



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:33 AM UTC

PDB ID : 1UF2 / pdb_00001uf2
Title : The Atomic Structure of Rice dwarf Virus (RDV)
Authors : Nakagawa, A.; Miyazaki, N.; Taka, J.; Naitow, H.; Ogawa, A.; Fujimoto, Z.; Mizuno, H.; Higashi, T.; Watanabe, Y.; Omura, T.; Cheng, R.H.; Tsukihara, T.
Deposited on : 2003-05-23
Resolution : 3.50 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

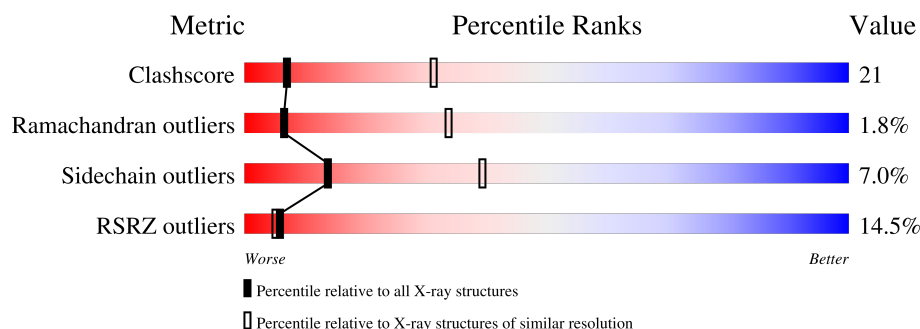
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1019	
1	B	1019	
2	C	421	
2	D	421	
2	E	421	
2	F	421	
2	G	421	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	421	5% 60% 34% 5%
2	I	421	15% 53% 39% 6%
2	J	421	17% 54% 40%
2	P	421	47% 57% 36% 5%
2	Q	421	17% 54% 40% 6%
2	R	421	7% 61% 34% 5%
2	S	421	15% 56% 36% 7%
2	T	421	2% 59% 35% 5%
3	K	506	% 98%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58130 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 Core protein P3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	967	Total	C	N	O	S	0	0	0
			7653	4885	1309	1427	32			
1	B	1019	Total	C	N	O	S	0	0	0
			8053	5138	1370	1512	33			

- Molecule 2 is a protein called Outer capsid protein P8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	414	Total	C	N	O	S	0	0	0
			3227	2060	542	608	17			
2	C	415	Total	C	N	O	S	0	0	0
			3234	2065	543	609	17			
2	D	417	Total	C	N	O	S	0	0	0
			3247	2073	545	612	17			
2	Q	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	E	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	F	415	Total	C	N	O	S	0	0	0
			3234	2065	543	609	17			
2	R	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	G	417	Total	C	N	O	S	0	0	0
			3253	2079	545	612	17			
2	H	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	S	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	I	419	Total	C	N	O	S	0	0	0
			3265	2085	547	616	17			
2	J	413	Total	C	N	O	S	0	0	0
			3221	2057	541	606	17			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	178	ALA	-	SEE REMARK 999	UNP P17379
C	178	ALA	-	SEE REMARK 999	UNP P17379
D	178	ALA	-	SEE REMARK 999	UNP P17379
Q	178	ALA	-	SEE REMARK 999	UNP P17379
E	178	ALA	-	SEE REMARK 999	UNP P17379
F	178	ALA	-	SEE REMARK 999	UNP P17379
R	178	ALA	-	SEE REMARK 999	UNP P17379
G	178	ALA	-	SEE REMARK 999	UNP P17379
H	178	ALA	-	SEE REMARK 999	UNP P17379
S	178	ALA	-	SEE REMARK 999	UNP P17379
I	178	ALA	-	SEE REMARK 999	UNP P17379
J	178	ALA	-	SEE REMARK 999	UNP P17379
T	178	ALA	-	SEE REMARK 999	UNP P17379

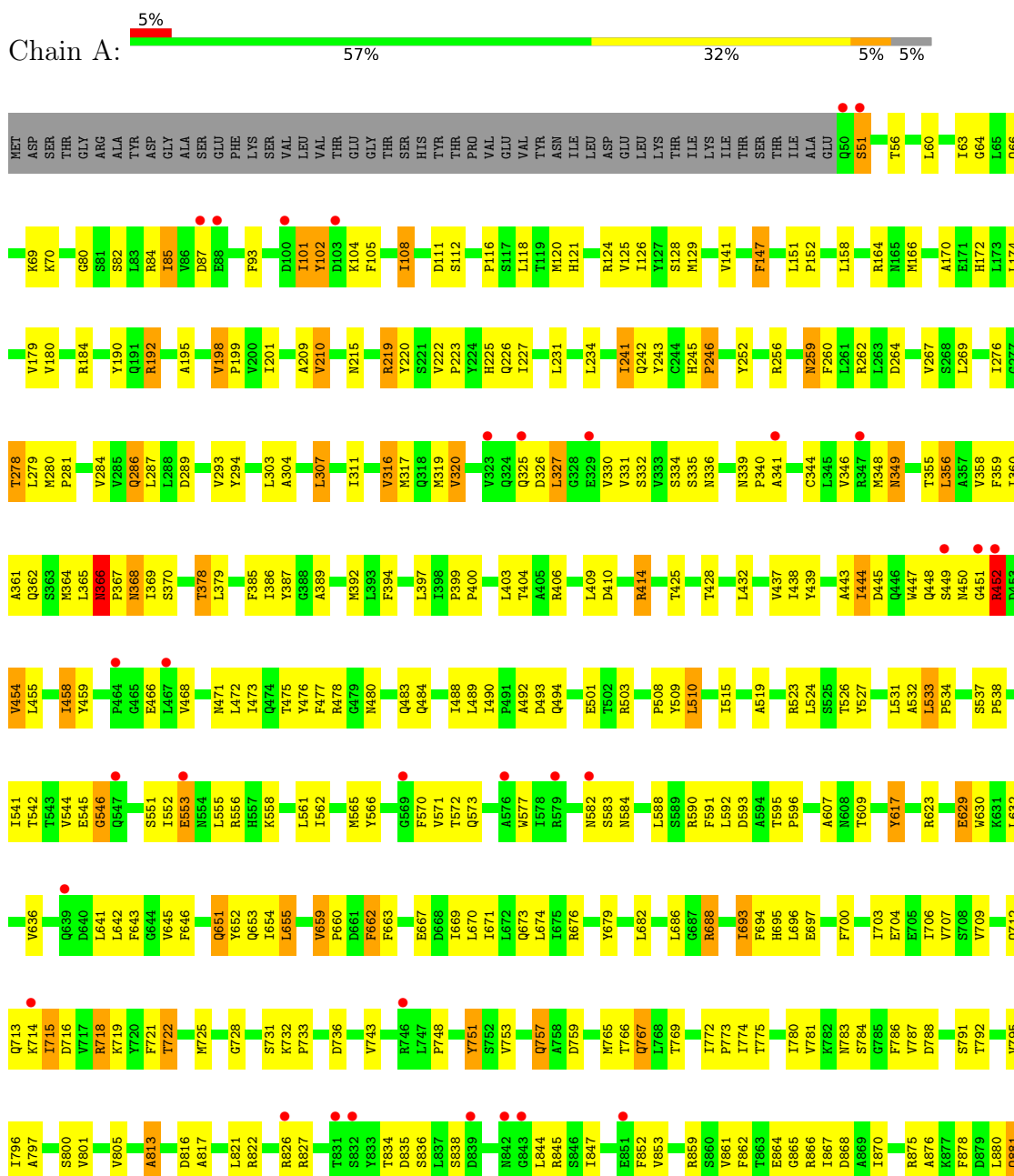
- Molecule 3 is a protein called Structural protein P7.

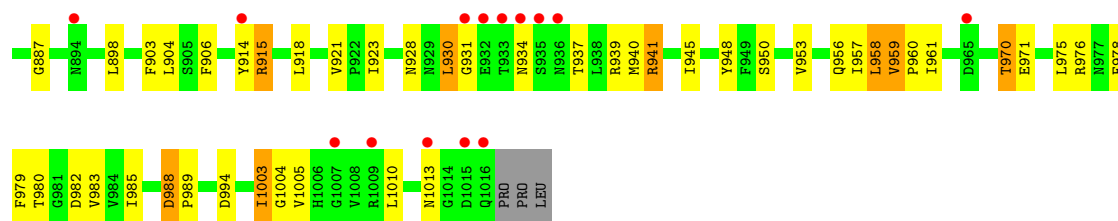
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	12	Total	C	N	O	0	0	0
			99	60	16	23			

3 Residue-property plots

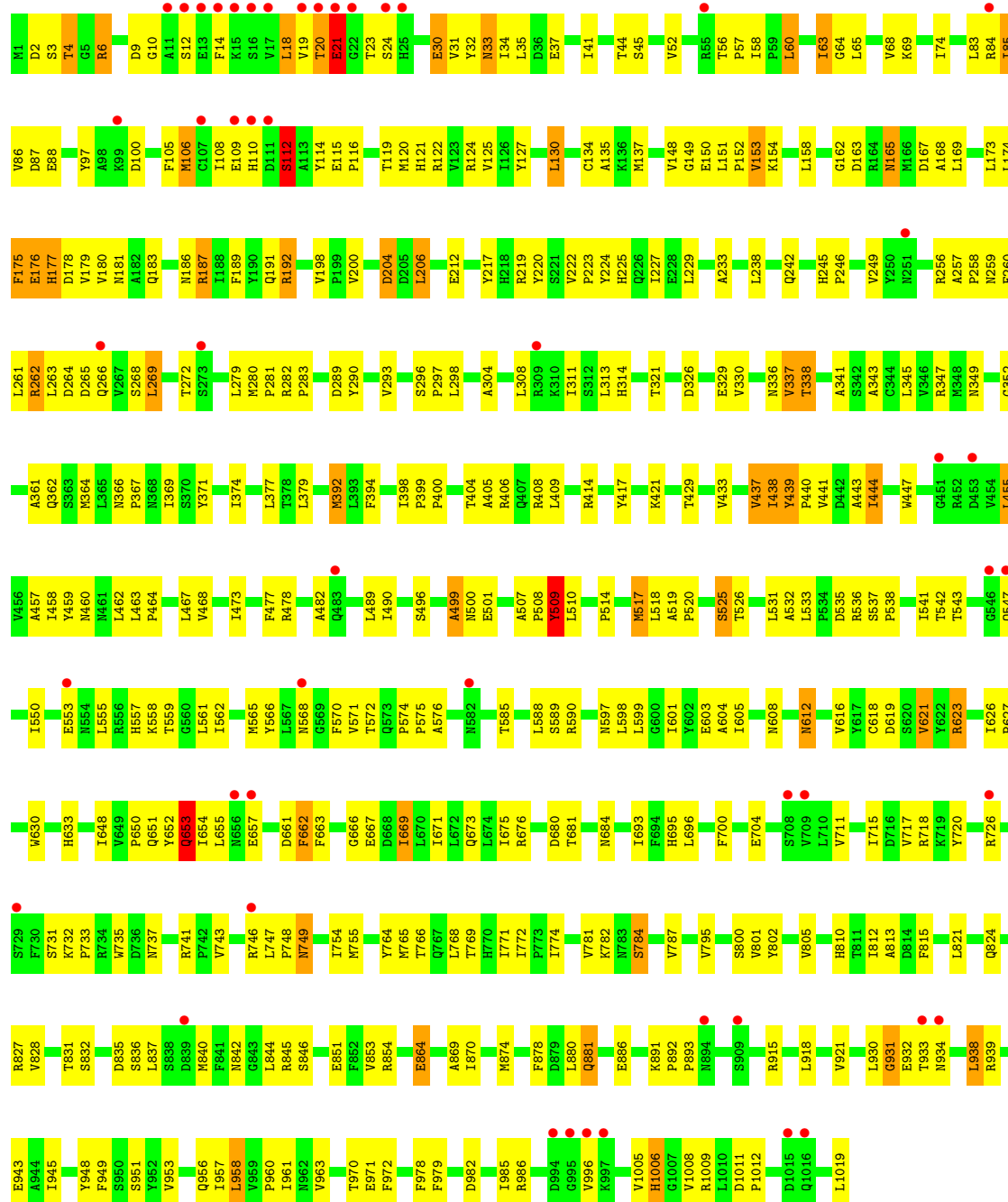
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Core protein P3

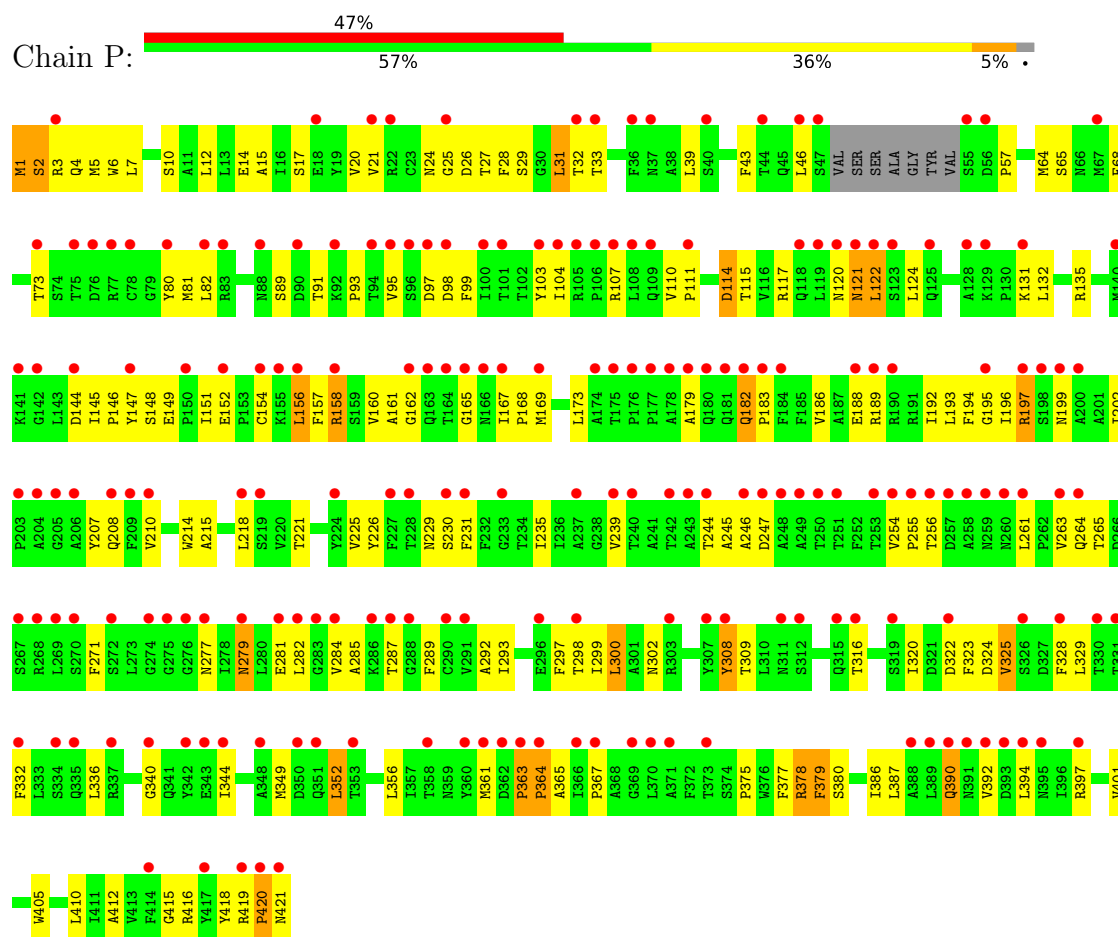




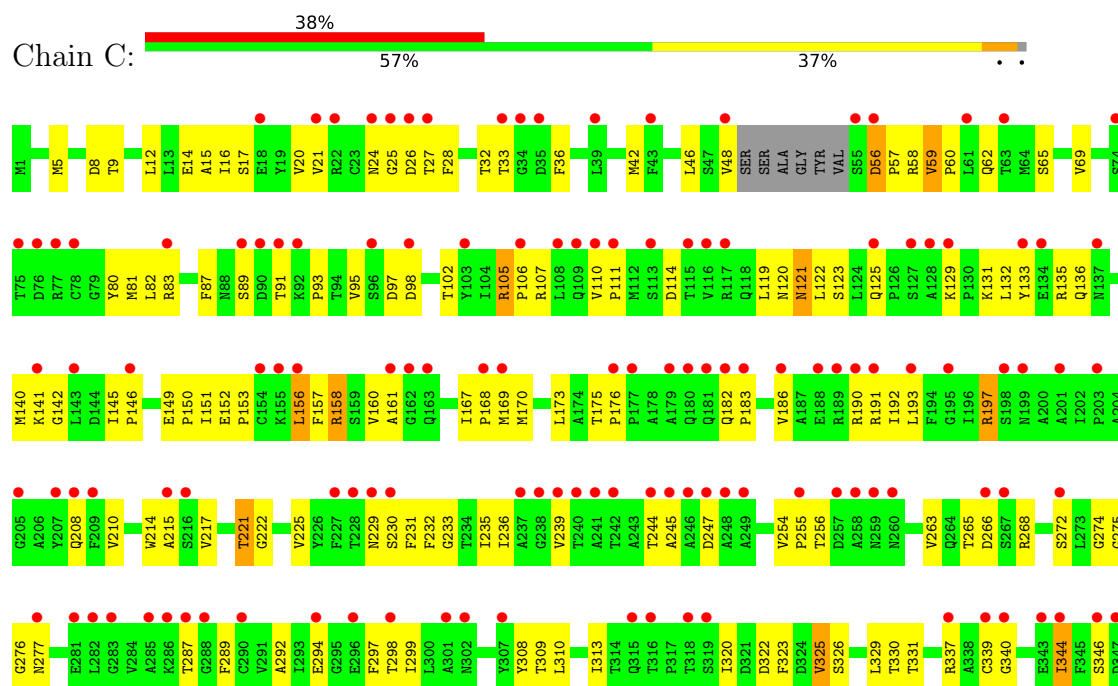
• Molecule 1: Core protein P3



- Molecule 2: Outer capsid protein P8

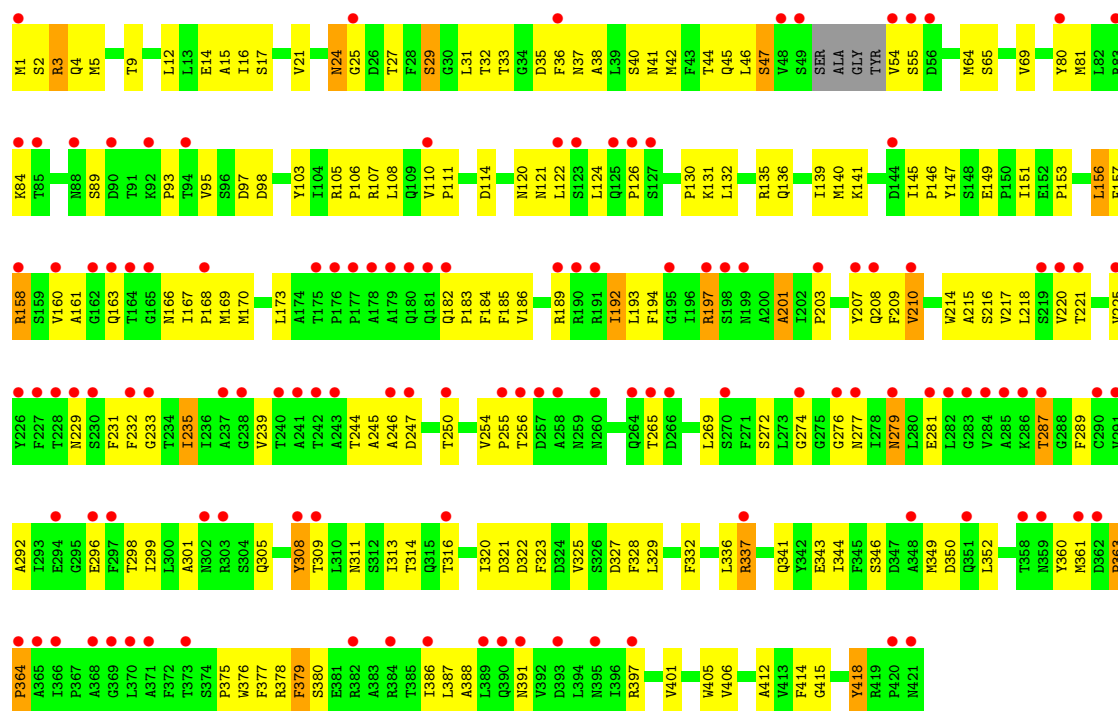


- Molecule 2: Outer capsid protein P8

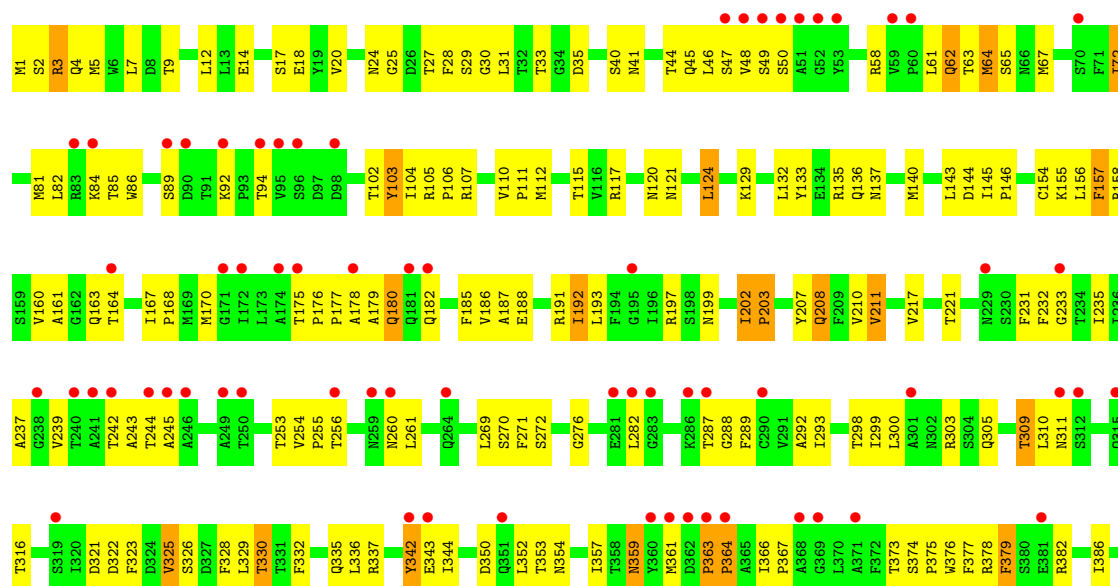




• Molecule 2: Outer capsid protein P8

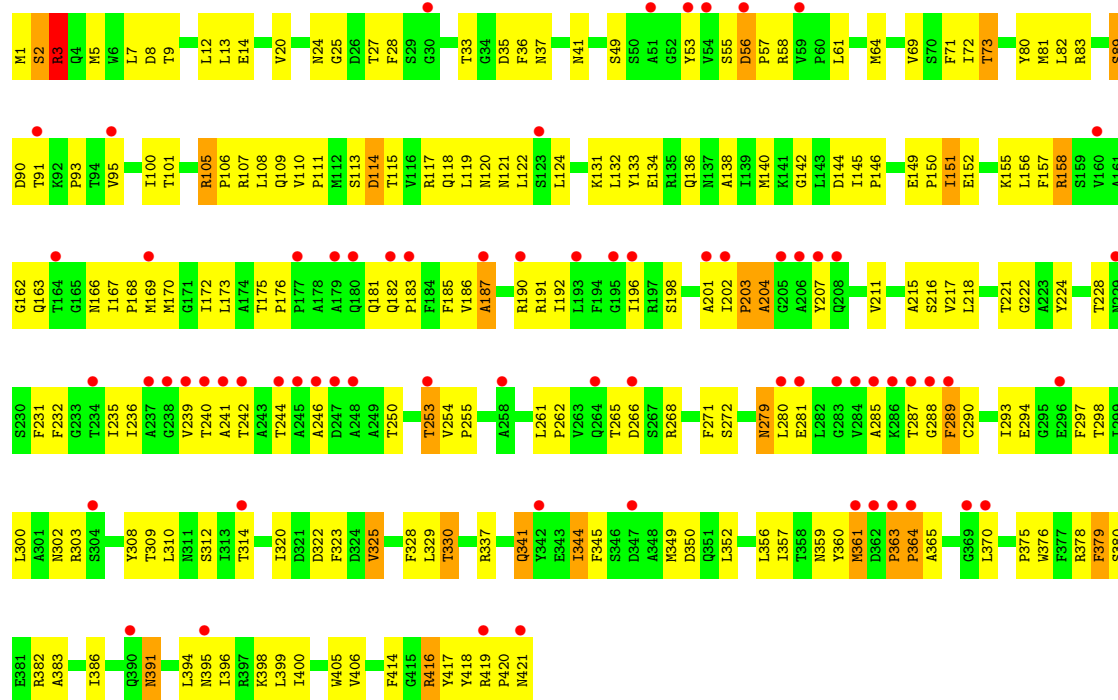


• Molecule 2: Outer capsid protein P8

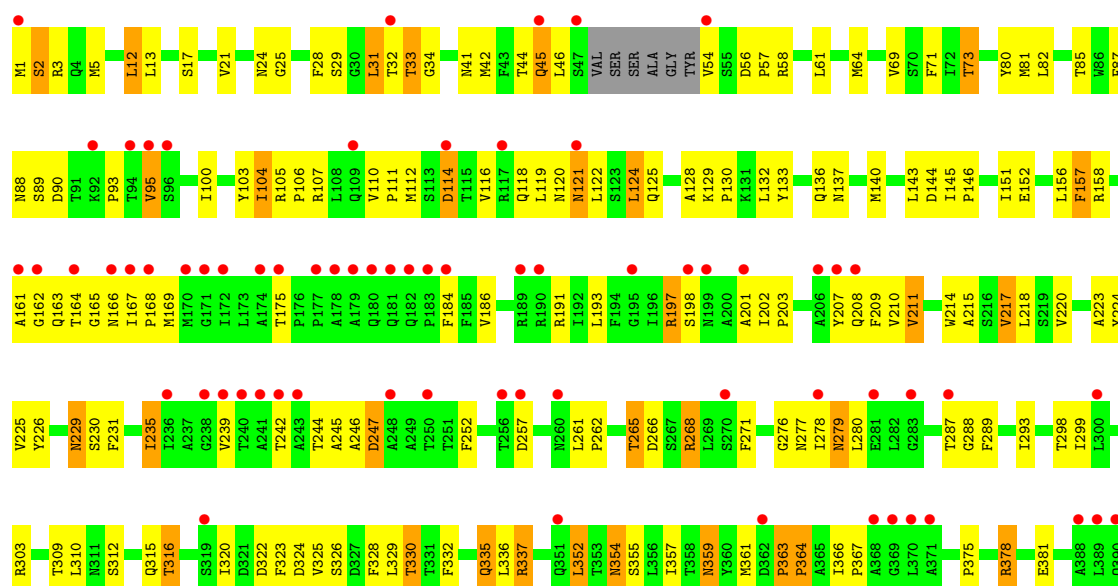




• Molecule 2: Outer capsid protein P8

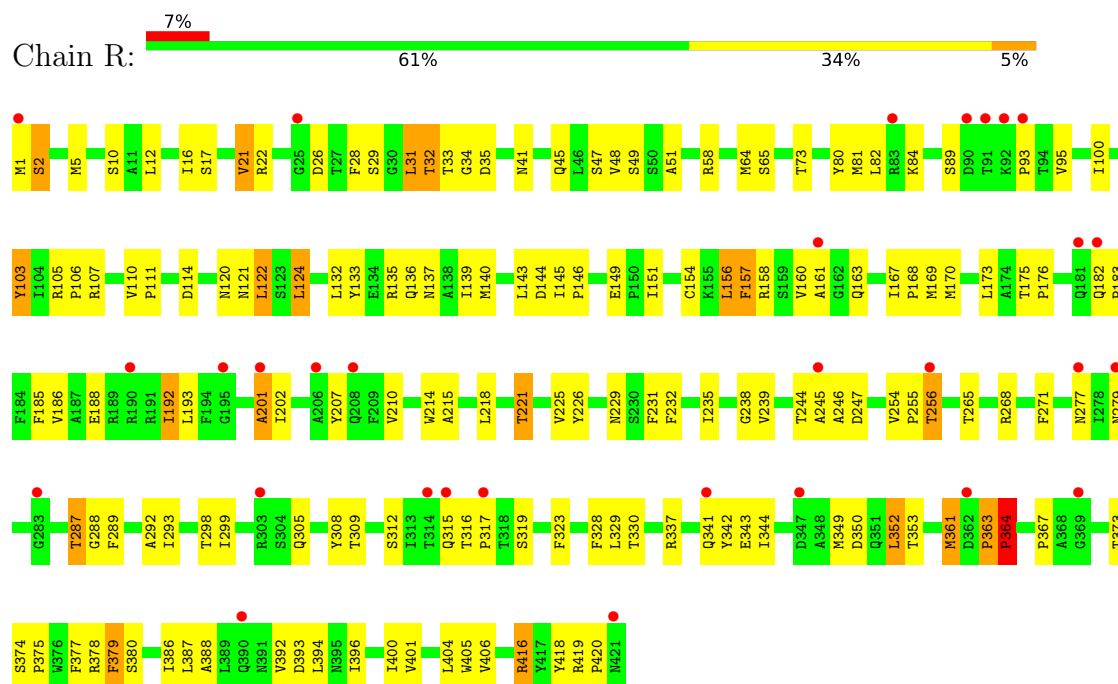


• Molecule 2: Outer capsid protein P8

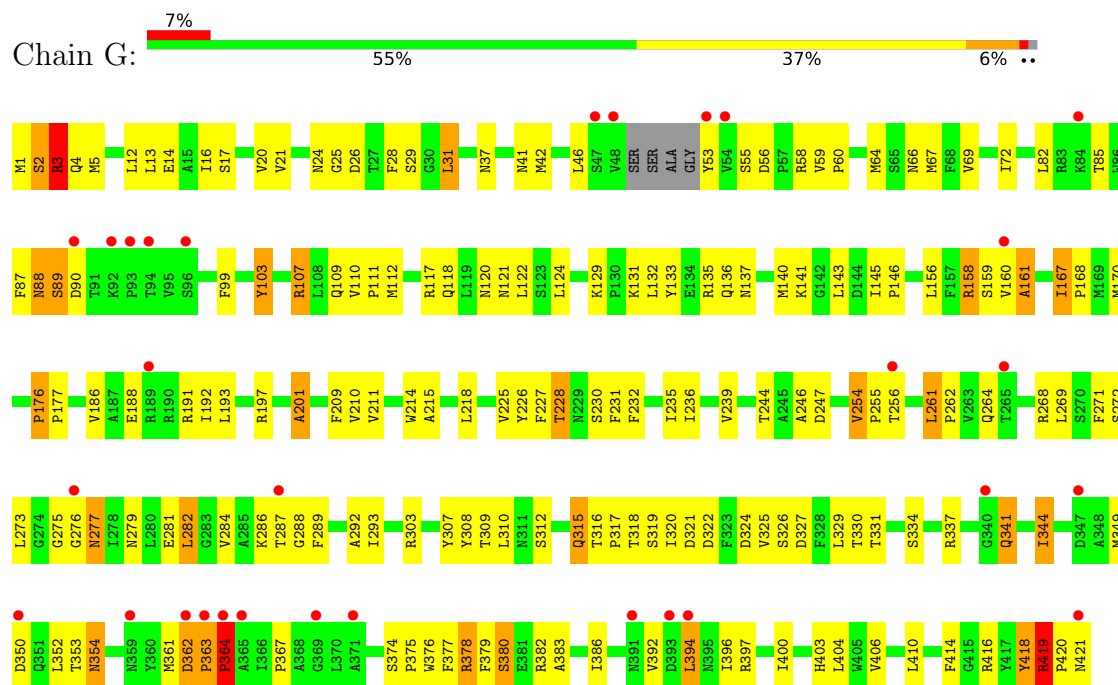




- Molecule 2: Outer capsid protein P8

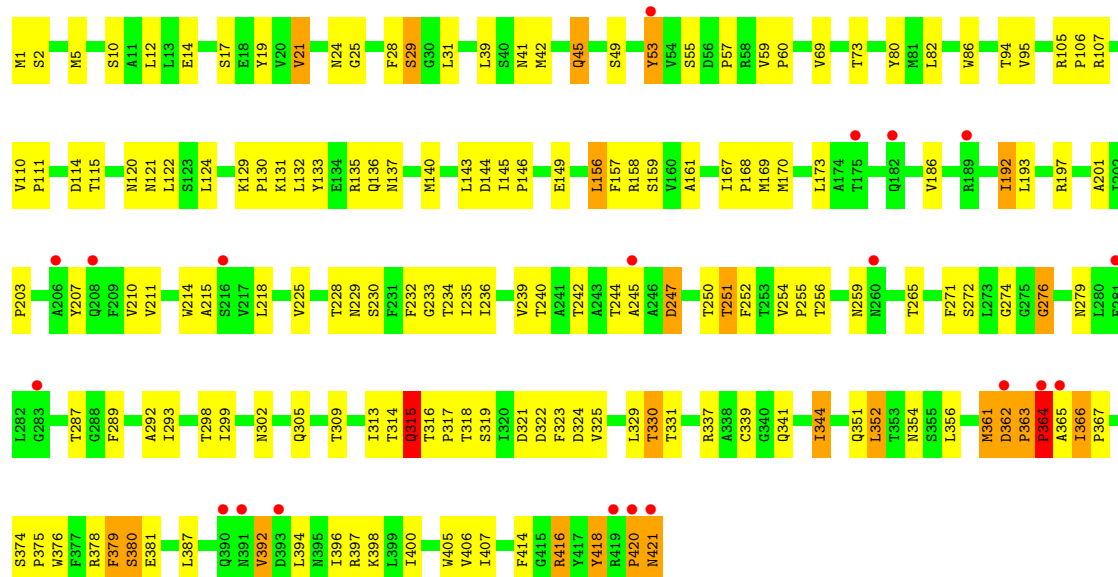


- Molecule 2: Outer capsid protein P8

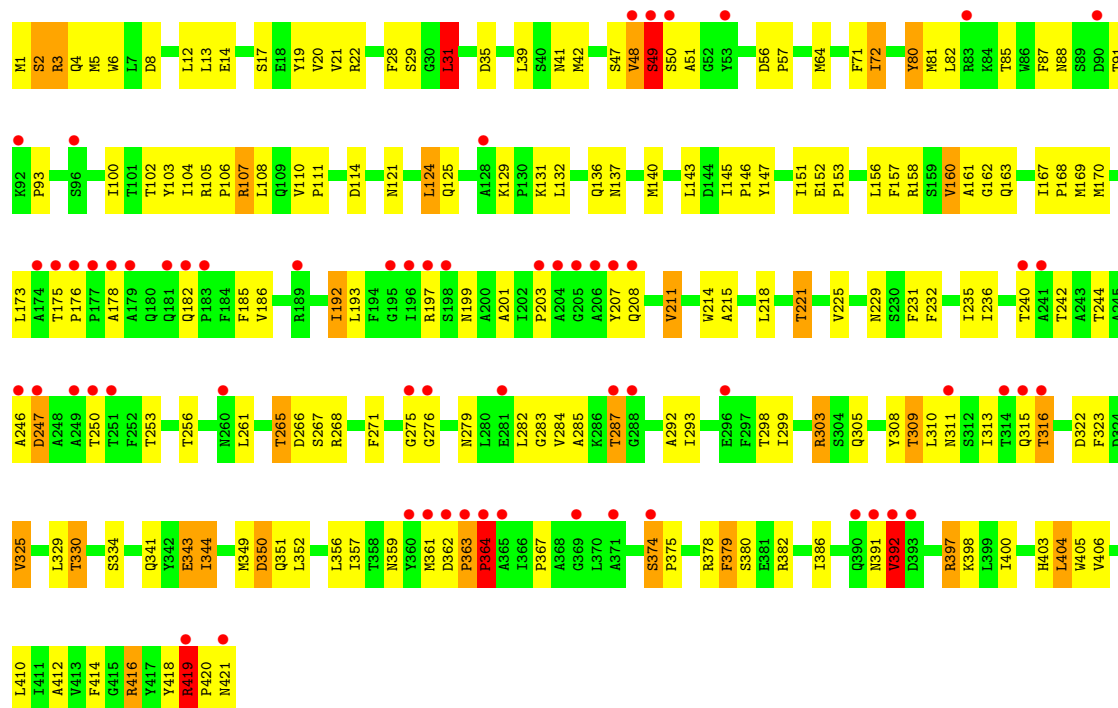


- Molecule 2: Outer capsid protein P8



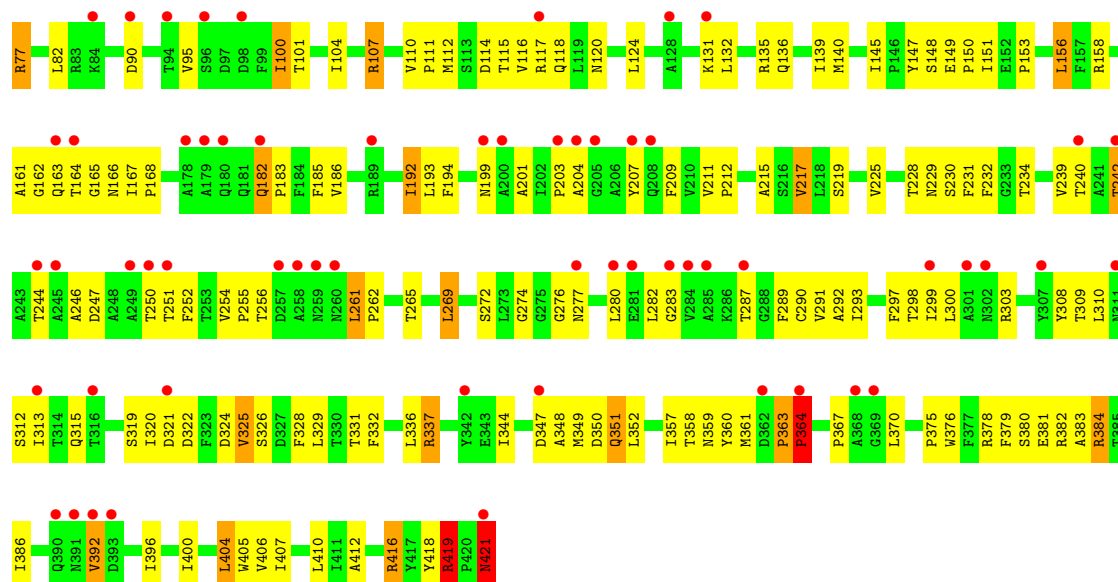


• Molecule 2: Outer capsid protein P8

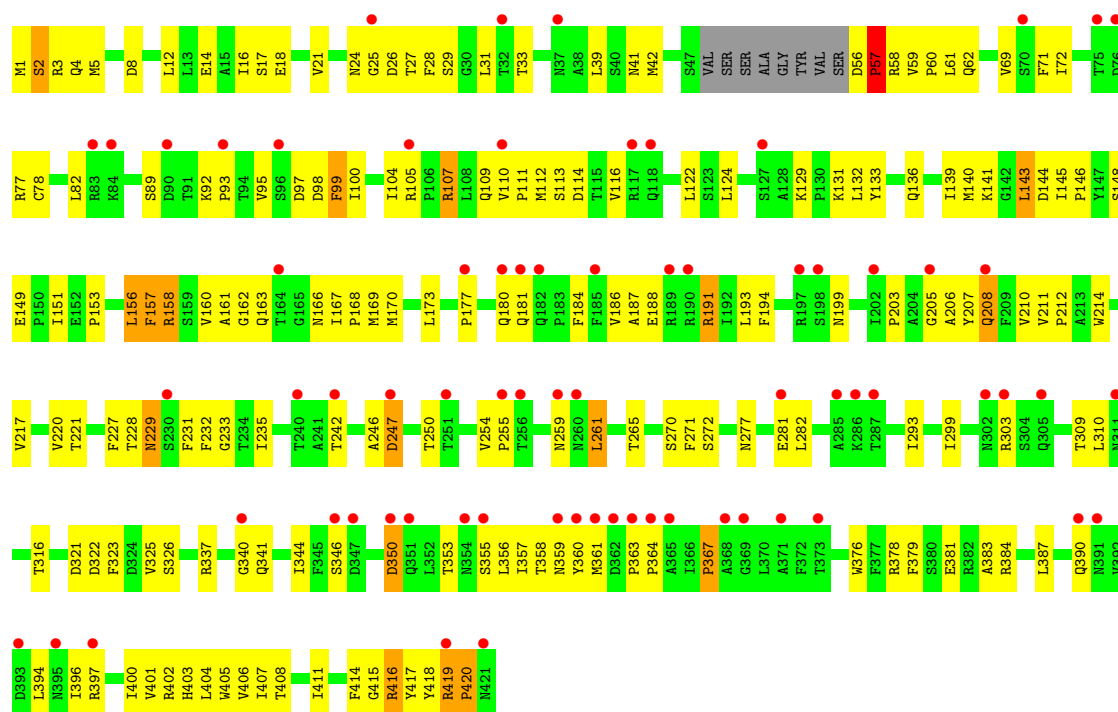


• Molecule 2: Outer capsid protein P8



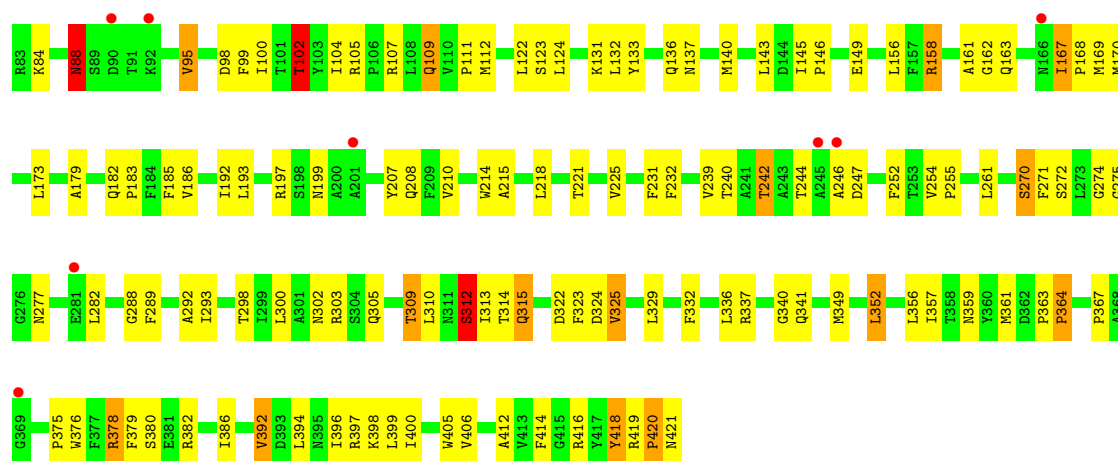


• Molecule 2: Outer capsid protein P8

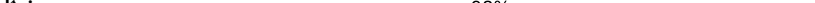


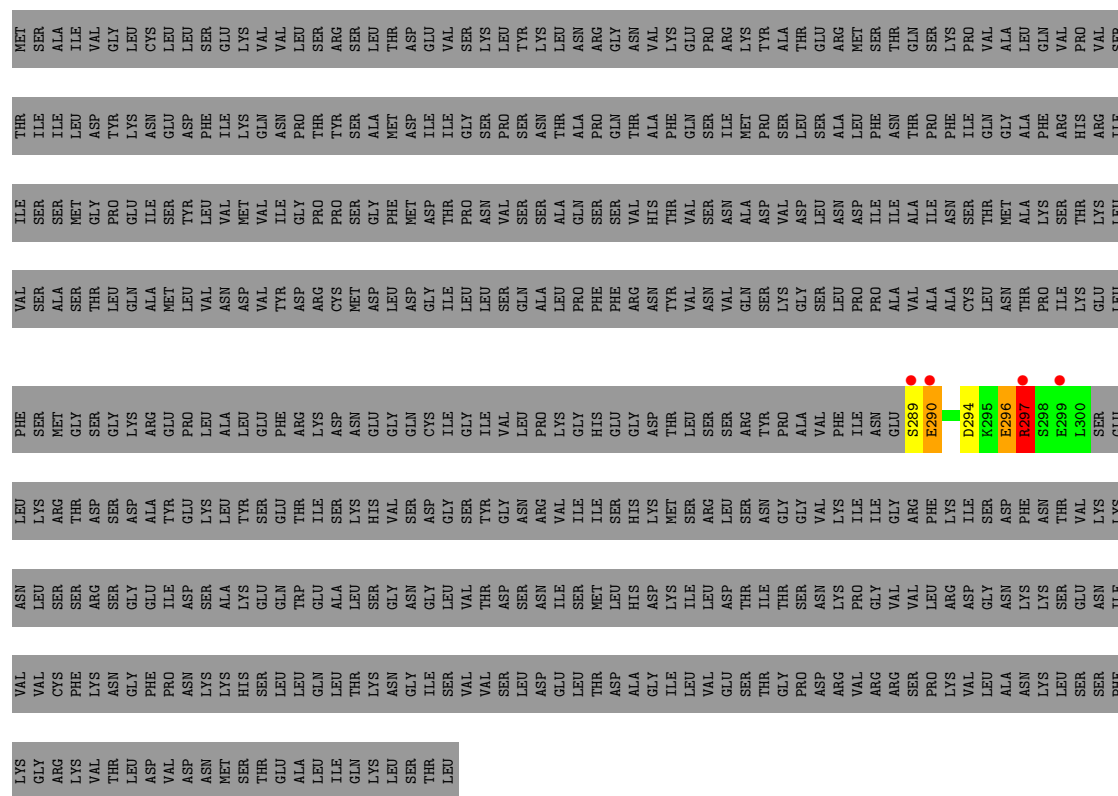
• Molecule 2: Outer capsid protein P8





- Molecule 3: Structural protein P7

Chain K:  98%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	770.00Å 795.00Å 814.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	228.74 – 3.50 228.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (228.74-3.50) 90.2 (228.74-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.49Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.303 , 0.306 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	58130	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.10% 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	0.64	0/7816	1.10	49/10641 (0.5%)
1	B	0.69	0/8224	1.10	63/11197 (0.6%)
2	C	0.49	0/3308	1.02	15/4508 (0.3%)
2	D	0.51	0/3321	1.04	19/4526 (0.4%)
2	E	0.57	0/3350	1.07	24/4567 (0.5%)
2	F	0.55	0/3308	1.09	28/4508 (0.6%)
2	G	0.61	0/3328	1.10	32/4536 (0.7%)
2	H	0.65	4/3350 (0.1%)	1.08	18/4567 (0.4%)
2	I	0.59	1/3340 (0.0%)	1.09	20/4552 (0.4%)
2	J	0.53	0/3295	1.06	16/4490 (0.4%)
2	P	0.49	0/3301	1.00	13/4498 (0.3%)
2	Q	0.57	0/3350	1.13	26/4567 (0.6%)
2	R	0.59	0/3350	1.05	16/4567 (0.4%)
2	S	0.54	0/3350	1.07	30/4567 (0.7%)
2	T	0.66	1/3350 (0.0%)	1.10	20/4567 (0.4%)
3	K	1.12	0/100	2.02	5/132 (3.8%)
All	All	0.60	6/59441 (0.0%)	1.08	394/80990 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	421	ASN	CA-CB	6.60	1.66	1.53
2	H	421	ASN	C-O	6.42	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	420	PRO	CA-C	5.44	1.58	1.52
2	I	421	ASN	CA-CB	5.32	1.64	1.53
2	T	1	MET	SD-CE	5.30	1.92	1.79
2	H	421	ASN	CB-CG	5.29	1.65	1.52

