



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 2AXU / pdb_00002axu
Title : Structure of PrgX
Authors : Shi, K.; Brown, C.K.; Gu, Z.Y.; Kozlowicz, B.K.; Dunny, G.M.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2005-09-06
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

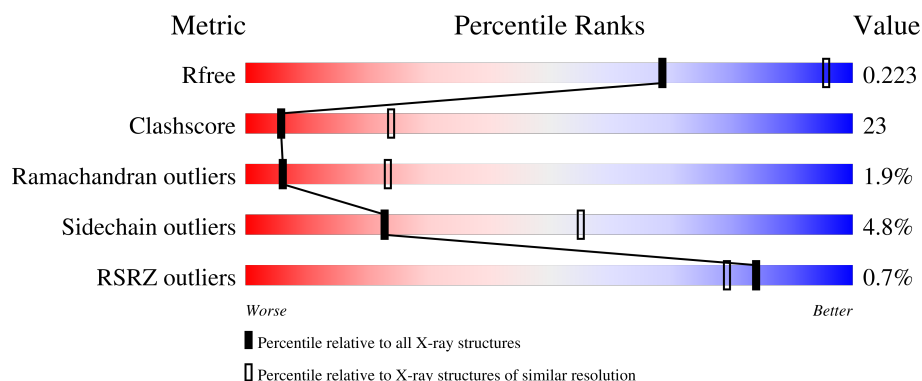
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	317	% 56% 33% 5% • 5%
1	G	317	% 49% 39% 7% •
1	H	317	% 53% 36% 5% 6%
1	I	317	% 46% 43% 5% 5%
1	J	317	% 51% 39% • 7%
1	K	317	54% 38% • 6%
1	L	317	53% 38% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30147 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 PrgX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2507	1630	402	469	1	5			
1	B	300	Total	C	N	O	S	Se	0	0	0
			2486	1616	399	466	1	4			
1	C	299	Total	C	N	O	S	Se	0	0	0
			2475	1607	398	465	1	4			
1	D	298	Total	C	N	O	S	Se	0	0	0
			2468	1602	397	464	1	4			
1	E	300	Total	C	N	O	S	Se	0	0	0
			2480	1610	399	466	1	4			
1	F	301	Total	C	N	O	S	Se	0	0	0
			2488	1616	400	467	1	4			
1	G	303	Total	C	N	O	S	Se	0	0	0
			2508	1630	402	471	1	4			
1	H	298	Total	C	N	O	S	Se	0	0	0
			2468	1602	397	464	1	4			
1	I	300	Total	C	N	O	S	Se	0	0	0
			2486	1616	399	466	1	4			
1	J	296	Total	C	N	O	S	Se	0	0	0
			2447	1587	394	461	1	4			
1	K	299	Total	C	N	O	S	Se	0	0	0
			2471	1604	397	465	1	4			
1	L	299	Total	C	N	O	S	Se	0	0	0
			2479	1611	398	465	1	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q04114
A	27	MSE	MET	modified residue	UNP Q04114
A	67	MSE	MET	modified residue	UNP Q04114
A	175	MSE	MET	modified residue	UNP Q04114
A	203	MSE	MET	modified residue	UNP Q04114

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	MET	modified residue	UNP Q04114
B	27	MSE	MET	modified residue	UNP Q04114
B	67	MSE	MET	modified residue	UNP Q04114
B	175	MSE	MET	modified residue	UNP Q04114
B	203	MSE	MET	modified residue	UNP Q04114
C	1	MSE	MET	modified residue	UNP Q04114
C	27	MSE	MET	modified residue	UNP Q04114
C	67	MSE	MET	modified residue	UNP Q04114
C	175	MSE	MET	modified residue	UNP Q04114
C	203	MSE	MET	modified residue	UNP Q04114
D	1	MSE	MET	modified residue	UNP Q04114
D	27	MSE	MET	modified residue	UNP Q04114
D	67	MSE	MET	modified residue	UNP Q04114
D	175	MSE	MET	modified residue	UNP Q04114
D	203	MSE	MET	modified residue	UNP Q04114
E	1	MSE	MET	modified residue	UNP Q04114
E	27	MSE	MET	modified residue	UNP Q04114
E	67	MSE	MET	modified residue	UNP Q04114
E	175	MSE	MET	modified residue	UNP Q04114
E	203	MSE	MET	modified residue	UNP Q04114
F	1	MSE	MET	modified residue	UNP Q04114
F	27	MSE	MET	modified residue	UNP Q04114
F	67	MSE	MET	modified residue	UNP Q04114
F	175	MSE	MET	modified residue	UNP Q04114
F	203	MSE	MET	modified residue	UNP Q04114
G	1	MSE	MET	modified residue	UNP Q04114
G	27	MSE	MET	modified residue	UNP Q04114
G	67	MSE	MET	modified residue	UNP Q04114
G	175	MSE	MET	modified residue	UNP Q04114
G	203	MSE	MET	modified residue	UNP Q04114
H	1	MSE	MET	modified residue	UNP Q04114
H	27	MSE	MET	modified residue	UNP Q04114
H	67	MSE	MET	modified residue	UNP Q04114
H	175	MSE	MET	modified residue	UNP Q04114
H	203	MSE	MET	modified residue	UNP Q04114
I	1	MSE	MET	modified residue	UNP Q04114
I	27	MSE	MET	modified residue	UNP Q04114
I	67	MSE	MET	modified residue	UNP Q04114
I	175	MSE	MET	modified residue	UNP Q04114
I	203	MSE	MET	modified residue	UNP Q04114
J	1	MSE	MET	modified residue	UNP Q04114
J	27	MSE	MET	modified residue	UNP Q04114

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	67	MSE	MET	modified residue	UNP Q04114
J	175	MSE	MET	modified residue	UNP Q04114
J	203	MSE	MET	modified residue	UNP Q04114
K	1	MSE	MET	modified residue	UNP Q04114
K	27	MSE	MET	modified residue	UNP Q04114
K	67	MSE	MET	modified residue	UNP Q04114
K	175	MSE	MET	modified residue	UNP Q04114
K	203	MSE	MET	modified residue	UNP Q04114
L	1	MSE	MET	modified residue	UNP Q04114
L	27	MSE	MET	modified residue	UNP Q04114
L	67	MSE	MET	modified residue	UNP Q04114
L	175	MSE	MET	modified residue	UNP Q04114
L	203	MSE	MET	modified residue	UNP Q04114

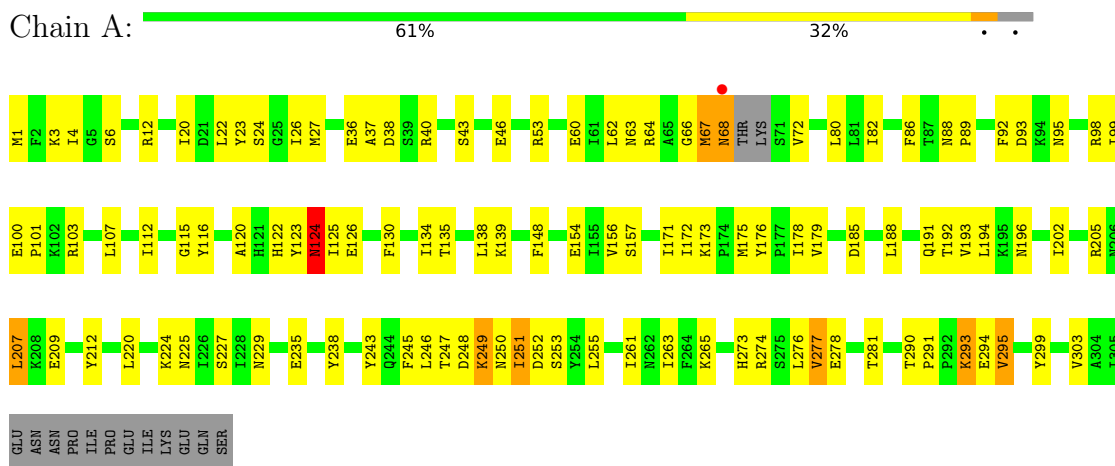
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	45	Total O 45 45	0	0
2	C	25	Total O 25 25	0	0
2	D	29	Total O 29 29	0	0
2	E	33	Total O 33 33	0	0
2	F	42	Total O 42 42	0	0
2	G	28	Total O 28 28	0	0
2	H	36	Total O 36 36	0	0
2	I	23	Total O 23 23	0	0
2	J	28	Total O 28 28	0	0
2	K	28	Total O 28 28	0	0
2	L	30	Total O 30 30	0	0

