	0.73
1:L:279:LYS:HE3	1:L:281:LYS:NZ	2.02	0.73
1:A:313:TYR:CD1	1:A:332:VAL:CG2	2.71	0.73
1:E:286:ILE:N	1:E:286:ILE:HD12	2.03	0.73
1:J:100:ARG:NH2	1:L:71:GLU:HG3	2.04	0.73
1:E:279:LYS:HE3	1:E:281:LYS:NZ	2.03	0.73
1:B:313:TYR:CD1	1:B:332:VAL:CG2	2.71	0.72
1:H:286:ILE:HD12	1:H:286:ILE:N	2.04	0.72
1:H:71:GLU:HG3	1:I:100:ARG:NH2	2.04	0.72
1:J:279:LYS:HE3	1:J:281:LYS:NZ	2.02	0.72
1:L:286:ILE:CG2	1:L:289:VAL:CG2	2.66	0.72
1:F:287:GLY:HA3	1:J:321:ASP:CG	2.15	0.72
1:K:286:ILE:HG21	1:K:289:VAL:CG2	2.19	0.72
1:B:279:LYS:HE3	1:B:281:LYS:NZ	2.04	0.72
1:K:286:ILE:CG2	1:K:289:VAL:CG2	2.68	0.72
1:I:286:ILE:HD12	1:I:286:ILE:N	2.05	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:NH2	1:C:71:GLU:HG3	2.05	0.72
1:J:286:ILE:N	1:J:286:ILE:HD12	2.05	0.72
1:D:313:TYR:CD1	1:D:332:VAL:CG2	2.73	0.72
1:I:160:LYS:HD3	1:I:162:GLU:OE2	1.88	0.72
1:I:286:ILE:HG21	1:I:289:VAL:CG2	2.19	0.72
1:G:313:TYR:CD1	1:G:332:VAL:CG2	2.70	0.71
1:F:279:LYS:HE3	1:F:281:LYS:NZ	2.04	0.71
1:A:286:ILE:HD12	1:A:286:ILE:N	2.04	0.71
1:C:111:TYR:OH	1:C:188:VAL:CG2	2.38	0.71
1:F:313:TYR:CD1	1:F:332:VAL:CG2	2.71	0.71
1:L:111:TYR:OH	1:L:188:VAL:CG2	2.39	0.71
1:D:286:ILE:HD12	1:D:286:ILE:N	2.05	0.71
1:K:111:TYR:OH	1:K:188:VAL:CG2	2.39	0.71
1:B:286:ILE:N	1:B:286:ILE:HD12	2.04	0.71
1:C:287:GLY:HA3	1:G:321:ASP:CG	2.15	0.71
1:F:286:ILE:HG21	1:F:289:VAL:CG2	2.21	0.71
1:L:286:ILE:N	1:L:286:ILE:HD12	2.05	0.71
1:F:286:ILE:CG2	1:F:289:VAL:CG2	2.69	0.71
1:G:100:ARG:NH2	1:I:71:GLU:HG3	2.06	0.71
1:G:286:ILE:N	1:G:286:ILE:HD12	2.06	0.71
1:K:286:ILE:HD12	1:K:286:ILE:N	2.04	0.71
1:E:321:ASP:CG	1:K:287:GLY:HA3	2.16	0.70
1:G:51:ILE:HD13	1:I:303:PHE:HB3	1.73	0.70
1:H:111:TYR:OH	1:H:188:VAL:CG2	2.38	0.70
1:G:111:TYR:OH	1:G:188:VAL:CG2	2.40	0.70
1:H:286:ILE:CG2	1:H:289:VAL:CG2	2.69	0.70
1:C:111:TYR:CZ	1:C:188:VAL:HG21	2.27	0.70
1:A:71:GLU:HG3	1:B:100:ARG:NH2	2.07	0.70
1:A:111:TYR:OH	1:A:188:VAL:CG2	2.39	0.70
1:C:286:ILE:N	1:C:286:ILE:HD12	2.06	0.70
1:E:286:ILE:CG2	1:E:289:VAL:CG2	2.69	0.70
1:H:286:ILE:HG21	1:H:289:VAL:CG2	2.21	0.70
1:F:287:GLY:HA3	1:J:321:ASP:OD1	1.87	0.70
1:C:286:ILE:HG21	1:C:289:VAL:CG2	2.21	0.70
1:J:286:ILE:HG21	1:J:289:VAL:CG2	2.21	0.70
1:E:244:PHE:CZ	1:K:285:GLY:HA3	2.27	0.70
1:D:286:ILE:HG21	1:D:289:VAL:CG2	2.22	0.70
1:B:286:ILE:HG21	1:B:289:VAL:CG2	2.21	0.69
1:C:286:ILE:CG2	1:C:289:VAL:CG2	2.70	0.69
1:D:286:ILE:CG2	1:D:289:VAL:CG2	2.70	0.69
1:E:286:ILE:HG21	1:E:289:VAL:CG2	2.21	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TYR:OH	1:B:188:VAL:CG2	2.41	0.69
1:B:286:ILE:CG2	1:B:289:VAL:CG2	2.70	0.69
1:H:111:TYR:CZ	1:H:188:VAL:HG21	2.26	0.69
1:A:111:TYR:CZ	1:A:188:VAL:HG21	2.28	0.69
1:G:111:TYR:CZ	1:G:188:VAL:HG21	2.27	0.69
1:J:111:TYR:OH	1:J:188:VAL:CG2	2.40	0.69
1:J:286:ILE:CG2	1:J:289:VAL:CG2	2.70	0.69
1:A:286:ILE:CG2	1:A:289:VAL:CG2	2.71	0.69
1:E:111:TYR:CZ	1:E:188:VAL:HG21	2.28	0.68
1:I:111:TYR:CZ	1:I:188:VAL:HG21	2.28	0.68
1:A:286:ILE:HG21	1:A:289:VAL:CG2	2.23	0.68
1:I:111:TYR:OH	1:I:188:VAL:CG2	2.41	0.68
1:B:111:TYR:CZ	1:B:188:VAL:HG21	2.29	0.68
1:H:111:TYR:CZ	1:H:188:VAL:HG23	2.28	0.68
1:E:111:TYR:OH	1:E:188:VAL:CG2	2.41	0.68
1:G:286:ILE:HG21	1:G:289:VAL:CG2	2.22	0.68
1:G:286:ILE:CG2	1:G:289:VAL:CG2	2.71	0.68
1:I:128:PHE:O	1:I:133:VAL:HG11	1.94	0.68
1:A:287:GLY:HA3	1:F:321:ASP:CG	2.19	0.68
1:F:111:TYR:OH	1:F:188:VAL:CG2	2.42	0.68
1:F:111:TYR:CZ	1:F:188:VAL:HG21	2.28	0.68
1:I:111:TYR:CZ	1:I:188:VAL:HG23	2.29	0.68
1:K:111:TYR:CZ	1:K:188:VAL:HG21	2.28	0.68
1:G:47:GLY:HA3	1:I:338:TYR:CZ	2.28	0.67
1:L:111:TYR:CZ	1:L:188:VAL:HG21	2.28	0.67
1:C:174:VAL:HG12	1:C:175:GLY:N	2.10	0.67
1:L:111:TYR:CZ	1:L:188:VAL:HG23	2.29	0.67
1:I:286:ILE:HG22	1:I:289:VAL:HG22	1.75	0.67
1:B:128:PHE:O	1:B:133:VAL:HG11	1.94	0.67
1:G:128:PHE:O	1:G:133:VAL:HG11	1.94	0.67
1:K:128:PHE:O	1:K:133:VAL:HG11	1.94	0.67
1:L:286:ILE:HG22	1:L:289:VAL:HG22	1.76	0.67
1:E:244:PHE:CZ	1:K:285:GLY:CA	2.77	0.67
1:J:128:PHE:O	1:J:133:VAL:HG11	1.95	0.67
1:K:111:TYR:CZ	1:K:188:VAL:HG23	2.29	0.67
1:D:71:GLU:HG3	1:E:100:ARG:NH2	2.10	0.67
1:K:286:ILE:HG22	1:K:289:VAL:HG22	1.77	0.67
1:B:287:GLY:HA3	1:L:321:ASP:OD2	1.94	0.66
1:C:128:PHE:O	1:C:133:VAL:HG11	1.96	0.66
1:D:128:PHE:O	1:D:133:VAL:HG11	1.94	0.66
1:G:71:GLU:HG3	1:H:100:ARG:NH2	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:262:GLN:OE1	1:H:270:ARG:NH1	2.29	0.66
1:J:111:TYR:CZ	1:J:188:VAL:HG21	2.28	0.66
1:D:111:TYR:CZ	1:D:188:VAL:HG21	2.31	0.66
1:E:111:TYR:CZ	1:E:188:VAL:HG23	2.31	0.66
1:E:174:VAL:HG12	1:E:175:GLY:N	2.10	0.66
1:K:174:VAL:HG12	1:K:175:GLY:N	2.11	0.66
1:G:111:TYR:CZ	1:G:188:VAL:HG23	2.29	0.66
1:G:338:TYR:CZ	1:H:47:GLY:HA3	2.31	0.66
1:J:174:VAL:HG12	1:J:175:GLY:N	2.11	0.66
1:C:111:TYR:CZ	1:C:188:VAL:HG23	2.30	0.66
1:D:111:TYR:OH	1:D:188:VAL:CG2	2.43	0.66
1:D:174:VAL:HG12	1:D:175:GLY:N	2.10	0.66
1:F:286:ILE:HG22	1:F:289:VAL:HG22	1.77	0.66
1:D:262:GLN:OE1	1:D:270:ARG:NH1	2.29	0.66
1:E:128:PHE:O	1:E:133:VAL:HG11	1.95	0.66
1:F:128:PHE:O	1:F:133:VAL:HG11	1.95	0.66
1:A:128:PHE:O	1:A:133:VAL:HG11	1.96	0.66
1:B:174:VAL:HG12	1:B:175:GLY:N	2.11	0.66
1:E:205:LEU:HG	1:E:247:THR:HG22	1.78	0.66
1:L:128:PHE:O	1:L:133:VAL:HG11	1.96	0.65
1:F:286:ILE:HD12	1:F:286:ILE:H	1.62	0.65
1:C:262:GLN:OE1	1:C:270:ARG:NH1	2.30	0.65
1:D:338:TYR:CZ	1:E:47:GLY:HA3	2.31	0.65
1:G:174:VAL:HG12	1:G:175:GLY:N	2.11	0.65
1:H:286:ILE:HG22	1:H:289:VAL:HG22	1.78	0.65
1:J:262:GLN:OE1	1:J:270:ARG:NH1	2.28	0.65
1:C:285:GLY:HA3	1:G:244:PHE:CZ	2.32	0.65
1:D:191:TYR:HD1	1:D:214:TRP:HB3	1.62	0.65
1:E:262:GLN:OE1	1:E:270:ARG:NH1	2.30	0.65
1:H:128:PHE:O	1:H:133:VAL:HG11	1.95	0.65
1:B:111:TYR:CZ	1:B:188:VAL:HG23	2.31	0.65
1:B:262:GLN:OE1	1:B:270:ARG:NH1	2.30	0.65
1:C:286:ILE:HG22	1:C:289:VAL:HG22	1.79	0.65
1:J:286:ILE:HG22	1:J:289:VAL:HG22	1.79	0.65
1:A:111:TYR:CZ	1:A:188:VAL:HG23	2.30	0.65
1:B:205:LEU:HG	1:B:247:THR:HG22	1.79	0.65
1:B:286:ILE:HG22	1:B:289:VAL:HG22	1.78	0.65
1:L:265:PHE:HB3	1:L:267:PHE:CE1	2.32	0.65
1:D:286:ILE:HG22	1:D:289:VAL:HG22	1.79	0.64
1:G:191:TYR:HD1	1:G:214:TRP:HB3	1.61	0.64
1:H:205:LEU:HG	1:H:247:THR:HG22	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:TYR:HD1	1:J:214:TRP:HB3	1.62	0.64
1:F:223:ASN:O	1:F:224:ASN:HB2	1.98	0.64
1:F:262:GLN:OE1	1:F:270:ARG:NH1	2.30	0.64
1:J:111:TYR:CZ	1:J:188:VAL:HG23	2.30	0.64
1:K:286:ILE:HD12	1:K:286:ILE:H	1.63	0.64
1:A:47:GLY:HA3	1:C:338:TYR:CZ	2.33	0.64
1:E:286:ILE:HG22	1:E:289:VAL:HG22	1.78	0.64
1:H:265:PHE:HB3	1:H:267:PHE:CE1	2.32	0.64
1:I:191:TYR:HD1	1:I:214:TRP:HB3	1.63	0.64
1:L:262:GLN:OE1	1:L:270:ARG:NH1	2.31	0.64
1:A:262:GLN:OE1	1:A:270:ARG:NH1	2.30	0.64
1:C:191:TYR:HD1	1:C:214:TRP:HB3	1.62	0.64
1:G:262:GLN:OE1	1:G:270:ARG:NH1	2.30	0.64
1:F:144:PHE:HB2	1:F:151:LEU:HD23	1.79	0.64
1:L:174:VAL:HG12	1:L:175:GLY:N	2.11	0.64
1:L:191:TYR:HD1	1:L:214:TRP:HB3	1.62	0.64
1:L:286:ILE:CG2	1:L:289:VAL:HG22	2.28	0.64
1:A:174:VAL:HG12	1:A:175:GLY:N	2.11	0.64
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.62	0.64
1:D:111:TYR:CZ	1:D:188:VAL:HG23	2.33	0.64
1:H:174:VAL:HG12	1:H:175:GLY:N	2.12	0.64
1:K:262:GLN:OE1	1:K:270:ARG:NH1	2.31	0.64
1:A:286:ILE:HG22	1:A:289:VAL:HG22	1.79	0.64
1:B:144:PHE:HB2	1:B:151:LEU:HD23	1.79	0.64
1:H:144:PHE:HB2	1:H:151:LEU:HD23	1.80	0.64
1:I:174:VAL:HG12	1:I:175:GLY:N	2.12	0.64
1:B:191:TYR:HD1	1:B:214:TRP:HB3	1.63	0.64
1:F:174:VAL:HG12	1:F:175:GLY:N	2.12	0.64
1:H:191:TYR:HD1	1:H:214:TRP:HB3	1.62	0.64
1:I:286:ILE:CG2	1:I:289:VAL:HG21	2.28	0.64
1:C:144:PHE:HB2	1:C:151:LEU:HD23	1.81	0.63
1:E:191:TYR:HD1	1:E:214:TRP:HB3	1.62	0.63
1:I:262:GLN:OE1	1:I:270:ARG:NH1	2.31	0.63
1:D:205:LEU:HG	1:D:247:THR:HG22	1.80	0.63
1:F:191:TYR:HD1	1:F:214:TRP:HB3	1.63	0.63
1:E:265:PHE:HB3	1:E:267:PHE:CE1	2.33	0.63
1:F:111:TYR:CZ	1:F:188:VAL:HG23	2.31	0.63
1:G:286:ILE:HG22	1:G:289:VAL:HG22	1.79	0.63
1:K:191:TYR:HD1	1:K:214:TRP:HB3	1.63	0.63
1:B:303:PHE:HB3	1:C:51:ILE:HD13	1.79	0.63
1:K:265:PHE:HB3	1:K:267:PHE:CE1	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:LEU:HG	1:G:247:THR:HG22	1.80	0.63
1:I:165:THR:HG21	1:I:167:ARG:HB3	1.81	0.63
1:I:286:ILE:CG2	1:I:289:VAL:HG22	2.28	0.63
1:F:265:PHE:HB3	1:F:267:PHE:CE1	2.33	0.63
1:L:205:LEU:HG	1:L:247:THR:HG22	1.80	0.63
1:A:144:PHE:HB2	1:A:151:LEU:HD23	1.80	0.63
1:G:18:VAL:HG13	1:G:337:VAL:HG22	1.80	0.63
1:G:144:PHE:HB2	1:G:151:LEU:HD23	1.81	0.63
1:J:18:VAL:HG13	1:J:337:VAL:HG22	1.80	0.63
1:K:18:VAL:HG13	1:K:337:VAL:HG22	1.81	0.63
1:K:286:ILE:CG2	1:K:289:VAL:HG22	2.29	0.63
1:I:144:PHE:HB2	1:I:151:LEU:HD23	1.80	0.63
1:J:265:PHE:HB3	1:J:267:PHE:CE1	2.33	0.63
1:K:165:THR:HG21	1:K:167:ARG:HB3	1.81	0.63
1:B:321:ASP:CG	1:H:287:GLY:CA	2.72	0.62
1:C:205:LEU:HG	1:C:247:THR:HG22	1.81	0.62
1:D:144:PHE:HB2	1:D:151:LEU:HD23	1.80	0.62