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	GLN	N-CA-C	-12.12	89.89	109.76
1	A	571	VAL	N-CA-C	-11.51	100.73	111.67
2	Q	363	PRO	CA-C-N	11.19	133.82	119.84
2	Q	363	PRO	C-N-CA	11.19	133.82	119.84
2	Q	129	LYS	CA-C-N	10.45	130.55	119.89
2	Q	129	LYS	C-N-CA	10.45	130.55	119.89
2	G	419	ARG	CA-C-N	10.28	130.05	118.85
2	G	419	ARG	C-N-CA	10.28	130.05	118.85
2	D	29	SER	N-CA-C	9.97	124.51	111.75
2	P	124	LEU	N-CA-C	9.90	121.76	110.97
2	P	29	SER	N-CA-C	9.68	122.72	111.11
2	S	3	ARG	N-CA-C	-9.44	100.99	111.28
1	B	813	ALA	N-CA-C	9.39	122.38	111.11
1	B	864	GLU	N-CA-C	9.34	124.48	112.34
2	E	3	ARG	N-CA-C	-9.22	101.11	111.71
2	Q	29	SER	N-CA-C	9.03	120.81	110.97
1	B	174	LEU	N-CA-C	9.01	121.03	111.03
1	A	449	SER	N-CA-C	8.90	122.46	110.35
2	R	124	LEU	N-CA-C	8.86	121.83	111.02
2	J	363	PRO	CA-C-N	8.72	130.74	119.84
2	J	363	PRO	C-N-CA	8.72	130.74	119.84
2	I	29	SER	N-CA-C	8.62	120.45	111.14
2	D	55	SER	N-CA-C	8.47	121.28	111.11
1	B	437	VAL	N-CA-C	-8.44	104.95	111.62
1	A	141	VAL	N-CA-C	-8.34	98.80	107.89
1	A	813	ALA	N-CA-C	8.28	121.05	111.11
1	B	741	ARG	CA-C-N	8.17	128.22	119.89
1	B	741	ARG	C-N-CA	8.17	128.22	119.89
2	Q	419	ARG	CA-C-N	8.11	129.97	119.84
2	Q	419	ARG	C-N-CA	8.11	129.97	119.84
2	C	419	ARG	CA-C-N	8.08	129.94	119.84
2	C	419	ARG	C-N-CA	8.08	129.94	119.84
2	I	419	ARG	CA-C-N	8.01	129.86	119.84
2	I	419	ARG	C-N-CA	8.01	129.86	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	363	PRO	CA-C-N	7.89	129.70	119.84
2	H	363	PRO	C-N-CA	7.89	129.70	119.84
1	A	959	VAL	CA-C-N	7.89	127.90	119.78
1	A	959	VAL	C-N-CA	7.89	127.90	119.78
1	A	1005	VAL	N-CA-C	-7.84	101.35	110.21
2	T	363	PRO	CA-C-N	7.80	129.59	119.84
2	T	363	PRO	C-N-CA	7.80	129.59	119.84
2	R	29	SER	N-CA-C	7.76	119.74	111.28
2	Q	202	ILE	CA-C-N	7.75	129.53	119.84
2	Q	202	ILE	C-N-CA	7.75	129.53	119.84
2	H	414	PHE	N-CA-C	7.73	120.78	111.82
2	G	312	SER	N-CA-C	-7.58	103.77	113.16
1	B	571	VAL	N-CA-C	-7.57	105.30	111.81
3	K	296	GLU	N-CA-C	7.54	122.12	109.76
1	A	437	VAL	N-CA-C	-7.50	104.47	111.45
2	F	419	ARG	CA-C-N	7.50	129.22	119.84
2	F	419	ARG	C-N-CA	7.50	129.22	119.84
2	R	363	PRO	CA-C-N	7.47	129.18	119.84
2	R	363	PRO	C-N-CA	7.47	129.18	119.84
2	F	363	PRO	CA-C-N	7.45	129.15	119.84
2	F	363	PRO	C-N-CA	7.45	129.15	119.84
2	S	29	SER	N-CA-C	7.44	120.10	111.02
1	A	174	LEU	N-CA-C	7.44	119.29	111.03
2	S	363	PRO	CA-C-N	7.39	129.08	119.84
2	S	363	PRO	C-N-CA	7.39	129.08	119.84
2	E	341	GLN	N-CA-C	-7.33	103.76	114.39
2	E	363	PRO	CA-C-N	7.29	128.95	119.84
2	E	363	PRO	C-N-CA	7.29	128.95	119.84
2	T	419	ARG	CA-C-N	7.26	128.91	119.84
2	T	419	ARG	C-N-CA	7.26	128.91	119.84
1	B	663	PHE	N-CA-C	7.24	122.29	113.17
2	J	129	LYS	CA-C-N	7.18	127.61	119.92
2	J	129	LYS	C-N-CA	7.18	127.61	119.92
1	A	519	ALA	CA-C-N	7.18	127.75	120.14
1	A	519	ALA	C-N-CA	7.18	127.75	120.14
2	C	89	SER	N-CA-C	7.16	120.05	109.24
2	I	363	PRO	CA-C-N	7.13	128.76	119.84
2	I	363	PRO	C-N-CA	7.13	128.76	119.84
1	A	370	SER	N-CA-C	7.05	119.79	109.07
2	H	129	LYS	CA-C-N	7.04	127.00	120.03
2	H	129	LYS	C-N-CA	7.04	127.00	120.03
2	G	129	LYS	CA-C-N	7.02	126.98	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	129	LYS	C-N-CA	7.02	126.98	120.03
2	S	20	VAL	N-CA-C	-7.02	104.02	110.82
2	J	376	TRP	N-CA-C	6.99	119.74	111.71
2	R	89	SER	N-CA-C	6.97	119.77	109.24
1	B	915	ARG	CA-C-N	6.96	127.55	120.38
1	B	915	ARG	C-N-CA	6.96	127.55	120.38
2	D	414	PHE	N-CA-C	6.96	118.94	111.36
2	G	363	PRO	CA-C-N	6.93	128.50	119.84
2	G	363	PRO	C-N-CA	6.93	128.50	119.84
1	B	467	LEU	N-CA-C	6.92	119.42	111.11
2	P	89	SER	N-CA-C	6.89	119.65	109.24
1	B	21	GLU	N-CA-C	6.87	119.72	108.52
2	J	99	PHE	N-CA-C	-6.85	102.30	111.96
2	J	3	ARG	N-CA-C	-6.83	103.91	111.36
1	B	499	ALA	N-CA-C	6.83	125.35	110.80
2	R	16	ILE	N-CA-C	-6.83	103.65	110.62
2	S	392	VAL	N-CA-C	6.80	118.46	109.21
1	A	510	LEU	CB-CA-C	-6.75	108.81	116.63
2	T	414	PHE	N-CA-C	6.73	119.63	111.82
1	B	510	LEU	CB-CA-C	-6.71	108.85	116.63
2	E	419	ARG	CA-C-N	6.71	128.22	119.84
2	E	419	ARG	C-N-CA	6.71	128.22	119.84
1	B	198	VAL	CA-C-N	6.68	126.14	118.85
1	B	198	VAL	C-N-CA	6.68	126.14	118.85
1	A	366	ASN	CA-C-N	6.64	126.33	119.56
1	A	366	ASN	C-N-CA	6.64	126.33	119.56
2	E	20	VAL	N-CA-C	-6.60	104.05	110.72
2	C	56	ASP	CA-C-N	6.59	126.29	119.56
2	C	56	ASP	C-N-CA	6.59	126.29	119.56
2	E	89	SER	N-CA-C	6.59	119.83	110.14
2	F	378	ARG	N-CA-C	-6.59	101.66	111.81
2	F	90	ASP	N-CA-C	-6.58	105.56	112.93
2	S	414	PHE	N-CA-C	6.56	119.43	111.82
1	A	452	ARG	N-CA-C	6.54	119.72	110.23
2	J	157	PHE	N-CA-C	6.54	119.77	109.96
2	S	124	LEU	N-CA-C	6.52	118.04	111.07
2	D	89	SER	N-CA-C	6.51	119.30	109.41
2	G	29	SER	N-CA-C	6.51	119.69	111.69
1	B	177	HIS	N-CA-C	6.50	118.45	111.36
2	G	31	LEU	N-CA-C	6.50	120.12	109.06
1	B	233	ALA	N-CA-C	-6.48	105.51	113.41
2	D	308	TYR	N-CA-C	6.47	119.33	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	277	ASN	N-CA-C	6.42	118.77	107.61
2	T	312	SER	N-CA-C	-6.41	104.38	111.82
2	F	95	VAL	N-CA-C	6.37	117.79	109.58
2	H	352	LEU	N-CA-C	-6.37	103.25	111.02
1	B	525	SER	N-CA-C	6.32	117.83	111.07
2	G	176	PRO	CA-C-N	6.30	126.27	119.78
2	G	176	PRO	C-N-CA	6.30	126.27	119.78
2	G	261	LEU	CA-C-N	6.30	126.25	119.76
2	G	261	LEU	C-N-CA	6.30	126.25	119.76
1	B	1019	LEU	CA-C-O	-6.29	102.13	121.00
2	R	103	TYR	N-CA-C	6.28	120.96	113.12
1	A	56	THR	CA-C-N	6.26	126.17	119.28
1	A	56	THR	C-N-CA	6.26	126.17	119.28
2	E	105	ARG	CA-C-N	6.24	127.64	119.84
2	E	105	ARG	C-N-CA	6.24	127.64	119.84
2	T	88	ASN	N-CA-C	6.22	121.04	113.38
2	G	89	SER	N-CA-C	6.22	119.33	109.81
2	T	20	VAL	N-CA-C	-6.22	104.28	110.62
1	A	617	TYR	N-CA-C	6.21	120.12	112.54
2	F	89	SER	N-CA-C	6.21	119.67	109.85
2	P	46	LEU	N-CA-C	-6.20	104.20	112.94
2	F	88	ASN	N-CA-C	6.20	117.83	111.14
1	B	112	SER	N-CA-C	6.19	123.99	110.80
2	G	414	PHE	N-CA-C	6.19	120.09	112.54
2	I	54	VAL	N-CA-C	6.17	122.17	109.34
2	S	129	LYS	CA-C-N	6.16	126.13	120.03
2	S	129	LYS	C-N-CA	6.16	126.13	120.03
2	C	363	PRO	CA-C-N	6.16	127.53	119.84
2	C	363	PRO	C-N-CA	6.16	127.53	119.84
2	Q	85	THR	N-CA-C	6.15	118.79	111.71
1	B	618	CYS	N-CA-C	-6.15	101.67	110.59
2	S	419	ARG	CA-C-N	6.15	127.53	119.84
2	S	419	ARG	C-N-CA	6.15	127.53	119.84
2	F	414	PHE	N-CA-C	6.13	118.93	111.82
2	Q	89	SER	N-CA-C	6.12	120.06	110.32
1	A	195	ALA	CA-C-N	6.11	125.67	119.19
1	A	195	ALA	C-N-CA	6.11	125.67	119.19
2	I	261	LEU	CA-C-N	6.11	126.07	119.78
2	I	261	LEU	C-N-CA	6.11	126.07	119.78
2	P	3	ARG	N-CA-C	-6.07	104.73	111.71
2	S	275	GLY	N-CA-C	6.04	121.88	114.69
2	E	414	PHE	N-CA-C	6.03	119.90	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ARG	N-CA-C	-6.02	104.59	112.41
1	B	158	LEU	N-CA-C	6.02	117.84	111.28
2	T	341	GLN	N-CA-C	-6.01	105.27	114.16
1	B	149	GLY	N-CA-C	-6.00	98.96	113.18
1	B	399	PRO	N-CA-C	-5.99	103.39	110.70
2	I	308	TYR	N-CA-C	5.99	120.19	113.01
1	A	368	ASN	N-CA-C	5.98	120.19	113.02
2	H	319	SER	N-CA-C	-5.98	100.55	110.17
2	S	103	TYR	N-CA-C	5.96	120.61	112.68
2	P	363	PRO	CA-C-N	5.96	127.28	119.84
2	P	363	PRO	C-N-CA	5.96	127.28	119.84
2	J	191	ARG	N-CA-C	5.96	117.91	108.79
2	R	350	ASP	N-CA-C	-5.95	104.79	111.28
3	K	297	ARG	N-CA-C	-5.95	98.13	110.80
1	A	693	ILE	CB-CA-C	-5.94	105.60	111.30
2	G	99	PHE	N-CA-C	-5.92	104.41	111.69
2	P	415	GLY	N-CA-C	5.92	119.36	112.50
2	H	416	ARG	N-CA-C	5.88	119.28	111.75
2	E	56	ASP	CA-C-N	5.88	125.50	119.56
2	E	56	ASP	C-N-CA	5.88	125.50	119.56
2	C	129	LYS	CA-C-N	5.86	125.77	119.85
2	C	129	LYS	C-N-CA	5.86	125.77	119.85
2	F	157	PHE	N-CA-C	5.84	118.70	110.23
2	H	418	TYR	N-CA-C	5.84	118.66	109.96
2	H	420	PRO	CA-C-N	5.83	132.19	121.70
2	H	420	PRO	C-N-CA	5.83	132.19	121.70
2	T	124	LEU	N-CA-C	5.83	117.31	111.07
1	A	662	PHE	CB-CA-C	-5.82	109.85	116.54
2	P	15	ALA	N-CA-C	-5.81	105.85	113.12
2	F	125	GLN	CA-C-N	5.81	125.78	120.21
2	F	125	GLN	C-N-CA	5.81	125.78	120.21
2	J	419	ARG	CA-C-N	5.80	127.09	119.84
2	J	419	ARG	C-N-CA	5.80	127.09	119.84
2	J	162	GLY	N-CA-C	5.79	119.65	112.64
2	F	261	LEU	CA-C-N	5.77	125.73	119.78
2	F	261	LEU	C-N-CA	5.77	125.73	119.78
2	T	3	ARG	N-CA-C	-5.77	104.99	111.28
3	K	290	GLU	CA-C-N	-5.76	112.63	119.84
3	K	290	GLU	C-N-CA	-5.76	112.63	119.84
2	F	235	ILE	N-CA-C	5.76	116.50	109.30
2	S	397	ARG	N-CA-C	-5.73	104.94	111.07
2	C	350	ASP	N-CA-C	-5.72	105.13	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	89	SER	N-CA-C	5.71	117.87	109.24
2	F	103	TYR	N-CA-C	5.71	120.38	113.41
2	C	414	PHE	N-CA-C	5.71	119.42	112.23
2	D	235	ILE	N-CA-C	5.69	116.61	108.93
2	H	315	GLN	N-CA-C	5.69	119.18	110.36
2	G	277	ASN	N-CA-C	5.69	117.74	108.76
2	G	394	LEU	N-CA-C	5.68	117.16	110.97
2	G	103	TYR	N-CA-C	5.67	120.70	113.55
1	A	82	SER	N-CA-C	-5.66	106.42	113.38
1	A	458	ILE	N-CA-C	-5.66	104.81	110.30
1	A	651	GLN	CA-C-N	-5.66	113.62	122.73
1	A	651	GLN	C-N-CA	-5.66	113.62	122.73
2	D	341	GLN	N-CA-C	-5.66	105.78	114.16
2	Q	47	SER	N-CA-C	5.66	117.91	109.59
1	B	661	ASP	N-CA-C	-5.65	98.77	110.80
2	T	39	LEU	N-CA-C	-5.64	105.23	111.71
2	R	374	SER	N-CA-C	5.63	114.78	108.25
2	G	88	ASN	N-CA-C	5.63	118.27	111.40
2	G	269	LEU	N-CA-C	5.61	119.11	110.42
2	Q	414	PHE	N-CA-C	5.60	118.32	111.82
1	B	978	PHE	N-CA-C	-5.60	105.10	111.14
2	F	85	THR	N-CA-C	5.60	117.38	111.28
2	T	102	THR	N-CA-C	5.59	120.16	113.23
2	T	378	ARG	N-CA-C	-5.59	103.90	111.55
2	Q	92	LYS	CA-C-N	5.58	125.49	119.85
2	Q	92	LYS	C-N-CA	5.58	125.49	119.85
1	B	828	VAL	N-CA-C	-5.57	106.38	111.67
2	F	124	LEU	N-CA-C	5.57	117.03	111.07
2	I	31	LEU	N-CA-C	5.56	117.11	107.93
2	T	313	ILE	N-CA-C	5.56	116.23	108.89
1	B	533	LEU	CA-C-N	5.55	125.50	119.78
1	B	533	LEU	C-N-CA	5.55	125.50	119.78
2	E	224	TYR	N-CA-C	-5.54	100.68	109.76
2	E	211	VAL	CA-C-N	5.53	125.48	119.78
2	E	211	VAL	C-N-CA	5.53	125.48	119.78
2	J	414	PHE	N-CA-C	5.53	119.74	112.89
2	P	10	SER	N-CA-C	-5.52	105.27	112.23
2	P	324	ASP	N-CA-C	5.50	119.82	113.38
1	A	259	ASN	N-CA-C	5.50	118.04	111.71
2	C	374	SER	CA-C-N	5.49	125.47	120.03
2	C	374	SER	C-N-CA	5.49	125.47	120.03
2	D	3	ARG	N-CA-C	-5.49	105.30	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	88	ASN	N-CA-C	5.48	119.67	112.92
2	I	312	SER	N-CA-C	-5.48	106.56	113.20
1	B	958	LEU	N-CA-C	5.48	117.13	108.96
2	F	191	ARG	N-CA-C	5.48	117.42	108.76
3	K	290	GLU	CB-CA-C	-5.48	104.11	113.04
2	T	95	VAL	N-CA-C	5.47	120.73	109.34
2	J	340	GLY	N-CA-C	-5.47	108.57	115.08
2	P	308	TYR	N-CA-C	5.47	119.67	112.89
2	S	211	VAL	CA-C-N	5.47	125.41	119.78
2	S	211	VAL	C-N-CA	5.47	125.41	119.78
1	A	198	VAL	CA-C-N	5.46	126.67	119.84
1	A	198	VAL	C-N-CA	5.46	126.67	119.84
1	B	366	ASN	CA-C-N	5.46	125.13	119.56
1	B	366	ASN	C-N-CA	5.46	125.13	119.56
2	H	29	SER	N-CA-C	5.46	120.37	111.37
1	A	51	SER	N-CA-C	5.45	117.00	109.15
1	B	566	TYR	N-CA-C	5.44	119.68	112.72
2	D	157	PHE	N-CA-C	5.43	118.11	110.23
2	Q	157	PHE	N-CA-C	5.43	117.30	110.24
1	A	399	PRO	N-CA-C	-5.42	104.08	110.70
1	A	454	VAL	N-CA-C	5.42	116.05	110.36
1	B	535	ASP	N-CA-C	5.41	116.98	111.14
2	F	29	SER	N-CA-C	5.41	117.25	111.36
2	R	319	SER	N-CA-C	-5.41	102.48	110.48
1	B	891	LYS	CA-C-N	5.41	125.95	120.38
1	B	891	LYS	C-N-CA	5.41	125.95	120.38
1	B	1011	ASP	CA-C-N	5.41	124.92	119.19
1	B	1011	ASP	C-N-CA	5.41	124.92	119.19
2	C	308	TYR	N-CA-C	5.41	119.50	113.01
2	G	167	ILE	CB-CA-C	-5.40	108.62	114.35
2	Q	191	ARG	N-CA-C	5.37	117.25	108.76
2	T	418	TYR	N-CA-C	5.37	117.97	109.96
1	B	953	VAL	N-CA-C	5.37	116.51	109.21
1	A	652	TYR	N-CA-C	5.37	118.84	112.72
2	G	20	VAL	N-CA-C	-5.37	105.30	110.72
2	D	363	PRO	CA-C-N	5.36	126.54	119.84
2	D	363	PRO	C-N-CA	5.36	126.54	119.84
2	G	392	VAL	N-CA-C	5.36	116.49	109.58
2	F	152	GLU	N-CA-C	-5.36	101.80	109.24
1	B	509	TYR	N-CA-C	5.35	117.99	109.96
2	S	308	TYR	N-CA-C	5.35	118.03	111.82
2	Q	211	VAL	CA-C-N	5.35	125.64	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	211	VAL	C-N-CA	5.35	125.64	119.92
2	P	378	ARG	N-CA-C	-5.34	106.53	112.57
1	A	693	ILE	N-CA-C	5.34	116.23	111.90
1	B	626	ILE	CB-CA-C	-5.34	105.97	110.94
2	Q	103	TYR	N-CA-C	5.34	121.20	114.31
1	A	958	LEU	N-CA-C	5.33	116.91	108.96
2	E	308	TYR	N-CA-C	5.33	119.41	113.01
2	R	47	SER	N-CA-C	5.33	118.23	109.76
2	D	103	TYR	N-CA-C	5.32	120.25	113.55
1	A	915	ARG	CA-C-N	5.32	125.86	120.38
1	A	915	ARG	C-N-CA	5.32	125.86	120.38
1	B	695	HIS	N-CA-C	-5.32	102.61	110.48
2	S	31	LEU	N-CA-C	5.31	117.33	108.99
2	D	15	ALA	N-CA-C	-5.31	105.41	111.14
2	Q	124	LEU	N-CA-C	5.31	116.87	111.14
2	D	415	GLY	N-CA-C	5.30	120.58	114.16
2	F	129	LYS	CA-C-N	5.30	125.24	119.78
2	F	129	LYS	C-N-CA	5.30	125.24	119.78
2	G	378	ARG	N-CA-C	-5.29	103.66	111.81
2	G	254	VAL	CA-C-N	5.29	125.35	119.32
2	G	254	VAL	C-N-CA	5.29	125.35	119.32
2	S	49	SER	N-CA-C	-5.29	99.54	110.80
2	T	84	LYS	N-CA-C	5.28	117.72	111.33
2	D	361	MET	N-CA-C	5.28	117.20	108.13
2	S	85	THR	N-CA-C	5.26	119.18	112.34
1	B	693	ILE	CB-CA-C	-5.24	105.51	110.70
2	F	104	ILE	N-CA-C	5.24	115.91	107.73
2	I	392	VAL	N-CA-C	5.24	116.78	109.55
1	B	175	PHE	N-CA-C	5.23	118.33	109.76
2	E	187	ALA	N-CA-C	5.23	117.33	109.23
1	B	150	GLU	N-CA-C	-5.22	106.77	112.72
2	D	350	ASP	N-CA-C	-5.22	105.01	111.33
2	T	167	ILE	CB-CA-C	-5.22	108.82	114.35
1	B	439	TYR	N-CA-C	-5.22	102.62	110.24
1	B	749	ASN	N-CA-C	5.21	119.97	111.37
2	C	102	THR	N-CA-C	5.21	117.86	111.82
2	S	283	GLY	N-CA-C	5.20	118.54	112.50
2	D	418	TYR	N-CA-C	5.20	117.71	109.96
2	S	176	PRO	CA-C-N	5.20	125.65	120.14
2	S	176	PRO	C-N-CA	5.20	125.65	120.14
1	A	934	ASN	N-CA-C	5.20	116.65	107.61
1	B	189	PHE	N-CA-C	5.19	119.67	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	VAL	N-CA-CB	-5.19	106.50	112.21
2	E	181	GLN	N-CA-C	5.19	116.79	110.41
1	A	721	PHE	N-CA-C	5.19	116.47	109.11
2	G	418	TYR	N-CA-C	5.18	117.86	110.24
2	J	181	GLN	N-CA-C	5.18	117.87	109.79
2	R	157	PHE	N-CA-C	5.18	117.73	110.23
1	B	574	PRO	N-CA-C	-5.17	105.50	110.47
2	I	274	GLY	N-CA-C	-5.17	105.47	112.14
1	B	519	ALA	CA-C-N	5.17	127.22	120.25
1	B	519	ALA	C-N-CA	5.17	127.22	120.25
1	A	978	PHE	N-CA-C	-5.16	105.10	111.40
2	R	21	VAL	CB-CA-C	-5.16	105.10	112.22
2	R	308	TYR	N-CA-C	5.16	119.29	112.89
2	Q	20	VAL	N-CA-C	-5.16	105.36	110.62
2	I	139	ILE	N-CA-C	5.16	116.50	110.62
2	S	374	SER	N-CA-C	5.15	112.86	108.22
2	G	3	ARG	N-CA-C	-5.15	105.67	111.28
2	I	90	ASP	N-CA-C	-5.15	105.46	112.26
2	R	26	ASP	N-CA-C	-5.14	104.82	111.71
2	I	199	ASN	N-CA-C	-5.14	106.85	113.23
1	B	52	VAL	N-CA-C	5.14	115.71	108.36
2	G	191	ARG	N-CA-C	5.13	116.08	108.60
2	S	309	THR	N-CA-C	-5.12	106.99	113.18
2	I	217	VAL	N-CA-C	-5.11	108.85	113.71
2	H	376	TRP	N-CA-C	5.11	118.98	112.34
1	B	832	SER	N-CA-C	5.11	117.44	109.52
2	Q	3	ARG	N-CA-C	-5.10	105.72	111.28
2	E	312	SER	N-CA-C	-5.10	105.90	111.82
2	S	350	ASP	N-CA-C	-5.10	105.16	111.33
2	H	276	GLY	N-CA-C	5.10	117.46	110.58
2	S	125	GLN	CA-C-N	5.09	125.10	120.21
2	S	125	GLN	C-N-CA	5.09	125.10	120.21
2	I	21	VAL	CB-CA-C	-5.09	105.46	111.97
1	A	327	LEU	N-CA-C	-5.08	105.83	111.36
2	G	26	ASP	N-CA-C	-5.08	104.55	111.56
1	A	573	GLN	N-CA-C	5.08	115.44	109.60
1	B	735	TRP	N-CA-C	-5.07	105.83	111.36
1	A	209	ALA	N-CA-C	5.07	117.47	111.33
2	D	54	VAL	CA-C-N	5.07	127.38	120.54
2	D	54	VAL	C-N-CA	5.07	127.38	120.54
2	E	221	THR	N-CA-C	-5.07	101.67	109.52
2	I	95	VAL	N-CA-C	5.07	115.41	108.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	312	SER	N-CA-C	-5.06	107.39	113.21
2	G	85	THR	N-CA-C	5.06	116.87	111.36
2	H	130	PRO	N-CA-C	5.06	119.00	111.41
2	F	162	GLY	N-CA-C	5.05	118.60	112.49
2	H	55	SER	N-CA-C	5.05	117.42	110.35
2	E	241	ALA	N-CA-C	-5.04	106.54	113.30
2	Q	178	ALA	N-CA-C	-5.04	105.43	111.03
2	Q	182	GLN	CA-C-N	5.04	125.03	119.89
2	Q	182	GLN	C-N-CA	5.04	125.03	119.89
1	B	367	PRO	N-CA-C	5.04	120.39	113.84
1	B	784	SER	N-CA-C	5.04	115.96	108.60
2	F	3	ARG	N-CA-C	-5.04	105.79	111.28
1	B	490	ILE	CA-C-N	5.04	124.94	119.85
1	B	490	ILE	C-N-CA	5.04	124.94	119.85
1	A	985	ILE	N-CA-C	5.03	115.51	108.17
2	F	312	SER	N-CA-C	-5.01	107.12	113.18
2	H	361	MET	N-CA-C	5.01	117.07	108.90
1	B	500	ASN	N-CA-C	-5.01	102.87	110.28
2	I	20	VAL	N-CA-C	-5.01	105.66	110.72
1	B	18	LEU	N-CA-C	5.01	118.65	112.54
1	B	932	GLU	N-CA-C	-5.01	103.07	110.48
2	E	261	LEU	CA-C-N	5.01	124.94	119.78
2	E	261	LEU	C-N-CA	5.01	124.94	119.78
1	B	192	ARG	N-CA-C	-5.00	100.36	108.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	751	TYR	Sidechain
1	B	509	TYR	Sidechain

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	7653	0	7664	300	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8053	0	8062	282	0
2	C	3234	0	3208	158	0
2	D	3247	0	3222	149	0
2	E	3274	0	3245	163	0
2	F	3234	0	3208	189	0
2	G	3253	0	3226	170	0
2	H	3274	0	3245	146	0
2	I	3265	0	3236	169	0
2	J	3221	0	3194	152	0
2	P	3227	0	3199	134	0
2	Q	3274	0	3245	176	0
2	R	3274	0	3245	146	0
2	S	3274	0	3245	160	0
2	T	3274	0	3245	128	0
3	K	99	0	89	2	0
All	All	58130	0	57778	2431	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 21.