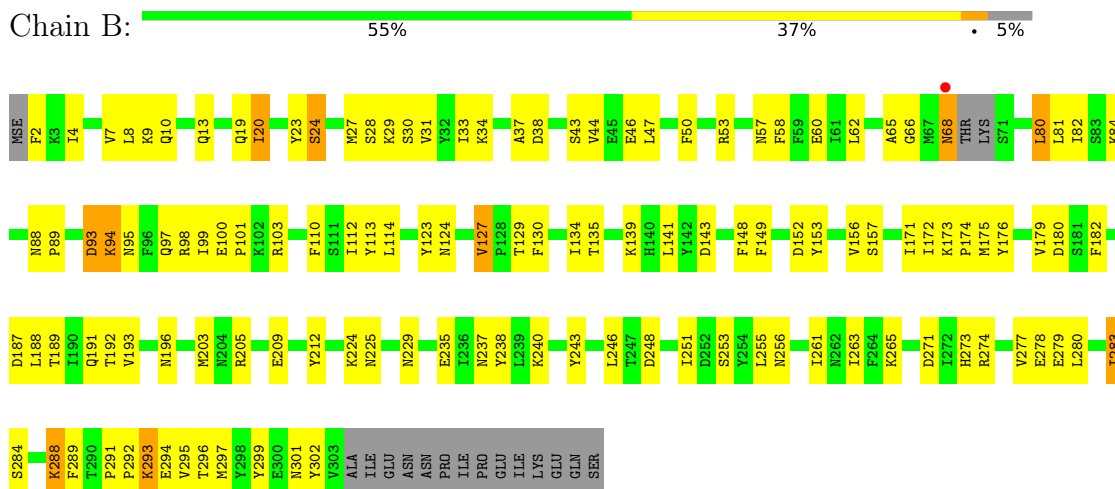
3 Residue-property plots

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

• Molecule 1: PrgX

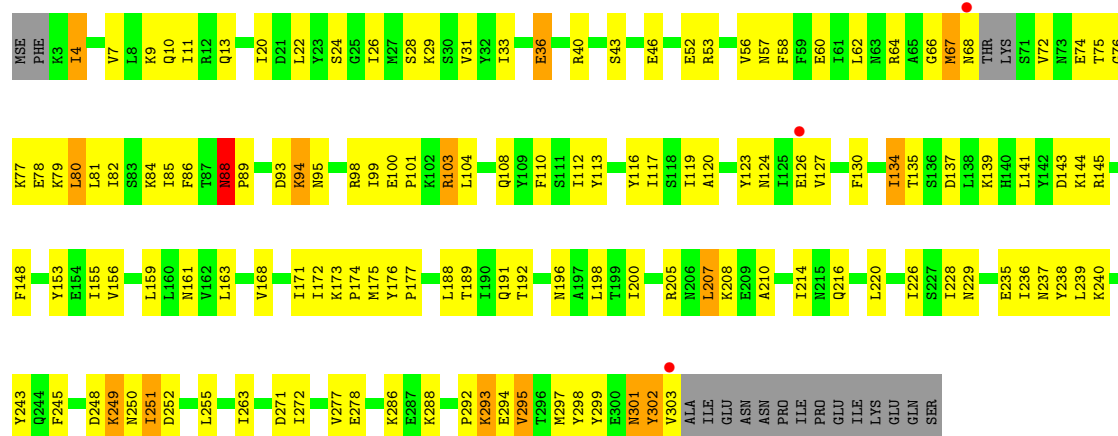


• Molecule 1: PrgX

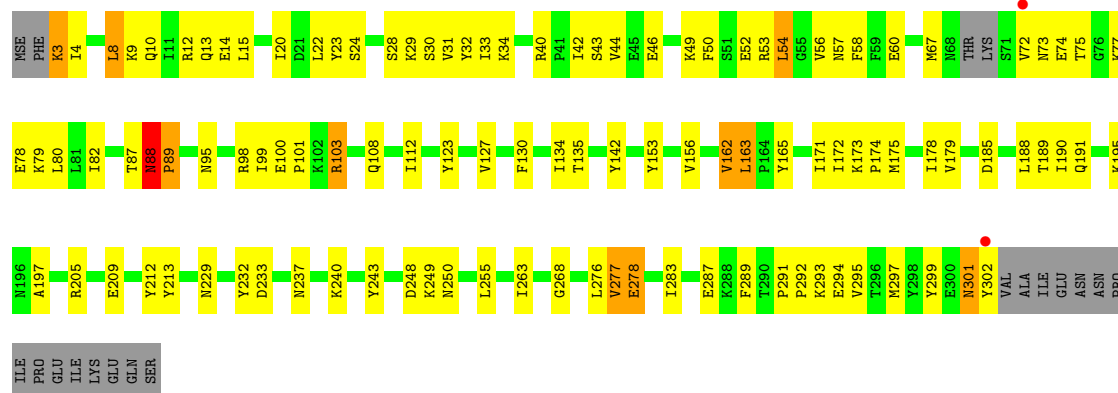


• Molecule 1: PrgX

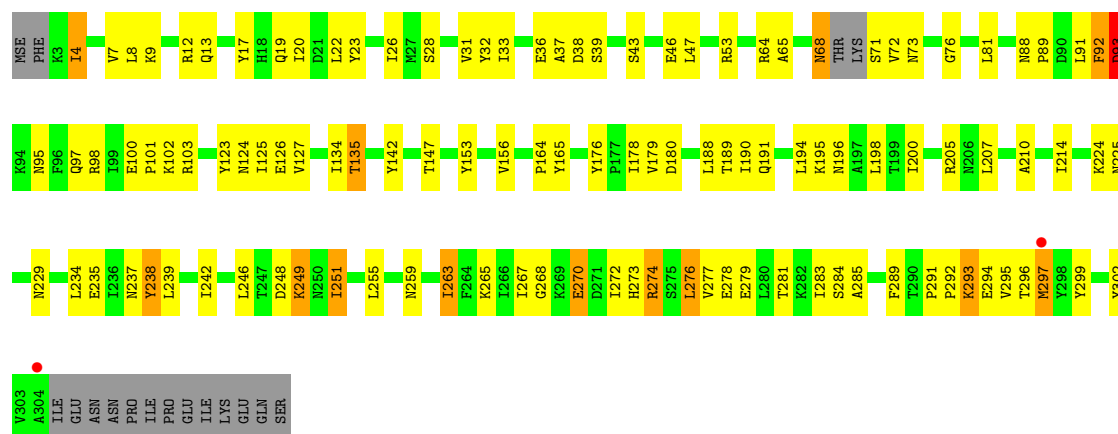




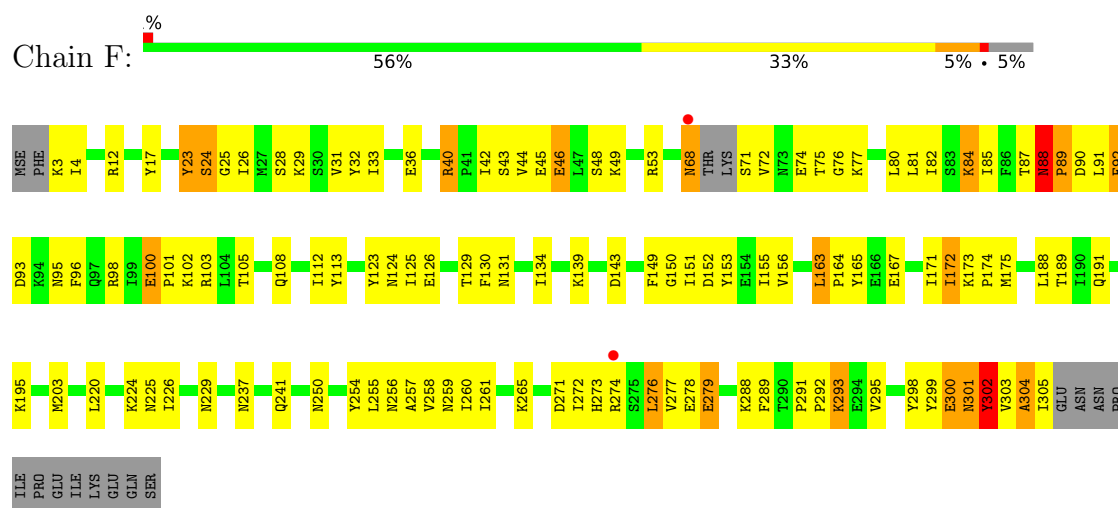
• Molecule 1: PrgX



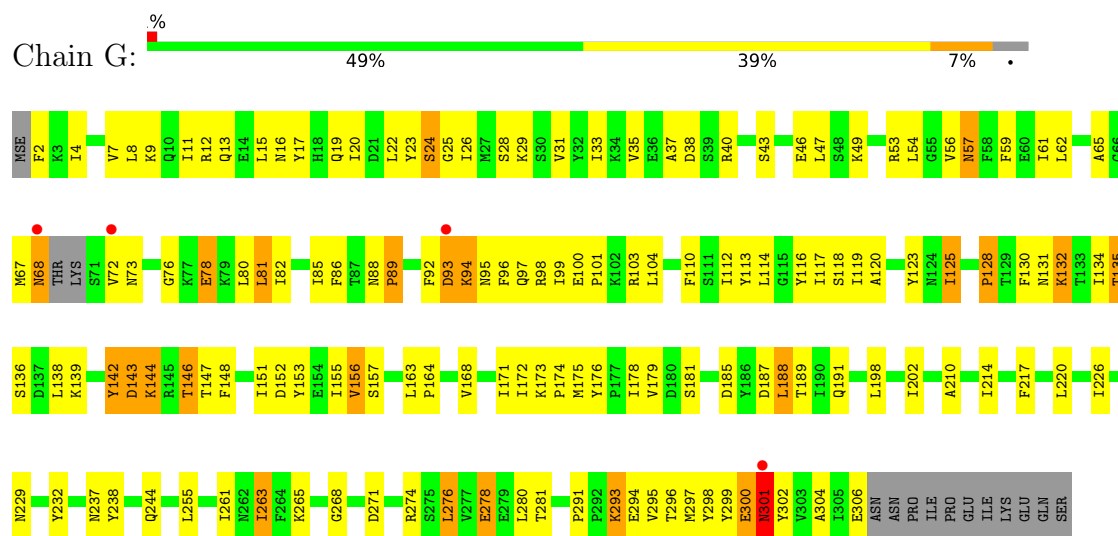
• Molecule 1: PrgX



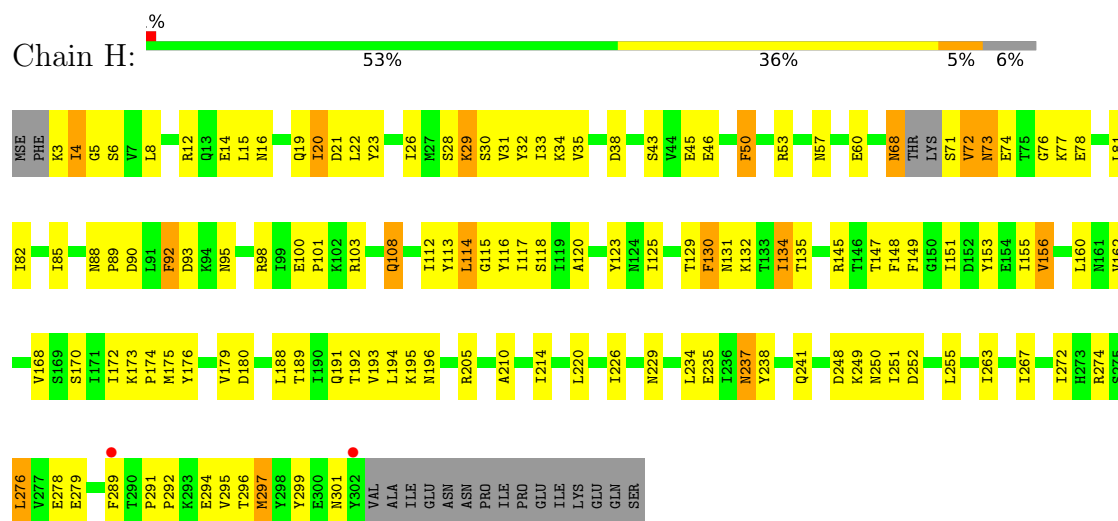
• Molecule 1: PrgX



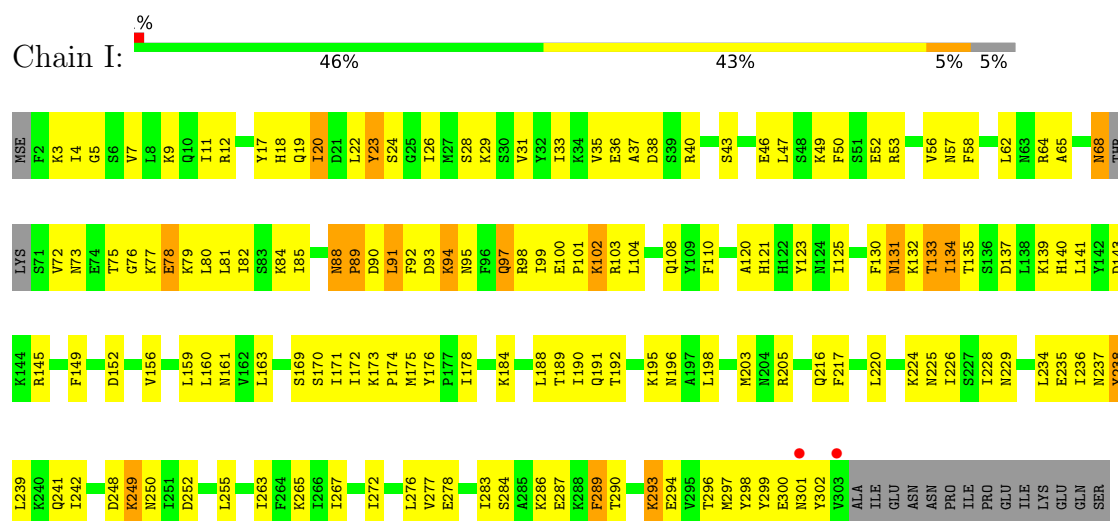
• Molecule 1: PrgX



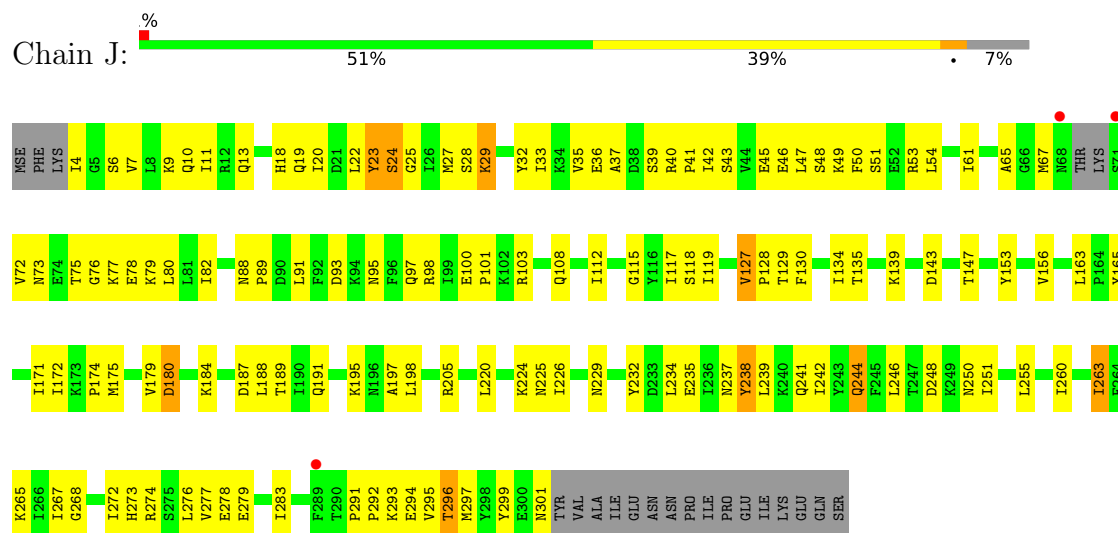
• Molecule 1: PrgX



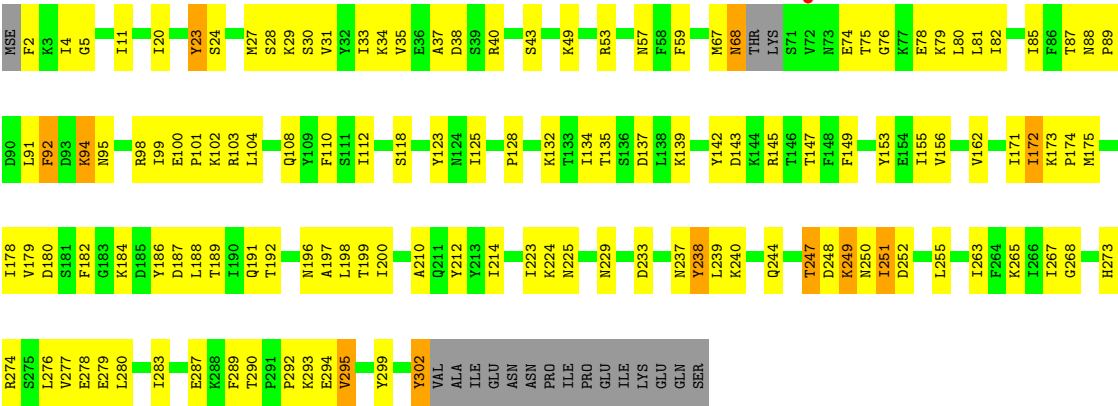
• Molecule 1: PrgX



• Molecule 1: PrgX



Chain L: 53% 38% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.65Å 134.72Å 195.93Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.90) 99.1 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.266 0.197 , 0.223	Depositor DCC
R_{free} test set	10564 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30147	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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	0.35	0/2554	0.87	6/3442 (0.2%)
1	B	0.34	0/2533	0.88	6/3414 (0.2%)
1	C	0.32	0/2521	0.84	1/3398 (0.0%)
1	D	0.34	0/2514	0.89	7/3388 (0.2%)
1	E	0.34	0/2526	0.88	9/3405 (0.3%)
1	F	0.32	0/2534	0.91	7/3416 (0.2%)
1	G	0.48	3/2555 (0.1%)	0.91	6/3444 (0.2%)
1	H	0.34	0/2514	0.89	2/3388 (0.1%)
1	I	0.32	0/2533	0.84	5/3414 (0.1%)
1	J	0.34	0/2492	0.87	3/3359 (0.1%)
1	K	0.34	0/2517	0.87	6/3394 (0.2%)
1	L	0.33	0/2526	0.88	5/3404 (0.1%)
All	All	0.35	3/30319 (0.0%)	0.88	63/40866 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	301	ASN	CA-C	-8.63	1.41	1.52
1	G	300	GLU	N-CA	-6.78	1.38	1.46
1	G	300	GLU	C-O	6.13	1.31	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	ALA	N-CA-C	-9.84	101.45	112.57
1	G	300	GLU	N-CA-C	-9.54	99.38	111.02
1	H	6	SER	N-CA-C	-9.35	100.97	111.82
1	F	172	ILE	N-CA-C	8.46	118.48	110.53
1	C	4	ILE	N-CA-C	8.38	119.17	110.62
1	F	91	LEU	N-CA-C	-6.97	104.85	113.15
1	L	88	ASN	CA-C-N	6.79	128.33	119.84
1	L	88	ASN	C-N-CA	6.79	128.33	119.84
1	F	302	TYR	N-CA-C	-6.58	96.79	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	VAL	CA-C-N	6.45	126.67	119.32
1	D	127	VAL	C-N-CA	6.45	126.67	119.32
1	A	207	LEU	N-CA-C	6.26	118.91	111.71
1	L	268	GLY	N-CA-C	6.26	122.53	115.08
1	E	142	TYR	N-CA-C	6.20	121.68	112.94
1	E	270	GLU	N-CA-C	6.13	117.96	111.28
1	G	81	LEU	N-CA-C	-6.11	105.59	113.16
1	G	268	GLY	N-CA-C	6.08	123.72	115.32
1	J	268	GLY	N-CA-C	6.04	123.62	114.61
1	A	88	ASN	CA-C-N	6.04	125.66	119.56
1	A	88	ASN	C-N-CA	6.04	125.66	119.56
1	K	185	ASP	N-CA-C	-6.04	104.78	111.36
1	F	88	ASN	CA-C-N	6.03	127.38	119.84
1	F	88	ASN	C-N-CA	6.03	127.38	119.84
1	K	87	THR	N-CA-C	-5.93	105.88	113.23
1	A	23	TYR	N-CA-C	5.83	119.58	112.23
1	E	207	LEU	N-CA-C	5.82	118.37	111.33
1	E	127	VAL	CA-C-N	5.74	125.59	119.28
1	E	127	VAL	C-N-CA	5.74	125.59	119.28
1	B	93	ASP	N-CA-C	5.73	118.26	111.33
1	L	142	TYR	N-CA-C	5.61	117.22	109.54
1	E	274	ARG	N-CA-C	-5.59	105.08	111.07
1	K	207	LEU	N-CA-C	5.59	118.31	111.82
1	L	172	ILE	N-CA-C	5.58	117.08	111.00
1	D	142	TYR	N-CA-C	5.56	119.71	111.87
1	E	268	GLY	N-CA-C	5.53	123.59	115.08
1	D	268	GLY	N-CA-C	5.48	122.89	115.32
1	J	127	VAL	CA-C-N	5.48	125.83	119.47
1	J	127	VAL	C-N-CA	5.48	125.83	119.47
1	A	154	GLU	N-CA-C	-5.35	105.36	111.14
1	I	88	ASN	CA-C-N	5.34	126.52	119.84
1	I	88	ASN	C-N-CA	5.34	126.52	119.84
1	B	99	ILE	N-CA-C	5.32	115.42	110.42
1	F	300	GLU	N-CA-C	-5.29	102.03	109.96
1	B	157	SER	N-CA-C	-5.27	105.43	111.07
1	E	39	SER	N-CA-C	-5.25	106.55	113.17
1	K	169	SER	N-CA-C	5.25	117.00	111.28
1	G	142	TYR	N-CA-C	5.20	119.37	112.72
1	B	127	VAL	CA-C-N	5.18	124.80	119.56
1	B	127	VAL	C-N-CA	5.18	124.80	119.56
1	I	110	PHE	N-CA-C	-5.18	105.82	111.82
1	D	88	ASN	CA-C-N	5.16	126.29	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	ASN	C-N-CA	5.16	126.29	119.84
1	G	88	ASN	CA-C-N	5.14	126.26	119.84
1	G	88	ASN	C-N-CA	5.14	126.26	119.84
1	K	157	SER	N-CA-C	-5.13	105.76	111.36
1	A	89	PRO	N-CA-C	5.13	120.27	113.86
1	E	297	MET	N-CA-C	-5.13	105.58	111.07
1	B	66	GLY	N-CA-C	5.13	123.27	115.63
1	D	278	GLU	N-CA-C	-5.09	105.73	111.28
1	I	296	THR	N-CA-C	-5.08	106.35	112.54
1	K	98	ARG	N-CA-C	-5.04	105.98	112.68
1	H	297	MET	N-CA-C	-5.02	105.50	110.97
1	I	238	TYR	N-CA-C	-5.02	105.72	111.14