1:J:47:GLY:HA3	1:L:338:TYR:CZ	2.34	0.62
1:C:265:PHE:HB3	1:C:267:PHE:CE1	2.34	0.62
1:A:265:PHE:HB3	1:A:267:PHE:CE1	2.34	0.62
1:D:303:PHE:HB3	1:E:51:ILE:HD13	1.81	0.62
1:A:18:VAL:HG13	1:A:337:VAL:HG22	1.80	0.62
1:I:265:PHE:HB3	1:I:267:PHE:CE1	2.34	0.62
1:L:223:ASN:O	1:L:224:ASN:HB2	1.99	0.62
1:J:144:PHE:HB2	1:J:151:LEU:HD23	1.81	0.62
1:B:18:VAL:HG13	1:B:337:VAL:HG22	1.82	0.62
1:D:51:ILE:HD13	1:F:303:PHE:HB3	1.81	0.62
1:G:265:PHE:HB3	1:G:267:PHE:CE1	2.34	0.62
1:I:223:ASN:O	1:I:224:ASN:HB2	2.00	0.62
1:A:286:ILE:HD12	1:A:286:ILE:H	1.65	0.62
1:B:265:PHE:HB3	1:B:267:PHE:CE1	2.34	0.62
1:B:286:ILE:HD12	1:B:286:ILE:H	1.63	0.62
1:H:296:GLU:OE2	1:H:312:ASP:OD1	2.18	0.62
1:A:205:LEU:HG	1:A:247:THR:HG22	1.81	0.62
1:E:303:PHE:HB3	1:F:51:ILE:HD13	1.80	0.62
1:L:286:ILE:HD12	1:L:286:ILE:H	1.64	0.62
1:B:338:TYR:CZ	1:C:47:GLY:HA3	2.35	0.62
1:E:205:LEU:HG	1:E:247:THR:CG2	2.30	0.62
1:K:144:PHE:HB2	1:K:151:LEU:HD23	1.81	0.62
1:L:18:VAL:HG13	1:L:337:VAL:HG22	1.82	0.62
1:B:205:LEU:HG	1:B:247:THR:CG2	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:GLY:HA3	1:J:244:PHE:CZ	2.35	0.62
1:G:296:GLU:OE2	1:G:312:ASP:OD1	2.18	0.62
1:L:144:PHE:HB2	1:L:151:LEU:HD23	1.80	0.62
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.81	0.61
1:I:205:LEU:HG	1:I:247:THR:HG22	1.80	0.61
1:K:205:LEU:HG	1:K:247:THR:HG22	1.82	0.61
1:L:165:THR:HG21	1:L:167:ARG:HB3	1.82	0.61
1:D:100:ARG:HH21	1:F:71:GLU:HG3	1.65	0.61
1:G:286:ILE:HD12	1:G:286:ILE:H	1.64	0.61
1:G:303:PHE:HB3	1:H:51:ILE:HD13	1.82	0.61
1:H:286:ILE:HD12	1:H:286:ILE:H	1.63	0.61
1:E:286:ILE:HD12	1:E:286:ILE:H	1.63	0.61
1:D:47:GLY:HA3	1:F:338:TYR:CZ	2.36	0.61
1:D:265:PHE:HB3	1:D:267:PHE:CE1	2.35	0.61
1:F:18:VAL:HG13	1:F:337:VAL:HG22	1.81	0.61
1:G:205:LEU:HG	1:G:247:THR:CG2	2.30	0.61
1:B:165:THR:HG21	1:B:167:ARG:HB3	1.83	0.61
1:B:223:ASN:O	1:B:224:ASN:HB2	2.01	0.61
1:F:205:LEU:HG	1:F:247:THR:HG22	1.82	0.61
1:J:165:THR:HG21	1:J:167:ARG:HB3	1.83	0.61
1:B:71:GLU:HG3	1:C:100:ARG:HH21	1.65	0.61
1:E:287:GLY:HA3	1:I:321:ASP:OD2	2.00	0.61
1:J:296:GLU:OE2	1:J:312:ASP:OD1	2.19	0.61
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.82	0.61
1:D:205:LEU:HG	1:D:247:THR:CG2	2.31	0.61
1:F:286:ILE:CG2	1:F:289:VAL:HG22	2.30	0.61
1:I:296:GLU:OE2	1:I:312:ASP:OD1	2.19	0.61
1:D:286:ILE:HD12	1:D:286:ILE:H	1.64	0.61
1:H:286:ILE:CG2	1:H:289:VAL:HG22	2.31	0.61
1:L:205:LEU:HG	1:L:247:THR:CG2	2.31	0.61
1:B:286:ILE:CG2	1:B:289:VAL:HG21	2.30	0.61
1:I:286:ILE:HD12	1:I:286:ILE:H	1.64	0.61
1:J:51:ILE:HD13	1:L:303:PHE:HB3	1.82	0.61
1:J:286:ILE:CG2	1:J:289:VAL:HG22	2.31	0.61
1:K:71:GLU:HG3	1:L:100:ARG:HH21	1.64	0.61
1:G:165:THR:HG21	1:G:167:ARG:HB3	1.83	0.61
1:H:18:VAL:HG13	1:H:337:VAL:HG22	1.83	0.61
1:H:165:THR:HG21	1:H:167:ARG:HB3	1.83	0.61
1:E:338:TYR:CZ	1:F:47:GLY:HA3	2.35	0.60
1:H:205:LEU:HG	1:H:247:THR:CG2	2.30	0.60
1:K:223:ASN:O	1:K:224:ASN:HB2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:CG2	1:B:289:VAL:HG22	2.31	0.60
1:C:286:ILE:CG2	1:C:289:VAL:HG22	2.31	0.60
1:D:165:THR:HG21	1:D:167:ARG:HB3	1.83	0.60
1:G:286:ILE:CG2	1:G:289:VAL:HG22	2.32	0.60
1:D:286:ILE:CG2	1:D:289:VAL:HG22	2.31	0.60
1:E:144:PHE:HB2	1:E:151:LEU:HD23	1.83	0.60
1:E:223:ASN:O	1:E:224:ASN:HB2	2.00	0.60
1:E:286:ILE:CG2	1:E:289:VAL:HG22	2.31	0.60
1:F:296:GLU:OE2	1:F:312:ASP:OD1	2.20	0.60
1:J:205:LEU:HG	1:J:247:THR:HG22	1.82	0.60
1:C:205:LEU:HG	1:C:247:THR:CG2	2.32	0.60
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.81	0.60
1:I:205:LEU:HG	1:I:247:THR:CG2	2.31	0.60
1:A:165:THR:HG21	1:A:167:ARG:HB3	1.84	0.60
1:B:321:ASP:CG	1:H:287:GLY:HA3	2.26	0.60
1:F:319:ASP:OD2	1:F:321:ASP:HB2	2.02	0.60
1:C:258:LEU:CD1	1:C:276:THR:HG23	2.32	0.60
1:D:286:ILE:CG2	1:D:289:VAL:HG21	2.31	0.60
1:E:258:LEU:CD1	1:E:276:THR:HG23	2.32	0.60
1:F:165:THR:HG21	1:F:167:ARG:HB3	1.83	0.60
1:K:27:ASN:HD22	1:K:29:GLU:HB2	1.67	0.60
1:L:286:ILE:CG2	1:L:289:VAL:HG21	2.28	0.60
1:L:296:GLU:OE2	1:L:312:ASP:OD1	2.20	0.60
1:A:338:TYR:CZ	1:B:47:GLY:HA3	2.37	0.60
1:C:287:GLY:CA	1:G:321:ASP:CG	2.67	0.60
1:C:296:GLU:OE2	1:C:312:ASP:OD1	2.19	0.60
1:F:205:LEU:HG	1:F:247:THR:CG2	2.32	0.59
1:J:286:ILE:HD12	1:J:286:ILE:H	1.64	0.59
1:A:205:LEU:HG	1:A:247:THR:CG2	2.32	0.59
1:F:286:ILE:CG2	1:F:289:VAL:HG21	2.29	0.59
1:G:286:ILE:CG2	1:G:289:VAL:HG21	2.32	0.59
1:I:18:VAL:HG13	1:I:337:VAL:HG22	1.82	0.59
1:A:223:ASN:O	1:A:224:ASN:HB2	2.02	0.59
1:A:286:ILE:CG2	1:A:289:VAL:HG22	2.31	0.59
1:J:307:MET:O	1:J:308:SER:HB3	2.02	0.59
1:D:223:ASN:O	1:D:224:ASN:HB2	2.01	0.59
1:K:205:LEU:HG	1:K:247:THR:CG2	2.32	0.59
1:B:258:LEU:CD1	1:B:276:THR:HG23	2.32	0.59
1:H:286:ILE:CG2	1:H:289:VAL:HG21	2.30	0.59
1:E:165:THR:HG21	1:E:167:ARG:HB3	1.84	0.59
1:J:205:LEU:HG	1:J:247:THR:CG2	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLU:OE2	1:B:312:ASP:OD1	2.21	0.59
1:C:286:ILE:HD12	1:C:286:ILE:H	1.65	0.59
1:F:258:LEU:CD1	1:F:276:THR:HG23	2.33	0.59
1:C:165:THR:HG21	1:C:167:ARG:HB3	1.84	0.59
1:G:307:MET:O	1:G:308:SER:HB3	2.03	0.59
1:G:319:ASP:OD2	1:G:321:ASP:HB2	2.03	0.59
1:K:258:LEU:CD1	1:K:276:THR:HG23	2.32	0.59
1:K:296:GLU:OE2	1:K:312:ASP:OD1	2.21	0.59
1:H:258:LEU:CD1	1:H:276:THR:HG23	2.33	0.59
1:D:258:LEU:CD1	1:D:276:THR:HG23	2.33	0.59
1:H:223:ASN:O	1:H:224:ASN:HB2	2.02	0.59
1:H:338:TYR:CZ	1:I:47:GLY:HA3	2.38	0.59
1:D:296:GLU:OE2	1:D:312:ASP:OD1	2.20	0.58
1:J:223:ASN:O	1:J:224:ASN:HB2	2.03	0.58
1:C:285:GLY:CA	1:G:244:PHE:CZ	2.85	0.58
1:F:307:MET:O	1:F:308:SER:HB3	2.02	0.58
1:J:286:ILE:CG2	1:J:289:VAL:HG21	2.31	0.58
1:A:303:PHE:HB3	1:B:51:ILE:HD13	1.85	0.58
1:I:287:GLY:HA3	1:K:321:ASP:OD2	2.03	0.58
1:B:319:ASP:OD2	1:B:321:ASP:HB2	2.02	0.58
1:C:319:ASP:OD2	1:C:321:ASP:HB2	2.04	0.58
1:I:258:LEU:CD1	1:I:276:THR:HG23	2.34	0.58
1:J:319:ASP:OD2	1:J:321:ASP:HB2	2.04	0.58
1:A:307:MET:O	1:A:308:SER:HB3	2.04	0.58
1:A:258:LEU:CD1	1:A:276:THR:HG23	2.32	0.58
1:A:296:GLU:OE2	1:A:312:ASP:OD1	2.21	0.58
1:L:307:MET:O	1:L:308:SER:HB3	2.03	0.58
1:H:45:PHE:O	1:H:45:PHE:CD1	2.57	0.58
1:C:104:VAL:HG22	1:C:156:GLN:OE1	2.04	0.58
1:I:319:ASP:OD2	1:I:321:ASP:HB2	2.02	0.58
1:J:71:GLU:HG3	1:K:100:ARG:HH21	1.69	0.58
1:J:258:LEU:CD1	1:J:276:THR:HG23	2.34	0.58
1:B:244:PHE:CZ	1:H:285:GLY:HA3	2.39	0.58
1:D:104:VAL:HG22	1:D:156:GLN:OE1	2.04	0.57
1:E:296:GLU:OE2	1:E:312:ASP:OD1	2.21	0.57
1:K:319:ASP:OD2	1:K:321:ASP:HB2	2.04	0.57
1:I:45:PHE:O	1:I:45:PHE:CD1	2.57	0.57
1:A:319:ASP:OD2	1:A:321:ASP:HB2	2.05	0.57
1:E:321:ASP:CG	1:K:287:GLY:CA	2.68	0.57
1:A:105:VAL:HG12	1:A:105:VAL:O	2.03	0.57
1:B:307:MET:O	1:B:308:SER:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASN:O	1:C:224:ASN:HB2	2.03	0.57
1:G:223:ASN:O	1:G:224:ASN:HB2	2.03	0.57
1:B:143:ASN:O	1:B:146:GLY:N	2.38	0.57
1:H:303:PHE:HB3	1:I:51:ILE:HD13	1.86	0.57
1:L:258:LEU:CD1	1:L:276:THR:HG23	2.34	0.57
1:G:105:VAL:HG12	1:G:105:VAL:O	2.04	0.57
1:G:47:GLY:HA3	1:I:338:TYR:CE2	2.40	0.57
1:A:45:PHE:CD1	1:A:45:PHE:O	2.58	0.56
1:G:104:VAL:HG22	1:G:156:GLN:OE1	2.04	0.56
1:H:319:ASP:OD2	1:H:321:ASP:HB2	2.05	0.56
1:D:240:ILE:HD13	1:D:251:ALA:HB2	1.87	0.56
1:L:319:ASP:OD2	1:L:321:ASP:HB2	2.04	0.56
1:A:286:ILE:CG2	1:A:289:VAL:HG21	2.33	0.56
1:H:307:MET:O	1:H:308:SER:HB3	2.05	0.56
1:I:286:ILE:HG22	1:I:289:VAL:CG2	2.34	0.56
1:K:307:MET:O	1:K:308:SER:HB3	2.05	0.56
1:B:45:PHE:O	1:B:45:PHE:CD1	2.58	0.56
1:C:270:ARG:O	1:C:270:ARG:HG2	2.05	0.56
1:D:307:MET:O	1:D:308:SER:HB3	2.04	0.56
1:E:143:ASN:O	1:E:146:GLY:N	2.38	0.56
1:I:104:VAL:HG22	1:I:156:GLN:OE1	2.05	0.56
1:I:307:MET:O	1:I:308:SER:HB3	2.04	0.56
1:D:105:VAL:HG12	1:D:105:VAL:O	2.05	0.56
1:D:319:ASP:OD2	1:D:321:ASP:HB2	2.04	0.56
1:E:319:ASP:OD2	1:E:321:ASP:HB2	2.05	0.56
1:B:303:PHE:CB	1:C:51:ILE:HD13	2.36	0.56
1:E:307:MET:O	1:E:308:SER:HB3	2.04	0.56
1:H:111:TYR:CE2	1:H:188:VAL:HG23	2.40	0.56
1:A:143:ASN:O	1:A:146:GLY:N	2.38	0.56
1:B:244:PHE:CZ	1:H:285:GLY:CA	2.89	0.56
1:C:143:ASN:O	1:C:146:GLY:N	2.39	0.56
1:D:143:ASN:O	1:D:146:GLY:N	2.38	0.56
1:E:45:PHE:O	1:E:45:PHE:CD1	2.58	0.56
1:G:45:PHE:O	1:G:45:PHE:CD1	2.59	0.56
1:B:104:VAL:HG22	1:B:156:GLN:OE1	2.06	0.56
1:B:130:VAL:HG13	1:B:213:GLN:CD	2.31	0.56
1:B:270:ARG:O	1:B:270:ARG:HG2	2.05	0.56
1:F:285:GLY:CA	1:J:244:PHE:CZ	2.89	0.56
1:A:104:VAL:HG22	1:A:156:GLN:OE1	2.06	0.56
1:G:11:VAL:HG21	1:I:340:PHE:HB2	1.88	0.56
1:C:307:MET:O	1:C:308:SER:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ILE:CG2	1:E:289:VAL:HG21	2.30	0.56
1:K:105:VAL:HG12	1:K:105:VAL:O	2.05	0.56
1:C:105:VAL:HG12	1:C:105:VAL:O	2.05	0.55
1:I:270:ARG:O	1:I:270:ARG:HG2	2.06	0.55
1:K:286:ILE:CG2	1:K:289:VAL:HG21	2.29	0.55
1:E:104:VAL:HG22	1:E:156:GLN:OE1	2.06	0.55
1:G:258:LEU:CD1	1:G:276:THR:HG23	2.36	0.55
1:J:45:PHE:O	1:J:45:PHE:CD1	2.59	0.55
1:K:165:THR:CG2	1:K:167:ARG:HB3	2.37	0.55
1:A:281:LYS:O	1:A:282:ASP:HB2	2.06	0.55