All (2431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:235:ILE:HD11	2:J:235:ILE:HD12	1.19	1.14
2:J:361:MET:HE1	2:J:367:PRO:HD3	1.15	1.14
2:P:235:ILE:HD13	2:D:229:ASN:HD21	1.06	1.09
2:S:344:ILE:H	2:S:344:ILE:HD12	1.20	1.07
1:B:225:HIS:ND1	1:B:227:ILE:HG22	1.71	1.05
2:Q:353:THR:HG22	2:Q:404:LEU:HD21	1.37	1.04
2:S:361:MET:HE1	2:S:367:PRO:HD3	1.34	1.03
1:B:106:MET:HG2	1:B:772:ILE:HG21	1.40	1.03
2:E:344:ILE:HD12	2:E:344:ILE:H	1.22	1.01
2:H:366:ILE:H	2:H:366:ILE:HD12	1.22	1.01
2:F:197:ARG:HG2	2:F:197:ARG:HH11	1.19	1.00
2:C:229:ASN:HD21	2:D:235:ILE:HD13	1.26	0.99
2:S:107:ARG:HG3	2:S:107:ARG:HH11	1.27	0.97
2:E:163:GLN:HE22	2:E:185:PHE:H	1.06	0.97
1:B:815:PHE:HA	1:B:874:MET:HE2	1.44	0.96
2:S:82:LEU:HD11	2:S:352:LEU:HD12	1.47	0.96
2:E:122:LEU:HD21	2:F:335:GLN:HE22	1.26	0.96
2:S:361:MET:CE	2:S:367:PRO:HD3	1.95	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:MET:HE3	2:E:106:PRO:HD3	1.49	0.94
2:T:361:MET:HE1	2:T:367:PRO:HD3	1.48	0.93
1:A:51:SER:HA	1:A:713:GLN:HE22	1.32	0.93
2:F:337:ARG:HH11	2:F:337:ARG:HG3	1.31	0.92
2:R:31:LEU:CD2	2:H:41:ASN:HB3	1.99	0.92
2:S:235:ILE:HD11	2:J:235:ILE:CD1	1.99	0.92
2:S:6:TRP:CZ2	2:S:81:MET:HE1	2.04	0.91
2:P:229:ASN:HD21	2:C:235:ILE:HD13	1.32	0.91
2:R:31:LEU:HD22	2:H:41:ASN:HB3	1.49	0.91
1:A:693:ILE:HG23	1:B:31:VAL:HG13	1.51	0.91
3:K:296:GLU:O	3:K:297:ARG:HB2	1.71	0.91
1:B:669:ILE:H	1:B:669:ILE:HD12	1.36	0.90
2:J:361:MET:CE	2:J:367:PRO:HD3	2.00	0.90
2:R:5:MET:HE3	2:R:106:PRO:HD3	1.51	0.90
2:J:361:MET:HE1	2:J:367:PRO:CD	2.02	0.90
2:G:362:ASP:OD1	2:G:362:ASP:O	1.90	0.90
2:C:142:GLY:HA3	2:Q:344:ILE:HD11	1.54	0.89
2:C:255:PRO:HG2	2:C:275:GLY:HA3	1.51	0.89
2:I:244:THR:HG22	2:I:246:ALA:H	1.37	0.88
2:F:361:MET:HE1	2:F:367:PRO:HD3	1.53	0.88
2:I:361:MET:HE1	2:I:367:PRO:HD3	1.53	0.88
2:H:344:ILE:HD12	2:H:344:ILE:H	1.37	0.88
2:J:62:GLN:HE21	2:J:419:ARG:HB3	1.39	0.87
2:S:240:THR:HG22	2:S:242:THR:H	1.40	0.87
2:T:6:TRP:CZ2	2:T:81:MET:HE1	2.08	0.87
2:D:5:MET:HE3	2:D:106:PRO:HD3	1.55	0.87
2:S:361:MET:HE1	2:S:367:PRO:CD	2.04	0.87
2:R:344:ILE:H	2:R:344:ILE:HD12	1.39	0.87
2:E:253:THR:HG22	2:E:279:ASN:HB2	1.56	0.86
2:P:182:GLN:HG3	2:P:183:PRO:HD2	1.57	0.86
2:C:208:GLN:OE1	2:F:210:VAL:HG21	1.75	0.86
2:C:344:ILE:H	2:C:344:ILE:HD12	1.41	0.86
1:B:616:VAL:HG23	1:B:662:PHE:O	1.75	0.86
2:T:244:THR:HG22	2:T:246:ALA:H	1.41	0.85
2:H:361:MET:HE1	2:H:367:PRO:HD3	1.57	0.85
2:F:197:ARG:HH11	2:F:197:ARG:CG	1.90	0.85
2:S:161:ALA:HA	2:S:315:GLN:HE22	1.41	0.85
1:A:349:ASN:H	1:A:349:ASN:HD22	1.24	0.85
2:E:391:ASN:H	2:E:391:ASN:ND2	1.71	0.85
1:B:60:LEU:H	1:B:60:LEU:HD12	1.41	0.84
1:B:684:ASN:HB3	2:R:32:THR:HG21	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ASN:HB3	2:F:31:LEU:HD22	1.57	0.84
1:B:364:MET:HE3	1:B:541:ILE:HB	1.59	0.84
2:P:235:ILE:HD13	2:D:229:ASN:ND2	1.91	0.84
2:P:344:ILE:HD12	2:P:344:ILE:H	1.42	0.83
2:S:375:PRO:HD2	2:S:378:ARG:HE	1.41	0.83
2:R:145:ILE:HG12	2:R:146:PRO:HD2	1.60	0.83
2:Q:3:ARG:HD2	2:Q:140:MET:HE3	1.60	0.83
2:D:349:MET:HE2	2:D:349:MET:HA	1.61	0.83
2:E:391:ASN:H	2:E:391:ASN:HD22	1.24	0.83
2:J:39:LEU:HA	2:J:42:MET:HE3	1.59	0.83
2:G:66:ASN:HD21	2:G:419:ARG:H	1.27	0.82
2:H:82:LEU:HD11	2:H:352:LEU:HD22	1.62	0.82
1:A:226:GLN:HE22	1:A:982:ASP:H	1.28	0.82
1:B:165:ASN:HD22	1:B:165:ASN:C	1.88	0.82
2:H:228:THR:HG22	2:H:229:ASN:H	1.43	0.82
2:P:20:VAL:HG23	2:P:39:LEU:HD11	1.60	0.81
1:B:696:LEU:HD23	1:B:700:PHE:HE1	1.43	0.81
2:P:2:SER:CB	2:P:5:MET:HE3	2.10	0.81
2:G:227:PHE:H	2:G:264:GLN:HE22	1.26	0.81
1:A:392:MET:HE2	1:A:392:MET:HA	1.61	0.80
1:A:438:ILE:HD11	1:A:447:TRP:CZ2	2.16	0.80
2:J:62:GLN:NE2	2:J:419:ARG:HB3	1.94	0.80
2:F:229:ASN:HD22	2:F:229:ASN:C	1.89	0.80
2:G:361:MET:SD	2:G:367:PRO:HG3	2.21	0.80
1:B:177:HIS:HA	1:B:180:VAL:HG12	1.63	0.80
1:A:226:GLN:NE2	1:A:982:ASP:H	1.79	0.80
2:F:316:THR:HG21	2:F:397:ARG:HH12	1.46	0.80
2:J:344:ILE:H	2:J:344:ILE:HD12	1.47	0.79
2:S:341:GLN:HA	2:S:344:ILE:HD13	1.64	0.79
2:C:323:PHE:HB2	2:C:405:TRP:HE1	1.47	0.79
2:J:378:ARG:HD2	2:J:381:GLU:OE1	1.82	0.79
2:F:322:ASP:HB2	2:F:325:VAL:HG12	1.63	0.79
2:H:107:ARG:HG3	2:H:107:ARG:HH11	1.48	0.79
2:E:118:GLN:HG2	2:G:421:ASN:O	1.81	0.79
2:F:337:ARG:HH11	2:F:337:ARG:CG	1.96	0.79
2:I:329:LEU:HD23	2:I:412:ALA:HB2	1.65	0.79
2:J:177:PRO:HG2	2:J:199:ASN:HB3	1.64	0.79
1:A:544:VAL:H	1:A:1013:ASN:ND2	1.81	0.79
2:S:2:SER:HB2	2:S:5:MET:HG3	1.64	0.78
1:A:286:GLN:HE21	1:A:287:LEU:N	1.81	0.78
2:H:159:SER:HB2	2:H:318:THR:HG22	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:ILE:HG22	2:H:293:ILE:HB	1.65	0.77
2:J:323:PHE:HB2	2:J:405:TRP:HE1	1.49	0.77
2:I:124:LEU:CD2	2:J:416:ARG:HD3	2.14	0.77
1:B:258:PRO:HG2	1:B:261:LEU:HD12	1.66	0.77
2:H:366:ILE:H	2:H:366:ILE:CD1	1.96	0.77
1:B:405:ALA:HA	1:B:408:ARG:NH1	1.99	0.76
2:H:173:LEU:HB3	2:H:236:ILE:HG23	1.65	0.76
2:D:255:PRO:HG3	2:D:276:GLY:H	1.49	0.76
2:C:5:MET:HE3	2:C:106:PRO:HD3	1.68	0.76
2:D:344:ILE:H	2:D:344:ILE:HD12	1.51	0.76
2:Q:217:VAL:HG12	2:Q:299:ILE:HG23	1.68	0.76
2:G:228:THR:HG22	2:H:234:THR:OG1	1.84	0.75
2:I:229:ASN:HD21	2:J:235:ILE:HG12	1.51	0.75
2:Q:322:ASP:O	2:Q:325:VAL:HG22	1.86	0.75
2:C:208:GLN:CD	2:F:210:VAL:HG21	2.11	0.75
2:E:122:LEU:CD2	2:F:335:GLN:HE22	1.98	0.75
2:H:362:ASP:C	2:H:362:ASP:OD1	2.30	0.75
2:S:235:ILE:HG13	2:J:229:ASN:HD21	1.51	0.75
2:I:256:THR:HB	2:J:337:ARG:HH12	1.51	0.75
2:J:163:GLN:NE2	2:J:169:MET:HG3	2.02	0.75
2:P:151:ILE:O	2:P:151:ILE:HD12	1.87	0.74
2:E:182:GLN:HE21	2:E:183:PRO:HD2	1.50	0.74
2:G:349:MET:CE	2:G:352:LEU:HD23	2.18	0.74
2:H:322:ASP:O	2:H:325:VAL:HG23	1.87	0.74
2:S:261:LEU:HD23	2:I:378:ARG:NH2	2.02	0.74
2:J:14:GLU:OE1	2:J:131:LYS:HB3	1.88	0.74
2:S:192:ILE:HG22	2:S:293:ILE:HB	1.70	0.74
2:P:2:SER:HB3	2:P:5:MET:HE3	1.69	0.73
2:C:375:PRO:HD2	2:C:378:ARG:HD3	1.69	0.73
2:Q:210:VAL:HG21	2:J:208:GLN:HG2	1.68	0.73
2:H:240:THR:HG22	2:H:242:THR:H	1.53	0.73
2:Q:145:ILE:HG12	2:Q:146:PRO:HD2	1.70	0.73
2:I:12:LEU:HD12	2:I:107:ARG:HG2	1.71	0.73
2:S:416:ARG:HD3	2:J:124:LEU:CD2	2.18	0.72
1:A:241:ILE:HG21	1:A:753:VAL:HG21	1.70	0.72
2:F:41:ASN:O	2:F:44:THR:HG22	1.89	0.72
2:F:140:MET:HE3	2:F:406:VAL:HG21	1.71	0.72
2:S:124:LEU:CD2	2:I:416:ARG:HD3	2.19	0.72
2:Q:192:ILE:HG22	2:Q:293:ILE:HB	1.72	0.72
2:H:339:CYS:HB3	2:H:421:ASN:HD21	1.54	0.72
2:I:250:THR:HG23	2:I:282:LEU:HA	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:418:TYR:CE1	2:H:420:PRO:HG3	2.25	0.72
2:T:357:ILE:HD13	2:T:400:ILE:HG21	1.69	0.72
2:Q:361:MET:HG2	2:Q:392:VAL:HG11	1.72	0.72
2:F:209:PHE:HB2	2:F:278:ILE:HG23	1.71	0.72
2:H:145:ILE:HG12	2:H:146:PRO:HD2	1.70	0.72
2:T:361:MET:CE	2:T:367:PRO:HD3	2.20	0.72
2:F:151:ILE:HD13	2:F:156:LEU:HD13	1.72	0.72
2:H:228:THR:HG22	2:H:229:ASN:N	2.04	0.72
2:R:31:LEU:HD22	2:H:41:ASN:CB	2.20	0.72
2:J:2:SER:HB3	2:J:5:MET:HB2	1.72	0.72
2:R:361:MET:HE1	2:R:367:PRO:HD3	1.71	0.71
2:R:349:MET:HE2	2:R:349:MET:HA	1.71	0.71
1:B:985:ILE:HD12	1:B:985:ILE:O	1.90	0.71
2:P:31:LEU:HD22	2:D:41:ASN:HB3	1.71	0.71
2:P:80:TYR:CE2	2:P:81:MET:HG3	2.25	0.71
2:E:391:ASN:HD22	2:E:391:ASN:N	1.86	0.71
2:F:361:MET:CE	2:F:367:PRO:HD3	2.19	0.71
2:S:82:LEU:HD11	2:S:352:LEU:CD1	2.18	0.71
2:S:344:ILE:HD12	2:S:344:ILE:N	2.02	0.71
2:I:361:MET:CE	2:I:367:PRO:HD3	2.20	0.71
1:B:187:ARG:HG2	1:B:187:ARG:HH11	1.56	0.71
1:B:222:VAL:HG13	1:B:223:PRO:HD2	1.71	0.71
2:G:159:SER:H	2:G:318:THR:HG23	1.55	0.71
1:B:280:MET:HE1	1:B:996:VAL:HG23	1.72	0.71
2:J:18:GLU:O	2:J:21:VAL:HG12	1.90	0.71
2:S:49:SER:C	2:S:51:ALA:H	1.98	0.71
1:A:210:VAL:HG23	1:A:276:ILE:HA	1.73	0.71
1:B:408:ARG:NH2	1:B:501:GLU:OE2	2.24	0.71
2:G:349:MET:HE1	2:G:352:LEU:CD2	2.21	0.70
1:A:304:ALA:HB2	1:A:369:ILE:HG13	1.73	0.70
2:C:231:PHE:O	2:C:232:PHE:HB2	1.92	0.70
2:G:41:ASN:HB3	2:H:31:LEU:CD2	2.22	0.70
2:S:357:ILE:HD11	2:S:386:ILE:HD12	1.74	0.70
2:S:416:ARG:HD3	2:J:124:LEU:HD21	1.74	0.70
2:P:375:PRO:HD2	2:P:378:ARG:HD3	1.74	0.70
2:I:24:ASN:C	2:I:24:ASN:HD22	1.99	0.70
2:J:205:GLY:O	2:J:281:GLU:HB2	1.91	0.70
2:J:396:ILE:O	2:J:400:ILE:HG13	1.91	0.70
1:A:316:VAL:HG21	1:A:651:GLN:NE2	2.07	0.70
1:B:2:ASP:OD2	1:B:4:THR:HG22	1.91	0.70
1:B:308:LEU:HD22	1:B:362:GLN:HB2	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:54:VAL:HG12	2:I:55:SER:N	2.06	0.70
1:A:286:GLN:HE21	1:A:287:LEU:H	1.39	0.70
2:C:142:GLY:CA	2:Q:344:ILE:HD11	2.22	0.70
2:I:344:ILE:H	2:I:344:ILE:HD12	1.56	0.70
2:R:157:PHE:O	2:R:158:ARG:HD2	1.91	0.70
1:A:289:ASP:H	1:A:673:GLN:NE2	1.90	0.70
2:P:229:ASN:ND2	2:C:235:ILE:HD13	2.06	0.70
2:T:59:VAL:HG13	2:T:60:PRO:HD3	1.73	0.70
2:F:110:VAL:CG2	2:F:111:PRO:HA	2.22	0.70
1:A:970:THR:HG21	2:J:41:ASN:OD1	1.91	0.69
1:B:787:VAL:HG21	1:B:853:VAL:HG12	1.73	0.69
2:J:59:VAL:HB	2:J:60:PRO:HD3	1.74	0.69
1:A:234:LEU:HD22	1:A:757:GLN:HE21	1.57	0.69
2:R:146:PRO:HG2	2:R:149:GLU:HB2	1.74	0.69
2:S:344:ILE:H	2:S:344:ILE:CD1	1.99	0.69
2:T:361:MET:HE1	2:T:367:PRO:CD	2.22	0.69
1:A:623:ARG:HG3	1:A:623:ARG:HH11	1.58	0.69
1:B:212:GLU:OE1	1:B:986:ARG:NH1	2.26	0.69
2:D:272:SER:C	2:D:274:GLY:H	1.98	0.69
2:Q:366:ILE:H	2:Q:366:ILE:HD12	1.58	0.69
2:P:158:ARG:NH2	2:P:320:ILE:HG13	2.07	0.69
2:D:80:TYR:CE2	2:D:81:MET:HG3	2.28	0.69
2:H:344:ILE:HD12	2:H:344:ILE:N	2.07	0.69
1:A:788:ASP:OD2	1:A:791:SER:HB2	1.92	0.69
2:R:235:ILE:HD13	2:H:229:ASN:HD21	1.58	0.69
2:I:124:LEU:HD21	2:J:416:ARG:HD3	1.73	0.69
2:R:254:VAL:HG13	2:R:255:PRO:HD2	1.74	0.69
2:Q:208:GLN:HG2	2:J:210:VAL:HG21	1.73	0.69
2:Q:137:ASN:HB3	2:Q:143:LEU:HD12	1.74	0.68
2:H:94:THR:HG23	2:H:94:THR:O	1.91	0.68
1:A:124:ARG:C	1:A:124:ARG:HD3	2.18	0.68
1:A:120:MET:HG3	1:A:682:LEU:HD11	1.76	0.68
2:D:140:MET:CE	2:D:406:VAL:HG11	2.23	0.68
2:I:24:ASN:HD22	2:I:25:GLY:N	1.90	0.68
2:H:254:VAL:HG12	2:H:256:THR:H	1.58	0.68
2:J:140:MET:HE1	2:J:406:VAL:HG11	1.75	0.68
1:B:655:LEU:HG	1:B:657:GLU:HG3	1.74	0.68
2:G:41:ASN:HB3	2:H:31:LEU:HD21	1.75	0.68
2:G:210:VAL:HA	2:G:277:ASN:HB3	1.75	0.68
2:E:344:ILE:HD12	2:E:344:ILE:N	2.04	0.68
2:F:82:LEU:HD11	2:F:352:LEU:HD22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:LEU:HD11	1:B:870:ILE:HG13	1.75	0.68
2:E:163:GLN:NE2	2:E:185:PHE:H	1.86	0.68
2:G:69:VAL:HG21	2:G:418:TYR:CE1	2.29	0.68
2:I:361:MET:HE1	2:I:367:PRO:CD	2.24	0.68
2:J:12:LEU:O	2:J:16:ILE:HG12	1.94	0.68
2:T:6:TRP:CE2	2:T:81:MET:HE1	2.29	0.68
1:A:219:ARG:HH11	1:A:219:ARG:HG3	1.59	0.67
2:J:156:LEU:HD21	2:J:299:ILE:HD11	1.76	0.67
1:A:280:MET:HG2	1:A:281:PRO:HD2	1.75	0.67
1:A:438:ILE:HD11	1:A:447:TRP:CH2	2.29	0.67
2:E:173:LEU:HB3	2:E:236:ILE:HG23	1.75	0.67
2:G:320:ILE:HD11	2:G:383:ALA:HB1	1.75	0.67
2:P:2:SER:HB2	2:P:5:MET:HE3	1.76	0.67
2:Q:394:LEU:HG	2:Q:398:LYS:HE3	1.77	0.67
2:F:197:ARG:HG2	2:F:197:ARG:NH1	2.01	0.67
2:R:239:VAL:HG13	2:R:289:PHE:HA	1.77	0.67
2:H:186:VAL:HG23	2:H:193:LEU:HB2	1.74	0.67
2:E:344:ILE:H	2:E:344:ILE:CD1	2.00	0.67
2:G:349:MET:HE1	2:G:352:LEU:HD23	1.75	0.67
2:H:361:MET:CE	2:H:367:PRO:HD3	2.24	0.67
2:I:322:ASP:O	2:I:325:VAL:HG22	1.95	0.67
2:P:323:PHE:HB2	2:P:405:TRP:NE1	2.09	0.67
2:D:69:VAL:HG21	2:D:418:TYR:CD1	2.30	0.67
2:Q:261:LEU:HD23	2:E:378:ARG:NH2	2.10	0.67
2:S:266:ASP:HB2	2:I:319:SER:HB3	1.76	0.67
1:A:108:ILE:HG22	1:A:774:ILE:HD11	1.76	0.67
2:C:361:MET:CE	2:C:367:PRO:HD3	2.25	0.67
2:D:309:THR:HG22	2:D:309:THR:O	1.95	0.67
2:E:204:ALA:HB2	2:E:285:ALA:N	2.09	0.67
2:G:344:ILE:H	2:G:344:ILE:HD12	1.59	0.67
2:H:344:ILE:H	2:H:344:ILE:CD1	2.08	0.67
2:I:419:ARG:HE	2:I:421:ASN:HD21	1.43	0.67
1:B:732:LYS:N	1:B:733:PRO:HD2	2.10	0.67
2:C:374:SER:HB2	2:C:375:PRO:HD2	1.76	0.67
2:F:186:VAL:HG23	2:F:193:LEU:HB2	1.77	0.67
2:C:26:ASP:HA	2:C:28:PHE:HE1	1.60	0.66
2:S:378:ARG:HH12	2:J:261:LEU:HD22	1.59	0.66
1:A:561:LEU:HG	1:A:565:MET:CE	2.25	0.66
2:F:54:VAL:O	2:F:54:VAL:HG12	1.94	0.66
2:G:3:ARG:HG2	2:G:4:GLN:N	2.11	0.66
2:Q:180:GLN:HE21	2:Q:202:ILE:HG22	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ILE:HD13	1:A:1003:ILE:H	1.61	0.66
2:F:361:MET:HE1	2:F:367:PRO:CD	2.23	0.66
1:B:444:ILE:CD1	1:B:444:ILE:H	2.07	0.66
2:D:158:ARG:NH2	2:D:320:ILE:HG13	2.10	0.66
2:G:353:THR:HG22	2:G:404:LEU:HD11	1.77	0.66
2:G:418:TYR:CZ	2:G:420:PRO:HG3	2.30	0.66
2:H:378:ARG:HD2	2:H:381:GLU:OE2	1.95	0.66
2:I:49:SER:O	2:I:50:SER:HB3	1.93	0.66
2:I:320:ILE:HD11	2:I:383:ALA:HB1	1.77	0.66
2:T:33:THR:HG22	2:T:35:ASP:H	1.59	0.66
1:A:349:ASN:HD22	1:A:349:ASN:N	1.92	0.66
2:I:261:LEU:HD23	2:J:378:ARG:CZ	2.26	0.66
1:A:781:VAL:HG23	1:A:868:ASP:O	1.96	0.66
2:S:12:LEU:HD22	2:S:107:ARG:HD2	1.76	0.66
2:S:107:ARG:HH11	2:S:107:ARG:CG	2.03	0.66
2:J:353:THR:O	2:J:357:ILE:HG13	1.96	0.66
2:I:230:SER:HB3	2:J:233:GLY:O	1.96	0.66
1:B:616:VAL:HG22	1:B:662:PHE:CE2	2.31	0.66
2:C:323:PHE:HB2	2:C:405:TRP:NE1	2.10	0.66
1:B:153:VAL:HG21	1:B:191:GLN:CD	2.19	0.66
1:B:669:ILE:H	1:B:669:ILE:CD1	2.09	0.65
2:Q:210:VAL:HG21	2:J:208:GLN:CG	2.26	0.65
2:T:255:PRO:HB2	2:T:275:GLY:HA3	1.78	0.65
1:A:976:ARG:O	1:A:980:THR:HG23	1.96	0.65
2:E:7:LEU:CD2	2:E:136:GLN:HE21	2.09	0.65
2:Q:366:ILE:HD12	2:Q:366:ILE:N	2.11	0.65
2:F:120:ASN:O	2:F:122:LEU:N	2.30	0.65
2:F:239:VAL:HA	2:F:288:GLY:HA3	1.78	0.65
2:J:24:ASN:HD22	2:J:25:GLY:N	1.93	0.65
1:B:438:ILE:HD11	1:B:458:ILE:HG12	1.78	0.65
2:H:239:VAL:HG13	2:H:289:PHE:HA	1.78	0.65
2:T:19:TYR:CD1	2:T:42:MET:HE1	2.31	0.65
2:T:375:PRO:HD2	2:T:378:ARG:HD3	1.79	0.65
2:P:239:VAL:HG13	2:P:289:PHE:HA	1.77	0.65
2:R:309:THR:HG22	2:R:309:THR:O	1.95	0.65
2:G:110:VAL:HG22	2:G:111:PRO:HA	1.79	0.65
2:G:244:THR:HG22	2:G:246:ALA:H	1.60	0.65
2:J:112:MET:HE3	2:J:116:VAL:CG2	2.27	0.65
2:T:349:MET:CE	2:T:352:LEU:HG	2.27	0.65
1:B:930:LEU:O	1:B:931:GLY:O	2.14	0.65
2:P:12:LEU:HD22	2:P:107:ARG:HD2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:254:VAL:HG11	2:J:272:SER:O	1.97	0.65
1:B:958:LEU:C	1:B:958:LEU:HD12	2.22	0.65
2:P:82:LEU:HD11	2:P:352:LEU:HD22	1.77	0.65
2:Q:357:ILE:HG23	2:Q:400:ILE:HD13	1.78	0.65
2:G:244:THR:HB	2:G:247:ASP:OD1	1.95	0.65
2:D:24:ASN:HD22	2:D:24:ASN:C	2.03	0.65
2:I:329:LEU:CD2	2:I:412:ALA:HB2	2.27	0.65
1:B:60:LEU:HD12	1:B:60:LEU:N	2.12	0.64
1:B:669:ILE:HD12	1:B:669:ILE:N	2.10	0.64
2:P:165:GLY:O	2:P:169:MET:HG2	1.96	0.64
2:C:309:THR:O	2:C:309:THR:HG22	1.96	0.64
2:Q:7:LEU:HD11	2:Q:140:MET:HE2	1.79	0.64
1:B:165:ASN:C	1:B:165:ASN:ND2	2.56	0.64
2:P:254:VAL:HG13	2:P:255:PRO:HD2	1.79	0.64
2:E:115:THR:HG21	2:F:57:PRO:HD2	1.80	0.64
2:E:391:ASN:ND2	2:E:391:ASN:N	2.42	0.64
2:G:137:ASN:HB3	2:G:143:LEU:HD12	1.79	0.64
2:G:211:VAL:HG22	2:G:276:GLY:O	1.98	0.64
2:G:362:ASP:OD1	2:G:362:ASP:C	2.40	0.64
2:J:140:MET:CE	2:J:406:VAL:HG11	2.27	0.64
2:T:158:ARG:HD2	2:T:312:SER:HB3	1.79	0.64
2:C:59:VAL:HB	2:C:60:PRO:CD	2.27	0.64
1:A:102:TYR:CG	1:A:765:MET:HE1	2.32	0.64
1:A:844:LEU:HD11	1:A:870:ILE:HG13	1.79	0.64
2:E:132:LEU:O	2:E:136:GLN:HG3	1.96	0.64
2:F:209:PHE:HB2	2:F:278:ILE:CG2	2.26	0.64
1:B:337:VAL:O	1:B:338:THR:C	2.41	0.64
2:C:337:ARG:HH11	2:C:337:ARG:HG3	1.61	0.64
2:Q:115:THR:HG23	2:E:58:ARG:HG2	1.79	0.64
2:G:110:VAL:CG2	2:G:111:PRO:HA	2.27	0.64
1:A:544:VAL:H	1:A:1013:ASN:HD22	1.45	0.64
2:D:110:VAL:CG2	2:D:111:PRO:HA	2.27	0.64
2:D:201:ALA:HA	2:D:287:THR:HA	1.79	0.64
2:Q:133:TYR:HA	2:Q:136:GLN:OE1	1.97	0.64
2:H:140:MET:HE3	2:H:406:VAL:HG21	1.79	0.64
2:P:24:ASN:HD22	2:P:25:GLY:N	1.96	0.64
1:B:85:ILE:HG12	1:B:933:THR:OG1	1.98	0.63
2:S:124:LEU:HD23	2:I:416:ARG:HD3	1.79	0.63
1:A:915:ARG:HA	1:B:1005:VAL:HG23	1.80	0.63
1:B:19:VAL:O	1:B:21:GLU:N	2.31	0.63
1:B:151:LEU:HD12	1:B:152:PRO:HD2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:95:VAL:CG2	2:E:100:ILE:HG21	2.28	0.63
2:E:157:PHE:C	2:E:158:ARG:HD2	2.23	0.63
2:G:192:ILE:HD11	2:G:218:LEU:CD1	2.29	0.63
2:P:323:PHE:HB2	2:P:405:TRP:HE1	1.64	0.63
2:F:316:THR:HG21	2:F:397:ARG:NH1	2.13	0.63
2:G:107:ARG:HH11	2:G:107:ARG:HG3	1.61	0.63
2:S:382:ARG:O	2:S:386:ILE:HG12	1.98	0.63
2:Q:58:ARG:HG2	2:F:119:LEU:HD13	1.80	0.63
2:Q:163:GLN:HE22	2:Q:185:PHE:H	1.47	0.63
2:F:167:ILE:N	2:F:168:PRO:HD2	2.13	0.63
2:T:24:ASN:HD22	2:T:25:GLY:N	1.97	0.63
1:B:377:LEU:O	1:B:414:ARG:NH1	2.32	0.63
2:G:239:VAL:HG13	2:G:289:PHE:HA	1.81	0.63
2:T:163:GLN:NE2	2:T:185:PHE:O	2.27	0.63
2:Q:33:THR:HG22	2:Q:35:ASP:H	1.63	0.63
2:Q:353:THR:O	2:Q:357:ILE:HG13	1.98	0.63
2:G:315:GLN:HE21	2:G:315:GLN:CA	2.12	0.63
2:T:56:ASP:C	2:T:58:ARG:H	2.05	0.63
2:T:64:MET:HE2	2:T:65:SER:N	2.14	0.63
1:A:432:LEU:HB3	1:A:438:ILE:HG22	1.81	0.63
1:A:366:ASN:C	1:A:366:ASN:HD22	2.07	0.63
2:C:12:LEU:HD22	2:C:107:ARG:HD3	1.81	0.63
2:C:33:THR:HG23	2:C:36:PHE:HB3	1.80	0.63
2:F:69:VAL:O	2:F:73:THR:HB	1.99	0.63
1:B:304:ALA:HB2	1:B:369:ILE:HB	1.79	0.63
2:C:210:VAL:HG21	2:F:208:GLN:NE2	2.14	0.63
2:H:361:MET:HE1	2:H:367:PRO:CD	2.28	0.63
2:Q:379:PHE:CE1	2:Q:404:LEU:HD12	2.34	0.62
1:B:269:LEU:HA	1:B:272:THR:HG22	1.80	0.62
2:Q:342:TYR:O	2:Q:342:TYR:HD2	1.83	0.62
1:A:531:LEU:O	1:A:532:ALA:HB3	2.00	0.62
2:H:214:TRP:CZ3	2:H:215:ALA:HB2	2.34	0.62
2:I:217:VAL:HG13	2:I:303:ARG:HB3	1.79	0.62
1:B:115:GLU:HB3	1:B:116:PRO:HD3	1.81	0.62
1:B:619:ASP:OD1	1:B:621:VAL:HG23	1.98	0.62
2:P:309:THR:O	2:P:309:THR:HG22	1.98	0.62
2:E:124:LEU:CD2	2:F:416:ARG:HD3	2.30	0.62
2:F:208:GLN:HG2	2:F:279:ASN:HD21	1.64	0.62
2:G:24:ASN:HD22	2:G:25:GLY:N	1.97	0.62
2:S:186:VAL:HG23	2:S:193:LEU:HB2	1.82	0.62
2:S:303:ARG:HB3	2:S:303:ARG:HH11	1.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:VAL:HG12	2:C:161:ALA:H	1.64	0.62
2:T:357:ILE:HD11	2:T:386:ILE:HD12	1.81	0.62
1:A:480:ASN:ND2	1:A:503:ARG:HD3	2.14	0.62
1:B:553:GLU:HG2	2:Q:30:GLY:HA2	1.82	0.62
2:C:420:PRO:O	2:C:421:ASN:OXT	2.17	0.62
2:Q:197:ARG:HG2	2:Q:239:VAL:HG23	1.81	0.62
2:Q:379:PHE:HE1	2:Q:404:LEU:HD12	1.62	0.62
2:S:6:TRP:CE2	2:S:81:MET:HE1	2.35	0.62
1:A:769:THR:O	1:A:772:ILE:HG12	2.00	0.62
1:A:835:ASP:OD1	1:A:838:SER:HB2	2.00	0.62
1:B:782:LYS:HG2	1:B:846:SER:HB2	1.79	0.62
2:Q:235:ILE:HD11	2:E:235:ILE:HD11	1.82	0.62
1:B:313:LEU:HD22	1:B:604:ALA:HB1	1.81	0.62
2:C:140:MET:CE	2:C:406:VAL:HG11	2.29	0.62
2:D:24:ASN:HD22	2:D:25:GLY:N	1.96	0.62
2:G:255:PRO:HB2	2:G:275:GLY:HA3	1.80	0.62
1:A:286:GLN:NE2	1:A:287:LEU:H	1.98	0.62
1:B:268:SER:O	1:B:272:THR:HG22	1.99	0.62
2:Q:167:ILE:N	2:Q:168:PRO:HD2	2.15	0.62
2:Q:271:PHE:HZ	2:Q:293:ILE:HD13	1.63	0.62
2:F:110:VAL:HG22	2:F:111:PRO:HA	1.80	0.62
1:B:33:ASN:H	1:B:33:ASN:HD22	1.47	0.61
2:R:375:PRO:HD3	2:H:259:ASN:HD22	1.65	0.61
2:S:329:LEU:HD23	2:S:412:ALA:HB2	1.81	0.61
2:J:323:PHE:HB2	2:J:405:TRP:NE1	2.14	0.61
1:A:355:THR:O	1:A:358:VAL:HG12	2.00	0.61
1:A:660:PRO:HG2	1:A:662:PHE:CE1	2.35	0.61
2:C:151:ILE:HD12	2:C:151:ILE:O	2.00	0.61
2:C:255:PRO:CG	2:C:275:GLY:HA3	2.27	0.61
1:A:366:ASN:HD22	1:A:368:ASN:H	1.46	0.61
2:D:329:LEU:HD23	2:D:412:ALA:HB2	1.82	0.61
2:S:107:ARG:HG3	2:S:107:ARG:NH1	2.07	0.61
1:B:31:VAL:HG12	1:B:32:TYR:N	2.14	0.61
2:J:160:VAL:HG22	2:J:161:ALA:H	1.64	0.61
1:A:669:ILE:HD12	1:A:669:ILE:N	2.14	0.61
2:Q:271:PHE:CZ	2:Q:293:ILE:HD13	2.34	0.61
2:F:1:MET:HG3	2:F:100:ILE:HG21	1.81	0.61
2:D:151:ILE:HD12	2:D:151:ILE:O	1.99	0.61
2:J:167:ILE:N	2:J:168:PRO:HD2	2.15	0.61
1:A:595:THR:HA	1:A:645:VAL:HG13	1.83	0.61
2:C:230:SER:HB3	2:D:233:GLY:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:145:ILE:CG1	2:R:146:PRO:HD2	2.30	0.61
2:G:309:THR:HG22	2:G:309:THR:O	2.00	0.61
1:B:746:ARG:HD3	2:G:37:ASN:HD21	1.64	0.61
2:P:344:ILE:H	2:P:344:ILE:CD1	2.12	0.61
2:I:298:THR:HG22	2:I:299:ILE:N	2.14	0.61
2:J:140:MET:HE3	2:J:406:VAL:HG21	1.83	0.61
1:A:80:GLY:HA3	1:A:930:LEU:O	2.01	0.60
1:B:361:ALA:HA	1:B:605:ILE:HD12	1.83	0.60
2:F:329:LEU:HD13	2:F:412:ALA:HB2	1.82	0.60
1:B:227:ILE:HD11	1:B:768:LEU:HD21	1.83	0.60
2:S:145:ILE:HG12	2:S:146:PRO:HD2	1.82	0.60
2:J:383:ALA:O	2:J:387:LEU:HD23	2.01	0.60
1:A:60:LEU:HD22	1:A:60:LEU:N	2.16	0.60
1:B:696:LEU:HD23	1:B:700:PHE:CE1	2.31	0.60
2:Q:5:MET:HE3	2:Q:106:PRO:HD3	1.82	0.60
2:Q:48:VAL:HG23	2:Q:102:THR:O	2.01	0.60
2:C:42:MET:HG2	2:D:31:LEU:HD21	1.82	0.60
2:Q:167:ILE:HB	2:F:266:ASP:OD1	2.01	0.60
2:Q:211:VAL:HG12	2:Q:276:GLY:C	2.26	0.60
2:F:166:ASN:C	2:F:168:PRO:HD2	2.26	0.60
2:S:48:VAL:HG22	2:S:102:THR:HG23	1.82	0.60
1:B:63:ILE:HG22	1:B:137:MET:O	2.01	0.60
2:C:362:ASP:OD2	2:Q:366:ILE:HD13	2.02	0.60
1:A:533:LEU:HB3	1:A:534:PRO:HD2	1.83	0.60
2:F:24:ASN:HD22	2:F:25:GLY:N	2.00	0.60
2:G:361:MET:HE1	2:G:367:PRO:HG3	1.83	0.60
2:S:41:ASN:HB3	2:I:31:LEU:CD1	2.30	0.60
1:A:108:ILE:HD12	1:A:108:ILE:N	2.17	0.60
2:E:235:ILE:HD11	2:F:235:ILE:HD11	1.83	0.60
2:F:140:MET:HE1	2:F:406:VAL:HG11	1.82	0.60
2:G:209:PHE:O	2:G:277:ASN:HB2	2.02	0.60
2:G:254:VAL:HG13	2:G:255:PRO:HD2	1.84	0.60
2:S:378:ARG:NH1	2:J:261:LEU:HD22	2.17	0.60
1:A:85:ILE:H	1:A:85:ILE:HD12	1.67	0.60
2:P:145:ILE:HG12	2:P:146:PRO:HD2	1.84	0.60
1:B:438:ILE:HD11	1:B:458:ILE:CG1	2.30	0.60
1:B:985:ILE:HD12	1:B:985:ILE:C	2.26	0.60
2:I:186:VAL:CG2	2:I:193:LEU:HB2	2.32	0.60
1:B:30:GLU:HB3	1:B:35:LEU:HG	1.83	0.60
2:C:145:ILE:HD11	2:C:149:GLU:OE2	2.01	0.60
2:C:167:ILE:HB	2:C:168:PRO:HD3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:115:THR:CG2	2:E:58:ARG:HG2	2.32	0.59
2:G:4:GLN:HE22	2:G:141:LYS:HE3	1.67	0.59
1:B:65:LEU:O	1:B:68:VAL:HG23	2.02	0.59
1:B:468:VAL:HG23	2:D:98:ASP:OD1	2.02	0.59
2:P:43:PHE:CE1	2:P:57:PRO:HB3	2.37	0.59
2:Q:361:MET:SD	2:Q:367:PRO:HG3	2.43	0.59
2:E:202:ILE:HD13	2:E:288:GLY:H	1.66	0.59
2:E:203:PRO:HG2	2:E:207:TYR:OH	2.01	0.59
2:F:13:LEU:HD21	2:F:64:MET:HE2	1.84	0.59
2:Q:110:VAL:CG2	2:Q:111:PRO:HA	2.32	0.59
2:F:193:LEU:HD12	2:F:231:PHE:HD1	1.66	0.59
1:A:438:ILE:HD12	1:A:439:TYR:H	1.68	0.59
2:D:145:ILE:HG12	2:D:146:PRO:HD2	1.84	0.59
2:G:344:ILE:HD12	2:G:344:ILE:N	2.17	0.59
2:G:361:MET:CE	2:G:367:PRO:HG3	2.32	0.59
2:S:157:PHE:O	2:S:158:ARG:HD2	2.02	0.59
2:T:244:THR:HB	2:T:247:ASP:OD1	2.02	0.59
1:A:303:LEU:HD23	1:A:303:LEU:C	2.27	0.59
2:Q:217:VAL:CG1	2:Q:299:ILE:HG23	2.33	0.59
2:J:61:LEU:HD12	2:J:417:TYR:CE1	2.37	0.59
1:A:392:MET:O	1:A:558:LYS:HD2	2.03	0.59
1:A:813:ALA:HB2	2:E:101:THR:HB	1.85	0.59
2:F:214:TRP:CZ3	2:F:215:ALA:HB2	2.37	0.59
2:R:256:THR:CG2	2:G:337:ARG:NH1	2.65	0.59
2:T:69:VAL:HG21	2:T:418:TYR:CD1	2.38	0.59
2:P:31:LEU:HD21	2:D:45:GLN:CG	2.33	0.59
2:E:13:LEU:HD21	2:E:64:MET:HE2	1.83	0.59
2:J:1:MET:HG2	2:J:93:PRO:HD2	1.85	0.59
1:A:366:ASN:ND2	1:A:368:ASN:H	2.00	0.59
2:Q:124:LEU:CD2	2:E:416:ARG:HD3	2.33	0.59
1:A:346:VAL:C	1:A:348:MET:H	2.10	0.59
1:B:371:TYR:CE2	1:B:633:HIS:HB3	2.38	0.59
2:C:344:ILE:HD12	2:C:344:ILE:N	2.15	0.59
2:S:235:ILE:CD1	2:J:235:ILE:HD12	2.12	0.59
1:B:392:MET:HG2	1:B:565:MET:HE1	1.85	0.58
1:B:414:ARG:N	1:B:414:ARG:HD3	2.18	0.58
2:R:235:ILE:HD13	2:H:229:ASN:ND2	2.18	0.58
2:R:337:ARG:NH1	2:H:256:THR:HG22	2.18	0.58
2:H:145:ILE:HG12	2:H:146:PRO:CD	2.33	0.58
2:H:396:ILE:O	2:H:400:ILE:HG13	2.03	0.58
2:J:77:ARG:NE	2:J:97:ASP:OD1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:122:LEU:N	2:T:122:LEU:HD12	2.18	0.58
1:A:475:THR:CG2	1:A:561:LEU:HD13	2.33	0.58
1:B:835:ASP:O	1:B:837:LEU:N	2.36	0.58
2:C:16:ILE:HG12	2:C:42:MET:HE2	1.85	0.58
2:F:145:ILE:HG12	2:F:146:PRO:HD2	1.84	0.58
2:T:14:GLU:OE2	2:T:131:LYS:HB3	2.03	0.58
2:C:160:VAL:HG12	2:C:161:ALA:N	2.18	0.58
2:G:145:ILE:HG12	2:G:146:PRO:HD2	1.85	0.58
1:A:262:ARG:HD3	1:A:1003:ILE:HG22	1.85	0.58
1:A:688:ARG:NH2	2:E:37:ASN:OD1	2.36	0.58
2:E:7:LEU:HD22	2:E:136:GLN:HE21	1.67	0.58
2:I:54:VAL:O	2:I:55:SER:CB	2.51	0.58
2:I:167:ILE:N	2:I:168:PRO:CD	2.66	0.58
2:I:182:GLN:CG	2:I:183:PRO:HD2	2.32	0.58
2:J:112:MET:HE3	2:J:116:VAL:HG23	1.86	0.58
2:T:221:THR:HA	2:T:270:SER:HB3	1.83	0.58
2:Q:14:GLU:OE2	2:Q:132:LEU:N	2.25	0.58
2:E:254:VAL:CG1	2:E:255:PRO:HD2	2.34	0.58
2:F:224:TYR:CE2	2:F:268:ARG:HD3	2.39	0.58
2:R:80:TYR:CE2	2:R:100:ILE:HD11	2.38	0.58
2:S:163:GLN:NE2	2:S:185:PHE:O	2.36	0.58
2:S:169:MET:O	2:S:173:LEU:HG	2.03	0.58
2:S:244:THR:N	2:S:247:ASP:OD2	2.25	0.58
1:A:958:LEU:HD12	1:A:958:LEU:C	2.27	0.58
1:B:206:LEU:HD12	1:B:206:LEU:H	1.67	0.58
1:B:945:ILE:O	1:B:948:TYR:HB3	2.04	0.58
2:P:192:ILE:HD11	2:P:218:LEU:CD1	2.34	0.58
2:G:4:GLN:HE22	2:G:141:LYS:CE	2.15	0.58
2:H:254:VAL:HG13	2:H:255:PRO:HD2	1.84	0.58
2:I:396:ILE:HD12	2:I:396:ILE:N	2.18	0.58
2:T:98:ASP:O	2:T:102:THR:HG23	2.02	0.58
1:B:165:ASN:HD21	1:B:167:ASP:HB2	1.69	0.58
1:B:290:TYR:O	1:B:293:VAL:HG23	2.03	0.58
1:B:400:PRO:HG3	1:B:509:TYR:HB2	1.86	0.58
1:B:438:ILE:HG23	1:B:447:TRP:HZ2	1.69	0.58
2:Q:180:GLN:HE21	2:Q:202:ILE:CG2	2.16	0.58
2:R:41:ASN:ND2	2:G:31:LEU:HB2	2.18	0.58
1:A:475:THR:HG22	1:A:561:LEU:HD13	1.84	0.58
2:C:24:ASN:C	2:C:24:ASN:HD22	2.11	0.58
2:C:157:PHE:C	2:C:158:ARG:HD2	2.29	0.58
2:T:161:ALA:HA	2:T:315:GLN:NE2	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:H	1:B:33:ASN:ND2	2.02	0.58
2:P:64:MET:HE2	2:P:65:SER:N	2.19	0.58
2:E:254:VAL:HG13	2:E:255:PRO:HD2	1.86	0.58
2:E:337:ARG:HH11	2:E:337:ARG:HG3	1.66	0.58
2:R:151:ILE:HD12	2:R:151:ILE:O	2.03	0.58
2:T:161:ALA:HA	2:T:315:GLN:HE22	1.67	0.58
1:A:527:TYR:CZ	1:A:531:LEU:HD11	2.39	0.58
2:P:322:ASP:O	2:P:325:VAL:HG22	2.03	0.58
2:P:361:MET:HE3	2:P:392:VAL:HG22	1.86	0.58
2:C:65:SER:OG	2:C:417:TYR:HB2	2.04	0.58
2:Q:361:MET:HE1	2:Q:367:PRO:HG3	1.85	0.58
2:E:228:THR:O	2:E:290:CYS:HB3	2.04	0.58
2:F:355:SER:O	2:F:359:ASN:ND2	2.36	0.58
2:I:261:LEU:HD23	2:J:378:ARG:NH1	2.18	0.58
2:J:110:VAL:HG23	2:J:111:PRO:HA	1.85	0.58
2:E:382:ARG:O	2:E:386:ILE:HG12	2.04	0.57
2:T:309:THR:O	2:T:310:LEU:HB2	2.04	0.57
2:D:239:VAL:HG13	2:D:289:PHE:HA	1.86	0.57
2:E:360:TYR:HB2	2:E:400:ILE:HD11	1.87	0.57
2:H:12:LEU:HD22	2:H:107:ARG:HD2	1.86	0.57
1:B:781:VAL:HG12	1:B:869:ALA:HB2	1.85	0.57
2:C:254:VAL:HG11	2:C:272:SER:O	2.04	0.57
2:C:344:ILE:H	2:C:344:ILE:CD1	2.13	0.57
2:F:326:SER:HA	2:F:329:LEU:HD23	1.85	0.57
2:I:12:LEU:HD13	2:I:46:LEU:HD11	1.85	0.57
2:H:394:LEU:HG	2:H:398:LYS:HE3	1.87	0.57
1:A:392:MET:HE1	1:A:476:TYR:HE1	1.68	0.57
1:A:632:LEU:N	1:A:632:LEU:HD12	2.19	0.57
2:E:145:ILE:HD11	2:E:149:GLU:OE2	2.05	0.57
2:R:22:ARG:HD3	2:R:35:ASP:OD2	2.04	0.57
2:R:182:GLN:HB3	2:R:183:PRO:HD2	1.86	0.57
2:S:6:TRP:HZ2	2:S:81:MET:HE1	1.67	0.57
2:S:316:THR:HG21	2:S:397:ARG:NH1	2.18	0.57
1:A:307:LEU:O	1:A:307:LEU:HD13	2.03	0.57
1:A:406:ARG:O	1:A:409:LEU:HB3	2.04	0.57
2:Q:155:LYS:HE2	2:F:268:ARG:HH21	1.70	0.57
1:A:286:GLN:HE21	1:A:286:GLN:CA	2.18	0.57
2:C:5:MET:HG2	2:C:106:PRO:HG3	1.85	0.57
2:R:175:THR:OG1	2:H:242:THR:HG23	2.05	0.57
2:S:110:VAL:CG2	2:S:111:PRO:HA	2.34	0.57
1:A:334:SER:C	1:A:336:ASN:H	2.13	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:HH11	1:B:187:ARG:CG	2.17	0.57
1:B:192:ARG:HG3	1:B:220:TYR:CE2	2.40	0.57
2:P:229:ASN:ND2	2:P:229:ASN:O	2.38	0.57
2:F:197:ARG:CG	2:F:197:ARG:NH1	2.59	0.57
2:I:350:ASP:OD1	2:I:382:ARG:NH2	2.34	0.57
2:T:394:LEU:HG	2:T:398:LYS:HE3	1.86	0.57
1:B:731:SER:OG	1:B:733:PRO:HG2	2.05	0.57
2:C:110:VAL:CG2	2:C:111:PRO:HA	2.34	0.57
2:F:375:PRO:HD2	2:F:378:ARG:HG3	1.86	0.57
2:G:239:VAL:HA	2:G:288:GLY:O	2.05	0.57
2:J:316:THR:HG21	2:J:397:ARG:HH12	1.70	0.57
1:A:508:PRO:HG2	1:A:509:TYR:CE1	2.40	0.57
1:B:204:ASP:OD1	1:B:282:ARG:NH1	2.38	0.57
2:P:239:VAL:HG13	2:P:289:PHE:CA	2.35	0.57
2:E:124:LEU:HD21	2:F:416:ARG:HD3	1.86	0.57
2:G:419:ARG:HD2	2:G:421:ASN:ND2	2.20	0.57
2:S:225:VAL:HA	2:S:292:ALA:O	2.05	0.57
2:I:41:ASN:HB3	2:J:31:LEU:CD1	2.35	0.57
2:D:145:ILE:CG1	2:D:146:PRO:HD2	2.34	0.56
2:Q:124:LEU:HD21	2:E:416:ARG:HD3	1.86	0.56
2:Q:254:VAL:HG13	2:Q:255:PRO:HD2	1.87	0.56
2:G:82:LEU:HD11	2:G:352:LEU:HD12	1.87	0.56
2:H:24:ASN:HD22	2:H:25:GLY:N	2.03	0.56
2:H:145:ILE:HD11	2:H:149:GLU:OE2	2.04	0.56
2:S:132:LEU:O	2:S:136:GLN:HG3	2.05	0.56
2:S:231:PHE:O	2:S:232:PHE:HB2	2.05	0.56
2:J:16:ILE:CD1	2:J:42:MET:HB3	2.35	0.56
2:J:403:HIS:CD2	2:J:407:ILE:HD11	2.39	0.56
2:T:305:GLN:O	2:T:309:THR:HB	2.04	0.56
1:A:129:MET:HE1	1:A:765:MET:HE2	1.87	0.56
1:A:151:LEU:HD12	1:A:152:PRO:HD2	1.85	0.56
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.20	0.56
1:B:60:LEU:H	1:B:60:LEU:CD1	2.08	0.56
1:B:364:MET:HE3	1:B:541:ILE:CB	2.33	0.56
2:C:140:MET:HE3	2:C:406:VAL:HG11	1.86	0.56
2:E:95:VAL:HG21	2:E:100:ILE:HG21	1.87	0.56
2:G:344:ILE:H	2:G:344:ILE:CD1	2.18	0.56
2:T:64:MET:HE2	2:T:65:SER:CA	2.36	0.56
1:A:331:VAL:O	1:A:332:SER:HB3	2.05	0.56
1:A:361:ALA:O	1:A:364:MET:HE3	2.05	0.56
1:B:654:ILE:N	1:B:654:ILE:HD12	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:PRO:HB3	2:F:32:THR:O	2.05	0.56
2:P:344:ILE:HD12	2:P:344:ILE:N	2.17	0.56
2:D:46:LEU:O	2:D:47:SER:HB3	2.03	0.56
2:G:24:ASN:HD22	2:G:24:ASN:C	2.13	0.56
2:T:145:ILE:HG12	2:T:146:PRO:HD2	1.87	0.56
1:A:105:PHE:CE2	1:A:765:MET:HB3	2.41	0.56
1:A:112:SER:HB3	1:A:118:LEU:HD23	1.85	0.56
1:B:2:ASP:O	1:B:4:THR:N	2.38	0.56
1:B:19:VAL:C	1:B:21:GLU:H	2.13	0.56
2:Q:31:LEU:HD11	2:F:42:MET:HG2	1.86	0.56
2:Q:305:GLN:O	2:Q:309:THR:HB	2.05	0.56
2:R:156:LEU:HD21	2:R:299:ILE:HD11	1.86	0.56
1:B:112:SER:HB3	1:B:918:LEU:CB	2.36	0.56
2:P:64:MET:HG3	2:P:103:TYR:CD2	2.41	0.56
2:Q:309:THR:O	2:Q:310:LEU:HB2	2.05	0.56
2:Q:342:TYR:HD2	2:Q:342:TYR:C	2.14	0.56
2:G:109:GLN:HE21	2:G:112:MET:HB3	1.71	0.56
2:J:344:ILE:H	2:J:344:ILE:CD1	2.18	0.56
2:D:151:ILE:HD12	2:D:151:ILE:C	2.30	0.56
2:Q:359:ASN:HD22	2:Q:359:ASN:N	2.03	0.56
2:R:256:THR:HG21	2:G:337:ARG:NH1	2.21	0.56
2:H:325:VAL:CG2	2:H:405:TRP:NE1	2.69	0.56
2:I:110:VAL:HG23	2:I:111:PRO:HA	1.87	0.56
2:I:269:LEU:N	2:I:269:LEU:HD22	2.21	0.56
1:A:124:ARG:HD3	1:A:124:ARG:O	2.06	0.56
2:Q:361:MET:HG2	2:Q:392:VAL:CG1	2.35	0.56
2:I:375:PRO:HD2	2:I:378:ARG:HD3	1.87	0.56
1:B:361:ALA:CA	1:B:605:ILE:HD12	2.36	0.56
1:B:444:ILE:H	1:B:444:ILE:HD12	1.70	0.56
2:F:420:PRO:O	2:F:421:ASN:C	2.48	0.56
2:T:322:ASP:O	2:T:325:VAL:HG22	2.04	0.56
2:T:349:MET:HE1	2:T:352:LEU:HG	1.88	0.56
1:A:210:VAL:HG21	1:A:245:HIS:NE2	2.21	0.56
1:B:537:SER:HB3	1:B:538:PRO:HD2	1.88	0.56
2:E:2:SER:HB2	2:E:5:MET:H	1.71	0.56
2:R:122:LEU:O	2:G:331:THR:HG21	2.06	0.56
2:T:252:PHE:CE1	2:T:261:LEU:HD12	2.41	0.56
2:C:17:SER:O	2:C:21:VAL:HG23	2.06	0.56
2:D:17:SER:O	2:D:21:VAL:HG23	2.06	0.56
2:E:33:THR:HG22	2:E:35:ASP:H	1.69	0.56
2:E:309:THR:O	2:E:309:THR:HG22	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:MET:O	2:F:2:SER:C	2.48	0.56
2:T:64:MET:HE2	2:T:65:SER:HA	1.87	0.56
1:B:392:MET:HE3	1:B:561:LEU:HD21	1.88	0.55
2:R:361:MET:HE1	2:R:367:PRO:CD	2.34	0.55
2:J:407:ILE:N	2:J:407:ILE:HD12	2.21	0.55
2:T:323:PHE:HB2	2:T:405:TRP:NE1	2.21	0.55
1:A:930:LEU:HD22	1:A:930:LEU:N	2.21	0.55
2:D:209:PHE:O	2:D:277:ASN:HB3	2.05	0.55
2:Q:5:MET:HB3	2:Q:104:ILE:HG22	1.88	0.55
2:Q:24:ASN:HD22	2:Q:25:GLY:N	2.04	0.55
2:Q:239:VAL:HG13	2:Q:289:PHE:HA	1.88	0.55
2:E:152:GLU:OE1	2:E:155:LYS:HE3	2.05	0.55
2:E:231:PHE:O	2:E:232:PHE:HB2	2.06	0.55
2:F:244:THR:HG22	2:F:246:ALA:H	1.71	0.55
2:G:109:GLN:HE21	2:G:112:MET:CB	2.20	0.55
2:H:137:ASN:HB3	2:H:143:LEU:HD12	1.87	0.55
2:I:124:LEU:HD23	2:J:416:ARG:HD3	1.87	0.55
2:I:337:ARG:HH11	2:I:337:ARG:HG3	1.70	0.55
2:J:344:ILE:HD12	2:J:344:ILE:N	2.20	0.55
2:E:201:ALA:HA	2:E:287:THR:HA	1.86	0.55
2:I:337:ARG:HG3	2:I:337:ARG:NH1	2.21	0.55
1:A:796:ILE:HG23	1:A:928:ASN:HB2	1.89	0.55
2:E:192:ILE:HG22	2:E:293:ILE:HB	1.87	0.55
2:H:225:VAL:HA	2:H:292:ALA:O	2.07	0.55
1:A:108:ILE:HD12	1:A:108:ILE:H	1.70	0.55
1:A:243:TYR:HB3	1:A:279:LEU:HB3	1.88	0.55
1:B:112:SER:HB3	1:B:918:LEU:HB2	1.88	0.55
1:B:304:ALA:CB	1:B:369:ILE:HB	2.36	0.55
2:D:337:ARG:HH11	2:D:337:ARG:HB3	1.71	0.55
2:Q:416:ARG:HD3	2:F:124:LEU:HD21	1.89	0.55
2:R:244:THR:HG22	2:R:245:ALA:N	2.22	0.55
2:R:361:MET:CE	2:R:367:PRO:HD3	2.35	0.55
2:I:192:ILE:HG22	2:I:293:ILE:HB	1.88	0.55
1:B:206:LEU:HD12	1:B:206:LEU:N	2.21	0.55
1:B:666:GLY:HA2	1:B:669:ILE:HD13	1.88	0.55
2:P:186:VAL:HG23	2:P:193:LEU:HB2	1.88	0.55
2:C:191:ARG:HB3	2:C:294:GLU:HG3	1.87	0.55
2:D:12:LEU:CD2	2:D:107:ARG:HD3	2.36	0.55
2:G:124:LEU:CD2	2:H:416:ARG:HD3	2.37	0.55
1:A:339:ASN:HD21	1:A:341:ALA:HB3	1.71	0.55
2:Q:5:MET:CE	2:Q:105:ARG:HA	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:342:TYR:C	2:Q:342:TYR:CD2	2.84	0.55
2:G:394:LEU:O	2:G:397:ARG:HB2	2.07	0.55
2:S:329:LEU:CD2	2:S:412:ALA:HB2	2.37	0.55
1:A:561:LEU:HG	1:A:565:MET:HE3	1.89	0.55
1:A:800:SER:OG	1:A:801:VAL:N	2.40	0.55
2:P:120:ASN:O	2:P:122:LEU:N	2.40	0.55
2:R:64:MET:HG3	2:R:103:TYR:CD2	2.42	0.55
2:H:110:VAL:CG2	2:H:111:PRO:HA	2.36	0.55
1:A:866:ARG:NH1	2:J:92:LYS:HD2	2.22	0.55
2:P:329:LEU:HD23	2:P:412:ALA:HB2	1.88	0.55
2:C:244:THR:HB	2:C:247:ASP:OD1	2.07	0.55
2:D:244:THR:HB	2:D:247:ASP:OD1	2.06	0.55
2:F:2:SER:CB	2:F:5:MET:HE3	2.37	0.55
2:F:140:MET:CE	2:F:406:VAL:HG21	2.37	0.55
2:R:254:VAL:HG12	2:R:256:THR:H	1.71	0.55
2:I:69:VAL:HG21	2:I:418:TYR:CD1	2.42	0.55
1:A:801:VAL:O	1:A:961:ILE:HG13	2.07	0.55
1:B:121:HIS:O	1:B:125:VAL:HG23	2.07	0.55
2:C:26:ASP:HA	2:C:28:PHE:CE1	2.42	0.55
2:Q:350:ASP:OD1	2:Q:382:ARG:NH2	2.39	0.55
1:A:700:PHE:O	1:A:704:GLU:HG3	2.07	0.54
1:A:791:SER:HB2	1:A:859:ARG:HH12	1.71	0.54
1:B:105:PHE:CE2	1:B:765:MET:HB3	2.42	0.54
1:B:821:LEU:HD13	1:B:840:MET:HE1	1.89	0.54
2:R:344:ILE:H	2:R:344:ILE:CD1	2.16	0.54
2:R:416:ARG:HD3	2:H:124:LEU:CD2	2.37	0.54
2:G:318:THR:HG22	2:G:319:SER:N	2.21	0.54
2:J:403:HIS:HD2	2:J:407:ILE:HD11	1.72	0.54
2:C:361:MET:HE1	2:C:367:PRO:HD3	1.89	0.54
2:D:158:ARG:NH2	2:D:321:ASP:OD2	2.41	0.54
2:D:225:VAL:HA	2:D:292:ALA:O	2.07	0.54
2:Q:155:LYS:HE2	2:F:268:ARG:NH2	2.22	0.54
2:R:1:MET:HE3	2:R:5:MET:HE1	1.88	0.54
2:J:141:LYS:HB2	2:J:143:LEU:CD2	2.37	0.54
2:J:145:ILE:HG12	2:J:146:PRO:HD2	1.89	0.54
1:B:153:VAL:HG22	1:B:154:LYS:N	2.22	0.54
1:B:392:MET:HG2	1:B:565:MET:CE	2.37	0.54
2:Q:233:GLY:O	2:F:230:SER:HB2	2.06	0.54
2:R:225:VAL:HA	2:R:292:ALA:O	2.07	0.54
2:R:416:ARG:HD3	2:H:124:LEU:HD21	1.88	0.54
2:G:2:SER:HB2	2:G:5:MET:HE3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:69:VAL:HG21	2:J:418:TYR:CD1	2.43	0.54
2:T:382:ARG:O	2:T:386:ILE:HG12	2.07	0.54
1:A:158:LEU:HD13	1:A:166:MET:HB2	1.89	0.54
1:A:286:GLN:HG3	1:A:748:PRO:HA	1.90	0.54
1:B:374:ILE:HD11	1:B:394:PHE:HE2	1.72	0.54
2:G:16:ILE:HD13	2:G:42:MET:HB3	1.90	0.54
2:H:418:TYR:CZ	2:H:420:PRO:HG3	2.41	0.54
2:S:151:ILE:C	2:S:151:ILE:HD12	2.32	0.54
1:A:225:HIS:ND1	1:A:227:ILE:HG12	2.23	0.54
1:A:339:ASN:HB2	1:A:340:PRO:HD2	1.90	0.54
1:B:960:PRO:O	1:B:963:VAL:HG12	2.06	0.54
2:P:151:ILE:HD12	2:P:151:ILE:C	2.32	0.54
2:D:146:PRO:HG2	2:D:149:GLU:HB2	1.89	0.54
2:D:215:ALA:C	2:D:217:VAL:H	2.16	0.54
2:Q:186:VAL:HB	2:Q:231:PHE:CE1	2.43	0.54
2:F:337:ARG:CG	2:F:337:ARG:NH1	2.63	0.54
2:R:31:LEU:HD23	2:H:41:ASN:HB3	1.86	0.54
2:J:110:VAL:CG2	2:J:111:PRO:HA	2.38	0.54
2:J:217:VAL:HG12	2:J:303:ARG:HD2	1.89	0.54
2:C:322:ASP:O	2:C:325:VAL:HG22	2.08	0.54
2:D:145:ILE:HD11	2:D:149:GLU:OE2	2.07	0.54
2:Q:110:VAL:HG23	2:Q:111:PRO:HA	1.89	0.54
2:Q:158:ARG:NH2	2:Q:321:ASP:OD1	2.41	0.54
2:F:80:TYR:HB3	2:F:95:VAL:HG21	1.89	0.54
2:R:2:SER:HB3	2:R:5:MET:HG3	1.90	0.54
2:G:375:PRO:HD2	2:G:378:ARG:HD3	1.89	0.54
2:T:30:GLY:O	2:T:31:LEU:C	2.50	0.54
2:C:349:MET:HE2	2:C:349:MET:HA	1.90	0.54
2:Q:323:PHE:HB2	2:Q:405:TRP:HE1	1.72	0.54
2:G:227:PHE:H	2:G:264:GLN:NE2	2.02	0.54
2:I:14:GLU:OE1	2:I:131:LYS:HB3	2.07	0.54
2:T:182:GLN:HG3	2:T:183:PRO:HD2	1.89	0.54
2:T:214:TRP:CZ3	2:T:215:ALA:HB2	2.42	0.54
1:B:536:ARG:NH1	1:B:616:VAL:O	2.40	0.54
2:C:244:THR:HG22	2:C:245:ALA:N	2.22	0.54
2:G:382:ARG:O	2:G:386:ILE:HG12	2.08	0.54
2:S:140:MET:HE3	2:S:406:VAL:HG11	1.89	0.54
2:S:156:LEU:HD22	2:S:218:LEU:HD21	1.89	0.54
2:I:228:THR:O	2:I:290:CYS:HB3	2.07	0.54
2:T:145:ILE:CG1	2:T:146:PRO:HD2	2.38	0.54
2:T:156:LEU:HD12	2:T:218:LEU:HD21	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:ILE:CG2	1:A:928:ASN:HB2	2.38	0.54
2:P:24:ASN:HD22	2:P:24:ASN:C	2.14	0.54
2:P:329:LEU:CD2	2:P:412:ALA:HB2	2.37	0.54
2:F:121:ASN:HA	2:F:146:PRO:HA	1.90	0.54
2:R:110:VAL:CG2	2:R:111:PRO:HA	2.38	0.54
2:H:107:ARG:HH11	2:H:107:ARG:CG	2.17	0.54
2:H:133:TYR:HA	2:H:136:GLN:NE2	2.23	0.54
2:H:374:SER:HB2	2:H:375:PRO:HD2	1.90	0.54
2:I:229:ASN:ND2	2:J:235:ILE:HG12	2.21	0.54
1:A:428:THR:HG23	1:A:466:GLU:OE2	2.08	0.54