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	2507	0	2543	93	0
1	B	2486	0	2515	112	0
1	C	2475	0	2506	126	0
1	D	2468	0	2497	94	0
1	E	2480	0	2511	101	0
1	F	2488	0	2522	129	0
1	G	2508	0	2537	159	0
1	H	2468	0	2497	135	0
1	I	2486	0	2515	153	0
1	J	2447	0	2475	122	0
1	K	2471	0	2498	102	0
1	L	2479	0	2506	117	0
2	A	37	0	0	11	0
2	B	45	0	0	6	0
2	C	25	0	0	11	0
2	D	29	0	0	6	0
2	E	33	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	42	0	0	6	0
2	G	28	0	0	19	0
2	H	36	0	0	5	0
2	I	23	0	0	10	0
2	J	28	0	0	5	0
2	K	28	0	0	12	0
2	L	30	0	0	6	0
All	All	30147	0	30122	1380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1380) 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:156:VAL:HG21	1:B:175:MSE:HE1	1.21	1.19
1:I:93:ASP:HB3	1:I:97:GLN:HE22	1.21	1.03
1:H:4:ILE:HG21	1:H:38:ASP:HA	1.38	1.01
1:C:263:ILE:HG13	1:D:263:ILE:HG13	1.42	1.01
1:B:20:ILE:HD12	1:B:20:ILE:H	1.24	0.99
1:H:191:GLN:HE22	1:H:229:ASN:H	0.99	0.99
1:C:82:ILE:HD11	1:C:112:ILE:HG23	1.45	0.98
1:K:191:GLN:NE2	1:K:229:ASN:H	1.62	0.98
1:H:4:ILE:HG22	1:H:5:GLY:H	1.29	0.97
1:A:263:ILE:HG13	1:B:263:ILE:HG13	1.46	0.97
1:L:82:ILE:HD11	1:L:112:ILE:HG23	1.47	0.96
1:C:95:ASN:HD22	1:C:98:ARG:HH22	0.98	0.96
1:G:43:SER:HA	1:H:43:SER:HA	1.45	0.95
1:G:298:TYR:HA	1:G:301:ASN:ND2	1.81	0.95
1:E:191:GLN:HE22	1:E:229:ASN:H	1.14	0.94
1:I:20:ILE:HD12	1:I:20:ILE:H	1.29	0.94
1:K:263:ILE:HG13	1:L:263:ILE:HG13	1.50	0.93
1:F:156:VAL:HG21	1:F:175:MSE:HE1	1.49	0.93
1:H:72:VAL:HG22	1:H:73:ASN:H	1.34	0.93
1:G:191:GLN:HE22	1:G:229:ASN:H	1.16	0.93
1:L:191:GLN:HE22	1:L:229:ASN:H	1.17	0.92
1:K:191:GLN:HE22	1:K:229:ASN:N	1.66	0.92
1:G:263:ILE:HG13	1:H:263:ILE:HG13	1.51	0.92
1:D:191:GLN:HE22	1:D:229:ASN:H	1.16	0.92
1:G:72:VAL:HG13	1:G:73:ASN:H	1.33	0.92
1:A:191:GLN:HE22	1:A:229:ASN:H	0.97	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ILE:HD12	1:E:20:ILE:H	1.36	0.90
1:F:191:GLN:HE22	1:F:229:ASN:H	1.17	0.89
1:G:298:TYR:HA	1:G:301:ASN:HD21	1.36	0.89
1:F:28:SER:HB3	1:F:31:VAL:HG23	1.55	0.89
1:F:300:GLU:O	1:F:301:ASN:HB2	1.72	0.88
1:H:4:ILE:HG22	1:H:5:GLY:N	1.88	0.88
1:B:172:ILE:HA	1:B:175:MSE:HE3	1.55	0.87
1:D:255:LEU:HD21	1:L:255:LEU:HD21	1.54	0.87
1:D:82:ILE:HD11	1:D:112:ILE:HG23	1.54	0.86
1:A:191:GLN:NE2	1:A:229:ASN:H	1.73	0.86
1:K:82:ILE:HD11	1:K:112:ILE:HG23	1.56	0.85
1:E:100:GLU:HB3	1:E:101:PRO:HD3	1.57	0.85
1:F:172:ILE:HA	1:F:175:MSE:HE3	1.58	0.85
1:F:29:LYS:O	1:F:33:ILE:HG12	1.77	0.85
1:J:4:ILE:HD11	1:J:7:VAL:HG23	1.59	0.85
1:A:255:LEU:HD21	1:F:255:LEU:HD21	1.56	0.84
1:C:68:ASN:HB2	2:C:329:HOH:O	1.76	0.84
1:C:95:ASN:HD22	1:C:98:ARG:NH2	1.76	0.83
1:F:172:ILE:HA	1:F:175:MSE:CE	2.08	0.83
1:I:283:ILE:HG13	2:I:323:HOH:O	1.78	0.83
1:A:251:ILE:HG21	1:F:292:PRO:HD3	1.61	0.83
1:B:297:MET:HE2	1:B:301:ASN:HD21	1.44	0.83
1:B:156:VAL:CG2	1:B:175:MSE:HE1	2.08	0.83
1:G:82:ILE:HD11	1:G:112:ILE:HG23	1.59	0.83
1:I:134:ILE:HG23	1:I:135:THR:H	1.43	0.82
1:D:294:GLU:O	1:D:297:MET:HB3	1.80	0.82
1:G:172:ILE:HD13	2:G:321:HOH:O	1.78	0.81
1:A:191:GLN:HE22	1:A:229:ASN:N	1.78	0.81
1:J:82:ILE:HD11	1:J:112:ILE:HG23	1.62	0.81
1:L:20:ILE:HD12	1:L:20:ILE:H	1.45	0.81
1:F:293:LYS:HD3	1:F:293:LYS:N	1.95	0.80
1:C:43:SER:HA	1:D:43:SER:HA	1.63	0.80
1:F:304:ALA:O	1:F:305:ILE:HG13	1.82	0.80
1:G:146:THR:HG23	1:H:14:GLU:OE1	1.81	0.80
1:D:54:LEU:HB3	2:D:319:HOH:O	1.81	0.79
1:B:82:ILE:HD11	1:B:112:ILE:HG23	1.63	0.79
1:E:292:PRO:O	1:E:295:VAL:HG22	1.83	0.79
1:F:259:ASN:HB2	2:F:341:HOH:O	1.82	0.78
1:I:7:VAL:HG21	1:I:65:ALA:HA	1.64	0.78
1:E:293:LYS:HD3	1:E:293:LYS:N	1.99	0.78
1:I:191:GLN:HE22	1:I:229:ASN:H	1.31	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.49	0.78
1:B:29:LYS:O	1:B:33:ILE:HG12	1.83	0.77
1:E:278:GLU:HG2	1:E:299:TYR:CE2	2.19	0.77
1:H:255:LEU:HD21	1:I:255:LEU:HD21	1.63	0.77
1:I:220:LEU:O	1:I:226:ILE:HG21	1.84	0.77
1:I:265:LYS:HG3	2:I:321:HOH:O	1.84	0.77
1:A:100:GLU:HB3	1:A:101:PRO:HD3	1.65	0.77
1:B:191:GLN:HE22	1:B:229:ASN:H	1.33	0.76
2:A:348:HOH:O	1:B:182:PHE:HA	1.84	0.76
1:H:4:ILE:CG2	1:H:5:GLY:H	1.98	0.76
1:K:57:ASN:HB3	2:K:338:HOH:O	1.85	0.76
1:H:191:GLN:HE22	1:H:229:ASN:N	1.80	0.76
1:F:293:LYS:HD3	1:F:293:LYS:H	1.51	0.76
1:B:156:VAL:HG21	1:B:175:MSE:CE	2.11	0.76
1:I:263:ILE:HG13	1:J:263:ILE:HG13	1.68	0.76
1:K:95:ASN:HD22	1:K:98:ARG:HH12	1.34	0.76
1:G:255:LEU:HD11	1:J:255:LEU:HD21	1.67	0.75
1:B:20:ILE:H	1:B:20:ILE:CD1	2.00	0.75
1:G:20:ILE:O	1:G:24:SER:HB3	1.84	0.75
1:F:4:ILE:HD12	1:F:4:ILE:H	1.51	0.75
1:L:91:LEU:HA	1:L:94:LYS:HD3	1.67	0.75
1:B:20:ILE:HD12	1:B:20:ILE:N	2.02	0.74
1:L:292:PRO:HG2	1:L:295:VAL:HG13	1.67	0.74
2:A:354:HOH:O	1:F:250:ASN:HA	1.86	0.74
1:B:171:ILE:O	1:B:175:MSE:HE2	1.86	0.74
1:H:103:ARG:HG2	1:H:103:ARG:HH11	1.51	0.74
1:B:179:VAL:HG23	1:B:180:ASP:OD1	1.87	0.74
1:J:95:ASN:HD22	1:J:98:ARG:HH12	1.35	0.74
1:C:74:GLU:HB3	1:D:52:GLU:OE1	1.87	0.74
1:H:294:GLU:O	1:H:297:MET:HB3	1.86	0.74
1:C:134:ILE:HG12	1:C:163:LEU:HD11	1.68	0.74
1:I:20:ILE:HA	1:I:23:TYR:CE2	2.22	0.74
1:D:78:GLU:OE1	1:D:99:ILE:HD11	1.88	0.74
1:L:171:ILE:O	1:L:175:MSE:HE3	1.87	0.74
1:C:153:TYR:HB2	1:C:189:THR:HG22	1.70	0.73
1:G:156:VAL:HG21	1:G:172:ILE:HG12	1.68	0.73
1:J:156:VAL:CG2	1:J:175:MSE:HE1	2.18	0.73
1:H:191:GLN:NE2	1:H:229:ASN:H	1.82	0.73
1:I:100:GLU:HB3	1:I:101:PRO:HD3	1.70	0.73
1:B:278:GLU:HG2	1:B:299:TYR:CE2	2.22	0.73
1:H:20:ILE:HG13	1:H:23:TYR:OH	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:PHE:HA	2:G:338:HOH:O	1.88	0.73
1:D:100:GLU:HB3	1:D:101:PRO:HD3	1.68	0.73
1:H:23:TYR:CZ	1:H:29:LYS:HB3	2.24	0.73
1:B:293:LYS:HD3	1:B:293:LYS:N	2.04	0.72
1:I:4:ILE:HD12	1:I:4:ILE:H	1.54	0.72
1:J:20:ILE:HA	1:J:23:TYR:CE2	2.24	0.72
1:C:191:GLN:HE22	1:C:229:ASN:H	1.37	0.72
1:G:293:LYS:HD3	1:G:293:LYS:N	2.05	0.72
1:L:79:LYS:HD2	1:L:112:ILE:HG12	1.69	0.72
1:C:292:PRO:HG2	1:C:295:VAL:HG13	1.71	0.72
1:K:89:PRO:HB3	1:K:123:TYR:CD2	2.24	0.72
1:B:292:PRO:HG3	1:E:251:ILE:HG21	1.71	0.71
1:G:76:GLY:O	1:G:80:LEU:HD23	1.90	0.71
1:H:278:GLU:HG2	1:H:299:TYR:CE2	2.25	0.71
1:D:30:SER:HA	1:D:33:ILE:HG12	1.73	0.71
1:I:20:ILE:H	1:I:20:ILE:CD1	2.04	0.71
1:I:43:SER:OG	1:I:46:GLU:HG3	1.90	0.71
1:J:156:VAL:HG21	1:J:175:MSE:HE1	1.72	0.71
1:I:298:TYR:HA	1:I:301:ASN:HB2	1.72	0.71
1:K:191:GLN:HE22	1:K:229:ASN:H	0.82	0.71
1:L:98:ARG:HB3	1:L:98:ARG:NH1	2.06	0.71
1:D:87:THR:O	1:D:88:ASN:HB2	1.90	0.71
1:F:291:PRO:HB2	1:F:295:VAL:HG21	1.73	0.71
1:H:82:ILE:HD11	1:H:112:ILE:HG23	1.73	0.70
1:K:139:LYS:O	1:K:143:ASP:HB2	1.90	0.70
1:C:255:LEU:HD21	1:K:255:LEU:HD21	1.71	0.70
1:E:234:LEU:HD21	1:E:263:ILE:HG21	1.74	0.70
1:L:68:ASN:N	1:L:68:ASN:HD22	1.89	0.70
1:I:278:GLU:HG2	1:I:299:TYR:CE2	2.26	0.70
1:C:148:PHE:HA	2:C:342:HOH:O	1.91	0.70
1:C:251:ILE:HD13	1:C:251:ILE:O	1.90	0.70
1:I:293:LYS:HD3	1:I:294:GLU:H	1.57	0.70
1:I:81:LEU:HD12	1:I:84:LYS:HB3	1.73	0.70
1:I:173:LYS:HB2	1:I:174:PRO:HD3	1.74	0.70
1:K:293:LYS:HD3	1:K:293:LYS:N	2.06	0.70
1:G:188:LEU:HD21	1:G:229:ASN:HD22	1.56	0.70
1:A:293:LYS:HD3	1:A:293:LYS:N	2.07	0.70
1:G:152:ASP:O	1:G:156:VAL:HG12	1.90	0.70
1:J:224:LYS:O	1:J:225:ASN:HB2	1.90	0.70
1:J:4:ILE:CD1	1:J:7:VAL:HG23	2.22	0.69
1:A:95:ASN:HA	1:A:98:ARG:HH12	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ASN:O	1:C:303:VAL:N	2.25	0.69
1:G:98:ARG:NH1	1:G:98:ARG:HB3	2.07	0.69
1:L:98:ARG:HB3	1:L:98:ARG:HH11	1.55	0.69
1:A:43:SER:OG	1:A:46:GLU:HG3	1.92	0.69
1:B:93:ASP:O	1:B:97:GLN:HG3	1.93	0.69
1:E:8:LEU:HD13	2:E:319:HOH:O	1.93	0.69
1:J:191:GLN:HE22	1:J:229:ASN:H	1.38	0.69
1:K:279:GLU:HG3	2:K:339:HOH:O	1.92	0.69
1:B:224:LYS:HG2	1:B:225:ASN:ND2	2.08	0.69
1:C:26:ILE:HD11	1:C:53:ARG:NH1	2.07	0.69
1:J:291:PRO:HG2	1:J:296:THR:HG23	1.74	0.69
1:G:210:ALA:HB1	2:G:323:HOH:O	1.92	0.69
1:I:26:ILE:HD11	1:I:53:ARG:NH1	2.08	0.69
1:F:156:VAL:HG21	1:F:175:MSE:CE	2.23	0.69
1:E:224:LYS:HE2	1:E:225:ASN:HD21	1.58	0.68
1:C:220:LEU:O	1:C:226:ILE:HG21	1.92	0.68
1:B:100:GLU:HB3	1:B:101:PRO:HD3	1.73	0.68
1:H:21:ASP:O	1:H:53:ARG:HD3	1.93	0.68
1:E:95:ASN:HA	1:E:98:ARG:HH12	1.58	0.68
1:I:52:GLU:CD	1:J:73:ASN:HD22	2.00	0.68
1:I:98:ARG:O	1:I:101:PRO:HD2	1.94	0.68
1:F:100:GLU:HB3	1:F:101:PRO:HD3	1.76	0.68
1:K:265:LYS:HB2	1:K:273:HIS:CD2	2.29	0.68
1:H:20:ILE:H	1:H:20:ILE:HD12	1.57	0.68
1:A:1:MSE:HE2	1:A:72:VAL:HG22	1.74	0.68
1:H:210:ALA:O	1:H:214:ILE:HG13	1.94	0.68
1:F:220:LEU:O	1:F:226:ILE:HG21	1.94	0.67
1:C:100:GLU:HB3	1:C:101:PRO:HD3	1.76	0.67
1:I:43:SER:HA	1:J:43:SER:HA	1.77	0.67
1:G:57:ASN:N	1:G:57:ASN:HD22	1.91	0.67
1:L:265:LYS:HB2	1:L:273:HIS:CD2	2.29	0.67
1:A:95:ASN:HD22	1:A:98:ARG:HH12	1.43	0.67
1:B:172:ILE:HA	1:B:175:MSE:CE	2.24	0.67
1:F:301:ASN:HA	1:F:304:ALA:HB3	1.75	0.67
1:B:28:SER:OG	1:B:31:VAL:HG23	1.94	0.67
1:K:148:PHE:CD2	1:K:175:MSE:HE2	2.29	0.67
1:D:293:LYS:HD3	1:D:293:LYS:N	2.09	0.67
1:A:139:LYS:HD3	2:A:351:HOH:O	1.93	0.67
1:H:22:LEU:O	1:H:26:ILE:HD12	1.94	0.67
1:E:9:LYS:HG2	1:E:13:GLN:HE21	1.60	0.67
1:L:128:PRO:O	1:L:132:LYS:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG23	2:A:327:HOH:O	1.93	0.66
1:I:248:ASP:O	1:I:249:LYS:C	2.39	0.66
1:L:76:GLY:O	1:L:80:LEU:HD23	1.95	0.66
1:F:81:LEU:O	1:F:85:ILE:HG13	1.94	0.66
1:A:224:LYS:HG2	1:A:225:ASN:ND2	2.11	0.66
1:F:265:LYS:HB2	1:F:273:HIS:CD2	2.31	0.66
1:C:176:TYR:HB3	1:C:216:GLN:OE1	1.96	0.66
1:E:103:ARG:HG2	1:E:103:ARG:HH11	1.60	0.66
1:L:20:ILE:HA	1:L:23:TYR:CE2	2.30	0.66
1:D:229:ASN:HB3	1:D:232:TYR:HB2	1.78	0.65
1:J:95:ASN:ND2	1:J:98:ARG:HH22	1.94	0.65
1:H:4:ILE:CG2	1:H:5:GLY:N	2.58	0.65
1:H:235:GLU:O	1:H:238:TYR:HB3	1.96	0.65
1:K:292:PRO:HG2	1:K:295:VAL:HG22	1.77	0.65
1:K:224:LYS:O	1:K:225:ASN:HB2	1.96	0.65
1:A:250:ASN:HB3	1:A:253:SER:HB2	1.76	0.65
1:D:28:SER:HB3	1:D:31:VAL:HG23	1.79	0.65
1:H:89:PRO:HG3	1:H:123:TYR:CE2	2.32	0.65
1:L:171:ILE:HG22	1:L:175:MSE:CE	2.26	0.65
1:F:273:HIS:O	1:F:277:VAL:HG23	1.97	0.65
1:L:95:ASN:HA	1:L:98:ARG:HH12	1.60	0.65
1:L:23:TYR:HD2	1:L:24:SER:N	1.94	0.65
1:L:95:ASN:HD22	1:L:98:ARG:HH22	1.43	0.65
1:L:278:GLU:HG2	1:L:299:TYR:CE2	2.32	0.65
1:I:294:GLU:O	1:I:297:MET:HB3	1.97	0.65
1:K:82:ILE:CD1	1:K:112:ILE:HG23	2.26	0.65
1:K:43:SER:HA	1:L:43:SER:HA	1.77	0.65
1:C:75:THR:HG21	1:C:108:GLN:HB3	1.77	0.64
1:C:95:ASN:ND2	1:C:98:ARG:HH22	1.83	0.64
1:D:153:TYR:HB2	1:D:189:THR:HG22	1.79	0.64
1:I:94:LYS:NZ	1:I:94:LYS:H	1.94	0.64
1:K:283:ILE:HG13	2:K:320:HOH:O	1.96	0.64
1:A:82:ILE:HD11	1:A:112:ILE:HG23	1.78	0.64
1:I:235:GLU:O	1:I:238:TYR:HB3	1.97	0.64
1:B:43:SER:OG	1:B:46:GLU:HG3	1.98	0.64
1:C:79:LYS:HD2	1:C:112:ILE:HG12	1.78	0.64
1:F:171:ILE:HG22	1:F:175:MSE:HE2	1.79	0.64
1:G:81:LEU:O	1:G:85:ILE:HG13	1.98	0.64
1:K:99:ILE:HG13	1:K:116:TYR:CE1	2.32	0.64
1:K:293:LYS:HD3	1:K:293:LYS:H	1.62	0.64
1:B:293:LYS:HD3	1:B:293:LYS:H	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ARG:O	1:F:278:GLU:HG3	1.96	0.64
1:I:156:VAL:CG1	1:I:172:ILE:HG12	2.27	0.64
1:L:100:GLU:HB3	1:L:101:PRO:HD3	1.79	0.64
1:F:292:PRO:HG2	1:F:295:VAL:HG22	1.79	0.64
1:G:43:SER:OG	1:G:46:GLU:HG3	1.96	0.64
1:L:98:ARG:O	1:L:102:LYS:HD3	1.98	0.64
1:C:86:PHE:CD1	1:C:119:ILE:HG12	2.33	0.64
1:I:20:ILE:HD12	1:I:20:ILE:N	2.08	0.64
1:I:170:SER:OG	1:I:171:ILE:HD12	1.98	0.64
1:I:191:GLN:NE2	1:I:229:ASN:H	1.96	0.64
1:B:153:TYR:HB2	1:B:189:THR:HG22	1.80	0.64
1:J:278:GLU:HG3	1:J:299:TYR:HE2	1.62	0.64
1:C:293:LYS:HD3	1:C:294:GLU:H	1.64	0.63
1:D:4:ILE:HG22	2:D:338:HOH:O	1.97	0.63
1:D:57:ASN:HB2	1:D:60:GLU:HB2	1.81	0.63
1:J:100:GLU:HB3	1:J:101:PRO:HD3	1.81	0.63
1:L:98:ARG:HH11	1:L:98:ARG:CB	2.11	0.63
1:G:132:LYS:NZ	1:G:132:LYS:HB3	2.14	0.63
1:H:205:ARG:HG2	1:H:205:ARG:HH11	1.64	0.63
1:J:4:ILE:HD13	1:J:6:SER:OG	1.99	0.63
1:L:27:MSE:HE1	1:L:40:ARG:HH22	1.63	0.63
1:H:20:ILE:HD12	1:H:20:ILE:N	2.12	0.63
1:I:23:TYR:HD2	1:I:24:SER:N	1.96	0.63
1:E:178:ILE:HG13	1:E:190:ILE:HD12	1.80	0.63
1:H:26:ILE:HD11	1:H:53:ARG:HE	1.63	0.63
1:H:68:ASN:HD22	1:H:68:ASN:N	1.95	0.63
1:K:178:ILE:O	1:K:223:ILE:HD11	1.99	0.63
1:B:23:TYR:OH	1:B:29:LYS:HE3	1.98	0.63
1:E:191:GLN:NE2	1:E:229:ASN:H	1.91	0.63
1:G:299:TYR:O	1:G:300:GLU:C	2.40	0.63
1:C:171:ILE:O	1:C:174:PRO:HD2	1.98	0.63
1:G:156:VAL:CG2	1:G:172:ILE:HG12	2.28	0.63
1:L:292:PRO:HG2	1:L:295:VAL:CG1	2.29	0.63
1:L:110:PHE:HD2	1:L:155:ILE:HD13	1.64	0.62
1:L:171:ILE:HG22	1:L:175:MSE:HE3	1.81	0.62
1:B:278:GLU:HG2	1:B:299:TYR:HE2	1.63	0.62
1:J:153:TYR:HB2	1:J:189:THR:HG22	1.81	0.62
1:F:43:SER:OG	1:F:46:GLU:HB2	2.00	0.62
1:G:20:ILE:HD12	1:G:20:ILE:H	1.63	0.62
1:L:4:ILE:HD12	1:L:4:ILE:H	1.64	0.62
1:G:20:ILE:HA	1:G:23:TYR:CE1	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:PRO:HG3	1:E:123:TYR:CE2	2.34	0.62
1:L:94:LYS:NZ	1:L:94:LYS:HB3	2.14	0.62
1:G:138:LEU:HD13	1:G:171:ILE:HD11	1.81	0.62
1:L:134:ILE:HG23	1:L:135:THR:N	2.15	0.62
1:H:148:PHE:CD1	1:H:175:MSE:HG2	2.35	0.62
1:J:265:LYS:HB2	1:J:273:HIS:CD2	2.35	0.62
1:A:274:ARG:HG2	1:A:274:ARG:NH1	2.15	0.61
1:F:272:ILE:HG22	1:F:276:LEU:HD22	1.81	0.61
1:J:79:LYS:HG3	1:J:112:ILE:HD11	1.81	0.61
1:B:68:ASN:H	1:B:68:ASN:HD22	1.47	0.61
1:E:4:ILE:HD11	1:F:44:VAL:HG11	1.81	0.61
1:H:279:GLU:HB3	2:H:328:HOH:O	2.00	0.61
1:F:82:ILE:HD11	1:F:112:ILE:HG23	1.81	0.61
1:H:172:ILE:HA	1:H:175:MSE:HE3	1.80	0.61
1:L:81:LEU:O	1:L:85:ILE:HG13	1.99	0.61
1:F:23:TYR:C	1:F:23:TYR:HD2	2.09	0.61
1:G:301:ASN:O	1:G:304:ALA:N	2.33	0.61
1:L:20:ILE:HD12	1:L:20:ILE:N	2.14	0.61
1:E:12:ARG:HG3	1:E:17:TYR:HB2	1.81	0.61
1:I:76:GLY:O	1:I:80:LEU:HG	2.00	0.61
1:K:43:SER:OG	1:K:46:GLU:HG3	2.01	0.61
1:L:49:LYS:O	1:L:53:ARG:HG2	1.99	0.61
1:A:263:ILE:CG1	1:B:263:ILE:HG13	2.28	0.61
1:A:277:VAL:HG13	1:A:299:TYR:HB2	1.81	0.61
1:C:191:GLN:HE22	1:C:228:ILE:HA	1.65	0.61
1:J:172:ILE:HA	1:J:175:MSE:HE3	1.83	0.61
1:A:68:ASN:N	1:A:68:ASN:HD22	1.99	0.61
1:A:293:LYS:HD3	1:A:294:GLU:H	1.64	0.61
1:E:191:GLN:HE22	1:E:229:ASN:N	1.93	0.61
1:I:102:LYS:H	1:I:102:LYS:HD3	1.66	0.61
1:I:134:ILE:HG23	1:I:135:THR:N	2.15	0.61
1:C:137:ASP:O	1:C:141:LEU:HG	2.01	0.61
1:E:267:ILE:HA	1:F:237:ASN:ND2	2.15	0.61
1:G:26:ILE:HD11	1:G:53:ARG:NH1	2.16	0.61
1:I:49:LYS:O	1:I:53:ARG:HG2	2.00	0.61
1:K:156:VAL:HG11	1:K:172:ILE:HG12	1.83	0.61
1:A:43:SER:HA	1:B:43:SER:HA	1.83	0.61
1:E:20:ILE:H	1:E:20:ILE:CD1	2.12	0.61
1:G:23:TYR:OH	1:G:29:LYS:HD2	2.01	0.61
1:J:20:ILE:O	1:J:24:SER:HB3	2.01	0.61
1:L:187:ASP:O	1:L:191:GLN:HG3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:ASN:N	1:L:68:ASN:ND2	2.45	0.60
1:G:68:ASN:H	1:G:68:ASN:HD22	1.48	0.60
1:C:67:MSE:HE3	2:C:322:HOH:O	2.01	0.60
1:D:95:ASN:ND2	1:D:98:ARG:HH12	2.00	0.60
1:E:293:LYS:HD3	1:E:294:GLU:H	1.65	0.60
1:H:134:ILE:HG23	1:H:135:THR:N	2.16	0.60
1:L:293:LYS:HD3	1:L:294:GLU:H	1.67	0.60
1:F:49:LYS:O	1:F:53:ARG:HG2	2.01	0.60
1:E:72:VAL:HG13	1:E:73:ASN:N	2.15	0.60
1:J:171:ILE:HG22	1:J:175:MSE:CE	2.31	0.60
1:D:134:ILE:HG23	1:D:135:THR:N	2.17	0.60
1:G:173:LYS:HB2	1:G:174:PRO:HD3	1.83	0.60
1:K:237:ASN:ND2	1:L:267:ILE:HA	2.16	0.60
1:G:198:LEU:HD11	2:G:323:HOH:O	2.00	0.60
1:H:272:ILE:HG22	1:H:276:LEU:HD22	1.83	0.60
1:K:99:ILE:HG13	1:K:116:TYR:CZ	2.37	0.60
1:F:3:LYS:HB3	1:F:4:ILE:HD12	1.83	0.60
1:G:72:VAL:HG13	1:G:73:ASN:N	2.13	0.60
1:I:156:VAL:HG13	1:I:172:ILE:HG12	1.83	0.60
1:G:143:ASP:O	1:G:144:LYS:HB2	2.02	0.60
1:K:184:LYS:HB3	1:L:184:LYS:HD3	1.84	0.60
1:L:28:SER:OG	1:L:31:VAL:HG23	2.01	0.60
