



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:38 PM EDT

PDB ID : 2YKS / pdb_00002yks
Title : PENTAMERIC LIGAND GATED ION CHANNEL ELIC MUTANT F246A
Authors : Zimmermann, I.; Dutzler, R.
Deposited on : 2011-05-30
Resolution : 3.30 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

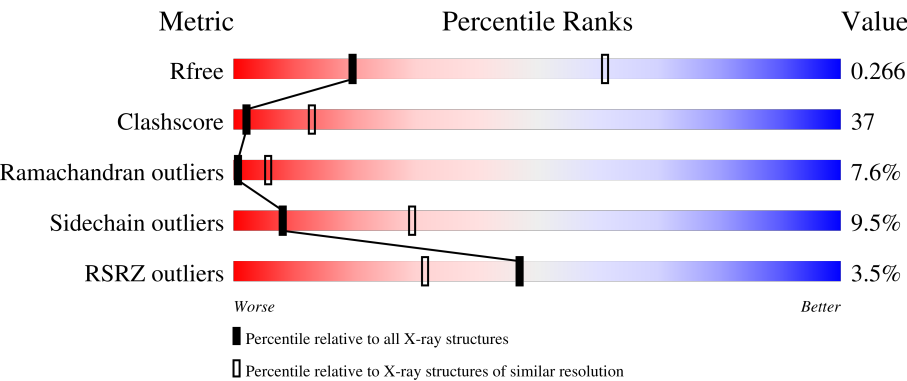
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	321	4% 39% 44% 11% 5%
1	B	321	4% 43% 40% 11% 5%
1	C	321	2% 42% 40% 12% 5%
1	D	321	4% 41% 43% 11% 5%
1	E	321	2% 40% 41% 12% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	321	2%41%40%13%• 5%
1	G	321	5%42%41%11%• 5%
1	H	321	2%40%43%12%• 5%
1	I	321	6%40%43%11%• 5%
1	J	321	3%40%42%12%• 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24950 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 CYS-LOOP LIGAND-GATED ION CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	B	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	C	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	D	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	E	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	F	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	G	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	H	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	I	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	J	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ALA	PHE	engineered mutation	UNP P0C7B7
A	288	ASN	MET	conflict	UNP P0C7B7
B	246	ALA	PHE	engineered mutation	UNP P0C7B7
B	288	ASN	MET	conflict	UNP P0C7B7
C	246	ALA	PHE	engineered mutation	UNP P0C7B7
C	288	ASN	MET	conflict	UNP P0C7B7
D	246	ALA	PHE	engineered mutation	UNP P0C7B7
D	288	ASN	MET	conflict	UNP P0C7B7
E	246	ALA	PHE	engineered mutation	UNP P0C7B7

Continued on next page...

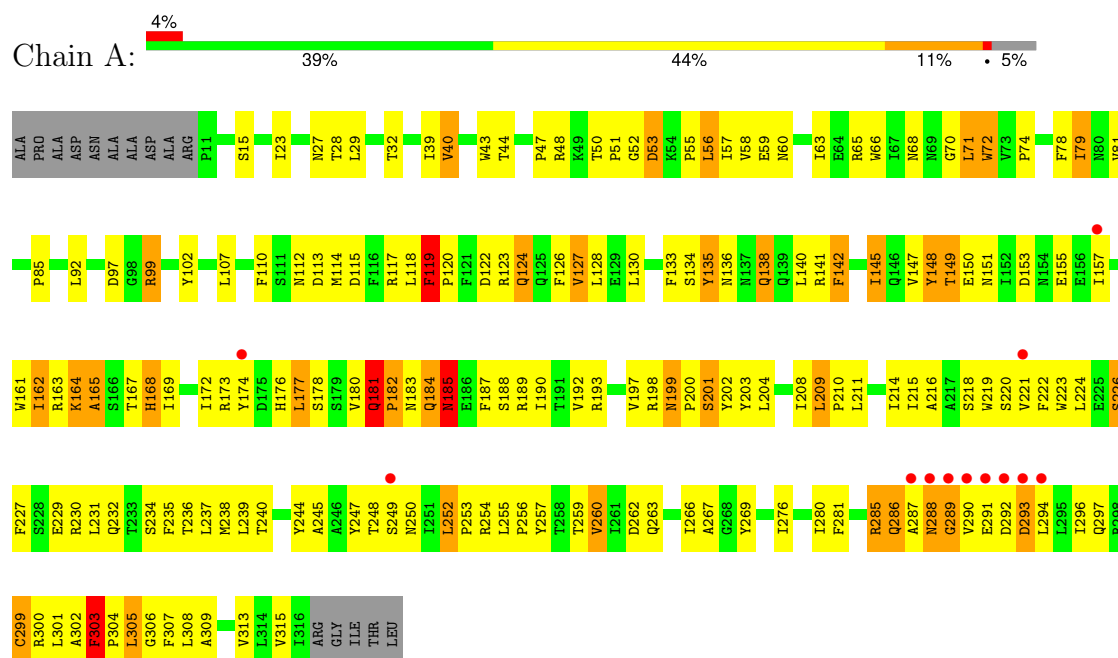
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	288	ASN	MET	conflict	UNP P0C7B7
F	246	ALA	PHE	engineered mutation	UNP P0C7B7
F	288	ASN	MET	conflict	UNP P0C7B7
G	246	ALA	PHE	engineered mutation	UNP P0C7B7
G	288	ASN	MET	conflict	UNP P0C7B7
H	246	ALA	PHE	engineered mutation	UNP P0C7B7
H	288	ASN	MET	conflict	UNP P0C7B7
I	246	ALA	PHE	engineered mutation	UNP P0C7B7
I	288	ASN	MET	conflict	UNP P0C7B7
J	246	ALA	PHE	engineered mutation	UNP P0C7B7
J	288	ASN	MET	conflict	UNP P0C7B7

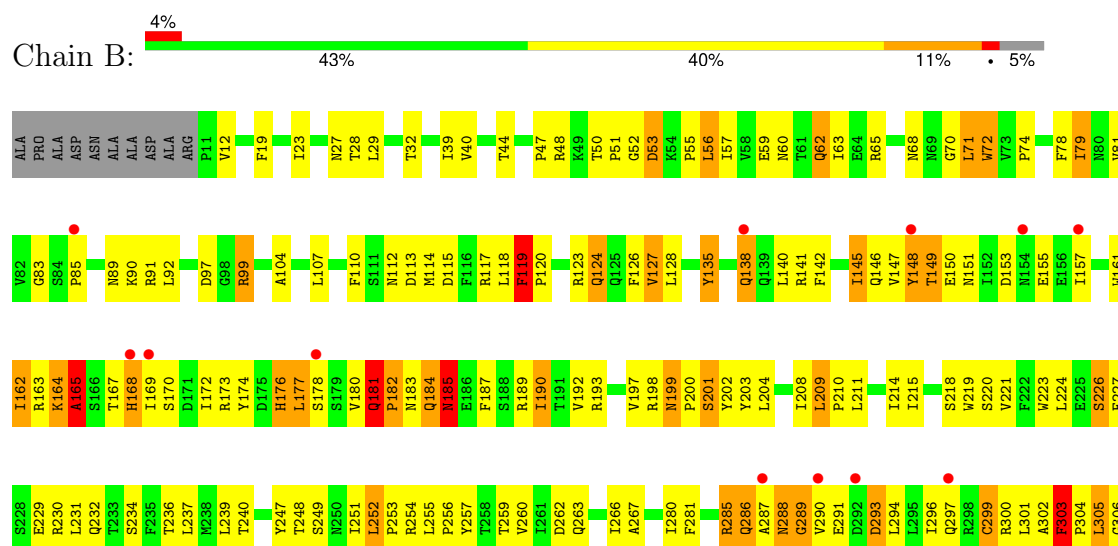
3 Residue-property plots

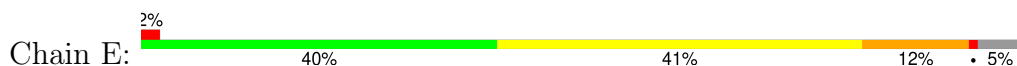
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

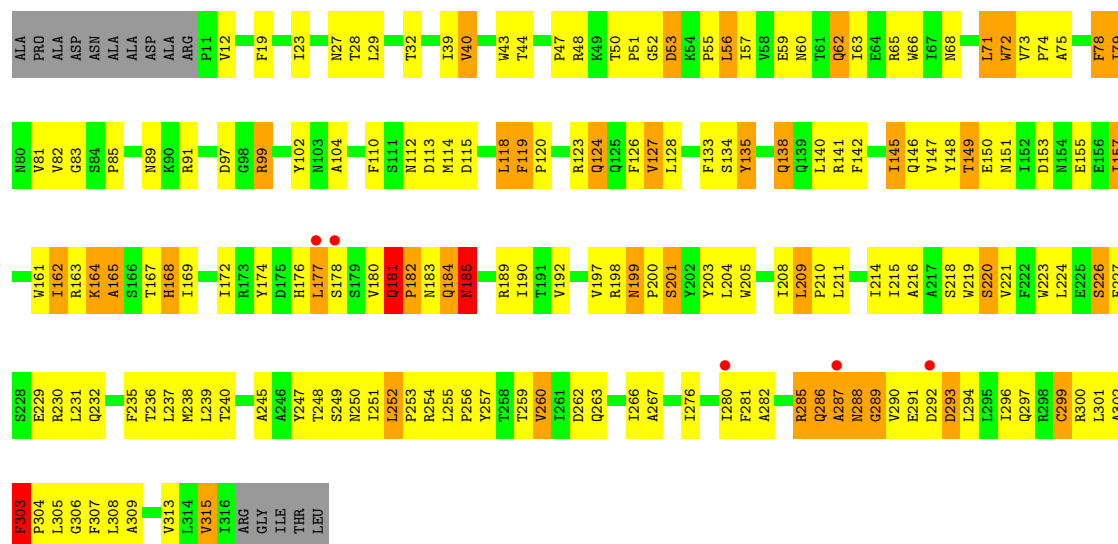
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



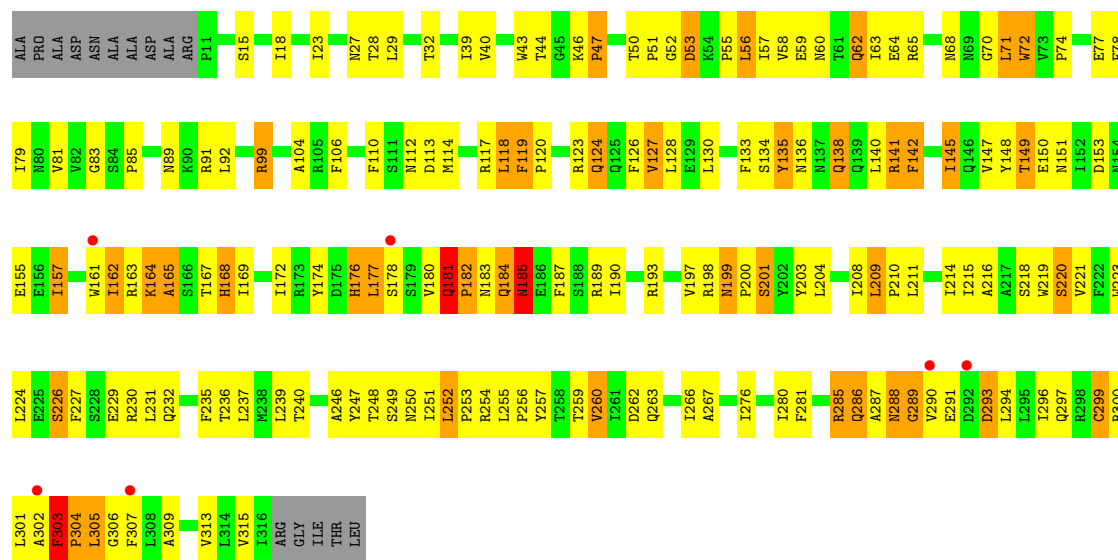
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



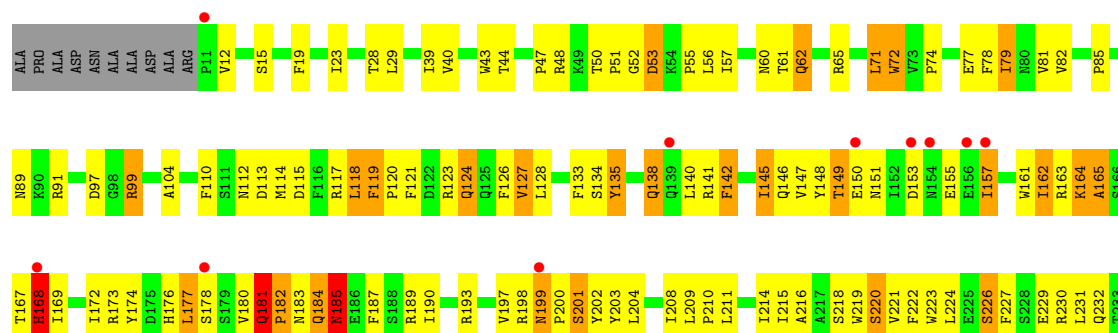


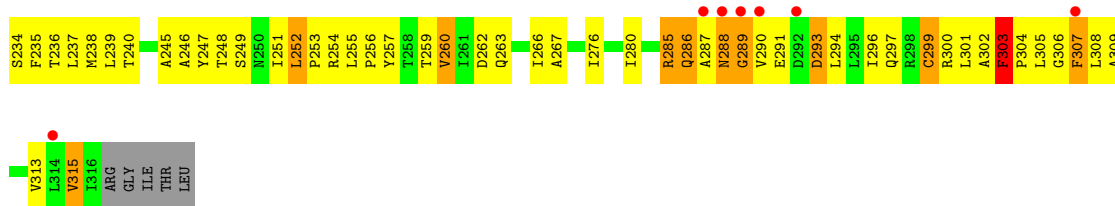


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

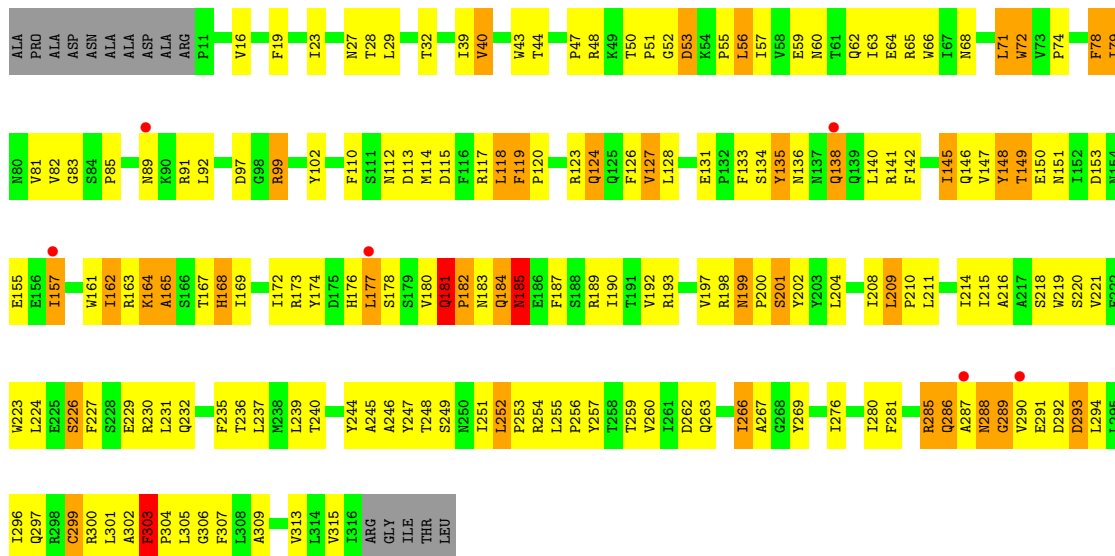


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

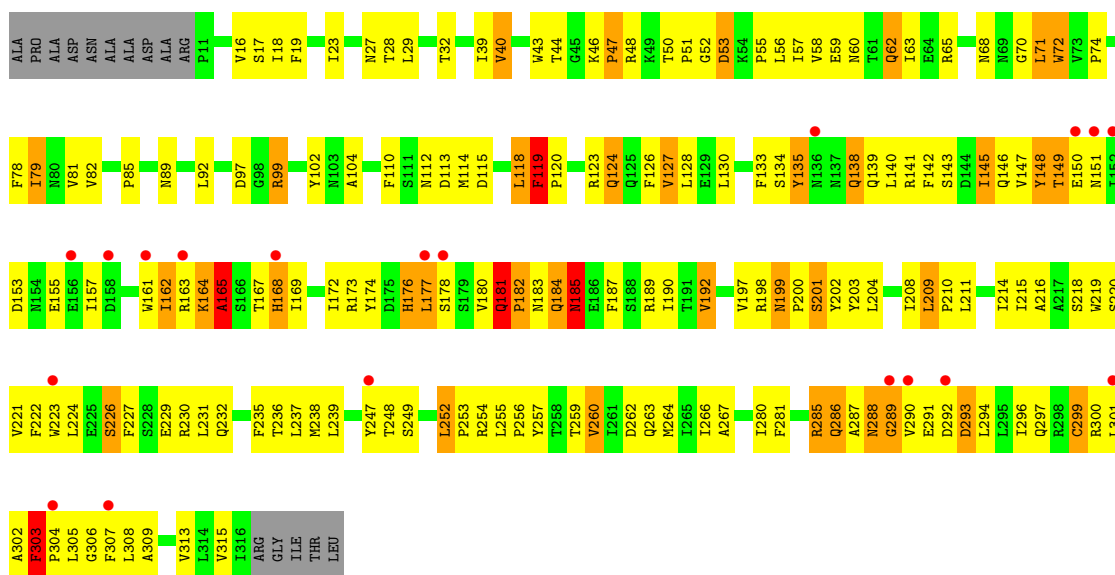




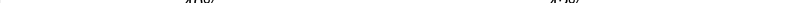
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