1:A:923:ILE:HG23	1:A:923:ILE:O	2.07	0.54
2:Q:160:VAL:HG12	2:Q:161:ALA:N	2.23	0.54
2:E:352:LEU:HD23	2:E:352:LEU:C	2.32	0.54
2:I:82:LEU:HD21	2:I:352:LEU:HD11	1.89	0.54
2:I:82:LEU:HD11	2:I:352:LEU:HD12	1.89	0.54
2:J:61:LEU:HD12	2:J:417:TYR:CD1	2.42	0.54
2:T:282:LEU:HD11	2:T:289:PHE:CD2	2.43	0.54
1:B:105:PHE:CE1	1:B:122:ARG:HB3	2.43	0.53
1:B:311:ILE:HD11	1:B:362:GLN:HA	1.90	0.53
1:B:349:ASN:OD1	1:B:352:GLY:N	2.38	0.53
2:P:120:ASN:C	2:P:122:LEU:N	2.66	0.53
2:D:147:TYR:CE1	2:D:301:ALA:HB1	2.43	0.53
2:D:156:LEU:HD21	2:D:299:ILE:HD11	1.89	0.53
2:E:345:PHE:CZ	2:E:349:MET:HE3	2.43	0.53
2:F:262:PRO:HB2	2:F:265:THR:OG1	2.08	0.53
2:R:1:MET:O	2:R:2:SER:C	2.50	0.53
2:G:225:VAL:HA	2:G:292:ALA:O	2.09	0.53
2:H:69:VAL:HG21	2:H:418:TYR:CD1	2.43	0.53
1:B:827:ARG:NH1	1:B:827:ARG:HB3	2.24	0.53
2:C:151:ILE:HD12	2:C:151:ILE:C	2.32	0.53
2:E:156:LEU:HD12	2:E:218:LEU:HD21	1.89	0.53
2:E:167:ILE:N	2:E:168:PRO:CD	2.71	0.53
2:T:239:VAL:HG13	2:T:289:PHE:HA	1.91	0.53
2:C:132:LEU:O	2:C:136:GLN:HG3	2.08	0.53
2:G:228:THR:CG2	2:H:234:THR:OG1	2.56	0.53
2:H:105:ARG:O	2:H:107:ARG:HG2	2.08	0.53
2:H:211:VAL:HG22	2:H:276:GLY:O	2.08	0.53
2:J:16:ILE:HD13	2:J:42:MET:HB3	1.91	0.53
2:T:254:VAL:HG11	2:T:272:SER:O	2.08	0.53
2:R:80:TYR:CE2	2:R:81:MET:HG3	2.43	0.53
2:R:163:GLN:NE2	2:R:185:PHE:H	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:214:TRP:CZ3	2:R:215:ALA:HB2	2.42	0.53
2:H:161:ALA:HA	2:H:315:GLN:NE2	2.22	0.53
2:H:313:ILE:HD13	2:H:387:LEU:HD13	1.90	0.53
2:I:382:ARG:O	2:I:386:ILE:HG13	2.08	0.53
1:B:374:ILE:HD11	1:B:394:PHE:CE2	2.43	0.53
2:C:197:ARG:HG3	2:C:197:ARG:HH11	1.74	0.53
2:Q:366:ILE:H	2:Q:366:ILE:CD1	2.20	0.53
2:E:222:GLY:HA3	2:E:268:ARG:NH1	2.23	0.53
2:R:161:ALA:HA	2:R:315:GLN:NE2	2.22	0.53
2:I:231:PHE:O	2:I:232:PHE:HB2	2.07	0.53
1:B:19:VAL:C	1:B:21:GLU:N	2.66	0.53
2:C:24:ASN:HD22	2:C:25:GLY:N	2.06	0.53
2:D:124:LEU:O	2:D:126:PRO:HD3	2.09	0.53
2:Q:416:ARG:HD3	2:F:124:LEU:CD2	2.39	0.53
2:F:157:PHE:O	2:F:158:ARG:HD3	2.08	0.53
2:I:240:THR:HB	2:I:242:THR:HG22	1.89	0.53
1:A:51:SER:HA	1:A:713:GLN:NE2	2.14	0.53
1:A:293:VAL:HG23	1:A:294:TYR:N	2.24	0.53
2:C:80:TYR:CE2	2:C:81:MET:HG3	2.43	0.53
2:D:214:TRP:CZ3	2:D:215:ALA:HB2	2.43	0.53
2:R:145:ILE:HD11	2:R:149:GLU:OE2	2.09	0.53
2:G:418:TYR:CE1	2:G:420:PRO:HG3	2.44	0.53
2:S:203:PRO:HG2	2:S:207:TYR:OH	2.08	0.53
2:I:151:ILE:HD12	2:I:151:ILE:O	2.08	0.53
2:P:31:LEU:HD21	2:D:45:GLN:HG3	1.91	0.53
2:Q:282:LEU:HD11	2:Q:289:PHE:CE2	2.42	0.53
2:R:239:VAL:HG13	2:R:289:PHE:CA	2.39	0.53
2:I:329:LEU:HD23	2:I:412:ALA:CB	2.36	0.53
1:A:945:ILE:O	1:A:948:TYR:HB3	2.08	0.53
1:B:280:MET:HB2	1:B:281:PRO:HD2	1.91	0.53
2:P:225:VAL:HG12	2:P:263:VAL:HG13	1.91	0.53
2:D:9:THR:HA	2:D:107:ARG:HD2	1.90	0.53
2:D:140:MET:HE1	2:D:406:VAL:HG11	1.89	0.53
2:D:167:ILE:N	2:D:168:PRO:CD	2.71	0.53
2:Q:239:VAL:HA	2:Q:288:GLY:O	2.09	0.53
2:E:144:ASP:OD1	2:E:302:ASN:HA	2.08	0.53
2:I:219:SER:HB2	2:I:300:LEU:CD2	2.39	0.53
1:A:362:GLN:C	1:A:364:MET:H	2.16	0.53
2:P:146:PRO:HG2	2:P:149:GLU:HB2	1.91	0.53
2:E:122:LEU:CD2	2:F:335:GLN:NE2	2.71	0.53
2:E:242:THR:HG23	2:F:175:THR:OG1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:VAL:HG12	2:G:60:PRO:HD3	1.91	0.53
2:H:167:ILE:HB	2:H:168:PRO:HD3	1.91	0.53
2:S:5:MET:HE2	2:S:106:PRO:HD3	1.91	0.53
2:T:1:MET:O	2:T:2:SER:C	2.52	0.53
1:A:326:ASP:O	1:A:330:VAL:HG23	2.08	0.52
1:A:386:ILE:HG22	1:A:387:TYR:N	2.24	0.52
1:B:623:ARG:HG2	1:B:623:ARG:NH1	2.24	0.52
2:E:240:THR:HG22	2:E:242:THR:H	1.75	0.52
2:E:322:ASP:O	2:E:325:VAL:HG22	2.10	0.52
2:R:107:ARG:HG2	2:R:107:ARG:HH11	1.73	0.52
2:G:3:ARG:HD2	2:G:89:SER:O	2.09	0.52
1:A:450:ASN:O	1:A:452:ARG:N	2.42	0.52
1:B:666:GLY:O	1:B:667:GLU:C	2.52	0.52
2:C:121:ASN:HA	2:C:146:PRO:HA	1.90	0.52
2:C:277:ASN:ND2	2:F:210:VAL:HB	2.23	0.52
2:D:107:ARG:HG2	2:D:107:ARG:HH11	1.75	0.52
2:Q:107:ARG:HG2	2:Q:107:ARG:HH11	1.73	0.52
2:Q:197:ARG:HD2	2:Q:237:ALA:O	2.08	0.52
2:E:82:LEU:HD11	2:E:352:LEU:HG	1.92	0.52
2:R:229:ASN:HD21	2:G:235:ILE:H	1.57	0.52
2:G:268:ARG:HD2	2:H:321:ASP:HB2	1.91	0.52
1:A:378:THR:HG22	1:A:379:LEU:N	2.24	0.52
1:B:1006:HIS:CD2	1:B:1006:HIS:N	2.77	0.52
2:C:208:GLN:NE2	2:F:210:VAL:HG21	2.24	0.52
2:D:12:LEU:HD23	2:D:107:ARG:HD3	1.90	0.52
2:E:110:VAL:CG2	2:E:111:PRO:HA	2.39	0.52
2:E:337:ARG:HG3	2:E:337:ARG:NH1	2.24	0.52
2:R:160:VAL:C	2:R:315:GLN:HE21	2.17	0.52
2:G:192:ILE:HD11	2:G:218:LEU:HD13	1.90	0.52
2:H:230:SER:HA	2:H:234:THR:O	2.09	0.52
1:B:489:LEU:HD13	1:B:514:PRO:HB3	1.92	0.52
1:B:531:LEU:O	1:B:532:ALA:HB3	2.10	0.52
2:J:407:ILE:HD12	2:J:407:ILE:H	1.73	0.52
1:B:851:GLU:OE2	1:B:854:ARG:NH1	2.42	0.52
2:D:210:VAL:HA	2:D:277:ASN:OD1	2.10	0.52
2:Q:14:GLU:HG3	2:F:124:LEU:HD12	1.92	0.52
2:F:1:MET:HG3	2:F:100:ILE:CG2	2.40	0.52
2:F:151:ILE:C	2:F:151:ILE:HD12	2.34	0.52
2:F:244:THR:HB	2:F:247:ASP:OD1	2.09	0.52
2:R:239:VAL:HA	2:R:288:GLY:O	2.09	0.52
2:G:158:ARG:HG3	2:G:318:THR:HG21	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:151:ILE:HD13	2:S:156:LEU:HD13	1.91	0.52
2:S:214:TRP:CZ3	2:S:215:ALA:HB2	2.45	0.52
2:T:31:LEU:HD23	2:T:36:PHE:CZ	2.44	0.52
1:B:970:THR:HG23	1:B:971:GLU:HG2	1.91	0.52
2:P:121:ASN:HA	2:P:146:PRO:HA	1.91	0.52
2:P:349:MET:HA	2:P:349:MET:HE2	1.91	0.52
2:P:419:ARG:HD2	2:P:421:ASN:HD22	1.75	0.52
2:Q:197:ARG:HG2	2:Q:239:VAL:CG2	2.40	0.52
2:Q:211:VAL:HG12	2:Q:276:GLY:O	2.09	0.52
2:R:110:VAL:HG23	2:R:111:PRO:HA	1.91	0.52
2:I:64:MET:HE2	2:I:65:SER:HA	1.91	0.52
1:A:565:MET:HG3	1:A:566:TYR:CD1	2.44	0.52
2:F:120:ASN:O	2:F:121:ASN:C	2.53	0.52
2:F:229:ASN:C	2:F:229:ASN:ND2	2.60	0.52
2:F:244:THR:C	2:F:246:ALA:N	2.68	0.52
2:F:332:PHE:CE2	2:F:336:LEU:HD11	2.45	0.52
2:F:393:ASP:HB3	2:F:396:ILE:HG12	1.91	0.52
2:H:316:THR:CG2	2:H:397:ARG:HH12	2.23	0.52
2:S:1:MET:HB2	2:S:5:MET:SD	2.49	0.52
2:T:255:PRO:CB	2:T:275:GLY:HA3	2.40	0.52
1:A:340:PRO:HG2	1:A:341:ALA:H	1.75	0.52
2:P:80:TYR:CZ	2:P:81:MET:HG3	2.45	0.52
2:P:202:ILE:HG22	2:P:207:TYR:OH	2.10	0.52
2:D:121:ASN:HA	2:D:146:PRO:HA	1.91	0.52
2:E:24:ASN:HD22	2:E:25:GLY:N	2.07	0.52
2:E:350:ASP:OD2	2:E:382:ARG:NH2	2.39	0.52
2:J:57:PRO:O	2:J:61:LEU:HD23	2.10	0.52
1:A:124:ARG:NH1	1:A:128:SER:HB3	2.25	0.52
1:A:623:ARG:HG3	1:A:623:ARG:NH1	2.25	0.52
2:D:192:ILE:HD11	2:D:218:LEU:CD1	2.39	0.52
2:Q:170:MET:HE1	2:F:226:TYR:HD1	1.74	0.52
2:E:80:TYR:CE2	2:E:81:MET:HG3	2.44	0.52
2:F:252:PHE:CD1	2:F:278:ILE:HD11	2.45	0.52
2:G:349:MET:CE	2:G:352:LEU:CD2	2.83	0.52
2:G:379:PHE:HE1	2:G:404:LEU:HD22	1.74	0.52
2:T:137:ASN:HB3	2:T:143:LEU:HD12	1.90	0.52
2:T:225:VAL:HA	2:T:292:ALA:O	2.10	0.52
2:T:239:VAL:HA	2:T:288:GLY:O	2.09	0.52
1:B:127:TYR:OH	1:B:755:MET:HG2	2.10	0.52
2:P:169:MET:O	2:P:173:LEU:HD13	2.09	0.52
2:C:329:LEU:CD2	2:C:412:ALA:HB2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:242:THR:HG23	2:E:175:THR:OG1	2.09	0.52
2:Q:323:PHE:HB2	2:Q:405:TRP:NE1	2.24	0.52
2:E:191:ARG:HB3	2:E:294:GLU:HG3	1.91	0.52
2:E:386:ILE:HG21	2:E:400:ILE:CG2	2.40	0.52
2:F:244:THR:C	2:F:246:ALA:H	2.17	0.52
2:G:69:VAL:HA	2:G:72:ILE:HG22	1.92	0.52
2:G:160:VAL:HG22	2:G:161:ALA:H	1.75	0.52
2:T:271:PHE:CZ	2:T:293:ILE:HD13	2.45	0.52
2:T:361:MET:HG2	2:T:392:VAL:HG11	1.90	0.52
1:A:695:HIS:HE1	1:B:653:GLN:HG3	1.74	0.51
1:A:767:GLN:C	1:A:769:THR:H	2.18	0.51
1:B:37:GLU:O	1:B:41:ILE:HD13	2.10	0.51
2:P:148:SER:OG	2:C:331:THR:HG23	2.10	0.51
2:P:186:VAL:CG2	2:P:193:LEU:HB2	2.40	0.51
2:P:386:ILE:O	2:P:397:ARG:HG2	2.11	0.51
2:Q:82:LEU:HD11	2:Q:352:LEU:HD12	1.92	0.51
2:F:325:VAL:HG22	2:F:329:LEU:HD21	1.92	0.51
2:G:239:VAL:HG13	2:G:289:PHE:CA	2.40	0.51
2:S:28:PHE:HB2	2:S:31:LEU:CD2	2.41	0.51
2:I:161:ALA:HA	2:I:315:GLN:OE1	2.10	0.51
2:T:186:VAL:HG23	2:T:193:LEU:HB2	1.91	0.51
1:A:116:PRO:HB3	2:E:53:TYR:CD2	2.46	0.51
1:A:404:THR:HG22	1:A:406:ARG:H	1.76	0.51
1:A:714:LYS:HG3	1:B:18:LEU:HD21	1.91	0.51
1:B:269:LEU:HA	1:B:272:THR:CG2	2.40	0.51
2:P:157:PHE:C	2:P:158:ARG:HD2	2.35	0.51
2:C:274:GLY:C	2:C:276:GLY:H	2.18	0.51
2:G:124:LEU:HD21	2:H:416:ARG:HD3	1.92	0.51
2:H:110:VAL:HG23	2:H:111:PRO:HA	1.91	0.51
2:H:201:ALA:HA	2:H:287:THR:HA	1.92	0.51
2:H:339:CYS:CB	2:H:421:ASN:HD21	2.23	0.51
2:T:420:PRO:O	2:T:421:ASN:C	2.53	0.51
2:C:12:LEU:CD2	2:C:107:ARG:HD3	2.40	0.51
2:C:375:PRO:CD	2:C:378:ARG:HD3	2.39	0.51
2:D:24:ASN:C	2:D:24:ASN:ND2	2.68	0.51
2:D:110:VAL:HG22	2:D:111:PRO:HA	1.91	0.51
2:G:170:MET:HE2	2:G:232:PHE:HB2	1.91	0.51
2:S:137:ASN:HB3	2:S:143:LEU:HD12	1.91	0.51
2:I:6:TRP:CE3	2:I:410:LEU:HD13	2.45	0.51
2:T:43:PHE:HZ	2:T:60:PRO:HG3	1.74	0.51
2:C:9:THR:O	2:C:12:LEU:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:MET:CE	2:E:105:ARG:HA	2.40	0.51
2:F:1:MET:CA	2:F:93:PRO:HG2	2.40	0.51
2:S:121:ASN:HA	2:S:146:PRO:HA	1.93	0.51
2:I:332:PHE:CE2	2:I:336:LEU:HD11	2.46	0.51
2:T:170:MET:HE2	2:T:232:PHE:HB2	1.93	0.51
1:A:225:HIS:CE1	1:A:227:ILE:HG12	2.45	0.51
2:Q:203:PRO:HG2	2:Q:207:TYR:OH	2.10	0.51
2:F:166:ASN:HD22	2:F:167:ILE:HD12	1.76	0.51
2:G:133:TYR:HA	2:G:136:GLN:OE1	2.11	0.51
2:I:381:GLU:O	2:I:384:ARG:HB3	2.11	0.51
2:T:109:GLN:HG3	2:T:112:MET:HB3	1.92	0.51
1:A:780:ILE:HB	1:A:870:ILE:HB	1.91	0.51
2:C:132:LEU:HA	2:C:135:ARG:HD2	1.92	0.51
2:D:97:ASP:O	2:D:98:ASP:C	2.53	0.51
2:Q:12:LEU:HA	2:E:28:PHE:CZ	2.46	0.51
2:Q:186:VAL:HG23	2:Q:193:LEU:HB2	1.92	0.51
2:E:235:ILE:CD1	2:F:235:ILE:HD11	2.41	0.51
2:S:107:ARG:CG	2:S:107:ARG:NH1	2.67	0.51
2:I:261:LEU:CD2	2:J:378:ARG:CZ	2.89	0.51
2:I:320:ILE:HD11	2:I:383:ALA:CB	2.40	0.51
2:T:56:ASP:C	2:T:58:ARG:N	2.66	0.51
1:A:880:LEU:HG	1:A:881:GLN:N	2.26	0.51
2:Q:329:LEU:O	2:Q:330:THR:C	2.54	0.51
2:E:182:GLN:NE2	2:E:183:PRO:HD2	2.22	0.51
2:G:132:LEU:O	2:G:136:GLN:HG3	2.10	0.51
2:G:309:THR:O	2:G:310:LEU:HB2	2.10	0.51
2:H:161:ALA:HA	2:H:315:GLN:HE22	1.76	0.51
2:J:211:VAL:HG23	2:J:277:ASN:HA	1.93	0.51
2:P:115:THR:HG22	2:C:58:ARG:NH1	2.26	0.51
2:F:137:ASN:HB3	2:F:143:LEU:HD12	1.91	0.51
2:H:133:TYR:HA	2:H:136:GLN:HE21	1.75	0.51
2:S:323:PHE:HB2	2:S:405:TRP:NE1	2.26	0.51
2:J:403:HIS:HD2	2:J:407:ILE:CD1	2.24	0.51
2:T:140:MET:HE3	2:T:406:VAL:HG21	1.92	0.51
1:A:784:SER:HA	1:A:852:PHE:CZ	2.45	0.51
1:B:650:PRO:HB2	1:B:652:TYR:CE1	2.46	0.51
2:C:394:LEU:HG	2:C:398:LYS:HE3	1.92	0.51
2:Q:117:ARG:O	2:Q:120:ASN:HB3	2.11	0.51
2:H:1:MET:O	2:H:2:SER:C	2.53	0.51
1:A:241:ILE:CD1	1:A:242:GLN:HG3	2.41	0.51
1:B:336:ASN:O	1:B:337:VAL:HG13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ILE:HD12	1:B:444:ILE:N	2.24	0.51
2:P:145:ILE:CG1	2:P:146:PRO:HD2	2.41	0.51
2:C:33:THR:HG23	2:C:36:PHE:CB	2.41	0.51
2:G:396:ILE:O	2:G:400:ILE:HG13	2.11	0.51
2:S:211:VAL:HG12	2:S:276:GLY:O	2.11	0.51
2:S:356:LEU:HD23	2:S:404:LEU:HD23	1.93	0.51
2:I:54:VAL:HG12	2:I:56:ASP:N	2.26	0.51
2:I:357:ILE:HD13	2:I:400:ILE:HG21	1.93	0.51
1:A:129:MET:SD	1:A:765:MET:HE2	2.51	0.50
1:B:153:VAL:CG2	1:B:154:LYS:N	2.73	0.50
2:P:244:THR:HG22	2:P:245:ALA:N	2.26	0.50
2:E:138:ALA:O	2:E:142:GLY:HA2	2.11	0.50
2:F:105:ARG:HB2	2:F:106:PRO:HD2	1.94	0.50
2:R:163:GLN:HE22	2:R:185:PHE:H	1.59	0.50
2:R:254:VAL:CG1	2:R:255:PRO:HD2	2.39	0.50
2:J:208:GLN:HE21	2:J:208:GLN:N	2.09	0.50
1:A:432:LEU:CB	1:A:438:ILE:HG22	2.40	0.50
1:A:928:ASN:C	1:A:928:ASN:OD1	2.55	0.50
1:B:175:PHE:O	1:B:176:GLU:C	2.54	0.50
2:C:142:GLY:HA3	2:Q:344:ILE:CD1	2.36	0.50
2:D:140:MET:HE3	2:D:406:VAL:HG11	1.93	0.50
2:D:329:LEU:CD2	2:D:412:ALA:HB2	2.40	0.50
2:E:185:PHE:HE2	2:E:192:ILE:HD11	1.76	0.50
2:S:48:VAL:O	2:S:49:SER:HB3	2.10	0.50
2:I:352:LEU:HD21	2:I:407:ILE:HG21	1.93	0.50
2:I:357:ILE:HA	2:I:400:ILE:HD13	1.93	0.50
1:B:259:ASN:O	1:B:260:PHE:HB2	2.10	0.50
2:E:151:ILE:HG12	2:E:152:GLU:N	2.25	0.50
2:F:112:MET:O	2:F:116:VAL:HG23	2.11	0.50
2:I:19:TYR:CG	2:I:42:MET:HE1	2.45	0.50
1:A:508:PRO:HG2	1:A:509:TYR:CD1	2.47	0.50
1:A:607:ALA:HA	1:A:654:ILE:HD13	1.92	0.50
1:A:822:ARG:HH12	1:A:904:LEU:HD13	1.75	0.50
1:B:20:THR:O	1:B:20:THR:HG22	2.11	0.50
2:S:124:LEU:HD21	2:I:416:ARG:HD3	1.92	0.50
2:J:394:LEU:HA	2:J:397:ARG:NE	2.26	0.50
1:A:85:ILE:HD12	1:A:85:ILE:N	2.26	0.50
1:A:108:ILE:HG22	1:A:774:ILE:CD1	2.40	0.50
2:D:220:VAL:HA	2:D:296:GLU:O	2.11	0.50
2:E:163:GLN:HE22	2:E:185:PHE:N	1.90	0.50
2:E:254:VAL:HG11	2:E:272:SER:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:375:PRO:HD2	2:E:378:ARG:HD3	1.93	0.50
2:F:167:ILE:N	2:F:167:ILE:HD12	2.26	0.50
2:H:2:SER:OG	2:H:5:MET:HG3	2.12	0.50
1:A:210:VAL:CG2	1:A:276:ILE:HA	2.40	0.50
1:B:815:PHE:CA	1:B:874:MET:HE2	2.31	0.50
2:Q:170:MET:HE1	2:F:226:TYR:HB2	1.92	0.50
2:F:163:GLN:HG2	2:F:169:MET:HE2	1.94	0.50
2:H:323:PHE:HB2	2:H:405:TRP:HE1	1.77	0.50
2:S:47:SER:HB2	2:S:51:ALA:CB	2.41	0.50
2:I:310:LEU:HD22	2:I:313:ILE:HD11	1.93	0.50
2:T:167:ILE:N	2:T:168:PRO:CD	2.75	0.50
1:A:307:LEU:C	1:A:307:LEU:CD1	2.85	0.50
1:A:389:ALA:HB1	1:A:562:ILE:HD13	1.92	0.50
2:P:110:VAL:CG2	2:P:111:PRO:HA	2.42	0.50
2:C:87:PHE:CE1	2:C:140:MET:HG3	2.46	0.50
2:G:107:ARG:HH11	2:G:107:ARG:CG	2.23	0.50
2:S:28:PHE:HB2	2:S:31:LEU:HD21	1.92	0.50
2:I:203:PRO:HG2	2:I:207:TYR:OH	2.12	0.50
2:I:309:THR:O	2:I:310:LEU:HB2	2.12	0.50
2:J:104:ILE:N	2:J:104:ILE:HD12	2.27	0.50
2:P:254:VAL:HG12	2:P:256:THR:H	1.76	0.50
2:R:151:ILE:HD12	2:R:151:ILE:C	2.35	0.50
2:R:229:ASN:OD1	2:G:235:ILE:HG12	2.11	0.50
2:G:82:LEU:HD11	2:G:352:LEU:CD1	2.42	0.50
2:G:353:THR:CG2	2:G:404:LEU:HD11	2.39	0.50
2:S:91:THR:O	2:S:93:PRO:HD3	2.12	0.50
2:S:362:ASP:C	2:S:362:ASP:OD1	2.51	0.50
2:I:225:VAL:HA	2:I:292:ALA:O	2.11	0.50
2:I:251:THR:O	2:I:280:LEU:HD12	2.12	0.50
2:T:337:ARG:HH11	2:T:337:ARG:HG3	1.76	0.50
1:B:85:ILE:CD1	1:B:933:THR:OG1	2.60	0.50
1:B:406:ARG:O	1:B:409:LEU:HB3	2.12	0.50
2:P:378:ARG:O	2:P:380:SER:N	2.45	0.50
2:E:175:THR:O	2:E:176:PRO:C	2.55	0.50
2:F:225:VAL:HG11	2:F:252:PHE:HE2	1.76	0.50
2:R:120:ASN:O	2:R:121:ASN:C	2.55	0.50
2:R:375:PRO:HD2	2:R:378:ARG:HD3	1.94	0.50
2:G:230:SER:HB3	2:H:233:GLY:O	2.11	0.50
2:G:315:GLN:HE21	2:G:315:GLN:HA	1.77	0.50
2:J:355:SER:O	2:J:358:THR:HB	2.12	0.50
1:B:392:MET:HE3	1:B:561:LEU:CD2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:PHE:CE2	1:B:398:ILE:HD13	2.47	0.49
1:B:414:ARG:HG3	1:B:414:ARG:HH11	1.77	0.49
2:D:151:ILE:HD13	2:D:156:LEU:HD23	1.93	0.49
2:E:1:MET:O	2:E:2:SER:C	2.53	0.49
2:E:7:LEU:CD2	2:E:136:GLN:NE2	2.73	0.49
2:I:135:ARG:NH1	2:I:324:ASP:OD2	2.45	0.49
2:I:163:GLN:HE22	2:I:185:PHE:H	1.59	0.49
2:I:252:PHE:CE1	2:I:261:LEU:HD12	2.47	0.49
2:I:344:ILE:HD12	2:I:344:ILE:N	2.23	0.49
1:A:400:PRO:HG3	1:A:509:TYR:HB2	1.95	0.49
1:A:533:LEU:HD13	1:A:663:PHE:CE2	2.47	0.49
2:G:109:GLN:HB2	2:H:29:SER:HA	1.94	0.49
2:J:139:ILE:O	2:J:402:ARG:NH1	2.45	0.49
2:T:64:MET:HE2	2:T:64:MET:C	2.37	0.49
1:A:147:PHE:N	1:A:147:PHE:CD1	2.80	0.49
1:A:654:ILE:HD12	1:A:1010:LEU:HD21	1.93	0.49
1:A:716:ASP:O	1:A:719:LYS:HG2	2.12	0.49
1:A:731:SER:O	1:A:732:LYS:C	2.55	0.49
1:A:822:ARG:NH1	1:A:904:LEU:HD13	2.27	0.49
2:Q:374:SER:HB2	2:Q:375:PRO:HD2	1.94	0.49
2:E:239:VAL:HG13	2:E:289:PHE:HA	1.94	0.49
2:G:110:VAL:HG22	2:G:111:PRO:CA	2.42	0.49
1:A:125:VAL:O	1:A:126:ILE:C	2.55	0.49
1:A:170:ALA:C	1:A:172:HIS:H	2.20	0.49
1:B:177:HIS:O	1:B:178:ASP:C	2.55	0.49
2:C:120:ASN:O	2:C:122:LEU:N	2.46	0.49
2:D:132:LEU:O	2:D:136:GLN:HG3	2.12	0.49
2:E:360:TYR:CB	2:E:400:ILE:HD11	2.42	0.49
2:S:247:ASP:OD1	2:S:284:VAL:HG21	2.12	0.49
2:S:378:ARG:NH1	2:J:261:LEU:HD13	2.27	0.49
2:J:322:ASP:O	2:J:325:VAL:HG23	2.11	0.49
2:T:221:THR:HG22	2:T:270:SER:HB3	1.95	0.49
1:A:64:GLY:HA3	1:A:66:GLN:HE21	1.76	0.49
1:A:786:PHE:O	1:A:797:ALA:HA	2.13	0.49
1:B:623:ARG:HG2	1:B:623:ARG:HH11	1.77	0.49
2:P:244:THR:HB	2:P:247:ASP:OD1	2.12	0.49
2:C:277:ASN:HD21	2:F:210:VAL:HB	1.77	0.49
2:Q:361:MET:CE	2:Q:367:PRO:HG3	2.43	0.49
2:E:169:MET:O	2:E:173:LEU:HG	2.12	0.49
2:R:12:LEU:HD22	2:R:107:ARG:HD3	1.95	0.49
2:S:357:ILE:HD13	2:S:400:ILE:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:71:PHE:CZ	2:T:81:MET:HE3	2.47	0.49
1:B:298:LEU:C	1:B:298:LEU:HD23	2.37	0.49
2:P:235:ILE:HD11	2:D:235:ILE:HD11	1.93	0.49
2:C:142:GLY:N	2:Q:344:ILE:HD11	2.27	0.49
2:H:53:TYR:N	2:H:53:TYR:CD2	2.79	0.49
2:S:87:PHE:HB2	2:S:403:HIS:CE1	2.47	0.49
1:A:307:LEU:HD21	1:A:365:LEU:HB3	1.94	0.49
2:P:82:LEU:O	2:P:356:LEU:HD12	2.13	0.49
2:P:131:LYS:NZ	2:C:26:ASP:OD1	2.45	0.49
2:P:379:PHE:CE1	2:P:405:TRP:HA	2.47	0.49
2:C:156:LEU:HD21	2:C:299:ILE:HD11	1.93	0.49
2:G:1:MET:HB2	2:G:5:MET:SD	2.52	0.49
2:G:316:THR:HA	2:G:317:PRO:C	2.37	0.49
2:H:19:TYR:CD1	2:H:42:MET:HE1	2.48	0.49
2:S:80:TYR:CE2	2:S:81:MET:HE2	2.48	0.49
2:I:107:ARG:HH11	2:I:107:ARG:HG3	1.77	0.49
2:J:24:ASN:HD22	2:J:24:ASN:C	2.20	0.49
2:J:100:ILE:HD12	2:J:100:ILE:N	2.26	0.49
1:A:278:THR:O	1:A:279:LEU:HD23	2.13	0.49
1:A:284:VAL:HG23	1:A:284:VAL:O	2.13	0.49
1:A:362:GLN:C	1:A:364:MET:N	2.68	0.49
2:P:120:ASN:O	2:P:121:ASN:C	2.55	0.49
2:P:361:MET:HE1	2:P:367:PRO:HB3	1.94	0.49
2:C:107:ARG:HG2	2:C:107:ARG:HH11	1.77	0.49
2:E:361:MET:HE2	2:E:365:ALA:O	2.13	0.49
2:S:14:GLU:OE1	2:S:131:LYS:HB3	2.13	0.49
2:I:145:ILE:HD11	2:I:149:GLU:OE2	2.12	0.49
2:I:147:TYR:O	2:I:298:THR:HG21	2.11	0.49
2:J:158:ARG:NH2	2:J:321:ASP:OD1	2.46	0.49
1:B:110:HIS:C	1:B:112:SER:H	2.21	0.49
2:P:192:ILE:HD11	2:P:218:LEU:HD12	1.95	0.49
2:C:133:TYR:HA	2:C:136:GLN:OE1	2.13	0.49
2:D:36:PHE:O	2:D:40:SER:HB2	2.12	0.49
2:Q:175:THR:OG1	2:F:242:THR:HG23	2.12	0.49
2:F:280:LEU:CD2	2:F:289:PHE:HE1	2.25	0.49
2:R:419:ARG:O	2:R:419:ARG:HG2	2.13	0.49
2:I:112:MET:HE3	2:I:115:THR:HB	1.94	0.49
2:J:97:ASP:C	2:J:99:PHE:H	2.20	0.49
2:J:309:THR:O	2:J:310:LEU:HB2	2.13	0.49
2:J:358:THR:O	2:J:360:TYR:N	2.45	0.49
1:A:385:PHE:HA	1:A:566:TYR:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:H	1:A:555:LEU:HD12	1.78	0.49
1:A:783:ASN:ND2	1:A:784:SER:H	2.11	0.49
1:B:109:GLU:H	1:B:109:GLU:CD	2.20	0.49
1:B:439:TYR:O	1:B:440:PRO:C	2.56	0.49
2:P:91:THR:O	2:P:93:PRO:HD3	2.12	0.49
2:Q:5:MET:HE2	2:Q:105:ARG:HA	1.94	0.49
2:R:337:ARG:NH1	2:R:342:TYR:CE2	2.80	0.49
2:H:239:VAL:HG13	2:H:289:PHE:CA	2.43	0.49
2:S:253:THR:HG22	2:S:279:ASN:HB3	1.95	0.49
2:P:31:LEU:HD21	2:D:45:GLN:HG2	1.95	0.48
2:E:132:LEU:HG	2:E:328:PHE:CE1	2.48	0.48
2:F:186:VAL:HB	2:F:231:PHE:CE1	2.48	0.48
2:F:202:ILE:N	2:F:202:ILE:HD12	2.28	0.48
2:F:357:ILE:HG23	2:F:400:ILE:HD13	1.95	0.48
2:R:244:THR:HG22	2:R:246:ALA:H	1.78	0.48
2:S:71:PHE:HZ	2:S:81:MET:HE3	1.78	0.48
1:B:585:THR:O	1:B:589:SER:HB2	2.13	0.48
1:B:696:LEU:O	1:B:700:PHE:HD1	1.96	0.48
2:P:24:ASN:C	2:P:24:ASN:ND2	2.70	0.48
2:Q:253:THR:HG22	2:Q:260:ASN:HA	1.94	0.48
2:Q:332:PHE:CE2	2:Q:336:LEU:HD11	2.49	0.48
2:F:167:ILE:N	2:F:168:PRO:CD	2.76	0.48
2:F:396:ILE:O	2:F:400:ILE:HG13	2.13	0.48
2:H:169:MET:O	2:H:173:LEU:HG	2.12	0.48
2:T:396:ILE:O	2:T:400:ILE:HG13	2.13	0.48
1:A:591:PHE:HE1	1:A:642:LEU:HD12	1.76	0.48
1:B:675:ILE:HD13	1:B:717:VAL:HG13	1.94	0.48
2:C:329:LEU:HD23	2:C:412:ALA:HB2	1.93	0.48
2:G:56:ASP:OD1	2:G:58:ARG:HB2	2.12	0.48
2:H:323:PHE:HB2	2:H:405:TRP:NE1	2.29	0.48
1:B:443:ALA:O	1:B:444:ILE:C	2.57	0.48
1:B:561:LEU:O	1:B:565:MET:HG3	2.13	0.48
2:D:14:GLU:OE2	2:D:131:LYS:HB3	2.13	0.48
2:D:163:GLN:NE2	2:D:185:PHE:O	2.46	0.48
2:F:164:THR:HG23	2:F:165:GLY:N	2.29	0.48
2:J:387:LEU:HD21	2:J:401:VAL:HG21	1.94	0.48
2:T:271:PHE:HZ	2:T:293:ILE:HD13	1.78	0.48
1:A:641:LEU:HG	1:A:641:LEU:O	2.13	0.48
1:B:219:ARG:HD2	1:B:982:ASP:CG	2.38	0.48
1:B:404:THR:HG22	1:B:406:ARG:H	1.78	0.48
1:B:459:TYR:CG	1:B:473:ILE:HG21	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:28:PHE:CZ	2:F:12:LEU:HA	2.48	0.48
2:Q:186:VAL:HB	2:Q:231:PHE:CZ	2.49	0.48
2:E:121:ASN:HA	2:E:146:PRO:HA	1.96	0.48
2:R:167:ILE:N	2:R:168:PRO:CD	2.76	0.48
2:G:12:LEU:O	2:G:16:ILE:HG12	2.12	0.48
2:H:45:GLN:HE21	2:H:45:GLN:HB2	1.47	0.48
2:S:356:LEU:O	2:S:357:ILE:C	2.54	0.48
2:I:185:PHE:CD2	2:I:212:PRO:HD2	2.49	0.48
2:T:356:LEU:HD12	2:T:400:ILE:HG23	1.95	0.48
1:A:523:ARG:NH2	1:A:609:THR:HG23	2.28	0.48
2:P:31:LEU:CD2	2:D:41:ASN:HB3	2.41	0.48
2:C:105:ARG:HG3	2:C:106:PRO:N	2.28	0.48
2:D:145:ILE:HD12	2:D:308:TYR:HE1	1.78	0.48
2:E:140:MET:CE	2:E:406:VAL:HG11	2.43	0.48
2:E:363:PRO:HA	2:E:364:PRO:HD3	1.71	0.48
2:F:2:S:SER:HB3	2:F:5:MET:HE3	1.96	0.48
2:F:325:VAL:HG13	2:F:326:SER:N	2.29	0.48
2:S:13:LEU:HD21	2:S:64:MET:HE2	1.96	0.48
2:S:49:SER:C	2:S:51:ALA:N	2.67	0.48
2:S:158:ARG:HG3	2:S:313:ILE:HD13	1.96	0.48
2:S:379:PHE:CE1	2:S:404:LEU:HD12	2.49	0.48
2:S:379:PHE:O	2:S:380:SER:C	2.55	0.48
2:I:47:SER:O	2:I:49:SER:N	2.47	0.48
2:I:325:VAL:HG13	2:I:405:TRP:CZ2	2.48	0.48
2:P:132:LEU:HG	2:P:328:PHE:CE2	2.48	0.48
2:P:261:LEU:HD22	2:P:271:PHE:CD2	2.48	0.48
2:Q:235:ILE:HG12	2:F:229:ASN:HD21	1.78	0.48
2:F:239:VAL:HG13	2:F:288:GLY:O	2.13	0.48
2:F:378:ARG:NE	2:F:381:GLU:OE2	2.41	0.48
2:G:419:ARG:HD2	2:G:421:ASN:HD22	1.77	0.48
2:H:24:ASN:HD22	2:H:24:ASN:C	2.22	0.48
2:S:1:MET:O	2:S:2:SER:C	2.55	0.48
2:S:173:LEU:HB3	2:S:236:ILE:HG23	1.95	0.48
2:J:353:THR:HG22	2:J:404:LEU:HD11	1.95	0.48
1:A:468:VAL:O	1:A:472:LEU:HD23	2.13	0.48
1:B:597:ASN:C	1:B:599:LEU:N	2.70	0.48
2:D:121:ASN:HA	2:D:146:PRO:HB3	1.95	0.48
2:E:61:LEU:HD22	2:E:417:TYR:CE1	2.48	0.48
2:R:121:ASN:HA	2:R:146:PRO:HA	1.95	0.48
2:R:256:THR:HG22	2:G:337:ARG:NH1	2.28	0.48
2:R:361:MET:CE	2:R:367:PRO:HB3	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:156:LEU:HD21	2:G:307:TYR:HB2	1.95	0.48
2:S:309:THR:O	2:S:309:THR:HG22	2.14	0.48
2:T:332:PHE:CE2	2:T:336:LEU:HD11	2.49	0.48
1:B:165:ASN:ND2	1:B:168:ALA:H	2.12	0.48
2:C:225:VAL:HA	2:C:292:ALA:O	2.13	0.48
2:D:3:ARG:HG3	2:D:4:GLN:N	2.27	0.48
2:D:160:VAL:HG12	2:D:161:ALA:N	2.29	0.48
2:D:272:SER:C	2:D:274:GLY:N	2.69	0.48
2:Q:282:LEU:HD11	2:Q:289:PHE:CD2	2.49	0.48
2:E:186:VAL:HG21	2:E:231:PHE:CZ	2.49	0.48
2:G:282:LEU:HD21	2:G:286:LYS:HD2	1.96	0.48
2:I:100:ILE:HG22	2:I:101:THR:N	2.28	0.48
2:I:104:ILE:HD12	2:I:104:ILE:N	2.28	0.48
2:P:390:GLN:H	2:P:390:GLN:HG2	1.35	0.48
2:C:14:GLU:HG2	2:C:131:LYS:HD3	1.94	0.48
2:D:121:ASN:HA	2:D:146:PRO:CB	2.44	0.48
2:D:166:ASN:N	2:D:168:PRO:HD2	2.29	0.48
2:D:254:VAL:HG12	2:D:256:THR:H	1.79	0.48
2:F:110:VAL:HG23	2:F:111:PRO:HA	1.96	0.48
2:G:69:VAL:HG21	2:G:418:TYR:CZ	2.48	0.48
2:R:41:ASN:HD21	2:R:45:GLN:HE21	1.62	0.47
2:G:140:MET:HE3	2:G:406:VAL:HG11	1.96	0.47
2:I:239:VAL:HG13	2:I:289:PHE:HA	1.96	0.47
2:J:341:GLN:HA	2:J:344:ILE:HD13	1.95	0.47
1:B:297:PRO:HB3	1:B:630:TRP:CE2	2.48	0.47
2:P:114:ASP:CG	2:P:117:ARG:HH12	2.22	0.47
2:C:59:VAL:HB	2:C:60:PRO:HD3	1.95	0.47
2:C:254:VAL:HG12	2:C:256:THR:H	1.78	0.47
2:D:182:GLN:HB3	2:D:183:PRO:HD2	1.96	0.47
2:D:239:VAL:HG13	2:D:289:PHE:CA	2.44	0.47
2:F:239:VAL:HG13	2:F:289:PHE:HA	1.97	0.47
2:R:64:MET:HE2	2:R:65:SER:N	2.30	0.47
2:H:14:GLU:OE2	2:H:131:LYS:HB3	2.14	0.47
2:S:378:ARG:HH11	2:J:261:LEU:HD13	1.78	0.47
2:Q:1:MET:HB2	2:Q:5:MET:SD	2.55	0.47
2:E:122:LEU:HD21	2:F:335:GLN:NE2	2.10	0.47
2:G:363:PRO:HA	2:G:364:PRO:HD3	1.76	0.47
2:H:379:PHE:O	2:H:381:GLU:N	2.47	0.47
2:I:219:SER:HB2	2:I:300:LEU:HD23	1.97	0.47
2:T:2:SER:CB	2:T:5:MET:HE3	2.44	0.47
2:T:255:PRO:HG2	2:T:275:GLY:HA3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ASP:OD2	1:B:1005:VAL:HG12	2.13	0.47
1:A:861:VAL:HG12	1:A:862:PHE:N	2.29	0.47
1:B:245:HIS:CD2	1:B:246:PRO:HD2	2.50	0.47
1:B:541:ILE:HG23	1:B:542:THR:HG22	1.97	0.47
1:B:558:LYS:O	1:B:562:ILE:HG13	2.14	0.47
2:C:274:GLY:C	2:C:276:GLY:N	2.71	0.47
2:F:325:VAL:O	2:F:329:LEU:HD22	2.15	0.47
2:G:117:ARG:NH2	2:G:118:GLN:HE21	2.13	0.47
2:H:140:MET:HE1	2:H:406:VAL:HG11	1.95	0.47
2:H:170:MET:HE2	2:H:232:PHE:HB2	1.95	0.47
2:H:272:SER:C	2:H:274:GLY:H	2.22	0.47
2:S:316:THR:HG21	2:S:397:ARG:HH12	1.79	0.47
2:I:46:LEU:N	2:I:46:LEU:HD12	2.28	0.47
2:J:99:PHE:HD2	2:J:100:ILE:HD12	1.78	0.47
2:J:206:ALA:C	2:J:207:TYR:CD1	2.92	0.47
2:J:358:THR:C	2:J:360:TYR:H	2.22	0.47
1:A:334:SER:O	1:A:336:ASN:N	2.47	0.47
1:A:400:PRO:HB2	1:A:515:ILE:HG12	1.96	0.47
1:B:31:VAL:HG12	1:B:32:TYR:H	1.79	0.47
2:Q:272:SER:OG	2:Q:300:LEU:HD11	2.15	0.47
2:R:186:VAL:HG23	2:R:193:LEU:HB2	1.95	0.47
2:S:416:ARG:O	2:J:122:LEU:HD13	2.15	0.47
2:J:193:LEU:HD12	2:J:231:PHE:HD1	1.79	0.47
2:J:309:THR:O	2:J:309:THR:HG22	2.15	0.47
1:A:558:LYS:O	1:A:562:ILE:HG13	2.15	0.47
1:A:653:GLN:HG3	1:A:653:GLN:O	2.13	0.47
2:C:120:ASN:C	2:C:122:LEU:N	2.71	0.47
2:Q:377:PHE:C	2:Q:377:PHE:CD1	2.93	0.47
2:R:192:ILE:HD11	2:R:218:LEU:CD1	2.45	0.47
2:R:231:PHE:O	2:R:232:PHE:HB2	2.13	0.47
2:I:110:VAL:CG2	2:I:111:PRO:HA	2.44	0.47
2:I:357:ILE:HD13	2:I:400:ILE:HD13	1.96	0.47
1:A:104:LYS:HD3	1:B:23:THR:HG22	1.96	0.47
1:A:490:ILE:HB	1:A:501:GLU:HB2	1.96	0.47
1:B:673:GLN:HE21	1:B:747:LEU:HD12	1.80	0.47
2:P:225:VAL:HA	2:P:292:ALA:O	2.15	0.47
2:P:363:PRO:HA	2:P:364:PRO:HD3	1.83	0.47
2:C:16:ILE:O	2:C:20:VAL:HG23	2.14	0.47
2:C:190:ARG:O	2:C:190:ARG:HG2	2.14	0.47
2:D:64:MET:HE2	2:D:65:SER:N	2.30	0.47
2:Q:82:LEU:HD11	2:Q:352:LEU:CD1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:VAL:HG22	2:E:187:ALA:N	2.29	0.47
2:E:280:LEU:CD2	2:E:289:PHE:HE1	2.28	0.47
2:F:45:GLN:O	2:F:107:ARG:NH1	2.46	0.47
2:F:156:LEU:HD22	2:F:218:LEU:HD21	1.97	0.47
2:F:184:PHE:CD1	2:F:184:PHE:C	2.93	0.47
2:G:13:LEU:HD21	2:G:64:MET:HE2	1.95	0.47
2:G:14:GLU:OE1	2:G:131:LYS:HB3	2.15	0.47
2:H:82:LEU:HD22	2:H:356:LEU:HD23	1.97	0.47
2:H:271:PHE:CZ	2:H:293:ILE:HD13	2.50	0.47
2:S:158:ARG:CG	2:S:313:ILE:HD13	2.44	0.47
2:S:221:THR:HG21	2:I:326:SER:O	2.15	0.47
2:S:416:ARG:HD3	2:J:124:LEU:HD23	1.96	0.47
2:I:2:SER:OG	2:I:5:MET:HE3	2.15	0.47
2:I:24:ASN:C	2:I:24:ASN:ND2	2.72	0.47
2:J:169:MET:O	2:J:173:LEU:HG	2.14	0.47
2:T:133:TYR:HA	2:T:136:GLN:OE1	2.14	0.47
1:A:241:ILE:HD12	1:A:242:GLN:N	2.30	0.47
1:A:303:LEU:HD22	1:A:369:ILE:HD11	1.97	0.47
1:A:356:LEU:O	1:A:360:ILE:HG13	2.14	0.47
1:A:492:ALA:C	1:A:494:GLN:H	2.22	0.47
1:B:2:ASP:C	1:B:4:THR:H	2.23	0.47
1:B:222:VAL:CG1	1:B:224:TYR:HD1	2.28	0.47
1:B:444:ILE:CD1	1:B:444:ILE:N	2.73	0.47
2:P:230:SER:HB3	2:C:233:GLY:O	2.14	0.47
2:P:418:TYR:CE1	2:P:420:PRO:HG3	2.50	0.47
2:C:123:SER:HB2	2:D:17:SER:OG	2.15	0.47
2:D:110:VAL:HG23	2:D:111:PRO:HA	1.97	0.47
2:D:363:PRO:HA	2:D:364:PRO:HD3	1.81	0.47
2:F:56:ASP:OD1	2:F:58:ARG:HB2	2.15	0.47
2:F:203:PRO:HG2	2:F:207:TYR:OH	2.15	0.47
2:R:235:ILE:HD12	2:R:235:ILE:N	2.29	0.47
2:G:135:ARG:NH1	2:G:324:ASP:OD2	2.47	0.47
2:G:350:ASP:O	2:G:354:ASN:HB2	2.14	0.47
2:S:322:ASP:O	2:S:325:VAL:HG22	2.15	0.47
2:I:211:VAL:HG22	2:I:276:GLY:O	2.13	0.47
2:J:166:ASN:OD1	2:J:186:VAL:CG2	2.62	0.47
2:T:132:LEU:O	2:T:136:GLN:HG3	2.14	0.47
1:A:484:GLN:NE2	2:D:29:SER:O	2.48	0.47
1:A:551:SER:OG	1:A:553:GLU:HB2	2.14	0.47
2:P:361:MET:CE	2:P:392:VAL:HG22	2.44	0.47
2:Q:168:PRO:C	2:Q:170:MET:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:SER:CB	2:G:5:MET:HE3	2.45	0.47
2:H:379:PHE:O	2:H:380:SER:C	2.57	0.47
2:S:379:PHE:HE1	2:S:404:LEU:HD12	1.80	0.47
2:I:186:VAL:HG23	2:I:193:LEU:HB2	1.96	0.47
2:T:255:PRO:CG	2:T:275:GLY:HA3	2.45	0.47
1:A:222:VAL:HB	1:A:223:PRO:HD2	1.96	0.47
1:B:177:HIS:H	1:B:177:HIS:CD2	2.33	0.47
1:B:183:GLN:O	1:B:186:ASN:HB2	2.16	0.47
2:F:323:PHE:O	2:F:324:ASP:HB2	2.15	0.47
2:G:167:ILE:N	2:G:168:PRO:CD	2.78	0.47
2:T:59:VAL:N	2:T:60:PRO:HD2	2.30	0.47
2:T:349:MET:HE3	2:T:352:LEU:HG	1.96	0.47
1:A:679:TYR:CD1	1:A:703:ILE:HD11	2.50	0.46
1:B:514:PRO:HB2	1:B:517:MET:HE3	1.97	0.46
1:B:956:GLN:C	1:B:957:ILE:HD12	2.40	0.46
2:Q:84:LYS:HE2	2:S:351:GLN:HE22	1.79	0.46
2:F:164:THR:HG23	2:F:165:GLY:H	1.80	0.46
2:R:154:CYS:HB3	2:R:188:GLU:O	2.14	0.46
2:G:322:ASP:HB2	2:G:325:VAL:HG12	1.97	0.46
2:G:349:MET:HE3	2:G:352:LEU:HD23	1.96	0.46
2:H:122:LEU:HD12	2:H:122:LEU:N	2.30	0.46
2:I:349:MET:HE2	2:I:376:TRP:CE3	2.51	0.46
2:I:396:ILE:N	2:I:396:ILE:CD1	2.78	0.46
2:J:361:MET:HE3	2:J:361:MET:HB2	1.87	0.46
2:T:349:MET:HG2	2:T:376:TRP:CD2	2.51	0.46
2:C:337:ARG:HG3	2:C:337:ARG:NH1	2.28	0.46
2:Q:382:ARG:O	2:Q:386:ILE:HG12	2.15	0.46
2:E:9:THR:HA	2:E:107:ARG:HG3	1.97	0.46
2:S:22:ARG:HD3	2:S:35:ASP:OD2	2.15	0.46
1:A:170:ALA:C	1:A:172:HIS:N	2.74	0.46
1:A:787:VAL:HG21	1:A:853:VAL:HG12	1.97	0.46
1:B:63:ILE:HG12	1:B:64:GLY:N	2.29	0.46
1:B:74:ILE:HD11	1:B:979:PHE:CE1	2.50	0.46
2:C:83:ARG:HG2	2:C:359:ASN:ND2	2.30	0.46
2:F:226:TYR:N	2:F:226:TYR:CD2	2.82	0.46
2:R:271:PHE:CZ	2:R:293:ILE:HD13	2.50	0.46
2:R:337:ARG:HH12	2:H:256:THR:HG22	1.79	0.46
2:R:361:MET:HE1	2:R:367:PRO:CG	2.46	0.46
2:H:140:MET:CE	2:H:406:VAL:HG11	2.45	0.46
2:S:329:LEU:O	2:S:330:THR:C	2.58	0.46
2:T:156:LEU:CD1	2:T:218:LEU:HD21	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:254:VAL:HG13	2:T:255:PRO:HD2	1.97	0.46
1:B:438:ILE:HG23	1:B:447:TRP:CZ2	2.48	0.46
2:D:16:ILE:HD11	2:D:42:MET:HB3	1.97	0.46
2:D:311:ASN:C	2:D:313:ILE:H	2.24	0.46
2:E:386:ILE:HG21	2:E:400:ILE:HG21	1.96	0.46
2:E:420:PRO:O	2:E:421:ASN:OXT	2.34	0.46
2:I:378:ARG:HB3	2:I:381:GLU:OE1	2.16	0.46
2:T:272:SER:C	2:T:274:GLY:H	2.24	0.46
1:B:217:TYR:CE2	1:B:986:ARG:HB2	2.50	0.46
2:P:167:ILE:N	2:P:168:PRO:CD	2.78	0.46
2:C:239:VAL:HG13	2:C:289:PHE:HA	1.98	0.46
2:Q:145:ILE:HG12	2:Q:146:PRO:CD	2.42	0.46
2:F:69:VAL:HG21	2:F:418:TYR:CD1	2.51	0.46
2:F:217:VAL:HG22	2:F:303:ARG:HH21	1.81	0.46
2:F:271:PHE:CZ	2:F:293:ILE:HD13	2.50	0.46
2:H:5:MET:SD	2:H:106:PRO:HD3	2.56	0.46
2:H:361:MET:HE3	2:H:361:MET:HB2	1.70	0.46
2:S:271:PHE:CZ	2:S:293:ILE:HD13	2.50	0.46
2:J:250:THR:HG23	2:J:282:LEU:HA	1.98	0.46
1:A:591:PHE:HD2	1:A:592:LEU:HD23	1.80	0.46
1:A:805:VAL:O	1:A:805:VAL:HG12	2.16	0.46
1:B:429:THR:O	1:B:433:VAL:HG23	2.16	0.46
2:P:95:VAL:HG23	2:P:95:VAL:O	2.15	0.46
2:D:332:PHE:CE2	2:D:336:LEU:HD11	2.50	0.46
2:E:379:PHE:O	2:E:380:SER:C	2.59	0.46
2:G:214:TRP:CZ3	2:G:215:ALA:HB2	2.50	0.46
2:H:363:PRO:HA	2:H:364:PRO:HD3	1.73	0.46
2:J:97:ASP:O	2:J:99:PHE:N	2.48	0.46
2:J:156:LEU:O	2:J:214:TRP:HB2	2.15	0.46
1:A:455:LEU:HD23	1:A:477:PHE:CZ	2.50	0.46
1:B:437:VAL:HG13	1:B:457:ALA:HB1	1.98	0.46
2:P:316:THR:HG21	2:P:397:ARG:HH12	1.81	0.46
2:P:377:PHE:CD1	2:P:377:PHE:C	2.94	0.46
2:D:95:VAL:O	2:D:95:VAL:HG23	2.15	0.46
2:E:14:GLU:OE2	2:E:131:LYS:HB3	2.15	0.46
2:F:128:ALA:O	2:F:130:PRO:HD3	2.16	0.46
2:R:170:MET:HE2	2:R:232:PHE:HB2	1.98	0.46
2:G:158:ARG:NH2	2:G:321:ASP:OD2	2.45	0.46
2:S:110:VAL:HG22	2:S:111:PRO:HA	1.97	0.46
2:T:9:THR:HG21	2:T:104:ILE:HA	1.98	0.46
2:T:379:PHE:O	2:T:380:SER:C	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG23	1:A:276:ILE:CA	2.44	0.46
1:A:327:LEU:O	1:A:331:VAL:HG22	2.15	0.46
1:B:262:ARG:NH1	1:B:262:ARG:HB3	2.29	0.46
1:B:769:THR:C	1:B:771:ILE:H	2.24	0.46
1:B:878:PHE:HA	1:B:921:VAL:O	2.16	0.46
2:C:110:VAL:HG23	2:C:111:PRO:HA	1.97	0.46
2:C:158:ARG:NH2	2:C:320:ILE:HG13	2.31	0.46
2:C:231:PHE:HB2	2:C:236:ILE:HD11	1.97	0.46
2:Q:378:ARG:NH1	2:F:257:ASP:OD1	2.46	0.46
2:F:87:PHE:HB2	2:F:403:HIS:ND1	2.31	0.46
2:G:318:THR:CG2	2:G:319:SER:N	2.78	0.46
2:H:156:LEU:HD22	2:H:218:LEU:HD21	1.97	0.46
2:S:363:PRO:HA	2:S:364:PRO:HD3	1.74	0.46
2:J:227:PHE:HZ	2:J:250:THR:HG21	1.80	0.46
2:T:45:GLN:O	2:T:46:LEU:C	2.59	0.46
1:A:93:PHE:CD2	1:A:975:LEU:HD22	2.51	0.46
1:A:108:ILE:H	1:A:108:ILE:CD1	2.22	0.46
1:A:129:MET:HE1	1:A:765:MET:CE	2.46	0.46
1:A:349:ASN:N	1:A:349:ASN:ND2	2.63	0.46
1:A:537:SER:HB3	1:A:538:PRO:CD	2.46	0.46
1:B:60:LEU:HA	1:B:135:ALA:HB1	1.98	0.46
1:B:732:LYS:N	1:B:733:PRO:CD	2.79	0.46
2:D:69:VAL:HG21	2:D:418:TYR:CG	2.50	0.46
2:E:150:PRO:HA	2:E:297:PHE:O	2.16	0.46
2:F:140:MET:CE	2:F:406:VAL:HG11	2.45	0.46
2:S:211:VAL:HG13	2:S:211:VAL:O	2.15	0.46
2:T:396:ILE:HD12	2:T:396:ILE:N	2.31	0.46
1:A:410:ASP:O	1:A:414:ARG:HG2	2.16	0.46
1:B:212:GLU:CD	1:B:986:ARG:HH12	2.24	0.46
1:B:810:HIS:CD2	1:B:840:MET:HG3	2.51	0.46
2:P:68:PHE:HB2	2:P:99:PHE:CE1	2.51	0.46
2:F:211:VAL:HG23	2:F:276:GLY:C	2.41	0.46
2:R:160:VAL:HG12	2:R:161:ALA:N	2.30	0.46
1:A:245:HIS:CD2	1:A:246:PRO:HD2	2.51	0.45
1:A:773:PRO:O	1:A:774:ILE:HG13	2.16	0.45
1:B:308:LEU:CD2	1:B:362:GLN:HB2	2.43	0.45
1:B:362:GLN:C	1:B:364:MET:H	2.24	0.45
1:B:478:ARG:HD2	1:B:557:HIS:NE2	2.31	0.45
2:D:4:GLN:HE22	2:D:141:LYS:NZ	2.14	0.45
2:D:135:ARG:NH1	2:D:323:PHE:O	2.49	0.45
2:Q:64:MET:HE2	2:Q:65:SER:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:LEU:HD22	2:E:136:GLN:NE2	2.30	0.45
2:F:215:ALA:C	2:F:217:VAL:H	2.25	0.45
2:R:12:LEU:HA	2:G:28:PHE:CZ	2.51	0.45
2:I:310:LEU:HB3	2:I:313:ILE:HD12	1.98	0.45
2:I:322:ASP:HB2	2:I:325:VAL:CG2	2.47	0.45
2:T:56:ASP:O	2:T:58:ARG:N	2.49	0.45
2:T:240:THR:HB	2:T:242:THR:CG2	2.46	0.45
1:A:630:TRP:O	1:A:725:MET:HE2	2.16	0.45
1:A:847:ILE:HG23	1:A:864:GLU:HG3	1.99	0.45
1:B:127:TYR:O	1:B:130:LEU:HB2	2.16	0.45
2:P:28:PHE:CZ	2:D:12:LEU:HA	2.51	0.45
2:C:82:LEU:HD11	2:C:352:LEU:HD22	1.97	0.45
2:C:266:ASP:OD1	2:D:166:ASN:HB3	2.16	0.45
2:C:277:ASN:OD1	2:F:210:VAL:HG12	2.15	0.45
2:E:24:ASN:HD22	2:E:24:ASN:C	2.24	0.45
2:E:203:PRO:O	2:E:204:ALA:C	2.59	0.45
2:F:1:MET:HB3	2:F:93:PRO:HG2	1.98	0.45
2:F:33:THR:O	2:F:34:GLY:C	2.60	0.45
2:G:53:TYR:C	2:G:55:SER:N	2.73	0.45
2:S:192:ILE:HG21	2:S:293:ILE:HD12	1.98	0.45
2:I:153:PRO:O	2:I:156:LEU:N	2.48	0.45
2:J:378:ARG:HB3	2:J:381:GLU:OE1	2.16	0.45
2:T:26:ASP:HA	2:T:28:PHE:CE1	2.52	0.45
2:T:111:PRO:O	2:T:112:MET:C	2.58	0.45
1:A:286:GLN:HE21	1:A:286:GLN:C	2.23	0.45
1:A:360:ILE:HG23	1:A:397:LEU:O	2.15	0.45
1:A:697:GLU:HG3	1:A:718:ARG:NH2	2.31	0.45
1:B:227:ILE:HD11	1:B:768:LEU:CD2	2.46	0.45
2:C:125:GLN:HE22	2:D:131:LYS:HA	1.81	0.45
2:D:120:ASN:O	2:D:121:ASN:C	2.59	0.45
2:D:387:LEU:HG	2:D:401:VAL:HG21	1.98	0.45
2:Q:81:MET:HE1	2:Q:410:LEU:HD23	1.99	0.45
2:Q:261:LEU:HD23	2:E:378:ARG:CZ	2.46	0.45
2:F:193:LEU:HD12	2:F:231:PHE:CD1	2.50	0.45
2:R:161:ALA:N	2:R:315:GLN:HE21	2.15	0.45
2:R:323:PHE:HB2	2:R:405:TRP:NE1	2.31	0.45
2:R:344:ILE:HD12	2:R:344:ILE:N	2.20	0.45
1:B:177:HIS:C	1:B:179:VAL:N	2.73	0.45
1:B:518:LEU:O	1:B:520:PRO:HD3	2.17	0.45
2:Q:31:LEU:CD1	2:F:42:MET:HG2	2.45	0.45
2:Q:112:MET:HE3	2:E:36:PHE:HZ	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ILE:HG12	2:F:146:PRO:CD	2.46	0.45
2:F:211:VAL:HG23	2:F:277:ASN:N	2.32	0.45
2:R:337:ARG:NH1	2:H:256:THR:CG2	2.80	0.45
2:G:13:LEU:HD21	2:G:64:MET:CE	2.47	0.45
2:J:133:TYR:HA	2:J:136:GLN:OE1	2.16	0.45
2:J:381:GLU:O	2:J:384:ARG:N	2.50	0.45
2:T:169:MET:O	2:T:173:LEU:HD13	2.17	0.45
1:A:307:LEU:HD13	1:A:307:LEU:C	2.42	0.45
1:A:340:PRO:CG	1:A:584:ASN:HD21	2.30	0.45
1:A:392:MET:HA	1:A:392:MET:CE	2.41	0.45
1:A:545:GLU:O	1:A:546:GLY:O	2.34	0.45
1:A:706:ILE:O	1:A:707:VAL:C	2.58	0.45
1:A:712:GLN:O	1:A:713:GLN:HB2	2.17	0.45
2:C:254:VAL:HG13	2:C:255:PRO:HD2	1.98	0.45
2:C:329:LEU:O	2:C:330:THR:C	2.59	0.45
2:D:387:LEU:HD23	2:D:397:ARG:HB3	1.97	0.45
2:E:69:VAL:HG21	2:E:418:TYR:CD1	2.51	0.45
2:E:394:LEU:HG	2:E:398:LYS:HE3	1.98	0.45
2:F:244:THR:O	2:F:246:ALA:N	2.49	0.45
2:F:322:ASP:HB2	2:F:325:VAL:CG1	2.40	0.45
2:R:341:GLN:O	2:R:342:TYR:C	2.59	0.45
2:G:349:MET:HE1	2:G:352:LEU:HD22	1.95	0.45
2:I:244:THR:HB	2:I:247:ASP:OD1	2.17	0.45
2:J:188:GLU:HA	2:J:232:PHE:CE1	2.51	0.45
2:J:346:SER:O	2:J:350:ASP:OD1	2.34	0.45
2:T:207:TYR:N	2:T:207:TYR:CD1	2.84	0.45
1:A:531:LEU:O	1:A:532:ALA:CB	2.64	0.45
1:A:570:PHE:HE1	1:A:577:TRP:CE3	2.34	0.45
1:B:704:GLU:HG3	1:B:717:VAL:HG23	1.98	0.45
1:B:772:ILE:HD12	1:B:772:ILE:O	2.17	0.45
2:C:157:PHE:HD1	2:C:214:TRP:CE2	2.35	0.45
2:C:210:VAL:HG23	2:C:210:VAL:O	2.16	0.45
2:F:421:ASN:HA	2:R:144:ASP:OD2	2.16	0.45
2:G:66:ASN:HD22	2:G:418:TYR:HD1	1.64	0.45
2:H:157:PHE:HD1	2:H:214:TRP:CE2	2.35	0.45
2:S:175:THR:OG1	2:J:242:THR:HG23	2.16	0.45
2:I:118:GLN:C	2:I:120:ASN:N	2.73	0.45
2:J:59:VAL:O	2:J:62:GLN:HB3	2.16	0.45
2:T:5:MET:HB3	2:T:104:ILE:HG22	1.98	0.45
2:T:24:ASN:HD22	2:T:24:ASN:C	2.22	0.45
1:A:340:PRO:HG3	1:A:584:ASN:HD21	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:O	1:B:282:ARG:HG3	2.16	0.45
1:B:772:ILE:CD1	1:B:774:ILE:HB	2.47	0.45
2:D:1:MET:HE3	2:D:5:MET:HE1	1.98	0.45
2:D:120:ASN:C	2:D:122:LEU:N	2.74	0.45
2:Q:61:LEU:HD12	2:F:119:LEU:HD21	1.99	0.45
2:Q:193:LEU:HD21	2:Q:292:ALA:HB2	1.99	0.45
2:R:82:LEU:HD11	2:R:352:LEU:HD22	1.98	0.45
2:R:124:LEU:CD2	2:G:416:ARG:HD3	2.47	0.45
2:H:244:THR:HB	2:H:247:ASP:OD1	2.17	0.45