1:E:270:ARG:O	1:E:270:ARG:HG2	2.06	0.55
1:I:27:ASN:HD22	1:I:29:GLU:CB	2.12	0.55
1:L:45:PHE:O	1:L:45:PHE:CD1	2.59	0.55
1:B:281:LYS:O	1:B:282:ASP:HB2	2.07	0.55
1:F:111:TYR:CE2	1:F:188:VAL:HG23	2.42	0.55
1:H:221:ASP:O	1:H:222:ALA:HB2	2.05	0.55
1:K:130:VAL:HG13	1:K:213:GLN:CD	2.32	0.55
1:L:143:ASN:HA	1:L:148:VAL:O	2.07	0.55
1:G:51:ILE:HD13	1:I:303:PHE:CB	2.34	0.55
1:I:165:THR:CG2	1:I:167:ARG:HB3	2.37	0.55
1:B:309:THR:HG22	1:B:336:ILE:CA	2.35	0.55
1:E:130:VAL:HG13	1:E:213:GLN:CD	2.32	0.55
1:H:130:VAL:HG13	1:H:213:GLN:CD	2.32	0.55
1:I:105:VAL:HG12	1:I:105:VAL:O	2.07	0.55
1:I:221:ASP:O	1:I:222:ALA:HB2	2.07	0.55
1:J:303:PHE:HB3	1:K:51:ILE:HD13	1.89	0.55
1:J:338:TYR:CZ	1:K:47:GLY:HA3	2.42	0.55
1:K:143:ASN:O	1:K:146:GLY:N	2.39	0.55
1:L:286:ILE:HG22	1:L:289:VAL:CG2	2.34	0.55
1:J:105:VAL:HG12	1:J:105:VAL:O	2.06	0.55
1:K:71:GLU:CG	1:L:100:ARG:HH21	2.19	0.55
1:F:130:VAL:HG13	1:F:213:GLN:CD	2.32	0.55
1:F:143:ASN:O	1:F:146:GLY:N	2.39	0.55
1:F:281:LYS:O	1:F:282:ASP:HB2	2.07	0.55
1:J:111:TYR:CE2	1:J:188:VAL:HG23	2.42	0.55
1:A:221:ASP:O	1:A:222:ALA:HB2	2.06	0.55
1:H:286:ILE:HG22	1:H:289:VAL:CG2	2.36	0.55
1:J:104:VAL:HG22	1:J:156:GLN:OE1	2.07	0.55
1:J:294:TYR:CD1	1:J:294:TYR:C	2.85	0.55
1:K:104:VAL:HG22	1:K:156:GLN:OE1	2.06	0.55
1:K:281:LYS:O	1:K:282:ASP:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:111:TYR:CE2	1:L:188:VAL:HG23	2.41	0.55
1:E:111:TYR:CE2	1:E:188:VAL:HG23	2.42	0.54
1:H:281:LYS:O	1:H:282:ASP:HB2	2.07	0.54
1:I:111:TYR:CE2	1:I:188:VAL:HG23	2.41	0.54
1:I:143:ASN:HA	1:I:148:VAL:O	2.07	0.54
1:K:45:PHE:CD1	1:K:45:PHE:O	2.59	0.54
1:A:111:TYR:CE2	1:A:188:VAL:HG23	2.43	0.54
1:A:321:ASP:OD2	1:J:287:GLY:HA3	2.06	0.54
1:B:235:ARG:HH21	1:B:253:LYS:HZ2	1.56	0.54
1:B:338:TYR:CE2	1:C:47:GLY:HA3	2.43	0.54
1:K:294:TYR:CD1	1:K:294:TYR:C	2.85	0.54
1:L:143:ASN:O	1:L:146:GLY:N	2.41	0.54
1:G:111:TYR:CE2	1:G:188:VAL:HG23	2.41	0.54
1:G:143:ASN:HA	1:G:148:VAL:O	2.07	0.54
1:L:221:ASP:O	1:L:222:ALA:HB2	2.07	0.54
1:D:221:ASP:O	1:D:222:ALA:HB2	2.07	0.54
1:F:105:VAL:HG12	1:F:105:VAL:O	2.08	0.54
1:H:143:ASN:O	1:H:146:GLY:N	2.40	0.54
1:I:141:ASN:HB3	1:I:153:PHE:CE1	2.43	0.54
1:A:294:TYR:CD1	1:A:294:TYR:C	2.85	0.54
1:C:111:TYR:CE2	1:C:188:VAL:HG23	2.42	0.54
1:D:100:ARG:HH21	1:F:71:GLU:CG	2.21	0.54
1:J:281:LYS:O	1:J:282:ASP:HB2	2.08	0.54
1:F:45:PHE:CD1	1:F:45:PHE:O	2.60	0.54
1:F:104:VAL:HG22	1:F:156:GLN:OE1	2.07	0.54
1:F:165:THR:CG2	1:F:167:ARG:HB3	2.38	0.54
1:G:143:ASN:O	1:G:146:GLY:N	2.41	0.54
1:H:104:VAL:HG22	1:H:156:GLN:OE1	2.08	0.54
1:A:240:ILE:HD13	1:A:251:ALA:HB2	1.90	0.54
1:B:143:ASN:HA	1:B:148:VAL:O	2.08	0.54
1:F:221:ASP:O	1:F:222:ALA:HB2	2.07	0.54
1:H:143:ASN:HA	1:H:148:VAL:O	2.08	0.54
1:L:165:THR:CG2	1:L:167:ARG:HB3	2.37	0.54
1:A:51:ILE:HD13	1:C:303:PHE:HB3	1.89	0.53
1:E:281:LYS:O	1:E:282:ASP:HB2	2.07	0.53
1:F:270:ARG:O	1:F:270:ARG:HG2	2.07	0.53
1:K:111:TYR:CE2	1:K:188:VAL:HG23	2.43	0.53
1:K:144:PHE:O	1:K:145:PHE:HB2	2.08	0.53
1:B:105:VAL:HG12	1:B:105:VAL:O	2.08	0.53
1:H:165:THR:CG2	1:H:167:ARG:HB3	2.38	0.53
1:I:143:ASN:O	1:I:146:GLY:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:270:ARG:O	1:K:270:ARG:HG2	2.08	0.53
1:B:111:TYR:CE2	1:B:188:VAL:HG23	2.43	0.53
1:B:221:ASP:O	1:B:222:ALA:HB2	2.07	0.53
1:H:105:VAL:HG12	1:H:105:VAL:O	2.08	0.53
1:L:130:VAL:HG13	1:L:213:GLN:CD	2.32	0.53
1:B:240:ILE:HD13	1:B:251:ALA:HB2	1.91	0.53
1:C:174:VAL:CG1	1:C:175:GLY:N	2.72	0.53
1:D:45:PHE:O	1:D:45:PHE:CD1	2.61	0.53
1:G:144:PHE:O	1:G:145:PHE:HB2	2.09	0.53
1:K:221:ASP:O	1:K:222:ALA:HB2	2.07	0.53
1:C:294:TYR:CD1	1:C:294:TYR:C	2.87	0.53
1:D:165:THR:CG2	1:D:167:ARG:HB3	2.39	0.53
1:I:130:VAL:HG13	1:I:213:GLN:CD	2.34	0.53
1:L:294:TYR:C	1:L:294:TYR:CD1	2.86	0.53
1:C:281:LYS:O	1:C:282:ASP:HB2	2.08	0.53
1:F:286:ILE:H	1:F:286:ILE:CD1	2.22	0.53
1:G:3:ILE:HD12	1:I:3:ILE:HG21	1.91	0.53
1:G:141:ASN:HB3	1:G:153:PHE:CE1	2.44	0.53
1:G:165:THR:CG2	1:G:167:ARG:HB3	2.38	0.53
1:J:221:ASP:O	1:J:222:ALA:HB2	2.08	0.53
1:A:270:ARG:O	1:A:270:ARG:HG2	2.08	0.53
1:C:221:ASP:O	1:C:222:ALA:HB2	2.08	0.53
1:D:281:LYS:O	1:D:282:ASP:HB2	2.08	0.53
1:E:221:ASP:O	1:E:222:ALA:HB2	2.08	0.53
1:K:174:VAL:CG1	1:K:175:GLY:N	2.72	0.53
1:A:144:PHE:O	1:A:145:PHE:HB2	2.09	0.53
1:C:286:ILE:HG22	1:C:289:VAL:CG2	2.37	0.53
1:F:143:ASN:HA	1:F:148:VAL:O	2.08	0.53
1:K:240:ILE:HD13	1:K:251:ALA:HB2	1.91	0.53
1:L:144:PHE:O	1:L:145:PHE:HB2	2.09	0.53
1:B:294:TYR:CD1	1:B:294:TYR:C	2.86	0.53
1:C:45:PHE:O	1:C:45:PHE:CD1	2.62	0.53
1:C:130:VAL:HG13	1:C:213:GLN:CD	2.33	0.53
1:D:321:ASP:OD2	1:G:287:GLY:HA3	2.09	0.53
1:E:143:ASN:HA	1:E:148:VAL:O	2.09	0.53
1:I:281:LYS:O	1:I:282:ASP:HB2	2.09	0.53
1:I:294:TYR:CD1	1:I:294:TYR:C	2.87	0.53
1:J:144:PHE:O	1:J:145:PHE:HB2	2.08	0.53
1:B:340:PHE:HB2	1:C:11:VAL:HG21	1.91	0.52
1:D:111:TYR:CE2	1:D:188:VAL:HG23	2.44	0.52
1:D:130:VAL:HG13	1:D:213:GLN:CD	2.34	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:VAL:CG1	1:D:175:GLY:N	2.71	0.52
1:E:105:VAL:HG12	1:E:105:VAL:O	2.08	0.52
1:E:294:TYR:CD1	1:E:294:TYR:C	2.86	0.52
1:F:286:ILE:HG22	1:F:289:VAL:CG2	2.36	0.52
1:F:294:TYR:CD1	1:F:294:TYR:C	2.86	0.52
1:G:222:ALA:O	1:G:223:ASN:HB2	2.09	0.52
1:B:71:GLU:CG	1:C:100:ARG:HH21	2.23	0.52
1:B:165:THR:CG2	1:B:167:ARG:HB3	2.39	0.52
1:C:165:THR:CG2	1:C:167:ARG:HB3	2.39	0.52
1:E:286:ILE:N	1:E:286:ILE:CD1	2.72	0.52
1:G:281:LYS:O	1:G:282:ASP:HB2	2.09	0.52
1:G:338:TYR:CE2	1:H:47:GLY:HA3	2.45	0.52
1:H:270:ARG:O	1:H:270:ARG:HG2	2.08	0.52
1:J:130:VAL:HG13	1:J:213:GLN:CD	2.34	0.52
1:J:143:ASN:HA	1:J:148:VAL:O	2.09	0.52
1:L:105:VAL:HG12	1:L:105:VAL:O	2.10	0.52
1:L:174:VAL:CG1	1:L:175:GLY:N	2.72	0.52
1:L:270:ARG:O	1:L:270:ARG:HG2	2.09	0.52
1:A:309:THR:HG22	1:A:336:ILE:CA	2.34	0.52
1:H:144:PHE:O	1:H:145:PHE:HB2	2.08	0.52
1:D:294:TYR:CD1	1:D:294:TYR:C	2.88	0.52
1:G:130:VAL:HG13	1:G:213:GLN:CD	2.33	0.52
1:C:143:ASN:HA	1:C:148:VAL:O	2.08	0.52
1:D:143:ASN:HA	1:D:148:VAL:O	2.09	0.52
1:E:174:VAL:CG1	1:E:175:GLY:N	2.72	0.52
1:H:141:ASN:HB3	1:H:153:PHE:CE1	2.45	0.52
1:I:144:PHE:O	1:I:145:PHE:HB2	2.10	0.52
1:I:264:GLN:OE1	1:I:270:ARG:HB2	2.09	0.52
1:J:165:THR:CG2	1:J:167:ARG:HB3	2.38	0.52
1:J:174:VAL:CG1	1:J:175:GLY:N	2.72	0.52
1:J:222:ALA:O	1:J:223:ASN:HB2	2.09	0.52
1:L:281:LYS:O	1:L:282:ASP:HB2	2.09	0.52
1:C:222:ALA:O	1:C:223:ASN:HB2	2.09	0.52
1:C:286:ILE:CG2	1:C:289:VAL:HG21	2.31	0.52
1:D:309:THR:HG22	1:D:336:ILE:CA	2.34	0.52
1:A:143:ASN:HA	1:A:148:VAL:O	2.09	0.52
1:B:174:VAL:CG1	1:B:175:GLY:N	2.73	0.52
1:B:303:PHE:CG	1:C:51:ILE:HD13	2.45	0.52
1:G:309:THR:HG22	1:G:336:ILE:CA	2.35	0.52
1:H:240:ILE:HD13	1:H:251:ALA:HB2	1.92	0.52
1:J:309:THR:HG22	1:J:336:ILE:CA	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:ASN:HA	1:K:148:VAL:O	2.08	0.52
1:L:104:VAL:HG22	1:L:156:GLN:OE1	2.08	0.52
1:A:130:VAL:HG13	1:A:213:GLN:CD	2.35	0.52
1:D:51:ILE:HD13	1:F:303:PHE:CB	2.39	0.52
1:E:165:THR:CG2	1:E:167:ARG:HB3	2.39	0.52
1:F:258:LEU:HD13	1:F:276:THR:HG23	1.92	0.52
1:E:286:ILE:H	1:E:286:ILE:CD1	2.23	0.52
1:A:165:THR:CG2	1:A:167:ARG:HB3	2.39	0.52
1:E:143:ASN:O	1:E:144:PHE:C	2.53	0.52
1:E:303:PHE:CB	1:F:51:ILE:HD13	2.40	0.52
1:F:161:ASN:HB2	1:F:170:ASN:OD1	2.11	0.52
1:F:286:ILE:N	1:F:286:ILE:CD1	2.71	0.52
1:H:294:TYR:CD1	1:H:294:TYR:C	2.87	0.52
1:K:154:ALA:O	1:K:176:GLY:HA2	2.10	0.52
1:G:174:VAL:CG1	1:G:175:GLY:N	2.73	0.51
1:A:174:VAL:CG1	1:A:175:GLY:N	2.73	0.51
1:B:141:ASN:HB3	1:B:153:PHE:CE1	2.46	0.51
1:B:154:ALA:O	1:B:176:GLY:HA2	2.11	0.51
1:G:270:ARG:HG2	1:G:270:ARG:O	2.10	0.51
1:I:161:ASN:HB2	1:I:170:ASN:OD1	2.09	0.51
1:I:240:ILE:HD13	1:I:251:ALA:HB2	1.92	0.51
1:I:309:THR:HG22	1:I:336:ILE:CA	2.38	0.51
1:K:286:ILE:H	1:K:286:ILE:CD1	2.23	0.51
1:D:141:ASN:HB3	1:D:153:PHE:CE1	2.45	0.51
1:F:144:PHE:O	1:F:145:PHE:HB2	2.10	0.51
1:G:221:ASP:O	1:G:222:ALA:HB2	2.09	0.51
1:H:244:PHE:CZ	1:L:285:GLY:HA3	2.45	0.51
1:J:270:ARG:O	1:J:270:ARG:HG2	2.09	0.51
1:A:141:ASN:HB3	1:A:153:PHE:CE1	2.45	0.51
1:D:270:ARG:O	1:D:270:ARG:HG2	2.08	0.51
1:F:240:ILE:HD13	1:F:251:ALA:HB2	1.92	0.51
1:J:141:ASN:HB3	1:J:153:PHE:CE1	2.45	0.51
1:K:264:GLN:OE1	1:K:270:ARG:HB2	2.10	0.51
1:B:340:PHE:CB	1:C:11:VAL:HG21	2.40	0.51
1:C:258:LEU:HD13	1:C:276:THR:HG23	1.93	0.51
1:D:47:GLY:HA3	1:F:338:TYR:CE2	2.45	0.51
1:E:154:ALA:O	1:E:176:GLY:HA2	2.10	0.51
1:F:174:VAL:CG1	1:F:175:GLY:N	2.73	0.51
1:G:204:PRO:HD2	1:G:248:SER:O	2.10	0.51
1:H:143:ASN:O	1:H:144:PHE:C	2.54	0.51
1:L:141:ASN:HB3	1:L:153:PHE:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PHE:O	1:D:145:PHE:HB2	2.10	0.51
1:E:144:PHE:O	1:E:145:PHE:HB2	2.09	0.51
1:E:222:ALA:O	1:E:223:ASN:HB2	2.09	0.51
1:H:174:VAL:CG1	1:H:175:GLY:N	2.73	0.51
1:K:141:ASN:HB3	1:K:153:PHE:CE1	2.46	0.51
1:K:204:PRO:HB2	1:K:247:THR:CG2	2.41	0.51
1:A:154:ALA:O	1:A:176:GLY:HA2	2.10	0.51