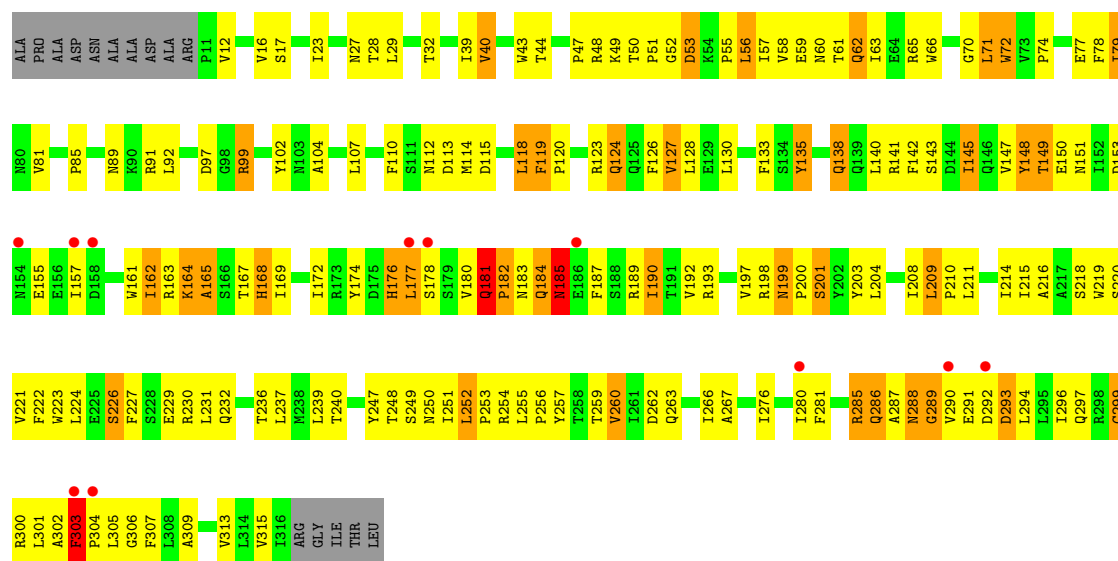


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.50Å 266.15Å 110.85Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	19.97 – 3.30 19.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.97-3.30) 97.6 (19.97-3.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.242 , 0.265 0.246 , 0.266	Depositor DCC
R_{free} test set	4322 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24950	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.82	0/2562	1.07	13/3493 (0.4%)
1	B	0.93	2/2562 (0.1%)	1.12	14/3493 (0.4%)
1	C	0.89	2/2562 (0.1%)	1.10	11/3493 (0.3%)
1	D	0.95	1/2562 (0.0%)	1.10	12/3493 (0.3%)
1	E	0.88	1/2562 (0.0%)	1.10	13/3493 (0.4%)
1	F	0.83	0/2562	1.09	12/3493 (0.3%)
1	G	0.95	3/2562 (0.1%)	1.12	15/3493 (0.4%)
1	H	0.88	0/2562	1.10	16/3493 (0.5%)
1	I	0.97	3/2562 (0.1%)	1.12	16/3493 (0.5%)
1	J	0.85	1/2562 (0.0%)	1.09	11/3493 (0.3%)
All	All	0.90	13/25620 (0.1%)	1.10	133/34930 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	82	VAL	CA-C	6.55	1.60	1.53
1	C	86	ASP	C-N	6.19	1.42	1.33
1	B	165	ALA	CA-CB	-5.66	1.44	1.53
1	D	197	VAL	CA-CB	-5.63	1.47	1.54
1	I	18	ILE	C-O	-5.48	1.17	1.24
1	G	246	ALA	CA-CB	-5.42	1.44	1.53
1	I	165	ALA	CA-CB	-5.25	1.44	1.53
1	J	190	ILE	CA-CB	-5.25	1.47	1.54
1	B	190	ILE	CA-CB	-5.22	1.47	1.54
1	G	168	HIS	CA-C	5.13	1.59	1.52
1	I	192	VAL	CA-CB	-5.08	1.48	1.54
1	C	57	ILE	CA-CB	-5.07	1.47	1.53
1	G	135	TYR	CA-C	5.06	1.58	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	GLY	O-C-N	-9.09	117.17	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	127	VAL	N-CA-C	8.09	120.13	108.48
1	A	127	VAL	N-CA-C	7.86	119.80	108.48
1	I	127	VAL	N-CA-C	7.63	119.47	108.48
1	B	127	VAL	N-CA-C	7.59	119.41	108.48
1	C	127	VAL	N-CA-C	7.59	119.41	108.48
1	F	299	CYS	N-CA-C	-7.56	104.02	112.57
1	E	287	ALA	N-CA-C	-7.56	102.12	112.03
1	A	299	CYS	N-CA-C	-7.41	104.20	112.57
1	J	299	CYS	N-CA-C	-7.35	104.27	112.57
1	G	127	VAL	N-CA-C	7.33	119.03	108.48
1	J	127	VAL	N-CA-C	7.33	119.03	108.48
1	J	236	THR	N-CA-C	-7.32	104.15	113.23
1	H	127	VAL	N-CA-C	7.28	118.97	108.48
1	I	299	CYS	N-CA-C	-7.26	104.36	112.57
1	I	199	ASN	CA-C-N	7.23	127.57	119.32
1	I	199	ASN	C-N-CA	7.23	127.57	119.32
1	G	299	CYS	N-CA-C	-7.16	104.48	112.57
1	H	287	ALA	N-CA-C	-7.13	102.68	112.03
1	J	287	ALA	N-CA-C	-7.12	102.70	112.03
1	D	127	VAL	N-CA-C	7.10	118.70	108.48
1	B	287	ALA	N-CA-C	-7.09	102.75	112.03
1	A	287	ALA	N-CA-C	-7.03	102.82	112.03
1	I	287	ALA	N-CA-C	-7.01	102.84	112.03
1	E	83	GLY	O-C-N	-6.98	118.55	123.08
1	D	287	ALA	N-CA-C	-6.96	102.91	112.03
1	B	299	CYS	N-CA-C	-6.95	104.72	112.57
1	C	287	ALA	N-CA-C	-6.94	102.94	112.03
1	F	287	ALA	N-CA-C	-6.91	102.98	112.03
1	C	299	CYS	N-CA-C	-6.89	104.79	112.57
1	D	299	CYS	N-CA-C	-6.88	104.79	112.57
1	I	82	VAL	CA-C-N	-6.88	116.02	121.86
1	I	82	VAL	C-N-CA	-6.88	116.02	121.86
1	G	287	ALA	N-CA-C	-6.87	103.03	112.03
1	H	266	ILE	N-CA-C	-6.85	103.80	110.72
1	E	127	VAL	N-CA-C	6.82	118.30	108.48
1	H	299	CYS	N-CA-C	-6.76	104.93	112.57
1	C	199	ASN	CA-C-N	6.73	126.99	119.32
1	C	199	ASN	C-N-CA	6.73	126.99	119.32
1	E	299	CYS	N-CA-C	-6.58	105.13	112.57
1	D	199	ASN	CA-C-N	6.48	126.71	119.32
1	D	199	ASN	C-N-CA	6.48	126.71	119.32
1	B	149	THR	N-CA-C	-6.39	101.00	110.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	THR	N-CA-C	-6.38	101.03	110.46
1	J	149	THR	N-CA-C	-6.28	101.16	110.46
1	F	149	THR	N-CA-C	-6.27	101.18	110.46
1	B	135	TYR	N-CA-C	6.21	119.07	108.02
1	C	236	THR	N-CA-C	-6.21	105.53	113.23
1	B	138	GLN	N-CA-C	-6.16	97.17	107.32
1	D	135	TYR	N-CA-C	6.15	118.96	108.02
1	D	236	THR	N-CA-C	-6.14	105.62	113.23
1	E	62	GLN	N-CA-C	6.13	117.97	111.28
1	B	62	GLN	N-CA-C	6.11	117.94	111.28
1	G	149	THR	N-CA-C	-6.11	101.42	110.46
1	G	135	TYR	N-CA-C	6.11	118.90	108.02
1	C	149	THR	N-CA-C	-6.10	101.43	110.46
1	A	281	PHE	N-CA-C	-6.08	103.97	112.12
1	I	62	GLN	N-CA-C	6.08	117.91	111.28
1	G	82	VAL	CA-C-N	-6.04	116.73	121.86
1	G	82	VAL	C-N-CA	-6.04	116.73	121.86
1	G	62	GLN	N-CA-C	6.03	117.85	111.28
1	F	135	TYR	N-CA-C	6.03	118.75	108.02
1	I	236	THR	N-CA-C	-6.01	105.78	113.23
1	I	149	THR	N-CA-C	-5.99	101.59	110.46
1	A	138	GLN	N-CA-C	-5.98	97.45	107.32
1	E	149	THR	N-CA-C	-5.98	101.61	110.46
1	B	199	ASN	CA-C-N	5.96	126.11	119.32
1	B	199	ASN	C-N-CA	5.96	126.11	119.32
1	A	135	TYR	N-CA-C	5.92	118.56	108.02
1	J	135	TYR	N-CA-C	5.89	118.50	108.02
1	C	138	GLN	N-CA-C	-5.87	97.63	107.32
1	E	199	ASN	CA-C-N	5.84	125.98	119.32
1	E	199	ASN	C-N-CA	5.84	125.98	119.32
1	H	135	TYR	N-CA-C	5.84	118.42	108.02
1	H	138	GLN	N-CA-C	-5.83	97.70	107.32
1	I	281	PHE	N-CA-C	-5.82	104.33	112.12
1	H	149	THR	N-CA-C	-5.81	101.86	110.46
1	I	135	TYR	N-CA-C	5.80	118.34	108.02
1	I	138	GLN	N-CA-C	-5.78	97.79	107.32
1	F	62	GLN	N-CA-C	5.76	117.56	111.28
1	A	149	THR	N-CA-C	-5.73	101.98	110.46
1	E	135	TYR	N-CA-C	5.70	118.16	108.02
1	F	199	ASN	CA-C-N	5.69	125.81	119.32
1	F	199	ASN	C-N-CA	5.69	125.81	119.32
1	C	135	TYR	N-CA-C	5.64	118.07	108.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	THR	N-CA-C	-5.59	106.30	113.23
1	H	281	PHE	N-CA-C	-5.57	104.65	112.12
1	H	82	VAL	CA-C-N	-5.52	117.17	121.86
1	H	82	VAL	C-N-CA	-5.52	117.17	121.86
1	F	236	THR	N-CA-C	-5.50	106.42	113.23
1	J	138	GLN	N-CA-C	-5.50	98.25	107.32
1	A	119	PHE	N-CA-C	5.48	121.92	109.81
1	E	138	GLN	N-CA-C	-5.48	98.28	107.32
1	A	199	ASN	CA-C-N	5.48	125.56	119.32
1	A	199	ASN	C-N-CA	5.48	125.56	119.32
1	J	281	PHE	N-CA-C	-5.46	104.81	112.12
1	H	236	THR	N-CA-C	-5.44	106.48	113.23
1	G	236	THR	N-CA-C	-5.36	106.58	113.23
1	J	199	ASN	CA-C-N	5.36	125.43	119.32
1	J	199	ASN	C-N-CA	5.36	125.43	119.32
1	E	236	THR	N-CA-C	-5.34	106.61	113.23
1	G	315	VAL	N-CA-C	-5.33	107.11	112.17
1	A	236	THR	N-CA-C	-5.32	106.63	113.23
1	H	131	GLU	CA-C-N	5.31	125.61	119.93
1	H	131	GLU	C-N-CA	5.31	125.61	119.93
1	G	199	ASN	CA-C-N	5.30	125.36	119.32
1	G	199	ASN	C-N-CA	5.30	125.36	119.32
1	C	281	PHE	N-CA-C	-5.29	105.03	112.12
1	D	281	PHE	N-CA-C	-5.28	105.04	112.12
1	B	119	PHE	N-CA-C	5.26	121.44	109.81
1	J	62	GLN	N-CA-C	5.26	117.01	111.28
1	E	308	LEU	N-CA-C	-5.25	106.87	113.28
1	B	90	LYS	N-CA-C	-5.25	102.28	110.42
1	A	308	LEU	N-CA-C	-5.23	106.90	113.28
1	B	305	LEU	N-CA-C	-5.22	107.08	113.50
1	I	308	LEU	N-CA-C	-5.21	106.92	113.28
1	D	138	GLN	N-CA-C	-5.17	98.79	107.32
1	G	138	GLN	N-CA-C	-5.15	98.83	107.32
1	D	119	PHE	N-CA-C	5.14	121.17	109.81
1	G	308	LEU	N-CA-C	-5.12	107.03	113.28
1	B	281	PHE	N-CA-C	-5.11	105.28	112.12
1	I	119	PHE	N-CA-C	5.10	121.08	109.81
1	I	238	MET	N-CA-C	-5.07	105.64	111.07
1	A	305	LEU	N-CA-C	-5.06	107.28	113.50
1	F	138	GLN	N-CA-C	-5.06	98.97	107.32
1	F	304	PRO	N-CA-C	-5.04	106.97	113.57
1	F	305	LEU	N-CA-C	-5.04	107.30	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	307	PHE	N-CA-C	-5.04	107.31	113.50
1	D	24	TYR	N-CA-C	5.03	114.93	108.34
1	C	62	GLN	N-CA-C	5.03	116.76	111.28
1	H	199	ASN	CA-C-N	5.01	125.04	119.32
1	H	199	ASN	C-N-CA	5.01	125.04	119.32
1	E	315	VAL	N-CA-C	-5.00	107.42	112.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2495	0	2471	211	1
1	B	2495	0	2471	206	0
1	C	2495	0	2471	205	0
1	D	2495	0	2471	208	2
1	E	2495	0	2471	208	1
1	F	2495	0	2471	202	1
1	G	2495	0	2471	217	2
1	H	2495	0	2471	200	0
1	I	2495	0	2471	219	0
1	J	2495	0	2471	202	1
All	All	24950	0	24710	1855	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (1855) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:HG2	1:I:163:ARG:HB3	1.28	1.16
1:B:164:LYS:HZ2	1:B:165:ALA:N	1.48	1.11
1:I:164:LYS:NZ	1:I:165:ALA:H	1.52	1.06
1:D:164:LYS:NZ	1:D:165:ALA:H	1.54	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:NZ	1:B:165:ALA:H	1.52	1.05
1:G:164:LYS:HZ2	1:G:165:ALA:N	1.55	1.03
1:G:164:LYS:NZ	1:G:165:ALA:H	1.58	1.01
1:I:164:LYS:HZ2	1:I:165:ALA:N	1.60	1.00
1:B:173:ARG:HH22	1:I:139:GLN:NE2	1.62	0.97
1:J:164:LYS:HZ2	1:J:165:ALA:H	0.97	0.95
1:J:164:LYS:NZ	1:J:165:ALA:H	1.65	0.95
1:F:164:LYS:HZ2	1:F:165:ALA:N	1.65	0.94
1:F:164:LYS:NZ	1:F:165:ALA:H	1.66	0.93
1:A:164:LYS:HZ2	1:A:165:ALA:H	1.10	0.93
1:A:164:LYS:NZ	1:A:165:ALA:H	1.67	0.92
1:H:223:TRP:HE1	1:H:300:ARG:HB3	1.33	0.92
1:J:223:TRP:HE1	1:J:300:ARG:HB3	1.35	0.92
1:I:164:LYS:HZ2	1:I:165:ALA:H	0.93	0.91
1:C:164:LYS:HZ2	1:C:165:ALA:N	1.67	0.91
1:H:164:LYS:NZ	1:H:165:ALA:H	1.67	0.91
1:C:223:TRP:HE1	1:C:300:ARG:HB3	1.33	0.90
1:A:223:TRP:HE1	1:A:300:ARG:HB3	1.36	0.90
1:E:164:LYS:NZ	1:E:165:ALA:H	1.70	0.90
1:H:164:LYS:HZ2	1:H:165:ALA:H	1.18	0.89
1:J:145:ILE:H	1:J:145:ILE:HD12	1.36	0.89
1:A:249:SER:HB3	1:E:251:ILE:HG13	1.53	0.89
1:H:162:ILE:HG22	1:H:163:ARG:H	1.37	0.89
1:A:288:ASN:CG	1:A:289:GLY:H	1.81	0.89
1:E:167:THR:HG22	1:E:168:HIS:H	1.37	0.89
1:A:167:THR:HG22	1:A:168:HIS:H	1.38	0.89
1:I:167:THR:HG22	1:I:168:HIS:H	1.36	0.89
1:I:145:ILE:H	1:I:145:ILE:HD12	1.36	0.89
1:I:223:TRP:HE1	1:I:300:ARG:HB3	1.38	0.89
1:J:164:LYS:HZ2	1:J:165:ALA:N	1.71	0.89
1:G:223:TRP:HE1	1:G:300:ARG:HB3	1.36	0.88
1:E:223:TRP:HE1	1:E:300:ARG:HB3	1.39	0.88
1:B:167:THR:HG22	1:B:168:HIS:H	1.39	0.88
1:D:164:LYS:HZ1	1:D:165:ALA:N	1.71	0.87
1:H:167:THR:HG22	1:H:168:HIS:H	1.37	0.87
1:D:164:LYS:HZ1	1:D:165:ALA:H	0.87	0.87
1:F:164:LYS:HZ2	1:F:165:ALA:H	0.89	0.87
1:B:145:ILE:H	1:B:145:ILE:HD12	1.39	0.87
1:D:223:TRP:HE1	1:D:300:ARG:HB3	1.40	0.87
1:A:140:LEU:HD13	1:A:190:ILE:HG13	1.56	0.87
1:E:164:LYS:HZ2	1:E:165:ALA:H	1.22	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASN:CG	1:G:289:GLY:H	1.83	0.86
1:B:181:GLN:HG3	1:B:182:PRO:HD3	1.57	0.86
1:C:164:LYS:NZ	1:C:165:ALA:H	1.73	0.86
1:E:181:GLN:HG3	1:E:182:PRO:HD3	1.57	0.86
1:H:288:ASN:CG	1:H:289:GLY:H	1.83	0.86
1:B:168:HIS:ND1	1:I:167:THR:HB	1.91	0.86
1:C:288:ASN:CG	1:C:289:GLY:H	1.84	0.86
1:D:72:TRP:CZ2	1:D:74:PRO:HG3	2.11	0.86
1:F:181:GLN:HG3	1:F:182:PRO:HD3	1.58	0.86
1:H:145:ILE:HD12	1:H:145:ILE:H	1.40	0.86
1:J:288:ASN:CG	1:J:289:GLY:H	1.83	0.86
1:B:288:ASN:CG	1:B:289:GLY:H	1.84	0.86
1:B:173:ARG:HH22	1:I:139:GLN:HE22	1.22	0.85
1:E:288:ASN:CG	1:E:289:GLY:H	1.84	0.85
1:I:288:ASN:CG	1:I:289:GLY:H	1.84	0.85
1:F:237:LEU:HD13	1:G:235:PHE:CD2	2.09	0.85
1:I:224:LEU:HD21	1:J:231:LEU:HD22	1.58	0.85
1:D:181:GLN:HG3	1:D:182:PRO:HD3	1.59	0.85
1:C:145:ILE:HD12	1:C:145:ILE:H	1.41	0.85
1:G:181:GLN:HG3	1:G:182:PRO:HD3	1.57	0.85
1:D:288:ASN:CG	1:D:289:GLY:H	1.85	0.85
1:F:288:ASN:CG	1:F:289:GLY:H	1.83	0.85
1:A:72:TRP:CZ2	1:A:74:PRO:HG3	2.11	0.85
1:A:181:GLN:HG3	1:A:182:PRO:HD3	1.58	0.84
1:H:181:GLN:HG3	1:H:182:PRO:HD3	1.59	0.84
1:J:167:THR:HG22	1:J:168:HIS:H	1.42	0.84
1:C:164:LYS:HZ2	1:C:165:ALA:H	0.85	0.84
1:C:181:GLN:HG3	1:C:182:PRO:HD3	1.59	0.83
1:I:215:ILE:O	1:I:218:SER:HB3	1.78	0.83
1:E:145:ILE:H	1:E:145:ILE:HD12	1.43	0.83
1:F:145:ILE:H	1:F:145:ILE:HD12	1.41	0.83
1:G:294:LEU:HA	1:G:297:GLN:HE21	1.43	0.83
1:E:162:ILE:HG22	1:E:163:ARG:H	1.44	0.83
1:I:181:GLN:HG3	1:I:182:PRO:HD3	1.58	0.83
1:J:181:GLN:HG3	1:J:182:PRO:HD3	1.58	0.83
1:A:145:ILE:H	1:A:145:ILE:HD12	1.43	0.83
1:F:256:PRO:HG2	1:F:257:TYR:HD1	1.43	0.82
1:H:256:PRO:HG2	1:H:257:TYR:HD1	1.44	0.82
1:F:215:ILE:O	1:F:218:SER:HB3	1.80	0.82
1:A:162:ILE:HG22	1:A:163:ARG:H	1.44	0.82
1:F:167:THR:HG22	1:F:168:HIS:H	1.43	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ILE:HG22	1:G:163:ARG:H	1.44	0.82
1:B:223:TRP:HE1	1:B:300:ARG:HB3	1.43	0.82
1:F:198:ARG:O	1:F:200:PRO:HD3	1.80	0.82
1:B:164:LYS:HD3	1:I:163:ARG:HD2	1.61	0.82
1:C:256:PRO:HG2	1:C:257:TYR:HD1	1.45	0.82
1:D:44:THR:HA	1:D:99:ARG:HA	1.62	0.81
1:A:293:ASP:HB2	1:A:296:ILE:HG22	1.61	0.81
1:F:72:TRP:CZ2	1:F:74:PRO:HG3	2.14	0.81
1:H:223:TRP:NE1	1:H:300:ARG:HB3	1.95	0.81
1:I:198:ARG:O	1:I:200:PRO:HD3	1.79	0.81
1:J:215:ILE:O	1:J:218:SER:HB3	1.80	0.81
1:G:145:ILE:H	1:G:145:ILE:HD12	1.43	0.81
1:H:140:LEU:HD13	1:H:190:ILE:HG13	1.63	0.81
1:C:218:SER:HA	1:C:237:LEU:HD21	1.62	0.81
1:J:72:TRP:CZ2	1:J:74:PRO:HG3	2.15	0.81
1:J:119:PHE:HB3	1:J:120:PRO:HD3	1.61	0.81
1:B:119:PHE:HB3	1:B:120:PRO:HD3	1.63	0.81
1:I:256:PRO:HG2	1:I:257:TYR:HD1	1.44	0.81
1:J:294:LEU:HA	1:J:297:GLN:HE21	1.46	0.81
1:B:140:LEU:HD13	1:B:190:ILE:HG13	1.62	0.81
1:D:162:ILE:HG22	1:D:163:ARG:H	1.44	0.81
1:D:237:LEU:HD13	1:E:235:PHE:CD2	2.15	0.81
1:J:293:ASP:HB2	1:J:296:ILE:HG22	1.63	0.80
1:C:119:PHE:HB3	1:C:120:PRO:HD3	1.63	0.80
1:F:223:TRP:HE1	1:F:300:ARG:HB3	1.46	0.80
1:J:140:LEU:HD13	1:J:190:ILE:HG13	1.61	0.80
1:I:256:PRO:HG2	1:I:257:TYR:CD1	2.16	0.80
1:A:294:LEU:HA	1:A:297:GLN:HE21	1.46	0.80
1:D:198:ARG:O	1:D:200:PRO:HD3	1.81	0.80
1:A:164:LYS:HZ2	1:A:165:ALA:N	1.80	0.80
1:A:256:PRO:HG2	1:A:257:TYR:HD1	1.45	0.80
1:D:167:THR:HG22	1:D:168:HIS:H	1.47	0.80
1:E:256:PRO:HG2	1:E:257:TYR:HD1	1.46	0.80
1:G:167:THR:HG22	1:G:168:HIS:H	1.47	0.80
1:D:256:PRO:HG2	1:D:257:TYR:HD1	1.47	0.79
1:I:72:TRP:CZ2	1:I:74:PRO:HG3	2.17	0.79
1:G:119:PHE:HB3	1:G:120:PRO:HD3	1.64	0.79
1:G:256:PRO:HG2	1:G:257:TYR:HD1	1.46	0.79
1:D:140:LEU:HD13	1:D:190:ILE:HG13	1.64	0.79
1:D:215:ILE:O	1:D:218:SER:HB3	1.81	0.79
1:F:119:PHE:HB3	1:F:120:PRO:HD3	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:TRP:NE1	1:G:300:ARG:HB3	1.97	0.79
1:B:224:LEU:HD21	1:C:231:LEU:HD22	1.62	0.79
1:F:294:LEU:HA	1:F:297:GLN:HE21	1.46	0.79
1:D:294:LEU:HA	1:D:297:GLN:HE21	1.46	0.79
1:A:223:TRP:NE1	1:A:300:ARG:HB3	1.96	0.79
1:J:198:ARG:O	1:J:200:PRO:HD3	1.83	0.79
1:G:140:LEU:HD13	1:G:190:ILE:HG13	1.65	0.79
1:H:44:THR:HA	1:H:99:ARG:HA	1.63	0.79
1:C:293:ASP:HB2	1:C:296:ILE:HG22	1.65	0.79
1:H:218:SER:HA	1:H:237:LEU:HD21	1.64	0.79
1:E:294:LEU:HA	1:E:297:GLN:HE21	1.46	0.78
1:F:140:LEU:HD13	1:F:190:ILE:HG13	1.64	0.78
1:C:167:THR:HG22	1:C:168:HIS:H	1.48	0.78
1:B:162:ILE:HG22	1:B:163:ARG:H	1.48	0.78
1:A:239:LEU:HD23	1:E:240:THR:HA	1.65	0.78
1:F:256:PRO:HG2	1:F:257:TYR:CD1	2.19	0.78
1:H:294:LEU:HA	1:H:297:GLN:HE21	1.48	0.78
1:C:198:ARG:O	1:C:200:PRO:HD3	1.84	0.78
1:J:223:TRP:NE1	1:J:300:ARG:HB3	1.99	0.78
1:A:235:PHE:CD2	1:E:237:LEU:HD13	2.19	0.78
1:F:249:SER:HB3	1:J:251:ILE:HG13	1.65	0.78
1:H:256:PRO:HG2	1:H:257:TYR:CD1	2.19	0.78
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.47	0.78
1:H:119:PHE:HB3	1:H:120:PRO:HD3	1.65	0.78
1:H:198:ARG:O	1:H:200:PRO:HD3	1.84	0.77
1:C:162:ILE:HG22	1:C:163:ARG:H	1.48	0.77
1:E:140:LEU:HD13	1:E:190:ILE:HG13	1.64	0.77
1:I:294:LEU:HA	1:I:297:GLN:HE21	1.49	0.77
1:C:223:TRP:NE1	1:C:300:ARG:HB3	1.98	0.77
1:G:256:PRO:HG2	1:G:257:TYR:CD1	2.20	0.77
1:I:293:ASP:HB2	1:I:296:ILE:HG22	1.65	0.77
1:F:68:ASN:ND2	1:J:65:ARG:HD2	1.99	0.77
1:H:224:LEU:HD21	1:I:231:LEU:HD22	1.66	0.77
1:G:294:LEU:HA	1:G:297:GLN:NE2	1.99	0.77
1:B:198:ARG:O	1:B:200:PRO:HD3	1.84	0.77
1:D:145:ILE:H	1:D:145:ILE:HD12	1.49	0.77
1:I:140:LEU:HD13	1:I:190:ILE:HG13	1.67	0.77
1:E:293:ASP:HB2	1:E:296:ILE:HG22	1.66	0.77
1:J:28:THR:HB	1:J:255:LEU:HD21	1.68	0.77
1:C:256:PRO:HG2	1:C:257:TYR:CD1	2.20	0.76
1:F:162:ILE:HG22	1:F:163:ARG:H	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:LEU:HB3	1:I:210:PRO:CD	2.13	0.76
1:J:123:ARG:HD2	1:J:197:VAL:HG22	1.67	0.76
1:J:256:PRO:HG2	1:J:257:TYR:HD1	1.50	0.76
1:C:28:THR:HB	1:C:255:LEU:HD21	1.67	0.76
1:F:293:ASP:HB2	1:F:296:ILE:HG22	1.66	0.76
1:I:119:PHE:HB3	1:I:120:PRO:HD3	1.67	0.76
1:B:293:ASP:HB2	1:B:296:ILE:HG22	1.67	0.76
1:D:293:ASP:HB2	1:D:296:ILE:HG22	1.68	0.76
1:I:44:THR:HA	1:I:99:ARG:HA	1.67	0.76
1:I:223:TRP:NE1	1:I:300:ARG:HB3	2.00	0.76
1:A:44:THR:HA	1:A:99:ARG:HA	1.67	0.76
1:C:140:LEU:HD13	1:C:190:ILE:HG13	1.66	0.76
1:A:224:LEU:HD21	1:B:231:LEU:HD22	1.67	0.76
1:D:256:PRO:HG2	1:D:257:TYR:CD1	2.20	0.76
1:E:227:PHE:HA	1:E:230:ARG:HH11	1.49	0.76
1:E:256:PRO:HG2	1:E:257:TYR:CD1	2.21	0.76
1:E:223:TRP:NE1	1:E:300:ARG:HB3	1.99	0.76
1:G:28:THR:HB	1:G:255:LEU:HD21	1.68	0.76
1:J:227:PHE:HA	1:J:230:ARG:HH11	1.51	0.76
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.51	0.76
1:A:198:ARG:O	1:A:200:PRO:HD3	1.86	0.75
1:G:293:ASP:HB2	1:G:296:ILE:HG22	1.66	0.75
1:A:119:PHE:HB3	1:A:120:PRO:HD3	1.67	0.75
1:I:162:ILE:HG22	1:I:163:ARG:H	1.49	0.75
1:A:148:TYR:OH	1:B:176:HIS:CE1	2.39	0.75
1:E:119:PHE:HB3	1:E:120:PRO:HD3	1.68	0.75
1:E:198:ARG:O	1:E:200:PRO:HD3	1.86	0.75
1:C:227:PHE:HA	1:C:230:ARG:HH11	1.51	0.75
1:H:293:ASP:HB2	1:H:296:ILE:HG22	1.68	0.75
1:E:72:TRP:CZ2	1:E:74:PRO:HG3	2.22	0.75
1:C:72:TRP:CZ2	1:C:74:PRO:HG3	2.22	0.75
1:C:215:ILE:O	1:C:218:SER:HB3	1.87	0.75
1:A:294:LEU:HA	1:A:297:GLN:NE2	2.02	0.74
1:G:44:THR:HA	1:G:99:ARG:HA	1.67	0.74
1:H:28:THR:HB	1:H:255:LEU:HD21	1.70	0.74
1:J:218:SER:HA	1:J:237:LEU:HD21	1.68	0.74
1:C:294:LEU:HA	1:C:297:GLN:HE21	1.51	0.74
1:E:215:ILE:O	1:E:218:SER:HB3	1.87	0.74
1:J:44:THR:HA	1:J:99:ARG:HA	1.67	0.74
1:J:256:PRO:HG2	1:J:257:TYR:CD1	2.22	0.74
1:H:72:TRP:CZ2	1:H:74:PRO:HG3	2.23	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:OH	1:B:176:HIS:NE2	2.20	0.74
1:H:215:ILE:O	1:H:218:SER:HB3	1.87	0.74
1:E:294:LEU:HA	1:E:297:GLN:NE2	2.02	0.74
1:J:294:LEU:HA	1:J:297:GLN:NE2	2.03	0.74
1:B:294:LEU:HA	1:B:297:GLN:HE21	1.52	0.74
1:D:218:SER:HA	1:D:237:LEU:HD21	1.69	0.74
1:B:223:TRP:NE1	1:B:300:ARG:HB3	2.03	0.74
1:D:294:LEU:HA	1:D:297:GLN:NE2	2.02	0.74
1:G:237:LEU:HD13	1:H:235:PHE:CD2	2.23	0.74
1:F:223:TRP:NE1	1:F:300:ARG:HB3	2.02	0.73
1:G:72:TRP:CZ2	1:G:74:PRO:HG3	2.22	0.73
1:A:256:PRO:HG2	1:A:257:TYR:CD1	2.22	0.73
1:E:123:ARG:HD2	1:E:197:VAL:HG22	1.70	0.73
1:F:218:SER:HA	1:F:237:LEU:HD21	1.68	0.73
1:G:198:ARG:O	1:G:200:PRO:HD3	1.87	0.73
1:I:148:TYR:OH	1:J:176:HIS:CE1	2.41	0.73
1:B:227:PHE:HA	1:B:230:ARG:HH11	1.52	0.73
1:D:28:THR:HB	1:D:255:LEU:HD21	1.70	0.73
1:A:39:ILE:HD11	1:A:78:PHE:CZ	2.23	0.73
1:A:227:PHE:HA	1:A:230:ARG:HH11	1.52	0.73
1:E:44:THR:HA	1:E:99:ARG:HA	1.70	0.73
1:F:44:THR:HA	1:F:99:ARG:HA	1.68	0.73
1:F:239:LEU:HD23	1:J:240:THR:HA	1.71	0.73
1:C:44:THR:HA	1:C:99:ARG:HA	1.71	0.73
1:D:164:LYS:HZ2	1:D:164:LYS:HA	1.54	0.73
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.69	0.73
1:G:114:MET:HE2	1:G:124:GLN:HG2	1.71	0.73
1:G:218:SER:HA	1:G:237:LEU:HD21	1.70	0.73
1:F:220:SER:HB2	1:G:280:ILE:HD13	1.71	0.73