2:I:150:PRO:HA	2:I:297:PHE:O	2.17	0.45
2:T:145:ILE:HD11	2:T:149:GLU:OE2	2.17	0.45
1:B:263:LEU:O	1:B:264:ASP:C	2.60	0.45
2:C:225:VAL:HG12	2:C:263:VAL:HG13	1.98	0.45
2:Q:17:SER:O	2:Q:18:GLU:C	2.58	0.45
2:Q:154:CYS:HB3	2:Q:187:ALA:O	2.17	0.45
2:E:156:LEU:CD1	2:E:218:LEU:HD21	2.47	0.45
2:E:198:SER:HB3	2:E:202:ILE:HD11	1.99	0.45
2:R:1:MET:HB3	2:R:93:PRO:HD2	1.99	0.45
2:S:374:SER:HB2	2:S:375:PRO:HD2	1.99	0.45
2:J:188:GLU:CD	2:J:191:ARG:HE	2.25	0.45
1:B:58:ILE:CG1	1:B:754:ILE:HD13	2.47	0.45
1:B:65:LEU:HD21	1:B:222:VAL:HG11	1.99	0.45
2:P:195:GLY:C	2:P:196:ILE:HG13	2.42	0.45
2:C:62:GLN:HG3	2:C:419:ARG:HB3	1.98	0.45
2:D:309:THR:O	2:D:309:THR:CG2	2.63	0.45
2:Q:1:MET:O	2:Q:2:SER:C	2.60	0.45
2:E:320:ILE:HD11	2:E:383:ALA:HB1	1.99	0.45
2:F:201:ALA:HA	2:F:287:THR:HA	1.98	0.45
2:R:132:LEU:O	2:R:136:GLN:HG3	2.17	0.45
2:R:363:PRO:HA	2:R:364:PRO:HD3	1.85	0.45
2:H:156:LEU:HD11	2:H:299:ILE:HD11	1.99	0.45
2:J:254:VAL:HG13	2:J:255:PRO:HD2	1.98	0.45
1:A:286:GLN:CG	1:A:748:PRO:HA	2.46	0.45
1:A:311:ILE:HD11	1:A:362:GLN:HB3	1.98	0.45
1:A:669:ILE:N	1:A:669:ILE:CD1	2.79	0.45
1:A:914:TYR:O	1:B:1005:VAL:HG23	2.17	0.45
1:A:915:ARG:HH22	1:B:30:GLU:CD	2.25	0.45
1:B:222:VAL:HG13	1:B:223:PRO:CD	2.46	0.45
1:B:249:VAL:HG21	1:B:280:MET:HE2	1.99	0.45
1:B:256:ARG:O	1:B:257:ALA:C	2.60	0.45
2:C:169:MET:O	2:C:173:LEU:HD13	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:ASN:CB	2:D:146:PRO:HA	2.47	0.45
2:D:132:LEU:HG	2:D:328:PHE:CE2	2.51	0.45
2:D:244:THR:HG22	2:D:245:ALA:N	2.31	0.45
2:D:346:SER:O	2:D:349:MET:N	2.50	0.45
2:Q:72:ILE:O	2:Q:72:ILE:HD13	2.17	0.45
2:E:57:PRO:O	2:E:58:ARG:C	2.60	0.45
2:F:104:ILE:HD12	2:F:104:ILE:N	2.32	0.45
2:R:167:ILE:HB	2:R:168:PRO:HD3	1.99	0.45
2:S:323:PHE:HB2	2:S:405:TRP:HE1	1.82	0.45
2:I:74:SER:HB3	2:I:77:ARG:HG3	1.99	0.45
2:I:117:ARG:O	2:I:120:ASN:HB3	2.17	0.45
2:I:182:GLN:HG2	2:I:183:PRO:HD2	1.99	0.45
2:I:204:ALA:HB1	2:I:283:GLY:O	2.17	0.45
1:A:84:ARG:HA	1:A:84:ARG:HD2	1.82	0.44
1:B:627:PRO:HG2	1:B:630:TRP:CG	2.52	0.44
2:Q:49:SER:O	2:Q:50:SER:HB3	2.17	0.44
2:Q:193:LEU:HD23	2:Q:292:ALA:HA	1.99	0.44
2:R:139:ILE:HD12	2:R:405:TRP:CE3	2.51	0.44
2:R:235:ILE:HD11	2:H:235:ILE:CD1	2.46	0.44
2:H:17:SER:O	2:H:21:VAL:HG23	2.17	0.44
2:S:17:SER:O	2:S:21:VAL:HG23	2.16	0.44
2:S:56:ASP:C	2:S:56:ASP:OD2	2.60	0.44
2:S:311:ASN:C	2:S:313:ILE:H	2.25	0.44
2:I:186:VAL:HB	2:I:231:PHE:CZ	2.51	0.44
2:I:298:THR:HG22	2:I:299:ILE:H	1.79	0.44
2:I:348:ALA:O	2:I:351:GLN:HB3	2.17	0.44
1:A:311:ILE:CD1	1:A:362:GLN:HB3	2.47	0.44
1:A:327:LEU:HD11	1:A:646:PHE:CD1	2.53	0.44
1:B:329:GLU:O	1:B:330:VAL:C	2.61	0.44
1:B:408:ARG:HH22	1:B:501:GLU:CD	2.24	0.44
1:B:463:LEU:HB3	1:B:464:PRO:HD2	2.00	0.44
1:B:550:ILE:HB	1:B:599:LEU:HD11	1.99	0.44
2:P:12:LEU:HA	2:C:28:PHE:CZ	2.52	0.44
2:P:14:GLU:OE2	2:P:131:LYS:HB3	2.17	0.44
2:Q:396:ILE:O	2:Q:400:ILE:HG13	2.18	0.44
2:E:3:ARG:HD3	2:E:89:SER:O	2.17	0.44
2:E:172:ILE:N	2:E:172:ILE:HD12	2.32	0.44
2:E:329:LEU:O	2:E:330:THR:C	2.61	0.44
2:R:140:MET:CE	2:R:406:VAL:HG11	2.47	0.44
2:H:1:MET:HB2	2:H:5:MET:SD	2.57	0.44
2:H:19:TYR:CG	2:H:42:MET:HE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:151:ILE:HG12	2:S:299:ILE:HG13	2.00	0.44
2:I:254:VAL:HG13	2:I:255:PRO:HD2	1.98	0.44
2:T:109:GLN:CG	2:T:112:MET:HB3	2.47	0.44
1:A:362:GLN:O	1:A:364:MET:N	2.50	0.44
1:A:834:THR:HG23	1:A:835:ASP:N	2.32	0.44
1:B:282:ARG:HA	1:B:283:PRO:HD3	1.85	0.44
1:B:800:SER:OG	1:B:801:VAL:N	2.50	0.44
2:C:141:LYS:C	2:Q:344:ILE:HD11	2.42	0.44
2:D:107:ARG:HG2	2:D:107:ARG:NH1	2.32	0.44
2:Q:62:GLN:O	2:Q:63:THR:C	2.60	0.44
2:Q:107:ARG:HG2	2:Q:107:ARG:NH1	2.32	0.44
2:Q:157:PHE:CG	2:Q:158:ARG:N	2.85	0.44
2:E:49:SER:HB3	2:E:105:ARG:NH1	2.33	0.44
2:F:239:VAL:HA	2:F:288:GLY:CA	2.47	0.44
2:R:120:ASN:C	2:R:122:LEU:N	2.75	0.44
2:R:137:ASN:HB3	2:R:143:LEU:HD12	1.99	0.44
2:R:175:THR:O	2:R:176:PRO:C	2.59	0.44
2:R:221:THR:HB	2:G:327:ASP:OD1	2.18	0.44
2:R:377:PHE:CD1	2:R:377:PHE:C	2.95	0.44
2:H:39:LEU:HA	2:H:42:MET:HE3	1.99	0.44
2:H:361:MET:HG2	2:H:392:VAL:HG11	1.99	0.44
2:S:361:MET:HE1	2:S:367:PRO:N	2.32	0.44
2:J:100:ILE:HD12	2:J:100:ILE:H	1.83	0.44
2:T:3:ARG:HG3	2:T:4:GLN:N	2.33	0.44
2:T:5:MET:O	2:T:9:THR:HG23	2.18	0.44
2:T:24:ASN:C	2:T:24:ASN:ND2	2.76	0.44
1:A:102:TYR:CD1	1:A:765:MET:HE1	2.52	0.44
1:A:260:PHE:HA	1:A:1003:ILE:HD12	2.00	0.44
1:B:177:HIS:HA	1:B:180:VAL:CG1	2.42	0.44
1:B:949:PHE:C	1:B:951:SER:N	2.74	0.44
2:C:405:TRP:C	2:C:405:TRP:CE3	2.96	0.44
2:E:170:MET:HE2	2:E:232:PHE:HB2	1.98	0.44
2:E:271:PHE:CZ	2:E:293:ILE:HD13	2.53	0.44
2:F:2:SER:HB2	2:F:5:MET:HE3	1.98	0.44
2:F:252:PHE:CD1	2:F:252:PHE:C	2.95	0.44
2:G:17:SER:O	2:G:21:VAL:HG23	2.17	0.44
2:G:176:PRO:HA	2:G:177:PRO:HD2	1.84	0.44
2:G:188:GLU:HA	2:G:232:PHE:CE1	2.53	0.44
2:G:235:ILE:CD1	2:H:235:ILE:HD11	2.47	0.44
2:H:228:THR:CG2	2:H:229:ASN:H	2.21	0.44
2:I:164:THR:HG23	2:I:165:GLY:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:59:VAL:HG13	2:T:60:PRO:CD	2.45	0.44
2:T:356:LEU:O	2:T:357:ILE:C	2.61	0.44
1:A:264:ASP:HB3	1:A:267:VAL:HG23	2.00	0.44
1:A:286:GLN:NE2	1:A:286:GLN:CA	2.79	0.44
1:A:524:LEU:HD23	1:A:524:LEU:HA	1.85	0.44
1:A:958:LEU:C	1:A:958:LEU:CD1	2.91	0.44
1:B:86:VAL:HG22	1:B:88:GLU:H	1.81	0.44
1:B:293:VAL:HG22	1:B:669:ILE:HG13	1.99	0.44
1:B:459:TYR:CD2	1:B:482:ALA:HA	2.53	0.44
1:B:880:LEU:HG	1:B:881:GLN:N	2.33	0.44
1:B:949:PHE:C	1:B:951:SER:H	2.25	0.44
2:C:24:ASN:C	2:C:24:ASN:ND2	2.74	0.44
2:C:215:ALA:C	2:C:217:VAL:H	2.24	0.44
2:D:110:VAL:HG22	2:D:111:PRO:CA	2.48	0.44
2:E:71:PHE:C	2:E:73:THR:H	2.25	0.44
2:F:214:TRP:CE3	2:F:215:ALA:HB2	2.53	0.44
2:R:329:LEU:O	2:R:330:THR:C	2.60	0.44
2:H:337:ARG:HH11	2:H:337:ARG:HG3	1.83	0.44
2:I:64:MET:HE2	2:I:65:SER:N	2.32	0.44
2:I:132:LEU:HG	2:I:328:PHE:CE2	2.53	0.44
2:I:324:ASP:O	2:I:325:VAL:C	2.59	0.44
1:B:65:LEU:HD21	1:B:222:VAL:CG1	2.47	0.44
1:B:601:ILE:HG13	1:B:648:ILE:HD13	1.99	0.44
1:B:711:VAL:O	1:B:711:VAL:HG12	2.18	0.44
2:P:31:LEU:HD22	2:D:41:ASN:CB	2.45	0.44
2:E:110:VAL:HG23	2:E:111:PRO:HA	2.00	0.44
2:F:71:PHE:CE2	2:F:81:MET:HE2	2.53	0.44
2:G:201:ALA:HA	2:G:287:THR:HA	2.00	0.44
2:S:151:ILE:HD12	2:S:151:ILE:O	2.18	0.44
2:I:344:ILE:H	2:I:344:ILE:CD1	2.26	0.44
1:A:63:ILE:HG13	1:A:64:GLY:N	2.33	0.44
1:A:179:VAL:O	1:A:180:VAL:C	2.60	0.44
1:A:307:LEU:HD21	1:A:365:LEU:CB	2.48	0.44
1:A:348:MET:CG	1:A:643:PHE:HB2	2.48	0.44
1:A:732:LYS:HD3	1:A:736:ASP:OD2	2.17	0.44
1:B:525:SER:O	1:B:526:THR:C	2.59	0.44
2:P:12:LEU:HA	2:C:28:PHE:CE2	2.53	0.44
2:P:186:VAL:HB	2:P:231:PHE:CE1	2.53	0.44
2:P:254:VAL:CG1	2:P:255:PRO:HD2	2.46	0.44
2:P:299:ILE:O	2:P:300:LEU:C	2.60	0.44
2:Q:64:MET:HG3	2:Q:103:TYR:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:341:GLN:HA	2:E:344:ILE:HD13	2.00	0.44
2:R:28:PHE:CD1	2:R:28:PHE:N	2.86	0.44
2:R:186:VAL:HB	2:R:231:PHE:CE1	2.53	0.44
2:G:341:GLN:HE21	2:G:341:GLN:HB3	1.53	0.44
2:S:39:LEU:HA	2:S:42:MET:HE3	1.98	0.44
2:S:132:LEU:HD23	2:S:132:LEU:HA	1.78	0.44
2:S:271:PHE:HZ	2:S:293:ILE:HD13	1.83	0.44
2:S:284:VAL:O	2:S:285:ALA:C	2.61	0.44
1:A:591:PHE:CE1	1:A:642:LEU:HD12	2.53	0.44
2:P:179:ALA:HA	2:P:199:ASN:OD1	2.18	0.44
2:D:153:PRO:HD2	2:D:189:ARG:O	2.17	0.44
2:H:135:ARG:NH1	2:H:324:ASP:HB2	2.32	0.44
2:S:72:ILE:O	2:S:72:ILE:HG23	2.17	0.44
2:S:419:ARG:NH1	2:S:419:ARG:HG2	2.33	0.44
2:J:56:ASP:OD1	2:J:58:ARG:N	2.41	0.44
2:J:254:VAL:CG1	2:J:255:PRO:HD2	2.48	0.44
2:T:394:LEU:O	2:T:397:ARG:HB2	2.18	0.44
1:A:201:ILE:O	1:A:201:ILE:HG22	2.18	0.44
1:A:595:THR:OG1	1:A:596:PRO:HD3	2.18	0.44
1:B:671:ILE:O	1:B:675:ILE:HG13	2.18	0.44
1:B:958:LEU:C	1:B:958:LEU:CD1	2.91	0.44
2:C:394:LEU:O	2:C:397:ARG:HB2	2.17	0.44
2:D:1:MET:O	2:D:2:SER:C	2.60	0.44
2:E:114:ASP:OD2	2:E:117:ARG:NH2	2.51	0.44
2:S:71:PHE:CZ	2:S:81:MET:HE3	2.52	0.44
2:S:420:PRO:O	2:S:421:ASN:OXT	2.36	0.44
2:T:357:ILE:CD1	2:T:386:ILE:HD12	2.47	0.44
2:T:396:ILE:N	2:T:396:ILE:CD1	2.81	0.44
1:A:454:VAL:O	1:A:458:ILE:HG12	2.18	0.43
1:B:97:TYR:CE2	1:B:771:ILE:HD12	2.51	0.43
1:B:258:PRO:CG	1:B:261:LEU:HD12	2.43	0.43
2:D:225:VAL:HG23	2:D:269:LEU:HD12	2.00	0.43
2:Q:325:VAL:HG13	2:Q:405:TRP:CE2	2.53	0.43
2:E:91:THR:O	2:E:93:PRO:HD3	2.17	0.43
2:E:120:ASN:C	2:E:122:LEU:N	2.73	0.43
2:F:1:MET:C	2:F:93:PRO:HG2	2.43	0.43
2:R:132:LEU:HG	2:R:328:PHE:CE2	2.53	0.43
2:R:157:PHE:C	2:R:158:ARG:HD2	2.42	0.43
2:S:1:MET:HG2	2:S:93:PRO:HD2	2.00	0.43
2:I:6:TRP:CE2	2:I:104:ILE:HG12	2.53	0.43
1:A:939:ARG:HH11	1:A:939:ARG:HG2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:CG	1:B:187:ARG:NH1	2.77	0.43
2:C:186:VAL:HG23	2:C:193:LEU:HB2	2.00	0.43
2:D:84:LYS:HB3	2:D:360:TYR:CE2	2.53	0.43
2:G:24:ASN:C	2:G:24:ASN:ND2	2.76	0.43
2:G:53:TYR:C	2:G:55:SER:H	2.25	0.43
2:G:140:MET:CE	2:G:406:VAL:HG11	2.48	0.43
2:G:145:ILE:HD12	2:G:308:TYR:HE1	1.83	0.43
2:G:284:VAL:HG23	2:G:284:VAL:O	2.16	0.43
2:S:343:GLU:HG2	2:S:344:ILE:HD12	2.00	0.43
2:I:166:ASN:N	2:I:168:PRO:HD2	2.33	0.43
2:I:370:LEU:C	2:I:370:LEU:HD13	2.44	0.43
1:A:489:LEU:HD11	1:A:503:ARG:HA	2.00	0.43
1:A:653:GLN:NE2	1:A:655:LEU:CD1	2.81	0.43
1:B:180:VAL:HG13	1:B:181:ASN:N	2.33	0.43
1:B:597:ASN:C	1:B:599:LEU:H	2.25	0.43
1:B:772:ILE:HD12	1:B:772:ILE:C	2.43	0.43
2:C:91:THR:O	2:C:93:PRO:HD3	2.18	0.43
2:Q:24:ASN:ND2	2:Q:24:ASN:C	2.75	0.43
2:Q:121:ASN:HA	2:Q:146:PRO:HA	2.01	0.43
2:Q:221:THR:HA	2:Q:270:SER:HB3	1.99	0.43
2:E:202:ILE:HD12	2:E:202:ILE:N	2.33	0.43
2:E:250:THR:HG23	2:E:281:GLU:O	2.17	0.43
2:R:244:THR:HB	2:R:247:ASP:OD1	2.18	0.43
2:G:218:LEU:HA	2:G:218:LEU:HD23	1.85	0.43
2:G:226:TYR:HE1	2:G:228:THR:HG23	1.84	0.43
2:H:339:CYS:HB3	2:H:421:ASN:ND2	2.29	0.43
2:S:229:ASN:OD1	2:I:234:THR:HA	2.18	0.43
2:I:240:THR:HB	2:I:242:THR:CG2	2.49	0.43
2:J:71:PHE:CZ	2:J:78:CYS:HB3	2.53	0.43
1:A:66:GLN:CD	1:A:66:GLN:H	2.25	0.43
1:A:695:HIS:O	1:A:696:LEU:C	2.61	0.43
2:Q:24:ASN:HD22	2:Q:24:ASN:C	2.26	0.43
2:Q:361:MET:HB2	2:Q:361:MET:HE3	1.68	0.43
2:Q:363:PRO:HA	2:Q:364:PRO:HD3	1.52	0.43
2:F:24:ASN:HD22	2:F:24:ASN:C	2.26	0.43
2:H:157:PHE:C	2:H:158:ARG:HG2	2.43	0.43
2:S:167:ILE:HB	2:S:168:PRO:HD3	2.00	0.43
2:S:357:ILE:CD1	2:S:386:ILE:HD12	2.44	0.43
2:I:360:TYR:HB2	2:I:400:ILE:HD11	1.99	0.43
2:J:325:VAL:O	2:J:326:SER:C	2.62	0.43
2:J:415:GLY:O	2:J:418:TYR:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2:SER:HB2	2:T:5:MET:HE3	2.01	0.43
1:A:121:HIS:O	1:A:124:ARG:HB3	2.19	0.43
1:A:124:ARG:C	1:A:124:ARG:CD	2.91	0.43
1:B:14:PHE:CD1	1:B:14:PHE:C	2.97	0.43
1:B:802:TYR:O	1:B:805:VAL:HG12	2.18	0.43
2:P:144:ASP:OD1	2:P:302:ASN:HA	2.19	0.43
2:D:41:ASN:O	2:D:44:THR:HB	2.18	0.43
2:D:120:ASN:O	2:D:122:LEU:N	2.51	0.43
2:Q:352:LEU:HD21	2:Q:407:ILE:HG21	2.01	0.43
2:E:266:ASP:OD1	2:F:167:ILE:HD13	2.19	0.43
2:F:17:SER:O	2:F:21:VAL:HG23	2.18	0.43
2:R:418:TYR:CD1	2:R:420:PRO:HD3	2.54	0.43
2:G:1:MET:O	2:G:2:SER:C	2.62	0.43
2:G:261:LEU:HA	2:G:262:PRO:HD2	1.86	0.43
2:H:316:THR:HA	2:H:317:PRO:HA	1.88	0.43
2:I:310:LEU:HD22	2:I:313:ILE:CD1	2.48	0.43
2:J:82:LEU:HA	2:J:356:LEU:HD12	2.00	0.43
2:T:254:VAL:CG1	2:T:255:PRO:HD2	2.48	0.43
1:A:220:TYR:N	1:A:220:TYR:CD1	2.86	0.43
1:A:358:VAL:HG13	1:A:359:PHE:N	2.33	0.43
1:A:488:ILE:HD12	1:A:488:ILE:N	2.33	0.43
1:A:903:PHE:O	1:A:906:PHE:HB3	2.19	0.43
2:C:5:MET:CE	2:C:106:PRO:HD3	2.43	0.43
2:C:346:SER:O	2:C:350:ASP:OD1	2.35	0.43
2:D:5:MET:HE2	2:D:105:ARG:HA	2.01	0.43
2:D:184:PHE:O	2:D:194:PHE:HA	2.19	0.43
2:Q:254:VAL:HG12	2:Q:256:THR:H	1.84	0.43
2:Q:309:THR:O	2:Q:309:THR:CG2	2.66	0.43
2:F:337:ARG:HG3	2:F:337:ARG:NH1	2.12	0.43
2:F:359:ASN:ND2	2:F:359:ASN:H	2.14	0.43
2:G:325:VAL:HG13	2:G:326:SER:N	2.34	0.43
2:G:379:PHE:CE1	2:G:404:LEU:HD22	2.52	0.43
2:H:252:PHE:HA	2:H:279:ASN:O	2.18	0.43
2:H:329:LEU:O	2:H:330:THR:C	2.61	0.43
2:S:201:ALA:HA	2:S:287:THR:HA	1.99	0.43
2:S:313:ILE:HB	2:S:398:LYS:HE2	2.01	0.43
2:I:217:VAL:O	2:I:300:LEU:HG	2.18	0.43
2:T:71:PHE:HZ	2:T:81:MET:HE3	1.84	0.43
2:T:302:ASN:C	2:T:303:ARG:HG2	2.44	0.43
2:T:329:LEU:HD13	2:T:412:ALA:HB2	2.00	0.43
1:A:307:LEU:HD22	1:A:617:TYR:HD1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ILE:HD12	1:A:715:ILE:HA	1.74	0.43
1:B:588:LEU:HD12	1:B:588:LEU:O	2.18	0.43
2:C:16:ILE:CG1	2:C:42:MET:HE2	2.47	0.43
2:C:69:VAL:HG21	2:C:418:TYR:CD1	2.54	0.43
2:D:344:ILE:H	2:D:344:ILE:CD1	2.27	0.43
2:Q:316:THR:HG21	2:Q:397:ARG:HH12	1.83	0.43
2:E:3:ARG:HH11	2:E:90:ASP:CG	2.26	0.43
2:E:83:ARG:HG2	2:E:359:ASN:HD22	1.83	0.43
2:E:320:ILE:HD11	2:E:383:ALA:CB	2.49	0.43
2:F:220:VAL:CG1	2:F:223:ALA:HB2	2.49	0.43
2:R:386:ILE:C	2:R:388:ALA:H	2.27	0.43
2:G:16:ILE:CD1	2:G:42:MET:HB3	2.48	0.43
2:S:170:MET:HE2	2:S:231:PHE:O	2.19	0.43
2:S:244:THR:HG22	2:S:246:ALA:H	1.83	0.43
2:S:378:ARG:NH2	2:J:259:ASN:HB2	2.34	0.43
2:I:17:SER:O	2:I:21:VAL:HG23	2.19	0.43
2:J:145:ILE:HD11	2:J:149:GLU:OE2	2.18	0.43
1:B:44:THR:O	1:B:45:SER:C	2.61	0.43
1:B:225:HIS:ND1	1:B:227:ILE:CG2	2.62	0.43
2:P:156:LEU:HD21	2:P:299:ILE:HD11	2.01	0.43
2:P:194:PHE:CD1	2:P:194:PHE:C	2.96	0.43
2:C:235:ILE:HD12	2:C:235:ILE:N	2.33	0.43
2:E:190:ARG:HG2	2:E:190:ARG:O	2.19	0.43
2:R:95:VAL:HG23	2:R:95:VAL:O	2.19	0.43
2:R:373:THR:O	2:R:373:THR:HG22	2.19	0.43
2:H:378:ARG:O	2:H:379:PHE:C	2.61	0.43
2:I:262:PRO:HB2	2:I:265:THR:HG21	2.01	0.43
2:T:375:PRO:CD	2:T:378:ARG:HD3	2.48	0.43
1:A:252:TYR:CE1	1:A:256:ARG:NE	2.87	0.43
1:A:385:PHE:HA	1:A:566:TYR:CE2	2.54	0.43
1:B:845:ARG:NH2	1:B:864:GLU:OE1	2.42	0.43
2:C:379:PHE:O	2:C:380:SER:C	2.62	0.43
2:D:197:ARG:HH11	2:D:197:ARG:HG3	1.84	0.43
2:Q:242:THR:HG22	2:Q:243:ALA:N	2.34	0.43
2:Q:325:VAL:HG13	2:Q:405:TRP:CZ2	2.54	0.43
2:F:46:LEU:HD12	2:F:46:LEU:HA	1.80	0.43
2:R:132:LEU:O	2:R:133:TYR:C	2.62	0.43
2:S:303:ARG:HH11	2:S:303:ARG:CB	2.31	0.43
2:I:349:MET:O	2:I:350:ASP:C	2.62	0.43
2:T:99:PHE:O	2:T:100:ILE:C	2.62	0.43
1:A:190:TYR:CE1	1:A:976:ARG:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:NE2	1:A:286:GLN:HA	2.34	0.43
1:A:366:ASN:HA	1:A:367:PRO:HD2	1.89	0.43
1:A:670:LEU:HD21	1:A:751:TYR:CE1	2.54	0.43
1:B:608:ASN:HA	1:B:612:ASN:HB2	2.00	0.43
1:B:764:TYR:O	1:B:765:MET:C	2.62	0.43
1:B:781:VAL:HG21	1:B:784:SER:HB3	2.01	0.43
2:P:284:VAL:HG12	2:P:285:ALA:N	2.34	0.43
2:D:377:PHE:CD1	2:D:377:PHE:C	2.97	0.43
2:Q:111:PRO:O	2:Q:112:MET:C	2.62	0.43
2:F:110:VAL:HG22	2:F:111:PRO:CA	2.47	0.43
2:R:107:ARG:HG2	2:R:107:ARG:NH1	2.33	0.43
2:H:120:ASN:O	2:H:121:ASN:C	2.62	0.43
2:H:341:GLN:HA	2:H:344:ILE:HD13	2.00	0.43
2:S:361:MET:HG2	2:S:392:VAL:HG11	2.01	0.43
2:I:151:ILE:HD12	2:I:151:ILE:C	2.44	0.43
2:J:100:ILE:H	2:J:100:ILE:CD1	2.32	0.43
2:J:109:GLN:O	2:J:113:SER:CB	2.67	0.43
1:A:817:ALA:O	1:A:821:LEU:HG	2.18	0.42
1:A:887:GLY:HA2	1:A:930:LEU:CD1	2.48	0.42
1:B:265:ASP:O	1:B:266:GLN:C	2.61	0.42
2:P:363:PRO:O	2:P:365:ALA:N	2.52	0.42
2:C:175:THR:O	2:C:176:PRO:C	2.60	0.42
2:C:310:LEU:HB3	2:C:313:ILE:HD12	2.01	0.42
2:D:214:TRP:CE3	2:D:215:ALA:HB2	2.53	0.42
2:Q:41:ASN:O	2:Q:44:THR:HB	2.19	0.42
2:Q:177:PRO:HG2	2:Q:199:ASN:HB3	2.01	0.42
2:E:186:VAL:HG22	2:E:187:ALA:H	1.83	0.42
2:R:135:ARG:HG3	2:R:135:ARG:HH11	1.82	0.42
2:H:210:VAL:HG23	2:H:210:VAL:O	2.18	0.42
2:T:82:LEU:HD11	2:T:352:LEU:HD22	2.01	0.42
2:T:186:VAL:HB	2:T:231:PHE:CE1	2.53	0.42
1:A:722:THR:CG2	1:A:728:GLY:HA2	2.49	0.42
1:A:781:VAL:HG21	1:A:867:ILE:HG22	2.01	0.42
1:B:179:VAL:O	1:B:180:VAL:C	2.60	0.42
2:D:316:THR:HG21	2:D:397:ARG:HH12	1.84	0.42
2:Q:179:ALA:O	2:Q:180:GLN:C	2.62	0.42
2:Q:254:VAL:HG11	2:Q:272:SER:O	2.19	0.42
2:E:357:ILE:HD11	2:E:386:ILE:HD12	2.01	0.42
2:F:325:VAL:O	2:F:329:LEU:CD2	2.68	0.42
2:R:379:PHE:O	2:R:380:SER:C	2.60	0.42
2:H:365:ALA:O	2:H:366:ILE:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:112:MET:HE2	2:I:116:VAL:HG23	2.01	0.42
1:A:447:TRP:O	1:A:448:GLN:C	2.62	0.42
1:A:667:GLU:O	1:A:671:ILE:HG12	2.19	0.42
1:B:31:VAL:HG21	1:B:1008:VAL:HG22	2.01	0.42
2:C:107:ARG:HG2	2:C:107:ARG:NH1	2.34	0.42
2:D:108:LEU:HA	2:D:108:LEU:HD23	1.84	0.42
2:D:244:THR:HG22	2:D:246:ALA:H	1.85	0.42
2:E:12:LEU:HA	2:F:28:PHE:CZ	2.54	0.42
2:F:114:ASP:C	2:F:116:VAL:N	2.74	0.42
2:R:210:VAL:HA	2:R:277:ASN:OD1	2.19	0.42
2:G:3:ARG:HH11	2:G:90:ASP:CG	2.28	0.42
2:G:67:MET:HE2	2:G:67:MET:HB3	1.93	0.42
2:G:231:PHE:HB2	2:G:236:ILE:HD11	2.00	0.42
2:G:329:LEU:O	2:G:330:THR:C	2.62	0.42
2:H:24:ASN:C	2:H:24:ASN:ND2	2.77	0.42
2:H:59:VAL:HG13	2:H:60:PRO:HD3	2.01	0.42
2:I:19:TYR:CD1	2:I:42:MET:HE1	2.54	0.42
2:J:166:ASN:OD1	2:J:186:VAL:HG22	2.18	0.42
2:J:418:TYR:CD1	2:J:420:PRO:HD3	2.55	0.42
2:T:323:PHE:HB2	2:T:405:TRP:HE1	1.84	0.42
1:B:311:ILE:HD12	1:B:362:GLN:HB3	2.02	0.42
1:B:599:LEU:O	1:B:603:GLU:HG3	2.19	0.42
2:P:152:GLU:OE1	2:P:189:ARG:HG2	2.19	0.42
2:C:221:THR:HB	2:D:327:ASP:OD2	2.19	0.42
2:D:186:VAL:HG23	2:D:193:LEU:HB2	2.01	0.42
2:E:215:ALA:C	2:E:217:VAL:H	2.27	0.42
2:E:309:THR:O	2:E:310:LEU:HB2	2.20	0.42
2:F:87:PHE:CE1	2:F:403:HIS:HA	2.54	0.42
2:G:121:ASN:HA	2:G:146:PRO:HA	2.00	0.42
2:S:147:TYR:HB2	2:I:331:THR:HG22	2.01	0.42
2:I:132:LEU:O	2:I:136:GLN:HG3	2.20	0.42
2:I:215:ALA:C	2:I:217:VAL:H	2.27	0.42
2:I:363:PRO:HA	2:I:364:PRO:HD3	1.74	0.42
2:J:1:MET:O	2:J:2:SER:C	2.62	0.42
2:T:9:THR:HA	2:T:107:ARG:HG3	2.02	0.42
1:A:767:GLN:C	1:A:769:THR:N	2.76	0.42
1:A:988:ASP:HA	1:A:989:PRO:HD3	1.86	0.42
2:P:1:MET:HE3	2:P:5:MET:SD	2.59	0.42
2:P:6:TRP:CD1	2:P:104:ILE:HG21	2.54	0.42
2:Q:337:ARG:HH21	2:Q:342:TYR:HE1	1.67	0.42
2:E:300:LEU:HA	2:E:300:LEU:HD23	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:399:LEU:O	2:E:400:ILE:C	2.62	0.42
2:R:135:ARG:HG3	2:R:135:ARG:NH1	2.35	0.42
2:S:421:ASN:O	2:S:421:ASN:OD1	2.38	0.42
2:I:1:MET:O	2:I:2:SER:C	2.62	0.42
2:I:112:MET:HE2	2:I:116:VAL:CG2	2.49	0.42
1:A:192:ARG:HG3	1:A:220:TYR:CE2	2.55	0.42
1:A:245:HIS:O	1:A:246:PRO:C	2.63	0.42
1:A:319:MET:O	1:A:320:VAL:C	2.62	0.42
1:A:459:TYR:CG	1:A:473:ILE:HG21	2.54	0.42
1:A:492:ALA:C	1:A:494:GLN:N	2.78	0.42
1:B:35:LEU:HA	1:B:35:LEU:HD23	1.81	0.42
1:B:58:ILE:HG13	1:B:754:ILE:HD13	2.01	0.42
2:P:160:VAL:HG22	2:P:161:ALA:H	1.85	0.42
2:C:97:ASP:O	2:C:98:ASP:C	2.62	0.42
2:D:140:MET:HE3	2:D:406:VAL:HG21	2.01	0.42
2:D:375:PRO:HD2	2:D:378:ARG:HD3	2.01	0.42
2:Q:410:LEU:HD12	2:Q:410:LEU:HA	1.83	0.42
2:E:122:LEU:HA	2:E:122:LEU:HD23	1.82	0.42
2:E:375:PRO:CG	2:E:378:ARG:HD3	2.49	0.42
2:F:309:THR:O	2:F:310:LEU:HB2	2.20	0.42
2:F:363:PRO:HA	2:F:364:PRO:HD3	1.66	0.42
2:R:343:GLU:N	2:R:343:GLU:OE2	2.52	0.42
2:G:13:LEU:HD23	2:G:13:LEU:HA	1.85	0.42
2:G:186:VAL:HG23	2:G:193:LEU:HB2	2.02	0.42
2:S:418:TYR:CZ	2:S:420:PRO:HG3	2.55	0.42
2:I:12:LEU:HA	2:J:28:PHE:CZ	2.55	0.42
2:J:24:ASN:C	2:J:24:ASN:ND2	2.77	0.42
2:J:157:PHE:HD1	2:J:214:TRP:CE2	2.36	0.42
1:A:126:ILE:HD13	1:A:126:ILE:HA	1.79	0.42
2:P:64:MET:HG3	2:P:103:TYR:CE2	2.55	0.42
2:P:154:CYS:HB3	2:P:188:GLU:O	2.19	0.42
2:P:160:VAL:HG22	2:P:161:ALA:N	2.35	0.42
2:P:210:VAL:HA	2:P:277:ASN:OD1	2.19	0.42
2:C:15:ALA:C	2:C:42:MET:HE1	2.44	0.42
2:F:132:LEU:HD21	2:F:328:PHE:CD1	2.54	0.42
2:F:198:SER:HB3	2:F:202:ILE:HD11	2.01	0.42
2:R:105:ARG:O	2:R:107:ARG:HG3	2.18	0.42
2:R:305:GLN:O	2:R:309:THR:HB	2.20	0.42
2:R:396:ILE:O	2:R:400:ILE:HG13	2.19	0.42
2:H:57:PRO:C	2:H:60:PRO:HD2	2.45	0.42
2:S:152:GLU:HA	2:S:153:PRO:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:419:ARG:HG2	2:S:419:ARG:HH11	1.85	0.42
2:I:298:THR:CG2	2:I:299:ILE:N	2.81	0.42
2:J:221:THR:HA	2:J:270:SER:HB3	2.01	0.42
2:J:246:ALA:O	2:J:247:ASP:C	2.63	0.42
1:A:492:ALA:O	1:A:494:GLN:N	2.53	0.42
1:A:783:ASN:HD22	1:A:784:SER:H	1.66	0.42
1:A:878:PHE:HA	1:A:921:VAL:O	2.18	0.42
1:A:941:ARG:H	1:A:941:ARG:HG3	1.71	0.42
2:P:6:TRP:CE3	2:P:410:LEU:HD13	2.54	0.42
2:P:394:LEU:O	2:P:397:ARG:HB2	2.20	0.42
2:D:121:ASN:HA	2:D:146:PRO:CA	2.50	0.42
2:Q:244:THR:HG22	2:Q:245:ALA:N	2.35	0.42
2:F:246:ALA:O	2:F:247:ASP:C	2.62	0.42
2:S:322:ASP:O	2:S:323:PHE:HB2	2.20	0.42
2:I:46:LEU:N	2:I:46:LEU:CD1	2.82	0.42
2:J:184:PHE:O	2:J:194:PHE:HA	2.20	0.42
1:B:362:GLN:C	1:B:364:MET:N	2.77	0.42
2:C:56:ASP:HA	2:C:57:PRO:HD2	1.79	0.42
2:C:110:VAL:HG22	2:C:111:PRO:HA	2.02	0.42
2:E:119:LEU:HA	2:E:119:LEU:HD23	1.83	0.42
2:E:133:TYR:O	2:E:134:GLU:C	2.63	0.42
2:R:238:GLY:C	2:R:239:VAL:HG23	2.45	0.42
2:R:316:THR:HA	2:R:317:PRO:C	2.44	0.42
2:G:120:ASN:C	2:G:122:LEU:N	2.76	0.42
2:H:107:ARG:CG	2:H:107:ARG:NH1	2.80	0.42
2:H:144:ASP:OD1	2:H:302:ASN:HA	2.20	0.42
2:S:170:MET:HE2	2:S:232:PHE:HB2	2.01	0.42
2:I:131:LYS:NZ	2:J:26:ASP:OD1	2.52	0.42
2:I:309:THR:O	2:I:309:THR:HG22	2.20	0.42
2:T:17:SER:O	2:T:18:GLU:C	2.62	0.42
2:T:88:ASN:C	2:T:88:ASN:ND2	2.78	0.42
1:A:344:CYS:C	1:A:346:VAL:H	2.28	0.42
1:A:826:ARG:HH11	1:A:826:ARG:HG2	1.85	0.42
1:B:119:THR:O	1:B:120:MET:C	2.62	0.42
1:B:308:LEU:HD22	1:B:362:GLN:CB	2.45	0.42
1:B:769:THR:O	1:B:772:ILE:HG13	2.19	0.42
1:B:892:PRO:HA	1:B:893:PRO:HD3	1.88	0.42
2:P:110:VAL:HG23	2:P:111:PRO:HA	2.01	0.42
2:P:135:ARG:HG2	2:P:308:TYR:CE2	2.55	0.42
2:C:56:ASP:O	2:C:60:PRO:HD2	2.19	0.42
2:C:419:ARG:HA	2:C:420:PRO:HD2	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:THR:HG22	2:D:35:ASP:H	1.83	0.42
2:D:38:ALA:C	2:D:40:SER:N	2.77	0.42
2:D:386:ILE:C	2:D:388:ALA:H	2.28	0.42
2:Q:168:PRO:C	2:Q:170:MET:N	2.76	0.42
2:E:5:MET:HE3	2:E:105:ARG:HA	2.01	0.42
2:E:118:GLN:C	2:E:120:ASN:N	2.77	0.42
2:F:133:TYR:HA	2:F:136:GLN:OE1	2.20	0.42
2:F:166:ASN:N	2:F:168:PRO:HD2	2.34	0.42
2:F:329:LEU:O	2:F:330:THR:C	2.63	0.42
2:R:418:TYR:CG	2:R:420:PRO:HD3	2.55	0.42
2:G:107:ARG:CG	2:G:107:ARG:NH1	2.81	0.42
2:G:244:THR:C	2:G:246:ALA:N	2.78	0.42
2:S:268:ARG:HD2	2:I:321:ASP:HB2	2.02	0.42
2:I:269:LEU:HD22	2:I:269:LEU:H	1.85	0.42
2:J:163:GLN:HE21	2:J:169:MET:HG3	1.77	0.42
2:J:168:PRO:C	2:J:170:MET:H	2.28	0.42
2:T:15:ALA:HB1	2:T:42:MET:HE3	2.02	0.42
2:T:361:MET:HE3	2:T:361:MET:HB2	1.84	0.42
1:A:471:ASN:O	1:A:472:LEU:C	2.62	0.41
1:A:533:LEU:CB	1:A:534:PRO:HD2	2.50	0.41
1:B:455:LEU:HD13	1:B:477:PHE:CZ	2.55	0.41
1:B:458:ILE:O	1:B:462:LEU:HG	2.20	0.41
2:P:264:GLN:O	2:C:168:PRO:HG3	2.19	0.41
2:C:119:LEU:HD23	2:C:119:LEU:HA	1.90	0.41
2:C:309:THR:HG21	2:Q:343:GLU:HB3	2.01	0.41
2:E:109:GLN:O	2:E:113:SER:CB	2.67	0.41
2:F:278:ILE:HG23	2:F:278:ILE:O	2.19	0.41
2:R:12:LEU:HA	2:G:28:PHE:CE2	2.55	0.41
2:R:169:MET:HE3	2:R:173:LEU:CD1	2.49	0.41
2:R:186:VAL:CG2	2:R:193:LEU:HB2	2.50	0.41
2:G:379:PHE:O	2:G:380:SER:C	2.62	0.41
2:H:214:TRP:CE3	2:H:215:ALA:HB2	2.54	0.41
2:H:351:GLN:O	2:H:352:LEU:C	2.63	0.41
2:J:17:SER:O	2:J:18:GLU:C	2.63	0.41
2:J:228:THR:OG1	2:J:229:ASN:N	2.52	0.41
2:T:239:VAL:HG13	2:T:289:PHE:CA	2.50	0.41
1:A:151:LEU:HD12	1:A:152:PRO:CD	2.49	0.41
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.84	0.41
1:A:783:ASN:ND2	1:A:784:SER:N	2.68	0.41
1:A:898:LEU:HD23	1:A:957:ILE:HG21	2.02	0.41
1:B:938:LEU:CD2	1:B:938:LEU:H	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:192:ILE:HD12	2:P:297:PHE:HE2	1.84	0.41
2:C:12:LEU:O	2:C:15:ALA:HB3	2.20	0.41
2:C:339:CYS:SG	2:C:420:PRO:HG3	2.61	0.41
2:Q:5:MET:HE3	2:Q:105:ARG:HA	2.01	0.41
2:E:5:MET:HE2	2:E:105:ARG:HA	2.01	0.41
2:E:8:ASP:OD2	2:E:108:LEU:HD12	2.21	0.41
2:F:118:GLN:C	2:F:120:ASN:N	2.77	0.41
2:F:271:PHE:HZ	2:F:293:ILE:HD13	1.84	0.41
2:G:374:SER:HB2	2:G:375:PRO:HD2	2.02	0.41
2:S:3:ARG:HG3	2:S:4:GLN:N	2.35	0.41
2:I:209:PHE:O	2:I:277:ASN:HB3	2.20	0.41
1:A:394:PHE:CZ	1:A:636:VAL:HG11	2.55	0.41
1:A:552:ILE:HD11	1:A:556:ARG:HH21	1.86	0.41
1:A:653:GLN:NE2	1:A:655:LEU:HD11	2.35	0.41
1:A:732:LYS:N	1:A:733:PRO:CD	2.83	0.41
1:A:915:ARG:HA	1:B:1005:VAL:CG2	2.48	0.41
1:A:959:VAL:HA	1:A:960:PRO:HD3	1.85	0.41
1:B:296:SER:HB2	1:B:720:TYR:O	2.20	0.41
1:B:417:TYR:OH	1:B:421:LYS:HE3	2.21	0.41
1:B:747:LEU:HG	1:B:748:PRO:HD2	2.02	0.41
2:P:17:SER:O	2:P:21:VAL:HG23	2.20	0.41
2:P:120:ASN:C	2:P:122:LEU:H	2.27	0.41
2:C:152:GLU:HA	2:C:153:PRO:HD2	1.87	0.41
2:C:378:ARG:O	2:C:379:PHE:C	2.63	0.41
2:D:46:LEU:HD12	2:D:46:LEU:HA	1.80	0.41
2:D:147:TYR:CE1	2:D:301:ALA:CB	3.04	0.41
2:D:215:ALA:O	2:D:217:VAL:N	2.53	0.41
2:E:271:PHE:HZ	2:E:293:ILE:HD13	1.85	0.41
2:H:203:PRO:HG2	2:H:207:TYR:OH	2.20	0.41
2:H:250:THR:HG22	2:H:251:THR:N	2.34	0.41
2:H:396:ILE:N	2:H:396:ILE:HD12	2.35	0.41
2:S:1:MET:O	2:S:2:SER:O	2.39	0.41
2:T:179:ALA:HA	2:T:199:ASN:OD1	2.21	0.41
2:T:349:MET:HG2	2:T:376:TRP:CG	2.55	0.41
1:A:241:ILE:HD13	1:A:242:GLN:HG3	2.03	0.41
1:A:443:ALA:O	1:A:445:ASP:N	2.53	0.41
1:B:33:ASN:O	1:B:34:ILE:C	2.61	0.41
1:B:623:ARG:HH11	1:B:623:ARG:CG	2.33	0.41
2:P:97:ASP:O	2:P:98:ASP:C	2.63	0.41
2:Q:175:THR:O	2:Q:176:PRO:C	2.59	0.41
2:E:262:PRO:HB2	2:E:265:THR:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:ASN:C	2:F:122:LEU:N	2.77	0.41
2:F:361:MET:HE3	2:F:361:MET:HB2	1.86	0.41
2:G:186:VAL:HB	2:G:231:PHE:CE1	2.55	0.41
2:H:158:ARG:HD2	2:H:313:ILE:HG12	2.01	0.41
2:H:244:THR:HG22	2:H:245:ALA:N	2.35	0.41
2:S:8:ASP:OD2	2:S:108:LEU:HB2	2.20	0.41
2:I:217:VAL:HG12	2:I:299:ILE:HG23	2.03	0.41
2:I:379:PHE:CE1	2:I:404:LEU:HD12	2.54	0.41
2:J:403:HIS:O	2:J:407:ILE:CD1	2.68	0.41
1:A:260:PHE:HA	1:A:1003:ILE:CD1	2.50	0.41
1:A:443:ALA:O	1:A:444:ILE:C	2.62	0.41
1:A:781:VAL:HG21	1:A:867:ILE:CG2	2.50	0.41
1:A:876:ALA:HA	1:A:918:LEU:HD12	2.03	0.41
1:B:459:TYR:HB2	1:B:473:ILE:HG21	2.01	0.41
1:B:731:SER:C	1:B:733:PRO:HD2	2.45	0.41
2:P:226:TYR:CD1	2:C:170:MET:HE1	2.56	0.41
2:D:305:GLN:O	2:D:309:THR:HB	2.20	0.41
2:Q:239:VAL:HG13	2:Q:289:PHE:CA	2.50	0.41
2:F:156:LEU:HD11	2:F:299:ILE:HD11	2.02	0.41
2:R:58:ARG:HG3	2:H:115:THR:HG23	2.03	0.41
2:R:124:LEU:HD21	2:G:416:ARG:HD3	2.03	0.41
2:R:202:ILE:HG22	2:R:207:TYR:OH	2.20	0.41
2:R:235:ILE:N	2:R:235:ILE:CD1	2.83	0.41
2:R:392:VAL:O	2:R:393:ASP:C	2.64	0.41
2:G:377:PHE:CD1	2:G:377:PHE:C	2.99	0.41
2:H:59:VAL:N	2:H:60:PRO:HD2	2.36	0.41
2:S:1:MET:HB3	2:S:2:SER:H	1.49	0.41
2:I:44:THR:O	2:I:44:THR:CG2	2.66	0.41
2:I:64:MET:HE2	2:I:65:SER:CA	2.49	0.41
2:J:132:LEU:HD23	2:J:132:LEU:HA	1.92	0.41
1:A:129:MET:CE	1:A:765:MET:HE2	2.50	0.41
1:A:198:VAL:HG13	1:A:199:PRO:HD2	2.02	0.41
1:A:219:ARG:HH11	1:A:219:ARG:CG	2.29	0.41
1:A:316:VAL:HG21	1:A:651:GLN:HE21	1.82	0.41
1:A:950:SER:O	1:A:953:VAL:HG22	2.20	0.41
1:B:31:VAL:CG1	1:B:32:TYR:N	2.81	0.41
1:B:56:THR:HA	1:B:57:PRO:HD3	1.89	0.41
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.80	0.41
1:B:570:PHE:CD1	1:B:570:PHE:N	2.89	0.41
1:B:812:ILE:HD11	1:B:840:MET:HE3	2.03	0.41
2:D:343:GLU:HB3	2:F:309:THR:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:163:GLN:NE2	2:Q:185:PHE:H	2.13	0.41
2:Q:239:VAL:HA	2:Q:288:GLY:C	2.46	0.41
2:E:151:ILE:HD11	2:E:156:LEU:HG	2.02	0.41
2:E:244:THR:C	2:E:246:ALA:N	2.79	0.41
2:E:323:PHE:HB2	2:E:405:TRP:HE1	1.85	0.41
2:F:61:LEU:HD12	2:F:61:LEU:HA	1.91	0.41
2:F:354:ASN:ND2	2:F:366:ILE:HD13	2.36	0.41
2:R:17:SER:O	2:R:21:VAL:HG23	2.20	0.41
2:G:12:LEU:HA	2:H:28:PHE:CZ	2.55	0.41
2:G:210:VAL:HA	2:G:277:ASN:CB	2.48	0.41
2:S:178:ALA:O	2:S:199:ASN:ND2	2.53	0.41
1:A:102:TYR:CB	1:A:765:MET:HE1	2.50	0.41
1:A:111:ASP:OD2	1:A:875:ARG:HD2	2.21	0.41
1:A:404:THR:C	1:A:406:ARG:N	2.78	0.41
1:B:85:ILE:CG1	1:B:933:THR:OG1	2.66	0.41
1:B:115:GLU:O	1:B:116:PRO:C	2.64	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.82	0.41
1:B:507:ALA:HB3	1:B:508:PRO:HD3	2.03	0.41
1:B:598:LEU:O	1:B:599:LEU:C	2.64	0.41
2:P:332:PHE:CE2	2:P:336:LEU:HD11	2.56	0.41
2:D:169:MET:O	2:D:173:LEU:HD13	2.21	0.41
2:D:208:GLN:HG2	2:D:279:ASN:OD1	2.20	0.41
2:Q:46:LEU:HD23	2:Q:46:LEU:HA	1.81	0.41
2:Q:132:LEU:HG	2:Q:328:PHE:CE2	2.56	0.41
2:Q:404:LEU:HD22	2:Q:404:LEU:HA	1.91	0.41
2:G:41:ASN:HB3	2:H:31:LEU:HD22	1.99	0.41
2:S:250:THR:HG23	2:S:282:LEU:HA	2.03	0.41
2:J:153:PRO:HB2	2:J:187:ALA:HB1	2.03	0.41
1:A:438:ILE:CD1	1:A:447:TRP:CZ2	2.96	0.41
1:A:541:ILE:HG23	1:A:542:THR:HG22	2.03	0.41
1:B:377:LEU:HD23	1:B:377:LEU:HA	1.84	0.41
1:B:801:VAL:O	1:B:961:ILE:HG13	2.20	0.41
2:P:147:TYR:N	2:P:147:TYR:CD1	2.89	0.41
2:C:46:LEU:N	2:C:46:LEU:HD12	2.36	0.41
2:C:222:GLY:HA2	2:C:268:ARG:HB3	2.02	0.41
2:D:139:ILE:HD12	2:D:405:TRP:CE3	2.56	0.41
2:D:170:MET:HE2	2:D:232:PHE:HB2	2.02	0.41
2:Q:9:THR:HA	2:Q:107:ARG:HD2	2.02	0.41
2:E:166:ASN:N	2:E:168:PRO:HD2	2.36	0.41
2:E:185:PHE:CE2	2:E:192:ILE:HD11	2.54	0.41
2:F:325:VAL:HB	2:F:405:TRP:HE1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1:MET:O	2:R:2:SER:O	2.39	0.41
2:R:268:ARG:HD2	2:G:321:ASP:HB2	2.02	0.41
2:G:309:THR:O	2:G:309:THR:CG2	2.68	0.41
2:H:59:VAL:CG1	2:H:60:PRO:HD3	2.50	0.41
2:S:160:VAL:HG12	2:S:161:ALA:H	1.86	0.41
2:J:132:LEU:O	2:J:136:GLN:HG3	2.21	0.41
1:A:101:ILE:O	1:A:102:TYR:C	2.64	0.41
1:A:307:LEU:HD22	1:A:617:TYR:CD1	2.55	0.41
1:A:317:MET:CE	3:K:294:ASP:OD2	2.69	0.41
1:A:582:ASN:O	1:A:583:SER:C	2.62	0.41
1:A:676:ARG:HG2	1:A:676:ARG:HH11	1.86	0.41
1:B:313:LEU:HD23	1:B:608:ASN:ND2	2.36	0.41
1:B:341:ALA:C	1:B:343:ALA:N	2.76	0.41
1:B:971:GLU:O	1:B:972:PHE:C	2.64	0.41
2:P:214:TRP:CZ3	2:P:215:ALA:HB2	2.55	0.41
2:P:271:PHE:CZ	2:P:293:ILE:HD13	2.55	0.41
2:P:316:THR:HG21	2:P:397:ARG:NH1	2.35	0.41
2:C:95:VAL:HG23	2:C:95:VAL:O	2.21	0.41
2:C:110:VAL:HG22	2:C:111:PRO:CA	2.51	0.41
2:C:150:PRO:HA	2:C:297:PHE:O	2.21	0.41
2:D:1:MET:HB3	2:D:93:PRO:HD2	2.03	0.41
2:D:203:PRO:HG2	2:D:207:TYR:OH	2.20	0.41
2:D:250:THR:HG23	2:D:281:GLU:O	2.21	0.41
2:D:328:PHE:CD1	2:D:328:PHE:N	2.89	0.41
2:Q:217:VAL:HG13	2:Q:303:ARG:HB3	2.02	0.41
2:Q:366:ILE:N	2:Q:366:ILE:CD1	2.79	0.41
2:E:196:ILE:HB	2:E:289:PHE:HE2	1.86	0.41
2:F:24:ASN:C	2:F:24:ASN:ND2	2.79	0.41
2:F:80:TYR:CE2	2:F:81:MET:HG3	2.56	0.41
2:F:309:THR:O	2:F:309:THR:HG22	2.20	0.41
2:R:256:THR:CG2	2:G:337:ARG:HH12	2.33	0.41
2:R:393:ASP:OD2	2:R:394:LEU:N	2.53	0.41
2:G:87:PHE:HB2	2:G:403:HIS:CE1	2.56	0.41
2:G:349:MET:HG2	2:G:376:TRP:CG	2.56	0.41
2:S:13:LEU:HD23	2:S:13:LEU:HA	1.87	0.41
2:S:41:ASN:CB	2:I:31:LEU:HD11	2.51	0.41
2:S:56:ASP:HA	2:S:57:PRO:HD2	1.88	0.41
2:S:124:LEU:HD12	2:I:14:GLU:HG3	2.03	0.41
2:S:170:MET:CE	2:S:232:PHE:HB2	2.51	0.41
2:I:147:TYR:N	2:I:147:TYR:CD1	2.89	0.41
2:I:201:ALA:HA	2:I:287:THR:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:396:ILE:CD1	2:I:396:ILE:H	2.34	0.41
2:T:82:LEU:HD22	2:T:356:LEU:HD23	2.03	0.41
2:T:186:VAL:CG2	2:T:193:LEU:HB2	2.51	0.41
2:T:324:ASP:O	2:T:325:VAL:C	2.63	0.41
1:A:223:PRO:HA	1:A:979:PHE:O	2.20	0.41
2:P:208:GLN:HG2	2:P:279:ASN:OD1	2.20	0.41
2:C:387:LEU:HG	2:C:401:VAL:HG21	2.03	0.41
2:D:160:VAL:HG12	2:D:161:ALA:H	1.86	0.41
2:Q:3:ARG:HG3	2:Q:4:GLN:N	2.36	0.41
2:Q:326:SER:HA	2:Q:329:LEU:HD12	2.03	0.41
2:E:82:LEU:HA	2:E:356:LEU:HD23	2.01	0.41
2:R:48:VAL:HB	2:R:49:SER:H	1.68	0.41
2:R:201:ALA:HA	2:R:287:THR:HA	2.03	0.41
2:G:64:MET:HG3	2:G:103:TYR:CD2	2.55	0.41
2:G:145:ILE:HD12	2:G:308:TYR:CE1	2.55	0.41
2:G:272:SER:O	2:G:272:SER:OG	2.38	0.41
2:H:352:LEU:HD11	2:H:407:ILE:HG21	2.02	0.41
2:I:14:GLU:OE1	2:I:132:LEU:N	2.40	0.41
2:I:57:PRO:C	2:I:60:PRO:HD2	2.46	0.41
2:I:239:VAL:HG13	2:I:289:PHE:CA	2.51	0.41
2:J:271:PHE:CZ	2:J:293:ILE:HD13	2.56	0.41
2:J:415:GLY:O	2:J:416:ARG:C	2.63	0.41
2:T:1:MET:HB3	2:T:2:SER:H	1.58	0.41
2:T:231:PHE:O	2:T:232:PHE:HB2	2.20	0.41
1:A:659:VAL:H	1:A:659:VAL:HG23	1.62	0.40
1:B:289:ASP:O	1:B:290:TYR:C	2.64	0.40
1:B:651:GLN:O	1:B:652:TYR:C	2.65	0.40
2:C:325:VAL:O	2:C:326:SER:C	2.64	0.40
2:D:325:VAL:HG13	2:D:405:TRP:NE1	2.36	0.40
2:Q:81:MET:HE3	2:Q:86:TRP:CZ2	2.55	0.40
2:Q:132:LEU:O	2:Q:133:TYR:C	2.64	0.40
2:E:24:ASN:C	2:E:24:ASN:ND2	2.79	0.40
2:R:387:LEU:HG	2:R:401:VAL:HG21	2.03	0.40
2:G:254:VAL:HG12	2:G:256:THR:H	1.86	0.40
2:S:265:THR:C	2:S:267:SER:H	2.29	0.40
2:J:408:THR:O	2:J:411:ILE:HB	2.20	0.40
1:A:629:GLU:CD	1:B:590:ARG:HH12	2.30	0.40
1:A:679:TYR:HD1	1:A:703:ILE:HD11	1.85	0.40
1:A:706:ILE:O	1:A:709:VAL:N	2.50	0.40
1:B:326:ASP:O	1:B:330:VAL:HG23	2.21	0.40
1:B:718:ARG:NH1	1:B:718:ARG:HG2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:4:GLN:O	2:P:7:LEU:N	2.54	0.40
2:P:167:ILE:HB	2:P:168:PRO:HD3	2.03	0.40
2:C:48:VAL:HG21	2:C:105:ARG:NH2	2.37	0.40
2:C:379:PHE:CE1	2:C:404:LEU:HD22	2.56	0.40
2:D:121:ASN:CA	2:D:146:PRO:HA	2.52	0.40
2:D:379:PHE:O	2:D:380:SER:C	2.63	0.40
2:Q:188:GLU:HA	2:Q:232:PHE:CE1	2.56	0.40
2:Q:254:VAL:CG1	2:Q:255:PRO:HD2	2.50	0.40
2:Q:418:TYR:CZ	2:Q:420:PRO:HG3	2.56	0.40
2:E:396:ILE:O	2:E:400:ILE:HG12	2.20	0.40
2:R:5:MET:HE3	2:R:105:ARG:HA	2.03	0.40
2:R:353:THR:HG23	2:R:404:LEU:HD11	2.04	0.40
2:G:271:PHE:CZ	2:G:293:ILE:HD13	2.56	0.40
2:H:316:THR:HG23	2:H:397:ARG:HH12	1.87	0.40
2:I:158:ARG:HA	2:I:158:ARG:HD3	1.88	0.40
2:I:254:VAL:HG11	2:I:272:SER:O	2.20	0.40
1:A:60:LEU:N	1:A:60:LEU:CD2	2.82	0.40
1:B:489:LEU:CD1	1:B:514:PRO:HB3	2.50	0.40
1:B:555:LEU:HD12	1:B:555:LEU:N	2.36	0.40
2:P:26:ASP:OD1	2:D:131:LYS:NZ	2.54	0.40
2:P:387:LEU:HG	2:P:401:VAL:HG21	2.03	0.40
2:C:120:ASN:O	2:C:121:ASN:C	2.61	0.40
2:C:121:ASN:HA	2:C:146:PRO:HB3	2.03	0.40
2:C:182:GLN:HB3	2:C:183:PRO:HD2	2.03	0.40
2:C:309:THR:O	2:C:309:THR:CG2	2.67	0.40
2:C:323:PHE:HD1	2:C:405:TRP:CD1	2.39	0.40
2:C:363:PRO:HA	2:C:364:PRO:HD3	1.85	0.40
2:D:322:ASP:O	2:D:325:VAL:HG22	2.20	0.40
2:D:325:VAL:HG13	2:D:405:TRP:CE2	2.57	0.40
2:D:344:ILE:HD12	2:D:344:ILE:N	2.27	0.40
2:Q:135:ARG:O	2:Q:136:GLN:C	2.64	0.40
2:Q:359:ASN:N	2:Q:359:ASN:ND2	2.68	0.40
2:G:361:MET:HE1	2:G:367:PRO:CG	2.51	0.40
2:S:157:PHE:HD1	2:S:214:TRP:CE2	2.39	0.40
2:I:358:THR:C	2:I:360:TYR:H	2.30	0.40
2:J:105:ARG:O	2:J:107:ARG:HG2	2.21	0.40
2:T:9:THR:HG22	2:T:107:ARG:HE	1.86	0.40
1:B:6:ARG:HH11	1:B:6:ARG:CB	2.35	0.40
1:B:108:ILE:HG12	1:B:109:GLU:N	2.37	0.40
1:B:114:TYR:O	1:B:115:GLU:C	2.63	0.40
1:B:364:MET:CE	1:B:541:ILE:HD12	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:197:ARG:HG3	2:P:197:ARG:HH11	1.86	0.40
2:P:244:THR:HG22	2:P:246:ALA:H	1.87	0.40
2:P:299:ILE:O	2:P:300:LEU:O	2.39	0.40
2:C:235:ILE:N	2:C:235:ILE:CD1	2.84	0.40
2:C:373:THR:HG22	2:C:373:THR:O	2.20	0.40
2:Q:396:ILE:HD12	2:Q:396:ILE:N	2.37	0.40
2:F:163:GLN:HE21	2:F:169:MET:HG3	1.86	0.40
2:R:33:THR:O	2:R:34:GLY:C	2.63	0.40
2:R:226:TYR:CD1	2:G:170:MET:HE1	2.57	0.40
2:G:87:PHE:HB2	2:G:403:HIS:ND1	2.36	0.40
2:H:121:ASN:HA	2:H:146:PRO:HA	2.04	0.40
2:H:132:LEU:HD23	2:H:132:LEU:HA	1.91	0.40
2:S:100:ILE:HG23	2:S:104:ILE:HB	2.03	0.40
2:S:349:MET:O	2:S:350:ASP:C	2.65	0.40
2:I:58:ARG:O	2:I:62:GLN:HB2	2.22	0.40
2:I:72:ILE:HD12	2:I:72:ILE:HA	1.86	0.40
2:I:194:PHE:CZ	2:I:291:VAL:HG11	2.56	0.40
2:I:261:LEU:HA	2:I:262:PRO:HD2	1.85	0.40
2:I:358:THR:O	2:I:360:TYR:N	2.54	0.40
2:J:418:TYR:CE1	2:J:420:PRO:HD3	2.57	0.40
2:T:282:LEU:HD11	2:T:289:PHE:CE2	2.57	0.40
1:B:345:LEU:HA	1:B:345:LEU:HD23	1.84	0.40
1:B:575:PRO:HG2	1:B:576:ALA:H	1.86	0.40
2:D:186:VAL:HB	2:D:231:PHE:CZ	2.57	0.40
2:Q:167:ILE:N	2:Q:168:PRO:CD	2.82	0.40
2:Q:170:MET:HE1	2:F:226:TYR:CD1	2.56	0.40
2:E:239:VAL:HA	2:E:288:GLY:C	2.47	0.40
2:F:279:ASN:HD22	2:F:279:ASN:HA	1.51	0.40
2:F:310:LEU:HD21	2:F:320:ILE:HD11	2.03	0.40
2:R:64:MET:HG3	2:R:103:TYR:CE2	2.56	0.40
2:R:309:THR:O	2:R:309:THR:CG2	2.65	0.40
2:G:120:ASN:O	2:G:121:ASN:C	2.64	0.40
2:S:19:TYR:CG	2:S:42:MET:HE1	2.56	0.40
2:I:140:MET:CE	2:I:406:VAL:HG11	2.50	0.40
2:J:72:ILE:O	2:J:72:ILE:HG13	2.20	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	965/1019 (95%)	845 (88%)	105 (11%)	15 (2%)	7	36
1	B	1017/1019 (100%)	901 (89%)	97 (10%)	19 (2%)	6	33
2	C	411/421 (98%)	367 (89%)	38 (9%)	6 (2%)	8	37
2	D	413/421 (98%)	361 (87%)	46 (11%)	6 (2%)	8	37
2	E	419/421 (100%)	368 (88%)	41 (10%)	10 (2%)	4	29
2	F	411/421 (98%)	370 (90%)	34 (8%)	7 (2%)	7	35
2	G	413/421 (98%)	364 (88%)	43 (10%)	6 (2%)	8	37
2	H	419/421 (100%)	379 (90%)	34 (8%)	6 (1%)	9	38
2	I	415/421 (99%)	375 (90%)	34 (8%)	6 (1%)	9	38
2	J	409/421 (97%)	348 (85%)	47 (12%)	14 (3%)	3	23
2	P	410/421 (97%)	361 (88%)	40 (10%)	9 (2%)	5	30
2	Q	419/421 (100%)	365 (87%)	47 (11%)	7 (2%)	7	35
2	R	419/421 (100%)	376 (90%)	37 (9%)	6 (1%)	9	38
2	S	419/421 (100%)	366 (87%)	44 (10%)	9 (2%)	5	31
2	T	419/421 (100%)	369 (88%)	41 (10%)	9 (2%)	5	31
3	K	10/506 (2%)	8 (80%)	1 (10%)	1 (10%)	0	6
All	All	7388/8017 (92%)	6523 (88%)	729 (10%)	136 (2%)	6	34

