Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:40 PM GMT

PDB ID	:	1PMA
Title	:	PROTEASOME FROM THERMOPLASMA ACIDOPHILUM
Authors	:	Loewe, J.; Stock, D.; Jap, B.; Zwickl, P.; Baumeister, W.; Huber, R.
Deposited on	:	1994-12-19
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

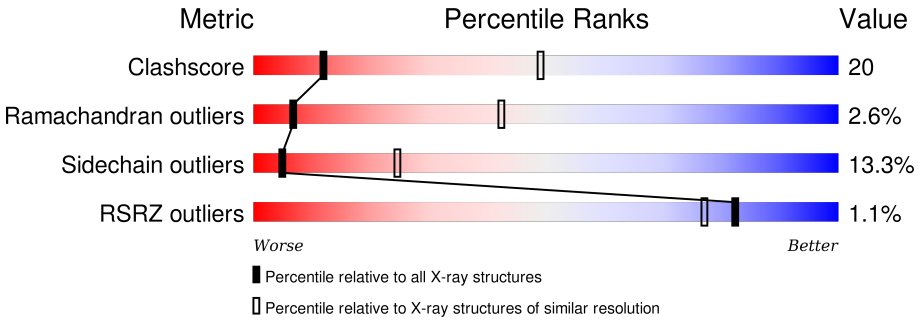
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	233	2% 48% 42% 5% 5%
1	C	233	% 51% 35% 8% 5%
1	D	233	3% 49% 39% 7% 5%
1	E	233	2% 49% 37% 9% 5%
1	F	233	2% 45% 42% 7% 5%
1	G	233	3% 44% 44% 7% 5%
1	H	233	2% 48% 41% 5% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	233	3% 49% 38% 7% 5%
1	J	233	3% 51% 37% 6% 5%
1	K	233	2% 54% 35% 6% 5%
1	L	233	2% 51% 37% 6% 5%
1	M	233	2% 51% 39% 5% 5%
1	N	233	2% 55% 32% 7% 5%
1	O	233	% 50% 36% 9% 5%
2	1	211	54% 34% 9%
2	2	211	55% 33% 8%
2	B	211	51% 37% 9%
2	P	211	57% 31% 8%
2	Q	211	58% 31% 7%
2	R	211	51% 37% 8%
2	S	211	52% 36% 8%
2	T	211	59% 31% 7%
2	U	211	54% 35% 8%
2	V	211	53% 36% 8%
2	W	211	54% 34% 9%
2	X	211	57% 33% 6%
2	Y	211	58% 30% 8%
2	Z	211	55% 35% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 56294 atoms, of which 10402 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 PROTEASOME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	C	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	D	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	E	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	F	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	G	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	H	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	I	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	J	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	K	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	L	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	M	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	N	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	O	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			

- Molecule 2 is a protein called PROTEASOME.

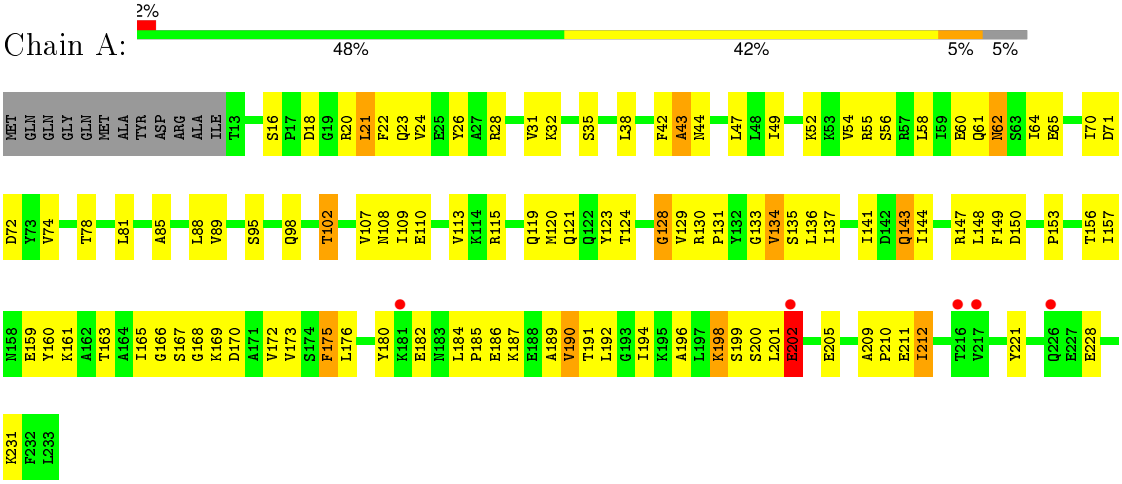
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	P	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	Q	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	R	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	S	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	T	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	U	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	V	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	W	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	X	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	Y	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	Z	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	1	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			
2	2	203	Total	C	H	N	O	S	0	0	0
			1908	985	350	264	298	11			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