1:D:223:TRP:NE1	1:D:300:ARG:HB3	2.02	0.72
1:D:227:PHE:HA	1:D:230:ARG:HH11	1.52	0.72
1:G:251:ILE:HG13	1:H:249:SER:HB3	1.71	0.72
1:B:173:ARG:NH2	1:I:139:GLN:HE22	1.87	0.72
1:F:237:LEU:HD13	1:G:235:PHE:CE2	2.24	0.72
1:H:164:LYS:HZ2	1:H:165:ALA:N	1.87	0.72
1:F:28:THR:HB	1:F:255:LEU:HD21	1.72	0.72
1:J:209:LEU:HB3	1:J:210:PRO:CD	2.20	0.72
1:D:119:PHE:HB3	1:D:120:PRO:HD3	1.72	0.72
1:G:227:PHE:HA	1:G:230:ARG:HH11	1.55	0.72
1:A:293:ASP:HB2	1:A:296:ILE:CG2	2.19	0.71
1:E:209:LEU:HB3	1:E:210:PRO:CD	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:LEU:HA	1:F:297:GLN:NE2	2.04	0.71
1:A:215:ILE:O	1:A:218:SER:HB3	1.90	0.71
1:C:123:ARG:HD2	1:C:197:VAL:HG22	1.73	0.71
1:I:227:PHE:HA	1:I:230:ARG:HH11	1.55	0.71
1:E:28:THR:HB	1:E:255:LEU:HD21	1.71	0.71
1:B:44:THR:HA	1:B:99:ARG:HA	1.72	0.71
1:E:39:ILE:HD11	1:E:78:PHE:CZ	2.25	0.71
1:J:162:ILE:HG22	1:J:163:ARG:H	1.54	0.71
1:A:78:PHE:HB3	1:A:81:VAL:HG23	1.71	0.71
1:D:91:ARG:HB2	1:E:133:PHE:CE2	2.26	0.71
1:F:227:PHE:HA	1:F:230:ARG:HH11	1.55	0.71
1:B:148:TYR:OH	1:C:176:HIS:NE2	2.24	0.71
1:E:226:SER:O	1:E:230:ARG:HD3	1.91	0.71
1:A:28:THR:HB	1:A:255:LEU:HD21	1.72	0.71
1:B:224:LEU:O	1:B:230:ARG:HD2	1.90	0.71
1:C:39:ILE:HD11	1:C:78:PHE:CZ	2.25	0.71
1:E:150:GLU:HB3	1:E:153:ASP:HB2	1.73	0.71
1:F:78:PHE:HB3	1:F:81:VAL:HG23	1.73	0.71
1:I:294:LEU:HA	1:I:297:GLN:NE2	2.06	0.71
1:E:78:PHE:HB3	1:E:81:VAL:HG23	1.73	0.70
1:H:209:LEU:HB3	1:H:210:PRO:CD	2.21	0.70
1:F:150:GLU:HB3	1:F:153:ASP:HB2	1.74	0.70
1:J:293:ASP:HB2	1:J:296:ILE:CG2	2.21	0.70
1:D:301:LEU:HD23	1:D:301:LEU:O	1.91	0.70
1:H:227:PHE:HA	1:H:230:ARG:HH11	1.57	0.70
1:I:28:THR:HB	1:I:255:LEU:HD21	1.72	0.70
1:H:52:GLY:O	1:H:53:ASP:HB2	1.91	0.70
1:H:294:LEU:HA	1:H:297:GLN:NE2	2.05	0.70
1:I:78:PHE:HB3	1:I:81:VAL:HG23	1.73	0.70
1:I:293:ASP:HB2	1:I:296:ILE:CG2	2.21	0.70
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.74	0.70
1:E:301:LEU:O	1:E:301:LEU:HD23	1.91	0.70
1:F:254:ARG:O	1:F:255:LEU:HD23	1.91	0.70
1:A:162:ILE:HD12	1:A:162:ILE:N	2.07	0.70
1:I:148:TYR:CE2	1:J:176:HIS:NE2	2.60	0.69
1:D:224:LEU:O	1:D:230:ARG:HD2	1.92	0.69
1:H:226:SER:O	1:H:230:ARG:HD3	1.91	0.69
1:I:202:TYR:HB2	1:J:256:PRO:O	1.93	0.69
1:J:211:LEU:O	1:J:215:ILE:HG12	1.91	0.69
1:C:293:ASP:HB2	1:C:296:ILE:CG2	2.22	0.69
1:D:52:GLY:O	1:D:53:ASP:HB2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:GLU:HB3	1:G:153:ASP:HB2	1.73	0.69
1:H:39:ILE:HD11	1:H:78:PHE:CZ	2.26	0.69
1:H:254:ARG:O	1:H:255:LEU:HD23	1.92	0.69
1:H:150:GLU:HB3	1:H:153:ASP:HB2	1.74	0.69
1:D:78:PHE:HB3	1:D:81:VAL:HG23	1.72	0.69
1:G:162:ILE:HD12	1:G:162:ILE:N	2.07	0.69
1:C:301:LEU:O	1:C:301:LEU:HD23	1.93	0.69
1:D:209:LEU:HB3	1:D:210:PRO:CD	2.23	0.69
1:I:148:TYR:HE2	1:J:176:HIS:HE2	1.38	0.69
1:E:52:GLY:O	1:E:53:ASP:HB2	1.92	0.69
1:F:301:LEU:O	1:F:301:LEU:HD23	1.92	0.69
1:G:164:LYS:HZ2	1:G:165:ALA:H	0.76	0.69
1:J:39:ILE:HD11	1:J:78:PHE:CZ	2.28	0.69
1:D:150:GLU:HB3	1:D:153:ASP:HB2	1.75	0.69
1:B:215:ILE:O	1:B:218:SER:HB3	1.93	0.69
1:D:226:SER:O	1:D:230:ARG:HD3	1.93	0.69
1:E:114:MET:HE2	1:E:124:GLN:HG2	1.75	0.69
1:A:150:GLU:HB3	1:A:153:ASP:HB2	1.74	0.68
1:C:150:GLU:HB3	1:C:153:ASP:HB2	1.73	0.68
1:E:293:ASP:HB2	1:E:296:ILE:CG2	2.23	0.68
1:G:215:ILE:O	1:G:218:SER:HB3	1.93	0.68
1:J:150:GLU:HB3	1:J:153:ASP:HB2	1.73	0.68
1:B:209:LEU:HB3	1:B:210:PRO:CD	2.24	0.68
1:I:218:SER:HA	1:I:237:LEU:HD21	1.74	0.68
1:B:218:SER:HA	1:B:237:LEU:HD21	1.73	0.68
1:J:162:ILE:N	1:J:162:ILE:HD12	2.08	0.68
1:B:72:TRP:CZ2	1:B:74:PRO:HG3	2.28	0.68
1:B:167:THR:HG22	1:B:168:HIS:N	2.08	0.68
1:D:72:TRP:O	1:D:72:TRP:CD1	2.47	0.68
1:E:227:PHE:HA	1:E:230:ARG:NH1	2.08	0.68
1:G:240:THR:HA	1:H:239:LEU:HD23	1.75	0.68
1:I:167:THR:HG22	1:I:168:HIS:N	2.08	0.68
1:C:114:MET:HE2	1:C:124:GLN:HG2	1.74	0.68
1:G:78:PHE:HB3	1:G:81:VAL:HG23	1.76	0.68
1:A:123:ARG:HD2	1:A:197:VAL:HG22	1.74	0.68
1:B:39:ILE:HD11	1:B:78:PHE:CZ	2.29	0.68
1:F:114:MET:HE2	1:F:124:GLN:HG2	1.75	0.68
1:A:52:GLY:O	1:A:53:ASP:HB2	1.94	0.68
1:A:301:LEU:HD23	1:A:301:LEU:O	1.94	0.68
1:B:167:THR:O	1:B:168:HIS:HB2	1.94	0.68
1:E:218:SER:HA	1:E:237:LEU:HD21	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:VAL:C	1:G:128:LEU:HD12	2.19	0.68
1:G:167:THR:O	1:G:168:HIS:HB2	1.93	0.68
1:A:202:TYR:HB2	1:B:256:PRO:O	1.94	0.67
1:A:226:SER:O	1:A:230:ARG:HD3	1.94	0.67
1:B:150:GLU:HB3	1:B:153:ASP:HB2	1.75	0.67
1:C:226:SER:O	1:C:230:ARG:HD3	1.93	0.67
1:C:294:LEU:HA	1:C:297:GLN:NE2	2.08	0.67
1:G:293:ASP:HB2	1:G:296:ILE:CG2	2.23	0.67
1:B:168:HIS:HD1	1:I:167:THR:HB	1.58	0.67
1:A:231:LEU:HD23	1:A:231:LEU:C	2.19	0.67
1:B:28:THR:HB	1:B:255:LEU:HD21	1.76	0.67
1:C:209:LEU:HB3	1:C:210:PRO:CD	2.24	0.67
1:D:164:LYS:NZ	1:D:165:ALA:N	2.36	0.67
1:G:127:VAL:O	1:G:128:LEU:HD12	1.93	0.67
1:H:78:PHE:HB3	1:H:81:VAL:HG23	1.74	0.67
1:B:256:PRO:HG2	1:B:257:TYR:CD1	2.29	0.67
1:G:288:ASN:CG	1:G:289:GLY:N	2.52	0.67
1:A:114:MET:HE2	1:A:124:GLN:HG2	1.74	0.67
1:B:294:LEU:HA	1:B:297:GLN:NE2	2.09	0.67
1:C:91:ARG:CD	1:D:134:SER:HB3	2.25	0.67
1:D:293:ASP:HB2	1:D:296:ILE:CG2	2.24	0.67
1:E:164:LYS:HZ2	1:E:165:ALA:N	1.91	0.67
1:A:288:ASN:CG	1:A:289:GLY:N	2.52	0.67
1:F:123:ARG:HD2	1:F:197:VAL:HG22	1.77	0.67
1:G:72:TRP:HZ3	1:G:135:TYR:CZ	2.11	0.67
1:F:157:ILE:HD11	1:G:115:ASP:OD2	1.94	0.67
1:F:293:ASP:HB2	1:F:296:ILE:CG2	2.24	0.67
1:A:148:TYR:CE2	1:B:176:HIS:NE2	2.62	0.67
1:D:211:LEU:O	1:D:215:ILE:HG12	1.95	0.67
1:B:256:PRO:HG2	1:B:257:TYR:HD1	1.59	0.67
1:I:150:GLU:HB3	1:I:153:ASP:HB2	1.75	0.67
1:F:231:LEU:HD23	1:F:231:LEU:C	2.20	0.67
1:J:259:THR:O	1:J:263:GLN:HG3	1.95	0.67
1:A:218:SER:HA	1:A:237:LEU:HD21	1.77	0.66
1:E:72:TRP:HZ3	1:E:135:TYR:CZ	2.12	0.66
1:B:114:MET:HE2	1:B:124:GLN:HG2	1.76	0.66
1:B:226:SER:O	1:B:230:ARG:HD3	1.95	0.66
1:F:288:ASN:CG	1:F:289:GLY:N	2.54	0.66
1:G:52:GLY:O	1:G:53:ASP:HB2	1.96	0.66
1:F:211:LEU:O	1:F:215:ILE:HG12	1.96	0.66
1:J:78:PHE:HB3	1:J:81:VAL:HG23	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASP:HB2	1:B:296:ILE:CG2	2.24	0.66
1:H:293:ASP:HB2	1:H:296:ILE:CG2	2.25	0.66
1:B:123:ARG:HD2	1:B:197:VAL:HG22	1.76	0.66
1:H:301:LEU:O	1:H:301:LEU:HD23	1.96	0.66
1:I:231:LEU:HD23	1:I:231:LEU:C	2.20	0.66
1:A:115:ASP:OD2	1:E:157:ILE:HD11	1.95	0.66
1:A:254:ARG:O	1:A:255:LEU:HD23	1.96	0.66
1:D:127:VAL:O	1:D:128:LEU:HD12	1.96	0.66
1:D:220:SER:HB2	1:E:280:ILE:HD13	1.76	0.66
1:F:247:TYR:CE1	1:G:245:ALA:HB1	2.30	0.66
1:G:219:TRP:C	1:G:221:VAL:H	2.04	0.66
1:I:301:LEU:HD23	1:I:301:LEU:O	1.95	0.66
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.31	0.66
1:J:301:LEU:HD23	1:J:301:LEU:O	1.95	0.66
1:B:301:LEU:HD23	1:B:301:LEU:O	1.96	0.65
1:J:72:TRP:HZ3	1:J:135:TYR:CZ	2.14	0.65
1:B:226:SER:HB3	1:B:229:GLU:HG3	1.77	0.65
1:B:247:TYR:HE1	1:C:249:SER:HG	1.42	0.65
1:H:239:LEU:CD1	1:I:239:LEU:HD21	2.26	0.65
1:H:72:TRP:HZ3	1:H:135:TYR:CZ	2.14	0.65
1:H:288:ASN:CG	1:H:289:GLY:N	2.54	0.65
1:I:226:SER:HB3	1:I:229:GLU:HG3	1.78	0.65
1:A:209:LEU:HB3	1:A:210:PRO:CD	2.26	0.65
1:B:169:ILE:HB	1:I:168:HIS:ND1	2.12	0.65
1:J:226:SER:O	1:J:230:ARG:HD3	1.96	0.65
1:A:148:TYR:CZ	1:B:176:HIS:NE2	2.65	0.65
1:I:288:ASN:CG	1:I:289:GLY:N	2.54	0.65
1:A:204:LEU:HD23	1:A:208:ILE:HG13	1.78	0.65
1:B:162:ILE:N	1:B:162:ILE:HD12	2.10	0.65
1:E:167:THR:HG22	1:E:168:HIS:N	2.08	0.65
1:E:288:ASN:CG	1:E:289:GLY:N	2.54	0.65
1:A:259:THR:O	1:A:263:GLN:HG3	1.97	0.65
1:J:78:PHE:HB3	1:J:81:VAL:CG2	2.27	0.65
1:A:162:ILE:HD12	1:A:162:ILE:H	1.61	0.65
1:E:254:ARG:O	1:E:255:LEU:HD23	1.96	0.65
1:G:254:ARG:O	1:G:255:LEU:HD23	1.96	0.65
1:H:204:LEU:HD23	1:H:208:ILE:HG13	1.79	0.65
1:D:114:MET:HE2	1:D:124:GLN:HG2	1.79	0.64
1:H:226:SER:HB3	1:H:229:GLU:HG3	1.79	0.64
1:H:239:LEU:HD13	1:I:239:LEU:HD21	1.79	0.64
1:B:288:ASN:CG	1:B:289:GLY:N	2.54	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:HD13	1:E:235:PHE:CE2	2.31	0.64
1:G:204:LEU:HD23	1:G:208:ILE:HG13	1.79	0.64
1:G:226:SER:HB3	1:G:229:GLU:HG3	1.78	0.64
1:G:301:LEU:HD23	1:G:301:LEU:O	1.97	0.64
1:J:231:LEU:C	1:J:231:LEU:HD23	2.22	0.64
1:A:78:PHE:HB3	1:A:81:VAL:CG2	2.27	0.64
1:D:254:ARG:O	1:D:255:LEU:HD23	1.97	0.64
1:F:209:LEU:HB3	1:F:210:PRO:CD	2.28	0.64
1:F:91:ARG:HB2	1:G:133:PHE:HE2	1.60	0.64
1:D:78:PHE:HB3	1:D:81:VAL:CG2	2.28	0.64
1:D:247:TYR:CE1	1:E:245:ALA:HB1	2.33	0.64
1:G:209:LEU:HB3	1:G:210:PRO:CD	2.26	0.64
1:H:211:LEU:O	1:H:215:ILE:HG12	1.96	0.64
1:I:52:GLY:O	1:I:53:ASP:HB2	1.97	0.64
1:E:204:LEU:HD23	1:E:208:ILE:HG13	1.80	0.64
1:H:167:THR:HG22	1:H:168:HIS:N	2.07	0.64
1:I:72:TRP:HZ3	1:I:135:TYR:CZ	2.15	0.64
1:A:247:TYR:HE1	1:B:249:SER:HG	1.46	0.64
1:B:127:VAL:C	1:B:128:LEU:HD12	2.23	0.64
1:F:134:SER:HB3	1:J:91:ARG:CD	2.28	0.64
1:H:112:ASN:OD1	1:H:113:ASP:N	2.30	0.64
1:J:227:PHE:HA	1:J:230:ARG:NH1	2.13	0.64
1:J:254:ARG:O	1:J:255:LEU:HD23	1.98	0.64
1:C:72:TRP:HZ3	1:C:135:TYR:CZ	2.16	0.64
1:C:254:ARG:O	1:C:255:LEU:HD23	1.96	0.64
1:E:226:SER:HB3	1:E:229:GLU:HG3	1.80	0.64
1:H:224:LEU:O	1:H:230:ARG:HD2	1.97	0.64
1:I:254:ARG:O	1:I:255:LEU:HD23	1.98	0.64
1:A:167:THR:HG22	1:A:168:HIS:N	2.10	0.64
1:E:78:PHE:HB3	1:E:81:VAL:CG2	2.28	0.64
1:F:162:ILE:HD12	1:F:162:ILE:N	2.12	0.64
1:D:226:SER:HB3	1:D:229:GLU:HG3	1.79	0.63
1:C:237:LEU:HD13	1:D:235:PHE:CD2	2.33	0.63
1:H:78:PHE:HB3	1:H:81:VAL:CG2	2.29	0.63
1:D:227:PHE:HA	1:D:230:ARG:NH1	2.14	0.63
1:D:39:ILE:HD11	1:D:78:PHE:CZ	2.32	0.63
1:D:231:LEU:HD23	1:D:231:LEU:C	2.24	0.63
1:F:78:PHE:HB3	1:F:81:VAL:CG2	2.28	0.63
1:G:123:ARG:HD2	1:G:197:VAL:HG22	1.78	0.63
1:B:227:PHE:HA	1:B:230:ARG:NH1	2.13	0.63
1:D:72:TRP:CD1	1:D:72:TRP:C	2.76	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:SER:HB3	1:C:229:GLU:HG3	1.81	0.63
1:B:224:LEU:HB2	1:B:230:ARG:HG3	1.79	0.63
1:G:91:ARG:HB2	1:H:133:PHE:CE2	2.34	0.63
1:I:39:ILE:HD11	1:I:78:PHE:CZ	2.32	0.63
1:D:123:ARG:HD2	1:D:197:VAL:HG22	1.80	0.63
1:B:204:LEU:HD23	1:B:208:ILE:HG13	1.79	0.63
1:E:162:ILE:N	1:E:162:ILE:HD12	2.14	0.63
1:G:226:SER:O	1:G:230:ARG:HD3	1.98	0.63
1:G:91:ARG:CD	1:H:134:SER:HB3	2.28	0.62
1:B:223:TRP:CE3	1:C:280:ILE:HG22	2.34	0.62
1:G:162:ILE:HD12	1:G:162:ILE:H	1.61	0.62
1:B:148:TYR:OH	1:C:176:HIS:CE1	2.52	0.62
1:C:52:GLY:O	1:C:53:ASP:HB2	1.97	0.62
1:C:78:PHE:HB3	1:C:81:VAL:HG23	1.80	0.62
1:D:59:GLU:O	1:D:63:ILE:HG13	1.99	0.62
1:F:72:TRP:CH2	1:F:74:PRO:HG3	2.34	0.62
1:F:220:SER:HB2	1:G:280:ILE:CD1	2.30	0.62
1:I:169:ILE:HD12	1:I:190:ILE:HG12	1.82	0.62
1:A:134:SER:HB3	1:E:91:ARG:CD	2.29	0.62
1:C:231:LEU:HD23	1:C:231:LEU:C	2.24	0.62
1:D:251:ILE:HG13	1:E:249:SER:HB3	1.80	0.62
1:F:52:GLY:O	1:F:53:ASP:HB2	1.99	0.62
1:G:224:LEU:O	1:G:230:ARG:HD2	1.98	0.62
1:J:162:ILE:HD12	1:J:162:ILE:H	1.63	0.62
1:A:249:SER:HB3	1:E:251:ILE:CG1	2.29	0.62
1:F:167:THR:HG22	1:F:168:HIS:N	2.14	0.62
1:G:169:ILE:HD12	1:G:190:ILE:HG12	1.82	0.62
1:A:226:SER:HB3	1:A:229:GLU:HG3	1.82	0.62
1:A:280:ILE:CD1	1:E:220:SER:HB2	2.29	0.62
1:D:56:LEU:HD13	1:D:57:ILE:N	2.15	0.62
1:E:231:LEU:C	1:E:231:LEU:HD23	2.25	0.62
1:F:162:ILE:HD12	1:F:162:ILE:H	1.65	0.62
1:B:127:VAL:O	1:B:128:LEU:HD12	2.00	0.62
1:F:226:SER:HB3	1:F:229:GLU:HG3	1.80	0.62
1:G:167:THR:O	1:G:168:HIS:CB	2.48	0.62
1:F:305:LEU:C	1:F:305:LEU:HD12	2.25	0.62
1:A:72:TRP:CH2	1:A:74:PRO:HG3	2.35	0.61
1:A:227:PHE:HA	1:A:230:ARG:NH1	2.15	0.61
1:C:162:ILE:HD12	1:C:162:ILE:N	2.15	0.61
1:C:211:LEU:O	1:C:215:ILE:HG12	2.00	0.61
1:F:239:LEU:CD2	1:J:240:THR:HA	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LEU:O	1:I:230:ARG:HD2	2.00	0.61
1:D:162:ILE:HD12	1:D:162:ILE:N	2.14	0.61
1:E:224:LEU:O	1:E:230:ARG:HD2	2.01	0.61
1:G:227:PHE:HA	1:G:230:ARG:NH1	2.15	0.61
1:C:227:PHE:HA	1:C:230:ARG:NH1	2.14	0.61
1:F:224:LEU:O	1:F:230:ARG:HD2	2.00	0.61
1:J:204:LEU:HD23	1:J:208:ILE:HG13	1.83	0.61
1:I:226:SER:O	1:I:230:ARG:HD3	2.01	0.61
1:J:167:THR:HG22	1:J:168:HIS:N	2.13	0.61
1:C:78:PHE:HB3	1:C:81:VAL:CG2	2.30	0.61
1:E:305:LEU:HD12	1:E:305:LEU:C	2.26	0.61
1:A:112:ASN:OD1	1:A:113:ASP:N	2.34	0.61
1:C:204:LEU:HD23	1:C:208:ILE:HG13	1.82	0.61
1:I:148:TYR:OH	1:J:176:HIS:NE2	2.33	0.61
1:B:52:GLY:O	1:B:53:ASP:HB2	1.99	0.61
1:B:202:TYR:HB2	1:C:256:PRO:O	2.00	0.61
1:C:224:LEU:O	1:C:230:ARG:HD2	2.00	0.61
1:F:39:ILE:HD11	1:F:78:PHE:CZ	2.36	0.61
1:J:114:MET:HE2	1:J:124:GLN:HG2	1.83	0.61
1:B:251:ILE:HG13	1:C:249:SER:HB3	1.82	0.61
1:D:305:LEU:C	1:D:305:LEU:HD12	2.26	0.61
1:E:211:LEU:O	1:E:215:ILE:HG12	2.01	0.61
1:B:305:LEU:C	1:B:305:LEU:HD12	2.26	0.60
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.34	0.60
1:F:240:THR:HA	1:G:239:LEU:HD23	1.83	0.60
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.36	0.60
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.36	0.60
1:H:231:LEU:HD23	1:H:231:LEU:C	2.26	0.60
1:I:162:ILE:HD12	1:I:162:ILE:N	2.16	0.60
1:D:162:ILE:HD12	1:D:162:ILE:H	1.66	0.60
1:D:224:LEU:HB2	1:D:230:ARG:HG3	1.84	0.60
1:J:210:PRO:O	1:J:214:ILE:HG12	2.00	0.60
1:D:259:THR:O	1:D:263:GLN:HG3	2.02	0.60
1:A:305:LEU:C	1:A:305:LEU:HD12	2.27	0.60
1:F:169:ILE:HD12	1:F:190:ILE:HG12	1.84	0.60
1:F:255:LEU:HB3	1:F:256:PRO:HD2	1.83	0.60
1:G:72:TRP:CD1	1:G:72:TRP:O	2.55	0.60
1:H:72:TRP:O	1:H:72:TRP:CD1	2.55	0.60
1:A:210:PRO:O	1:A:214:ILE:HG12	2.01	0.60
1:B:72:TRP:HZ3	1:B:135:TYR:CZ	2.19	0.60
1:B:162:ILE:HD12	1:B:162:ILE:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:HH22	1:I:139:GLN:CD	2.09	0.60
1:D:127:VAL:C	1:D:128:LEU:HD12	2.26	0.60
1:F:91:ARG:HB2	1:G:133:PHE:CE2	2.35	0.60
1:F:239:LEU:HD23	1:J:240:THR:OG1	2.01	0.60
1:G:39:ILE:HD11	1:G:78:PHE:CZ	2.35	0.60
1:J:226:SER:HB3	1:J:229:GLU:HG3	1.83	0.60
1:A:211:LEU:O	1:A:215:ILE:HG12	2.01	0.60
1:I:211:LEU:O	1:I:215:ILE:HG12	2.01	0.60
1:J:51:PRO:HD2	1:J:56:LEU:HD23	1.83	0.60
1:D:72:TRP:HZ3	1:D:135:TYR:CZ	2.20	0.60
1:D:112:ASN:OD1	1:D:113:ASP:N	2.35	0.60
1:F:226:SER:O	1:F:230:ARG:HD3	2.02	0.60
1:G:199:ASN:HD22	1:G:199:ASN:C	2.10	0.60
1:B:65:ARG:HD2	1:C:68:ASN:ND2	2.16	0.60
1:D:72:TRP:CH2	1:D:74:PRO:HG3	2.37	0.60
1:A:269:TYR:CD2	1:E:210:PRO:HB3	2.36	0.59
1:F:251:ILE:HG13	1:G:249:SER:HB3	1.81	0.59
1:G:91:ARG:HD2	1:H:134:SER:CB	2.31	0.59
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.37	0.59
1:I:78:PHE:HB3	1:I:81:VAL:CG2	2.33	0.59
1:I:114:MET:HE2	1:I:124:GLN:HG2	1.83	0.59
1:J:127:VAL:O	1:J:128:LEU:HD12	2.02	0.59
1:A:148:TYR:HE2	1:B:176:HIS:HE2	1.49	0.59
1:D:255:LEU:HB3	1:D:256:PRO:HD2	1.84	0.59
1:G:211:LEU:O	1:G:215:ILE:HG12	2.02	0.59
1:A:280:ILE:HG22	1:E:223:TRP:CE3	2.37	0.59
1:A:240:THR:OG1	1:B:239:LEU:HD23	2.03	0.59
1:C:240:THR:HA	1:D:239:LEU:HD23	1.83	0.59
1:D:185:ASN:N	1:D:185:ASN:HD22	2.00	0.59
1:F:72:TRP:HZ3	1:F:135:TYR:CZ	2.20	0.59
1:F:259:THR:O	1:F:263:GLN:HG3	2.03	0.59
1:I:290:VAL:O	1:I:290:VAL:HG12	2.02	0.59
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.37	0.59
1:B:112:ASN:OD1	1:B:113:ASP:N	2.36	0.59
1:G:231:LEU:HD23	1:G:231:LEU:C	2.27	0.59
1:F:219:TRP:C	1:F:221:VAL:H	2.11	0.59
1:I:123:ARG:HD2	1:I:197:VAL:HG22	1.85	0.59
1:I:224:LEU:HB2	1:I:230:ARG:HG3	1.84	0.59
1:C:51:PRO:HD2	1:C:56:LEU:HD23	1.85	0.59
1:F:134:SER:CB	1:J:91:ARG:HD2	2.32	0.59
1:H:145:ILE:HD12	1:H:145:ILE:N	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:ILE:HD13	1:G:238:MET:HE3	1.85	0.59
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.84	0.58
1:A:235:PHE:HD2	1:E:237:LEU:HD13	1.65	0.58
1:G:210:PRO:HB3	1:H:269:TYR:CD2	2.37	0.58
1:I:185:ASN:N	1:I:185:ASN:HD22	2.00	0.58
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.38	0.58
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.38	0.58
1:A:285:ARG:HA	1:A:285:ARG:NE	2.18	0.58
1:A:290:VAL:O	1:A:290:VAL:HG12	2.04	0.58
1:B:107:LEU:HD23	1:C:83:GLY:HA2	1.85	0.58
1:F:227:PHE:HA	1:F:230:ARG:NH1	2.19	0.58
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.38	0.58
1:A:127:VAL:O	1:A:128:LEU:HD12	2.04	0.58
1:B:78:PHE:HB3	1:B:81:VAL:HG23	1.86	0.58
1:C:72:TRP:O	1:C:72:TRP:CD1	2.55	0.58
1:C:305:LEU:C	1:C:305:LEU:HD12	2.29	0.58
1:E:162:ILE:HD12	1:E:162:ILE:H	1.67	0.58
1:G:285:ARG:NE	1:G:285:ARG:HA	2.17	0.58
1:H:162:ILE:N	1:H:162:ILE:HD12	2.18	0.58
1:I:72:TRP:O	1:I:72:TRP:CD1	2.57	0.58
1:I:227:PHE:HA	1:I:230:ARG:NH1	2.17	0.58
1:J:52:GLY:O	1:J:53:ASP:HB2	2.02	0.58
1:E:185:ASN:HD22	1:E:185:ASN:N	1.99	0.58
1:H:305:LEU:C	1:H:305:LEU:HD12	2.28	0.58
1:D:91:ARG:CD	1:E:134:SER:HB3	2.34	0.58
1:F:224:LEU:HB2	1:F:230:ARG:HG3	1.86	0.58
1:I:285:ARG:HA	1:I:285:ARG:NE	2.19	0.58
1:J:224:LEU:HB2	1:J:230:ARG:HG3	1.86	0.58
1:A:231:LEU:HD22	1:E:224:LEU:HD21	1.86	0.58
1:F:112:ASN:OD1	1:F:113:ASP:N	2.37	0.58
1:H:174:TYR:O	1:H:177:LEU:HD11	2.04	0.58
1:C:162:ILE:HD12	1:C:162:ILE:H	1.68	0.58
1:C:219:TRP:C	1:C:221:VAL:H	2.12	0.58
1:H:148:TYR:OH	1:I:176:HIS:NE2	2.36	0.58
1:I:204:LEU:HD23	1:I:208:ILE:HG13	1.86	0.58
1:A:140:LEU:HD22	1:A:190:ILE:HD11	1.86	0.58
1:A:299:CYS:HB2	1:A:302:ALA:CB	2.34	0.58
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.85	0.58
1:C:127:VAL:C	1:C:128:LEU:HD12	2.28	0.58
1:C:251:ILE:HG13	1:D:249:SER:HB3	1.84	0.58
1:E:219:TRP:C	1:E:221:VAL:H	2.11	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:VAL:O	1:E:290:VAL:HG12	2.04	0.58
1:J:288:ASN:CG	1:J:289:GLY:N	2.54	0.58
1:C:285:ARG:NE	1:C:285:ARG:HA	2.18	0.57
1:G:305:LEU:C	1:G:305:LEU:HD12	2.29	0.57
1:H:290:VAL:O	1:H:290:VAL:HG12	2.04	0.57
1:I:72:TRP:CD1	1:I:72:TRP:C	2.82	0.57
1:F:64:GLU:HG3	1:J:61:THR:HG21	1.84	0.57
1:G:299:CYS:HB2	1:G:302:ALA:CB	2.34	0.57
1:I:305:LEU:C	1:I:305:LEU:HD12	2.30	0.57
1:A:224:LEU:O	1:A:230:ARG:HD2	2.05	0.57
1:E:164:LYS:HZ2	1:E:164:LYS:HA	1.69	0.57
1:C:185:ASN:HD22	1:C:185:ASN:N	2.03	0.57
1:D:290:VAL:O	1:D:290:VAL:HG12	2.04	0.57
1:E:127:VAL:O	1:E:128:LEU:HD12	2.04	0.57
1:F:51:PRO:HD2	1:F:56:LEU:HD23	1.85	0.57
1:G:290:VAL:O	1:G:290:VAL:HG12	2.04	0.57
1:H:164:LYS:HZ2	1:H:164:LYS:HA	1.70	0.57
1:H:199:ASN:C	1:H:199:ASN:HD22	2.11	0.57
1:B:169:ILE:HD12	1:B:190:ILE:HG12	1.86	0.57
1:F:204:LEU:HD23	1:F:208:ILE:HG13	1.87	0.57
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.69	0.57
1:C:224:LEU:HB2	1:C:230:ARG:HG3	1.87	0.57
1:H:91:ARG:CD	1:I:134:SER:HB3	2.35	0.57