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	451	GLY
1	A	546	GLY
1	B	24	SER
1	B	112	SER
1	B	379	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	444	ILE
1	B	836	SER
1	B	931	GLY
1	B	934	ASN
2	P	364	PRO
2	P	379	PHE
2	P	416	ARG
2	C	364	PRO
2	C	379	PHE
2	D	47	SER
2	D	216	SER
2	Q	364	PRO
2	Q	379	PHE
2	Q	416	ARG
2	F	121	ASN
2	R	364	PRO
2	R	379	PHE
2	G	364	PRO
2	H	247	ASP
2	H	364	PRO
2	I	55	SER
2	J	98	ASP
2	T	95	VAL
3	K	297	ARG
1	A	215	ASN
1	A	335	SER
1	A	836	SER
1	A	1004	GLY
1	B	3	SER
1	B	10	GLY
1	B	20	THR
1	B	162	GLY
1	B	338	THR
1	B	612	ASN
1	B	662	PHE
2	P	300	LEU
2	C	340	GLY
2	D	364	PRO
2	D	376	TRP
2	D	379	PHE
2	E	162	GLY
2	E	364	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	376	TRP
2	E	379	PHE
2	F	161	ALA
2	F	247	ASP
2	F	364	PRO
2	H	380	SER
2	S	2	SER
2	S	49	SER
2	S	364	PRO
2	I	364	PRO
2	J	57	PRO
2	J	359	ASN
2	J	364	PRO
2	J	416	ARG
2	T	364	PRO
2	T	416	ARG
1	A	493	ASP
1	A	931	GLY
1	B	499	ALA
1	B	653	GLN
2	P	121	ASN
2	C	121	ASN
2	Q	180	GLN
2	Q	203	PRO
2	E	330	THR
2	E	416	ARG
2	R	2	SER
2	R	51	ALA
2	R	201	ALA
2	G	161	ALA
2	G	201	ALA
2	H	86	TRP
2	H	330	THR
2	H	379	PHE
2	S	162	GLY
2	I	2	SER
2	I	359	ASN
2	I	416	ARG
2	J	180	GLN
2	T	29	SER
1	A	102	TYR
2	P	340	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	420	PRO
2	C	420	PRO
2	D	201	ALA
2	F	2	SER
2	R	416	ARG
2	G	2	SER
2	S	330	THR
2	S	379	PHE
2	S	416	ARG
2	J	2	SER
2	T	359	ASN
1	A	378	THR
1	A	444	ILE
1	A	553	GLU
1	A	865	GLY
1	B	9	ASP
2	Q	376	TRP
2	E	2	SER
2	E	204	ALA
2	F	245	ALA
2	F	420	PRO
2	G	46	LEU
2	G	380	SER
2	S	50	SER
2	I	162	GLY
2	J	29	SER
2	J	212	PRO
2	J	247	ASP
2	J	367	PRO
2	J	379	PHE
1	B	824	GLN
2	P	2	SER
2	Q	330	THR
2	E	216	SER
2	S	359	ASN
2	T	300	LEU
1	B	148	VAL
2	E	203	PRO
2	T	162	GLY
2	T	420	PRO
2	P	162	GLY
2	J	203	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	340	GLY
1	A	246	PRO
2	C	59	VAL
2	J	420	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	854/900 (95%)	788 (92%)	66 (8%)	12	37
1	B	900/900 (100%)	830 (92%)	70 (8%)	11	36
2	C	356/360 (99%)	338 (95%)	18 (5%)	21	48
2	D	358/360 (99%)	338 (94%)	20 (6%)	19	46
2	E	360/360 (100%)	339 (94%)	21 (6%)	18	44
2	F	356/360 (99%)	333 (94%)	23 (6%)	15	42
2	G	358/360 (99%)	338 (94%)	20 (6%)	19	46
2	H	360/360 (100%)	334 (93%)	26 (7%)	13	38
2	I	360/360 (100%)	332 (92%)	28 (8%)	11	36
2	J	354/360 (98%)	333 (94%)	21 (6%)	18	44
2	P	355/360 (99%)	333 (94%)	22 (6%)	16	43
2	Q	360/360 (100%)	331 (92%)	29 (8%)	11	35
2	R	360/360 (100%)	342 (95%)	18 (5%)	22	48
2	S	360/360 (100%)	328 (91%)	32 (9%)	9	32
2	T	360/360 (100%)	328 (91%)	32 (9%)	9	32
3	K	12/450 (3%)	9 (75%)	3 (25%)	0	4
All	All	6423/6930 (93%)	5974 (93%)	449 (7%)	14	39