1:E:286:ILE:HG22	1:E:289:VAL:CG2	2.37	0.51
1:F:154:ALA:O	1:F:176:GLY:HA2	2.11	0.51
1:G:240:ILE:HD13	1:G:251:ALA:HB2	1.92	0.51
1:J:143:ASN:O	1:J:146:GLY:N	2.43	0.51
1:L:165:THR:CG2	1:L:167:ARG:H	2.13	0.51
1:A:258:LEU:HD13	1:A:276:THR:HG23	1.93	0.51
1:B:264:GLN:OE1	1:B:270:ARG:HB2	2.11	0.51
1:D:258:LEU:HD13	1:D:276:THR:HG23	1.92	0.51
1:D:338:TYR:CE2	1:E:47:GLY:HA3	2.46	0.51
1:E:141:ASN:HB3	1:E:153:PHE:CE1	2.46	0.51
1:E:258:LEU:HD13	1:E:276:THR:HG23	1.92	0.51
1:I:174:VAL:CG1	1:I:175:GLY:N	2.73	0.51
1:A:143:ASN:O	1:A:144:PHE:C	2.54	0.51
1:B:143:ASN:O	1:B:144:PHE:C	2.53	0.51
1:B:144:PHE:O	1:B:145:PHE:HB2	2.11	0.51
1:F:143:ASN:O	1:F:144:PHE:C	2.54	0.51
1:G:11:VAL:HG21	1:I:340:PHE:CB	2.41	0.51
1:H:222:ALA:O	1:H:223:ASN:HB2	2.11	0.51
1:J:258:LEU:HD13	1:J:276:THR:HG23	1.93	0.51
1:J:286:ILE:N	1:J:286:ILE:CD1	2.74	0.51
1:L:222:ALA:O	1:L:223:ASN:HB2	2.11	0.51
1:C:144:PHE:O	1:C:145:PHE:HB2	2.10	0.50
1:J:240:ILE:HD13	1:J:251:ALA:HB2	1.92	0.50
1:L:136:VAL:CG1	1:L:158:LEU:HD13	2.41	0.50
1:D:143:ASN:O	1:D:144:PHE:C	2.55	0.50
1:D:222:ALA:O	1:D:223:ASN:HB2	2.11	0.50
1:E:240:ILE:HD13	1:E:251:ALA:HB2	1.91	0.50
1:G:136:VAL:CG1	1:G:158:LEU:HD13	2.42	0.50
1:H:321:ASP:OD2	1:L:287:GLY:HA3	2.11	0.50
1:I:154:ALA:O	1:I:176:GLY:HA2	2.11	0.50
1:J:154:ALA:O	1:J:176:GLY:HA2	2.11	0.50
1:C:309:THR:HG22	1:C:336:ILE:CA	2.36	0.50
1:H:136:VAL:CG1	1:H:158:LEU:HD13	2.41	0.50
1:L:154:ALA:O	1:L:176:GLY:HA2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:O	1:A:223:ASN:HB2	2.11	0.50
1:D:154:ALA:O	1:D:176:GLY:HA2	2.11	0.50
1:F:309:THR:HG22	1:F:336:ILE:CA	2.36	0.50
1:G:294:TYR:C	1:G:294:TYR:CD1	2.88	0.50
1:G:340:PHE:HB2	1:H:11:VAL:HG21	1.93	0.50
1:H:161:ASN:HB2	1:H:170:ASN:OD1	2.11	0.50
1:I:204:PRO:HB2	1:I:247:THR:CG2	2.42	0.50
1:J:286:ILE:HG22	1:J:289:VAL:CG2	2.38	0.50
1:J:286:ILE:H	1:J:286:ILE:CD1	2.25	0.50
1:G:286:ILE:N	1:G:286:ILE:CD1	2.74	0.50
1:K:161:ASN:HB2	1:K:170:ASN:OD1	2.12	0.50
1:A:286:ILE:H	1:A:286:ILE:CD1	2.25	0.50
1:B:286:ILE:H	1:B:286:ILE:CD1	2.24	0.50
1:G:154:ALA:O	1:G:176:GLY:HA2	2.11	0.50
1:I:258:LEU:HD13	1:I:276:THR:HG23	1.93	0.50
1:J:161:ASN:HB2	1:J:170:ASN:OD1	2.11	0.50
1:B:286:ILE:N	1:B:286:ILE:CD1	2.73	0.50
1:C:143:ASN:O	1:C:144:PHE:C	2.54	0.50
1:I:286:ILE:H	1:I:286:ILE:CD1	2.24	0.50
1:L:204:PRO:HD2	1:L:248:SER:O	2.11	0.50
1:E:153:PHE:HA	1:E:177:SER:O	2.12	0.50
1:E:204:PRO:HB2	1:E:247:THR:CG2	2.42	0.50
1:G:286:ILE:H	1:G:286:ILE:CD1	2.25	0.50
1:I:136:VAL:CG1	1:I:158:LEU:HD13	2.41	0.50
1:J:71:GLU:CG	1:K:100:ARG:HH21	2.25	0.50
1:L:286:ILE:H	1:L:286:ILE:CD1	2.25	0.50
1:E:161:ASN:HB2	1:E:170:ASN:OD1	2.12	0.50
1:G:105:VAL:HA	1:G:190:ALA:HB1	1.94	0.50
1:G:153:PHE:HA	1:G:177:SER:O	2.12	0.50
1:G:161:ASN:HB2	1:G:170:ASN:OD1	2.11	0.50
1:G:313:TYR:HD1	1:G:332:VAL:CG2	2.18	0.50
1:H:204:PRO:HD2	1:H:248:SER:O	2.12	0.50
1:I:286:ILE:N	1:I:286:ILE:CD1	2.74	0.50
1:C:154:ALA:O	1:C:176:GLY:HA2	2.12	0.49
1:C:204:PRO:HD2	1:C:248:SER:O	2.12	0.49
1:D:11:VAL:HG21	1:F:340:PHE:HB2	1.93	0.49
1:D:204:PRO:HB2	1:D:247:THR:CG2	2.42	0.49
1:H:286:ILE:H	1:H:286:ILE:CD1	2.24	0.49
1:L:240:ILE:HD13	1:L:251:ALA:HB2	1.92	0.49
1:L:264:GLN:OE1	1:L:270:ARG:HB2	2.12	0.49
1:B:161:ASN:HB2	1:B:170:ASN:OD1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:HD13	1:C:251:ALA:HB2	1.94	0.49
1:C:321:ASP:OD2	1:D:287:GLY:HA3	2.12	0.49
1:F:153:PHE:HA	1:F:177:SER:O	2.13	0.49
1:H:154:ALA:O	1:H:176:GLY:HA2	2.11	0.49
1:I:204:PRO:HD2	1:I:248:SER:O	2.12	0.49
1:B:303:PHE:HB3	1:C:51:ILE:HG21	1.94	0.49
1:D:286:ILE:HG22	1:D:289:VAL:CG2	2.38	0.49
1:F:141:ASN:HB3	1:F:153:PHE:CE1	2.47	0.49
1:I:143:ASN:O	1:I:144:PHE:C	2.55	0.49
1:J:153:PHE:HA	1:J:177:SER:O	2.12	0.49
1:K:309:THR:HG22	1:K:336:ILE:CA	2.37	0.49
1:L:309:THR:HG22	1:L:336:ILE:CA	2.37	0.49
1:C:136:VAL:CG1	1:C:158:LEU:HD13	2.42	0.49
1:I:66:GLN:HG3	1:I:78:GLY:HA3	1.94	0.49
1:J:51:ILE:HD13	1:L:303:PHE:CB	2.43	0.49
1:J:136:VAL:CG1	1:J:158:LEU:HD13	2.42	0.49
1:K:143:ASN:O	1:K:144:PHE:C	2.56	0.49
1:K:222:ALA:O	1:K:223:ASN:HB2	2.12	0.49
1:K:236:ASN:OD1	1:K:252:ASN:HA	2.12	0.49
1:K:286:ILE:N	1:K:286:ILE:CD1	2.73	0.49
1:K:338:TYR:CZ	1:L:47:GLY:HA3	2.48	0.49
1:L:258:LEU:HD13	1:L:276:THR:HG23	1.94	0.49
1:C:236:ASN:OD1	1:C:252:ASN:HA	2.13	0.49
1:E:136:VAL:CG1	1:E:158:LEU:HD13	2.42	0.49
1:K:204:PRO:HD2	1:K:248:SER:O	2.12	0.49
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.47	0.49
1:D:340:PHE:HB2	1:E:11:VAL:HG21	1.94	0.49
1:H:66:GLN:HG3	1:H:78:GLY:HA3	1.94	0.49
1:I:267:PHE:H	1:I:267:PHE:HD1	1.61	0.49
1:L:286:ILE:N	1:L:286:ILE:CD1	2.73	0.49
1:A:47:GLY:HA3	1:C:338:TYR:CE2	2.48	0.49
1:B:204:PRO:HB2	1:B:247:THR:CG2	2.43	0.49
1:K:136:VAL:CG1	1:K:158:LEU:HD13	2.43	0.49
1:L:161:ASN:HB2	1:L:170:ASN:OD1	2.13	0.49
1:B:153:PHE:HA	1:B:177:SER:O	2.13	0.49
1:B:258:LEU:HD13	1:B:276:THR:HG23	1.94	0.49
1:D:161:ASN:HB2	1:D:170:ASN:OD1	2.12	0.49
1:E:244:PHE:HZ	1:K:285:GLY:CA	2.26	0.49
1:H:258:LEU:HD13	1:H:276:THR:HG23	1.94	0.49
1:I:222:ALA:O	1:I:223:ASN:HB2	2.11	0.49
1:K:258:LEU:HD13	1:K:276:THR:HG23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:GLU:HG3	1:F:100:ARG:HH21	1.77	0.49
1:E:264:GLN:OE1	1:E:270:ARG:HB2	2.13	0.49
1:F:31:SER:CA	1:F:329:ASP:HB2	2.40	0.49
1:H:264:GLN:OE1	1:H:270:ARG:HB2	2.12	0.49
1:L:143:ASN:O	1:L:144:PHE:C	2.56	0.49
1:L:269:LEU:HG	1:L:271:PRO:HD3	1.95	0.49
1:A:286:ILE:HG22	1:A:289:VAL:CG2	2.39	0.49
1:B:283:VAL:O	1:B:284:GLU:C	2.56	0.49
1:E:236:ASN:OD1	1:E:252:ASN:HA	2.13	0.49
1:G:204:PRO:HB2	1:G:247:THR:CG2	2.43	0.49
1:H:309:THR:HG22	1:H:336:ILE:CA	2.37	0.49
1:J:204:PRO:HB2	1:J:247:THR:CG2	2.43	0.49
1:A:100:ARG:HH21	1:C:71:GLU:HG3	1.76	0.48
1:G:267:PHE:HD1	1:G:267:PHE:H	1.61	0.48
1:I:165:THR:CG2	1:I:167:ARG:H	2.15	0.48
1:A:153:PHE:HA	1:A:177:SER:O	2.12	0.48
1:B:105:VAL:HA	1:B:190:ALA:HB1	1.94	0.48
1:C:204:PRO:HB2	1:C:247:THR:CG2	2.43	0.48
1:C:286:ILE:H	1:C:286:ILE:CD1	2.26	0.48
1:D:286:ILE:H	1:D:286:ILE:CD1	2.25	0.48
1:F:204:PRO:HD2	1:F:248:SER:O	2.13	0.48
1:I:153:PHE:HA	1:I:177:SER:O	2.13	0.48
1:I:236:ASN:OD1	1:I:252:ASN:HA	2.13	0.48
1:J:143:ASN:O	1:J:144:PHE:C	2.56	0.48
1:K:66:GLN:HG3	1:K:78:GLY:HA3	1.95	0.48
1:A:3:ILE:HD12	1:C:3:ILE:HG21	1.95	0.48
1:A:11:VAL:HG21	1:C:340:PHE:HB2	1.95	0.48
1:H:61:TRP:CZ2	1:H:63:TYR:HB2	2.48	0.48
1:H:236:ASN:OD1	1:H:252:ASN:HA	2.13	0.48
1:J:269:LEU:HG	1:J:271:PRO:HD3	1.95	0.48
1:A:31:SER:CA	1:A:329:ASP:HB2	2.40	0.48
1:A:161:ASN:HB2	1:A:170:ASN:OD1	2.13	0.48
1:A:264:GLN:OE1	1:A:270:ARG:HB2	2.12	0.48
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.48	0.48
1:K:165:THR:CG2	1:K:167:ARG:H	2.14	0.48
1:K:283:VAL:O	1:K:284:GLU:C	2.56	0.48
1:L:204:PRO:HB2	1:L:247:THR:CG2	2.42	0.48
1:A:66:GLN:HG3	1:A:78:GLY:HA3	1.96	0.48
1:A:204:PRO:HB2	1:A:247:THR:CG2	2.43	0.48
1:E:267:PHE:HD1	1:E:267:PHE:H	1.62	0.48
1:F:136:VAL:CG1	1:F:158:LEU:HD13	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:PRO:HB2	1:E:247:THR:HG23	1.95	0.48
1:H:31:SER:CA	1:H:329:ASP:HB2	2.39	0.48
1:H:204:PRO:HB2	1:H:247:THR:CG2	2.43	0.48
1:I:61:TRP:CZ2	1:I:63:TYR:HB2	2.48	0.48
1:J:105:VAL:HA	1:J:190:ALA:HB1	1.96	0.48
1:L:153:PHE:HA	1:L:177:SER:O	2.13	0.48
1:L:236:ASN:OD1	1:L:252:ASN:HA	2.14	0.48
1:E:313:TYR:HD1	1:E:332:VAL:CG2	2.19	0.48
1:K:204:PRO:HB2	1:K:247:THR:HG23	1.95	0.48
1:B:136:VAL:CG1	1:B:158:LEU:HD13	2.44	0.48
1:B:222:ALA:O	1:B:223:ASN:HB2	2.12	0.48
1:E:31:SER:CA	1:E:329:ASP:HB2	2.39	0.48
1:F:267:PHE:HD1	1:F:267:PHE:H	1.60	0.48
1:G:66:GLN:HG3	1:G:78:GLY:HA3	1.96	0.48
1:H:269:LEU:HG	1:H:271:PRO:HD3	1.96	0.48
1:D:66:GLN:HG3	1:D:78:GLY:HA3	1.96	0.48
1:D:236:ASN:OD1	1:D:252:ASN:HA	2.14	0.48
1:F:283:VAL:O	1:F:284:GLU:C	2.56	0.48
1:G:143:ASN:O	1:G:144:PHE:C	2.57	0.48
1:J:47:GLY:HA3	1:L:338:TYR:CE2	2.48	0.48
1:L:272:SER:N	1:L:298:GLY:O	2.44	0.48
1:A:236:ASN:OD1	1:A:252:ASN:HA	2.14	0.48
1:C:66:GLN:HG3	1:C:78:GLY:HA3	1.96	0.48
1:C:153:PHE:HA	1:C:177:SER:O	2.14	0.48
1:C:264:GLN:OE1	1:C:270:ARG:HB2	2.14	0.48
1:D:204:PRO:HD2	1:D:248:SER:O	2.13	0.48
1:G:236:ASN:OD1	1:G:252:ASN:HA	2.13	0.48
1:J:165:THR:CG2	1:J:167:ARG:H	2.16	0.48
1:J:204:PRO:HD2	1:J:248:SER:O	2.13	0.48
1:L:267:PHE:HD1	1:L:267:PHE:H	1.60	0.48
1:B:66:GLN:HG3	1:B:78:GLY:HA3	1.96	0.47
1:D:105:VAL:HA	1:D:190:ALA:HB1	1.96	0.47
1:F:264:GLN:OE1	1:F:270:ARG:HB2	2.14	0.47
1:F:269:LEU:HG	1:F:271:PRO:HD3	1.96	0.47
1:F:313:TYR:HD1	1:F:332:VAL:CG2	2.19	0.47
1:G:165:THR:HG22	1:G:166:ALA:N	2.28	0.47
1:D:204:PRO:HB2	1:D:247:THR:HG23	1.96	0.47
1:D:264:GLN:OE1	1:D:270:ARG:HB2	2.13	0.47
1:F:204:PRO:HB2	1:F:247:THR:CG2	2.43	0.47
1:F:222:ALA:O	1:F:223:ASN:HB2	2.13	0.47
1:G:340:PHE:CB	1:H:11:VAL:HG21	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:PHE:CD1	1:I:45:PHE:C	2.92	0.47
1:I:105:VAL:HA	1:I:190:ALA:HB1	1.96	0.47