1:B:173:ARG:NH2	1:I:139:GLN:NE2	2.43	0.57
1:C:112:ASN:OD1	1:C:113:ASP:N	2.37	0.57
1:D:199:ASN:HD22	1:D:199:ASN:C	2.12	0.57
1:J:145:ILE:HD12	1:J:145:ILE:N	2.13	0.57
1:A:202:TYR:HB2	1:B:256:PRO:C	2.30	0.57
1:B:240:THR:HA	1:C:239:LEU:HD23	1.85	0.57
1:D:240:THR:HA	1:E:239:LEU:HD23	1.86	0.57
1:F:290:VAL:O	1:F:290:VAL:HG12	2.04	0.57
1:H:251:ILE:HG13	1:I:249:SER:HB3	1.87	0.57
1:C:91:ARG:HD2	1:D:134:SER:CB	2.35	0.57
1:C:223:TRP:CE2	1:C:300:ARG:HD3	2.40	0.57
1:H:227:PHE:HA	1:H:230:ARG:NH1	2.18	0.57
1:A:59:GLU:O	1:A:63:ILE:HG13	2.05	0.57
1:B:23:ILE:HG21	1:B:126:PHE:CD2	2.41	0.56
1:C:255:LEU:HB3	1:C:256:PRO:HD2	1.87	0.56
1:C:290:VAL:HG12	1:C:290:VAL:O	2.04	0.56
1:F:72:TRP:O	1:F:72:TRP:CD1	2.58	0.56
1:J:255:LEU:HB3	1:J:256:PRO:HD2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:290:VAL:O	1:J:290:VAL:HG12	2.04	0.56
1:A:56:LEU:HD13	1:A:57:ILE:N	2.20	0.56
1:A:65:ARG:HD2	1:B:68:ASN:ND2	2.20	0.56
1:B:167:THR:O	1:B:168:HIS:CB	2.51	0.56
1:D:167:THR:HG22	1:D:168:HIS:N	2.19	0.56
1:D:219:TRP:C	1:D:221:VAL:H	2.13	0.56
1:G:167:THR:HG22	1:G:168:HIS:N	2.17	0.56
1:G:259:THR:O	1:G:263:GLN:HG3	2.05	0.56
1:I:59:GLU:O	1:I:63:ILE:HG13	2.05	0.56
1:J:219:TRP:C	1:J:221:VAL:H	2.14	0.56
1:B:115:ASP:H	1:B:124:GLN:HE22	1.53	0.56
1:B:290:VAL:O	1:B:290:VAL:HG12	2.04	0.56
1:E:112:ASN:OD1	1:E:113:ASP:N	2.38	0.56
1:G:112:ASN:OD1	1:G:113:ASP:N	2.38	0.56
1:G:224:LEU:HB2	1:G:230:ARG:HG3	1.85	0.56
1:B:211:LEU:O	1:B:215:ILE:HG12	2.05	0.56
1:B:223:TRP:CE3	1:C:280:ILE:CG2	2.88	0.56
1:C:288:ASN:CG	1:C:289:GLY:N	2.54	0.56
1:D:288:ASN:CG	1:D:289:GLY:N	2.55	0.56
1:G:185:ASN:HD22	1:G:185:ASN:N	2.02	0.56
1:J:305:LEU:C	1:J:305:LEU:HD12	2.31	0.56
1:F:285:ARG:NE	1:F:285:ARG:HA	2.21	0.56
1:H:252:LEU:HG	1:H:253:PRO:HD2	1.87	0.56
1:E:224:LEU:HB2	1:E:230:ARG:HG3	1.88	0.56
1:E:262:ASP:O	1:E:266:ILE:HG12	2.06	0.56
1:F:299:CYS:HB2	1:F:302:ALA:CB	2.36	0.56
1:H:145:ILE:HG21	1:H:192:VAL:HG11	1.88	0.56
1:I:127:VAL:O	1:I:128:LEU:HD12	2.05	0.56
1:A:167:THR:O	1:A:168:HIS:HB2	2.05	0.56
1:A:262:ASP:O	1:A:266:ILE:HG12	2.06	0.56
1:G:294:LEU:CA	1:G:297:GLN:HE21	2.18	0.56
1:I:174:TYR:O	1:I:177:LEU:HD11	2.06	0.56
1:J:112:ASN:OD1	1:J:113:ASP:N	2.39	0.56
1:J:285:ARG:NE	1:J:285:ARG:HA	2.20	0.56
1:D:204:LEU:HD23	1:D:208:ILE:HG13	1.86	0.56
1:G:237:LEU:HD13	1:H:235:PHE:HD2	1.68	0.56
1:I:148:TYR:CZ	1:J:176:HIS:NE2	2.73	0.56
1:J:223:TRP:CE2	1:J:300:ARG:HD3	2.41	0.56
1:B:226:SER:HB3	1:B:229:GLU:CG	2.36	0.55
1:C:259:THR:O	1:C:263:GLN:HG3	2.06	0.55
1:E:285:ARG:NE	1:E:285:ARG:HA	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:C	1:B:231:LEU:HD23	2.31	0.55
1:H:219:TRP:C	1:H:221:VAL:H	2.14	0.55
1:I:209:LEU:HB3	1:I:210:PRO:HD3	1.85	0.55
1:D:285:ARG:HA	1:D:285:ARG:NE	2.21	0.55
1:H:56:LEU:HD13	1:H:57:ILE:N	2.21	0.55
1:H:202:TYR:HB2	1:I:256:PRO:O	2.05	0.55
1:H:255:LEU:HB3	1:H:256:PRO:HD2	1.88	0.55
1:J:231:LEU:HD23	1:J:232:GLN:N	2.21	0.55
1:F:303:PHE:N	1:F:304:PRO:CD	2.70	0.55
1:I:162:ILE:HD12	1:I:162:ILE:H	1.69	0.55
1:B:219:TRP:C	1:B:221:VAL:H	2.14	0.55
1:F:200:PRO:O	1:F:201:SER:C	2.50	0.55
1:G:78:PHE:HB3	1:G:81:VAL:CG2	2.36	0.55
1:B:259:THR:O	1:B:263:GLN:HG3	2.07	0.55
1:I:299:CYS:HB2	1:I:302:ALA:CB	2.37	0.55
1:A:185:ASN:N	1:A:185:ASN:HD22	2.05	0.55
1:D:51:PRO:HD2	1:D:56:LEU:HD23	1.89	0.55
1:D:57:ILE:HD13	1:E:134:SER:O	2.06	0.55
1:H:59:GLU:O	1:H:63:ILE:HG13	2.07	0.55
1:H:210:PRO:O	1:H:214:ILE:HG12	2.06	0.55
1:H:224:LEU:HB2	1:H:230:ARG:HG3	1.89	0.55
1:A:219:TRP:C	1:A:221:VAL:H	2.15	0.55
1:B:78:PHE:HB3	1:B:81:VAL:CG2	2.37	0.55
1:D:214:ILE:HD13	1:E:238:MET:HE3	1.87	0.55
1:F:185:ASN:HD22	1:F:185:ASN:N	2.04	0.55
1:H:223:TRP:CE2	1:H:300:ARG:HD3	2.42	0.55
1:J:127:VAL:C	1:J:128:LEU:HD12	2.31	0.55
1:J:224:LEU:O	1:J:230:ARG:HD2	2.07	0.55
1:B:72:TRP:CD1	1:B:72:TRP:O	2.60	0.54
1:E:72:TRP:CD1	1:E:72:TRP:O	2.59	0.54
1:G:65:ARG:HD2	1:H:68:ASN:ND2	2.22	0.54
1:H:162:ILE:HG22	1:H:163:ARG:N	2.16	0.54
1:H:299:CYS:HB2	1:H:302:ALA:CB	2.37	0.54
1:I:210:PRO:O	1:I:214:ILE:HG12	2.06	0.54
1:I:280:ILE:O	1:I:280:ILE:HG22	2.07	0.54
1:D:299:CYS:HB2	1:D:302:ALA:CB	2.38	0.54
1:H:162:ILE:HD12	1:H:162:ILE:H	1.71	0.54
1:H:259:THR:O	1:H:263:GLN:HG3	2.08	0.54
1:I:259:THR:O	1:I:263:GLN:HG3	2.07	0.54
1:J:167:THR:O	1:J:168:HIS:HB2	2.08	0.54
1:J:280:ILE:HG22	1:J:280:ILE:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PRO:HD2	1:B:56:LEU:HD23	1.87	0.54
1:B:174:TYR:O	1:B:177:LEU:HD11	2.07	0.54
1:C:167:THR:HG22	1:C:168:HIS:N	2.19	0.54
1:F:231:LEU:HD23	1:F:232:GLN:N	2.21	0.54
1:F:262:ASP:O	1:F:266:ILE:HG12	2.07	0.54
1:G:23:ILE:HG21	1:G:126:PHE:CD2	2.43	0.54
1:G:147:VAL:CG2	1:G:165:ALA:HB2	2.37	0.54
1:A:199:ASN:C	1:A:199:ASN:HD22	2.14	0.54
1:A:239:LEU:HD13	1:B:239:LEU:HD21	1.89	0.54
1:E:56:LEU:HD13	1:E:57:ILE:N	2.21	0.54
1:E:210:PRO:O	1:E:214:ILE:HG12	2.08	0.54
1:G:72:TRP:CD1	1:G:72:TRP:C	2.83	0.54
1:A:72:TRP:CD1	1:A:72:TRP:C	2.85	0.54
1:E:299:CYS:HB2	1:E:302:ALA:CB	2.37	0.54
1:B:185:ASN:HD22	1:B:185:ASN:N	2.05	0.54
1:B:199:ASN:HD22	1:B:199:ASN:C	2.14	0.54
1:B:202:TYR:HB2	1:C:256:PRO:C	2.32	0.54
1:B:285:ARG:NE	1:B:285:ARG:HA	2.22	0.54
1:F:127:VAL:C	1:F:128:LEU:HD12	2.33	0.54
1:G:255:LEU:HB3	1:G:256:PRO:HD2	1.90	0.54
1:I:219:TRP:C	1:I:221:VAL:H	2.14	0.54
1:A:72:TRP:HZ3	1:A:135:TYR:CZ	2.25	0.54
1:E:127:VAL:C	1:E:128:LEU:HD12	2.33	0.54
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.89	0.54
1:H:285:ARG:NE	1:H:285:ARG:HA	2.23	0.54
1:I:226:SER:HB3	1:I:229:GLU:CG	2.38	0.54
1:I:155:GLU:HB3	1:I:161:TRP:CD1	2.43	0.54
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.89	0.54
1:B:145:ILE:HD12	1:B:145:ILE:N	2.16	0.54
1:E:145:ILE:HD12	1:E:145:ILE:N	2.19	0.54
1:G:48:ARG:HB2	1:G:48:ARG:CZ	2.38	0.54
1:H:296:ILE:HG23	1:H:297:GLN:N	2.23	0.54
1:A:72:TRP:CD1	1:A:72:TRP:O	2.61	0.53
1:J:72:TRP:CH2	1:J:74:PRO:HG3	2.42	0.53
1:B:240:THR:OG1	1:C:239:LEU:HD23	2.08	0.53
1:B:254:ARG:O	1:B:255:LEU:HD23	2.09	0.53
1:E:305:LEU:HD12	1:E:306:GLY:N	2.24	0.53
1:H:185:ASN:HD22	1:H:185:ASN:N	2.05	0.53
1:I:145:ILE:H	1:I:145:ILE:CD1	2.13	0.53
1:A:134:SER:CB	1:E:91:ARG:HD2	2.38	0.53
1:F:91:ARG:CD	1:G:134:SER:HB3	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:MET:HE2	1:H:124:GLN:HG2	1.89	0.53
1:H:148:TYR:OH	1:I:176:HIS:CE1	2.61	0.53
1:J:97:ASP:OD1	1:J:99:ARG:HG2	2.09	0.53
1:A:239:LEU:CD1	1:B:239:LEU:HD21	2.37	0.53
1:A:245:ALA:HB1	1:E:247:TYR:CE1	2.43	0.53
1:C:72:TRP:CH2	1:C:74:PRO:HG3	2.43	0.53
1:C:72:TRP:CD1	1:C:72:TRP:C	2.85	0.53
1:D:251:ILE:CD1	1:E:249:SER:HB3	2.39	0.53
1:J:174:TYR:O	1:J:177:LEU:HD11	2.08	0.53
1:J:185:ASN:HD22	1:J:185:ASN:N	2.06	0.53
1:A:174:TYR:O	1:A:177:LEU:HD11	2.09	0.53
1:B:81:VAL:HG11	1:B:85:PRO:HD3	1.91	0.53
1:D:231:LEU:HD23	1:D:232:GLN:N	2.24	0.53
1:B:210:PRO:O	1:B:214:ILE:HG12	2.09	0.53
1:C:239:LEU:HD13	1:D:239:LEU:HD21	1.89	0.53
1:F:305:LEU:HD12	1:F:306:GLY:N	2.24	0.53
1:J:299:CYS:HB2	1:J:302:ALA:CB	2.39	0.53
1:A:303:PHE:C	1:A:303:PHE:HD1	2.17	0.53
1:D:251:ILE:CG1	1:E:249:SER:HB3	2.38	0.53
1:A:169:ILE:HD12	1:A:190:ILE:HG12	1.90	0.53
1:B:303:PHE:N	1:B:304:PRO:CD	2.72	0.53
1:D:81:VAL:HG11	1:D:85:PRO:HD3	1.91	0.53
1:D:303:PHE:C	1:D:303:PHE:HD1	2.17	0.53
1:G:267:ALA:HB1	1:G:307:PHE:HZ	1.74	0.53
1:I:303:PHE:N	1:I:304:PRO:CD	2.72	0.53
1:A:127:VAL:C	1:A:128:LEU:HD12	2.34	0.53
1:C:199:ASN:C	1:C:199:ASN:HD22	2.16	0.53
1:F:59:GLU:O	1:F:63:ILE:HG13	2.09	0.53
1:F:118:LEU:N	1:F:118:LEU:HD23	2.23	0.53
1:F:280:ILE:O	1:F:280:ILE:HG22	2.09	0.53
1:G:210:PRO:O	1:G:214:ILE:HG12	2.09	0.53
1:H:200:PRO:O	1:H:201:SER:C	2.51	0.53
1:H:303:PHE:N	1:H:304:PRO:CD	2.73	0.53
1:I:164:LYS:HZ2	1:I:164:LYS:HA	1.74	0.53
1:A:294:LEU:CA	1:A:297:GLN:HE21	2.21	0.52
1:D:200:PRO:O	1:D:201:SER:C	2.52	0.52
1:E:200:PRO:O	1:E:201:SER:C	2.51	0.52
1:F:210:PRO:O	1:F:214:ILE:HG12	2.08	0.52
1:H:123:ARG:HD2	1:H:197:VAL:HG22	1.90	0.52
1:A:172:ILE:HD13	1:A:189:ARG:HB3	1.91	0.52
1:A:255:LEU:HB3	1:A:256:PRO:HD2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:VAL:HG22	1:C:193:ARG:HG2	1.92	0.52
1:E:51:PRO:HD2	1:E:56:LEU:HD23	1.90	0.52
1:E:181:GLN:H	1:E:182:PRO:CD	2.22	0.52
1:G:157:ILE:HD11	1:H:115:ASP:CG	2.34	0.52
1:D:162:ILE:HG22	1:D:163:ARG:N	2.21	0.52
1:G:303:PHE:C	1:G:303:PHE:CD1	2.88	0.52
1:I:127:VAL:C	1:I:128:LEU:HD12	2.34	0.52
1:J:127:VAL:HG22	1:J:193:ARG:HG2	1.92	0.52
1:J:303:PHE:HD1	1:J:303:PHE:C	2.16	0.52
1:A:280:ILE:HD13	1:E:220:SER:HB2	1.91	0.52
1:G:303:PHE:C	1:G:303:PHE:HD1	2.16	0.52
1:I:172:ILE:HD13	1:I:189:ARG:HB3	1.90	0.52
1:I:231:LEU:HD23	1:I:232:GLN:N	2.24	0.52
1:A:81:VAL:HG11	1:A:85:PRO:HD3	1.91	0.52
1:A:239:LEU:CD2	1:E:240:THR:HA	2.38	0.52
1:A:299:CYS:HB2	1:A:302:ALA:HB3	1.92	0.52
1:B:255:LEU:HB3	1:B:256:PRO:HD2	1.90	0.52
1:B:280:ILE:HG22	1:B:280:ILE:O	2.09	0.52
1:C:91:ARG:HB2	1:D:133:PHE:HE2	1.74	0.52
1:C:315:VAL:O	1:C:315:VAL:HG12	2.10	0.52
1:D:169:ILE:HD12	1:D:190:ILE:HG12	1.91	0.52
1:D:203:TYR:O	1:D:208:ILE:HG12	2.09	0.52
1:H:51:PRO:HD2	1:H:56:LEU:HD23	1.91	0.52
1:H:91:ARG:HD3	1:I:134:SER:HB3	1.90	0.52
1:H:276:ILE:O	1:H:280:ILE:HG13	2.09	0.52
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.44	0.52
1:I:164:LYS:HZ2	1:I:164:LYS:CA	2.22	0.52
1:J:303:PHE:C	1:J:303:PHE:CD1	2.88	0.52
1:A:162:ILE:HG22	1:A:163:ARG:N	2.21	0.52
1:B:72:TRP:CD1	1:B:72:TRP:C	2.86	0.52
1:E:62:GLN:HE22	1:E:65:ARG:HH11	1.58	0.52
1:F:72:TRP:CD1	1:F:72:TRP:C	2.88	0.52
1:C:231:LEU:HD23	1:C:232:GLN:N	2.25	0.52
1:D:294:LEU:CA	1:D:297:GLN:HE21	2.21	0.52
1:H:72:TRP:CD1	1:H:72:TRP:C	2.85	0.52
1:I:247:TYR:HE1	1:J:249:SER:HG	1.58	0.52
1:I:262:ASP:O	1:I:266:ILE:HG12	2.08	0.52
1:C:303:PHE:HD1	1:C:303:PHE:C	2.18	0.52
1:F:181:GLN:H	1:F:182:PRO:CD	2.22	0.52
1:I:167:THR:CG2	1:I:168:HIS:H	2.14	0.52
1:A:200:PRO:O	1:A:201:SER:C	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASP:O	1:D:296:ILE:HG22	2.10	0.52
1:E:72:TRP:CH2	1:E:74:PRO:HG3	2.44	0.52
1:G:220:SER:HB2	1:H:280:ILE:HD13	1.91	0.52
1:H:91:ARG:HD2	1:I:134:SER:HB2	1.91	0.52
1:D:91:ARG:HD2	1:E:134:SER:CB	2.40	0.52
1:E:23:ILE:HG21	1:E:126:PHE:CD2	2.45	0.52
1:G:119:PHE:O	1:G:120:PRO:C	2.53	0.52
1:H:119:PHE:O	1:H:120:PRO:C	2.52	0.52
1:J:181:GLN:H	1:J:182:PRO:CD	2.23	0.52
1:A:181:GLN:H	1:A:182:PRO:CD	2.23	0.51
1:A:305:LEU:HD12	1:A:306:GLY:N	2.25	0.51
1:B:164:LYS:HZ2	1:B:165:ALA:H	0.69	0.51
1:C:220:SER:HB2	1:D:280:ILE:CD1	2.39	0.51
1:D:303:PHE:N	1:D:304:PRO:CD	2.72	0.51
1:D:305:LEU:HD12	1:D:306:GLY:N	2.26	0.51
1:G:72:TRP:CH2	1:G:74:PRO:HG3	2.44	0.51
1:I:301:LEU:C	1:I:304:PRO:HD2	2.35	0.51
1:C:174:TYR:O	1:C:177:LEU:HD11	2.09	0.51
1:D:167:THR:O	1:D:168:HIS:HB2	2.11	0.51
1:F:57:ILE:HD13	1:G:134:SER:O	2.09	0.51
1:G:51:PRO:HD2	1:G:56:LEU:HD23	1.93	0.51
1:I:72:TRP:CZ3	1:I:135:TYR:CZ	2.98	0.51
1:A:231:LEU:HD23	1:A:232:GLN:N	2.25	0.51
1:D:223:TRP:CE2	1:D:300:ARG:HD3	2.45	0.51
1:B:203:TYR:O	1:B:208:ILE:HG12	2.10	0.51
1:I:112:ASN:OD1	1:I:113:ASP:N	2.43	0.51
1:A:252:LEU:HG	1:A:253:PRO:HD2	1.92	0.51
1:C:172:ILE:HD13	1:C:189:ARG:HB3	1.93	0.51
1:D:303:PHE:C	1:D:303:PHE:CD1	2.89	0.51
1:F:276:ILE:O	1:F:280:ILE:HG13	2.11	0.51
1:J:140:LEU:HD22	1:J:190:ILE:HD11	1.93	0.51
1:J:169:ILE:HD12	1:J:190:ILE:HG12	1.92	0.51
1:A:303:PHE:C	1:A:303:PHE:CD1	2.88	0.51
1:B:305:LEU:HD12	1:B:306:GLY:N	2.25	0.51
1:D:181:GLN:H	1:D:182:PRO:CD	2.23	0.51
1:F:56:LEU:HD13	1:F:57:ILE:N	2.26	0.51
1:G:303:PHE:N	1:G:304:PRO:CD	2.74	0.51
1:H:91:ARG:HD2	1:I:134:SER:CB	2.40	0.51
1:H:303:PHE:HD1	1:H:303:PHE:C	2.18	0.51
1:J:180:VAL:HG21	1:J:184:GLN:HB2	1.93	0.51
1:A:115:ASP:CG	1:E:157:ILE:HD11	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:CYS:HB2	1:B:302:ALA:CB	2.40	0.51
1:C:157:ILE:HD11	1:D:115:ASP:OD2	2.09	0.51
1:C:210:PRO:O	1:C:214:ILE:HG12	2.10	0.51
1:C:276:ILE:O	1:C:280:ILE:HG13	2.11	0.51
1:D:118:LEU:N	1:D:118:LEU:HD23	2.26	0.51
1:E:276:ILE:O	1:E:280:ILE:HG13	2.10	0.51
1:G:199:ASN:C	1:G:199:ASN:ND2	2.66	0.51
1:H:167:THR:O	1:H:168:HIS:HB2	2.10	0.51
1:H:223:TRP:CE3	1:I:280:ILE:HG22	2.45	0.51
1:I:267:ALA:HB1	1:I:307:PHE:HZ	1.75	0.51
1:J:81:VAL:HG11	1:J:85:PRO:HD3	1.93	0.51
1:J:119:PHE:CB	1:J:120:PRO:HD3	2.37	0.51
1:B:56:LEU:HD13	1:B:57:ILE:N	2.26	0.51
1:B:223:TRP:CE2	1:B:300:ARG:HD3	2.46	0.51
1:D:115:ASP:H	1:D:124:GLN:HE22	1.59	0.51
1:D:209:LEU:HB3	1:D:210:PRO:HD3	1.93	0.51
1:E:223:TRP:CE2	1:E:300:ARG:HD3	2.46	0.51
1:F:226:SER:HB3	1:F:229:GLU:CG	2.41	0.51
1:C:303:PHE:N	1:C:304:PRO:CD	2.73	0.51
1:E:72:TRP:CD1	1:E:72:TRP:C	2.88	0.51
1:E:72:TRP:CZ3	1:E:135:TYR:CZ	2.96	0.51
1:F:239:LEU:HD23	1:J:240:THR:CA	2.39	0.51
1:G:28:THR:HB	1:G:255:LEU:CD2	2.39	0.51
1:G:219:TRP:C	1:G:221:VAL:N	2.68	0.51
1:G:226:SER:HB3	1:G:229:GLU:CG	2.41	0.51
1:G:299:CYS:HB2	1:G:302:ALA:HB3	1.93	0.51
1:G:305:LEU:HD12	1:G:306:GLY:N	2.25	0.51
1:A:72:TRP:CZ2	1:A:74:PRO:CG	2.90	0.50
1:C:305:LEU:HD12	1:C:306:GLY:N	2.27	0.50
1:D:252:LEU:HG	1:D:253:PRO:HD2	1.93	0.50
1:D:315:VAL:O	1:D:315:VAL:HG12	2.11	0.50
1:E:294:LEU:CA	1:E:297:GLN:HE21	2.21	0.50
1:G:248:THR:HG23	1:G:252:LEU:HD22	1.92	0.50
1:G:315:VAL:O	1:G:315:VAL:HG12	2.12	0.50
1:H:181:GLN:H	1:H:182:PRO:CD	2.23	0.50
1:A:117:ARG:HG2	1:A:117:ARG:HH11	1.76	0.50
1:C:62:GLN:HE22	1:C:65:ARG:HH11	1.58	0.50
1:D:157:ILE:HD11	1:E:115:ASP:OD2	2.11	0.50
1:E:248:THR:HG23	1:E:252:LEU:HD22	1.93	0.50
1:H:237:LEU:HD13	1:I:235:PHE:CD2	2.45	0.50
1:B:209:LEU:HB3	1:B:210:PRO:HD3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLN:HA	1:B:266:ILE:HG12	1.93	0.50
1:C:167:THR:O	1:C:168:HIS:HB2	2.11	0.50
1:E:119:PHE:O	1:E:120:PRO:C	2.54	0.50
1:G:181:GLN:H	1:G:182:PRO:CD	2.25	0.50
1:H:301:LEU:C	1:H:304:PRO:HD2	2.36	0.50
1:I:81:VAL:HG11	1:I:85:PRO:HD3	1.93	0.50
1:J:172:ILE:HD13	1:J:189:ARG:HB3	1.93	0.50
1:A:224:LEU:HB2	1:A:230:ARG:HG3	1.92	0.50
1:B:181:GLN:H	1:B:182:PRO:CD	2.24	0.50
1:C:303:PHE:C	1:C:303:PHE:CD1	2.89	0.50
1:D:27:ASN:HB3	1:D:32:THR:HB	1.93	0.50
1:G:223:TRP:CE2	1:G:300:ARG:HD3	2.46	0.50
1:G:247:TYR:CE1	1:H:245:ALA:HB1	2.47	0.50
1:H:172:ILE:HD13	1:H:189:ARG:HB3	1.93	0.50
1:H:226:SER:HB3	1:H:229:GLU:CG	2.40	0.50
1:I:255:LEU:HB3	1:I:256:PRO:HD2	1.93	0.50
1:J:199:ASN:HD22	1:J:199:ASN:C	2.17	0.50
1:J:200:PRO:O	1:J:201:SER:C	2.54	0.50
1:A:164:LYS:HZ2	1:A:164:LYS:HA	1.76	0.50
1:C:293:ASP:O	1:C:296:ILE:HG22	2.11	0.50
1:E:199:ASN:C	1:E:199:ASN:HD22	2.17	0.50
1:E:303:PHE:HD1	1:E:303:PHE:C	2.19	0.50
1:F:199:ASN:C	1:F:199:ASN:HD22	2.19	0.50
1:H:199:ASN:C	1:H:199:ASN:ND2	2.68	0.50
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.46	0.50
1:I:209:LEU:HD23	1:I:209:LEU:C	2.36	0.50
1:I:293:ASP:O	1:I:296:ILE:HG22	2.11	0.50
1:A:51:PRO:HD2	1:A:56:LEU:HD23	1.92	0.50
1:C:248:THR:HG23	1:C:252:LEU:HD22	1.94	0.50
1:F:237:LEU:HD13	1:G:235:PHE:HD2	1.72	0.50
1:F:237:LEU:CD1	1:G:235:PHE:CE2	2.93	0.50
1:G:240:THR:OG1	1:H:239:LEU:HD23	2.12	0.50
1:H:293:ASP:O	1:H:296:ILE:HG22	2.12	0.50
1:J:23:ILE:HG21	1:J:126:PHE:CD2	2.47	0.50
1:J:315:VAL:O	1:J:315:VAL:HG12	2.12	0.50
1:A:145:ILE:HG21	1:A:192:VAL:HG11	1.92	0.50
1:B:119:PHE:O	1:B:120:PRO:C	2.54	0.50
1:D:220:SER:HB2	1:E:280:ILE:CD1	2.41	0.50
1:I:119:PHE:O	1:I:120:PRO:C	2.55	0.50
1:J:263:GLN:HA	1:J:266:ILE:HG12	1.94	0.50
1:B:59:GLU:O	1:B:63:ILE:HG13	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLN:H	1:C:182:PRO:CD	2.24	0.50
1:E:209:LEU:HB3	1:E:210:PRO:HD3	1.92	0.50
1:H:72:TRP:CH2	1:H:74:PRO:HG3	2.47	0.50
1:I:181:GLN:H	1:I:182:PRO:CD	2.25	0.50
1:A:303:PHE:N	1:A:304:PRO:CD	2.74	0.50
1:C:59:GLU:O	1:C:63:ILE:HG13	2.11	0.50
1:C:127:VAL:O	1:C:128:LEU:HD12	2.12	0.50
1:D:120:PRO:HD2	1:D:260:VAL:HG23	1.94	0.50
1:D:180:VAL:HG21	1:D:184:GLN:HB2	1.93	0.50
1:E:231:LEU:HD23	1:E:232:GLN:N	2.26	0.50
1:H:65:ARG:HD2	1:I:68:ASN:ND2	2.26	0.50
1:B:91:ARG:CD	1:C:134:SER:HB3	2.42	0.49
1:B:303:PHE:HD1	1:B:303:PHE:C	2.20	0.49
1:C:119:PHE:CB	1:C:120:PRO:HD3	2.40	0.49
1:C:220:SER:HB2	1:D:280:ILE:HD13	1.94	0.49
1:C:223:TRP:NE1	1:C:300:ARG:HD3	2.27	0.49
1:D:89:ASN:O	1:D:104:ALA:HA	2.12	0.49
1:D:239:LEU:HD13	1:E:239:LEU:HD21	1.94	0.49
1:H:303:PHE:C	1:H:303:PHE:CD1	2.89	0.49
1:H:315:VAL:O	1:H:315:VAL:HG12	2.12	0.49
1:I:200:PRO:O	1:I:201:SER:C	2.54	0.49
1:A:167:THR:O	1:A:168:HIS:CB	2.60	0.49
1:F:77:GLU:O	1:F:130:LEU:HD23	2.11	0.49
1:I:145:ILE:HG21	1:I:192:VAL:HG11	1.93	0.49
1:B:148:TYR:CZ	1:C:176:HIS:NE2	2.80	0.49
1:B:262:ASP:O	1:B:266:ILE:HG12	2.12	0.49
1:E:303:PHE:N	1:E:304:PRO:CD	2.75	0.49
1:G:114:MET:CE	1:G:124:GLN:HG2	2.42	0.49
1:H:72:TRP:CZ3	1:H:135:TYR:CZ	2.96	0.49
1:H:209:LEU:HB3	1:H:210:PRO:HD3	1.93	0.49
1:B:147:VAL:C	1:B:149:THR:H	2.21	0.49
1:C:209:LEU:HD23	1:C:209:LEU:C	2.37	0.49
1:F:301:LEU:C	1:F:304:PRO:HD2	2.38	0.49
1:I:303:PHE:CD1	1:I:303:PHE:C	2.91	0.49
1:A:280:ILE:CG2	1:E:223:TRP:CE3	2.96	0.49
1:B:303:PHE:C	1:B:303:PHE:CD1	2.91	0.49
1:F:81:VAL:HG11	1:F:85:PRO:HD3	1.94	0.49
1:F:263:GLN:HA	1:F:266:ILE:HG12	1.94	0.49
1:G:120:PRO:HD2	1:G:260:VAL:HG23	1.93	0.49
1:H:296:ILE:CG2	1:H:297:GLN:N	2.75	0.49
1:I:199:ASN:C	1:I:199:ASN:HD22	2.19	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TRP:CE2	1:A:300:ARG:HD3	2.48	0.49
1:A:315:VAL:O	1:A:315:VAL:HG12	2.13	0.49
1:B:172:ILE:HD13	1:B:189:ARG:HB3	1.94	0.49
1:C:27:ASN:HB3	1:C:32:THR:HB	1.95	0.49
1:E:226:SER:HB3	1:E:229:GLU:CG	2.42	0.49
1:E:280:ILE:HG22	1:E:280:ILE:O	2.13	0.49
1:F:157:ILE:HD11	1:G:115:ASP:CG	2.38	0.49
1:F:251:ILE:CG1	1:G:249:SER:HB3	2.41	0.49
1:F:303:PHE:C	1:F:303:PHE:HD1	2.20	0.49
1:G:15:SER:HG	1:G:142:PHE:HD1	1.60	0.49
1:G:203:TYR:O	1:G:208:ILE:HG12	2.12	0.49
1:H:169:ILE:HD12	1:H:190:ILE:HG12	1.93	0.49
1:I:303:PHE:C	1:I:303:PHE:HD1	2.20	0.49
1:J:62:GLN:HE22	1:J:65:ARG:HH11	1.60	0.49
1:J:203:TYR:O	1:J:208:ILE:HG12	2.12	0.49
1:A:167:THR:CG2	1:A:168:HIS:H	2.19	0.49
1:C:72:TRP:CZ3	1:C:135:TYR:CZ	2.99	0.49
1:C:226:SER:HB3	1:C:229:GLU:CG	2.43	0.49
1:D:172:ILE:HD13	1:D:189:ARG:HB3	1.95	0.49
1:H:305:LEU:HD12	1:H:306:GLY:N	2.27	0.49
1:D:143:SER:HB3	1:D:167:THR:HG21	1.93	0.49
1:E:167:THR:O	1:E:168:HIS:HB2	2.13	0.49
1:E:303:PHE:C	1:E:303:PHE:CD1	2.91	0.49
1:A:133:PHE:CE2	1:E:91:ARG:HB2	2.48	0.49