All (449) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	70	LYS
1	A	85	ILE
1	A	87	ASP
1	A	108	ILE
1	A	147	PHE
1	A	184	ARG
1	A	192	ARG
1	A	219	ARG
1	A	241	ILE
1	A	259	ASN
1	A	269	LEU
1	A	278	THR
1	A	286	GLN
1	A	307	LEU
1	A	316	VAL
1	A	320	VAL
1	A	325	GLN
1	A	349	ASN
1	A	356	LEU
1	A	366	ASN
1	A	403	LEU
1	A	414	ARG
1	A	425	THR
1	A	452	ARG
1	A	478	ARG
1	A	483	GLN
1	A	510	LEU
1	A	526	THR
1	A	533	LEU
1	A	572	THR
1	A	588	LEU
1	A	590	ARG
1	A	593	ASP
1	A	629	GLU
1	A	655	LEU
1	A	659	VAL
1	A	674	LEU
1	A	686	LEU
1	A	688	ARG
1	A	694	PHE
1	A	715	ILE
1	A	718	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	722	THR
1	A	743	VAL
1	A	757	GLN
1	A	759	ASP
1	A	766	THR
1	A	767	GLN
1	A	775	THR
1	A	792	THR
1	A	795	VAL
1	A	827	ARG
1	A	845	ARG
1	A	881	GLN
1	A	930	LEU
1	A	937	THR
1	A	940	MET
1	A	941	ARG
1	A	956	GLN
1	A	970	THR
1	A	971	GLU
1	A	983	VAL
1	A	988	ASP
1	A	994	ASP
1	A	1003	ILE
1	B	4	THR
1	B	6	ARG
1	B	12	SER
1	B	21	GLU
1	B	30	GLU
1	B	33	ASN
1	B	60	LEU
1	B	63	ILE
1	B	69	LYS
1	B	83	LEU
1	B	84	ARG
1	B	85	ILE
1	B	87	ASP
1	B	100	ASP
1	B	106	MET
1	B	124	ARG
1	B	130	LEU
1	B	134	CYS
1	B	153	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	ASP
1	B	165	ASN
1	B	169	LEU
1	B	176	GLU
1	B	187	ARG
1	B	200	VAL
1	B	204	ASP
1	B	206	LEU
1	B	229	LEU
1	B	262	ARG
1	B	269	LEU
1	B	279	LEU
1	B	314	HIS
1	B	321	THR
1	B	337	VAL
1	B	347	ARG
1	B	392	MET
1	B	438	ILE
1	B	441	VAL
1	B	455	LEU
1	B	460	ASN
1	B	496	SER
1	B	517	MET
1	B	543	THR
1	B	547	GLN
1	B	559	THR
1	B	568	ASN
1	B	572	THR
1	B	621	VAL
1	B	623	ARG
1	B	653	GLN
1	B	669	ILE
1	B	676	ARG
1	B	680	ASP
1	B	681	THR
1	B	715	ILE
1	B	726	ARG
1	B	737	ASN
1	B	743	VAL
1	B	749	ASN
1	B	766	THR
1	B	795	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	831	THR
1	B	842	ASN
1	B	881	GLN
1	B	886	GLU
1	B	938	LEU
1	B	939	ARG
1	B	943	GLU
1	B	1006	HIS
1	B	1009	ARG
2	P	1	MET
2	P	27	THR
2	P	31	LEU
2	P	32	THR
2	P	33	THR
2	P	73	THR
2	P	114	ASP
2	P	122	LEU
2	P	156	LEU
2	P	158	ARG
2	P	182	GLN
2	P	197	ARG
2	P	221	THR
2	P	265	THR
2	P	279	ASN
2	P	281	GLU
2	P	282	LEU
2	P	287	THR
2	P	298	THR
2	P	325	VAL
2	P	352	LEU
2	P	390	GLN
2	C	8	ASP
2	C	27	THR
2	C	32	THR
2	C	105	ARG
2	C	114	ASP
2	C	156	LEU
2	C	158	ARG
2	C	192	ILE
2	C	197	ARG
2	C	221	THR
2	C	265	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	287	THR
2	C	298	THR
2	C	325	VAL
2	C	344	ILE
2	C	352	LEU
2	C	361	MET
2	C	364	PRO
2	D	24	ASN
2	D	27	THR
2	D	32	THR
2	D	37	ASN
2	D	114	ASP
2	D	130	PRO
2	D	156	LEU
2	D	158	ARG
2	D	192	ILE
2	D	197	ARG
2	D	210	VAL
2	D	221	THR
2	D	265	THR
2	D	279	ASN
2	D	287	THR
2	D	298	THR
2	D	314	THR
2	D	337	ARG
2	D	352	LEU
2	D	391	ASN
2	Q	27	THR
2	Q	40	SER
2	Q	45	GLN
2	Q	62	GLN
2	Q	64	MET
2	Q	67	MET
2	Q	72	ILE
2	Q	94	THR
2	Q	144	ASP
2	Q	156	LEU
2	Q	164	THR
2	Q	192	ILE
2	Q	208	GLN
2	Q	269	LEU
2	Q	287	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	298	THR
2	Q	309	THR
2	Q	311	ASN
2	Q	325	VAL
2	Q	335	GLN
2	Q	342	TYR
2	Q	354	ASN
2	Q	359	ASN
2	Q	373	THR
2	Q	392	VAL
2	Q	399	LEU
2	Q	404	LEU
2	Q	410	LEU
2	Q	421	ASN
2	E	3	ARG
2	E	27	THR
2	E	55	SER
2	E	56	ASP
2	E	72	ILE
2	E	73	THR
2	E	114	ASP
2	E	151	ILE
2	E	158	ARG
2	E	253	THR
2	E	279	ASN
2	E	289	PHE
2	E	298	THR
2	E	303	ARG
2	E	314	THR
2	E	325	VAL
2	E	344	ILE
2	E	361	MET
2	E	370	LEU
2	E	391	ASN
2	E	395	ASN
2	F	12	LEU
2	F	31	LEU
2	F	33	THR
2	F	45	GLN
2	F	73	THR
2	F	114	ASP
2	F	144	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	197	ARG
2	F	211	VAL
2	F	217	VAL
2	F	229	ASN
2	F	265	THR
2	F	268	ARG
2	F	279	ASN
2	F	298	THR
2	F	315	GLN
2	F	316	THR
2	F	330	THR
2	F	335	GLN
2	F	337	ARG
2	F	352	LEU
2	F	354	ASN
2	F	359	ASN
2	R	10	SER
2	R	31	LEU
2	R	32	THR
2	R	73	THR
2	R	84	LYS
2	R	114	ASP
2	R	122	LEU
2	R	156	LEU
2	R	192	ILE
2	R	221	THR
2	R	256	THR
2	R	265	THR
2	R	279	ASN
2	R	287	THR
2	R	298	THR
2	R	352	LEU
2	R	361	MET
2	R	364	PRO
2	G	3	ARG
2	G	88	ASN
2	G	107	ARG
2	G	158	ARG
2	G	197	ARG
2	G	228	THR
2	G	273	LEU
2	G	279	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	281	GLU
2	G	282	LEU
2	G	303	ARG
2	G	315	GLN
2	G	334	SER
2	G	341	GLN
2	G	344	ILE
2	G	354	ASN
2	G	362	ASP
2	G	364	PRO
2	G	410	LEU
2	G	419	ARG
2	H	10	SER
2	H	21	VAL
2	H	45	GLN
2	H	49	SER
2	H	53	TYR
2	H	73	THR
2	H	80	TYR
2	H	95	VAL
2	H	114	ASP
2	H	156	LEU
2	H	192	ILE
2	H	197	ARG
2	H	251	THR
2	H	265	THR
2	H	298	THR
2	H	305	GLN
2	H	309	THR
2	H	314	THR
2	H	315	GLN
2	H	331	THR
2	H	344	ILE
2	H	354	ASN
2	H	362	ASP
2	H	364	PRO
2	H	366	ILE
2	H	392	VAL
2	S	31	LEU
2	S	48	VAL
2	S	72	ILE
2	S	80	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	105	ARG
2	S	107	ARG
2	S	114	ASP
2	S	160	VAL
2	S	182	GLN
2	S	192	ILE
2	S	197	ARG
2	S	208	GLN
2	S	221	THR
2	S	247	ASP
2	S	256	THR
2	S	265	THR
2	S	287	THR
2	S	298	THR
2	S	303	ARG
2	S	305	GLN
2	S	310	LEU
2	S	316	THR
2	S	325	VAL
2	S	334	SER
2	S	343	GLU
2	S	344	ILE
2	S	364	PRO
2	S	391	ASN
2	S	392	VAL
2	S	404	LEU
2	S	410	LEU
2	S	419	ARG
2	I	4	GLN
2	I	12	LEU
2	I	24	ASN
2	I	33	THR
2	I	40	SER
2	I	64	MET
2	I	73	THR
2	I	77	ARG
2	I	100	ILE
2	I	107	ARG
2	I	114	ASP
2	I	148	SER
2	I	156	LEU
2	I	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	192	ILE
2	I	242	THR
2	I	269	LEU
2	I	325	VAL
2	I	337	ARG
2	I	347	ASP
2	I	351	GLN
2	I	364	PRO
2	I	380	SER
2	I	384	ARG
2	I	392	VAL
2	I	404	LEU
2	I	419	ARG
2	I	421	ASN
2	J	4	GLN
2	J	8	ASP
2	J	27	THR
2	J	33	THR
2	J	57	PRO
2	J	95	VAL
2	J	107	ARG
2	J	114	ASP
2	J	143	LEU
2	J	144	ASP
2	J	148	SER
2	J	151	ILE
2	J	156	LEU
2	J	158	ARG
2	J	208	GLN
2	J	220	VAL
2	J	229	ASN
2	J	261	LEU
2	J	265	THR
2	J	350	ASP
2	J	390	GLN
2	T	8	ASP
2	T	9	THR
2	T	27	THR
2	T	42	MET
2	T	54	VAL
2	T	55	SER
2	T	59	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	64	MET
2	T	73	THR
2	T	80	TYR
2	T	88	ASN
2	T	102	THR
2	T	105	ARG
2	T	109	GLN
2	T	123	SER
2	T	158	ARG
2	T	192	ILE
2	T	197	ARG
2	T	208	GLN
2	T	210	VAL
2	T	242	THR
2	T	270	SER
2	T	298	THR
2	T	309	THR
2	T	312	SER
2	T	314	THR
2	T	315	GLN
2	T	325	VAL
2	T	352	LEU
2	T	364	PRO
2	T	392	VAL
2	T	399	LEU
3	K	289	SER
3	K	290	GLU
3	K	297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (219) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	121	HIS
1	A	131	ASN
1	A	181	ASN
1	A	191	GLN
1	A	226	GLN
1	A	286	GLN
1	A	325	GLN
1	A	349	ASN
1	A	366	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	435	ASN
1	A	448	GLN
1	A	461	ASN
1	A	474	GLN
1	A	484	GLN
1	A	547	GLN
1	A	573	GLN
1	A	584	ASN
1	A	634	GLN
1	A	653	GLN
1	A	673	GLN
1	A	695	HIS
1	A	712	GLN
1	A	737	ASN
1	A	757	GLN
1	A	767	GLN
1	A	783	ASN
1	A	810	HIS
1	A	830	ASN
1	A	1013	ASN
1	B	121	HIS
1	B	165	ASN
1	B	177	HIS
1	B	226	GLN
1	B	236	ASN
1	B	318	GLN
1	B	324	GLN
1	B	325	GLN
1	B	351	GLN
1	B	362	GLN
1	B	395	GLN
1	B	435	ASN
1	B	483	GLN
1	B	547	GLN
1	B	633	HIS
1	B	639	GLN
1	B	651	GLN
1	B	653	GLN
1	B	760	HIS
1	B	810	HIS
1	B	1016	GLN
2	P	24	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	37	ASN
2	P	62	GLN
2	P	120	ASN
2	P	121	ASN
2	P	180	GLN
2	P	229	ASN
2	P	260	ASN
2	P	302	ASN
2	P	315	GLN
2	P	351	GLN
2	P	421	ASN
2	C	24	ASN
2	C	45	GLN
2	C	62	GLN
2	C	121	ASN
2	C	125	GLN
2	C	181	GLN
2	C	229	ASN
2	C	260	ASN
2	C	279	ASN
2	C	302	ASN
2	C	315	GLN
2	C	335	GLN
2	C	351	GLN
2	D	4	GLN
2	D	24	ASN
2	D	45	GLN
2	D	62	GLN
2	D	120	ASN
2	D	180	GLN
2	D	229	ASN
2	D	305	GLN
2	D	351	GLN
2	D	354	ASN
2	Q	24	ASN
2	Q	45	GLN
2	Q	118	GLN
2	Q	120	ASN
2	Q	121	ASN
2	Q	125	GLN
2	Q	163	GLN
2	Q	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	208	GLN
2	Q	259	ASN
2	Q	359	ASN
2	E	24	ASN
2	E	109	GLN
2	E	120	ASN
2	E	121	ASN
2	E	136	GLN
2	E	163	GLN
2	E	182	GLN
2	E	208	GLN
2	E	279	ASN
2	E	302	ASN
2	E	315	GLN
2	E	351	GLN
2	E	354	ASN
2	E	391	ASN
2	F	24	ASN
2	F	45	GLN
2	F	88	ASN
2	F	125	GLN
2	F	163	GLN
2	F	180	GLN
2	F	208	GLN
2	F	229	ASN
2	F	259	ASN
2	F	279	ASN
2	F	302	ASN
2	F	305	GLN
2	F	315	GLN
2	F	335	GLN
2	F	351	GLN
2	F	354	ASN
2	F	359	ASN
2	R	24	ASN
2	R	41	ASN
2	R	62	GLN
2	R	120	ASN
2	R	121	ASN
2	R	137	ASN
2	R	180	GLN
2	R	302	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	311	ASN
2	R	315	GLN
2	R	395	ASN
2	G	4	GLN
2	G	24	ASN
2	G	37	ASN
2	G	41	ASN
2	G	66	ASN
2	G	109	GLN
2	G	118	GLN
2	G	120	ASN
2	G	125	GLN
2	G	163	GLN
2	G	180	GLN
2	G	264	GLN
2	G	302	ASN
2	G	315	GLN
2	G	341	GLN
2	G	421	ASN
2	H	24	ASN
2	H	37	ASN
2	H	45	GLN
2	H	118	GLN
2	H	120	ASN
2	H	121	ASN
2	H	136	GLN
2	H	259	ASN
2	H	260	ASN
2	H	302	ASN
2	H	305	GLN
2	H	315	GLN
2	H	335	GLN
2	H	421	ASN
2	S	24	ASN
2	S	109	GLN
2	S	120	ASN
2	S	208	GLN
2	S	259	ASN
2	S	277	ASN
2	S	305	GLN
2	S	315	GLN
2	S	351	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	354	ASN
2	S	395	ASN
2	S	403	HIS
2	S	421	ASN
2	I	24	ASN
2	I	37	ASN
2	I	120	ASN
2	I	121	ASN
2	I	125	GLN
2	I	163	GLN
2	I	302	ASN
2	I	351	GLN
2	I	354	ASN
2	I	421	ASN
2	J	4	GLN
2	J	24	ASN
2	J	62	GLN
2	J	109	GLN
2	J	118	GLN
2	J	120	ASN
2	J	163	GLN
2	J	181	GLN
2	J	208	GLN
2	J	229	ASN
2	J	279	ASN
2	J	302	ASN
2	J	305	GLN
2	J	315	GLN
2	T	24	ASN
2	T	45	GLN
2	T	88	ASN
2	T	109	GLN
2	T	208	GLN
2	T	259	ASN
2	T	260	ASN
2	T	277	ASN
2	T	279	ASN
2	T	315	GLN
2	T	351	GLN
2	T	354	ASN
2	T	359	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	967/1019 (94%)	0.43	46 (4%)	35	19	1, 19, 50, 125	0
1	B	1019/1019 (100%)	0.37	50 (4%)	35	19	1, 15, 49, 115	0
2	C	415/421 (98%)	1.94	158 (38%)	1	1	44, 75, 99, 104	0
2	D	417/421 (99%)	1.59	125 (29%)	1	1	18, 68, 106, 112	0
2	E	421/421 (100%)	1.06	69 (16%)	4	4	3, 38, 71, 86	0
2	F	415/421 (98%)	1.16	74 (17%)	4	4	6, 42, 76, 82	0
2	G	417/421 (99%)	0.53	30 (7%)	21	14	1, 26, 59, 112	0
2	H	421/421 (100%)	0.44	20 (4%)	35	19	1, 26, 59, 89	0
2	I	419/421 (99%)	1.04	63 (15%)	5	5	12, 49, 82, 87	0
2	J	413/421 (98%)	1.21	71 (17%)	4	4	18, 51, 77, 93	0
2	P	414/421 (98%)	2.18	199 (48%)	0	1	49, 93, 113, 118	0
2	Q	421/421 (100%)	1.07	72 (17%)	4	4	11, 48, 76, 96	0
2	R	421/421 (100%)	0.56	30 (7%)	22	14	1, 27, 58, 70	0
2	S	421/421 (100%)	1.02	62 (14%)	6	5	6, 41, 72, 88	0
2	T	421/421 (100%)	0.13	8 (1%)	66	41	1, 15, 44, 74	0
3	K	12/506 (2%)	2.22	4 (33%)	1	1	61, 67, 74, 80	0
All	All	7434/8017 (92%)	0.89	1081 (14%)	6	5	1, 35, 92, 125	0