1:J:134:ILE:HG23	1:J:135:THR:N	2.17	0.59
1:A:26:ILE:HD11	1:A:53:ARG:HH12	1.67	0.59
1:B:273:HIS:O	1:B:277:VAL:HG23	2.01	0.59
1:H:103:ARG:HG2	1:H:103:ARG:NH1	2.17	0.59
1:I:88:ASN:ND2	1:I:91:LEU:HG	2.17	0.59
1:F:23:TYR:C	1:F:23:TYR:CD2	2.80	0.59
1:I:224:LYS:HE2	1:I:225:ASN:ND2	2.17	0.59
1:J:23:TYR:HE1	1:J:29:LYS:HA	1.67	0.59
1:C:24:SER:O	1:C:53:ARG:NH2	2.34	0.59
1:D:293:LYS:HD3	1:D:293:LYS:H	1.67	0.59
1:E:265:LYS:HB2	1:E:273:HIS:CD2	2.36	0.59
1:F:156:VAL:HG11	1:F:172:ILE:HG12	1.83	0.59
1:G:134:ILE:C	1:G:136:SER:H	2.10	0.59
1:F:23:TYR:HD2	1:F:24:SER:N	2.01	0.59
1:J:171:ILE:HG22	1:J:175:MSE:HE2	1.85	0.59
1:A:62:LEU:HB3	1:A:67:MSE:HG3	1.83	0.59
1:D:20:ILE:O	1:D:24:SER:HB3	2.02	0.59
1:L:78:GLU:OE2	1:L:99:ILE:HD11	2.02	0.59
1:C:168:VAL:O	1:C:172:ILE:HG13	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:HG2	1:C:299:TYR:CE2	2.38	0.59
1:F:71:SER:OG	1:F:80:LEU:HD21	2.02	0.59
1:G:293:LYS:HD3	1:G:294:GLU:H	1.67	0.59
1:C:271:ASP:HB2	2:C:326:HOH:O	2.03	0.59
1:I:37:ALA:O	1:I:38:ASP:HB2	2.03	0.59
1:I:293:LYS:HD3	1:I:293:LYS:N	2.17	0.59
1:C:11:ILE:HG21	1:C:56:VAL:HG21	1.83	0.59
1:D:233:ASP:O	1:D:237:ASN:HB2	2.02	0.59
1:F:90:ASP:C	1:F:92:PHE:H	2.09	0.59
1:G:86:PHE:HD1	1:G:119:ILE:HG23	1.68	0.59
1:H:129:THR:HA	1:H:132:LYS:HZ3	1.68	0.59
1:D:156:VAL:HG11	1:D:172:ILE:HG12	1.84	0.59
1:F:271:ASP:HB2	2:F:345:HOH:O	2.01	0.59
1:J:48:SER:O	1:J:51:SER:HB3	2.02	0.59
1:C:79:LYS:HG2	1:C:112:ILE:HD11	1.85	0.58
1:G:151:ILE:O	1:G:155:ILE:HG13	2.02	0.58
1:C:28:SER:OG	1:C:31:VAL:HG23	2.01	0.58
1:G:148:PHE:CG	1:G:175:MSE:HG2	2.39	0.58
1:B:94:LYS:HB3	1:B:94:LYS:HZ2	1.68	0.58
1:H:92:PHE:CZ	1:H:120:ALA:HB2	2.38	0.58
1:L:179:VAL:HG23	1:L:180:ASP:OD1	2.03	0.58
1:E:98:ARG:HB3	1:E:98:ARG:NH1	2.19	0.58
1:A:156:VAL:HG11	1:A:172:ILE:HG12	1.85	0.58
1:C:145:ARG:HA	1:D:14:GLU:OE2	2.04	0.58
1:F:89:PRO:HG3	1:F:123:TYR:CE2	2.39	0.58
1:H:5:GLY:O	1:H:8:LEU:HB2	2.03	0.58
1:B:246:LEU:HD21	1:B:283:ILE:CD1	2.33	0.58
1:F:68:ASN:O	1:F:71:SER:HB2	2.04	0.58
1:F:156:VAL:CG2	1:F:175:MSE:HE1	2.29	0.58
1:J:19:GLN:HE22	1:J:33:ILE:HD13	1.69	0.58
1:K:113:TYR:O	1:K:117:ILE:HG12	2.03	0.58
1:E:95:ASN:HA	1:E:98:ARG:NH1	2.19	0.58
1:H:176:TYR:CE2	1:H:194:LEU:HD21	2.38	0.58
1:K:85:ILE:O	1:K:85:ILE:HG22	2.04	0.58
1:K:274:ARG:HG2	1:K:274:ARG:HH11	1.68	0.58
1:I:31:VAL:O	1:I:35:VAL:HG23	2.04	0.57
1:B:95:ASN:HD22	1:B:98:ARG:HH22	1.52	0.57
1:F:171:ILE:O	1:F:175:MSE:HE2	2.03	0.57
1:I:3:LYS:O	1:I:3:LYS:HG3	2.03	0.57
1:J:4:ILE:HD12	1:J:4:ILE:O	2.04	0.57
1:B:81:LEU:HD12	1:B:84:LYS:HD2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:TYR:O	1:H:35:VAL:HB	2.04	0.57
1:I:92:PHE:CE2	1:I:125:ILE:HG21	2.39	0.57
1:E:72:VAL:HG13	1:E:73:ASN:H	1.68	0.57
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.69	0.57
1:H:4:ILE:N	1:H:4:ILE:HD12	2.18	0.57
1:I:91:LEU:HA	1:I:94:LYS:HE2	1.87	0.57
1:E:224:LYS:HE2	1:E:225:ASN:ND2	2.18	0.57
1:G:8:LEU:O	1:G:12:ARG:HB2	2.04	0.57
1:B:187:ASP:O	1:B:191:GLN:HG3	2.04	0.57
1:E:293:LYS:CD	1:E:294:GLU:H	2.17	0.57
1:I:4:ILE:HD12	1:I:4:ILE:N	2.19	0.57
1:J:278:GLU:HG3	1:J:299:TYR:CE2	2.39	0.57
1:B:297:MET:HE3	1:B:297:MET:HA	1.85	0.57
1:G:20:ILE:HD12	1:G:20:ILE:N	2.20	0.57
1:G:143:ASP:O	1:G:144:LYS:CB	2.52	0.57
1:C:123:TYR:O	1:C:124:ASN:HB2	2.05	0.57
1:D:50:PHE:O	1:D:54:LEU:HD12	2.05	0.57
1:C:9:LYS:HB2	1:C:36:GLU:HG2	1.87	0.57
1:F:98:ARG:HB3	1:F:98:ARG:NH1	2.20	0.57
1:G:95:ASN:N	1:G:95:ASN:HD22	2.02	0.57
1:G:271:ASP:HB2	2:G:324:HOH:O	2.05	0.57
1:K:155:ILE:HD13	2:K:319:HOH:O	2.04	0.57
1:D:34:LYS:HB3	1:D:40:ARG:HB2	1.87	0.56
1:D:277:VAL:HG21	2:D:318:HOH:O	2.03	0.56
1:J:156:VAL:HG21	1:J:175:MSE:CE	2.35	0.56
1:J:272:ILE:O	1:J:276:LEU:HD13	2.04	0.56
1:C:236:ILE:O	1:C:240:LYS:HG3	2.04	0.56
1:D:24:SER:OG	1:D:53:ARG:NH2	2.38	0.56
1:I:88:ASN:HD22	1:I:91:LEU:HG	1.71	0.56
1:J:274:ARG:HG3	2:J:337:HOH:O	2.04	0.56
1:L:75:THR:HG21	1:L:108:GLN:HB3	1.87	0.56
1:L:251:ILE:HD13	1:L:251:ILE:O	2.05	0.56
1:L:274:ARG:HA	1:L:302:TYR:CE1	2.40	0.56
1:C:135:THR:HG22	1:C:139:LYS:NZ	2.21	0.56
1:I:284:SER:HB3	1:I:289:PHE:HB3	1.87	0.56
1:K:242:ILE:HG21	2:K:320:HOH:O	2.05	0.56
1:B:130:PHE:CE1	1:B:134:ILE:HD13	2.41	0.56
1:I:75:THR:HG23	2:I:324:HOH:O	2.04	0.56
1:L:2:PHE:HB2	1:L:4:ILE:CD1	2.36	0.56
1:J:43:SER:OG	1:J:46:GLU:HG3	2.06	0.56
1:I:300:GLU:C	1:I:302:TYR:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:LEU:HD21	1:E:95:ASN:ND2	2.20	0.56
1:B:47:LEU:HG	1:B:58:PHE:CE1	2.41	0.56
1:C:43:SER:OG	1:C:46:GLU:HG3	2.06	0.56
1:G:20:ILE:H	1:G:20:ILE:CD1	2.19	0.56
1:G:96:PHE:O	1:G:100:GLU:HB2	2.05	0.56
1:I:139:LYS:O	1:I:143:ASP:HB2	2.06	0.56
1:C:191:GLN:NE2	1:C:229:ASN:H	2.04	0.55
1:D:49:LYS:O	1:D:53:ARG:HG2	2.06	0.55
1:D:248:ASP:O	1:D:249:LYS:C	2.48	0.55
1:G:15:LEU:O	1:G:16:ASN:HB2	2.06	0.55
1:G:78:GLU:OE2	1:G:99:ILE:HD11	2.07	0.55
1:H:3:LYS:N	1:H:4:ILE:HD12	2.21	0.55
1:H:30:SER:O	1:H:34:LYS:HG3	2.06	0.55
1:A:3:LYS:HB2	1:A:6:SER:OG	2.06	0.55
1:E:26:ILE:HD11	1:E:53:ARG:NH1	2.21	0.55
1:I:20:ILE:HA	1:I:23:TYR:CZ	2.40	0.55
1:K:75:THR:HG21	1:K:108:GLN:HB3	1.89	0.55
1:H:289:PHE:CE1	1:I:289:PHE:CE2	2.95	0.55
1:J:88:ASN:ND2	1:J:91:LEU:HG	2.22	0.55
1:L:20:ILE:H	1:L:20:ILE:CD1	2.18	0.55
1:C:293:LYS:HD3	1:C:293:LYS:N	2.21	0.55
1:E:293:LYS:HD3	1:E:293:LYS:H	1.69	0.55
1:G:23:TYR:CE2	1:G:29:LYS:HB2	2.42	0.55
1:H:98:ARG:O	1:H:101:PRO:HD2	2.06	0.55
1:I:108:GLN:HB3	2:I:324:HOH:O	2.06	0.55
1:E:12:ARG:HD3	1:E:22:LEU:HG	1.88	0.55
1:B:192:THR:HG22	1:B:196:ASN:ND2	2.22	0.55
1:C:210:ALA:O	1:C:214:ILE:HG13	2.06	0.55
1:F:85:ILE:HD11	1:F:95:ASN:OD1	2.07	0.55
1:H:156:VAL:CG2	1:H:175:MSE:HE1	2.37	0.55
1:C:29:LYS:O	1:C:33:ILE:HG13	2.07	0.55
1:C:66:GLY:O	1:C:68:ASN:N	2.40	0.55
1:C:153:TYR:CB	1:C:189:THR:HG22	2.36	0.55
1:G:274:ARG:HG3	1:G:302:TYR:CD1	2.41	0.55
1:I:149:PHE:CE2	1:J:11:ILE:HG12	2.41	0.55
1:L:279:GLU:HG2	2:L:322:HOH:O	2.06	0.55
1:F:88:ASN:N	1:F:89:PRO:HD3	2.22	0.55
1:C:78:GLU:CD	1:C:99:ILE:HD11	2.32	0.54
1:E:71:SER:N	1:E:76:GLY:HA3	2.22	0.54
1:F:28:SER:HB3	1:F:31:VAL:CG2	2.34	0.54
1:B:95:ASN:HA	1:B:98:ARG:NH1	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HB3	1:C:67:MSE:HG3	1.90	0.54
1:G:128:PRO:O	1:G:132:LYS:HE2	2.08	0.54
1:I:226:ILE:HG23	1:I:226:ILE:O	2.07	0.54
1:A:4:ILE:HD11	1:B:44:VAL:HG11	1.88	0.54
1:E:179:VAL:HG23	1:E:180:ASP:OD1	2.06	0.54
1:H:20:ILE:H	1:H:20:ILE:CD1	2.20	0.54
1:I:72:VAL:HG13	1:I:73:ASN:N	2.22	0.54
1:H:274:ARG:HG3	1:H:274:ARG:HH11	1.72	0.54
1:I:79:LYS:O	1:I:82:ILE:HG22	2.07	0.54
1:J:244:GLN:NE2	2:J:340:HOH:O	2.40	0.54
1:D:301:ASN:O	1:D:302:TYR:C	2.49	0.54
1:E:20:ILE:HD12	1:E:20:ILE:N	2.16	0.54
1:F:125:ILE:HG22	1:F:126:GLU:N	2.23	0.54
1:H:20:ILE:HA	1:H:23:TYR:CE1	2.43	0.54
1:A:92:PHE:CZ	1:A:120:ALA:HB2	2.43	0.54
1:C:77:LYS:O	1:C:81:LEU:HD13	2.08	0.54
1:D:12:ARG:HD3	1:D:22:LEU:HG	1.89	0.54
1:D:29:LYS:O	1:D:33:ILE:HG12	2.08	0.54
1:J:27:MSE:SE	1:J:35:VAL:HG21	2.57	0.54
1:K:20:ILE:O	1:K:24:SER:HB3	2.08	0.54
1:K:134:ILE:HG23	1:K:135:THR:N	2.23	0.54
1:L:103:ARG:HG2	1:L:103:ARG:HH11	1.73	0.54
1:E:88:ASN:ND2	1:E:91:LEU:HG	2.23	0.54
1:L:95:ASN:HA	1:L:98:ARG:NH1	2.22	0.54
1:I:4:ILE:H	1:I:4:ILE:CD1	2.19	0.54
1:I:26:ILE:HD11	1:I:53:ARG:HH11	1.73	0.54
1:L:81:LEU:HD21	1:L:95:ASN:ND2	2.23	0.54
1:L:280:LEU:HD22	2:L:321:HOH:O	2.07	0.54
1:D:291:PRO:HB2	1:D:295:VAL:CG2	2.37	0.54
1:G:54:LEU:HD11	2:G:322:HOH:O	2.08	0.54
1:H:129:THR:HA	1:H:132:LYS:NZ	2.23	0.54
1:C:60:GLU:HG2	1:C:64:ARG:HE	1.73	0.54
1:F:172:ILE:HA	1:F:175:MSE:HE2	1.88	0.54
1:K:153:TYR:HB2	1:K:189:THR:HG22	1.90	0.54
1:L:224:LYS:O	1:L:225:ASN:HB2	2.08	0.54
1:F:84:LYS:HB2	1:F:84:LYS:NZ	2.23	0.53
1:A:68:ASN:N	1:A:68:ASN:ND2	2.57	0.53
1:I:28:SER:OG	1:I:31:VAL:HG23	2.08	0.53
1:I:104:LEU:HD21	1:I:137:ASP:HB3	1.89	0.53
1:K:153:TYR:CB	1:K:189:THR:HG22	2.38	0.53
1:F:152:ASP:O	1:F:156:VAL:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:LEU:HB2	2:G:338:HOH:O	2.07	0.53
1:G:80:LEU:N	1:G:80:LEU:HD22	2.24	0.53
1:K:94:LYS:HB2	1:K:94:LYS:NZ	2.23	0.53
1:K:8:LEU:HD13	2:K:318:HOH:O	2.08	0.53
1:C:108:GLN:O	1:C:112:ILE:HG13	2.08	0.53
1:G:298:TYR:HB3	2:G:319:HOH:O	2.07	0.53
1:H:156:VAL:HG21	1:H:175:MSE:HE1	1.88	0.53
1:K:297:MET:HE3	1:K:297:MET:HA	1.90	0.53
1:F:191:GLN:NE2	1:F:229:ASN:H	1.97	0.53
1:F:257:ALA:O	1:F:261:ILE:HG13	2.08	0.53
1:G:119:ILE:HB	2:G:340:HOH:O	2.09	0.53
1:H:46:GLU:O	1:H:50:PHE:CD1	2.62	0.53
1:A:138:LEU:HD13	1:A:171:ILE:CD1	2.38	0.53
1:D:278:GLU:HG2	1:D:299:TYR:CE2	2.43	0.53
1:F:165:TYR:HE1	2:F:321:HOH:O	1.91	0.53
1:G:68:ASN:H	1:G:68:ASN:ND2	2.07	0.53
1:F:299:TYR:O	1:F:302:TYR:HB2	2.08	0.53
1:G:134:ILE:HG23	1:G:135:THR:N	2.24	0.53
1:B:37:ALA:O	1:B:38:ASP:HB2	2.09	0.53
1:B:89:PRO:HG3	1:B:123:TYR:CE2	2.43	0.53
1:G:7:VAL:HG21	1:G:65:ALA:HB2	1.91	0.53
1:G:28:SER:OG	1:G:31:VAL:HG23	2.09	0.53
1:L:134:ILE:HG23	1:L:135:THR:H	1.73	0.53
1:F:87:THR:O	1:F:88:ASN:HB2	2.09	0.53
1:I:205:ARG:HG2	1:I:205:ARG:HH11	1.74	0.53
1:B:209:GLU:O	1:B:212:TYR:HB3	2.09	0.52
1:G:85:ILE:HG22	1:G:85:ILE:O	2.07	0.52
1:G:98:ARG:NH1	1:G:98:ARG:CB	2.72	0.52
1:G:135:THR:HG22	1:G:135:THR:O	2.08	0.52
1:H:251:ILE:O	1:H:255:LEU:HG	2.08	0.52
1:A:176:TYR:CE2	1:A:194:LEU:HD21	2.44	0.52
1:C:80:LEU:HD12	1:C:84:LYS:NZ	2.24	0.52
1:D:278:GLU:HG2	1:D:299:TYR:HE2	1.73	0.52
1:H:26:ILE:CD1	1:H:53:ARG:HE	2.21	0.52
1:J:171:ILE:O	1:J:174:PRO:HD2	2.09	0.52
1:I:178:ILE:HG13	1:I:190:ILE:HD12	1.90	0.52
1:B:255:LEU:HD21	1:E:255:LEU:HD21	1.90	0.52
1:C:248:ASP:O	1:C:250:ASN:N	2.42	0.52
1:C:153:TYR:HB2	1:C:189:THR:CG2	2.39	0.52
1:G:153:TYR:HA	1:G:156:VAL:CG1	2.39	0.52
1:H:134:ILE:HG23	1:H:135:THR:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:LYS:O	1:J:13:GLN:HG3	2.08	0.52
1:K:19:GLN:OE1	1:K:33:ILE:HG12	2.10	0.52
1:D:23:TYR:HB3	1:D:32:TYR:CD2	2.45	0.52
1:G:188:LEU:CD2	1:G:229:ASN:HD22	2.21	0.52
1:K:115:GLY:O	1:K:118:SER:HB3	2.10	0.52
1:L:23:TYR:CD1	1:L:29:LYS:HA	2.44	0.52
1:L:197:ALA:HB1	2:L:319:HOH:O	2.08	0.52
1:D:173:LYS:HE3	2:D:330:HOH:O	2.08	0.52
1:D:292:PRO:HD3	1:L:251:ILE:HG21	1.91	0.52
1:E:103:ARG:HG2	1:E:103:ARG:NH1	2.24	0.52
1:G:278:GLU:HG2	1:G:299:TYR:CE2	2.44	0.52
1:H:192:THR:HG22	1:H:196:ASN:ND2	2.25	0.52
1:K:4:ILE:N	2:K:324:HOH:O	2.42	0.52
1:B:7:VAL:HG21	1:B:65:ALA:HA	1.91	0.52
1:B:203:MSE:C	1:B:205:ARG:H	2.18	0.52
1:G:29:LYS:O	1:G:33:ILE:HG13	2.09	0.52
1:J:23:TYR:C	1:J:23:TYR:CD2	2.85	0.52
1:J:27:MSE:HE3	1:J:46:GLU:OE2	2.10	0.52
1:L:238:TYR:HE2	2:L:321:HOH:O	1.92	0.52
1:G:98:ARG:HB3	1:G:98:ARG:CZ	2.39	0.52
1:H:8:LEU:O	1:H:12:ARG:HB2	2.10	0.52
1:H:71:SER:O	1:H:72:VAL:HG12	2.09	0.52
1:H:237:ASN:O	1:H:241:GLN:HG2	2.10	0.52
1:J:53:ARG:HG2	1:J:53:ARG:HH11	1.74	0.52
1:L:156:VAL:HG11	1:L:172:ILE:HG12	1.91	0.52
1:D:30:SER:HA	1:D:33:ILE:CG1	2.39	0.52
1:G:202:ILE:HG12	2:G:323:HOH:O	2.10	0.52
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.75	0.51
1:B:292:PRO:HG3	1:E:251:ILE:CG2	2.38	0.51
1:F:40:ARG:HG2	1:F:40:ARG:HH21	1.75	0.51
1:F:291:PRO:HB2	1:F:295:VAL:CG2	2.40	0.51
1:H:72:VAL:CG1	1:H:76:GLY:HA3	2.40	0.51
1:H:295:VAL:HG23	1:H:296:THR:N	2.25	0.51
1:I:29:LYS:O	1:I:33:ILE:HG12	2.11	0.51
1:B:57:ASN:HB3	1:B:60:GLU:HB2	1.91	0.51
1:F:96:PHE:O	1:F:100:GLU:HB2	2.09	0.51
1:F:171:ILE:O	1:F:174:PRO:HD2	2.10	0.51
1:G:217:PHE:O	1:G:220:LEU:HB2	2.10	0.51
1:H:72:VAL:HG22	1:H:73:ASN:N	2.14	0.51
1:J:238:TYR:HB2	1:J:260:ILE:HG21	1.91	0.51
1:A:156:VAL:CG1	1:A:172:ILE:HG12	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:TYR:HE1	2:J:318:HOH:O	1.92	0.51
1:B:288:LYS:HA	1:B:288:LYS:HE3	1.92	0.51
1:B:293:LYS:HD3	1:B:294:GLU:H	1.75	0.51
1:C:191:GLN:HE22	1:C:229:ASN:N	2.07	0.51
1:E:93:ASP:O	1:E:97:GLN:HG3	2.11	0.51
1:E:195:LYS:HD3	1:E:235:GLU:OE2	2.11	0.51
1:G:229:ASN:HB3	1:G:232:TYR:HB2	1.91	0.51
1:I:248:ASP:O	1:I:250:ASN:N	2.43	0.51
1:I:283:ILE:O	1:I:287:GLU:HG2	2.09	0.51
1:J:45:GLU:O	1:J:48:SER:HB3	2.11	0.51
1:K:100:GLU:HB3	1:K:101:PRO:HD3	1.92	0.51
1:A:66:GLY:C	1:A:68:ASN:H	2.19	0.51
1:F:153:TYR:HB2	1:F:189:THR:HG22	1.91	0.51
1:F:220:LEU:HB3	1:F:226:ILE:HD13	1.92	0.51
1:G:237:ASN:ND2	1:H:267:ILE:HA	2.25	0.51
1:J:72:VAL:O	1:J:77:LYS:HE3	2.09	0.51
1:K:59:PHE:HB2	2:K:338:HOH:O	2.11	0.51
1:G:293:LYS:CD	1:G:294:GLU:H	2.24	0.51
1:J:79:LYS:NZ	1:J:108:GLN:NE2	2.58	0.51
1:J:248:ASP:OD2	1:J:250:ASN:HB2	2.11	0.51
1:C:78:GLU:OE2	1:C:99:ILE:HD11	2.11	0.51
1:I:293:LYS:CD	1:I:294:GLU:H	2.24	0.51
1:K:248:ASP:O	1:K:249:LYS:C	2.54	0.51
1:K:293:LYS:H	1:K:293:LYS:CD	2.23	0.51
1:E:28:SER:OG	1:E:31:VAL:HG23	2.11	0.51
1:I:58:PHE:CD2	1:J:67:MSE:HE1	2.46	0.51
1:K:23:TYR:HB3	1:K:32:TYR:CD2	2.46	0.51
1:L:94:LYS:HB3	1:L:94:LYS:HZ2	1.76	0.51
1:B:53:ARG:HG2	1:B:53:ARG:HH11	1.76	0.51
1:B:297:MET:HE2	1:B:301:ASN:ND2	2.18	0.51
1:C:11:ILE:CG2	1:C:56:VAL:HG21	2.41	0.51
1:D:197:ALA:HB1	1:D:213:TYR:CZ	2.46	0.51
1:E:43:SER:OG	1:E:46:GLU:HG3	2.11	0.51
1:H:57:ASN:HB2	1:H:60:GLU:HB2	1.93	0.51
1:I:22:LEU:HD12	1:I:50:PHE:CD1	2.46	0.51
1:B:274:ARG:NH1	1:B:278:GLU:OE2	2.45	0.50
1:C:263:ILE:HG13	1:D:263:ILE:CG1	2.28	0.50
1:C:297:MET:HE3	1:C:297:MET:HA	1.93	0.50
1:D:171:ILE:O	1:D:174:PRO:HD2	2.11	0.50
1:I:169:SER:O	1:I:173:LYS:HG2	2.11	0.50
1:A:26:ILE:HD11	1:A:53:ARG:NH1	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:TYR:O	1:F:124:ASN:HB2	2.12	0.50
1:G:171:ILE:O	1:G:175:MSE:HE3	2.11	0.50
1:I:73:ASN:O	1:I:77:LYS:HG3	2.11	0.50
1:I:171:ILE:HD12	1:I:171:ILE:N	2.27	0.50
1:I:191:GLN:HE22	1:I:229:ASN:N	2.04	0.50
1:K:31:VAL:O	1:K:34:LYS:HB2	2.10	0.50
1:E:8:LEU:HD22	2:E:319:HOH:O	2.10	0.50
1:E:95:ASN:HD22	1:E:98:ARG:HH22	1.60	0.50
1:H:81:LEU:HD21	1:H:95:ASN:OD1	2.11	0.50
1:K:27:MSE:HE3	1:K:50:PHE:HZ	1.76	0.50
1:C:130:PHE:O	1:C:134:ILE:HG22	2.12	0.50
1:F:171:ILE:HG22	1:F:175:MSE:CE	2.40	0.50
1:C:85:ILE:HG22	1:C:85:ILE:O	2.12	0.50
1:H:5:GLY:HA3	1:H:8:LEU:HD12	1.94	0.50
1:L:89:PRO:HG3	1:L:123:TYR:CE2	2.47	0.50
1:G:26:ILE:HD11	1:G:53:ARG:HH12	1.76	0.50
1:H:289:PHE:CZ	1:I:289:PHE:CE2	2.99	0.50
1:H:289:PHE:HE1	1:I:289:PHE:HE2	1.60	0.50
1:I:23:TYR:HD2	1:I:23:TYR:C	2.19	0.50
1:K:151:ILE:O	1:K:155:ILE:HG13	2.12	0.50
1:A:125:ILE:HG22	1:A:126:GLU:N	2.26	0.50
1:C:156:VAL:HG11	1:C:172:ILE:HG12	1.93	0.50
1:D:130:PHE:CE1	1:D:134:ILE:HD13	2.47	0.50
1:G:261:ILE:HD12	1:G:280:LEU:HD22	1.92	0.50
1:H:151:ILE:O	1:H:155:ILE:HG13	2.12	0.50
1:I:160:LEU:HD21	1:I:172:ILE:HD11	1.94	0.50
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.76	0.50
1:C:298:TYR:HB3	2:C:318:HOH:O	2.12	0.50
1:F:32:TYR:CE1	1:F:36:GLU:HG3	2.47	0.50
1:H:289:PHE:CE1	1:I:289:PHE:HE2	2.29	0.50
1:D:156:VAL:CG1	1:D:172:ILE:HG12	2.42	0.49
1:G:98:ARG:CB	1:G:98:ARG:HH11	2.25	0.49
1:G:123:TYR:C	1:G:125:ILE:H	2.19	0.49
1:I:19:GLN:HE22	1:I:33:ILE:HD13	1.77	0.49
1:L:200:ILE:HD13	2:L:341:HOH:O	2.12	0.49
1:E:88:ASN:HD22	1:E:91:LEU:HG	1.77	0.49
1:J:23:TYR:C	1:J:23:TYR:HD2	2.20	0.49
1:L:23:TYR:HD2	1:L:23:TYR:C	2.20	0.49
1:L:210:ALA:O	1:L:214:ILE:HG13	2.12	0.49
1:B:31:VAL:O	1:B:34:LYS:HB2	2.12	0.49
1:B:141:LEU:HD13	2:B:320:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:LYS:NZ	1:E:102:LYS:HB3	2.27	0.49
1:G:95:ASN:N	1:G:95:ASN:ND2	2.60	0.49
1:I:64:ARG:NH1	2:I:326:HOH:O	2.45	0.49
1:I:156:VAL:HG21	1:I:175:MSE:SE	2.63	0.49
1:J:237:ASN:O	1:J:241:GLN:HG2	2.12	0.49
1:B:95:ASN:HA	1:B:98:ARG:HH12	1.76	0.49