1:A:199:ASN:C	1:A:199:ASN:ND2	2.71	0.49
1:B:72:TRP:CZ3	1:B:135:TYR:CZ	3.01	0.49
1:C:81:VAL:HG11	1:C:85:PRO:HD3	1.93	0.49
1:G:180:VAL:HG21	1:G:184:GLN:HB2	1.94	0.49
1:B:140:LEU:HD22	1:B:190:ILE:HD11	1.95	0.49
1:B:180:VAL:HG21	1:B:184:GLN:HB2	1.94	0.49
1:C:267:ALA:HB1	1:C:307:PHE:HZ	1.78	0.49
1:D:226:SER:HB3	1:D:229:GLU:CG	2.42	0.49
1:D:296:ILE:HG23	1:D:297:GLN:N	2.27	0.49
1:G:231:LEU:HD23	1:G:232:GLN:N	2.28	0.49
1:G:247:TYR:HD1	1:H:246:ALA:HA	1.76	0.49
1:D:119:PHE:O	1:D:120:PRO:C	2.57	0.48
1:D:299:CYS:HB2	1:D:302:ALA:HB3	1.95	0.48
1:G:262:ASP:O	1:G:266:ILE:HG12	2.13	0.48
1:J:72:TRP:CD1	1:J:72:TRP:O	2.66	0.48
1:B:293:ASP:O	1:B:296:ILE:HG22	2.13	0.48
1:D:210:PRO:O	1:D:214:ILE:HG12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:TRP:CZ2	1:F:74:PRO:CG	2.92	0.48
1:F:178:SER:C	1:F:180:VAL:H	2.21	0.48
1:F:239:LEU:HD21	1:J:239:LEU:HD13	1.95	0.48
1:H:81:VAL:HG11	1:H:85:PRO:HD3	1.95	0.48
1:I:296:ILE:HG23	1:I:297:GLN:N	2.28	0.48
1:C:263:GLN:HA	1:C:266:ILE:HG12	1.94	0.48
1:E:59:GLU:O	1:E:63:ILE:HG13	2.13	0.48
1:F:174:TYR:O	1:F:177:LEU:HD11	2.12	0.48
1:G:56:LEU:HD13	1:G:57:ILE:N	2.28	0.48
1:G:72:TRP:CZ3	1:G:135:TYR:CZ	2.97	0.48
1:I:164:LYS:HZ2	1:I:164:LYS:C	2.19	0.48
1:J:223:TRP:NE1	1:J:300:ARG:HD3	2.28	0.48
1:A:180:VAL:HG21	1:A:184:GLN:HB2	1.95	0.48
1:A:222:PHE:CE2	1:A:299:CYS:SG	3.06	0.48
1:C:56:LEU:HD13	1:C:57:ILE:N	2.28	0.48
1:C:280:ILE:HG22	1:C:280:ILE:O	2.13	0.48
1:E:167:THR:CG2	1:E:168:HIS:H	2.18	0.48
1:G:119:PHE:CB	1:G:120:PRO:HD3	2.38	0.48
1:J:145:ILE:HG21	1:J:192:VAL:HG11	1.95	0.48
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.48	0.48
1:A:66:TRP:HB3	1:A:71:LEU:HD12	1.95	0.48
1:E:97:ASP:OD1	1:E:99:ARG:HG2	2.13	0.48
1:E:255:LEU:HB3	1:E:256:PRO:HD2	1.94	0.48
1:F:117:ARG:HG2	1:F:117:ARG:HH11	1.79	0.48
1:F:252:LEU:HG	1:F:253:PRO:HD2	1.95	0.48
1:G:181:GLN:CG	1:G:182:PRO:HD3	2.38	0.48
1:J:72:TRP:CZ3	1:J:135:TYR:CZ	2.99	0.48
1:C:117:ARG:HG2	1:C:117:ARG:HH11	1.79	0.48
1:C:299:CYS:HB2	1:C:302:ALA:CB	2.42	0.48
1:E:162:ILE:HG22	1:E:163:ARG:N	2.22	0.48
1:E:293:ASP:O	1:E:296:ILE:HG22	2.13	0.48
1:G:204:LEU:HA	1:G:208:ILE:CG1	2.44	0.48
1:I:145:ILE:HD12	1:I:145:ILE:N	2.13	0.48
1:I:203:TYR:O	1:I:208:ILE:HG12	2.14	0.48
1:I:315:VAL:HG12	1:I:315:VAL:O	2.14	0.48
1:J:222:PHE:CE2	1:J:299:CYS:SG	3.06	0.48
1:J:288:ASN:OD1	1:J:291:GLU:HB3	2.14	0.48
1:J:303:PHE:N	1:J:304:PRO:CD	2.77	0.48
1:A:178:SER:C	1:A:180:VAL:H	2.22	0.48
1:F:62:GLN:HE22	1:F:65:ARG:HH11	1.61	0.48
1:F:267:ALA:HB1	1:F:307:PHE:HZ	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:VAL:C	1:I:149:THR:H	2.20	0.48
1:I:173:ARG:HA	1:I:185:ASN:O	2.13	0.48
1:I:223:TRP:CE2	1:I:300:ARG:HD3	2.49	0.48
1:I:299:CYS:HB2	1:I:302:ALA:HB3	1.95	0.48
1:J:294:LEU:CA	1:J:297:GLN:HE21	2.22	0.48
1:B:147:VAL:CG2	1:B:165:ALA:HB2	2.44	0.48
1:C:65:ARG:HD2	1:D:68:ASN:ND2	2.29	0.48
1:D:199:ASN:C	1:D:199:ASN:ND2	2.70	0.48
1:F:223:TRP:CE2	1:F:300:ARG:HD3	2.49	0.48
1:I:178:SER:C	1:I:180:VAL:H	2.21	0.48
1:I:181:GLN:CG	1:I:182:PRO:HD3	2.38	0.48
1:A:226:SER:HB3	1:A:229:GLU:CG	2.42	0.48
1:A:247:TYR:HE1	1:B:249:SER:OG	1.96	0.48
1:A:286:GLN:HB2	1:A:288:ASN:OD1	2.13	0.48
1:D:147:VAL:C	1:D:149:THR:H	2.21	0.48
1:E:315:VAL:O	1:E:315:VAL:HG12	2.14	0.48
1:F:296:ILE:HG23	1:F:297:GLN:N	2.29	0.48
1:F:303:PHE:C	1:F:303:PHE:CD1	2.91	0.48
1:G:263:GLN:HA	1:G:266:ILE:HG12	1.96	0.48
1:G:293:ASP:O	1:G:296:ILE:HG22	2.14	0.48
1:H:299:CYS:HB2	1:H:302:ALA:HB3	1.96	0.48
1:J:72:TRP:CD1	1:J:72:TRP:C	2.91	0.48
1:J:209:LEU:HB3	1:J:210:PRO:HD3	1.93	0.48
1:B:303:PHE:O	1:B:307:PHE:HB2	2.14	0.48
1:C:91:ARG:HD3	1:D:134:SER:HB3	1.96	0.48
1:D:59:GLU:OE2	1:E:75:ALA:HB3	2.14	0.48
1:D:178:SER:C	1:D:180:VAL:H	2.22	0.48
1:D:262:ASP:O	1:D:266:ILE:HG12	2.13	0.48
1:E:81:VAL:HG11	1:E:85:PRO:HD3	1.94	0.48
1:E:114:MET:CE	1:E:124:GLN:HG2	2.42	0.48
1:E:172:ILE:HD13	1:E:189:ARG:HB3	1.96	0.48
1:F:172:ILE:HD13	1:F:189:ARG:HB3	1.95	0.48
1:F:286:GLN:HB2	1:F:288:ASN:OD1	2.14	0.48
1:G:301:LEU:C	1:G:304:PRO:HD2	2.39	0.48
1:I:119:PHE:CB	1:I:120:PRO:HD3	2.43	0.48
1:I:252:LEU:HG	1:I:253:PRO:HD2	1.95	0.48
1:J:286:GLN:HB2	1:J:288:ASN:OD1	2.14	0.48
1:B:199:ASN:C	1:B:199:ASN:ND2	2.71	0.47
1:E:72:TRP:HZ3	1:E:135:TYR:CE1	2.32	0.47
1:F:27:ASN:HB3	1:F:32:THR:HB	1.95	0.47
1:F:147:VAL:C	1:F:149:THR:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:SER:HB2	1:H:280:ILE:CD1	2.43	0.47
1:J:303:PHE:O	1:J:307:PHE:HB2	2.14	0.47
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.49	0.47
1:B:62:GLN:HE22	1:B:65:ARG:HH11	1.62	0.47
1:E:27:ASN:HB3	1:E:32:THR:HB	1.96	0.47
1:I:89:ASN:HB3	1:J:133:PHE:CE2	2.49	0.47
1:B:178:SER:C	1:B:180:VAL:H	2.23	0.47
1:C:200:PRO:O	1:C:201:SER:C	2.57	0.47
1:E:178:SER:C	1:E:180:VAL:H	2.21	0.47
1:E:252:LEU:HG	1:E:253:PRO:HD2	1.96	0.47
1:G:288:ASN:OD1	1:G:291:GLU:HB3	2.14	0.47
1:G:296:ILE:HG23	1:G:297:GLN:N	2.30	0.47
1:A:114:MET:CE	1:A:124:GLN:HG2	2.44	0.47
1:A:119:PHE:CB	1:A:120:PRO:HD3	2.42	0.47
1:A:147:VAL:C	1:A:149:THR:H	2.21	0.47
1:C:115:ASP:H	1:C:124:GLN:HE22	1.61	0.47
1:C:303:PHE:O	1:C:307:PHE:HB2	2.14	0.47
1:D:62:GLN:HE22	1:D:65:ARG:HH11	1.63	0.47
1:E:299:CYS:HB2	1:E:302:ALA:HB3	1.95	0.47
1:F:288:ASN:OD1	1:F:291:GLU:HB3	2.15	0.47
1:G:178:SER:C	1:G:180:VAL:H	2.21	0.47
1:B:147:VAL:O	1:B:147:VAL:HG12	2.14	0.47
1:E:145:ILE:HG21	1:E:192:VAL:HG11	1.96	0.47
1:F:89:ASN:O	1:F:104:ALA:HA	2.15	0.47
1:F:299:CYS:HB2	1:F:302:ALA:HB3	1.95	0.47
1:J:262:ASP:O	1:J:266:ILE:HG12	2.13	0.47
1:A:140:LEU:HD13	1:A:190:ILE:CG1	2.37	0.47
1:B:301:LEU:C	1:B:304:PRO:HD2	2.39	0.47
1:C:91:ARG:HB2	1:D:133:PHE:CE2	2.49	0.47
1:C:120:PRO:HD2	1:C:260:VAL:HG23	1.96	0.47
1:D:72:TRP:CZ2	1:D:74:PRO:CG	2.90	0.47
1:E:267:ALA:HB1	1:E:307:PHE:HZ	1.80	0.47
1:E:303:PHE:O	1:E:307:PHE:HB2	2.14	0.47
1:A:293:ASP:O	1:A:296:ILE:HG22	2.14	0.47
1:A:301:LEU:C	1:A:304:PRO:HD2	2.39	0.47
1:B:200:PRO:O	1:B:201:SER:C	2.58	0.47
1:C:203:TYR:O	1:C:208:ILE:HG12	2.14	0.47
1:C:209:LEU:HB3	1:C:210:PRO:HD3	1.97	0.47
1:C:296:ILE:HG23	1:C:297:GLN:N	2.29	0.47
1:E:301:LEU:C	1:E:304:PRO:HD2	2.40	0.47
1:F:180:VAL:HG21	1:F:184:GLN:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:THR:HG21	1:H:64:GLU:HG3	1.95	0.47
1:G:81:VAL:HG11	1:G:85:PRO:HD3	1.96	0.47
1:G:117:ARG:HG2	1:G:117:ARG:HH11	1.80	0.47
1:G:276:ILE:O	1:G:280:ILE:HG13	2.14	0.47
1:J:187:PHE:CD1	1:J:187:PHE:N	2.83	0.47
1:B:288:ASN:OD1	1:B:291:GLU:HB3	2.15	0.47
1:C:301:LEU:C	1:C:304:PRO:HD2	2.40	0.47
1:F:58:VAL:HB	1:F:92:LEU:HB2	1.95	0.47
1:G:252:LEU:HG	1:G:253:PRO:HD2	1.96	0.47
1:I:294:LEU:CA	1:I:297:GLN:HE21	2.25	0.47
1:I:305:LEU:HD12	1:I:306:GLY:N	2.29	0.47
1:J:299:CYS:HB2	1:J:302:ALA:HB3	1.96	0.47
1:A:238:MET:HE3	1:E:214:ILE:HD13	1.97	0.47
1:A:303:PHE:O	1:A:307:PHE:HB2	2.14	0.47
1:D:120:PRO:HD2	1:D:260:VAL:CG2	2.44	0.47
1:D:303:PHE:O	1:D:307:PHE:HB2	2.14	0.47
1:E:172:ILE:N	1:E:172:ILE:HD12	2.30	0.47
1:F:127:VAL:O	1:F:128:LEU:HD12	2.15	0.47
1:F:172:ILE:HD12	1:F:172:ILE:N	2.30	0.47
1:J:252:LEU:HG	1:J:253:PRO:HD2	1.97	0.47
1:J:305:LEU:HD12	1:J:306:GLY:N	2.29	0.47
1:D:251:ILE:HD11	1:E:249:SER:HB3	1.97	0.47
1:E:259:THR:O	1:E:263:GLN:HG3	2.15	0.47
1:F:303:PHE:O	1:F:307:PHE:HB2	2.14	0.47
1:G:200:PRO:O	1:G:201:SER:C	2.58	0.47
1:G:240:THR:HA	1:H:239:LEU:CD2	2.43	0.47
1:G:285:ARG:C	1:G:285:ARG:HD3	2.40	0.47
1:H:288:ASN:OD1	1:H:291:GLU:HB3	2.15	0.47
1:A:107:LEU:HD23	1:B:83:GLY:HA2	1.97	0.46
1:B:147:VAL:O	1:B:149:THR:N	2.45	0.46
1:C:118:LEU:N	1:C:118:LEU:HD23	2.30	0.46
1:C:181:GLN:O	1:C:182:PRO:C	2.58	0.46
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.79	0.46
1:E:296:ILE:HG23	1:E:297:GLN:N	2.30	0.46
1:F:216:ALA:C	1:F:218:SER:N	2.73	0.46
1:F:315:VAL:HG12	1:F:315:VAL:O	2.14	0.46
1:H:148:TYR:CZ	1:I:176:HIS:NE2	2.82	0.46
1:H:178:SER:C	1:H:180:VAL:H	2.22	0.46
1:J:167:THR:CG2	1:J:168:HIS:H	2.22	0.46
1:J:257:TYR:CD1	1:J:257:TYR:N	2.83	0.46
1:B:248:THR:HG23	1:B:252:LEU:HD22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ALA:O	1:C:313:VAL:HG23	2.16	0.46
1:F:303:PHE:N	1:F:304:PRO:HD3	2.30	0.46
1:H:280:ILE:HG22	1:H:280:ILE:O	2.15	0.46
1:I:223:TRP:CE3	1:J:280:ILE:HG22	2.50	0.46
1:J:119:PHE:HB3	1:J:259:THR:HB	1.97	0.46
1:J:301:LEU:C	1:J:304:PRO:HD2	2.40	0.46
1:A:58:VAL:HB	1:A:92:LEU:HB2	1.97	0.46
1:A:97:ASP:OD1	1:A:99:ARG:HG2	2.15	0.46
1:C:178:SER:C	1:C:180:VAL:H	2.23	0.46
1:D:117:ARG:HG2	1:D:117:ARG:HH11	1.80	0.46
1:F:231:LEU:HD22	1:J:224:LEU:HD21	1.97	0.46
1:F:235:PHE:CD2	1:J:237:LEU:HD13	2.49	0.46
1:G:147:VAL:HG21	1:G:165:ALA:HB2	1.96	0.46
1:G:280:ILE:O	1:G:280:ILE:HG22	2.15	0.46
1:H:27:ASN:HB3	1:H:32:THR:HB	1.97	0.46
1:H:286:GLN:HB2	1:H:288:ASN:OD1	2.14	0.46
1:H:309:ALA:O	1:H:313:VAL:HG23	2.16	0.46
1:I:209:LEU:C	1:I:209:LEU:CD2	2.89	0.46
1:J:178:SER:C	1:J:180:VAL:H	2.22	0.46
1:J:293:ASP:O	1:J:296:ILE:HG22	2.15	0.46
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.41	0.46
1:C:204:LEU:HA	1:C:208:ILE:CG1	2.45	0.46
1:D:288:ASN:OD1	1:D:291:GLU:HB3	2.16	0.46
1:E:288:ASN:OD1	1:E:291:GLU:HB3	2.16	0.46
1:G:89:ASN:O	1:G:104:ALA:HA	2.15	0.46
1:H:97:ASP:OD1	1:H:99:ARG:HG2	2.14	0.46
1:H:115:ASP:H	1:H:124:GLN:HE22	1.62	0.46
1:I:286:GLN:HB2	1:I:288:ASN:OD1	2.15	0.46
1:A:296:ILE:HG23	1:A:297:GLN:N	2.30	0.46
1:B:91:ARG:HD2	1:C:134:SER:CB	2.46	0.46
1:B:247:TYR:HE1	1:C:249:SER:OG	1.98	0.46
1:F:209:LEU:HB3	1:F:210:PRO:HD3	1.98	0.46
1:F:250:ASN:HD22	1:J:250:ASN:ND2	2.13	0.46
1:G:97:ASP:OD1	1:G:99:ARG:HG2	2.16	0.46
1:J:120:PRO:HD2	1:J:260:VAL:HG23	1.98	0.46
1:A:27:ASN:HB3	1:A:32:THR:HB	1.96	0.46
1:C:147:VAL:C	1:C:149:THR:H	2.23	0.46
1:I:51:PRO:HD2	1:I:56:LEU:HD23	1.96	0.46
1:I:222:PHE:CE2	1:I:299:CYS:SG	3.08	0.46
1:J:172:ILE:N	1:J:172:ILE:HD12	2.30	0.46
1:B:309:ALA:O	1:B:313:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLN:CG	1:D:182:PRO:HD3	2.40	0.46
1:D:223:TRP:NE1	1:D:300:ARG:HD3	2.31	0.46
1:E:112:ASN:ND2	1:E:127:VAL:CG2	2.79	0.46
1:F:246:ALA:HA	1:J:247:TYR:HD1	1.80	0.46
1:F:293:ASP:O	1:F:296:ILE:HG22	2.16	0.46
1:G:219:TRP:O	1:G:221:VAL:N	2.49	0.46
1:H:231:LEU:HD23	1:H:232:GLN:N	2.30	0.46
1:H:262:ASP:O	1:H:266:ILE:HG12	2.16	0.46
1:I:56:LEU:HD13	1:I:57:ILE:N	2.30	0.46
1:I:185:ASN:N	1:I:185:ASN:ND2	2.63	0.46
1:I:288:ASN:OD1	1:I:291:GLU:HB3	2.16	0.46
1:J:167:THR:O	1:J:168:HIS:CB	2.64	0.46
1:B:92:LEU:HA	1:B:92:LEU:HD23	1.76	0.46
1:B:267:ALA:HB1	1:B:307:PHE:HZ	1.81	0.46
1:E:119:PHE:HB3	1:E:259:THR:HB	1.96	0.46
1:F:203:TYR:O	1:F:208:ILE:HG12	2.16	0.46
1:I:27:ASN:HB3	1:I:32:THR:HB	1.96	0.46
1:I:147:VAL:O	1:I:147:VAL:HG12	2.16	0.46
1:A:119:PHE:O	1:A:120:PRO:C	2.57	0.46
1:A:120:PRO:HD2	1:A:260:VAL:HG23	1.98	0.46
1:A:209:LEU:HB3	1:A:210:PRO:HD3	1.97	0.46
1:A:239:LEU:HD21	1:E:239:LEU:HD13	1.98	0.46
1:B:72:TRP:CH2	1:B:74:PRO:HG3	2.51	0.46
1:B:226:SER:HB3	1:B:229:GLU:CD	2.41	0.46
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.51	0.46
1:H:247:TYR:HE1	1:I:249:SER:HG	1.62	0.46
1:I:169:ILE:CD1	1:I:190:ILE:HG12	2.46	0.46
1:A:239:LEU:HD23	1:E:240:THR:CA	2.43	0.46
1:A:276:ILE:O	1:A:280:ILE:HG13	2.15	0.46
1:C:172:ILE:HD12	1:C:172:ILE:N	2.31	0.46
1:E:120:PRO:HD2	1:E:260:VAL:HG23	1.98	0.46
1:F:134:SER:HB3	1:J:91:ARG:HD3	1.98	0.46
1:F:167:THR:O	1:F:168:HIS:HB2	2.16	0.46
1:G:112:ASN:ND2	1:G:127:VAL:CG2	2.79	0.46
1:H:223:TRP:NE1	1:H:300:ARG:HD3	2.31	0.46
1:J:56:LEU:HD13	1:J:57:ILE:N	2.31	0.46
1:J:58:VAL:HB	1:J:92:LEU:HB2	1.98	0.46
1:D:174:TYR:O	1:D:177:LEU:HD11	2.15	0.45
1:E:185:ASN:N	1:E:185:ASN:ND2	2.64	0.45
1:F:219:TRP:O	1:F:221:VAL:N	2.49	0.45
1:F:249:SER:HG	1:J:247:TYR:HE1	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:ILE:CD1	1:G:190:ILE:HG12	2.46	0.45
1:G:174:TYR:O	1:G:177:LEU:HD11	2.15	0.45
1:H:167:THR:O	1:H:168:HIS:CB	2.64	0.45
1:H:173:ARG:HA	1:H:185:ASN:O	2.16	0.45
1:H:240:THR:OG1	1:I:239:LEU:HD23	2.15	0.45
1:H:303:PHE:O	1:H:307:PHE:HB2	2.16	0.45
1:J:89:ASN:O	1:J:104:ALA:HA	2.16	0.45
1:J:209:LEU:C	1:J:209:LEU:HD23	2.41	0.45
1:J:267:ALA:HB1	1:J:307:PHE:HZ	1.80	0.45
1:J:309:ALA:O	1:J:313:VAL:HG23	2.16	0.45
1:A:280:ILE:HG22	1:A:280:ILE:O	2.16	0.45
1:C:39:ILE:HD13	1:C:39:ILE:HG21	1.60	0.45
1:C:70:GLY:O	1:C:71:LEU:C	2.58	0.45
1:D:280:ILE:O	1:D:280:ILE:HG22	2.16	0.45
1:E:181:GLN:O	1:E:182:PRO:C	2.59	0.45
1:F:91:ARG:HD2	1:G:134:SER:CB	2.47	0.45
1:G:303:PHE:O	1:G:307:PHE:HB2	2.16	0.45
1:I:62:GLN:HE22	1:I:65:ARG:HH11	1.63	0.45
1:A:162:ILE:N	1:A:162:ILE:CD1	2.76	0.45
1:A:181:GLN:CG	1:A:182:PRO:HD3	2.39	0.45
1:B:70:GLY:O	1:B:71:LEU:C	2.59	0.45
1:C:77:GLU:O	1:C:130:LEU:HD23	2.16	0.45
1:C:145:ILE:HD12	1:C:145:ILE:N	2.15	0.45
1:D:72:TRP:CZ3	1:D:135:TYR:CZ	3.02	0.45
1:D:296:ILE:CG2	1:D:297:GLN:N	2.79	0.45
1:E:180:VAL:HG21	1:E:184:GLN:HB2	1.97	0.45
1:F:251:ILE:O	1:F:251:ILE:HG22	2.16	0.45
1:H:209:LEU:HD23	1:H:209:LEU:C	2.41	0.45
1:A:173:ARG:HA	1:A:185:ASN:O	2.16	0.45
1:A:286:GLN:HA	1:A:291:GLU:OE1	2.17	0.45
1:B:296:ILE:HG23	1:B:297:GLN:N	2.31	0.45
1:E:110:PHE:CD1	1:E:110:PHE:N	2.84	0.45
1:E:119:PHE:CB	1:E:120:PRO:HD3	2.43	0.45
1:F:119:PHE:O	1:F:120:PRO:C	2.58	0.45
1:H:127:VAL:HG22	1:H:193:ARG:HG2	1.96	0.45
1:H:267:ALA:HB1	1:H:307:PHE:HZ	1.80	0.45
1:J:226:SER:HB3	1:J:229:GLU:CG	2.47	0.45
1:B:247:TYR:HD1	1:C:246:ALA:HA	1.82	0.45
1:D:122:ASP:OD2	1:D:198:ARG:NE	2.36	0.45
1:D:286:GLN:HB2	1:D:288:ASN:OD1	2.16	0.45
1:F:15:SER:HG	1:F:142:PHE:HD1	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ILE:HD11	1:H:115:ASP:OD2	2.16	0.45
1:I:257:TYR:CD1	1:I:257:TYR:N	2.85	0.45
1:C:181:GLN:CG	1:C:182:PRO:HD3	2.40	0.45
1:C:199:ASN:C	1:C:199:ASN:ND2	2.73	0.45
1:D:181:GLN:O	1:D:182:PRO:C	2.59	0.45
1:E:231:LEU:HD12	1:E:280:ILE:HG12	1.98	0.45
1:E:237:LEU:HD12	1:E:237:LEU:HA	1.85	0.45
1:F:134:SER:HB2	1:J:91:ARG:HD2	1.99	0.45
1:F:249:SER:HB3	1:J:251:ILE:CG1	2.43	0.45
1:G:62:GLN:HE22	1:G:65:ARG:HH11	1.64	0.45
1:H:89:ASN:HB3	1:I:133:PHE:CD2	2.52	0.45
1:H:92:LEU:HA	1:H:92:LEU:HD23	1.75	0.45
1:H:127:VAL:O	1:H:128:LEU:HD12	2.16	0.45
1:J:147:VAL:C	1:J:149:THR:H	2.24	0.45
1:J:276:ILE:O	1:J:280:ILE:HG13	2.17	0.45
1:B:119:PHE:CB	1:B:120:PRO:HD3	2.38	0.45
1:B:204:LEU:HA	1:B:208:ILE:CG1	2.47	0.45
1:C:114:MET:CE	1:C:124:GLN:HG2	2.43	0.45
1:D:185:ASN:N	1:D:185:ASN:ND2	2.65	0.45
1:H:181:GLN:O	1:H:182:PRO:C	2.60	0.45
1:I:130:LEU:HD23	1:I:130:LEU:HA	1.71	0.45
1:I:296:ILE:CG2	1:I:297:GLN:N	2.79	0.45
1:A:267:ALA:HB1	1:A:307:PHE:HZ	1.82	0.45
1:B:286:GLN:HB2	1:B:288:ASN:OD1	2.16	0.45
1:C:180:VAL:HG21	1:C:184:GLN:HB2	1.99	0.45
1:C:219:TRP:C	1:C:221:VAL:N	2.75	0.45
1:C:288:ASN:OD1	1:C:291:GLU:HB3	2.16	0.45
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.52	0.45
1:D:301:LEU:C	1:D:304:PRO:HD2	2.42	0.45
1:F:181:GLN:N	1:F:182:PRO:CD	2.80	0.45
1:F:181:GLN:O	1:F:182:PRO:C	2.60	0.45
1:F:199:ASN:C	1:F:199:ASN:ND2	2.75	0.45
1:G:110:PHE:N	1:G:110:PHE:CD1	2.84	0.45
1:G:223:TRP:NE1	1:G:300:ARG:HD3	2.32	0.45
1:H:110:PHE:CD1	1:H:110:PHE:N	2.85	0.45
1:I:187:PHE:N	1:I:187:PHE:CD1	2.85	0.45
1:J:143:SER:HB3	1:J:167:THR:HG21	1.99	0.45
1:B:91:ARG:HD3	1:C:134:SER:HB3	1.99	0.45
1:B:117:ARG:HH11	1:B:117:ARG:HG2	1.81	0.45
1:B:127:VAL:HG22	1:B:193:ARG:HG2	1.99	0.45
1:C:209:LEU:C	1:C:209:LEU:CD2	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:CYS:HB2	1:C:302:ALA:HB3	1.99	0.45
1:E:286:GLN:HB2	1:E:288:ASN:OD1	2.17	0.45
1:F:110:PHE:N	1:F:110:PHE:CD1	2.84	0.45
1:G:140:LEU:HD13	1:G:190:ILE:CG1	2.43	0.45
1:I:263:GLN:HA	1:I:266:ILE:HG12	1.99	0.45
1:J:118:LEU:N	1:J:118:LEU:HD23	2.32	0.45
1:E:174:TYR:O	1:E:177:LEU:HD11	2.17	0.45
1:F:176:HIS:NE2	1:J:148:TYR:OH	2.50	0.45
1:G:167:THR:CG2	1:G:168:HIS:H	2.25	0.45
1:G:231:LEU:HD12	1:G:280:ILE:HG12	1.97	0.45
1:H:119:PHE:CB	1:H:120:PRO:HD3	2.41	0.45
1:I:112:ASN:ND2	1:I:127:VAL:CG2	2.79	0.45
1:B:181:GLN:O	1:B:182:PRO:C	2.60	0.44
1:C:119:PHE:O	1:C:120:PRO:C	2.58	0.44
1:C:285:ARG:HD3	1:C:285:ARG:C	2.42	0.44
1:E:115:ASP:H	1:E:124:GLN:HE22	1.65	0.44
1:E:199:ASN:C	1:E:199:ASN:ND2	2.75	0.44
1:E:263:GLN:HA	1:E:266:ILE:HG12	1.98	0.44
1:G:162:ILE:HG22	1:G:163:ARG:N	2.22	0.44
1:I:303:PHE:N	1:I:304:PRO:HD3	2.32	0.44
1:D:263:GLN:HA	1:D:266:ILE:HG12	2.00	0.44
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.52	0.44
1:G:119:PHE:HB3	1:G:259:THR:HB	1.99	0.44
1:H:117:ARG:HG2	1:H:117:ARG:HH11	1.81	0.44
1:I:118:LEU:O	1:I:119:PHE:C	2.60	0.44
1:I:140:LEU:HD13	1:I:190:ILE:CG1	2.43	0.44
1:A:78:PHE:O	1:A:79:ILE:C	2.59	0.44
1:A:209:LEU:HD23	1:A:209:LEU:C	2.42	0.44
1:A:248:THR:HG23	1:A:252:LEU:HD22	1.99	0.44
1:G:147:VAL:C	1:G:149:THR:H	2.25	0.44
1:G:172:ILE:N	1:G:172:ILE:HD12	2.32	0.44
1:H:62:GLN:HE22	1:H:65:ARG:HH11	1.64	0.44
1:H:66:TRP:HB3	1:H:71:LEU:HD12	1.98	0.44
1:H:72:TRP:HZ3	1:H:135:TYR:CE1	2.34	0.44
1:H:167:THR:CG2	1:H:168:HIS:H	2.19	0.44
1:H:180:VAL:HG21	1:H:184:GLN:HB2	1.99	0.44
1:I:303:PHE:O	1:I:307:PHE:HB2	2.17	0.44
1:J:296:ILE:HG23	1:J:297:GLN:N	2.31	0.44
1:A:134:SER:HB3	1:E:91:ARG:HD3	1.98	0.44
1:B:315:VAL:O	1:B:315:VAL:HG12	2.16	0.44
1:C:120:PRO:HD2	1:C:260:VAL:CG2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:PHE:N	1:D:110:PHE:CD1	2.85	0.44
1:F:114:MET:CE	1:F:124:GLN:HG2	2.45	0.44
1:F:187:PHE:N	1:F:187:PHE:CD1	2.85	0.44
1:F:296:ILE:CG2	1:F:297:GLN:N	2.80	0.44
1:I:145:ILE:CD1	1:I:145:ILE:N	2.77	0.44
1:I:147:VAL:O	1:I:149:THR:N	2.44	0.44
1:A:285:ARG:C	1:A:285:ARG:HD3	2.43	0.44
1:B:169:ILE:HG22	1:B:170:SER:N	2.32	0.44
1:B:204:LEU:HA	1:B:208:ILE:HG12	1.99	0.44
1:B:240:THR:HA	1:C:239:LEU:CD2	2.48	0.44
1:E:181:GLN:N	1:E:182:PRO:CD	2.81	0.44
1:G:172:ILE:HD13	1:G:189:ARG:HB3	1.99	0.44
1:G:286:GLN:HB2	1:G:288:ASN:OD1	2.17	0.44
1:I:110:PHE:CD1	1:I:110:PHE:N	2.86	0.44
1:J:140:LEU:HD13	1:J:190:ILE:CG1	2.41	0.44
1:B:145:ILE:N	1:B:145:ILE:CD1	2.79	0.44
1:B:181:GLN:CG	1:B:182:PRO:HD3	2.38	0.44
1:B:237:LEU:HD12	1:B:237:LEU:HA	1.87	0.44
1:C:286:GLN:HB2	1:C:288:ASN:OD1	2.17	0.44
1:D:172:ILE:HD12	1:D:172:ILE:N	2.32	0.44
1:D:309:ALA:O	1:D:313:VAL:HG23	2.18	0.44
1:E:216:ALA:C	1:E:218:SER:N	2.76	0.44
1:F:169:ILE:CD1	1:F:190:ILE:HG12	2.48	0.44
1:F:237:LEU:CD1	1:G:235:PHE:CD2	2.93	0.44