All (1081) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	369	GLY	12.8
2	R	369	GLY	10.7
2	E	421	ASN	9.2
2	P	393	ASP	9.1
2	C	347	ASP	8.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	233	GLY	8.4
2	E	247	ASP	8.2
2	E	246	ALA	8.1
2	E	195	GLY	7.9
2	P	362	ASP	7.7
2	P	204	ALA	7.7
2	P	275	GLY	7.5
2	C	369	GLY	7.3
2	J	362	ASP	7.2
2	I	421	ASN	7.1
2	F	238	GLY	7.0
2	C	362	ASP	7.0
2	P	182	GLN	7.0
2	C	238	GLY	7.0
2	E	208	GLN	6.9
2	F	182	GLN	6.9
2	C	421	ASN	6.9
2	S	391	ASN	6.9
2	I	257	ASP	6.7
3	K	289	SER	6.6
1	A	50	GLN	6.5
2	P	55	SER	6.4
2	D	182	GLN	6.4
2	P	246	ALA	6.4
2	F	369	GLY	6.3
2	S	393	ASP	6.3
2	I	259	ASN	6.2
2	S	362	ASP	6.2
2	Q	242	THR	6.1
2	C	390	GLN	6.0
2	C	180	GLN	5.9
2	S	182	GLN	5.8
2	S	315	GLN	5.8
2	P	286	LYS	5.8
2	C	247	ASP	5.7
2	J	421	ASN	5.7
2	C	55	SER	5.7
2	D	247	ASP	5.7
1	B	13	GLU	5.7
2	I	281	GLU	5.7
2	I	260	ASN	5.6
2	E	180	GLN	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	369	GLY	5.6
2	F	54	VAL	5.6
2	S	204	ALA	5.6
2	D	49	SER	5.6
2	J	364	PRO	5.5
2	P	395	ASN	5.5
2	Q	364	PRO	5.5
2	Q	369	GLY	5.4
2	C	76	ASP	5.4
2	C	283	GLY	5.4
2	I	204	ALA	5.4
2	D	48	VAL	5.4
2	Q	182	GLN	5.4
2	C	371	ALA	5.4
2	P	421	ASN	5.4
2	C	181	GLN	5.4
2	C	129	LYS	5.4
2	C	281	GLU	5.4
2	P	208	GLN	5.4
1	B	12	SER	5.3
2	Q	245	ALA	5.3
2	I	205	GLY	5.3
2	J	182	GLN	5.3
1	B	24	SER	5.3
2	D	177	PRO	5.3
2	F	171	GLY	5.3
1	A	1015	ASP	5.2
2	J	76	ASP	5.2
2	F	240	THR	5.2
2	J	281	GLU	5.2
2	P	178	ALA	5.2
2	C	90	ASP	5.2
1	A	1016	GLN	5.2
2	C	364	PRO	5.2
2	P	177	PRO	5.1
2	P	162	GLY	5.1
2	J	205	GLY	5.1
2	P	95	VAL	5.1
2	G	54	VAL	5.1
2	D	390	GLN	5.1
2	P	76	ASP	5.0
2	I	393	ASP	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	48	VAL	5.0
2	P	163	GLN	5.0
2	J	351	GLN	5.0
2	J	373	THR	5.0
2	D	258	ALA	5.0
2	C	239	VAL	5.0
2	P	78	CYS	5.0
2	S	176	PRO	4.9
2	F	95	VAL	4.9
2	Q	90	ASP	4.9
1	B	11	ALA	4.9
2	C	208	GLN	4.9
2	I	287	THR	4.9
2	D	179	ALA	4.9
2	E	364	PRO	4.9
2	F	177	PRO	4.9
2	P	256	THR	4.9
1	A	451	GLY	4.9
2	F	371	ALA	4.9
2	D	393	ASP	4.8
2	D	366	ILE	4.8
2	C	34	GLY	4.8
2	C	182	GLN	4.8
2	D	241	ALA	4.8
1	B	726	ARG	4.8
2	D	189	ARG	4.8
2	D	365	ALA	4.8
1	B	657	GLU	4.8
2	C	368	ALA	4.7
2	P	369	GLY	4.7
2	D	391	ASN	4.7
2	H	182	GLN	4.7
2	P	106	PRO	4.7
2	E	229	ASN	4.7
2	S	206	ALA	4.7
2	D	283	GLY	4.7
2	C	230	SER	4.7
2	P	125	GLN	4.7
2	C	391	ASN	4.6
2	S	419	ARG	4.6
2	C	354	ASN	4.6
2	P	203	PRO	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	351	GLN	4.6
2	S	50	SER	4.6
2	S	364	PRO	4.6
2	I	96	SER	4.6
2	P	284	VAL	4.6
2	C	48	VAL	4.6
2	P	390	GLN	4.6
2	P	205	GLY	4.6
2	P	283	GLY	4.6
2	C	163	GLN	4.5
2	E	244	THR	4.5
2	D	256	THR	4.5
2	P	199	ASN	4.5
2	D	56	ASP	4.5
2	D	208	GLN	4.5
2	D	246	ALA	4.5
2	Q	51	ALA	4.5
2	E	182	GLN	4.5
2	Q	92	LYS	4.5
2	D	238	GLY	4.5
2	F	287	THR	4.4
2	H	281	GLU	4.4
2	I	391	ASN	4.4
2	J	354	ASN	4.4
2	D	237	ALA	4.4
2	C	419	ARG	4.4
2	S	390	GLN	4.4
2	D	178	ALA	4.4
2	P	176	PRO	4.4
2	P	277	ASN	4.4
2	P	337	ARG	4.4
2	P	312	SER	4.4
2	Q	96	SER	4.4
2	S	260	ASN	4.3
2	D	162	GLY	4.3
2	P	83	ARG	4.3
2	P	260	ASN	4.3
2	F	421	ASN	4.3
2	P	281	GLU	4.3
2	C	83	ARG	4.3
2	E	239	VAL	4.3
2	D	371	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	S	181	GLN	4.3
2	D	250	THR	4.3
2	I	178	ALA	4.3
2	F	175	THR	4.3
2	P	183	PRO	4.3
2	C	205	GLY	4.2
2	F	162	GLY	4.2
2	S	276	GLY	4.2
2	C	191	ARG	4.2
2	F	362	ASP	4.2
1	B	546	GLY	4.2
2	E	206	ALA	4.2
1	B	15	LYS	4.2
2	P	290	CYS	4.2
2	P	181	GLN	4.2
2	E	207	TYR	4.2
3	K	290	GLU	4.2
1	B	995	GLY	4.1
2	D	257	ASP	4.1
2	P	233	GLY	4.1
2	P	276	GLY	4.1
2	I	90	ASP	4.1
2	C	92	LYS	4.1
2	F	178	ALA	4.1
2	J	361	MET	4.0
2	P	240	THR	4.0
2	C	190	ARG	4.0
2	F	391	ASN	4.0
2	J	371	ALA	4.0
2	D	264	GLN	4.0
2	I	390	GLN	4.0
2	D	54	VAL	4.0
2	J	347	ASP	4.0
2	D	198	SER	4.0
2	E	287	THR	4.0
2	S	96	SER	4.0
2	F	420	PRO	4.0
2	I	182	GLN	4.0
1	A	851	GLU	4.0
1	B	21	GLU	4.0
2	S	175	THR	4.0
2	E	285	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	179	ALA	4.0
2	P	190	ARG	4.0
2	P	257	ASP	3.9
2	C	161	ALA	3.9
2	D	243	ALA	3.9
2	Q	362	ASP	3.9
2	Q	246	ALA	3.9
2	D	190	ARG	3.9
2	Q	421	ASN	3.9
2	P	287	THR	3.9
2	J	260	ASN	3.9
2	Q	361	MET	3.8
2	F	168	PRO	3.8
2	C	110	VAL	3.8
2	D	163	GLN	3.8
1	A	933	THR	3.8
2	F	195	GLY	3.8
2	J	190	ARG	3.8
2	P	279	ASN	3.8
2	G	359	ASN	3.8
2	J	391	ASN	3.8
1	B	273	SER	3.8
2	J	90	ASP	3.8
2	C	287	THR	3.8
2	E	288	GLY	3.8
2	E	289	PHE	3.8
2	F	181	GLN	3.8
2	D	55	SER	3.8
2	F	260	ASN	3.8
2	P	342	TYR	3.8
3	K	299	GLU	3.8
2	D	180	GLN	3.8
2	Q	290	CYS	3.8
2	D	83	ARG	3.8
2	P	175	THR	3.8
2	J	346	SER	3.8
2	P	274	GLY	3.8
2	E	248	ALA	3.8
2	C	203	PRO	3.8
2	S	392	VAL	3.8
2	P	351	GLN	3.7
2	P	230	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	78	CYS	3.7
2	Q	95	VAL	3.7
2	I	280	LEU	3.7
2	J	359	ASN	3.7
2	C	179	ALA	3.7
2	J	242	THR	3.7
2	S	246	ALA	3.7
2	D	242	THR	3.7
2	C	21	VAL	3.7
2	P	219	SER	3.7
2	C	109	GLN	3.7
2	C	141	LYS	3.7
2	H	206	ALA	3.7
2	D	240	THR	3.6
2	D	181	GLN	3.6
2	H	390	GLN	3.6
1	A	932	GLU	3.6
2	D	90	ASP	3.6
2	G	369	GLY	3.6
2	S	92	LYS	3.6
2	D	364	PRO	3.6
2	P	350	ASP	3.6
2	J	368	ALA	3.6
2	P	88	ASN	3.6
2	D	191	ARG	3.6
2	D	229	ASN	3.6
2	S	207	TYR	3.6
2	P	288	GLY	3.6
2	D	362	ASP	3.6
2	J	419	ARG	3.6
2	D	290	CYS	3.6
1	B	994	ASP	3.6
2	D	287	THR	3.6
2	C	246	ALA	3.6
2	T	246	ALA	3.6
2	D	265	THR	3.6
2	R	92	LYS	3.5
2	E	59	VAL	3.5
2	C	266	ASP	3.5
2	E	362	ASP	3.5
2	S	208	GLN	3.5
2	P	92	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	195	GLY	3.5
1	B	16	SER	3.5
1	B	934	ASN	3.5
2	P	247	ASP	3.5
2	P	200	ALA	3.5
2	P	348	ALA	3.5
2	P	198	SER	3.5
2	D	175	THR	3.5
2	J	251	THR	3.5
2	C	125	GLN	3.5
2	J	181	GLN	3.5
2	C	189	ARG	3.5
1	B	451	GLY	3.5
2	P	142	GLY	3.5
2	D	276	GLY	3.5
2	F	161	ALA	3.5
2	G	53	TYR	3.5
1	B	746	ARG	3.5
2	P	100	ILE	3.4
2	E	286	LYS	3.4
2	F	172	ILE	3.4
2	P	90	ASP	3.4
2	E	240	THR	3.4
2	E	253	THR	3.4
2	C	378	ARG	3.4
2	P	388	ALA	3.4
1	B	111	ASP	3.4
2	P	18	GLU	3.4
2	C	198	SER	3.4
2	S	250	THR	3.4
2	S	251	THR	3.4
2	J	93	PRO	3.4
2	P	174	ALA	3.4
2	P	21	VAL	3.4
2	C	25	GLY	3.4
2	C	244	THR	3.4
2	H	393	ASP	3.4
2	F	92	LYS	3.4
2	C	420	PRO	3.4
2	P	243	ALA	3.4
2	C	346	SER	3.4
2	T	281	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	393	ASP	3.4
2	E	258	ALA	3.4
2	F	179	ALA	3.4
1	A	826	ARG	3.4
2	J	340	GLY	3.3
2	P	180	GLN	3.3
2	J	350	ASP	3.3
2	J	390	GLN	3.3
1	A	842	ASN	3.3
1	A	88	GLU	3.3
2	R	390	GLN	3.3
2	Q	371	ALA	3.3
2	I	203	PRO	3.3
2	D	286	LYS	3.3
2	E	419	ARG	3.3
2	F	370	LEU	3.3
2	E	238	GLY	3.3
2	Q	178	ALA	3.3
2	F	47	SER	3.3
2	P	147	TYR	3.3
2	D	125	GLN	3.3
2	P	22	ARG	3.3
2	C	337	ARG	3.3
2	D	127	SER	3.3
2	D	230	SER	3.3
2	P	120	ASN	3.3
2	I	180	GLN	3.3
2	P	156	LEU	3.2
2	D	395	ASN	3.2
2	D	421	ASN	3.2
2	P	308	TYR	3.2
2	C	75	THR	3.2
2	Q	174	ALA	3.2
1	B	709	VAL	3.2
2	F	319	SER	3.2
2	S	363	PRO	3.2
1	A	100	ASP	3.2
2	P	131	LYS	3.2
2	D	226	TYR	3.2
2	Q	419	ARG	3.2
2	D	368	ALA	3.2
2	R	90	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	281	GLU	3.2
2	F	174	ALA	3.2
2	I	249	ALA	3.2
2	J	363	PRO	3.2
2	Q	283	GLY	3.2
2	S	288	GLY	3.2
2	P	164	THR	3.2
2	D	221	THR	3.2
2	I	251	THR	3.2
2	C	257	ASP	3.2
2	C	201	ALA	3.2
2	C	61	LEU	3.2
1	B	547	GLN	3.2
2	Q	259	ASN	3.2
2	C	207	TYR	3.2
2	P	258	ALA	3.2
2	C	128	ALA	3.2
2	F	94	THR	3.1
2	R	91	THR	3.1
2	J	83	ARG	3.1
2	P	264	GLN	3.1
2	S	311	ASN	3.1
2	I	84	LYS	3.1
2	C	343	GLU	3.1
2	C	350	ASP	3.1
2	C	255	PRO	3.1
2	P	101	THR	3.1
2	J	164	THR	3.1
2	P	391	ASN	3.1
2	C	302	ASN	3.1
2	C	301	ALA	3.1
2	S	48	VAL	3.1
2	S	197	ARG	3.1
2	P	140	MET	3.1
2	I	164	THR	3.1
2	P	261	LEU	3.1
2	C	259	ASN	3.1
2	C	22	ARG	3.1
2	P	242	THR	3.1
2	P	370	LEU	3.1
2	J	75	THR	3.1
1	A	51	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	241	ALA	3.1
2	C	249	ALA	3.1
2	Q	50	SER	3.1
2	Q	241	ALA	3.1
2	G	393	ASP	3.1
2	C	340	GLY	3.1
2	I	250	THR	3.1
1	B	996	VAL	3.1
2	C	344	ILE	3.1
2	C	286	LYS	3.1
1	A	1009	ARG	3.1
2	C	168	PRO	3.1
2	P	392	VAL	3.0
2	P	231	PHE	3.0
2	R	347	ASP	3.0
2	I	362	ASP	3.0
2	P	73	THR	3.0
2	E	54	VAL	3.0
2	R	245	ALA	3.0
2	P	269	LEU	3.0
2	C	294	GLU	3.0
2	E	30	GLY	3.0
2	C	91	THR	3.0
2	F	250	THR	3.0
2	C	372	PHE	3.0
2	F	96	SER	3.0
2	J	70	SER	3.0
2	C	154	CYS	3.0
1	A	582	ASN	3.0
2	C	143	LEU	3.0
2	F	389	LEU	3.0
2	I	277	ASN	3.0
2	S	296	GLU	3.0
2	E	183	PRO	3.0
2	E	205	GLY	3.0
2	P	94	THR	3.0
2	F	164	THR	3.0
2	F	180	GLN	3.0
2	J	240	THR	3.0
2	J	256	THR	3.0
2	J	96	SER	3.0
2	P	206	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	277	ASN	3.0
2	I	369	GLY	3.0
2	I	240	THR	3.0
2	C	382	ARG	3.0
2	E	190	ARG	3.0
2	E	237	ALA	3.0
2	P	103	TYR	3.0
2	P	154	CYS	3.0
2	S	281	GLU	3.0
2	P	334	SER	3.0
2	F	239	VAL	3.0
2	D	176	PRO	2.9
2	D	420	PRO	2.9
2	P	36	PHE	2.9
2	S	195	GLY	2.9
2	P	210	VAL	2.9
2	C	127	SER	2.9
2	G	96	SER	2.9
2	C	285	ALA	2.9
2	I	313	ILE	2.9
2	P	282	LEU	2.9
2	P	326	SER	2.9
2	C	26	ASP	2.9
2	D	122	LEU	2.9
1	B	14	PHE	2.9
2	P	188	GLU	2.9
2	Q	311	ASN	2.9
2	C	288	GLY	2.9
2	F	390	GLN	2.9
2	H	208	GLN	2.9
2	I	283	GLY	2.9
2	J	198	SER	2.9
2	Q	250	THR	2.9
2	F	206	ALA	2.9
1	B	997	LYS	2.9
1	A	103	ASP	2.9
2	P	255	PRO	2.9
2	C	176	PRO	2.9
2	F	199	ASN	2.9
2	Q	244	THR	2.9
2	I	200	ALA	2.9
2	I	258	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	53	TYR	2.9
1	A	347	ARG	2.9
2	P	37	ASN	2.9
2	R	93	PRO	2.9
2	F	117	ARG	2.9
2	F	419	ARG	2.9
2	D	233	GLY	2.9
2	I	49	SER	2.9
2	J	118	GLN	2.9
2	Q	240	THR	2.9
2	E	242	THR	2.9
2	P	259	ASN	2.9
2	P	296	GLU	2.9
2	D	277	ASN	2.9
1	A	832	SER	2.8
2	C	96	SER	2.8
2	E	347	ASP	2.8
1	A	1007	GLY	2.8
2	P	25	GLY	2.8
2	C	162	GLY	2.8
2	F	109	GLN	2.8
2	R	303	ARG	2.8
2	Q	312	SER	2.8
2	E	160	VAL	2.8
2	Q	171	GLY	2.8
2	S	205	GLY	2.8
2	P	189	ARG	2.8
2	D	92	LYS	2.8
1	A	464	PRO	2.8
2	C	418	TYR	2.8
2	F	183	PRO	2.8
2	S	203	PRO	2.8
1	B	109	GLU	2.8
2	C	381	GLU	2.8
2	Q	282	LEU	2.8
2	H	260	ASN	2.8
1	B	107	CYS	2.8
2	I	208	GLN	2.8
1	A	965	ASP	2.8
2	I	368	ALA	2.8
2	C	361	MET	2.8
2	C	108	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	449	SER	2.8
2	P	96	SER	2.8
2	P	254	VAL	2.8
2	P	360	TYR	2.8
2	Q	49	SER	2.8
2	F	207	TYR	2.8
2	Q	181	GLN	2.8
2	E	245	ALA	2.8
2	G	94	THR	2.8
2	Q	393	ASP	2.8
2	Q	59	VAL	2.8
1	A	547	GLN	2.8
1	B	483	GLN	2.8
2	C	395	ASN	2.8
2	F	243	ALA	2.8
2	S	174	ALA	2.8
1	B	453	ASP	2.8
2	C	98	ASP	2.8
2	E	56	ASP	2.8
2	S	314	THR	2.8
2	S	316	THR	2.8
2	P	97	ASP	2.7
2	G	93	PRO	2.7
2	P	67	MET	2.7
2	G	265	THR	2.7
2	H	421	ASN	2.7
2	P	98	ASP	2.7
2	G	347	ASP	2.7
2	C	89	SER	2.7
2	P	150	PRO	2.7
2	G	363	PRO	2.7
1	B	22	GLY	2.7
2	P	75	THR	2.7
2	D	281	GLU	2.7
2	D	197	ARG	2.7
2	D	282	LEU	2.7
2	I	245	ALA	2.7
2	E	395	ASN	2.7
2	C	319	SER	2.7
2	P	367	PRO	2.7
2	P	82	LEU	2.7
2	P	195	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	207	TYR	2.7
2	Q	301	ALA	2.7
2	Q	360	TYR	2.7
2	R	206	ALA	2.7
2	P	44	THR	2.7
2	C	228	THR	2.7
2	E	234	THR	2.7
2	F	167	ILE	2.7
2	H	391	ASN	2.7
2	C	106	PRO	2.7
2	C	258	ALA	2.7
2	D	382	ARG	2.7
2	I	301	ALA	2.7
2	P	32	THR	2.7
2	P	358	THR	2.7
2	D	309	THR	2.7
2	F	242	THR	2.7
2	R	314	THR	2.7
2	C	24	ASN	2.7
2	D	302	ASN	2.7
2	P	129	LYS	2.7
2	C	113	SER	2.7
2	P	118	GLN	2.7
2	D	144	ASP	2.7
2	C	195	GLY	2.7
2	D	285	ALA	2.7
2	S	128	ALA	2.7
2	S	241	ALA	2.7
2	S	249	ALA	2.7
2	P	389	LEU	2.7
2	P	197	ARG	2.6
2	D	168	PRO	2.6
2	E	177	PRO	2.6
2	S	360	TYR	2.6
2	I	242	THR	2.6
2	C	199	ASN	2.6
2	P	394	LEU	2.6
2	F	45	GLN	2.6
2	Q	84	LYS	2.6
2	C	242	THR	2.6
2	C	307	TYR	2.6
2	D	316	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	53	TYR	2.6
2	E	164	THR	2.6
2	G	350	ASP	2.6
2	D	389	LEU	2.6
1	B	708	SER	2.6
1	A	452	ARG	2.6
2	C	77	ARG	2.6
2	C	363	PRO	2.6
2	R	341	GLN	2.6
2	C	63	THR	2.6
2	J	393	ASP	2.6
1	B	251	ASN	2.6
1	B	909	SER	2.6
2	D	210	VAL	2.6
2	D	384	ARG	2.6
2	P	119	LEU	2.6
2	Q	229	ASN	2.6
2	J	286	LYS	2.6
1	B	266	GLN	2.6
2	E	264	GLN	2.6
1	A	569	GLY	2.6
2	P	298	THR	2.6
2	P	316	THR	2.6
2	C	103	TYR	2.6
2	D	373	THR	2.6
2	Q	342	TYR	2.6
2	P	272	SER	2.6
2	J	127	SER	2.6
2	C	215	ALA	2.6
2	D	203	PRO	2.6
2	S	371	ALA	2.6
2	J	177	PRO	2.6
2	J	180	GLN	2.6
2	D	297	PHE	2.6
2	P	33	THR	2.5
2	D	164	THR	2.5
2	G	287	THR	2.5
2	C	155	LYS	2.5
2	D	160	VAL	2.5
2	P	166	ASN	2.5
2	G	90	ASP	2.5
2	I	98	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	37	ASN	2.5
2	T	201	ALA	2.5
2	D	25	GLY	2.5
2	Q	286	LYS	2.5
2	P	123	SER	2.5
2	P	268	ARG	2.5
2	P	263	VAL	2.5
2	Q	381	GLU	2.5
1	A	934	ASN	2.5
2	P	311	ASN	2.5
2	Q	315	GLN	2.5
2	E	241	ALA	2.5
1	B	933	THR	2.5
2	P	330	THR	2.5
2	C	316	THR	2.5
2	D	397	ARG	2.5
2	Q	89	SER	2.5
2	C	116	VAL	2.5
2	C	193	LEU	2.5
2	C	260	ASN	2.5
2	P	332	PHE	2.5
2	G	362	ASP	2.5
2	Q	368	ALA	2.5
2	F	248	ALA	2.5
2	C	177	PRO	2.5
2	E	283	GLY	2.5
2	S	196	ILE	2.5
2	P	419	ARG	2.5
2	F	256	THR	2.5
2	J	32	THR	2.5
2	C	282	LEU	2.5
2	D	270	SER	2.5
2	F	300	LEU	2.5
2	S	49	SER	2.5
2	S	198	SER	2.5
2	D	110	VAL	2.5
1	A	341	ALA	2.5
2	Q	390	GLN	2.5
2	R	201	ALA	2.5
2	S	90	ASP	2.5
2	S	178	ALA	2.5
1	A	843	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	369	GLY	2.5
2	C	39	LEU	2.5
2	E	280	LEU	2.5
2	F	190	ARG	2.5
2	D	386	ILE	2.5
2	J	302	ASN	2.5
2	S	179	ALA	2.5
2	S	365	ALA	2.5
2	I	128	ALA	2.5
2	P	340	GLY	2.5
2	Q	238	GLY	2.5
2	F	189	ARG	2.5
2	G	340	GLY	2.5
2	R	1	MET	2.5
1	B	110	HIS	2.4
2	T	92	LYS	2.4
2	E	196	ILE	2.4
2	P	248	ALA	2.4
2	Q	249	ALA	2.4
2	R	208	GLN	2.4
2	R	315	GLN	2.4
2	S	421	ASN	2.4
1	B	309	ARG	2.4
1	A	931	GLY	2.4
2	P	47	SER	2.4
2	D	220	VAL	2.4
2	P	155	LYS	2.4
2	D	80	TYR	2.4
2	R	83	ARG	2.4
2	J	189	ARG	2.4
2	J	311	ASN	2.4
2	Q	60	PRO	2.4
1	B	20	THR	2.4
2	Q	319	SER	2.4
2	J	247	ASP	2.4
1	B	19	VAL	2.4
2	P	307	TYR	2.4
2	E	342	TYR	2.4
2	H	53	TYR	2.4
2	P	343	GLU	2.4
2	C	188	GLU	2.4
2	E	193	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	281	GLU	2.4
2	P	109	GLN	2.4
2	P	128	ALA	2.4
2	P	303	ARG	2.4
2	C	248	ALA	2.4
2	F	208	GLN	2.4
2	J	303	ARG	2.4
2	R	279	ASN	2.4
2	F	1	MET	2.4
2	H	364	PRO	2.4
2	P	165	GLY	2.4
2	D	274	GLY	2.4
2	G	84	LYS	2.4
2	S	287	THR	2.4
2	D	291	VAL	2.4
2	F	257	ASP	2.4
2	H	365	ALA	2.4
2	J	197	ARG	2.4
1	A	325	GLN	2.4
2	E	390	GLN	2.4
2	E	363	PRO	2.4
2	F	121	ASN	2.4
2	P	244	THR	2.4
2	S	247	ASP	2.4
2	C	133	TYR	2.4
2	F	351	GLN	2.4
1	A	714	LYS	2.4
1	B	99	LYS	2.4
2	G	364	PRO	2.4
2	C	216	SER	2.4
2	P	104	ILE	2.4
2	D	94	THR	2.4
2	P	122	LEU	2.4
2	G	160	VAL	2.4
2	C	56	ASP	2.4
2	H	362	ASP	2.4
2	Q	343	GLU	2.4
2	J	285	ALA	2.4
2	C	267	SER	2.3
2	D	123	SER	2.3
2	C	186	VAL	2.3
2	G	256	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	579	ARG	2.3
2	C	117	ARG	2.3
2	D	158	ARG	2.3
2	S	83	ARG	2.3
2	P	80	TYR	2.3
2	P	169	MET	2.3
2	D	361	MET	2.3
2	J	360	TYR	2.3
1	A	329	GLU	2.3
2	P	249	ALA	2.3
2	D	296	GLU	2.3
2	H	245	ALA	2.3
2	I	285	ALA	2.3
1	B	729	SER	2.3
2	P	363	PRO	2.3
2	F	198	SER	2.3
1	A	1013	ASN	2.3
2	T	166	ASN	2.3
2	P	251	THR	2.3
2	I	244	THR	2.3
2	I	392	VAL	2.3
1	A	746	ARG	2.3
2	D	1	MET	2.3
2	J	117	ARG	2.3
2	G	365	ALA	2.3
2	P	46	LEU	2.3
2	C	352	LEU	2.3
2	G	394	LEU	2.3
2	I	299	ILE	2.3
2	D	165	GLY	2.3
1	A	894	ASN	2.3
2	P	121	ASN	2.3
2	C	115	THR	2.3
2	C	318	THR	2.3
2	D	85	THR	2.3
2	D	228	THR	2.3
2	P	108	LEU	2.3
2	D	232	PHE	2.3
1	A	87	ASP	2.3
1	B	553	GLU	2.3
2	J	305	GLN	2.3
2	P	40	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	283	GLY	2.3
1	B	582	ASN	2.3
2	P	253	THR	2.3
2	C	27	THR	2.3
2	D	303	ARG	2.3
2	I	131	LYS	2.3
2	P	179	ALA	2.3
2	P	328	PHE	2.3
2	C	383	ALA	2.3
2	C	417	TYR	2.3
2	E	187	ALA	2.3
1	A	639	GLN	2.3
2	P	152	GLU	2.3
2	C	18	GLU	2.3
1	B	17	VAL	2.3
2	Q	363	PRO	2.3
2	E	369	GLY	2.3
2	R	317	PRO	2.3
1	B	84	ARG	2.3
2	P	228	THR	2.3
2	D	337	ARG	2.3
2	Q	256	THR	2.3
2	G	189	ARG	2.3
2	I	311	ASN	2.3
2	J	105	ARG	2.3
2	F	241	ALA	2.3
1	A	553	GLU	2.3
2	P	267	SER	2.3
2	D	84	LYS	2.3
2	D	225	VAL	2.3
2	C	169	MET	2.3
2	T	90	ASP	2.3
2	P	331	THR	2.2
2	I	199	ASN	2.2
2	P	218	LEU	2.2
2	T	245	ALA	2.2
2	D	294	GLU	2.2
1	A	323	VAL	2.2
2	D	284	VAL	2.2
2	J	25	GLY	2.2
2	C	35	ASP	2.2
2	C	353	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	260	ASN	2.2
2	F	388	ALA	2.2
2	D	219	SER	2.2
2	E	304	SER	2.2
2	E	169	MET	2.2
2	P	158	ARG	2.2
2	J	110	VAL	2.2
2	D	126	PRO	2.2
2	C	290	CYS	2.2
2	D	358	THR	2.2
2	R	256	THR	2.2
1	A	839	ASP	2.2
2	Q	391	ASN	2.2
2	I	302	ASN	2.2
1	B	25	HIS	2.2
2	E	179	ALA	2.2
2	J	84	LYS	2.2
2	J	365	ALA	2.2
2	I	342	TYR	2.2
2	P	3	ARG	2.2
2	C	183	PRO	2.2
2	G	276	GLY	2.2
2	J	255	PRO	2.2
2	P	366	ILE	2.2
2	C	33	THR	2.2
2	E	91	THR	2.2
2	D	88	ASN	2.2
2	D	266	ASP	2.2
2	D	279	ASN	2.2
2	F	114	ASP	2.2
2	G	371	ALA	2.2
2	H	419	ARG	2.2
2	P	239	VAL	2.2
2	E	95	VAL	2.2
2	S	275	GLY	2.2
2	H	175	THR	2.2
2	Q	260	ASN	2.2
2	F	166	ASN	2.2
2	R	277	ASN	2.2
2	J	395	ASN	2.2
2	P	237	ALA	2.2
2	C	245	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	362	ASP	2.2
2	I	347	ASP	2.2
2	F	170	MET	2.2
1	A	935	SER	2.2
2	D	351	GLN	2.2
2	Q	264	GLN	2.2
2	H	216	SER	2.2
2	I	117	ARG	2.2
2	I	284	VAL	2.2
2	P	209	PHE	2.2
2	C	111	PRO	2.2
2	D	255	PRO	2.2
1	A	831	THR	2.2
2	Q	175	THR	2.2
2	E	314	THR	2.2
2	J	287	THR	2.2
2	P	361	MET	2.2
2	C	229	ASN	2.2
2	D	359	ASN	2.2
1	A	576	ALA	2.1
2	P	371	ALA	2.1
2	C	156	LEU	2.2
2	D	348	ALA	2.1
2	P	322	ASP	2.1
2	Q	403	HIS	2.1
2	H	189	ARG	2.1
2	S	374	SER	2.1
2	I	321	ASP	2.1
2	J	397	ARG	2.1
2	P	344	ILE	2.1
2	E	284	VAL	2.1
2	I	307	TYR	2.1
2	P	227	PHE	2.1
2	P	414	PHE	2.1
2	P	420	PRO	2.1
2	Q	52	GLY	2.1
2	C	134	GLU	2.1
2	S	177	PRO	2.1
2	I	364	PRO	2.1
2	P	353	THR	2.1
2	I	75	THR	2.1
2	I	94	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	467	LEU	2.1
2	E	361	MET	2.1
1	B	894	ASN	2.1
2	C	137	ASN	2.1
2	F	395	ASN	2.1
2	P	105	ARG	2.1
2	R	190	ARG	2.1
2	S	189	ARG	2.1
1	B	1016	GLN	2.1
2	P	315	GLN	2.1
2	P	335	GLN	2.1
2	Q	47	SER	2.1
2	E	123	SER	2.1
2	R	182	GLN	2.1
1	B	1015	ASP	2.1
2	C	339	CYS	2.1
2	C	209	PHE	2.1
2	D	227	PHE	2.1
2	J	185	PHE	2.1
2	Q	281	GLU	2.1
2	F	32	THR	2.1
2	P	107	ARG	2.1
2	E	201	ALA	2.1
2	R	181	GLN	2.1
2	R	25	GLY	2.1
2	S	369	GLY	2.1
2	P	364	PRO	2.1
2	P	250	THR	2.1
2	C	240	THR	2.1
2	Q	287	THR	2.1
2	I	316	THR	2.1
2	Q	83	ARG	2.1
3	K	297	ARG	2.1
2	F	270	SER	2.1
2	F	278	ILE	2.1
2	G	391	ASN	2.1
2	G	421	ASN	2.1
2	J	230	SER	2.1
2	P	141	LYS	2.1
2	C	43	PHE	2.1
2	F	184	PHE	2.1
2	G	48	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	308	TYR	2.1
2	E	266	ASP	2.1
2	R	195	GLY	2.1
2	H	283	GLY	2.1
2	S	53	TYR	2.1
2	C	373	THR	2.1
2	E	296	GLU	2.1
1	B	55	ARG	2.1
2	I	189	ARG	2.1
2	E	51	ALA	2.1
2	F	236	ILE	2.1
2	R	161	ALA	2.1
2	C	74	SER	2.1
2	C	272	SER	2.1
2	P	184	PHE	2.1
2	C	315	GLN	2.1
2	R	421	ASN	2.1
2	J	208	GLN	2.1
2	J	259	ASN	2.1
1	A	914	TYR	2.1
2	P	111	PRO	2.1
2	P	144	ASP	2.1
2	C	146	PRO	2.1
2	Q	164	THR	2.1
2	C	237	ALA	2.1
2	G	47	SER	2.1
2	J	355	SER	2.1
2	D	36	PHE	2.1
1	B	656	ASN	2.1
2	D	370	LEU	2.1
2	E	370	LEU	2.1
2	S	361	MET	2.1
2	P	224	TYR	2.0
2	P	417	TYR	2.0
1	B	839	ASP	2.0
2	P	56	ASP	2.0
2	P	77	ARG	2.0
2	P	397	ARG	2.0
2	Q	94	THR	2.0
2	Q	98	ASP	2.0
2	Q	172	ILE	2.0
2	F	368	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	227	PHE	2.0
2	I	2	SER	2.0
2	P	291	VAL	2.0
2	I	163	GLN	2.0
1	B	568	ASN	2.0
2	F	283	GLY	2.0
2	G	92	LYS	2.0
2	H	420	PRO	2.0
2	I	207	TYR	2.0
2	P	167	ILE	2.0
2	P	373	THR	2.0
2	E	202	ILE	2.0
2	J	202	ILE	2.0
2	P	319	SER	2.0
2	Q	70	SER	2.0
2	Q	351	GLN	2.0
1	A	936	ASN	2.0
2	D	199	ASN	2.0
2	D	195	GLY	2.0
2	S	183	PRO	2.0
2	I	3	ARG	2.0
2	C	298	THR	2.0
2	S	240	THR	2.0
2	C	296	GLU	2.0
2	P	270	SER	2.0
2	F	201	ALA	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.