1:B:291:PRO:HG2	1:B:296:THR:CG2	2.43	0.49
1:G:57:ASN:N	1:G:57:ASN:ND2	2.56	0.49
1:I:23:TYR:C	1:I:23:TYR:CD2	2.88	0.49
1:K:68:ASN:N	1:K:68:ASN:ND2	2.60	0.49
1:L:277:VAL:HG12	1:L:299:TYR:HB2	1.94	0.49
1:A:202:ILE:HD11	1:A:243:TYR:HB2	1.94	0.49
1:A:299:TYR:O	1:A:303:VAL:HG23	2.12	0.49
1:C:86:PHE:CE1	1:C:119:ILE:HG12	2.47	0.49
1:E:295:VAL:HG23	1:E:296:THR:N	2.27	0.49
1:B:148:PHE:CG	1:B:175:MSE:HG2	2.48	0.49
1:C:81:LEU:O	1:C:85:ILE:HG13	2.11	0.49
1:H:108:GLN:NE2	1:H:108:GLN:HA	2.26	0.49
1:K:141:LEU:HD13	2:K:319:HOH:O	2.12	0.49
1:K:205:ARG:HG2	2:K:332:HOH:O	2.10	0.49
1:A:138:LEU:HD13	1:A:171:ILE:HD11	1.94	0.49
1:A:53:ARG:HD3	2:A:331:HOH:O	2.13	0.49
1:A:72:VAL:HG22	1:A:72:VAL:O	2.13	0.49
1:A:291:PRO:HB2	1:A:295:VAL:CG2	2.43	0.49
1:B:134:ILE:HG23	1:B:135:THR:N	2.28	0.49
1:B:271:ASP:HB2	2:B:332:HOH:O	2.13	0.49
1:F:72:VAL:O	1:F:72:VAL:HG22	2.11	0.49
1:F:171:ILE:C	1:F:175:MSE:HE2	2.38	0.49
1:J:274:ARG:NH1	1:J:274:ARG:HG2	2.28	0.49
1:K:8:LEU:HD22	2:K:318:HOH:O	2.12	0.49
1:K:92:PHE:O	1:K:94:LYS:N	2.45	0.49
1:L:2:PHE:HB2	1:L:4:ILE:HD11	1.95	0.49
1:L:23:TYR:C	1:L:23:TYR:CD2	2.91	0.49
1:B:293:LYS:H	1:B:293:LYS:CD	2.26	0.49
1:E:23:TYR:HB3	1:E:32:TYR:CD2	2.48	0.49
1:G:296:THR:O	1:G:297:MET:C	2.56	0.49
1:D:289:PHE:CE1	1:L:251:ILE:HB	2.48	0.49
1:E:98:ARG:CB	1:E:98:ARG:HH11	2.26	0.49
1:F:23:TYR:O	1:F:25:GLY:N	2.46	0.49
1:H:248:ASP:O	1:H:249:LYS:C	2.56	0.49
1:J:4:ILE:HD12	1:J:4:ILE:C	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:VAL:C	1:J:37:ALA:H	2.19	0.49
1:E:251:ILE:HD13	1:E:251:ILE:O	2.13	0.48
1:F:125:ILE:HG22	1:F:126:GLU:H	1.77	0.48
1:G:281:THR:HA	1:G:291:PRO:HG2	1.95	0.48
1:I:133:THR:OG1	1:I:134:ILE:N	2.45	0.48
1:J:103:ARG:HG2	1:J:103:ARG:HH11	1.77	0.48
1:A:63:ASN:HB3	2:A:348:HOH:O	2.12	0.48
1:B:274:ARG:HH11	1:B:274:ARG:HG2	1.77	0.48
1:D:171:ILE:HG22	1:D:175:MSE:HE3	1.94	0.48
1:E:196:ASN:O	1:E:200:ILE:HG13	2.13	0.48
1:F:293:LYS:H	1:F:293:LYS:CD	2.22	0.48
1:H:4:ILE:CG2	1:H:38:ASP:HA	2.27	0.48
1:I:73:ASN:OD1	1:I:75:THR:HB	2.13	0.48
1:I:98:ARG:O	1:I:102:LYS:HE2	2.12	0.48
1:J:76:GLY:O	1:J:80:LEU:HG	2.13	0.48
1:A:98:ARG:HB3	1:A:98:ARG:NH1	2.29	0.48
1:B:68:ASN:H	1:B:68:ASN:ND2	2.10	0.48
1:H:73:ASN:O	1:H:77:LYS:HG3	2.13	0.48
1:J:42:ILE:HD12	1:J:46:GLU:OE1	2.13	0.48
1:A:60:GLU:OE2	1:A:64:ARG:NE	2.42	0.48
1:E:224:LYS:O	1:E:225:ASN:HB2	2.13	0.48
1:F:256:ASN:O	1:F:260:ILE:HG13	2.13	0.48
1:I:104:LEU:HD21	1:I:137:ASP:OD2	2.13	0.48
1:A:207:LEU:O	1:A:243:TYR:HE1	1.96	0.48
1:B:173:LYS:HB2	1:B:174:PRO:HD3	1.94	0.48
1:H:15:LEU:O	1:H:16:ASN:HB2	2.13	0.48
1:H:252:ASP:OD2	1:I:293:LYS:HD2	2.13	0.48
1:D:185:ASP:HB2	2:D:323:HOH:O	2.13	0.48
1:E:98:ARG:HB3	1:E:98:ARG:HH11	1.78	0.48
1:F:68:ASN:N	1:F:68:ASN:HD22	2.12	0.48
1:H:28:SER:OG	1:H:31:VAL:HG23	2.14	0.48
1:H:82:ILE:HD11	1:H:116:TYR:HE1	1.78	0.48
1:H:153:TYR:HB2	1:H:189:THR:HG22	1.94	0.48
1:I:68:ASN:N	1:I:68:ASN:HD22	2.11	0.48
1:J:32:TYR:CE1	1:J:36:GLU:HB2	2.49	0.48
1:L:247:THR:HG22	1:L:248:ASP:N	2.28	0.48
1:B:9:LYS:O	1:B:13:GLN:HG3	2.12	0.48
1:B:80:LEU:HD12	1:B:84:LYS:NZ	2.28	0.48
1:J:274:ARG:HG2	1:J:274:ARG:O	2.14	0.48
1:J:292:PRO:C	1:J:294:GLU:N	2.69	0.48
1:K:31:VAL:HG13	1:K:40:ARG:CD	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:PHE:O	1:K:100:GLU:HB2	2.12	0.48
1:A:265:LYS:HB2	1:A:273:HIS:CD2	2.49	0.48
1:E:4:ILE:HG22	1:E:8:LEU:CD1	2.44	0.48
1:F:42:ILE:HG22	2:F:350:HOH:O	2.14	0.48
1:F:156:VAL:HG21	1:F:175:MSE:SE	2.63	0.48
1:K:275:SER:O	1:K:279:GLU:HB2	2.14	0.48
1:K:277:VAL:HG12	1:K:299:TYR:HB2	1.96	0.48
1:L:173:LYS:HE2	1:L:212:TYR:CE2	2.48	0.48
1:C:171:ILE:O	1:C:175:MSE:HE3	2.12	0.48
1:C:205:ARG:HG2	1:C:205:ARG:HH11	1.79	0.48
1:I:141:LEU:HD13	2:I:325:HOH:O	2.13	0.48
1:J:297:MET:HE3	1:J:297:MET:HA	1.96	0.48
1:K:150:GLY:O	1:K:189:THR:HG21	2.14	0.48
1:K:293:LYS:N	1:K:293:LYS:CD	2.77	0.48
1:G:82:ILE:HG22	1:G:119:ILE:HD11	1.95	0.48
1:J:43:SER:HG	1:J:46:GLU:HG3	1.78	0.48
1:J:50:PHE:O	1:J:54:LEU:HG	2.13	0.48
1:B:81:LEU:HD21	1:B:95:ASN:ND2	2.29	0.47
1:I:92:PHE:CZ	1:I:120:ALA:HB2	2.49	0.47
1:I:198:LEU:HG	1:I:239:LEU:HD13	1.96	0.47
1:B:261:ILE:HD12	1:B:280:LEU:HD22	1.96	0.47
1:C:192:THR:HG22	1:C:196:ASN:ND2	2.29	0.47
1:D:209:GLU:O	1:D:212:TYR:HB3	2.15	0.47
1:E:68:ASN:N	1:E:68:ASN:HD22	2.12	0.47
1:H:72:VAL:CG2	1:H:73:ASN:H	2.15	0.47
1:H:274:ARG:HG3	1:H:274:ARG:NH1	2.29	0.47
1:I:237:ASN:O	1:I:241:GLN:HG2	2.15	0.47
1:A:134:ILE:HG23	1:A:135:THR:N	2.29	0.47
1:C:110:PHE:HD2	1:C:155:ILE:HD13	1.79	0.47
1:E:176:TYR:CE2	1:E:194:LEU:HD21	2.49	0.47
1:F:76:GLY:O	1:F:80:LEU:HD23	2.15	0.47
1:G:94:LYS:HE3	1:G:94:LYS:HA	1.97	0.47
1:H:68:ASN:N	1:H:68:ASN:ND2	2.61	0.47
1:I:300:GLU:C	1:I:302:TYR:N	2.73	0.47
1:L:30:SER:O	1:L:34:LYS:HG3	2.14	0.47
1:L:283:ILE:HG13	2:L:322:HOH:O	2.13	0.47
1:D:56:VAL:HG23	2:D:319:HOH:O	2.15	0.47
1:H:179:VAL:HG23	1:H:180:ASP:OD1	2.14	0.47
1:H:291:PRO:HB2	1:H:295:VAL:HG21	1.96	0.47
1:A:37:ALA:O	1:A:38:ASP:HB2	2.13	0.47
1:B:246:LEU:HD21	1:B:283:ILE:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PRO:HB3	1:D:123:TYR:CD2	2.49	0.47
1:J:187:ASP:O	1:J:191:GLN:HG3	2.13	0.47
1:A:251:ILE:HG21	1:F:292:PRO:CD	2.40	0.47
1:C:278:GLU:HA	1:C:299:TYR:CD2	2.50	0.47
1:E:198:LEU:HG	1:E:239:LEU:HD13	1.96	0.47
1:L:37:ALA:O	1:L:38:ASP:HB2	2.13	0.47
1:C:52:GLU:OE1	1:D:74:GLU:HB3	2.14	0.47
1:C:103:ARG:HG3	1:C:104:LEU:HG	1.96	0.47
1:C:176:TYR:HB3	1:C:177:PRO:HA	1.97	0.47
1:C:191:GLN:NE2	1:C:228:ILE:HA	2.29	0.47
1:D:292:PRO:HA	1:L:252:ASP:OD2	2.15	0.47
1:E:293:LYS:N	1:E:293:LYS:CD	2.75	0.47
1:F:191:GLN:HE22	1:F:229:ASN:N	1.99	0.47
1:G:57:ASN:ND2	1:G:57:ASN:H	2.13	0.47
1:G:198:LEU:CD1	2:G:323:HOH:O	2.60	0.47
1:G:293:LYS:HE2	1:G:294:GLU:HB2	1.96	0.47
1:H:88:ASN:C	1:H:90:ASP:H	2.22	0.47
1:H:160:LEU:HD21	1:H:172:ILE:HD11	1.97	0.47
1:I:23:TYR:CD2	1:I:24:SER:N	2.80	0.47
1:I:176:TYR:HB3	1:I:216:GLN:OE1	2.14	0.47
1:I:265:LYS:HD2	1:I:298:TYR:OH	2.15	0.47
1:J:117:ILE:HD12	1:J:130:PHE:HB2	1.97	0.47
1:K:274:ARG:HG2	1:K:274:ARG:NH1	2.30	0.47
1:L:178:ILE:O	1:L:223:ILE:HD11	2.15	0.47
1:C:94:LYS:NZ	1:C:94:LYS:HB3	2.30	0.47
1:F:23:TYR:HE1	1:F:29:LYS:HG3	1.78	0.47
1:F:164:PRO:HD2	1:F:167:GLU:OE2	2.14	0.47
1:F:288:LYS:HA	1:F:288:LYS:HD3	1.77	0.47
1:B:237:ASN:HB2	2:B:352:HOH:O	2.15	0.47
1:E:23:TYR:HB3	1:E:32:TYR:CG	2.49	0.47
1:G:26:ILE:HD13	1:G:49:LYS:HB3	1.97	0.47
1:H:74:GLU:OE2	1:H:77:LYS:HD2	2.14	0.47
1:J:293:LYS:O	1:J:297:MET:HB2	2.15	0.47
1:J:274:ARG:HG2	1:J:274:ARG:HH11	1.79	0.47
1:L:57:ASN:OD1	1:L:59:PHE:N	2.48	0.47
1:A:278:GLU:HG3	1:A:299:TYR:CE2	2.49	0.46
1:C:76:GLY:O	1:C:79:LYS:HB2	2.16	0.46
1:G:86:PHE:O	1:G:89:PRO:HD3	2.15	0.46
1:I:20:ILE:HG13	1:I:23:TYR:OH	2.15	0.46
1:J:28:SER:O	1:J:29:LYS:C	2.58	0.46
1:A:205:ARG:HG3	1:A:246:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLN:OE1	1:B:33:ILE:HD13	2.15	0.46
1:H:292:PRO:HA	1:I:252:ASP:OD2	2.15	0.46
1:K:86:PHE:HD1	1:K:119:ILE:HG12	1.79	0.46
1:K:299:TYR:O	1:K:303:VAL:HG23	2.15	0.46
1:A:148:PHE:CD2	1:A:175:MSE:HE2	2.51	0.46
1:A:290:THR:HB	2:A:354:HOH:O	2.15	0.46
1:E:100:GLU:HB3	1:E:101:PRO:CD	2.39	0.46
1:K:23:TYR:CE1	1:K:29:LYS:HG3	2.50	0.46
1:K:277:VAL:CG1	1:K:299:TYR:HB2	2.45	0.46
1:L:199:THR:HG23	1:L:279:GLU:OE2	2.16	0.46
1:L:240:LYS:O	1:L:244:GLN:HG3	2.16	0.46
1:A:251:ILE:O	1:A:251:ILE:HD13	2.15	0.46
1:D:72:VAL:HG13	1:D:73:ASN:N	2.30	0.46
1:D:293:LYS:H	1:D:293:LYS:CD	2.26	0.46
1:E:43:SER:HA	1:F:43:SER:HA	1.97	0.46
1:F:293:LYS:N	1:F:293:LYS:CD	2.74	0.46
1:G:12:ARG:HG2	1:G:17:TYR:O	2.16	0.46
1:G:92:PHE:O	1:G:93:ASP:C	2.58	0.46
1:J:4:ILE:N	1:J:65:ALA:HB1	2.30	0.46
1:B:68:ASN:HD22	1:B:68:ASN:N	2.08	0.46
1:F:237:ASN:O	1:F:241:GLN:HG2	2.15	0.46
1:G:103:ARG:HG3	1:G:104:LEU:HD23	1.98	0.46
1:G:135:THR:O	1:G:139:LYS:HE2	2.15	0.46
1:G:163:LEU:HD12	1:G:164:PRO:HD2	1.96	0.46
1:G:261:ILE:HG12	1:G:276:LEU:HB3	1.96	0.46
1:G:301:ASN:O	1:G:304:ALA:HB3	2.15	0.46
1:J:299:TYR:C	1:J:301:ASN:H	2.23	0.46
1:L:248:ASP:O	1:L:250:ASN:N	2.49	0.46
1:A:277:VAL:HG22	1:A:295:VAL:HB	1.98	0.46
1:B:23:TYR:CZ	1:B:29:LYS:HB2	2.51	0.46
1:D:82:ILE:HD11	1:D:112:ILE:CG2	2.35	0.46
1:D:292:PRO:O	1:D:295:VAL:HG22	2.15	0.46
1:F:173:LYS:HB2	1:F:174:PRO:HD3	1.98	0.46
1:K:89:PRO:HB3	1:K:123:TYR:CE2	2.50	0.46
1:L:94:LYS:H	1:L:94:LYS:HD2	1.81	0.46
1:C:156:VAL:CG1	1:C:172:ILE:HG12	2.45	0.46
1:E:248:ASP:O	1:E:249:LYS:C	2.58	0.46
1:K:163:LEU:HD12	1:K:164:PRO:HD2	1.98	0.46
1:A:192:THR:HG22	1:A:196:ASN:ND2	2.30	0.46
1:B:176:TYR:OH	1:B:193:VAL:HB	2.16	0.46
1:C:148:PHE:CG	1:C:175:MSE:HG2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:ILE:CG2	1:F:276:LEU:HD22	2.45	0.46
1:H:4:ILE:HG23	2:H:347:HOH:O	2.15	0.46
1:H:263:ILE:O	1:H:267:ILE:HG12	2.15	0.46
1:I:242:ILE:HG21	2:I:323:HOH:O	2.15	0.46
1:A:98:ARG:CB	1:A:98:ARG:HH11	2.29	0.46
1:A:293:LYS:CD	1:A:294:GLU:H	2.28	0.46
1:D:250:ASN:HA	1:L:290:THR:HB	1.97	0.46
1:H:100:GLU:HB3	1:H:101:PRO:HD3	1.96	0.46
1:H:205:ARG:HG2	1:H:205:ARG:NH1	2.28	0.46
1:J:23:TYR:HB2	1:J:27:MSE:HB2	1.97	0.46
1:H:46:GLU:O	1:H:50:PHE:HD1	1.98	0.46
1:H:113:TYR:CD2	1:H:114:LEU:HD23	2.51	0.46
1:I:18:HIS:HB3	1:I:20:ILE:HD13	1.97	0.46
1:J:127:VAL:N	1:J:128:PRO:CD	2.79	0.46
1:C:78:GLU:HA	1:C:78:GLU:OE1	2.16	0.45
1:D:87:THR:O	1:D:88:ASN:CB	2.62	0.45
1:E:272:ILE:HG22	1:E:276:LEU:HD22	1.98	0.45
1:F:151:ILE:O	1:F:155:ILE:HG13	2.16	0.45
1:G:35:VAL:HG22	1:G:40:ARG:NH2	2.31	0.45
1:G:68:ASN:HD22	1:G:68:ASN:N	2.08	0.45
1:H:130:PHE:O	1:H:132:LYS:N	2.49	0.45
1:I:5:GLY:HA3	1:I:38:ASP:OD2	2.16	0.45
1:F:203:MSE:HE3	1:F:203:MSE:O	2.16	0.45
1:F:224:LYS:O	1:F:225:ASN:HB2	2.16	0.45
1:G:67:MSE:HE3	1:G:67:MSE:O	2.16	0.45
1:H:115:GLY:O	1:H:118:SER:HB3	2.17	0.45
1:K:7:VAL:HG21	1:K:65:ALA:HA	1.97	0.45
1:E:195:LYS:C	1:E:195:LYS:HD2	2.42	0.45
1:E:297:MET:HE3	1:E:297:MET:HA	1.97	0.45
1:F:23:TYR:CD2	1:F:24:SER:N	2.83	0.45
1:F:26:ILE:HD11	1:F:53:ARG:HH11	1.81	0.45
1:G:176:TYR:CE2	1:G:178:ILE:HD11	2.50	0.45
1:I:90:ASP:C	1:I:92:PHE:N	2.74	0.45
1:A:100:GLU:HB3	1:A:101:PRO:CD	2.43	0.45
1:G:265:LYS:HD2	1:G:298:TYR:OH	2.16	0.45
1:I:192:THR:HG22	1:I:196:ASN:ND2	2.32	0.45
1:J:23:TYR:CE1	1:J:29:LYS:HA	2.50	0.45
1:C:60:GLU:HB2	2:C:321:HOH:O	2.17	0.45
1:D:205:ARG:HG2	1:D:205:ARG:HH11	1.81	0.45
1:E:205:ARG:HH11	1:E:205:ARG:HG2	1.81	0.45
1:F:153:TYR:CB	1:F:189:THR:HG22	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:GLU:HB3	1:G:101:PRO:HD3	1.97	0.45
1:I:40:ARG:HH21	1:I:40:ARG:HG3	1.82	0.45
1:I:191:GLN:HE22	1:I:228:ILE:HA	1.81	0.45
1:C:4:ILE:HD11	1:D:44:VAL:HG11	1.99	0.45
1:G:8:LEU:HD13	2:G:318:HOH:O	2.16	0.45
1:H:20:ILE:N	1:H:20:ILE:CD1	2.80	0.45
1:H:173:LYS:HB2	1:H:174:PRO:HD3	1.99	0.45
1:I:94:LYS:H	1:I:94:LYS:HZ1	1.64	0.45
1:J:229:ASN:HB3	1:J:232:TYR:HB2	1.97	0.45
1:J:279:GLU:O	1:J:283:ILE:HG12	2.16	0.45
1:B:279:GLU:O	1:B:283:ILE:HB	2.17	0.45
1:D:20:ILE:O	1:D:24:SER:CB	2.64	0.45
1:F:171:ILE:HD12	1:F:171:ILE:N	2.31	0.45
1:H:50:PHE:CD1	1:H:50:PHE:N	2.85	0.45
1:H:130:PHE:C	1:H:132:LYS:H	2.25	0.45
1:J:198:LEU:HG	1:J:239:LEU:HD13	1.97	0.45
1:K:88:ASN:HD21	1:K:91:LEU:HG	1.82	0.45
1:L:2:PHE:HB2	1:L:4:ILE:HD12	1.98	0.45
1:E:19:GLN:OE1	1:E:33:ILE:HD11	2.17	0.45
1:F:68:ASN:N	1:F:68:ASN:ND2	2.63	0.45
1:H:72:VAL:HG13	1:H:73:ASN:N	2.32	0.45
1:H:108:GLN:HE21	1:H:108:GLN:CA	2.30	0.45
1:L:108:GLN:O	1:L:112:ILE:HG13	2.17	0.45
1:L:233:ASP:O	1:L:237:ASN:HB2	2.16	0.45
1:E:210:ALA:O	1:E:214:ILE:HG13	2.17	0.45
1:F:75:THR:HG21	1:F:108:GLN:HB3	1.98	0.45
1:G:172:ILE:HG21	2:G:321:HOH:O	2.17	0.45
1:G:185:ASP:HB2	2:G:339:HOH:O	2.16	0.45
1:H:53:ARG:HG2	1:H:53:ARG:HH11	1.81	0.45
1:H:92:PHE:CE2	1:H:125:ILE:HG21	2.51	0.45
1:J:220:LEU:O	1:J:226:ILE:HG21	2.16	0.45
1:J:224:LYS:O	1:J:225:ASN:CB	2.63	0.45
1:K:198:LEU:HG	1:K:239:LEU:HD13	1.98	0.45
1:B:20:ILE:O	1:B:24:SER:HB3	2.17	0.45
1:B:149:PHE:O	1:B:152:ASP:HB2	2.17	0.45
1:C:301:ASN:O	1:C:302:TYR:HB2	2.17	0.45
1:D:3:LYS:HD3	1:D:3:LYS:N	2.32	0.45
1:E:278:GLU:HB3	2:E:347:HOH:O	2.16	0.45
1:F:74:GLU:HA	1:F:77:LYS:HE2	1.99	0.45
1:F:90:ASP:C	1:F:92:PHE:N	2.73	0.45
1:G:255:LEU:HD11	1:J:255:LEU:CD2	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:ASP:C	1:I:92:PHE:H	2.25	0.45
1:K:81:LEU:O	1:K:85:ILE:HG13	2.16	0.45
1:B:141:LEU:CB	2:B:320:HOH:O	2.65	0.44
1:D:240:LYS:O	1:D:243:TYR:HB3	2.17	0.44
1:E:134:ILE:HG23	1:E:135:THR:N	2.33	0.44
1:F:102:LYS:HB2	1:F:105:THR:OG1	2.17	0.44
1:F:139:LYS:O	1:F:143:ASP:HB2	2.17	0.44
1:K:85:ILE:O	1:K:85:ILE:CG2	2.65	0.44
1:L:85:ILE:HG22	1:L:85:ILE:O	2.17	0.44
1:A:130:PHE:CE1	1:A:134:ILE:HD13	2.53	0.44
1:B:261:ILE:CD1	1:B:280:LEU:HD22	2.47	0.44
1:C:57:ASN:ND2	2:C:324:HOH:O	2.51	0.44
1:D:249:LYS:HE2	1:D:287:GLU:OE1	2.17	0.44
1:I:93:ASP:C	1:I:95:ASN:N	2.75	0.44
1:I:133:THR:O	1:I:135:THR:N	2.50	0.44
1:J:179:VAL:HG23	1:J:180:ASP:OD1	2.18	0.44
1:J:205:ARG:HH11	1:J:205:ARG:HG2	1.81	0.44
1:L:78:GLU:CD	1:L:99:ILE:HD11	2.41	0.44
1:D:79:LYS:HE3	1:D:108:GLN:HE22	1.83	0.44
1:H:19:GLN:OE1	1:H:33:ILE:HG12	2.17	0.44
1:H:145:ARG:HH11	1:H:145:ARG:HG3	1.81	0.44
1:I:68:ASN:N	1:I:68:ASN:ND2	2.66	0.44
1:I:267:ILE:HG21	1:J:234:LEU:HD12	1.99	0.44
1:J:45:GLU:O	1:J:49:LYS:HG3	2.18	0.44
1:A:68:ASN:HD22	1:A:68:ASN:H	1.63	0.44
1:C:245:PHE:O	1:C:249:LYS:HD3	2.17	0.44
1:E:285:ALA:HB3	2:E:336:HOH:O	2.17	0.44
1:H:148:PHE:CG	1:H:175:MSE:HG2	2.52	0.44
1:J:82:ILE:HG23	1:J:119:ILE:HD11	1.98	0.44
1:J:134:ILE:CG2	1:J:135:THR:N	2.80	0.44
1:L:293:LYS:HD3	1:L:293:LYS:N	2.32	0.44
1:D:153:TYR:CB	1:D:189:THR:HG22	2.45	0.44
1:E:23:TYR:C	1:E:23:TYR:CD2	2.96	0.44
1:E:123:TYR:O	1:E:125:ILE:N	2.51	0.44
1:H:29:LYS:H	1:H:29:LYS:CD	2.31	0.44
1:A:248:ASP:O	1:A:249:LYS:C	2.60	0.44
1:F:254:TYR:O	1:F:258:VAL:HG23	2.17	0.44
1:F:265:LYS:HD2	1:F:298:TYR:OH	2.17	0.44
1:I:103:ARG:HG3	1:I:104:LEU:HG	2.00	0.44
1:J:40:ARG:HG3	1:J:41:PRO:HD2	1.99	0.44
1:J:156:VAL:HG11	1:J:172:ILE:HG12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:PRO:HB2	1:J:295:VAL:CG2	2.48	0.44
1:L:128:PRO:HB2	1:L:132:LYS:HE2	1.99	0.44
1:L:249:LYS:NZ	1:L:287:GLU:HB3	2.33	0.44
1:B:139:LYS:HD3	1:B:143:ASP:OD1	2.17	0.44
1:B:203:MSE:C	1:B:205:ARG:N	2.76	0.44
1:C:120:ALA:HB1	1:C:127:VAL:HG13	1.99	0.44
1:D:74:GLU:HA	1:D:77:LYS:HE2	2.00	0.44
1:D:134:ILE:CG2	1:D:135:THR:N	2.80	0.44
1:G:19:GLN:O	1:G:23:TYR:HD1	2.01	0.44
1:H:29:LYS:HD3	1:H:29:LYS:N	2.32	0.44
1:I:130:PHE:O	1:I:131:ASN:C	2.61	0.44
1:J:27:MSE:HE1	1:J:35:VAL:HG21	1.99	0.44
1:K:60:GLU:OE2	1:L:149:PHE:HB3	2.17	0.44
1:C:113:TYR:HE2	2:C:331:HOH:O	2.00	0.44
1:D:30:SER:CA	1:D:33:ILE:HG12	2.46	0.44
1:E:71:SER:HB2	2:E:350:HOH:O	2.18	0.44
1:E:265:LYS:HG3	2:E:318:HOH:O	2.18	0.44
1:F:131:ASN:N	1:F:131:ASN:HD22	2.13	0.44
1:G:72:VAL:HG22	1:G:73:ASN:N	2.32	0.44
1:H:176:TYR:OH	1:H:193:VAL:HB	2.17	0.44
1:J:139:LYS:O	1:J:143:ASP:HB2	2.17	0.44
1:K:238:TYR:HA	1:K:260:ILE:HD12	2.00	0.44
1:L:95:ASN:CA	1:L:98:ARG:HH12	2.30	0.44
1:A:22:LEU:HD12	2:A:318:HOH:O	2.18	0.44
1:A:185:ASP:HB2	2:A:341:HOH:O	2.18	0.44
1:A:251:ILE:HB	1:F:289:PHE:HE1	1.82	0.44
1:C:26:ILE:HD11	1:C:53:ARG:HH12	1.79	0.44
1:D:4:ILE:HG21	1:D:42:ILE:CG2	2.47	0.44
1:D:9:LYS:O	1:D:13:GLN:HG3	2.18	0.44
1:E:293:LYS:CD	1:E:293:LYS:H	2.31	0.44
1:F:303:VAL:C	1:F:305:ILE:H	2.25	0.44
1:J:47:LEU:HD11	1:J:61:ILE:HG21	2.00	0.44
1:K:27:MSE:HE3	1:K:50:PHE:CZ	2.52	0.44