1:I:300:ARG:O	1:I:304:PRO:HG2	2.17	0.44
1:J:199:ASN:C	1:J:199:ASN:ND2	2.74	0.44
1:A:181:GLN:N	1:A:182:PRO:CD	2.81	0.44
1:B:187:PHE:CD1	1:B:187:PHE:N	2.85	0.44
1:C:169:ILE:HD12	1:C:190:ILE:HG12	2.00	0.44
1:C:252:LEU:HG	1:C:253:PRO:HD2	1.99	0.44
1:D:39:ILE:HD13	1:D:39:ILE:HG21	1.61	0.44
1:D:70:GLY:O	1:D:71:LEU:C	2.60	0.44
1:E:169:ILE:HD12	1:E:190:ILE:HG12	2.00	0.44
1:H:118:LEU:HD23	1:H:118:LEU:N	2.32	0.44
1:H:147:VAL:C	1:H:149:THR:H	2.24	0.44
1:H:248:THR:HG23	1:H:252:LEU:HD22	2.00	0.44
1:I:70:GLY:O	1:I:71:LEU:C	2.61	0.44
1:I:239:LEU:CD1	1:J:239:LEU:HD21	2.48	0.44
1:J:223:TRP:CD1	1:J:300:ARG:HD3	2.53	0.44
1:A:204:LEU:HA	1:A:208:ILE:CG1	2.48	0.44
1:B:128:LEU:HD12	1:B:128:LEU:N	2.29	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ILE:CG2	1:C:297:GLN:N	2.81	0.44
1:E:48:ARG:CZ	1:E:48:ARG:HB2	2.47	0.44
1:G:201:SER:O	1:G:202:TYR:C	2.61	0.44
1:H:240:THR:HA	1:I:239:LEU:HD23	2.00	0.44
1:B:181:GLN:N	1:B:182:PRO:CD	2.81	0.44
1:D:119:PHE:CB	1:D:120:PRO:HD3	2.46	0.44
1:D:216:ALA:C	1:D:218:SER:N	2.74	0.44
1:E:40:VAL:HA	1:E:102:TYR:O	2.17	0.44
1:E:118:LEU:O	1:E:119:PHE:C	2.61	0.44
1:E:147:VAL:C	1:E:149:THR:H	2.25	0.44
1:E:164:LYS:HZ2	1:E:164:LYS:CA	2.30	0.44
1:E:292:ASP:O	1:E:297:GLN:NE2	2.51	0.44
1:I:216:ALA:C	1:I:218:SER:N	2.74	0.44
1:I:285:ARG:C	1:I:285:ARG:HD3	2.43	0.44
1:J:92:LEU:HD23	1:J:92:LEU:HA	1.75	0.44
1:J:181:GLN:CG	1:J:182:PRO:HD3	2.40	0.44
1:J:248:THR:HG23	1:J:252:LEU:HD22	2.00	0.44
1:A:70:GLY:O	1:A:71:LEU:C	2.60	0.43
1:A:187:PHE:N	1:A:187:PHE:CD1	2.86	0.43
1:B:167:THR:CG2	1:B:168:HIS:H	2.20	0.43
1:B:169:ILE:CD1	1:B:190:ILE:HG12	2.48	0.43
1:D:147:VAL:O	1:D:149:THR:N	2.46	0.43
1:D:237:LEU:CD1	1:E:235:PHE:CE2	2.99	0.43
1:E:296:ILE:CG2	1:E:297:GLN:N	2.81	0.43
1:H:216:ALA:C	1:H:218:SER:N	2.76	0.43
1:I:118:LEU:N	1:I:118:LEU:HD23	2.33	0.43
1:I:167:THR:O	1:I:168:HIS:HB2	2.17	0.43
1:J:145:ILE:H	1:J:145:ILE:CD1	2.14	0.43
1:J:181:GLN:N	1:J:182:PRO:CD	2.81	0.43
1:D:216:ALA:C	1:D:218:SER:H	2.27	0.43
1:F:150:GLU:HB3	1:F:153:ASP:CB	2.47	0.43
1:G:127:VAL:HG22	1:G:193:ARG:HG2	1.98	0.43
1:G:185:ASN:N	1:G:185:ASN:ND2	2.67	0.43
1:I:164:LYS:NZ	1:I:164:LYS:HA	2.33	0.43
1:J:119:PHE:O	1:J:120:PRO:C	2.58	0.43
1:A:309:ALA:O	1:A:313:VAL:HG23	2.18	0.43
1:F:119:PHE:CB	1:F:120:PRO:HD3	2.41	0.43
1:F:237:LEU:HD12	1:F:237:LEU:HA	1.91	0.43
1:F:251:ILE:CD1	1:G:249:SER:HB3	2.48	0.43
1:G:223:TRP:CD1	1:G:300:ARG:HD3	2.53	0.43
1:I:181:GLN:O	1:I:182:PRO:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:N	1:A:110:PHE:CD1	2.86	0.43
1:B:303:PHE:N	1:B:304:PRO:HD3	2.33	0.43
1:D:219:TRP:C	1:D:221:VAL:N	2.77	0.43
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.84	0.43
1:G:285:ARG:NE	1:G:285:ARG:CA	2.82	0.43
1:B:173:ARG:HA	1:B:185:ASN:O	2.19	0.43
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.99	0.43
1:C:167:THR:O	1:C:168:HIS:CB	2.67	0.43
1:C:214:ILE:HD13	1:D:238:MET:HE3	1.99	0.43
1:F:219:TRP:C	1:F:221:VAL:N	2.74	0.43
1:G:140:LEU:HD22	1:G:190:ILE:HD11	2.00	0.43
1:G:181:GLN:O	1:G:182:PRO:C	2.61	0.43
1:H:223:TRP:CD1	1:H:300:ARG:HD3	2.54	0.43
1:J:149:THR:HG22	1:J:150:GLU:N	2.33	0.43
1:J:181:GLN:O	1:J:182:PRO:C	2.61	0.43
1:A:145:ILE:H	1:A:145:ILE:CD1	2.19	0.43
1:B:234:SER:HA	1:B:237:LEU:HB2	2.01	0.43
1:B:299:CYS:HB2	1:B:302:ALA:HB3	1.99	0.43
1:E:149:THR:HG22	1:E:150:GLU:N	2.34	0.43
1:E:209:LEU:HD23	1:E:209:LEU:C	2.43	0.43
1:G:118:LEU:O	1:G:119:PHE:C	2.62	0.43
1:G:209:LEU:C	1:G:209:LEU:HD23	2.43	0.43
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.54	0.43
1:C:218:SER:CA	1:C:237:LEU:HD21	2.42	0.43
1:C:223:TRP:CD1	1:C:300:ARG:HD3	2.53	0.43
1:D:276:ILE:O	1:D:280:ILE:HG13	2.18	0.43
1:F:59:GLU:OE2	1:G:134:SER:OG	2.37	0.43
1:G:296:ILE:CG2	1:G:297:GLN:N	2.81	0.43
1:H:40:VAL:HA	1:H:102:TYR:O	2.19	0.43
1:H:149:THR:HG22	1:H:150:GLU:N	2.33	0.43
1:I:72:TRP:CZ2	1:I:74:PRO:CG	2.98	0.43
1:I:180:VAL:HG21	1:I:184:GLN:HB2	2.00	0.43
1:A:204:LEU:HA	1:A:208:ILE:HG12	2.00	0.43
1:C:119:PHE:HB3	1:C:259:THR:HB	2.01	0.43
1:C:150:GLU:CB	1:C:153:ASP:HB2	2.47	0.43
1:C:181:GLN:N	1:C:182:PRO:CD	2.81	0.43
1:D:119:PHE:HB3	1:D:259:THR:HB	2.00	0.43
1:D:292:ASP:O	1:D:297:GLN:NE2	2.52	0.43
1:F:72:TRP:CZ3	1:F:135:TYR:CZ	3.05	0.43
1:G:115:ASP:H	1:G:124:GLN:HE22	1.66	0.43
1:H:181:GLN:N	1:H:182:PRO:CD	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:TYR:HB2	1:I:256:PRO:C	2.44	0.43
1:I:16:VAL:HG12	1:I:17:SER:N	2.34	0.43
1:I:199:ASN:C	1:I:199:ASN:ND2	2.77	0.43
1:J:216:ALA:C	1:J:218:SER:N	2.73	0.43
1:A:296:ILE:CG2	1:A:297:GLN:N	2.82	0.43
1:B:119:PHE:HB3	1:B:120:PRO:CD	2.42	0.43
1:C:79:ILE:HD13	1:C:79:ILE:HA	1.87	0.43
1:C:262:ASP:O	1:C:266:ILE:HG12	2.18	0.43
1:D:223:TRP:CD1	1:D:300:ARG:HD3	2.54	0.43
1:E:309:ALA:O	1:E:313:VAL:HG23	2.18	0.43
1:F:176:HIS:CE1	1:J:148:TYR:OH	2.72	0.43
1:F:294:LEU:CA	1:F:297:GLN:HE21	2.22	0.43
1:F:305:LEU:C	1:F:305:LEU:CD1	2.92	0.43
1:G:145:ILE:H	1:G:145:ILE:CD1	2.17	0.43
1:G:204:LEU:HA	1:G:208:ILE:HG12	1.99	0.43
1:H:303:PHE:N	1:H:304:PRO:HD3	2.34	0.43
1:I:58:VAL:HB	1:I:92:LEU:HB2	2.01	0.43
1:J:150:GLU:HB3	1:J:153:ASP:CB	2.46	0.43
1:J:164:LYS:HZ2	1:J:164:LYS:HA	1.84	0.43
1:A:120:PRO:HD2	1:A:260:VAL:CG2	2.49	0.43
1:B:48:ARG:CZ	1:B:48:ARG:HB2	2.49	0.43
1:F:216:ALA:C	1:F:218:SER:H	2.27	0.43
1:F:248:THR:HG23	1:F:252:LEU:HD22	2.00	0.43
1:J:39:ILE:HG21	1:J:39:ILE:HD13	1.62	0.43
1:A:40:VAL:HA	1:A:102:TYR:O	2.19	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.73	0.42
1:C:187:PHE:CD1	1:C:187:PHE:N	2.86	0.42
1:D:303:PHE:N	1:D:304:PRO:HD3	2.33	0.42
1:E:150:GLU:CB	1:E:153:ASP:HB2	2.46	0.42
1:F:239:LEU:HD13	1:G:239:LEU:HD21	2.00	0.42
1:G:145:ILE:HD12	1:G:145:ILE:N	2.21	0.42
1:G:157:ILE:HD12	1:H:115:ASP:HA	2.00	0.42
1:I:140:LEU:HD22	1:I:190:ILE:HD11	2.01	0.42
1:I:181:GLN:N	1:I:182:PRO:CD	2.82	0.42
1:J:40:VAL:HA	1:J:102:TYR:O	2.19	0.42
1:J:300:ARG:O	1:J:304:PRO:HG2	2.19	0.42
1:D:112:ASN:ND2	1:D:127:VAL:CG2	2.82	0.42
1:D:127:VAL:HG22	1:D:193:ARG:HG2	2.01	0.42
1:D:167:THR:O	1:D:168:HIS:CB	2.66	0.42
1:E:204:LEU:HA	1:E:208:ILE:CG1	2.49	0.42
1:F:127:VAL:HG22	1:F:193:ARG:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:LEU:HD22	1:F:190:ILE:HD11	2.01	0.42
1:F:162:ILE:N	1:F:162:ILE:CD1	2.80	0.42
1:F:309:ALA:O	1:F:313:VAL:HG23	2.19	0.42
1:H:48:ARG:CZ	1:H:48:ARG:HB2	2.48	0.42
1:H:119:PHE:HB3	1:H:259:THR:HB	2.01	0.42
1:H:164:LYS:HZ2	1:H:164:LYS:CA	2.31	0.42
1:I:46:LYS:HA	1:I:47:PRO:HD2	1.78	0.42
1:I:89:ASN:O	1:I:104:ALA:HA	2.19	0.42
1:I:143:SER:HB3	1:I:167:THR:HG21	2.01	0.42
1:J:216:ALA:C	1:J:218:SER:H	2.27	0.42
1:A:231:LEU:HD12	1:A:280:ILE:HG12	2.01	0.42
1:A:250:ASN:HD22	1:E:250:ASN:ND2	2.18	0.42
1:B:97:ASP:OD1	1:B:99:ARG:HG2	2.19	0.42
1:C:167:THR:CG2	1:C:168:HIS:H	2.26	0.42
1:F:68:ASN:HA	1:J:65:ARG:NH1	2.34	0.42
1:F:147:VAL:CG2	1:F:165:ALA:HB2	2.49	0.42
1:A:181:GLN:O	1:A:182:PRO:C	2.62	0.42
1:A:223:TRP:NE1	1:A:300:ARG:HD3	2.34	0.42
1:A:234:SER:HA	1:A:237:LEU:HB2	2.02	0.42
1:C:300:ARG:O	1:C:304:PRO:HG2	2.18	0.42
1:F:251:ILE:O	1:F:251:ILE:CG2	2.67	0.42
1:G:118:LEU:N	1:G:118:LEU:HD23	2.35	0.42
1:I:292:ASP:O	1:I:297:GLN:NE2	2.53	0.42
1:J:27:ASN:HB3	1:J:32:THR:HB	2.01	0.42
1:J:59:GLU:O	1:J:63:ILE:HG13	2.19	0.42
1:B:252:LEU:HG	1:B:253:PRO:HD2	2.01	0.42
1:C:251:ILE:O	1:C:251:ILE:CG2	2.68	0.42
1:E:120:PRO:HD2	1:E:260:VAL:CG2	2.50	0.42
1:F:83:GLY:HA2	1:J:107:LEU:HD23	2.02	0.42
1:G:309:ALA:O	1:G:313:VAL:HG23	2.19	0.42
1:I:23:ILE:HG21	1:I:126:PHE:CD2	2.55	0.42
1:A:48:ARG:HB2	1:A:48:ARG:CZ	2.49	0.42
1:A:136:ASN:ND2	1:A:184:GLN:HG3	2.34	0.42
1:B:78:PHE:O	1:B:79:ILE:C	2.62	0.42
1:B:162:ILE:HG22	1:B:163:ARG:N	2.26	0.42
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.76	0.42
1:C:185:ASN:N	1:C:185:ASN:ND2	2.67	0.42
1:D:65:ARG:HD2	1:E:68:ASN:ND2	2.33	0.42
1:D:181:GLN:N	1:D:182:PRO:CD	2.81	0.42
1:E:150:GLU:HB3	1:E:153:ASP:CB	2.46	0.42
1:F:281:PHE:CZ	1:F:285:ARG:HG2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:PHE:CB	1:G:120:PRO:CD	2.98	0.42
1:G:149:THR:HG22	1:G:150:GLU:N	2.35	0.42
1:B:27:ASN:HB3	1:B:32:THR:HB	2.00	0.42
1:B:89:ASN:O	1:B:104:ALA:HA	2.19	0.42
1:B:226:SER:HB3	1:B:229:GLU:OE1	2.19	0.42
1:B:296:ILE:CG2	1:B:297:GLN:N	2.82	0.42
1:C:303:PHE:N	1:C:304:PRO:HD3	2.34	0.42
1:D:130:LEU:HA	1:D:130:LEU:HD23	1.87	0.42
1:G:150:GLU:CB	1:G:153:ASP:HB2	2.46	0.42
1:G:187:PHE:CD1	1:G:187:PHE:N	2.88	0.42
1:H:140:LEU:HD22	1:H:190:ILE:HD11	2.01	0.42
1:I:48:ARG:HB2	1:I:48:ARG:CZ	2.50	0.42
1:I:162:ILE:HG22	1:I:163:ARG:N	2.26	0.42
1:I:216:ALA:C	1:I:218:SER:H	2.27	0.42
1:J:48:ARG:CZ	1:J:48:ARG:HB2	2.49	0.42
1:J:285:ARG:C	1:J:285:ARG:HD3	2.45	0.42
1:J:296:ILE:CG2	1:J:297:GLN:N	2.83	0.42
1:A:145:ILE:HD12	1:A:145:ILE:N	2.19	0.42
1:A:300:ARG:O	1:A:304:PRO:HG2	2.19	0.42
1:C:28:THR:HB	1:C:255:LEU:CD2	2.41	0.42
1:C:97:ASP:OD1	1:C:99:ARG:HG2	2.20	0.42
1:D:48:ARG:HB2	1:D:48:ARG:CZ	2.50	0.42
1:D:204:LEU:HA	1:D:208:ILE:CG1	2.49	0.42
1:D:237:LEU:HD13	1:E:235:PHE:HD2	1.74	0.42
1:E:305:LEU:C	1:E:305:LEU:CD1	2.93	0.42
1:F:18:ILE:HB	1:F:145:ILE:HG22	2.02	0.42
1:I:120:PRO:HD2	1:I:260:VAL:CG2	2.50	0.42
1:I:226:SER:HB3	1:I:229:GLU:CD	2.45	0.42
1:A:79:ILE:HD13	1:A:79:ILE:HA	1.83	0.42
1:A:223:TRP:CE3	1:B:280:ILE:HG22	2.55	0.42
1:C:224:LEU:HD21	1:D:231:LEU:HD22	2.00	0.42
1:E:281:PHE:O	1:E:282:ALA:C	2.61	0.42
1:G:72:TRP:HZ3	1:G:135:TYR:CE1	2.38	0.42
1:G:181:GLN:N	1:G:182:PRO:CD	2.82	0.42
1:G:237:LEU:CD1	1:H:235:PHE:CD2	3.00	0.42
1:H:218:SER:CA	1:H:237:LEU:HD21	2.43	0.42
1:I:120:PRO:HD2	1:I:260:VAL:HG23	2.01	0.42
1:I:201:SER:O	1:I:202:TYR:C	2.62	0.42
1:I:208:ILE:HG23	1:I:264:MET:SD	2.59	0.42
1:A:288:ASN:OD1	1:A:291:GLU:HB3	2.19	0.42
1:D:46:LYS:HA	1:D:47:PRO:HD2	1.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ALA:C	1:E:218:SER:H	2.28	0.42
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.85	0.42
1:G:234:SER:HA	1:G:237:LEU:HB2	2.01	0.42
1:B:164:LYS:CD	1:I:163:ARG:HD2	2.41	0.41
1:C:204:LEU:HA	1:C:208:ILE:HG12	2.02	0.41
1:D:78:PHE:O	1:D:79:ILE:C	2.63	0.41
1:D:149:THR:HG22	1:D:150:GLU:N	2.35	0.41
1:E:167:THR:O	1:E:168:HIS:CB	2.68	0.41
1:H:219:TRP:C	1:H:221:VAL:N	2.78	0.41
1:I:219:TRP:C	1:I:221:VAL:N	2.78	0.41
1:J:119:PHE:CB	1:J:120:PRO:CD	2.98	0.41
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.84	0.41
1:A:140:LEU:HD12	1:A:188:SER:O	2.21	0.41
1:A:216:ALA:C	1:A:218:SER:N	2.78	0.41
1:B:164:LYS:HG2	1:I:163:ARG:CB	2.21	0.41
1:C:216:ALA:C	1:C:218:SER:N	2.75	0.41
1:C:231:LEU:HD12	1:C:280:ILE:HG12	2.02	0.41
1:C:251:ILE:O	1:C:251:ILE:HG22	2.18	0.41
1:F:119:PHE:HB3	1:F:259:THR:HB	2.02	0.41
1:F:149:THR:HG22	1:F:150:GLU:N	2.35	0.41
1:H:157:ILE:HD11	1:I:115:ASP:OD2	2.19	0.41
1:J:79:ILE:HD13	1:J:79:ILE:HA	1.83	0.41
1:J:115:ASP:H	1:J:124:GLN:HE22	1.68	0.41
1:A:303:PHE:N	1:A:304:PRO:HD3	2.35	0.41
1:B:140:LEU:HD13	1:B:190:ILE:CG1	2.41	0.41
1:G:39:ILE:HD13	1:G:39:ILE:HG21	1.73	0.41
1:G:120:PRO:HB2	1:G:121:PHE:CE2	2.56	0.41
1:G:285:ARG:HD3	1:G:285:ARG:O	2.20	0.41
1:H:62:GLN:O	1:H:65:ARG:HB2	2.19	0.41
1:J:130:LEU:HD23	1:J:130:LEU:HA	1.82	0.41
1:J:222:PHE:C	1:J:224:LEU:H	2.28	0.41
1:A:122:ASP:HB2	1:A:198:ARG:HB2	2.03	0.41
1:A:149:THR:HG22	1:A:150:GLU:N	2.35	0.41
1:A:223:TRP:CD1	1:A:300:ARG:HD3	2.55	0.41
1:A:292:ASP:O	1:A:297:GLN:NE2	2.54	0.41
1:B:150:GLU:HB3	1:B:153:ASP:CB	2.48	0.41
1:C:149:THR:HG22	1:C:150:GLU:N	2.35	0.41
1:F:70:GLY:O	1:F:71:LEU:C	2.62	0.41
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.65	0.41
1:F:285:ARG:HD3	1:F:285:ARG:C	2.46	0.41
1:H:150:GLU:CB	1:H:153:ASP:HB2	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:LEU:C	1:H:209:LEU:CD2	2.94	0.41
1:I:172:ILE:CD1	1:I:189:ARG:HB3	2.49	0.41
1:A:28:THR:HB	1:A:255:LEU:CD2	2.47	0.41
1:B:223:TRP:NE1	1:B:300:ARG:HD3	2.35	0.41
1:C:125:GLN:OE1	1:C:193:ARG:HD3	2.21	0.41
1:D:59:GLU:OE1	1:E:75:ALA:HB2	2.21	0.41
1:D:187:PHE:CD1	1:D:187:PHE:N	2.88	0.41
1:F:141:ARG:HD3	1:F:142:PHE:CZ	2.55	0.41
1:H:118:LEU:O	1:H:119:PHE:C	2.64	0.41
1:I:149:THR:HG22	1:I:150:GLU:N	2.34	0.41
1:I:239:LEU:HD13	1:J:239:LEU:HD21	2.02	0.41
1:J:110:PHE:N	1:J:110:PHE:CD1	2.89	0.41
1:B:219:TRP:C	1:B:221:VAL:N	2.78	0.41
1:C:58:VAL:HB	1:C:92:LEU:HB2	2.03	0.41
1:E:66:TRP:HB3	1:E:71:LEU:HD12	2.03	0.41
1:F:136:ASN:ND2	1:F:184:GLN:HG3	2.36	0.41
1:G:147:VAL:HG23	1:G:165:ALA:HB2	2.02	0.41
1:G:222:PHE:C	1:G:224:LEU:H	2.28	0.41
1:G:303:PHE:N	1:G:304:PRO:HD3	2.35	0.41
1:H:136:ASN:ND2	1:H:184:GLN:HG3	2.36	0.41
1:H:231:LEU:HD12	1:H:280:ILE:HG12	2.02	0.41
1:H:300:ARG:O	1:H:304:PRO:HG2	2.21	0.41
1:I:172:ILE:HD12	1:I:172:ILE:N	2.35	0.41
1:A:39:ILE:HG21	1:A:39:ILE:HD13	1.63	0.41
1:B:231:LEU:HD23	1:B:232:GLN:N	2.35	0.41
1:C:23:ILE:HG21	1:C:126:PHE:CD2	2.56	0.41
1:C:46:LYS:HA	1:C:47:PRO:HD2	1.86	0.41
1:C:91:ARG:HD2	1:D:134:SER:HB2	2.02	0.41
1:D:46:LYS:O	1:D:47:PRO:C	2.62	0.41
1:D:66:TRP:HB3	1:D:71:LEU:HD12	2.03	0.41
1:D:118:LEU:O	1:D:119:PHE:C	2.64	0.41
1:E:285:ARG:C	1:E:285:ARG:HD3	2.45	0.41
1:E:300:ARG:O	1:E:304:PRO:HG2	2.20	0.41
1:F:39:ILE:HG13	1:F:106:PHE:CE2	2.56	0.41
1:F:185:ASN:N	1:F:185:ASN:ND2	2.68	0.41
1:H:23:ILE:HG21	1:H:126:PHE:CD2	2.56	0.41
1:H:187:PHE:CD1	1:H:187:PHE:N	2.88	0.41
1:A:209:LEU:C	1:A:209:LEU:CD2	2.94	0.41
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.97	0.41
1:C:48:ARG:HB2	1:C:48:ARG:CZ	2.51	0.41
1:C:211:LEU:HD23	1:C:244:TYR:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:VAL:CG2	1:E:165:ALA:HB2	2.51	0.41
1:G:71:LEU:C	1:G:71:LEU:CD2	2.93	0.41
1:H:223:TRP:CE3	1:I:280:ILE:CG2	3.04	0.41
1:I:115:ASP:H	1:I:124:GLN:HE22	1.67	0.41
1:I:309:ALA:O	1:I:313:VAL:HG23	2.20	0.41
1:A:15:SER:HG	1:A:142:PHE:HD1	1.66	0.41
1:A:119:PHE:HB3	1:A:259:THR:HB	2.01	0.41
1:A:211:LEU:HD23	1:A:244:TYR:CE2	2.56	0.41
1:B:62:GLN:O	1:B:65:ARG:HB2	2.21	0.41
1:B:145:ILE:HG21	1:B:192:VAL:HG11	2.03	0.41
1:B:305:LEU:C	1:B:305:LEU:CD1	2.93	0.41
1:C:147:VAL:CG2	1:C:165:ALA:HB2	2.51	0.41
1:C:216:ALA:C	1:C:218:SER:H	2.29	0.41
1:C:237:LEU:HD12	1:C:237:LEU:HA	1.84	0.41
1:D:28:THR:HB	1:D:255:LEU:CD2	2.45	0.41
1:D:114:MET:CE	1:D:124:GLN:HG2	2.50	0.41
1:E:89:ASN:O	1:E:104:ALA:HA	2.20	0.41
1:G:78:PHE:O	1:G:79:ILE:C	2.63	0.41
1:G:120:PRO:HD2	1:G:260:VAL:CG2	2.51	0.41
1:G:209:LEU:HB3	1:G:210:PRO:HD3	2.00	0.41
1:H:44:THR:HG23	1:H:99:ARG:H	1.86	0.41
1:I:40:VAL:HA	1:I:102:TYR:O	2.21	0.41
1:I:79:ILE:HD13	1:I:79:ILE:HA	1.86	0.41
1:I:97:ASP:OD1	1:I:99:ARG:HG2	2.20	0.41
1:I:248:THR:HG23	1:I:252:LEU:HD22	2.02	0.41
1:J:208:ILE:HG12	1:J:208:ILE:H	1.67	0.41
1:J:209:LEU:C	1:J:209:LEU:CD2	2.94	0.41
1:A:285:ARG:NE	1:A:285:ARG:CA	2.83	0.41
1:C:257:TYR:CD1	1:C:257:TYR:N	2.88	0.41
1:D:125:GLN:OE1	1:D:193:ARG:HD3	2.21	0.41
1:D:164:LYS:HZ2	1:D:164:LYS:CA	2.30	0.41
1:D:197:VAL:HG12	1:D:198:ARG:N	2.35	0.41
1:D:201:SER:O	1:D:202:TYR:C	2.63	0.41
1:D:299:CYS:C	1:D:301:LEU:H	2.29	0.41
1:D:305:LEU:C	1:D:305:LEU:CD1	2.93	0.41
1:H:79:ILE:HD13	1:H:79:ILE:HA	1.81	0.41
1:I:285:ARG:NE	1:I:285:ARG:CA	2.84	0.41
1:J:237:LEU:HD12	1:J:237:LEU:HA	1.89	0.41
1:A:68:ASN:ND2	1:E:65:ARG:HD2	2.36	0.40
1:B:147:VAL:HG21	1:B:165:ALA:HB2	2.02	0.40
1:C:136:ASN:ND2	1:C:184:GLN:HG3	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ILE:O	1:D:251:ILE:HG22	2.20	0.40
1:E:162:ILE:N	1:E:162:ILE:CD1	2.81	0.40
1:E:223:TRP:NE1	1:E:300:ARG:HD3	2.36	0.40
1:F:120:PRO:HD2	1:F:260:VAL:HG23	2.03	0.40
1:A:127:VAL:HG22	1:A:193:ARG:HG2	2.02	0.40
1:A:203:TYR:O	1:A:208:ILE:HG12	2.22	0.40
1:A:266:ILE:HD12	1:E:205:TRP:O	2.21	0.40
1:D:266:ILE:O	1:D:269:TYR:HB2	2.22	0.40
1:D:286:GLN:HA	1:D:291:GLU:OE1	2.22	0.40
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.55	0.40
1:G:209:LEU:C	1:G:209:LEU:CD2	2.95	0.40
1:H:136:ASN:ND2	1:H:184:GLN:HA	2.36	0.40
1:H:292:ASP:O	1:H:297:GLN:NE2	2.54	0.40
1:I:46:LYS:HD3	1:I:46:LYS:N	2.36	0.40
1:I:148:TYR:HE2	1:J:176:HIS:NE2	2.09	0.40
1:I:286:GLN:HA	1:I:291:GLU:OE1	2.21	0.40
1:J:70:GLY:O	1:J:71:LEU:C	2.63	0.40
1:A:147:VAL:O	1:A:149:THR:N	2.47	0.40
1:F:286:GLN:HA	1:F:291:GLU:OE1	2.21	0.40
1:H:39:ILE:HD13	1:H:39:ILE:HG21	1.78	0.40
1:J:17:SER:O	1:J:40:VAL:HG23	2.20	0.40
1:J:147:VAL:CG2	1:J:165:ALA:HB2	2.51	0.40
1:B:110:PHE:CD1	1:B:110:PHE:N	2.88	0.40
1:B:149:THR:HG22	1:B:150:GLU:N	2.36	0.40
1:B:209:LEU:HD23	1:B:209:LEU:C	2.46	0.40
1:B:299:CYS:C	1:B:301:LEU:H	2.29	0.40
1:C:294:LEU:CA	1:C:297:GLN:HE21	2.27	0.40
1:D:285:ARG:HD3	1:D:285:ARG:C	2.46	0.40
1:E:73:VAL:HA	1:E:74:PRO:HD3	1.90	0.40
1:E:79:ILE:HD13	1:E:79:ILE:HA	1.84	0.40
1:F:46:LYS:HA	1:F:47:PRO:HD2	1.85	0.40
1:F:251:ILE:HD11	1:G:249:SER:HB3	2.03	0.40
1:G:77:GLU:CG	1:G:78:PHE:N	2.84	0.40
1:G:216:ALA:C	1:G:218:SER:N	2.78	0.40
1:H:16:VAL:HA	1:H:40:VAL:O	2.22	0.40
1:H:148:TYR:HD1	1:H:148:TYR:HA	1.72	0.40
1:H:211:LEU:HD23	1:H:244:TYR:CE2	2.56	0.40
1:J:292:ASP:O	1:J:297:GLN:NE2	2.54	0.40
1:B:148:TYR:CE2	1:C:176:HIS:NE2	2.85	0.40
1:C:110:PHE:CD1	1:C:110:PHE:N	2.88	0.40
1:D:147:VAL:O	1:D:147:VAL:HG12	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:TYR:O	1:E:208:ILE:HG12	2.21	0.40
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.56	0.40
1:J:16:VAL:HA	1:J:40:VAL:O	2.22	0.40
1:J:66:TRP:HB3	1:J:71:LEU:HD12	2.04	0.40
1:J:77:GLU:O	1:J:130:LEU:HD23	2.21	0.40
1:J:78:PHE:O	1:J:79:ILE:C	2.65	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASN:O	1:J:49:LYS:O[1_655]	1.93	0.27
1:D:139:GLN:NE2	1:G:173:ARG:NH2[2_354]	2.01	0.19
1:E:287:ALA:O	1:F:142:PHE:CD2[2_355]	2.12	0.08
1:A:291:GLU:OE1	1:D:49:LYS:NZ[1_556]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	B	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	C	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	D	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	E	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	F	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)	1	6
1	G	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)	1	6
1	H	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	I	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
All	All	3040/3210 (95%)	2371 (78%)	439 (14%)	230 (8%)	1	6