1:J:273:ILE:CD1	1:J:297:VAL:HG22	2.45	0.47
1:K:286:ILE:HG22	1:K:289:VAL:CG2	2.36	0.47
1:A:136:VAL:CG1	1:A:158:LEU:HD13	2.44	0.47
1:B:165:THR:HG22	1:B:166:ALA:N	2.29	0.47
1:B:204:PRO:HB2	1:B:247:THR:HG23	1.96	0.47
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.49	0.47
1:J:283:VAL:O	1:J:284:GLU:C	2.57	0.47
1:K:31:SER:CA	1:K:329:ASP:HB2	2.39	0.47
1:L:169:SER:O	1:L:170:ASN:HB3	2.15	0.47
1:A:267:PHE:HD1	1:A:267:PHE:H	1.60	0.47
1:C:31:SER:CA	1:C:329:ASP:HB2	2.39	0.47
1:D:31:SER:CA	1:D:329:ASP:HB2	2.41	0.47
1:D:153:PHE:HA	1:D:177:SER:O	2.13	0.47
1:E:338:TYR:CE2	1:F:47:GLY:HA3	2.49	0.47
1:H:267:PHE:HD1	1:H:267:PHE:H	1.60	0.47
1:L:283:VAL:O	1:L:284:GLU:C	2.57	0.47
1:B:286:ILE:HG22	1:B:289:VAL:CG2	2.37	0.47
1:C:267:PHE:HD1	1:C:267:PHE:H	1.61	0.47
1:D:165:THR:HG22	1:D:166:ALA:N	2.29	0.47
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.50	0.47
1:E:66:GLN:HG3	1:E:78:GLY:HA3	1.96	0.47
1:G:286:ILE:HG22	1:G:289:VAL:CG2	2.38	0.47
1:G:303:PHE:CB	1:H:51:ILE:HD13	2.42	0.47
1:J:144:PHE:O	1:J:144:PHE:CD2	2.68	0.47
1:L:22:TYR:OH	1:L:117:GLU:OE2	2.30	0.47
1:B:179:SER:HB3	1:B:188:VAL:HG13	1.96	0.47
1:B:236:ASN:OD1	1:B:252:ASN:HA	2.14	0.47
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.49	0.47
1:E:169:SER:O	1:E:170:ASN:HB3	2.15	0.47
1:H:283:VAL:O	1:H:284:GLU:C	2.57	0.47
1:H:313:TYR:HD1	1:H:332:VAL:CG2	2.17	0.47
1:L:61:TRP:CZ2	1:L:63:TYR:HB2	2.49	0.47
1:L:66:GLN:HG3	1:L:78:GLY:HA3	1.96	0.47
1:A:80:LYS:HD2	1:C:71:GLU:CB	2.28	0.47
1:A:283:VAL:O	1:A:284:GLU:C	2.58	0.47
1:B:31:SER:CA	1:B:329:ASP:HB2	2.41	0.47
1:B:303:PHE:HB3	1:C:51:ILE:CG2	2.44	0.47
1:C:161:ASN:HB2	1:C:170:ASN:OD1	2.13	0.47
1:D:169:SER:O	1:D:170:ASN:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:PHE:H	1:D:267:PHE:HD1	1.61	0.47
1:D:283:VAL:O	1:D:284:GLU:C	2.57	0.47
1:F:236:ASN:OD1	1:F:252:ASN:HA	2.14	0.47
1:G:144:PHE:O	1:G:144:PHE:CD2	2.68	0.47
1:H:153:PHE:HA	1:H:177:SER:O	2.13	0.47
1:H:258:LEU:N	1:H:258:LEU:HD22	2.30	0.47
1:J:267:PHE:H	1:J:267:PHE:HD1	1.62	0.47
1:L:165:THR:HG22	1:L:166:ALA:N	2.30	0.47
1:E:244:PHE:CZ	1:K:285:GLY:HA2	2.50	0.47
1:F:169:SER:O	1:F:170:ASN:HB3	2.14	0.47
1:G:264:GLN:OE1	1:G:270:ARG:HB2	2.14	0.47
1:H:105:VAL:HA	1:H:190:ALA:HB1	1.96	0.47
1:K:61:TRP:CZ2	1:K:63:TYR:HB2	2.50	0.47
1:K:105:VAL:HA	1:K:190:ALA:HB1	1.96	0.47
1:C:269:LEU:HG	1:C:271:PRO:HD3	1.97	0.47
1:G:71:GLU:HG3	1:H:100:ARG:HH21	1.80	0.47
1:I:269:LEU:HG	1:I:271:PRO:HD3	1.96	0.47
1:L:31:SER:CA	1:L:329:ASP:HB2	2.39	0.47
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.50	0.47
1:B:165:THR:CG2	1:B:167:ARG:H	2.15	0.47
1:B:204:PRO:HD2	1:B:248:SER:O	2.14	0.47
1:C:286:ILE:N	1:C:286:ILE:CD1	2.75	0.47
1:E:105:VAL:HA	1:E:190:ALA:HB1	1.96	0.47
1:E:283:VAL:O	1:E:284:GLU:C	2.58	0.47
1:G:283:VAL:O	1:G:284:GLU:C	2.57	0.47
1:H:286:ILE:N	1:H:286:ILE:CD1	2.73	0.47
1:K:153:PHE:HA	1:K:177:SER:O	2.14	0.47
1:L:204:PRO:HB2	1:L:247:THR:HG23	1.96	0.47
1:B:51:ILE:HB	1:B:55:LEU:HB3	1.98	0.46
1:C:204:PRO:HB2	1:C:247:THR:HG23	1.98	0.46
1:D:11:VAL:HG21	1:F:340:PHE:CB	2.45	0.46
1:E:269:LEU:HG	1:E:271:PRO:HD3	1.96	0.46
1:E:340:PHE:HB2	1:F:11:VAL:HG21	1.97	0.46
1:F:272:SER:N	1:F:298:GLY:O	2.46	0.46
1:G:204:PRO:HB2	1:G:247:THR:HG23	1.96	0.46
1:G:258:LEU:HD13	1:G:276:THR:HG23	1.96	0.46
1:J:3:ILE:HD12	1:L:3:ILE:HG21	1.97	0.46
1:J:165:THR:HG22	1:J:166:ALA:N	2.29	0.46
1:J:236:ASN:OD1	1:J:252:ASN:HA	2.15	0.46
1:K:303:PHE:HB3	1:L:51:ILE:HD13	1.98	0.46
1:L:313:TYR:HD1	1:L:332:VAL:CG2	2.17	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:CD1	1:A:297:VAL:HG22	2.44	0.46
1:C:283:VAL:O	1:C:284:GLU:C	2.58	0.46
1:E:165:THR:HG22	1:E:166:ALA:N	2.29	0.46
1:J:11:VAL:HG21	1:L:340:PHE:HB2	1.96	0.46
1:J:264:GLN:OE1	1:J:270:ARG:HB2	2.15	0.46
1:A:165:THR:HG22	1:A:166:ALA:N	2.29	0.46
1:D:303:PHE:CB	1:E:51:ILE:HD13	2.44	0.46
1:G:51:ILE:HD13	1:I:303:PHE:CG	2.50	0.46
1:G:100:ARG:HH21	1:I:71:GLU:HG3	1.76	0.46
1:H:45:PHE:CD1	1:H:45:PHE:C	2.93	0.46
1:H:204:PRO:HB2	1:H:247:THR:HG23	1.96	0.46
1:K:191:TYR:CD1	1:K:214:TRP:HB3	2.49	0.46
1:K:273:ILE:CD1	1:K:297:VAL:HG22	2.46	0.46
1:A:204:PRO:HD2	1:A:248:SER:O	2.15	0.46
1:D:3:ILE:HG21	1:E:3:ILE:HD12	1.97	0.46
1:D:136:VAL:CG1	1:D:158:LEU:HD13	2.45	0.46
1:D:340:PHE:CB	1:E:11:VAL:HG21	2.46	0.46
1:E:204:PRO:HD2	1:E:248:SER:O	2.15	0.46
1:G:3:ILE:HG21	1:H:3:ILE:HD12	1.98	0.46
1:G:191:TYR:CD1	1:G:214:TRP:HB3	2.48	0.46
1:H:273:ILE:CD1	1:H:297:VAL:HG22	2.45	0.46
1:K:144:PHE:O	1:K:144:PHE:CD2	2.69	0.46
1:K:165:THR:HG22	1:K:166:ALA:N	2.30	0.46
1:B:336:ILE:HG23	1:B:336:ILE:O	2.16	0.46
1:D:51:ILE:HD13	1:F:303:PHE:CG	2.50	0.46
1:D:52:ASN:OD1	1:D:53:SER:N	2.48	0.46
1:E:309:THR:HG22	1:E:336:ILE:CA	2.37	0.46
1:H:340:PHE:HB2	1:I:11:VAL:HG21	1.98	0.46
1:K:71:GLU:CD	1:L:100:ARG:HH21	2.24	0.46
1:K:169:SER:O	1:K:170:ASN:HB3	2.15	0.46
1:A:11:VAL:HG21	1:C:340:PHE:CB	2.46	0.46
1:E:144:PHE:O	1:E:144:PHE:CD2	2.69	0.46
1:I:204:PRO:HB2	1:I:247:THR:HG23	1.96	0.46
1:J:204:PRO:HB2	1:J:247:THR:HG23	1.97	0.46
1:L:105:VAL:HA	1:L:190:ALA:HB1	1.96	0.46
1:A:105:VAL:HA	1:A:190:ALA:HB1	1.96	0.46
1:A:204:PRO:HB2	1:A:247:THR:HG23	1.96	0.46
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.50	0.46
1:J:191:TYR:CD1	1:J:214:TRP:HB3	2.49	0.46
1:J:193:ALA:HA	1:J:211:ALA:O	2.16	0.46
1:A:191:TYR:CD1	1:A:214:TRP:HB3	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HA	1:C:190:ALA:HB1	1.97	0.46
1:D:3:ILE:HD12	1:F:3:ILE:HG21	1.97	0.46
1:D:286:ILE:N	1:D:286:ILE:CD1	2.74	0.46
1:E:193:ALA:HA	1:E:211:ALA:O	2.16	0.46
1:F:45:PHE:CD1	1:F:45:PHE:C	2.94	0.46
1:F:204:PRO:HB2	1:F:247:THR:HG23	1.97	0.46
1:G:61:TRP:CZ2	1:G:63:TYR:HB2	2.50	0.46
1:K:193:ALA:HA	1:K:211:ALA:O	2.16	0.46
1:L:45:PHE:CD1	1:L:45:PHE:C	2.93	0.46
1:A:45:PHE:CD1	1:A:45:PHE:C	2.93	0.46
1:F:309:THR:HG22	1:F:336:ILE:HG13	1.98	0.46
1:G:309:THR:HG22	1:G:336:ILE:HG13	1.98	0.46
1:H:169:SER:O	1:H:170:ASN:HB3	2.15	0.46
1:I:51:ILE:HB	1:I:55:LEU:HB3	1.97	0.46
1:I:165:THR:HG22	1:I:166:ALA:N	2.30	0.46
1:J:61:TRP:CZ2	1:J:63:TYR:HB2	2.50	0.46
1:J:100:ARG:HH21	1:L:71:GLU:HG3	1.77	0.46
1:J:169:SER:O	1:J:170:ASN:HB3	2.16	0.46
1:L:286:ILE:HG23	1:L:323:LYS:CB	2.46	0.46
1:I:144:PHE:O	1:I:144:PHE:CD2	2.69	0.46
1:I:179:SER:HB3	1:I:188:VAL:HG13	1.98	0.46
1:I:191:TYR:CD1	1:I:214:TRP:HB3	2.49	0.46
1:L:193:ALA:HA	1:L:211:ALA:O	2.16	0.46
1:B:45:PHE:CD1	1:B:45:PHE:C	2.94	0.45
1:B:193:ALA:HA	1:B:211:ALA:O	2.16	0.45
1:B:267:PHE:H	1:B:267:PHE:HD1	1.62	0.45
1:B:287:GLY:CA	1:L:321:ASP:OD2	2.61	0.45
1:C:165:THR:HG22	1:C:166:ALA:N	2.30	0.45
1:H:71:GLU:HG3	1:I:100:ARG:HH21	1.78	0.45
1:H:163:ARG:HD2	1:H:168:ARG:O	2.16	0.45
1:K:45:PHE:CD1	1:K:45:PHE:C	2.94	0.45
1:A:52:ASN:OD1	1:A:53:SER:N	2.50	0.45
1:F:165:THR:HG22	1:F:166:ALA:N	2.31	0.45
1:G:193:ALA:HA	1:G:211:ALA:O	2.17	0.45
1:I:169:SER:O	1:I:170:ASN:HB3	2.16	0.45
1:J:45:PHE:CD1	1:J:45:PHE:C	2.94	0.45
1:A:336:ILE:O	1:A:336:ILE:HG23	2.17	0.45
1:B:150:GLY:O	1:B:180:TYR:HA	2.17	0.45
1:E:273:ILE:CD1	1:E:297:VAL:HG22	2.46	0.45
1:F:66:GLN:HG3	1:F:78:GLY:HA3	1.96	0.45
1:H:191:TYR:CD1	1:H:214:TRP:HB3	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:O	1:A:144:PHE:CD2	2.70	0.45
1:A:169:SER:O	1:A:170:ASN:HB3	2.15	0.45
1:C:309:THR:HG22	1:C:336:ILE:HG13	1.98	0.45
1:D:272:SER:N	1:D:298:GLY:O	2.43	0.45
1:F:234:THR:OG1	1:F:254:THR:OG1	2.26	0.45
1:G:286:ILE:HG23	1:G:323:LYS:CB	2.47	0.45
1:I:193:ALA:HA	1:I:211:ALA:O	2.16	0.45
1:K:51:ILE:HB	1:K:55:LEU:HB3	1.99	0.45
1:K:71:GLU:CG	1:L:100:ARG:NH2	2.70	0.45
1:A:105:VAL:O	1:A:105:VAL:CG1	2.65	0.45
1:A:269:LEU:HG	1:A:271:PRO:HD3	1.99	0.45
1:B:269:LEU:HG	1:B:271:PRO:HD3	1.98	0.45
1:D:269:LEU:HG	1:D:271:PRO:HD3	1.98	0.45
1:E:258:LEU:N	1:E:258:LEU:HD22	2.32	0.45
1:F:51:ILE:HB	1:F:55:LEU:HB3	1.99	0.45
1:G:273:ILE:CD1	1:G:297:VAL:HG22	2.47	0.45
1:G:309:THR:CG2	1:G:336:ILE:HG13	2.46	0.45
1:H:193:ALA:HA	1:H:211:ALA:O	2.16	0.45
1:H:272:SER:N	1:H:298:GLY:O	2.46	0.45
1:J:52:ASN:OD1	1:J:53:SER:N	2.50	0.45
1:K:179:SER:HB3	1:K:188:VAL:HG13	1.97	0.45
1:D:144:PHE:O	1:D:144:PHE:CD2	2.70	0.45
1:E:45:PHE:CD1	1:E:45:PHE:C	2.93	0.45
1:F:105:VAL:HA	1:F:190:ALA:HB1	1.97	0.45
1:G:45:PHE:CD1	1:G:45:PHE:C	2.94	0.45
1:I:283:VAL:O	1:I:284:GLU:C	2.60	0.45
1:J:11:VAL:HG21	1:L:340:PHE:CB	2.47	0.45
1:J:66:GLN:HG3	1:J:78:GLY:HA3	1.98	0.45
1:J:338:TYR:CE2	1:K:47:GLY:HA3	2.52	0.45
1:K:336:ILE:HG23	1:K:336:ILE:O	2.17	0.45
1:B:3:ILE:HG21	1:C:3:ILE:HD12	1.99	0.45
1:B:273:ILE:CD1	1:B:297:VAL:HG22	2.47	0.45
1:F:193:ALA:HA	1:F:211:ALA:O	2.17	0.45
1:G:169:SER:O	1:G:170:ASN:HB3	2.16	0.45
1:K:206:GLY:H	1:K:284:GLU:CD	2.25	0.45
1:L:144:PHE:O	1:L:144:PHE:CD2	2.70	0.45
1:L:309:THR:HG22	1:L:336:ILE:HG13	1.99	0.45
1:D:273:ILE:CD1	1:D:297:VAL:HG22	2.46	0.45
1:D:286:ILE:HG23	1:D:323:LYS:CB	2.47	0.45
1:E:272:SER:N	1:E:298:GLY:O	2.45	0.45