1:K:47:LEU:HD23	1:K:58:PHE:CE1	2.53	0.44
1:L:238:TYR:HE1	1:L:279:GLU:OE1	2.01	0.44
1:B:205:ARG:HH11	1:B:205:ARG:HG2	1.83	0.43
1:C:251:ILE:HD13	1:C:255:LEU:HG	2.00	0.43
1:G:22:LEU:HD11	1:G:54:LEU:HG	2.00	0.43
1:G:123:TYR:C	1:G:125:ILE:N	2.75	0.43
1:G:153:TYR:CE2	1:G:175:MSE:HB3	2.53	0.43
1:H:250:ASN:HA	1:I:290:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:VAL:CG2	1:H:296:THR:N	2.80	0.43
1:I:184:LYS:HB3	1:J:184:LYS:HD2	2.00	0.43
1:C:113:TYR:CZ	1:C:117:ILE:HD11	2.53	0.43
1:D:293:LYS:N	1:D:293:LYS:CD	2.79	0.43
1:E:205:ARG:HG3	1:E:246:LEU:HD13	2.00	0.43
1:G:37:ALA:O	1:G:38:ASP:HB2	2.17	0.43
1:I:293:LYS:HD3	1:I:294:GLU:N	2.28	0.43
1:J:295:VAL:C	1:J:297:MET:H	2.25	0.43
1:K:12:ARG:HD3	1:K:22:LEU:HG	2.00	0.43
1:A:100:GLU:CB	1:A:101:PRO:HD3	2.43	0.43
1:C:145:ARG:NH2	2:C:342:HOH:O	2.50	0.43
1:E:284:SER:HB2	1:E:291:PRO:HG3	2.00	0.43
1:G:92:PHE:O	1:G:94:LYS:N	2.52	0.43
1:G:134:ILE:C	1:G:136:SER:N	2.75	0.43
1:G:187:ASP:O	1:G:191:GLN:HG3	2.18	0.43
1:I:100:GLU:CB	1:I:101:PRO:HD3	2.42	0.43
1:K:109:TYR:O	1:K:112:ILE:HB	2.18	0.43
1:L:118:SER:HA	1:L:162:VAL:HG11	2.00	0.43
1:D:20:ILE:HD13	1:D:23:TYR:CE1	2.53	0.43
1:E:125:ILE:HG22	1:E:126:GLU:N	2.32	0.43
1:H:117:ILE:HG13	1:H:130:PHE:CE1	2.53	0.43
1:I:40:ARG:HG3	1:I:40:ARG:O	2.18	0.43
1:I:287:GLU:HB3	2:I:320:HOH:O	2.18	0.43
1:A:12:ARG:HD3	1:A:22:LEU:HG	2.01	0.43
1:B:4:ILE:O	1:B:8:LEU:HG	2.17	0.43
1:B:89:PRO:HG3	1:B:123:TYR:CD2	2.53	0.43
1:B:235:GLU:O	1:B:238:TYR:HB3	2.18	0.43
1:C:250:ASN:OD1	1:C:252:ASP:HB2	2.19	0.43
1:D:249:LYS:HB3	1:L:289:PHE:CE1	2.52	0.43
1:E:92:PHE:O	1:E:93:ASP:C	2.61	0.43
1:G:54:LEU:HD21	2:G:322:HOH:O	2.18	0.43
1:I:89:PRO:HB3	1:I:123:TYR:CE2	2.53	0.43
1:J:23:TYR:O	1:J:25:GLY:N	2.42	0.43
1:K:95:ASN:HA	1:K:98:ARG:HH12	1.83	0.43
1:L:31:VAL:O	1:L:35:VAL:HG23	2.19	0.43
1:L:182:PHE:HB2	1:L:186:TYR:CG	2.53	0.43
1:B:127:VAL:HG23	1:B:127:VAL:O	2.19	0.43
1:C:272:ILE:HG13	2:C:326:HOH:O	2.18	0.43
1:D:8:LEU:HD11	1:D:50:PHE:HD2	1.83	0.43
1:G:89:PRO:HB3	1:G:123:TYR:CE2	2.54	0.43
1:I:19:GLN:NE2	1:I:33:ILE:HD13	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:TYR:HD2	1:J:24:SER:N	2.16	0.43
1:L:145:ARG:HG3	1:L:145:ARG:HH11	1.83	0.43
1:B:153:TYR:CE2	1:B:175:MSE:HB3	2.54	0.43
1:C:135:THR:HG22	1:C:139:LYS:HZ3	1.83	0.43
1:H:3:LYS:C	1:H:4:ILE:HD12	2.44	0.43
1:K:68:ASN:N	1:K:68:ASN:HD22	2.16	0.43
1:A:245:PHE:O	1:A:249:LYS:HD3	2.19	0.43
1:C:159:LEU:C	1:C:161:ASN:N	2.75	0.43
1:F:103:ARG:HG2	1:F:103:ARG:NH1	2.34	0.43
1:G:19:GLN:O	1:G:23:TYR:CD1	2.71	0.43
1:G:110:PHE:CE2	1:G:114:LEU:HD11	2.54	0.43
1:I:234:LEU:HD13	1:J:267:ILE:HG21	2.00	0.43
1:K:85:ILE:HD11	1:K:95:ASN:OD1	2.19	0.43
1:K:92:PHE:O	1:K:95:ASN:N	2.43	0.43
1:K:184:LYS:HE3	1:K:227:SER:OG	2.18	0.43
1:A:293:LYS:N	1:A:293:LYS:CD	2.80	0.43
1:F:81:LEU:O	1:F:85:ILE:CG1	2.66	0.43
1:G:100:GLU:C	1:G:100:GLU:CD	2.86	0.43
1:J:88:ASN:HD22	1:J:91:LEU:HG	1.83	0.43
1:L:87:THR:O	1:L:89:PRO:HD3	2.18	0.43
1:L:134:ILE:CG2	1:L:135:THR:N	2.81	0.43
1:A:122:HIS:C	1:A:124:ASN:H	2.27	0.43
1:B:293:LYS:N	1:B:293:LYS:CD	2.78	0.43
1:C:7:VAL:O	1:C:11:ILE:HG13	2.19	0.43
1:F:103:ARG:HD2	1:F:113:TYR:CE2	2.54	0.43
1:G:293:LYS:N	1:G:293:LYS:CD	2.79	0.43
1:K:98:ARG:O	1:K:101:PRO:HD2	2.19	0.43
1:C:139:LYS:HD2	1:C:139:LYS:N	2.34	0.42
1:C:156:VAL:CG2	1:C:175:MSE:HE1	2.49	0.42
1:C:278:GLU:HA	1:C:299:TYR:HD2	1.84	0.42
1:E:37:ALA:O	1:E:38:ASP:HB2	2.18	0.42
1:E:68:ASN:N	1:E:68:ASN:ND2	2.64	0.42
1:G:118:SER:C	1:G:120:ALA:N	2.77	0.42
1:G:130:PHE:CE1	1:G:134:ILE:HB	2.54	0.42
1:G:142:TYR:HE1	1:G:152:ASP:OD1	2.01	0.42
1:L:29:LYS:O	1:L:33:ILE:HG13	2.19	0.42
1:A:261:ILE:HG12	1:A:276:LEU:HB3	2.02	0.42
1:C:148:PHE:CD1	1:C:148:PHE:N	2.87	0.42
1:E:274:ARG:HA	1:E:302:TYR:CE1	2.54	0.42
1:H:45:GLU:HB2	2:H:348:HOH:O	2.18	0.42
1:H:220:LEU:O	1:H:226:ILE:HG21	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ARG:NH2	1:I:152:ASP:OD2	2.51	0.42
1:A:139:LYS:HG3	2:A:334:HOH:O	2.18	0.42
1:B:253:SER:HA	1:B:256:ASN:HD22	1.84	0.42
1:C:248:ASP:O	1:C:249:LYS:C	2.61	0.42
1:D:28:SER:HB3	1:D:31:VAL:CG2	2.47	0.42
1:D:75:THR:HG21	1:D:108:GLN:HB3	2.01	0.42
1:G:9:LYS:O	1:G:13:GLN:HG3	2.19	0.42
1:G:134:ILE:O	1:G:136:SER:N	2.51	0.42
1:H:88:ASN:C	1:H:90:ASP:N	2.77	0.42
1:J:23:TYR:HB3	1:J:32:TYR:CD2	2.55	0.42
1:J:171:ILE:O	1:J:175:MSE:CE	2.68	0.42
1:J:263:ILE:HD13	1:J:263:ILE:HA	1.89	0.42
1:K:229:ASN:HB3	1:K:232:TYR:HB2	2.01	0.42
1:K:256:ASN:O	1:K:260:ILE:HG13	2.19	0.42
1:L:95:ASN:HD22	1:L:98:ARG:NH2	2.13	0.42
1:C:28:SER:HG	1:C:31:VAL:HG23	1.83	0.42
1:C:78:GLU:OE1	1:C:81:LEU:HD22	2.19	0.42
1:C:145:ARG:NH2	1:D:15:LEU:HD21	2.35	0.42
1:D:162:VAL:O	1:D:163:LEU:HD12	2.20	0.42
1:D:292:PRO:HG2	1:D:295:VAL:HG13	2.00	0.42
1:F:23:TYR:CE1	1:F:29:LYS:HA	2.53	0.42
1:F:40:ARG:HG2	1:F:40:ARG:NH2	2.33	0.42
1:F:149:PHE:O	1:F:150:GLY:C	2.63	0.42
1:I:189:THR:C	1:I:191:GLN:N	2.77	0.42
1:L:4:ILE:HD12	1:L:4:ILE:N	2.32	0.42
1:L:89:PRO:HG3	1:L:123:TYR:CZ	2.53	0.42
1:A:224:LYS:O	1:A:225:ASN:HB2	2.20	0.42
1:B:153:TYR:HB2	1:B:189:THR:CG2	2.49	0.42
1:B:153:TYR:CB	1:B:189:THR:HG22	2.48	0.42
1:E:284:SER:CB	1:E:291:PRO:HG3	2.49	0.42
1:G:265:LYS:HE2	1:G:265:LYS:HB3	1.90	0.42
1:I:81:LEU:HD12	1:I:84:LYS:CB	2.44	0.42
1:L:192:THR:HG22	1:L:196:ASN:ND2	2.34	0.42
1:A:12:ARG:HH21	1:A:36:GLU:CD	2.28	0.42
1:B:240:LYS:O	1:B:243:TYR:HB3	2.20	0.42
1:F:276:LEU:HD12	1:F:276:LEU:HA	1.87	0.42
1:G:89:PRO:HB3	1:G:123:TYR:CD2	2.55	0.42
1:G:168:VAL:HG12	1:G:172:ILE:HD11	2.01	0.42
1:I:57:ASN:ND2	2:I:328:HOH:O	2.52	0.42
1:K:109:TYR:O	1:K:112:ILE:N	2.53	0.42
1:B:284:SER:HB3	1:B:289:PHE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:O	1:C:13:GLN:HG3	2.18	0.42
1:C:144:LYS:NZ	1:C:144:LYS:HB2	2.35	0.42
1:D:195:LYS:HD2	1:D:195:LYS:C	2.44	0.42
1:D:249:LYS:CE	1:D:287:GLU:OE1	2.68	0.42
1:E:164:PRO:O	1:E:165:TYR:C	2.63	0.42
1:F:272:ILE:HG13	2:F:345:HOH:O	2.19	0.42
1:G:95:ASN:C	1:G:97:GLN:H	2.27	0.42
1:H:130:PHE:C	1:H:132:LYS:N	2.78	0.42
1:A:99:ILE:HG13	1:A:116:TYR:CE1	2.54	0.42
1:A:107:LEU:HG	2:A:323:HOH:O	2.20	0.42
1:A:178:ILE:HG13	1:A:220:LEU:HD21	2.00	0.42
1:C:58:PHE:CD2	1:D:67:MSE:HE1	2.55	0.42
1:D:294:GLU:O	1:D:297:MET:CB	2.60	0.42
1:E:95:ASN:HD22	1:E:98:ARG:NH2	2.16	0.42
1:H:50:PHE:HD1	1:H:50:PHE:H	1.67	0.42
1:I:229:ASN:HA	2:I:337:HOH:O	2.19	0.42
1:J:23:TYR:C	1:J:25:GLY:H	2.26	0.42
1:J:242:ILE:O	1:J:246:LEU:HG	2.20	0.42
1:L:92:PHE:CD2	1:L:125:ILE:HG21	2.54	0.42
1:B:251:ILE:HD13	1:B:251:ILE:HA	1.94	0.42
1:B:289:PHE:CE2	1:E:289:PHE:HZ	2.37	0.42
1:C:171:ILE:HG22	1:C:175:MSE:CE	2.50	0.42
1:C:196:ASN:O	1:C:200:ILE:HG13	2.20	0.42
1:G:68:ASN:ND2	1:G:68:ASN:N	2.67	0.42
1:G:304:ALA:O	1:G:306:GLU:N	2.50	0.42
1:H:100:GLU:OE1	1:H:100:GLU:C	2.62	0.42
1:I:130:PHE:O	1:I:132:LYS:N	2.52	0.42
1:J:79:LYS:NZ	1:J:108:GLN:HE21	2.18	0.42
1:K:278:GLU:O	1:K:282:LYS:HG3	2.20	0.42
1:B:2:PHE:HB3	2:B:350:HOH:O	2.19	0.42
1:B:68:ASN:ND2	1:B:68:ASN:N	2.67	0.42
1:C:101:PRO:C	1:C:103:ARG:H	2.28	0.42
1:D:197:ALA:HB1	1:D:213:TYR:CE2	2.55	0.42
1:D:291:PRO:HB2	1:D:295:VAL:HG21	2.00	0.42
1:F:171:ILE:HD12	1:F:171:ILE:H	1.85	0.42
1:G:2:PHE:CZ	1:G:72:VAL:HG21	2.55	0.42
1:H:21:ASP:OD2	1:H:21:ASP:N	2.53	0.42
1:I:99:ILE:O	1:I:100:GLU:C	2.61	0.42
1:I:140:HIS:ND1	1:I:140:HIS:C	2.78	0.42
1:I:236:ILE:HA	1:I:239:LEU:HD12	2.02	0.42
1:J:78:GLU:OE1	1:J:78:GLU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:ILE:HG21	2:K:319:HOH:O	2.20	0.42
1:A:86:PHE:O	1:A:123:TYR:CE2	2.73	0.41
1:E:20:ILE:HA	1:E:23:TYR:CZ	2.54	0.41
1:F:130:PHE:CE1	1:F:134:ILE:HD13	2.55	0.41
1:G:134:ILE:HG23	1:G:135:THR:H	1.84	0.41
1:I:90:ASP:O	1:I:92:PHE:N	2.52	0.41
1:I:159:LEU:C	1:I:161:ASN:N	2.76	0.41
1:I:297:MET:HE2	1:I:301:ASN:OD1	2.20	0.41
1:L:173:LYS:HB2	1:L:174:PRO:HD3	2.02	0.41
1:L:198:LEU:HG	1:L:239:LEU:HD13	2.02	0.41
1:A:24:SER:O	1:A:53:ARG:NH2	2.54	0.41
1:A:64:ARG:NH1	1:A:64:ARG:HG2	2.35	0.41
1:B:94:LYS:HB3	1:B:94:LYS:NZ	2.34	0.41
1:C:56:VAL:HG13	2:C:324:HOH:O	2.20	0.41
1:D:10:GLN:NE2	1:D:10:GLN:C	2.79	0.41
1:F:88:ASN:C	1:F:90:ASP:H	2.28	0.41
1:G:19:GLN:HB2	2:G:326:HOH:O	2.19	0.41
1:G:163:LEU:HD12	1:G:164:PRO:CD	2.51	0.41
1:I:88:ASN:HD22	1:I:91:LEU:CD1	2.34	0.41
1:I:191:GLN:HG2	1:I:217:PHE:HE1	1.84	0.41
1:J:32:TYR:HE1	1:J:36:GLU:CD	2.27	0.41
1:K:92:PHE:O	1:K:93:ASP:C	2.63	0.41
1:L:278:GLU:HG2	1:L:299:TYR:CD2	2.56	0.41
1:C:40:ARG:HG2	1:C:40:ARG:HH21	1.86	0.41
1:E:265:LYS:HB3	1:E:265:LYS:HE2	1.81	0.41
1:G:92:PHE:CD2	1:G:125:ILE:HG21	2.55	0.41
1:I:11:ILE:CG2	1:I:56:VAL:HG21	2.51	0.41
1:L:5:GLY:HA3	1:L:38:ASP:OD2	2.20	0.41
1:A:99:ILE:HG22	1:A:100:GLU:N	2.34	0.41
1:B:134:ILE:HG22	2:B:356:HOH:O	2.19	0.41
1:C:99:ILE:HG13	1:C:116:TYR:CE1	2.55	0.41
1:C:207:LEU:HD13	1:C:243:TYR:CE1	2.56	0.41
1:D:178:ILE:HG13	1:D:190:ILE:HD12	2.01	0.41
1:E:4:ILE:HD13	1:E:47:LEU:HD22	2.01	0.41
1:E:64:ARG:HG2	1:E:64:ARG:HH11	1.86	0.41
1:F:85:ILE:HG22	1:F:85:ILE:O	2.19	0.41
1:G:4:ILE:HG21	1:G:47:LEU:HD13	2.03	0.41
1:I:62:LEU:O	1:I:65:ALA:HB3	2.20	0.41
1:J:22:LEU:HA	1:J:53:ARG:HD2	2.02	0.41
1:K:78:GLU:O	1:K:82:ILE:HG13	2.21	0.41
1:B:88:ASN:N	1:B:89:PRO:HD3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HD11	1:C:112:ILE:CG2	2.33	0.41
1:G:23:TYR:O	1:G:25:GLY:N	2.52	0.41
1:G:82:ILE:HG12	1:G:116:TYR:CE1	2.56	0.41
1:G:187:ASP:OD2	1:G:226:ILE:HD12	2.21	0.41
1:G:244:GLN:NE2	2:G:333:HOH:O	2.53	0.41
1:I:93:ASP:C	1:I:95:ASN:H	2.28	0.41
1:J:156:VAL:HG22	1:J:175:MSE:HE1	2.01	0.41
1:J:171:ILE:O	1:J:175:MSE:HE3	2.20	0.41
1:K:88:ASN:HD22	1:K:91:LEU:HD12	1.85	0.41
1:K:149:PHE:CE2	1:L:11:ILE:HG12	2.56	0.41
1:A:235:GLU:O	1:A:238:TYR:HB3	2.21	0.41
1:C:168:VAL:O	1:C:168:VAL:HG12	2.19	0.41
1:F:95:ASN:HA	1:F:98:ARG:HH12	1.86	0.41
1:G:56:VAL:HG12	1:G:61:ILE:HG13	2.01	0.41
1:G:132:LYS:HB3	1:G:132:LYS:HZ3	1.86	0.41
1:H:29:LYS:H	1:H:29:LYS:HD3	1.85	0.41
1:H:123:TYR:HB2	1:H:125:ILE:HG13	2.02	0.41
1:J:153:TYR:HB2	1:J:189:THR:CG2	2.50	0.41
1:K:210:ALA:O	1:K:214:ILE:HG13	2.21	0.41
1:E:72:VAL:CG1	1:E:73:ASN:N	2.83	0.41
1:G:57:ASN:HD22	1:G:57:ASN:H	1.66	0.41
1:G:237:ASN:HD21	1:H:267:ILE:HA	1.85	0.41
1:H:108:GLN:NE2	1:H:108:GLN:CA	2.82	0.41
1:I:293:LYS:HE2	1:I:294:GLU:HB2	2.01	0.41
1:J:278:GLU:HA	1:J:299:TYR:HD2	1.86	0.41
1:K:52:GLU:OE1	1:L:74:GLU:HB3	2.21	0.41
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.85	0.41
1:A:112:ILE:O	1:A:115:GLY:N	2.51	0.41
1:A:250:ASN:OD1	1:A:252:ASP:HB2	2.20	0.41
1:B:27:MSE:HE3	1:B:50:PHE:HZ	1.86	0.41
1:B:84:LYS:O	1:B:88:ASN:HB2	2.20	0.41
1:C:235:GLU:O	1:C:238:TYR:HB3	2.20	0.41
1:C:250:ASN:OD1	1:C:252:ASP:N	2.54	0.41
1:E:7:VAL:HG21	1:E:65:ALA:HA	2.03	0.41
1:F:195:LYS:HD2	2:F:344:HOH:O	2.20	0.41
1:G:11:ILE:HG12	1:H:149:PHE:CE2	2.56	0.41
1:G:35:VAL:HG22	1:G:40:ARG:HH21	1.86	0.41
1:I:103:ARG:HH21	1:I:133:THR:HB	1.86	0.41
1:J:195:LYS:HD3	1:J:235:GLU:OE2	2.21	0.41
1:K:261:ILE:HG12	1:K:276:LEU:HB3	2.02	0.41
1:A:27:MSE:HE1	1:A:40:ARG:HH22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:NH1	1:A:98:ARG:CB	2.83	0.41
1:A:251:ILE:O	1:A:255:LEU:HG	2.21	0.41
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.91	0.41
1:B:291:PRO:HB2	1:B:295:VAL:CG2	2.51	0.41
1:C:79:LYS:CD	1:C:112:ILE:HG12	2.49	0.41
1:C:86:PHE:C	1:C:88:ASN:H	2.29	0.41
1:D:58:PHE:CD2	1:D:58:PHE:C	2.99	0.41
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.86	0.41
1:E:12:ARG:HH21	1:E:36:GLU:CD	2.28	0.41
1:E:238:TYR:HE1	1:E:279:GLU:OE1	2.04	0.41
1:E:242:ILE:HG21	1:E:283:ILE:HD13	2.02	0.41
1:F:26:ILE:HD11	1:F:53:ARG:NH1	2.36	0.41
1:F:95:ASN:N	1:F:95:ASN:HD22	2.16	0.41
1:F:153:TYR:HB2	1:F:189:THR:CG2	2.51	0.41
1:G:85:ILE:O	1:G:85:ILE:CG2	2.68	0.41
1:G:136:SER:HA	1:G:139:LYS:HD2	2.03	0.41
1:I:4:ILE:HG21	1:I:47:LEU:HD13	2.02	0.41
1:I:12:ARG:HG3	1:I:17:TYR:HB2	2.03	0.41
1:I:203:MSE:HE3	1:I:286:LYS:HE2	2.02	0.41
1:I:272:ILE:O	1:I:276:LEU:HD13	2.21	0.41
1:J:197:ALA:HB1	2:J:318:HOH:O	2.20	0.41
1:L:104:LEU:HD21	1:L:137:ASP:OD1	2.21	0.41
1:L:224:LYS:HG2	1:L:225:ASN:ND2	2.35	0.41
1:B:30:SER:O	1:B:34:LYS:HG3	2.21	0.41
1:C:173:LYS:HB2	1:C:174:PRO:HD3	2.03	0.41
1:E:293:LYS:CG	1:E:294:GLU:N	2.84	0.41
1:G:135:THR:HG23	2:G:344:HOH:O	2.21	0.41
1:G:210:ALA:O	1:G:214:ILE:HG13	2.22	0.41
1:I:9:LYS:HB2	1:I:36:GLU:HB3	2.03	0.41
1:J:39:SER:O	1:J:40:ARG:HB2	2.21	0.41
1:J:75:THR:HG21	1:J:108:GLN:HB3	2.03	0.41
1:J:115:GLY:O	1:J:118:SER:HB3	2.21	0.41
1:K:91:LEU:HD22	1:K:95:ASN:OD1	2.21	0.41
1:K:220:LEU:O	1:K:226:ILE:HG21	2.21	0.41
1:L:139:LYS:O	1:L:143:ASP:HB2	2.21	0.41
1:A:172:ILE:O	1:A:173:LYS:C	2.64	0.40
1:B:113:TYR:OH	1:B:130:PHE:HD1	2.04	0.40
1:C:198:LEU:HG	1:C:239:LEU:HD13	2.03	0.40
1:F:45:GLU:O	1:F:48:SER:HB3	2.20	0.40
1:I:11:ILE:HG21	1:I:56:VAL:HG21	2.02	0.40
1:I:85:ILE:HG21	1:I:92:PHE:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:274:ARG:HB2	2:J:331:HOH:O	2.21	0.40
1:C:139:LYS:HA	1:C:143:ASP:OD2	2.20	0.40
1:D:40:ARG:NH2	1:D:46:GLU:OE1	2.49	0.40
1:E:153:TYR:CB	1:E:189:THR:HG22	2.51	0.40
1:F:26:ILE:CD1	1:F:53:ARG:NH1	2.84	0.40
1:F:81:LEU:HG	1:F:85:ILE:HD11	2.03	0.40
1:H:170:SER:HB3	2:H:336:HOH:O	2.21	0.40
1:J:35:VAL:C	1:J:37:ALA:N	2.79	0.40
1:K:12:ARG:HH11	1:K:12:ARG:HG2	1.85	0.40
1:L:100:GLU:C	1:L:100:GLU:CD	2.89	0.40
1:A:209:GLU:O	1:A:212:TYR:HB3	2.21	0.40
1:C:251:ILE:HD13	1:C:251:ILE:C	2.47	0.40
1:D:165:TYR:OH	1:D:209:GLU:OE1	2.38	0.40
1:E:4:ILE:HG22	1:E:8:LEU:HD11	2.03	0.40
1:G:113:TYR:CE1	1:G:117:ILE:HD11	2.56	0.40
1:H:78:GLU:O	1:H:82:ILE:CD1	2.69	0.40
1:H:78:GLU:O	1:H:82:ILE:HD13	2.21	0.40
1:H:81:LEU:O	1:H:85:ILE:HG13	2.22	0.40
1:H:274:ARG:NH2	1:H:301:ASN:O	2.52	0.40
1:J:79:LYS:HZ1	1:J:108:GLN:NE2	2.19	0.40
1:L:153:TYR:HB2	1:L:189:THR:HG22	2.03	0.40
1:B:110:PHE:O	1:B:114:LEU:HG	2.21	0.40
1:B:265:LYS:HB2	1:B:273:HIS:CD2	2.57	0.40
1:F:12:ARG:HG3	1:F:17:TYR:HB2	2.04	0.40
1:F:24:SER:OG	1:F:53:ARG:NH2	2.55	0.40
1:F:130:PHE:HZ	1:F:163:LEU:HD13	1.86	0.40
1:G:142:TYR:O	1:G:143:ASP:C	2.64	0.40
1:H:168:VAL:O	1:H:172:ILE:HG13	2.22	0.40
1:H:292:PRO:O	1:H:295:VAL:HG22	2.22	0.40
1:I:78:GLU:OE1	1:I:81:LEU:HD23	2.21	0.40
1:I:159:LEU:C	1:I:161:ASN:H	2.29	0.40
1:I:195:LYS:HE3	1:I:195:LYS:HB3	1.92	0.40
1:J:156:VAL:CG1	1:J:172:ILE:HG12	2.52	0.40
1:K:84:LYS:C	1:K:86:PHE:H	2.30	0.40
1:C:159:LEU:C	1:C:161:ASN:H	2.28	0.40
1:C:177:PRO:HA	1:C:216:GLN:OE1	2.20	0.40
1:F:279:GLU:OE1	1:F:279:GLU:C	2.64	0.40
1:G:153:TYR:HA	1:G:156:VAL:HG12	2.03	0.40
1:G:202:ILE:CG1	2:G:323:HOH:O	2.69	0.40
1:G:263:ILE:HG13	1:H:263:ILE:CG1	2.37	0.40
1:H:35:VAL:HG13	2:H:347:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:18:HIS:C	1:J:20:ILE:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/317 (94%)	273 (91%)	23 (8%)	3 (1%)	12	39
1	B	296/317 (93%)	279 (94%)	15 (5%)	2 (1%)	18	48
1	C	295/317 (93%)	251 (85%)	32 (11%)	12 (4%)	2	9
1	D	294/317 (93%)	275 (94%)	14 (5%)	5 (2%)	7	26
1	E	296/317 (93%)	271 (92%)	20 (7%)	5 (2%)	7	26
1	F	297/317 (94%)	266 (90%)	23 (8%)	8 (3%)	4	16
1	G	299/317 (94%)	257 (86%)	32 (11%)	10 (3%)	3	13
1	H	294/317 (93%)	268 (91%)	18 (6%)	8 (3%)	4	16
1	I	296/317 (93%)	257 (87%)	33 (11%)	6 (2%)	6	22
1	J	292/317 (92%)	259 (89%)	30 (10%)	3 (1%)	12	39
1	K	295/317 (93%)	274 (93%)	17 (6%)	4 (1%)	9	30
1	L	295/317 (93%)	269 (91%)	24 (8%)	2 (1%)	18	48
All	All	3548/3804 (93%)	3199 (90%)	281 (8%)	68 (2%)	6	23