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	119	PHE
1	A	141	ARG
1	A	151	ASN
1	A	168	HIS
1	A	201	SER
1	B	53	ASP
1	B	119	PHE
1	B	141	ARG
1	B	151	ASN
1	B	168	HIS
1	B	201	SER
1	C	53	ASP
1	C	119	PHE
1	C	141	ARG
1	C	151	ASN
1	C	168	HIS
1	C	201	SER
1	D	53	ASP
1	D	141	ARG
1	D	151	ASN
1	D	168	HIS
1	D	201	SER
1	E	53	ASP
1	E	119	PHE
1	E	141	ARG
1	E	151	ASN
1	E	168	HIS
1	E	201	SER
1	F	53	ASP
1	F	119	PHE
1	F	141	ARG
1	F	151	ASN
1	F	168	HIS
1	F	201	SER
1	G	53	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	119	PHE
1	G	141	ARG
1	G	151	ASN
1	G	168	HIS
1	G	201	SER
1	H	53	ASP
1	H	119	PHE
1	H	141	ARG
1	H	151	ASN
1	H	168	HIS
1	H	201	SER
1	I	53	ASP
1	I	119	PHE
1	I	141	ARG
1	I	151	ASN
1	I	168	HIS
1	I	201	SER
1	J	53	ASP
1	J	119	PHE
1	J	141	ARG
1	J	151	ASN
1	J	168	HIS
1	J	201	SER
1	A	99	ARG
1	A	165	ALA
1	A	183	ASN
1	B	99	ARG
1	B	183	ASN
1	B	288	ASN
1	C	99	ARG
1	C	165	ALA
1	C	183	ASN
1	C	288	ASN
1	D	99	ARG
1	D	119	PHE
1	D	183	ASN
1	D	288	ASN
1	E	99	ARG
1	E	165	ALA
1	E	183	ASN
1	E	288	ASN
1	F	99	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	165	ALA
1	F	183	ASN
1	F	288	ASN
1	G	99	ARG
1	G	165	ALA
1	G	183	ASN
1	G	220	SER
1	G	288	ASN
1	H	99	ARG
1	H	165	ALA
1	H	183	ASN
1	I	99	ARG
1	I	183	ASN
1	I	288	ASN
1	J	99	ARG
1	J	165	ALA
1	J	183	ASN
1	J	288	ASN
1	J	293	ASP
1	A	79	ILE
1	A	185	ASN
1	A	220	SER
1	A	226	SER
1	A	288	ASN
1	A	293	ASP
1	B	165	ALA
1	B	185	ASN
1	B	220	SER
1	B	226	SER
1	B	293	ASP
1	C	185	ASN
1	C	220	SER
1	C	226	SER
1	C	293	ASP
1	D	79	ILE
1	D	165	ALA
1	D	185	ASN
1	D	220	SER
1	D	226	SER
1	D	293	ASP
1	E	185	ASN
1	E	220	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	226	SER
1	E	293	ASP
1	F	185	ASN
1	F	220	SER
1	F	226	SER
1	F	293	ASP
1	G	185	ASN
1	G	226	SER
1	G	293	ASP
1	H	79	ILE
1	H	185	ASN
1	H	220	SER
1	H	226	SER
1	H	288	ASN
1	H	293	ASP
1	I	165	ALA
1	I	185	ASN
1	I	220	SER
1	I	226	SER
1	I	293	ASP
1	J	185	ASN
1	J	220	SER
1	J	226	SER
1	A	148	TYR
1	B	47	PRO
1	B	60	ASN
1	B	79	ILE
1	B	148	TYR
1	C	148	TYR
1	D	47	PRO
1	D	148	TYR
1	E	79	ILE
1	E	148	TYR
1	F	47	PRO
1	F	79	ILE
1	F	148	TYR
1	G	47	PRO
1	G	79	ILE
1	G	148	TYR
1	H	148	TYR
1	I	79	ILE
1	I	148	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	47	PRO
1	J	60	ASN
1	J	79	ILE
1	J	148	TYR
1	A	47	PRO
1	A	60	ASN
1	A	181	GLN
1	A	289	GLY
1	B	181	GLN
1	B	289	GLY
1	C	47	PRO
1	C	60	ASN
1	C	79	ILE
1	C	181	GLN
1	C	289	GLY
1	D	55	PRO
1	D	60	ASN
1	D	181	GLN
1	D	289	GLY
1	E	47	PRO
1	E	55	PRO
1	E	60	ASN
1	E	181	GLN
1	E	289	GLY
1	F	60	ASN
1	F	181	GLN
1	F	289	GLY
1	G	55	PRO
1	G	60	ASN
1	G	181	GLN
1	G	289	GLY
1	H	47	PRO
1	H	60	ASN
1	H	181	GLN
1	H	289	GLY
1	I	47	PRO
1	I	60	ASN
1	I	181	GLN
1	I	289	GLY
1	J	181	GLN
1	J	289	GLY
1	A	55	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	PRO
1	B	55	PRO
1	B	182	PRO
1	C	55	PRO
1	C	182	PRO
1	D	182	PRO
1	E	182	PRO
1	F	55	PRO
1	F	182	PRO
1	G	182	PRO
1	H	55	PRO
1	H	182	PRO
1	I	182	PRO
1	J	182	PRO
1	I	55	PRO
1	J	55	PRO
1	A	303	PHE
1	B	303	PHE
1	C	303	PHE
1	D	303	PHE
1	E	303	PHE
1	F	303	PHE
1	G	303	PHE
1	H	303	PHE
1	I	303	PHE
1	J	303	PHE