1:F:206:GLY:H	1:F:284:GLU:CD	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:GLY:O	1:I:180:TYR:HA	2.17	0.45
1:I:286:ILE:HG23	1:I:323:LYS:CB	2.47	0.45
1:K:163:ARG:HD2	1:K:168:ARG:O	2.15	0.45
1:B:286:ILE:HG23	1:B:323:LYS:CB	2.47	0.45
1:C:193:ALA:HA	1:C:211:ALA:O	2.17	0.45
1:H:179:SER:HB3	1:H:188:VAL:HG13	1.99	0.45
1:J:336:ILE:HG23	1:J:336:ILE:O	2.17	0.45
1:K:269:LEU:HG	1:K:271:PRO:HD3	1.97	0.45
1:L:179:SER:HB3	1:L:188:VAL:HG13	1.97	0.45
1:L:273:ILE:CD1	1:L:297:VAL:HG22	2.46	0.45
1:B:169:SER:O	1:B:170:ASN:HB3	2.16	0.45
1:B:191:TYR:CD1	1:B:214:TRP:HB3	2.49	0.45
1:C:163:ARG:HD2	1:C:168:ARG:O	2.17	0.45
1:C:206:GLY:H	1:C:284:GLU:CD	2.25	0.45
1:E:229:ALA:CB	1:E:259:LEU:HD23	2.47	0.45
1:G:258:LEU:N	1:G:258:LEU:HD22	2.32	0.45
1:I:234:THR:OG1	1:I:254:THR:OG1	2.28	0.45
1:I:273:ILE:CD1	1:I:297:VAL:HG22	2.47	0.45
1:J:179:SER:HB3	1:J:188:VAL:HG13	1.98	0.45
1:L:258:LEU:N	1:L:258:LEU:HD22	2.32	0.45
1:A:258:LEU:N	1:A:258:LEU:HD22	2.32	0.44
1:C:51:ILE:HB	1:C:55:LEU:HB3	1.99	0.44
1:C:165:THR:CG2	1:C:167:ARG:H	2.16	0.44
1:D:51:ILE:HB	1:D:55:LEU:HB3	1.99	0.44
1:D:206:GLY:H	1:D:284:GLU:CD	2.25	0.44
1:F:336:ILE:O	1:F:336:ILE:HG23	2.17	0.44
1:G:272:SER:N	1:G:298:GLY:O	2.44	0.44
1:H:165:THR:HG22	1:H:166:ALA:N	2.30	0.44
1:A:286:ILE:HG23	1:A:323:LYS:CB	2.47	0.44
1:C:258:LEU:N	1:C:258:LEU:HD22	2.33	0.44
1:E:3:ILE:HG21	1:F:3:ILE:HD12	1.99	0.44
1:E:309:THR:HG22	1:E:336:ILE:HG13	1.98	0.44
1:E:336:ILE:HG23	1:E:336:ILE:O	2.16	0.44
1:G:51:ILE:HB	1:G:55:LEU:HB3	1.99	0.44
1:K:272:SER:N	1:K:298:GLY:O	2.45	0.44
1:A:309:THR:CG2	1:A:336:ILE:HG13	2.48	0.44
1:C:45:PHE:CD1	1:C:45:PHE:C	2.95	0.44
1:D:45:PHE:CD1	1:D:45:PHE:C	2.95	0.44
1:H:51:ILE:HB	1:H:55:LEU:HB3	1.99	0.44
1:H:338:TYR:CE2	1:I:47:GLY:HA3	2.52	0.44
1:I:229:ALA:CB	1:I:259:LEU:HD23	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:90:TYR:CD2	1:J:93:VAL:HG21	2.52	0.44
1:A:51:ILE:HB	1:A:55:LEU:HB3	1.98	0.44
1:A:165:THR:CG2	1:A:167:ARG:H	2.15	0.44
1:A:229:ALA:CB	1:A:259:LEU:HD23	2.47	0.44
1:E:206:GLY:H	1:E:284:GLU:CD	2.26	0.44
1:E:309:THR:CG2	1:E:336:ILE:HG13	2.48	0.44
1:F:286:ILE:HG23	1:F:323:LYS:CB	2.48	0.44
1:G:206:GLY:H	1:G:284:GLU:CD	2.26	0.44
1:H:3:ILE:HG21	1:I:3:ILE:HD12	1.99	0.44
1:H:286:ILE:HG23	1:H:323:LYS:CB	2.47	0.44
1:H:303:PHE:CB	1:I:51:ILE:HD13	2.48	0.44
1:J:303:PHE:CB	1:K:51:ILE:HD13	2.47	0.44
1:K:258:LEU:HD22	1:K:258:LEU:N	2.32	0.44
1:A:193:ALA:HA	1:A:211:ALA:O	2.17	0.44
1:I:163:ARG:HD2	1:I:168:ARG:O	2.18	0.44
1:I:309:THR:HG22	1:I:336:ILE:HG13	1.98	0.44
1:L:51:ILE:HB	1:L:55:LEU:HB3	1.99	0.44
1:B:144:PHE:O	1:B:144:PHE:CD2	2.70	0.44
1:C:309:THR:CG2	1:C:336:ILE:HG13	2.47	0.44
1:D:51:ILE:HG21	1:F:303:PHE:HB3	2.00	0.44
1:D:71:GLU:HG3	1:E:100:ARG:HH21	1.81	0.44
1:F:309:THR:CG2	1:F:336:ILE:HG13	2.47	0.44
1:G:235:ARG:HA	1:G:235:ARG:HD3	1.79	0.44
1:H:206:GLY:H	1:H:284:GLU:CD	2.25	0.44
1:J:51:ILE:HB	1:J:55:LEU:HB3	2.00	0.44
1:J:54:ASP:HB3	1:J:91:ALA:HB2	2.00	0.44
1:J:309:THR:CG2	1:J:336:ILE:HG13	2.48	0.44
1:L:336:ILE:HG23	1:L:336:ILE:O	2.17	0.44
1:A:206:GLY:H	1:A:284:GLU:CD	2.26	0.44
1:E:71:GLU:CG	1:F:100:ARG:HH21	2.31	0.44
1:E:90:TYR:CD2	1:E:93:VAL:HG21	2.53	0.44
1:F:144:PHE:O	1:F:144:PHE:CD2	2.71	0.44
1:I:206:GLY:H	1:I:284:GLU:CD	2.26	0.44
1:I:235:ARG:HA	1:I:235:ARG:HD3	1.80	0.44
1:I:242:ASN:C	1:I:242:ASN:OD1	2.61	0.44
1:K:286:ILE:HG23	1:K:323:LYS:CB	2.48	0.44
1:C:105:VAL:O	1:C:105:VAL:CG1	2.66	0.44
1:C:191:TYR:CD1	1:C:214:TRP:HB3	2.48	0.44
1:D:336:ILE:HG23	1:D:336:ILE:O	2.17	0.44
1:E:286:ILE:HG23	1:E:323:LYS:CB	2.47	0.44
1:G:105:VAL:O	1:G:105:VAL:CG1	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:LEU:HG	1:G:271:PRO:HD3	1.99	0.44
1:I:31:SER:CA	1:I:329:ASP:HB2	2.40	0.44
1:I:336:ILE:HG23	1:I:336:ILE:O	2.17	0.44
1:K:309:THR:HG22	1:K:336:ILE:HG13	2.00	0.44
1:A:242:ASN:OD1	1:A:242:ASN:C	2.61	0.44
1:B:229:ALA:CB	1:B:259:LEU:HD23	2.48	0.44
1:C:179:SER:HB3	1:C:188:VAL:HG13	1.99	0.44
1:E:52:ASN:OD1	1:E:53:SER:N	2.51	0.44
1:H:257:VAL:C	1:H:258:LEU:HD22	2.43	0.44
1:I:313:TYR:HD1	1:I:332:VAL:CG2	2.17	0.44
1:J:206:GLY:H	1:J:284:GLU:CD	2.25	0.44
1:J:272:SER:N	1:J:298:GLY:O	2.46	0.44
1:L:273:ILE:HD13	1:L:273:ILE:HA	1.86	0.44
1:C:229:ALA:CB	1:C:259:LEU:HD23	2.47	0.43
1:E:51:ILE:HB	1:E:55:LEU:HB3	1.99	0.43
1:G:336:ILE:HG23	1:G:336:ILE:O	2.17	0.43
1:H:235:ARG:HA	1:H:235:ARG:HD3	1.80	0.43
1:J:286:ILE:HG23	1:J:323:LYS:CB	2.48	0.43
1:A:272:SER:N	1:A:298:GLY:O	2.46	0.43
1:A:286:ILE:N	1:A:286:ILE:CD1	2.73	0.43
1:B:52:ASN:OD1	1:B:53:SER:N	2.50	0.43
1:B:272:SER:N	1:B:298:GLY:O	2.44	0.43
1:C:272:SER:N	1:C:298:GLY:O	2.44	0.43
1:C:336:ILE:HG23	1:C:336:ILE:O	2.17	0.43
1:G:229:ALA:CB	1:G:259:LEU:HD23	2.48	0.43
1:G:303:PHE:CG	1:H:51:ILE:HD13	2.53	0.43
1:H:150:GLY:O	1:H:180:TYR:HA	2.19	0.43
1:A:309:THR:HG22	1:A:336:ILE:HG13	2.00	0.43
1:B:258:LEU:N	1:B:258:LEU:HD22	2.33	0.43
1:D:71:GLU:CB	1:E:80:LYS:HD2	2.26	0.43
1:E:286:ILE:HG23	1:E:323:LYS:HB3	2.00	0.43
1:H:242:ASN:OD1	1:H:242:ASN:C	2.61	0.43
1:J:309:THR:HG22	1:J:336:ILE:HG13	1.99	0.43
1:A:303:PHE:CB	1:B:51:ILE:HD13	2.48	0.43
1:H:144:PHE:O	1:H:144:PHE:CD2	2.71	0.43
1:B:22:TYR:OH	1:B:117:GLU:OE2	2.31	0.43
1:D:163:ARG:HD2	1:D:168:ARG:O	2.19	0.43
1:E:303:PHE:CG	1:F:51:ILE:HD13	2.54	0.43
1:A:111:TYR:OH	1:A:188:VAL:HG23	2.18	0.43
1:C:144:PHE:O	1:C:144:PHE:CD2	2.72	0.43
1:D:105:VAL:O	1:D:105:VAL:CG1	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLY:O	1:D:180:TYR:HA	2.19	0.43
1:G:90:TYR:CD2	1:G:93:VAL:HG21	2.54	0.43
1:G:179:SER:HB3	1:G:188:VAL:HG13	2.00	0.43
1:G:242:ASN:C	1:G:242:ASN:OD1	2.62	0.43
1:H:309:THR:HG22	1:H:336:ILE:HG13	2.00	0.43
1:K:229:ALA:CB	1:K:259:LEU:HD23	2.48	0.43
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.90	0.43
1:A:338:TYR:CE2	1:B:47:GLY:HA3	2.52	0.43
1:A:340:PHE:HB2	1:B:11:VAL:HG21	2.00	0.43
1:C:286:ILE:HG23	1:C:323:LYS:CB	2.48	0.43
1:D:179:SER:HB3	1:D:188:VAL:HG13	2.00	0.43
1:D:193:ALA:HA	1:D:211:ALA:O	2.18	0.43
1:D:229:ALA:CB	1:D:259:LEU:HD23	2.48	0.43
1:D:309:THR:HG22	1:D:336:ILE:HG13	2.00	0.43
1:E:163:ARG:HD2	1:E:168:ARG:O	2.19	0.43
1:F:52:ASN:OD1	1:F:53:SER:N	2.51	0.43
1:F:165:THR:CG2	1:F:167:ARG:H	2.16	0.43
1:F:273:ILE:CD1	1:F:297:VAL:HG22	2.49	0.43
1:H:229:ALA:CB	1:H:259:LEU:HD23	2.49	0.43
1:I:286:ILE:HG23	1:I:323:LYS:HB3	2.01	0.43
1:L:206:GLY:H	1:L:284:GLU:CD	2.26	0.43
1:B:115:LEU:HD21	1:B:274:ALA:HB2	2.01	0.43
1:B:206:GLY:H	1:B:284:GLU:CD	2.26	0.43
1:C:285:GLY:CA	1:G:244:PHE:HZ	2.31	0.43
1:D:242:ASN:C	1:D:242:ASN:OD1	2.61	0.43
1:E:340:PHE:CB	1:F:11:VAL:HG21	2.49	0.43
1:G:12:ASP:O	1:G:45:PHE:HA	2.18	0.43
1:H:336:ILE:HG23	1:H:336:ILE:O	2.19	0.43
1:K:309:THR:CG2	1:K:336:ILE:HG13	2.49	0.43
1:L:54:ASP:HB3	1:L:91:ALA:HB2	2.01	0.43
1:L:309:THR:CG2	1:L:336:ILE:HG13	2.49	0.43
1:C:235:ARG:HA	1:C:235:ARG:HD3	1.80	0.43
1:D:309:THR:CG2	1:D:336:ILE:HG13	2.48	0.43
1:F:235:ARG:HA	1:F:235:ARG:HD3	1.80	0.43
1:G:51:ILE:HG21	1:I:303:PHE:HB3	2.01	0.43
1:L:150:GLY:O	1:L:180:TYR:HA	2.19	0.43
1:B:286:ILE:HG23	1:B:323:LYS:HB3	2.00	0.43
1:B:309:THR:CG2	1:B:336:ILE:HG13	2.49	0.43
1:B:313:TYR:HD1	1:B:332:VAL:CG2	2.19	0.43
1:C:242:ASN:OD1	1:C:242:ASN:C	2.62	0.43
1:C:273:ILE:CD1	1:C:297:VAL:HG22	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:NH2	1:E:253:LYS:HZ3	2.17	0.43
1:F:229:ALA:CB	1:F:259:LEU:HD23	2.48	0.43
1:G:31:SER:CA	1:G:329:ASP:HB2	2.39	0.43
1:G:286:ILE:HG23	1:G:323:LYS:HB3	2.01	0.43
1:H:244:PHE:CZ	1:L:285:GLY:CA	3.02	0.43
1:I:12:ASP:O	1:I:45:PHE:HA	2.19	0.43
1:K:267:PHE:HD1	1:K:267:PHE:H	1.62	0.43
1:L:229:ALA:CB	1:L:259:LEU:HD23	2.49	0.43
1:C:169:SER:O	1:C:170:ASN:HB3	2.18	0.42
1:F:179:SER:HB3	1:F:188:VAL:HG13	2.01	0.42
1:G:165:THR:CG2	1:G:167:ARG:H	2.16	0.42
1:H:340:PHE:CB	1:I:11:VAL:HG21	2.49	0.42
1:I:22:TYR:OH	1:I:117:GLU:OE2	2.32	0.42
1:I:272:SER:N	1:I:298:GLY:O	2.45	0.42
1:J:229:ALA:CB	1:J:259:LEU:HD23	2.48	0.42
1:K:286:ILE:HG23	1:K:323:LYS:HB3	2.01	0.42
1:L:52:ASN:OD1	1:L:53:SER:N	2.52	0.42
1:A:71:GLU:HG3	1:B:100:ARG:HH21	1.80	0.42
1:C:54:ASP:HB3	1:C:91:ALA:HB2	2.01	0.42
1:D:100:ARG:NH2	1:F:71:GLU:CG	2.73	0.42
1:G:150:GLY:O	1:G:180:TYR:HA	2.19	0.42
1:J:286:ILE:HG23	1:J:323:LYS:HB3	2.01	0.42
1:J:313:TYR:HD1	1:J:332:VAL:CG2	2.17	0.42
1:L:90:TYR:CD2	1:L:93:VAL:HG21	2.54	0.42
1:B:287:GLY:N	1:L:321:ASP:OD1	2.45	0.42
1:E:235:ARG:NE	1:E:253:LYS:HG2	2.34	0.42
1:F:242:ASN:OD1	1:F:242:ASN:C	2.62	0.42
1:F:253:LYS:C	1:F:253:LYS:HD2	2.45	0.42
1:J:253:LYS:C	1:J:253:LYS:HD2	2.43	0.42
1:L:265:PHE:CB	1:L:267:PHE:CE1	3.02	0.42
1:A:150:GLY:O	1:A:180:TYR:HA	2.19	0.42
1:B:309:THR:HG22	1:B:336:ILE:HG13	2.00	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.89	0.42
1:E:242:ASN:OD1	1:E:242:ASN:C	2.60	0.42
1:H:235:ARG:NE	1:H:253:LYS:HG2	2.33	0.42
1:J:242:ASN:OD1	1:J:242:ASN:C	2.62	0.42