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	C	72	VAL
1	C	88	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	249	LYS
1	D	88	ASN
1	E	92	PHE
1	E	124	ASN
1	E	249	LYS
1	F	24	SER
1	F	93	ASP
1	G	144	LYS
1	H	4	ILE
1	H	72	VAL
1	I	133	THR
1	I	134	ILE
1	I	249	LYS
1	J	29	LYS
1	K	92	PHE
1	K	93	ASP
1	L	249	LYS
1	B	24	SER
1	C	67	MSE
1	C	103	ARG
1	C	126	GLU
1	D	103	ARG
1	F	88	ASN
1	F	301	ASN
1	G	93	ASP
1	G	135	THR
1	G	301	ASN
1	H	73	ASN
1	H	93	ASP
1	H	131	ASN
1	J	24	SER
1	K	24	SER
1	L	92	PHE
1	A	93	ASP
1	D	301	ASN
1	E	93	ASP
1	F	89	PRO
1	F	302	TYR
1	G	24	SER
1	H	92	PHE
1	I	131	ASN
1	A	249	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	93	ASP
1	C	301	ASN
1	C	302	TYR
1	G	143	ASP
1	H	130	PHE
1	H	134	ILE
1	I	91	LEU
1	K	124	ASN
1	C	89	PRO
1	C	134	ILE
1	C	208	LYS
1	E	4	ILE
1	G	89	PRO
1	G	131	ASN
1	I	89	PRO
1	J	89	PRO
1	B	248	ASP
1	F	92	PHE
1	G	128	PRO
1	D	162	VAL
1	D	89	PRO
1	G	125	ILE
1	F	40	ARG