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	274/283 (97%)	248 (90%)	26 (10%)	8	29
1	B	274/283 (97%)	248 (90%)	26 (10%)	8	29
1	C	274/283 (97%)	248 (90%)	26 (10%)	8	29
1	D	274/283 (97%)	249 (91%)	25 (9%)	9	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	274/283 (97%)	246 (90%)	28 (10%)	7	26
1	F	274/283 (97%)	248 (90%)	26 (10%)	8	29
1	G	274/283 (97%)	249 (91%)	25 (9%)	9	31
1	H	274/283 (97%)	247 (90%)	27 (10%)	7	27
1	I	274/283 (97%)	249 (91%)	25 (9%)	9	31
1	J	274/283 (97%)	247 (90%)	27 (10%)	7	27
All	All	2740/2830 (97%)	2479 (90%)	261 (10%)	8	29

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	40	VAL
1	A	43	TRP
1	A	50	THR
1	A	56	LEU
1	A	71	LEU
1	A	72	TRP
1	A	118	LEU
1	A	124	GLN
1	A	138	GLN
1	A	142	PHE
1	A	145	ILE
1	A	157	ILE
1	A	162	ILE
1	A	164	LYS
1	A	176	HIS
1	A	177	LEU
1	A	181	GLN
1	A	184	GLN
1	A	185	ASN
1	A	209	LEU
1	A	252	LEU
1	A	260	VAL
1	A	285	ARG
1	A	286	GLN
1	A	303	PHE
1	B	12	VAL
1	B	29	LEU
1	B	40	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	50	THR
1	B	56	LEU
1	B	71	LEU
1	B	72	TRP
1	B	118	LEU
1	B	124	GLN
1	B	138	GLN
1	B	142	PHE
1	B	145	ILE
1	B	157	ILE
1	B	162	ILE
1	B	164	LYS
1	B	176	HIS
1	B	177	LEU
1	B	181	GLN
1	B	184	GLN
1	B	185	ASN
1	B	209	LEU
1	B	252	LEU
1	B	260	VAL
1	B	285	ARG
1	B	286	GLN
1	B	303	PHE
1	C	29	LEU
1	C	40	VAL
1	C	43	TRP
1	C	50	THR
1	C	56	LEU
1	C	71	LEU
1	C	72	TRP
1	C	118	LEU
1	C	124	GLN
1	C	138	GLN
1	C	142	PHE
1	C	145	ILE
1	C	157	ILE
1	C	162	ILE
1	C	164	LYS
1	C	176	HIS
1	C	177	LEU
1	C	181	GLN
1	C	184	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	185	ASN
1	C	209	LEU
1	C	252	LEU
1	C	260	VAL
1	C	285	ARG
1	C	286	GLN
1	C	303	PHE
1	D	12	VAL
1	D	29	LEU
1	D	40	VAL
1	D	43	TRP
1	D	50	THR
1	D	71	LEU
1	D	72	TRP
1	D	118	LEU
1	D	124	GLN
1	D	138	GLN
1	D	142	PHE
1	D	145	ILE
1	D	157	ILE
1	D	162	ILE
1	D	164	LYS
1	D	176	HIS
1	D	177	LEU
1	D	181	GLN
1	D	184	GLN
1	D	185	ASN
1	D	252	LEU
1	D	260	VAL
1	D	285	ARG
1	D	286	GLN
1	D	303	PHE
1	E	12	VAL
1	E	29	LEU
1	E	40	VAL
1	E	43	TRP
1	E	50	THR
1	E	56	LEU
1	E	71	LEU
1	E	72	TRP
1	E	78	PHE
1	E	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	124	GLN
1	E	138	GLN
1	E	142	PHE
1	E	145	ILE
1	E	157	ILE
1	E	162	ILE
1	E	164	LYS
1	E	176	HIS
1	E	177	LEU
1	E	181	GLN
1	E	184	GLN
1	E	185	ASN
1	E	209	LEU
1	E	252	LEU
1	E	260	VAL
1	E	285	ARG
1	E	286	GLN
1	E	303	PHE
1	F	29	LEU
1	F	40	VAL
1	F	43	TRP
1	F	50	THR
1	F	56	LEU
1	F	71	LEU
1	F	72	TRP
1	F	118	LEU
1	F	124	GLN
1	F	138	GLN
1	F	142	PHE
1	F	145	ILE
1	F	157	ILE
1	F	162	ILE
1	F	164	LYS
1	F	176	HIS
1	F	177	LEU
1	F	181	GLN
1	F	184	GLN
1	F	185	ASN
1	F	209	LEU
1	F	252	LEU
1	F	260	VAL
1	F	285	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	286	GLN
1	F	303	PHE
1	G	12	VAL
1	G	29	LEU
1	G	40	VAL
1	G	43	TRP
1	G	50	THR
1	G	71	LEU
1	G	72	TRP
1	G	118	LEU
1	G	124	GLN
1	G	138	GLN
1	G	142	PHE
1	G	145	ILE
1	G	157	ILE
1	G	162	ILE
1	G	164	LYS
1	G	176	HIS
1	G	177	LEU
1	G	181	GLN
1	G	184	GLN
1	G	185	ASN
1	G	252	LEU
1	G	260	VAL
1	G	285	ARG
1	G	286	GLN
1	G	303	PHE
1	H	29	LEU
1	H	40	VAL
1	H	43	TRP
1	H	50	THR
1	H	56	LEU
1	H	71	LEU
1	H	72	TRP
1	H	78	PHE
1	H	118	LEU
1	H	124	GLN
1	H	138	GLN
1	H	142	PHE
1	H	145	ILE
1	H	157	ILE
1	H	162	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	164	LYS
1	H	176	HIS
1	H	177	LEU
1	H	181	GLN
1	H	184	GLN
1	H	185	ASN
1	H	209	LEU
1	H	252	LEU
1	H	260	VAL
1	H	285	ARG
1	H	286	GLN
1	H	303	PHE
1	I	29	LEU
1	I	40	VAL
1	I	43	TRP
1	I	50	THR
1	I	71	LEU
1	I	72	TRP
1	I	118	LEU
1	I	124	GLN
1	I	138	GLN
1	I	142	PHE
1	I	145	ILE
1	I	157	ILE
1	I	162	ILE
1	I	164	LYS
1	I	176	HIS
1	I	177	LEU
1	I	181	GLN
1	I	184	GLN
1	I	185	ASN
1	I	209	LEU
1	I	252	LEU
1	I	260	VAL
1	I	285	ARG
1	I	286	GLN
1	I	303	PHE
1	J	12	VAL
1	J	29	LEU
1	J	40	VAL
1	J	43	TRP
1	J	50	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	56	LEU
1	J	71	LEU
1	J	72	TRP
1	J	118	LEU
1	J	124	GLN
1	J	138	GLN
1	J	142	PHE
1	J	145	ILE
1	J	157	ILE
1	J	162	ILE
1	J	164	LYS
1	J	176	HIS
1	J	177	LEU
1	J	181	GLN
1	J	184	GLN
1	J	185	ASN
1	J	209	LEU
1	J	252	LEU
1	J	260	VAL
1	J	285	ARG
1	J	286	GLN
1	J	303	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	62	GLN
1	A	124	GLN
1	A	136	ASN
1	A	151	ASN
1	A	154	ASN
1	A	181	GLN
1	A	185	ASN
1	A	199	ASN
1	A	250	ASN
1	A	283	HIS
1	A	297	GLN
1	B	42	GLN
1	B	62	GLN
1	B	68	ASN
1	B	124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	ASN
1	B	151	ASN
1	B	154	ASN
1	B	185	ASN
1	B	199	ASN
1	B	297	GLN
1	C	42	GLN
1	C	62	GLN
1	C	124	GLN
1	C	136	ASN
1	C	151	ASN
1	C	154	ASN
1	C	181	GLN
1	C	185	ASN
1	C	199	ASN
1	C	250	ASN
1	C	283	HIS
1	C	284	HIS
1	C	297	GLN
1	D	42	GLN
1	D	62	GLN
1	D	68	ASN
1	D	124	GLN
1	D	136	ASN
1	D	151	ASN
1	D	154	ASN
1	D	168	HIS
1	D	181	GLN
1	D	185	ASN
1	D	199	ASN
1	D	283	HIS
1	D	297	GLN
1	E	42	GLN
1	E	62	GLN
1	E	68	ASN
1	E	124	GLN
1	E	136	ASN
1	E	151	ASN
1	E	154	ASN
1	E	181	GLN
1	E	185	ASN
1	E	199	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	250	ASN
1	E	283	HIS
1	E	297	GLN
1	F	42	GLN
1	F	62	GLN
1	F	124	GLN
1	F	136	ASN
1	F	151	ASN
1	F	154	ASN
1	F	168	HIS
1	F	181	GLN
1	F	185	ASN
1	F	199	ASN
1	F	250	ASN
1	F	283	HIS
1	F	284	HIS
1	F	297	GLN
1	G	42	GLN
1	G	62	GLN
1	G	124	GLN
1	G	136	ASN
1	G	151	ASN
1	G	154	ASN
1	G	181	GLN
1	G	185	ASN
1	G	199	ASN
1	G	283	HIS
1	G	297	GLN
1	H	42	GLN
1	H	62	GLN
1	H	124	GLN
1	H	136	ASN
1	H	151	ASN
1	H	154	ASN
1	H	181	GLN
1	H	185	ASN
1	H	199	ASN
1	H	250	ASN
1	H	283	HIS
1	H	297	GLN
1	I	42	GLN
1	I	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	68	ASN
1	I	124	GLN
1	I	136	ASN
1	I	139	GLN
1	I	151	ASN
1	I	154	ASN
1	I	181	GLN
1	I	185	ASN
1	I	199	ASN
1	I	283	HIS
1	I	297	GLN
1	J	42	GLN
1	J	62	GLN
1	J	124	GLN
1	J	136	ASN
1	J	151	ASN
1	J	154	ASN
1	J	181	GLN
1	J	185	ASN
1	J	199	ASN
1	J	250	ASN
1	J	283	HIS
1	J	284	HIS
1	J	297	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	306/321 (95%)	-0.02	12 (3%)	43	29	64, 105, 278, 412	0
1	B	306/321 (95%)	0.08	13 (4%)	40	26	60, 103, 278, 412	0
1	C	306/321 (95%)	-0.05	6 (1%)	65	46	60, 104, 278, 412	0
1	D	306/321 (95%)	0.06	13 (4%)	40	26	59, 103, 277, 401	0
1	E	306/321 (95%)	0.00	5 (1%)	70	52	62, 105, 278, 413	0
1	F	306/321 (95%)	-0.04	6 (1%)	65	46	62, 105, 277, 412	0
1	G	306/321 (95%)	0.08	17 (5%)	30	20	59, 104, 277, 412	0
1	H	306/321 (95%)	-0.08	6 (1%)	65	46	63, 104, 278, 413	0
1	I	306/321 (95%)	0.22	19 (6%)	26	18	56, 102, 278, 407	0
1	J	306/321 (95%)	0.06	11 (3%)	46	31	62, 105, 278, 412	0
All	All	3060/3210 (95%)	0.03	108 (3%)	47	31	56, 104, 287, 413	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	314	LEU	5.1
1	A	292	ASP	5.0
1	G	290	VAL	4.7
1	A	291	GLU	4.5
1	A	290	VAL	4.4
1	A	288	ASN	4.4
1	E	292	ASP	4.3
1	G	157	ILE	4.3
1	F	178	SER	4.2
1	B	290	VAL	4.1
1	B	292	ASP	4.0
1	B	157	ILE	3.9
1	G	288	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	287	ALA	3.8
1	H	290	VAL	3.7
1	I	290	VAL	3.6
1	D	178	SER	3.6
1	G	154	ASN	3.6
1	H	138	GLN	3.5
1	F	302	ALA	3.5
1	D	151	ASN	3.5
1	E	178	SER	3.4
1	I	289	GLY	3.4
1	J	304	PRO	3.3
1	J	290	VAL	3.3
1	F	307	PHE	3.2
1	I	177	LEU	3.2
1	G	292	ASP	3.1
1	A	289	GLY	3.1
1	J	292	ASP	3.1
1	I	292	ASP	3.1
1	H	157	ILE	3.1
1	A	174	TYR	3.0
1	G	287	ALA	3.0
1	E	287	ALA	2.9
1	I	156	GLU	2.9
1	A	157	ILE	2.9
1	B	287	ALA	2.9
1	I	178	SER	2.8
1	D	290	VAL	2.8
1	D	158	ASP	2.8
1	I	304	PRO	2.8
1	H	89	ASN	2.7
1	C	178	SER	2.7
1	C	177	LEU	2.7
1	C	157	ILE	2.7
1	D	296	ILE	2.6
1	I	301	LEU	2.6
1	B	178	SER	2.6
1	B	154	ASN	2.6
1	G	199	ASN	2.6
1	G	307	PHE	2.6
1	J	303	PHE	2.6
1	I	136	ASN	2.6
1	J	158	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	294	LEU	2.6
1	H	287	ALA	2.6
1	A	293	ASP	2.5
1	F	290	VAL	2.5
1	I	158	ASP	2.5
1	B	307	PHE	2.5
1	J	177	LEU	2.5
1	J	178	SER	2.5
1	I	163	ARG	2.5
1	H	177	LEU	2.4
1	B	168	HIS	2.4
1	A	249	SER	2.4
1	I	307	PHE	2.4
1	E	177	LEU	2.4
1	J	154	ASN	2.4
1	I	152	ILE	2.4
1	B	297	GLN	2.3
1	G	156	GLU	2.3
1	A	221	VAL	2.3
1	D	11	PRO	2.3
1	D	49	LYS	2.3
1	G	150	GLU	2.3
1	I	223	TRP	2.3
1	G	168	HIS	2.3
1	J	280	ILE	2.3
1	I	168	HIS	2.3
1	J	157	ILE	2.2
1	C	154	ASN	2.2
1	I	161	TRP	2.2
1	D	220	SER	2.2
1	G	289	GLY	2.2
1	I	247	TYR	2.2
1	D	234	SER	2.2
1	D	156	GLU	2.2
1	B	85	PRO	2.2
1	B	148	TYR	2.1
1	D	22	LYS	2.1
1	I	150	GLU	2.1
1	J	186	GLU	2.1
1	G	153	ASP	2.1
1	G	139	GLN	2.1
1	C	289	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	136	ASN	2.1
1	I	151	ASN	2.1
1	F	161	TRP	2.1
1	E	280	ILE	2.1
1	G	11	PRO	2.1
1	F	292	ASP	2.1
1	G	178	SER	2.0
1	D	157	ILE	2.0
1	B	169	ILE	2.0
1	B	138	GLN	2.0
1	C	290	VAL	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.