1:K:90:TYR:CD2	1:K:93:VAL:HG21	2.54	0.42
1:K:179:SER:HB2	1:K:188:VAL:HG22	2.02	0.42
1:L:12:ASP:O	1:L:45:PHE:HA	2.19	0.42
1:E:150:GLY:O	1:E:180:TYR:HA	2.19	0.42
1:E:179:SER:HB3	1:E:188:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:ARG:NH2	1:H:253:LYS:HZ3	2.17	0.42
1:I:258:LEU:N	1:I:258:LEU:HD22	2.34	0.42
1:K:235:ARG:NH2	1:K:253:LYS:HZ3	2.18	0.42
1:L:136:VAL:CG1	1:L:158:LEU:CD1	2.98	0.42
1:A:179:SER:HB3	1:A:188:VAL:HG13	2.01	0.42
1:B:242:ASN:OD1	1:B:242:ASN:C	2.62	0.42
1:H:90:TYR:CD2	1:H:93:VAL:HG21	2.54	0.42
1:I:285:GLY:HA3	1:K:244:PHE:CZ	2.54	0.42
1:I:309:THR:CG2	1:I:336:ILE:HG13	2.49	0.42
1:K:242:ASN:OD1	1:K:242:ASN:C	2.63	0.42
1:B:12:ASP:O	1:B:45:PHE:HA	2.20	0.42
1:C:52:ASN:OD1	1:C:53:SER:N	2.53	0.42
1:D:258:LEU:HD22	1:D:258:LEU:N	2.35	0.42
1:D:273:ILE:HD13	1:D:273:ILE:HA	1.86	0.42
1:E:303:PHE:HB3	1:F:51:ILE:HG21	2.01	0.42
1:F:258:LEU:N	1:F:258:LEU:HD22	2.34	0.42
1:H:309:THR:CG2	1:H:336:ILE:HG13	2.50	0.42
1:K:253:LYS:HD2	1:K:253:LYS:C	2.45	0.42
1:L:231:TYR:HD1	1:L:257:VAL:HG22	1.85	0.42
1:L:286:ILE:HG23	1:L:323:LYS:HB3	2.00	0.42
1:F:54:ASP:HB3	1:F:91:ALA:HB2	2.02	0.42
1:H:71:GLU:CG	1:I:100:ARG:HH21	2.32	0.42
1:K:54:ASP:HB3	1:K:91:ALA:HB2	2.02	0.42
1:K:235:ARG:NE	1:K:253:LYS:HG2	2.35	0.42
1:A:253:LYS:C	1:A:253:LYS:HD2	2.45	0.42
1:A:286:ILE:HG23	1:A:323:LYS:HB3	2.00	0.42
1:D:54:ASP:HB3	1:D:91:ALA:HB2	2.02	0.42
1:D:253:LYS:HD2	1:D:253:LYS:C	2.45	0.42
1:F:235:ARG:NE	1:F:253:LYS:HG2	2.35	0.42
1:G:54:ASP:HB3	1:G:91:ALA:HB2	2.02	0.42
1:J:100:ARG:HH21	1:L:71:GLU:CG	2.32	0.42
1:J:303:PHE:CG	1:K:51:ILE:HD13	2.55	0.42
1:K:12:ASP:O	1:K:45:PHE:HA	2.20	0.42
1:A:54:ASP:HB3	1:A:91:ALA:HB2	2.02	0.42
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.91	0.42
1:F:150:GLY:O	1:F:180:TYR:HA	2.20	0.42
1:A:90:TYR:CD2	1:A:93:VAL:HG21	2.55	0.41
1:B:179:SER:HB2	1:B:188:VAL:HG22	2.02	0.41
1:F:90:TYR:CD2	1:F:93:VAL:HG21	2.55	0.41
1:H:52:ASN:OD1	1:H:53:SER:N	2.53	0.41
1:H:253:LYS:HD2	1:H:253:LYS:C	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:PHE:CB	1:H:267:PHE:CE1	3.02	0.41
1:H:286:ILE:HG23	1:H:323:LYS:HB3	2.01	0.41
1:K:52:ASN:OD1	1:K:53:SER:N	2.53	0.41
1:K:105:VAL:O	1:K:105:VAL:CG1	2.67	0.41
1:L:191:TYR:CD1	1:L:214:TRP:HB3	2.49	0.41
1:A:163:ARG:HD2	1:A:168:ARG:O	2.20	0.41
1:C:1:ALA:N	1:C:340:PHE:OXT	2.42	0.41
1:C:253:LYS:C	1:C:253:LYS:HD2	2.45	0.41
1:D:286:ILE:HG23	1:D:323:LYS:HB3	2.01	0.41
1:G:163:ARG:HD2	1:G:168:ARG:O	2.20	0.41
1:J:105:VAL:O	1:J:105:VAL:CG1	2.67	0.41
1:K:150:GLY:O	1:K:180:TYR:HA	2.19	0.41
1:K:257:VAL:C	1:K:258:LEU:HD22	2.45	0.41
1:B:54:ASP:HB3	1:B:91:ALA:HB2	2.01	0.41
1:C:150:GLY:O	1:C:180:TYR:HA	2.19	0.41
1:E:12:ASP:O	1:E:45:PHE:HA	2.20	0.41
1:G:22:TYR:OH	1:G:117:GLU:OE2	2.33	0.41
1:G:100:ARG:HH21	1:I:71:GLU:CG	2.34	0.41
1:G:115:LEU:HD21	1:G:274:ALA:HB2	2.02	0.41
1:G:284:GLU:CD	1:G:284:GLU:H	2.28	0.41
1:H:12:ASP:O	1:H:45:PHE:HA	2.19	0.41
1:I:180:TYR:CE2	1:I:182:TYR:HB2	2.55	0.41
1:J:309:THR:HG22	1:J:336:ILE:CB	2.51	0.41
1:L:223:ASN:O	1:L:224:ASN:CB	2.68	0.41
1:B:163:ARG:HD2	1:B:168:ARG:O	2.20	0.41
1:E:265:PHE:CB	1:E:267:PHE:CE1	3.02	0.41
1:E:284:GLU:CD	1:E:284:GLU:H	2.28	0.41
1:G:203:GLN:HA	1:G:204:PRO:HD3	1.86	0.41
1:J:303:PHE:HB3	1:K:51:ILE:HG21	2.01	0.41
1:L:163:ARG:HD2	1:L:168:ARG:O	2.20	0.41
1:A:170:ASN:ND2	1:A:170:ASN:C	2.79	0.41
1:A:309:THR:HG22	1:A:336:ILE:CB	2.50	0.41
1:C:174:VAL:CG1	1:C:175:GLY:H	2.34	0.41
1:C:286:ILE:HG23	1:C:323:LYS:HB3	2.03	0.41
1:D:142:SER:HA	1:D:152:ASN:OD1	2.21	0.41
1:E:54:ASP:HB3	1:E:91:ALA:HB2	2.01	0.41
1:F:253:LYS:HD2	1:F:254:THR:N	2.36	0.41
1:H:104:VAL:HG13	1:H:156:GLN:HB2	2.03	0.41
1:I:235:ARG:NE	1:I:253:LYS:HG2	2.35	0.41
1:K:115:LEU:HD21	1:K:274:ALA:HB2	2.03	0.41
1:C:257:VAL:C	1:C:258:LEU:HD22	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:ASN:OD1	1:G:53:SER:N	2.53	0.41
1:G:257:VAL:C	1:G:258:LEU:HD22	2.45	0.41
1:H:235:ARG:NH2	1:H:253:LYS:NZ	2.69	0.41
1:I:52:ASN:OD1	1:I:53:SER:N	2.53	0.41
1:I:90:TYR:CD2	1:I:93:VAL:HG21	2.55	0.41
1:K:170:ASN:ND2	1:K:170:ASN:C	2.79	0.41
1:A:235:ARG:HA	1:A:235:ARG:HD3	1.80	0.41
1:A:244:PHE:CZ	1:J:285:GLY:HA3	2.55	0.41
1:G:104:VAL:HG13	1:G:156:GLN:HB2	2.03	0.41
1:G:235:ARG:NE	1:G:253:LYS:HG2	2.36	0.41
1:I:284:GLU:CD	1:I:284:GLU:H	2.28	0.41
1:A:100:ARG:HH21	1:C:71:GLU:CG	2.32	0.41
1:A:179:SER:HB2	1:A:188:VAL:HG22	2.03	0.41
1:B:235:ARG:NE	1:B:253:LYS:HG2	2.35	0.41
1:D:51:ILE:CG2	1:F:303:PHE:HB3	2.50	0.41
1:D:253:LYS:HD2	1:D:254:THR:N	2.36	0.41
1:E:257:VAL:C	1:E:258:LEU:HD22	2.46	0.41
1:F:105:VAL:O	1:F:105:VAL:CG1	2.69	0.41
1:I:115:LEU:HD13	1:I:296:GLU:HG3	2.03	0.41
1:J:31:SER:CA	1:J:329:ASP:HB2	2.40	0.41
1:J:51:ILE:HG21	1:L:303:PHE:HB3	2.03	0.41
1:J:258:LEU:N	1:J:258:LEU:HD22	2.36	0.41
1:J:340:PHE:HB2	1:K:11:VAL:HG21	2.03	0.41
1:L:235:ARG:NE	1:L:253:LYS:HG2	2.35	0.41
1:A:235:ARG:NE	1:A:253:LYS:HG2	2.36	0.41
1:B:90:TYR:CD2	1:B:93:VAL:HG21	2.55	0.41
1:B:115:LEU:HD13	1:B:296:GLU:HG3	2.02	0.41
1:B:253:LYS:HD2	1:B:253:LYS:C	2.46	0.41
1:B:257:VAL:C	1:B:258:LEU:HD22	2.46	0.41
1:B:284:GLU:CD	1:B:284:GLU:H	2.29	0.41
1:B:309:THR:HG22	1:B:336:ILE:CB	2.51	0.41
1:D:55:LEU:HD12	1:D:55:LEU:HA	1.90	0.41
1:D:174:VAL:HG12	1:D:175:GLY:H	1.84	0.41
1:D:174:VAL:CG1	1:D:175:GLY:H	2.33	0.41
1:D:284:GLU:CD	1:D:284:GLU:H	2.29	0.41
1:F:286:ILE:HG23	1:F:323:LYS:HB3	2.02	0.41
1:G:143:ASN:CA	1:G:148:VAL:O	2.69	0.41
1:G:170:ASN:ND2	1:G:170:ASN:C	2.79	0.41
1:H:24:SER:H	1:H:35:ASN:ND2	2.19	0.41
1:I:115:LEU:HD21	1:I:274:ALA:HB2	2.02	0.41
1:I:136:VAL:CG1	1:I:158:LEU:CD1	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:150:GLY:O	1:J:180:TYR:HA	2.20	0.41
1:J:170:ASN:C	1:J:170:ASN:ND2	2.78	0.41
1:K:313:TYR:HD1	1:K:332:VAL:CG2	2.18	0.41
1:L:309:THR:HG22	1:L:336:ILE:CB	2.51	0.41
1:E:124:TYR:O	1:E:131:GLY:HA3	2.21	0.41
1:E:174:VAL:CG1	1:E:175:GLY:H	2.35	0.41
1:F:163:ARG:HD2	1:F:168:ARG:O	2.21	0.41
1:H:54:ASP:HB3	1:H:91:ALA:HB2	2.02	0.41
1:I:54:ASP:HB3	1:I:91:ALA:HB2	2.02	0.41
1:J:163:ARG:HD2	1:J:168:ARG:O	2.21	0.41
1:K:284:GLU:CD	1:K:284:GLU:H	2.29	0.41
1:L:64:ASN:O	1:L:79:ASN:HA	2.21	0.41
1:L:115:LEU:HD21	1:L:274:ALA:HB2	2.03	0.41
1:L:242:ASN:C	1:L:242:ASN:OD1	2.62	0.41
1:A:253:LYS:HD2	1:A:254:THR:N	2.36	0.40
1:F:231:TYR:HD1	1:F:257:VAL:HG22	1.86	0.40
1:G:71:GLU:CB	1:H:80:LYS:HD2	2.25	0.40
1:G:253:LYS:HD2	1:G:253:LYS:C	2.45	0.40
1:I:105:VAL:O	1:I:105:VAL:CG1	2.68	0.40
1:I:124:TYR:O	1:I:131:GLY:HA3	2.21	0.40
1:B:105:VAL:O	1:B:105:VAL:CG1	2.68	0.40
1:D:111:TYR:OH	1:D:188:VAL:HG23	2.21	0.40
1:D:170:ASN:ND2	1:D:170:ASN:C	2.79	0.40
1:E:203:GLN:HA	1:E:204:PRO:HD3	1.86	0.40
1:E:253:LYS:HD2	1:E:253:LYS:C	2.46	0.40
1:I:265:PHE:CB	1:I:267:PHE:CE1	3.04	0.40
1:A:257:VAL:C	1:A:258:LEU:HD22	2.46	0.40
1:D:100:ARG:HH21	1:F:71:GLU:CD	2.29	0.40
1:F:170:ASN:ND2	1:F:170:ASN:C	2.79	0.40
1:G:265:PHE:CB	1:G:267:PHE:CE1	3.04	0.40
1:H:136:VAL:CG1	1:H:158:LEU:CD1	2.99	0.40
1:I:231:TYR:HD1	1:I:257:VAL:HG22	1.86	0.40
1:I:253:LYS:HD2	1:I:253:LYS:C	2.46	0.40
1:J:180:TYR:CE2	1:J:182:TYR:HB2	2.56	0.40
1:A:115:LEU:N	1:A:115:LEU:HD23	2.36	0.40
1:A:340:PHE:CB	1:B:11:VAL:HG21	2.52	0.40
1:D:12:ASP:O	1:D:45:PHE:HA	2.22	0.40
1:D:115:LEU:HD21	1:D:274:ALA:HB2	2.04	0.40
1:F:64:ASN:O	1:F:79:ASN:HA	2.22	0.40
1:G:136:VAL:CG1	1:G:158:LEU:CD1	3.00	0.40
1:J:51:ILE:HD13	1:L:303:PHE:CG	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:265:PHE:CB	1:K:267:PHE:CE1	3.03	0.40
1:K:309:THR:HG22	1:K:336:ILE:CB	2.51	0.40
1:A:3:ILE:HG21	1:B:3:ILE:HD12	2.03	0.40
1:A:12:ASP:O	1:A:45:PHE:HA	2.21	0.40
1:B:180:TYR:CE2	1:B:182:TYR:HB2	2.56	0.40
1:C:12:ASP:O	1:C:45:PHE:HA	2.21	0.40
1:C:309:THR:HG22	1:C:336:ILE:CB	2.52	0.40
1:D:235:ARG:HD3	1:D:235:ARG:HA	1.79	0.40
1:F:12:ASP:O	1:F:45:PHE:HA	2.20	0.40
1:F:191:TYR:CD1	1:F:214:TRP:HB3	2.49	0.40
1:G:309:THR:HG22	1:G:336:ILE:CB	2.51	0.40
1:J:340:PHE:CB	1:K:11:VAL:HG21	2.52	0.40
1:K:111:TYR:OH	1:K:188:VAL:HG23	2.17	0.40
1:L:115:LEU:HD13	1:L:296:GLU:HG3	2.03	0.40
1:L:126:ASP:HA	1:L:133:VAL:HG12	2.04	0.40
1:L:143:ASN:CA	1:L:148:VAL:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	36	67
1	B	338/340 (99%)	312 (92%)	25 (7%)	1 (0%)	36	67
1	C	338/340 (99%)	311 (92%)	25 (7%)	2 (1%)	21	54
1	D	338/340 (99%)	312 (92%)	25 (7%)	1 (0%)	36	67
1	E	338/340 (99%)	312 (92%)	25 (7%)	1 (0%)	36	67
1	F	338/340 (99%)	311 (92%)	25 (7%)	2 (1%)	21	54
1	G	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	36	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	36	67
1	I	338/340 (99%)	311 (92%)	25 (7%)	2 (1%)	21	54
1	J	338/340 (99%)	310 (92%)	27 (8%)	1 (0%)	36	67
1	K	338/340 (99%)	313 (93%)	24 (7%)	1 (0%)	36	67
1	L	338/340 (99%)	311 (92%)	26 (8%)	1 (0%)	36	67
All	All	4056/4080 (99%)	3736 (92%)	305 (8%)	15 (0%)	30	62

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	ALA