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	285/294 (97%)	270 (95%)	15 (5%)	20	52
1	B	283/294 (96%)	271 (96%)	12 (4%)	26	60
1	C	282/294 (96%)	266 (94%)	16 (6%)	18	49
1	D	281/294 (96%)	271 (96%)	10 (4%)	31	65
1	E	282/294 (96%)	266 (94%)	16 (6%)	18	49
1	F	283/294 (96%)	271 (96%)	12 (4%)	26	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	285/294 (97%)	265 (93%)	20 (7%)	14	40
1	H	281/294 (96%)	267 (95%)	14 (5%)	22	53
1	I	283/294 (96%)	270 (95%)	13 (5%)	24	57
1	J	279/294 (95%)	264 (95%)	15 (5%)	20	51
1	K	281/294 (96%)	272 (97%)	9 (3%)	34	68
1	L	282/294 (96%)	270 (96%)	12 (4%)	26	60
All	All	3387/3528 (96%)	3223 (95%)	164 (5%)	23	55

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	67	MSE
1	A	68	ASN
1	A	80	LEU
1	A	124	ASN
1	A	157	SER
1	A	179	VAL
1	A	188	LEU
1	A	227	SER
1	A	247	THR
1	A	251	ILE
1	A	277	VAL
1	A	281	THR
1	A	293	LYS
1	A	295	VAL
1	B	10	GLN
1	B	20	ILE
1	B	68	ASN
1	B	80	LEU
1	B	94	LYS
1	B	124	ASN
1	B	129	THR
1	B	188	LEU
1	B	283	ILE
1	B	288	LYS
1	B	293	LYS
1	B	302	TYR
1	C	10	GLN
1	C	20	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	22	LEU
1	C	36	GLU
1	C	80	LEU
1	C	88	ASN
1	C	94	LYS
1	C	188	LEU
1	C	207	LEU
1	C	237	ASN
1	C	251	ILE
1	C	277	VAL
1	C	286	LYS
1	C	288	LYS
1	C	293	LYS
1	C	295	VAL
1	D	3	LYS
1	D	8	LEU
1	D	54	LEU
1	D	80	LEU
1	D	163	LEU
1	D	179	VAL
1	D	188	LEU
1	D	276	LEU
1	D	277	VAL
1	D	283	ILE
1	E	68	ASN
1	E	93	ASP
1	E	135	THR
1	E	147	THR
1	E	156	VAL
1	E	188	LEU
1	E	237	ASN
1	E	238	TYR
1	E	251	ILE
1	E	259	ASN
1	E	263	ILE
1	E	270	GLU
1	E	276	LEU
1	E	277	VAL
1	E	281	THR
1	E	293	LYS
1	F	23	TYR
1	F	46	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	68	ASN
1	F	84	LYS
1	F	100	GLU
1	F	129	THR
1	F	163	LEU
1	F	188	LEU
1	F	276	LEU
1	F	279	GLU
1	F	293	LYS
1	F	302	TYR
1	G	57	ASN
1	G	68	ASN
1	G	78	GLU
1	G	94	LYS
1	G	132	LYS
1	G	146	THR
1	G	147	THR
1	G	156	VAL
1	G	157	SER
1	G	179	VAL
1	G	181	SER
1	G	188	LEU
1	G	189	THR
1	G	238	TYR
1	G	263	ILE
1	G	276	LEU
1	G	278	GLU
1	G	293	LYS
1	G	295	VAL
1	G	301	ASN
1	H	20	ILE
1	H	29	LYS
1	H	50	PHE
1	H	68	ASN
1	H	108	GLN
1	H	114	LEU
1	H	147	THR
1	H	156	VAL
1	H	162	VAL
1	H	188	LEU
1	H	195	LYS
1	H	234	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	237	ASN
1	H	276	LEU
1	I	20	ILE
1	I	23	TYR
1	I	68	ASN
1	I	78	GLU
1	I	94	LYS
1	I	97	GLN
1	I	102	LYS
1	I	121	HIS
1	I	163	LEU
1	I	188	LEU
1	I	277	VAL
1	I	289	PHE
1	I	293	LYS
1	J	10	GLN
1	J	23	TYR
1	J	93	ASP
1	J	97	GLN
1	J	129	THR
1	J	147	THR
1	J	163	LEU
1	J	180	ASP
1	J	188	LEU
1	J	238	TYR
1	J	244	GLN
1	J	251	ILE
1	J	263	ILE
1	J	277	VAL
1	J	296	THR
1	K	68	ASN
1	K	94	LYS
1	K	131	ASN
1	K	143	ASP
1	K	147	THR
1	K	188	LEU
1	K	270	GLU
1	K	281	THR
1	K	302	TYR
1	L	23	TYR
1	L	67	MSE
1	L	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	94	LYS
1	L	147	THR
1	L	188	LEU
1	L	238	TYR
1	L	247	THR
1	L	251	ILE
1	L	276	LEU
1	L	295	VAL
1	L	302	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	68	ASN
1	A	88	ASN
1	A	95	ASN
1	A	97	GLN
1	A	108	GLN
1	A	122	HIS
1	A	158	ASN
1	A	161	ASN
1	A	191	GLN
1	A	211	GLN
1	A	215	ASN
1	A	225	ASN
1	A	244	GLN
1	B	16	ASN
1	B	68	ASN
1	B	73	ASN
1	B	95	ASN
1	B	97	GLN
1	B	108	GLN
1	B	158	ASN
1	B	161	ASN
1	B	191	GLN
1	B	215	ASN
1	B	225	ASN
1	B	256	ASN
1	B	301	ASN
1	C	10	GLN
1	C	19	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	88	ASN
1	C	95	ASN
1	C	97	GLN
1	C	108	GLN
1	C	124	ASN
1	C	158	ASN
1	C	191	GLN
1	C	215	ASN
1	C	219	HIS
1	C	225	ASN
1	C	241	GLN
1	D	10	GLN
1	D	88	ASN
1	D	97	GLN
1	D	108	GLN
1	D	158	ASN
1	D	161	ASN
1	D	191	GLN
1	D	215	ASN
1	D	241	GLN
1	E	10	GLN
1	E	13	GLN
1	E	16	ASN
1	E	68	ASN
1	E	88	ASN
1	E	95	ASN
1	E	97	GLN
1	E	108	GLN
1	E	131	ASN
1	E	158	ASN
1	E	161	ASN
1	E	191	GLN
1	E	211	GLN
1	E	215	ASN
1	E	219	HIS
1	E	225	ASN
1	E	244	GLN
1	E	301	ASN
1	F	10	GLN
1	F	63	ASN
1	F	68	ASN
1	F	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	122	HIS
1	F	131	ASN
1	F	158	ASN
1	F	191	GLN
1	F	211	GLN
1	F	215	ASN
1	F	225	ASN
1	F	237	ASN
1	F	244	GLN
1	F	262	ASN
1	G	10	GLN
1	G	57	ASN
1	G	68	ASN
1	G	88	ASN
1	G	97	GLN
1	G	108	GLN
1	G	122	HIS
1	G	131	ASN
1	G	158	ASN
1	G	161	ASN
1	G	191	GLN
1	G	215	ASN
1	G	229	ASN
1	G	237	ASN
1	G	244	GLN
1	G	250	ASN
1	G	259	ASN
1	H	68	ASN
1	H	88	ASN
1	H	97	GLN
1	H	108	GLN
1	H	122	HIS
1	H	191	GLN
1	H	196	ASN
1	H	215	ASN
1	H	219	HIS
1	H	244	GLN
1	H	273	HIS
1	I	13	GLN
1	I	19	GLN
1	I	63	ASN
1	I	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	88	ASN
1	I	95	ASN
1	I	97	GLN
1	I	121	HIS
1	I	131	ASN
1	I	191	GLN
1	I	211	GLN
1	I	215	ASN
1	I	225	ASN
1	I	237	ASN
1	I	244	GLN
1	J	10	GLN
1	J	16	ASN
1	J	73	ASN
1	J	88	ASN
1	J	95	ASN
1	J	108	GLN
1	J	131	ASN
1	J	191	GLN
1	J	196	ASN
1	J	211	GLN
1	J	215	ASN
1	J	244	GLN
1	J	250	ASN
1	K	63	ASN
1	K	68	ASN
1	K	88	ASN
1	K	97	GLN
1	K	108	GLN
1	K	131	ASN
1	K	158	ASN
1	K	161	ASN
1	K	191	GLN
1	K	211	GLN
1	K	215	ASN
1	K	237	ASN
1	K	244	GLN
1	K	259	ASN
1	L	68	ASN
1	L	88	ASN
1	L	95	ASN
1	L	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	108	GLN
1	L	131	ASN
1	L	158	ASN
1	L	191	GLN
1	L	211	GLN
1	L	215	ASN
1	L	225	ASN
1	L	237	ASN
1	L	244	GLN
1	L	259	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	298/317 (94%)	-0.58	1 (0%) 90 87	19, 42, 99, 133	0
1	B	296/317 (93%)	-0.55	1 (0%) 90 87	15, 42, 95, 193	0
1	C	295/317 (93%)	-0.26	3 (1%) 79 73	19, 60, 121, 160	0
1	D	294/317 (92%)	-0.44	2 (0%) 84 79	19, 56, 110, 189	0
1	E	296/317 (93%)	-0.53	2 (0%) 84 79	16, 47, 98, 132	0
1	F	297/317 (93%)	-0.36	2 (0%) 84 79	18, 53, 116, 167	0
1	G	299/317 (94%)	-0.28	4 (1%) 75 67	23, 57, 121, 159	0
1	H	294/317 (92%)	-0.41	2 (0%) 84 79	18, 52, 111, 169	0
1	I	296/317 (93%)	-0.27	2 (0%) 84 79	28, 66, 134, 169	0
1	J	292/317 (92%)	-0.42	3 (1%) 79 73	24, 56, 119, 171	0
1	K	295/317 (93%)	-0.36	1 (0%) 90 87	17, 51, 112, 169	0
1	L	295/317 (93%)	-0.46	1 (0%) 90 87	16, 52, 103, 149	0
All	All	3547/3804 (93%)	-0.41	24 (0%) 84 79	15, 53, 114, 193	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	VAL	3.1
1	G	301	ASN	2.9
1	J	289	PHE	2.8
1	G	72	VAL	2.8
1	E	304	ALA	2.7
1	J	68	ASN	2.7
1	H	302	TYR	2.7
1	J	71	SER	2.6
1	B	68	ASN	2.5
1	D	302	TYR	2.4
1	F	68	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	303	VAL	2.4
1	K	304	ALA	2.4
1	I	301	ASN	2.3
1	F	274	ARG	2.3
1	G	68	ASN	2.3
1	E	297	MET	2.2
1	A	68	ASN	2.2
1	C	126	GLU	2.1
1	C	68	ASN	2.1
1	L	72	VAL	2.0
1	G	93	ASP	2.0
1	H	289	PHE	2.0
1	C	303	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.