1	I	222	ALA
1	L	222	ALA
1	A	222	ALA
1	B	222	ALA
1	C	222	ALA
1	E	222	ALA
1	F	222	ALA
1	G	222	ALA
1	H	222	ALA
1	J	222	ALA
1	K	222	ALA
1	C	284	GLU
1	F	284	GLU
1	I	284	GLU

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	263/263 (100%)	255 (97%)	8 (3%)	36	57
1	B	263/263 (100%)	255 (97%)	8 (3%)	36	57
1	C	263/263 (100%)	254 (97%)	9 (3%)	32	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	263/263 (100%)	255 (97%)	8 (3%)	36	57
1	E	263/263 (100%)	255 (97%)	8 (3%)	36	57
1	F	263/263 (100%)	256 (97%)	7 (3%)	39	59
1	G	263/263 (100%)	256 (97%)	7 (3%)	39	59
1	H	263/263 (100%)	255 (97%)	8 (3%)	36	57
1	I	263/263 (100%)	256 (97%)	7 (3%)	39	59
1	J	263/263 (100%)	256 (97%)	7 (3%)	39	59
1	K	263/263 (100%)	255 (97%)	8 (3%)	36	57
1	L	263/263 (100%)	255 (97%)	8 (3%)	36	57
All	All	3156/3156 (100%)	3063 (97%)	93 (3%)	37	58

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	170	ASN
1	A	218	LEU
1	A	253	LYS
1	A	279	LYS
1	A	284	GLU
1	A	286	ILE
1	A	289	VAL
1	B	104	VAL
1	B	170	ASN
1	B	218	LEU
1	B	253	LYS
1	B	279	LYS
1	B	284	GLU
1	B	286	ILE
1	B	289	VAL
1	C	27	ASN
1	C	104	VAL
1	C	170	ASN
1	C	218	LEU
1	C	253	LYS
1	C	279	LYS
1	C	284	GLU
1	C	286	ILE
1	C	289	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	104	VAL
1	D	170	ASN
1	D	218	LEU
1	D	253	LYS
1	D	279	LYS
1	D	284	GLU
1	D	286	ILE
1	D	289	VAL
1	E	104	VAL
1	E	170	ASN
1	E	218	LEU
1	E	253	LYS
1	E	279	LYS
1	E	284	GLU
1	E	286	ILE
1	E	289	VAL
1	F	104	VAL
1	F	218	LEU
1	F	253	LYS
1	F	279	LYS
1	F	284	GLU
1	F	286	ILE
1	F	289	VAL
1	G	104	VAL
1	G	218	LEU
1	G	253	LYS
1	G	279	LYS
1	G	284	GLU
1	G	286	ILE
1	G	289	VAL
1	H	104	VAL
1	H	170	ASN
1	H	218	LEU
1	H	253	LYS
1	H	279	LYS
1	H	284	GLU
1	H	286	ILE
1	H	289	VAL
1	I	104	VAL
1	I	218	LEU
1	I	253	LYS
1	I	279	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	284	GLU
1	I	286	ILE
1	I	289	VAL
1	J	104	VAL
1	J	218	LEU
1	J	253	LYS
1	J	279	LYS
1	J	284	GLU
1	J	286	ILE
1	J	289	VAL
1	K	104	VAL
1	K	170	ASN
1	K	218	LEU
1	K	253	LYS
1	K	279	LYS
1	K	284	GLU
1	K	286	ILE
1	K	289	VAL
1	L	104	VAL
1	L	170	ASN
1	L	218	LEU
1	L	253	LYS
1	L	279	LYS
1	L	284	GLU
1	L	286	ILE
1	L	289	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	35	ASN
1	A	60	GLN
1	A	203	GLN
1	A	223	ASN
1	A	246	ASN
1	A	255	GLN
1	B	9	ASN
1	B	35	ASN
1	B	60	GLN
1	B	203	GLN
1	B	223	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	246	ASN
1	B	255	GLN
1	C	35	ASN
1	C	60	GLN
1	C	203	GLN
1	C	223	ASN
1	C	246	ASN
1	C	255	GLN
1	D	9	ASN
1	D	35	ASN
1	D	60	GLN
1	D	223	ASN
1	D	246	ASN
1	D	255	GLN
1	E	9	ASN
1	E	35	ASN
1	E	60	GLN
1	E	203	GLN
1	E	223	ASN
1	E	246	ASN
1	E	255	GLN
1	F	35	ASN
1	F	60	GLN
1	F	203	GLN
1	F	223	ASN
1	F	246	ASN
1	F	255	GLN
1	G	35	ASN
1	G	60	GLN
1	G	203	GLN
1	G	223	ASN
1	G	246	ASN
1	G	255	GLN
1	H	9	ASN
1	H	35	ASN
1	H	60	GLN
1	H	203	GLN
1	H	223	ASN
1	H	246	ASN
1	H	255	GLN
1	I	9	ASN
1	I	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	35	ASN
1	I	60	GLN
1	I	203	GLN
1	I	223	ASN
1	I	246	ASN
1	I	255	GLN
1	J	35	ASN
1	J	60	GLN
1	J	223	ASN
1	J	246	ASN
1	J	255	GLN
1	K	27	ASN
1	K	35	ASN
1	K	60	GLN
1	K	223	ASN
1	K	246	ASN
1	K	255	GLN
1	L	35	ASN
1	L	60	GLN
1	L	203	GLN
1	L	223	ASN
1	L	246	ASN
1	L	255	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	339/340 (99%)	0.79	21 (6%)	26	22	76, 78, 80, 81	0
1	B	340/340 (100%)	0.75	23 (6%)	23	20	76, 78, 80, 82	0
1	C	340/340 (100%)	0.75	21 (6%)	26	22	76, 78, 80, 81	0
1	D	339/340 (99%)	0.85	31 (9%)	15	16	76, 78, 80, 81	0
1	E	340/340 (100%)	0.70	14 (4%)	41	30	76, 78, 80, 81	0
1	F	340/340 (100%)	0.73	21 (6%)	26	22	76, 78, 80, 82	0
1	G	339/340 (99%)	0.78	19 (5%)	30	23	76, 78, 80, 81	0
1	H	340/340 (100%)	0.80	20 (5%)	28	23	76, 78, 80, 82	0
1	I	340/340 (100%)	0.87	28 (8%)	17	17	76, 78, 80, 82	0
1	J	339/340 (99%)	0.73	19 (5%)	30	23	76, 78, 80, 81	0
1	K	340/340 (100%)	0.76	24 (7%)	22	19	76, 78, 80, 82	0
1	L	340/340 (100%)	0.86	29 (8%)	16	17	76, 78, 80, 82	0
All	All	4076/4080 (99%)	0.78	270 (6%)	24	21	76, 78, 80, 82	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLY	5.7
1	B	157	TYR	4.6
1	J	157	TYR	4.6
1	G	321	ASP	4.5
1	E	157	TYR	4.5
1	F	101	ASN	4.5
1	H	157	TYR	4.4
1	F	157	TYR	4.4
1	I	59	GLY	4.3
1	A	157	TYR	4.1
1	K	157	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	221	ASP	4.1
1	L	319	ASP	4.0
1	I	74	ASP	4.0
1	H	8	GLY	4.0
1	A	7	ASP	3.9
1	D	110	GLY	3.9
1	J	15	GLY	3.9
1	I	157	TYR	3.8
1	F	8	GLY	3.8
1	L	321	ASP	3.7
1	A	321	ASP	3.6
1	G	107	ASP	3.6
1	C	157	TYR	3.6
1	K	319	ASP	3.6
1	H	321	ASP	3.6
1	G	106	TYR	3.5
1	B	321	ASP	3.5
1	G	7	ASP	3.5
1	B	319	ASP	3.5
1	G	201	GLU	3.5
1	H	244	PHE	3.4
1	D	243	LYS	3.4
1	L	229	ALA	3.4
1	B	101	ASN	3.4
1	G	157	TYR	3.4
1	J	26	GLY	3.4
1	E	209	LYS	3.4
1	K	134	GLY	3.3
1	G	164	ASP	3.3
1	D	126	ASP	3.3
1	C	201	GLU	3.3
1	D	157	TYR	3.3
1	E	201	GLU	3.3
1	C	33	GLY	3.3
1	G	74	ASP	3.2
1	I	99	GLY	3.2
1	J	28	GLY	3.2
1	H	60	GLN	3.2
1	C	164	ASP	3.2
1	K	189	GLY	3.2
1	G	183	GLU	3.2
1	F	29	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	306	ASN	3.1
1	L	157	TYR	3.1
1	L	201	GLU	3.1
1	B	102	TYR	3.1
1	H	319	ASP	3.1
1	G	140	ARG	3.1
1	D	221	ASP	3.1
1	B	106	TYR	3.0
1	K	244	PHE	3.0
1	J	290	ASP	3.0
1	K	164	ASP	3.0
1	L	288	ASP	3.0
1	C	29	GLU	3.0
1	J	164	ASP	3.0
1	C	286	ILE	3.0
1	E	102	TYR	3.0
1	F	319	ASP	3.0
1	D	319	ASP	3.0
1	J	340	PHE	2.9
1	A	230	ASN	2.9
1	L	230	ASN	2.9
1	H	122	THR	2.9
1	F	220	TYR	2.9
1	I	250	PHE	2.9
1	H	59	GLY	2.9
1	H	67	GLY	2.9
1	B	69	ASN	2.9
1	K	317	GLN	2.9
1	J	77	THR	2.9
1	K	1	ALA	2.9
1	B	288	ASP	2.9
1	H	7	ASP	2.9
1	J	89	LYS	2.9
1	K	67	GLY	2.9
1	G	59	GLY	2.8
1	B	67	GLY	2.8
1	C	321	ASP	2.8
1	D	285	GLY	2.8
1	K	101	ASN	2.8
1	D	46	LYS	2.8
1	D	162	GLU	2.8
1	J	67	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	135	GLY	2.8
1	A	53	SER	2.8
1	E	29	GLU	2.7
1	L	286	ILE	2.7
1	A	305	LYS	2.7
1	E	275	TYR	2.7
1	L	287	GLY	2.7
1	L	253	LYS	2.7
1	L	27	ASN	2.7
1	L	93	VAL	2.7
1	K	149	ASP	2.7
1	I	48	GLU	2.7
1	B	25	LYS	2.7
1	A	28	GLY	2.6
1	C	54	ASP	2.6
1	D	249	GLY	2.6
1	D	180	TYR	2.6
1	G	241	THR	2.6
1	A	162	GLU	2.6
1	G	29	GLU	2.6
1	C	1	ALA	2.6
1	B	290	ASP	2.6
1	C	319	ASP	2.6
1	E	290	ASP	2.6
1	L	136	VAL	2.6
1	D	106	TYR	2.6
1	D	244	PHE	2.6
1	H	1	ALA	2.6
1	I	134	GLY	2.6
1	D	77	THR	2.6
1	D	108	ALA	2.6
1	I	10	LYS	2.5
1	I	47	GLY	2.5
1	C	48	GLU	2.5
1	C	218	LEU	2.5
1	H	29	GLU	2.5
1	C	7	ASP	2.5
1	A	108	ALA	2.5
1	D	215	ALA	2.5
1	D	321	ASP	2.5
1	F	273	ILE	2.5
1	I	98	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	182	TYR	2.5
1	B	10	LYS	2.5
1	F	73	ALA	2.5
1	L	336	ILE	2.5
1	H	2	GLU	2.4
1	I	29	GLU	2.4
1	J	319	ASP	2.4
1	D	201	GLU	2.4
1	K	89	LYS	2.4
1	D	164	ASP	2.4
1	H	37	ASP	2.4
1	I	102	TYR	2.4
1	K	314	ILE	2.4
1	L	7	ASP	2.4
1	H	134	GLY	2.4
1	K	340	PHE	2.4
1	L	218	LEU	2.4
1	E	106	TYR	2.4
1	H	17	ALA	2.4
1	J	201	GLU	2.4
1	B	33	GLY	2.3
1	C	279	LYS	2.3
1	A	229	ALA	2.3
1	H	50	GLN	2.3
1	F	223	ASN	2.3
1	G	101	ASN	2.3
1	D	102	TYR	2.3
1	H	229	ALA	2.3
1	L	280	ALA	2.3
1	A	164	ASP	2.3
1	F	7	ASP	2.3
1	C	323	LYS	2.3
1	A	17	ALA	2.3
1	F	244	PHE	2.3
1	K	321	ASP	2.3
1	K	243	LYS	2.3
1	K	323	LYS	2.3
1	C	188	VAL	2.3
1	D	26	GLY	2.3
1	I	135	GLY	2.3
1	I	321	ASP	2.3
1	A	304	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	269	LEU	2.3
1	A	201	GLU	2.3
1	L	29	GLU	2.3
1	C	189	GLY	2.3
1	E	89	LYS	2.3
1	I	67	GLY	2.3
1	K	36	GLY	2.3
1	A	306	ASN	2.2
1	I	60	GLN	2.2
1	B	7	ASP	2.2
1	H	216	THR	2.2
1	C	306	ASN	2.2
1	F	21	HIS	2.2
1	D	98	TYR	2.2
1	I	305	LYS	2.2
1	D	71	GLU	2.2
1	B	120	GLY	2.2
1	C	19	GLY	2.2
1	B	282	ASP	2.2
1	C	127	ASP	2.2
1	J	248	SER	2.2
1	B	132	ARG	2.2
1	D	324	LEU	2.2
1	F	77	THR	2.2
1	F	27	ASN	2.2
1	G	242	ASN	2.2
1	I	290	ASP	2.2
1	D	21	HIS	2.2
1	K	16	LYS	2.2
1	F	222	ALA	2.2
1	J	60	GLN	2.2
1	I	20	LEU	2.2
1	L	98	TYR	2.2
1	K	286	ILE	2.2
1	E	48	GLU	2.2
1	A	76	GLN	2.1
1	F	70	SER	2.1
1	L	105	VAL	2.1
1	G	28	GLY	2.1
1	I	2	GLU	2.1
1	L	48	GLU	2.1
1	A	77	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	2.1
1	A	74	ASP	2.1
1	L	290	ASP	2.1
1	L	289	VAL	2.1
1	D	340	PHE	2.1
1	B	36	GLY	2.1
1	D	28	GLY	2.1
1	E	2	GLU	2.1
1	I	162	GLU	2.1
1	J	181	GLU	2.1
1	I	77	THR	2.1
1	I	69	ASN	2.1
1	I	333	ALA	2.1
1	F	63	TYR	2.1
1	G	248	SER	2.1
1	L	255	GLN	2.1
1	B	136	VAL	2.1
1	K	21	HIS	2.1
1	G	149	ASP	2.1
1	I	8	GLY	2.1
1	J	217	GLY	2.1
1	C	117	GLU	2.1
1	I	201	GLU	2.1
1	E	187	ILE	2.1
1	D	246	ASN	2.1
1	G	69	ASN	2.1
1	L	238	THR	2.1
1	F	243	LYS	2.1
1	J	243	LYS	2.1
1	L	323	LYS	2.1
1	B	27	ASN	2.1
1	L	186	GLY	2.0
1	A	221	ASP	2.0
1	D	290	ASP	2.0
1	H	81	THR	2.0
1	J	84	ALA	2.0
1	D	36	GLY	2.0
1	K	135	GLY	2.0
1	E	25	LYS	2.0
1	J	25	LYS	2.0
1	A	29	GLU	2.0
1	L	256	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	2.0
1	B	292	VAL	2.0
1	I	136	VAL	2.0
1	F	238	THR	2.0
1	F	181	GLU	2.0
1	E	321	ASP	2.0
1	K	259	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.