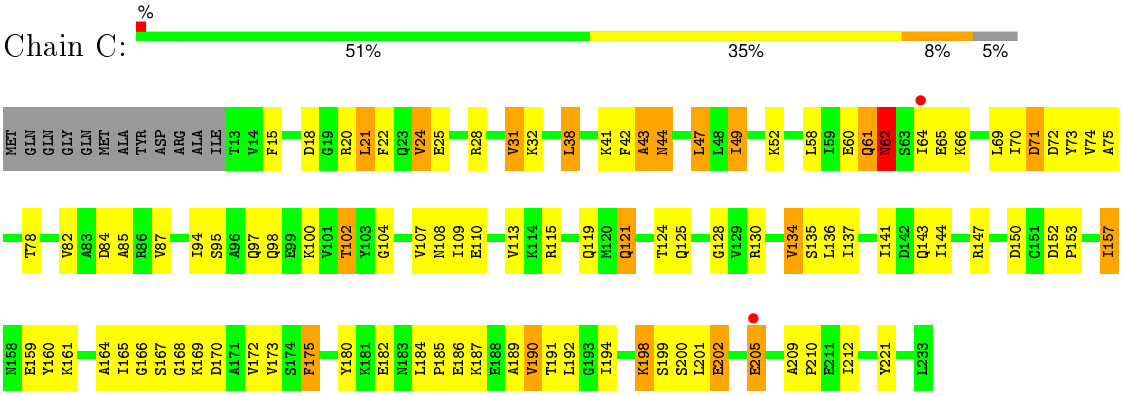
- Molecule 1: PROTEASOME

Chain A:



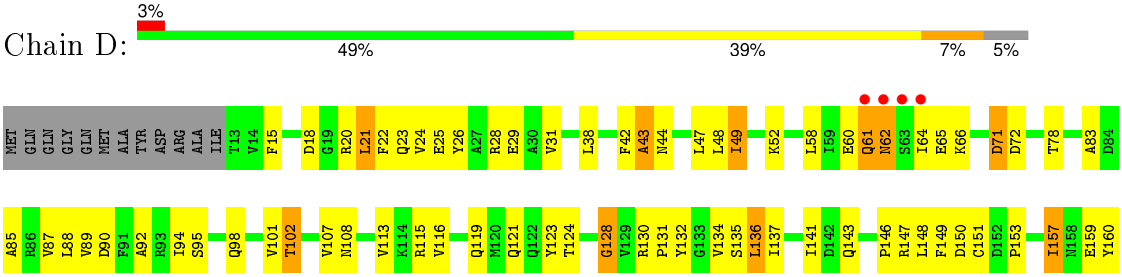
- Molecule 1: PROTEASOME

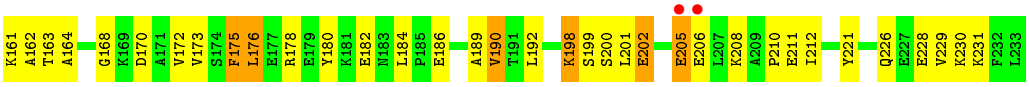
Chain C:



- Molecule 1: PROTEASOME

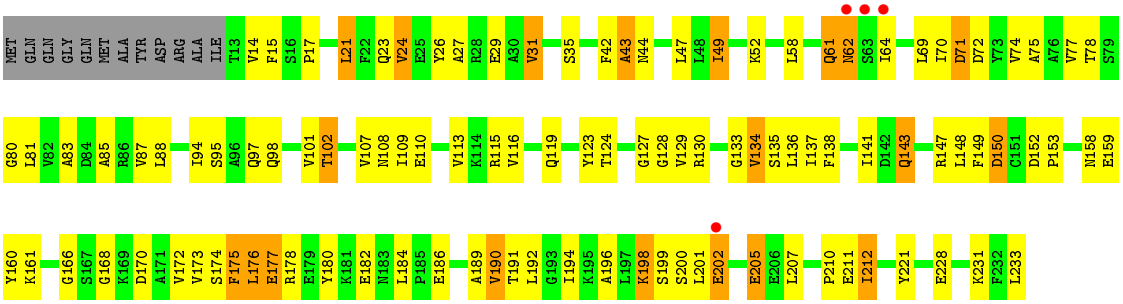
Chain D:





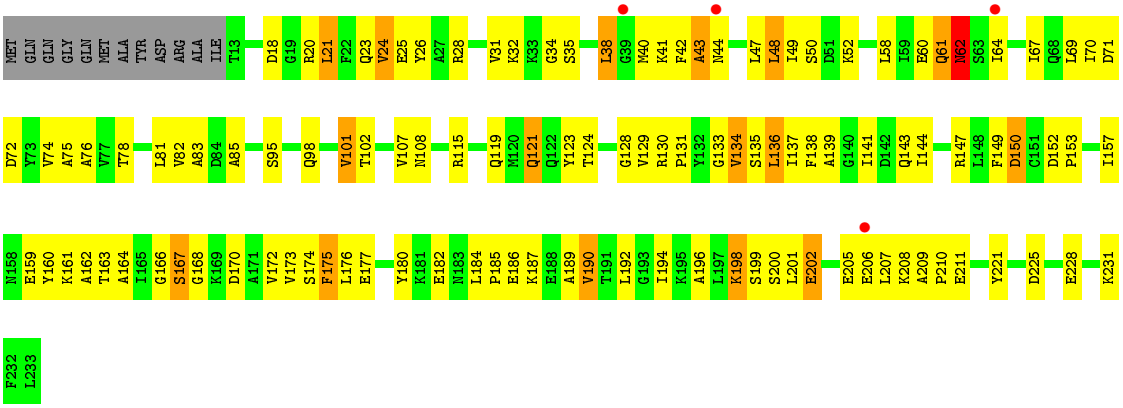
• Molecule 1: PROTEASOME

Chain E:



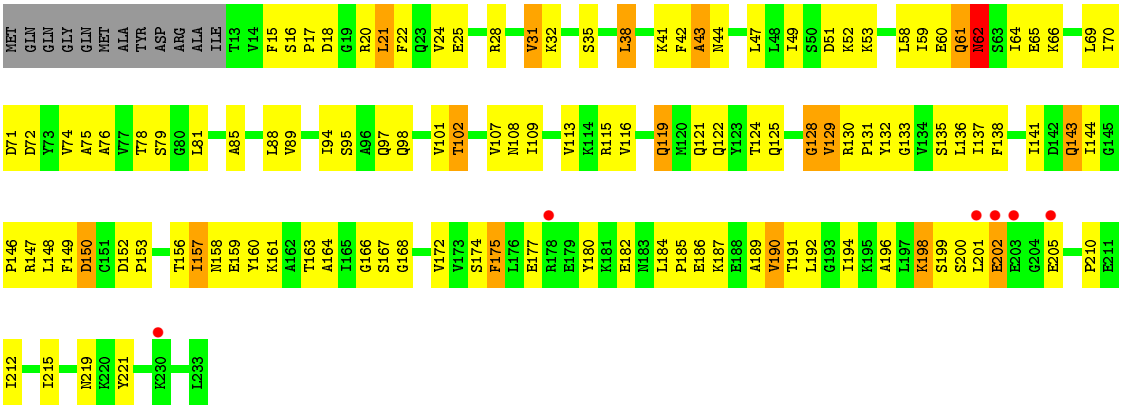
• Molecule 1: PROTEASOME

Chain F:



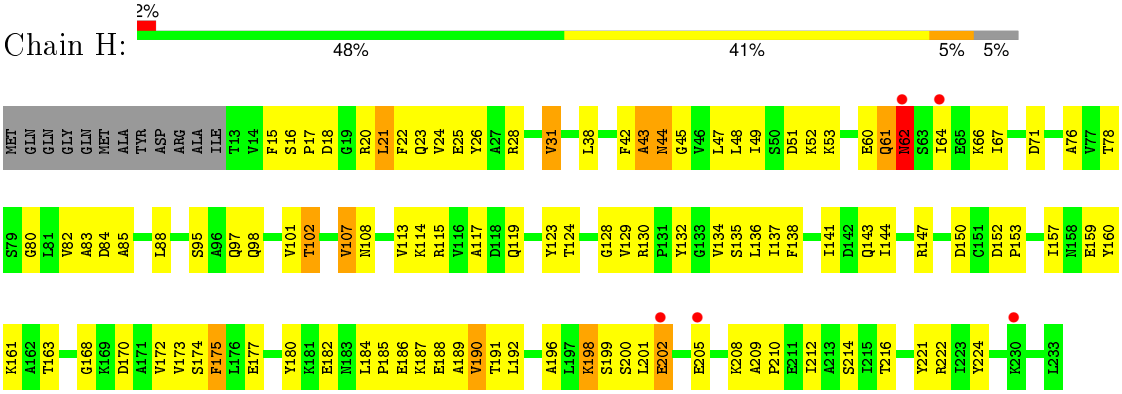
• Molecule 1: PROTEASOME

Chain G:



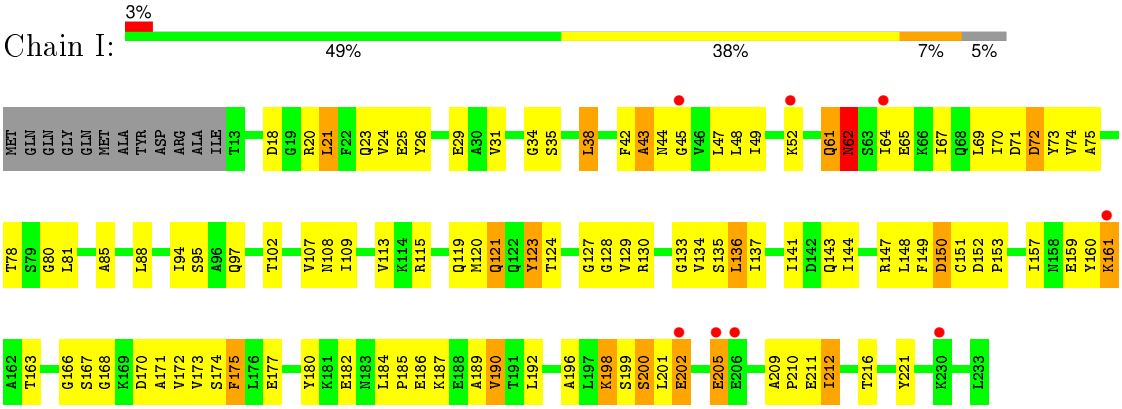
• Molecule 1: PROTEASOME

Chain H:



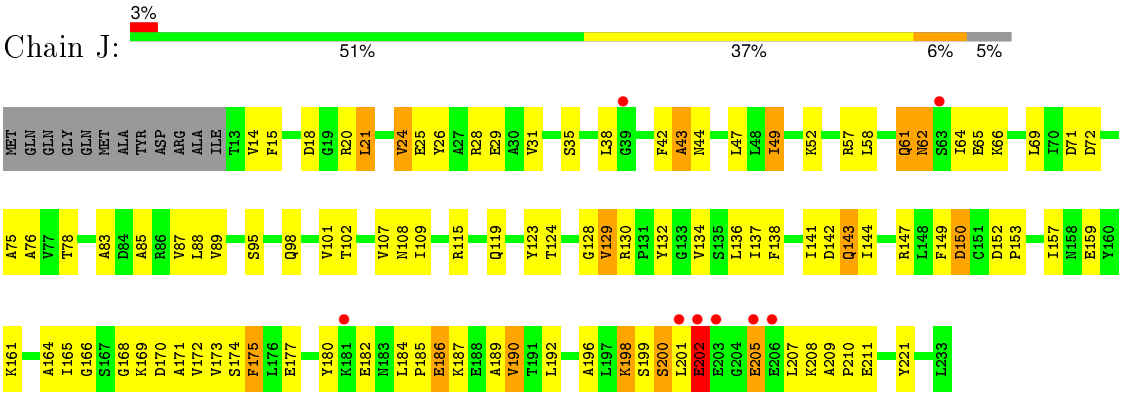
• Molecule 1: PROTEASOME

Chain I:



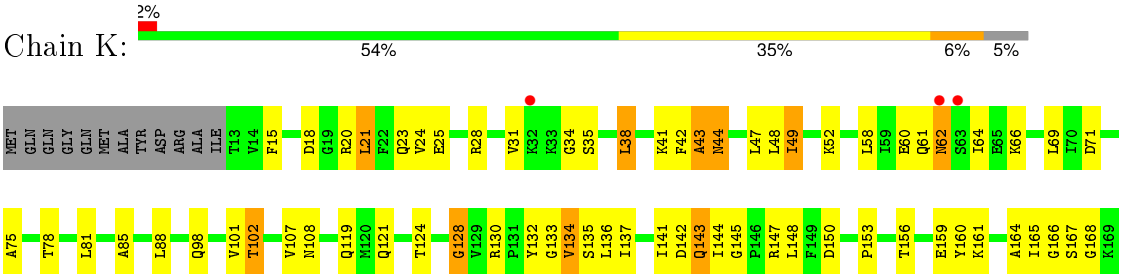
• Molecule 1: PROTEASOME

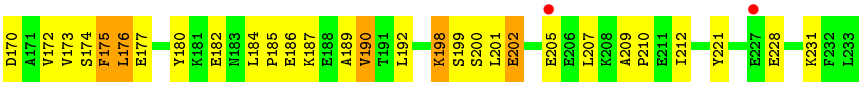
Chain J:



• Molecule 1: PROTEASOME

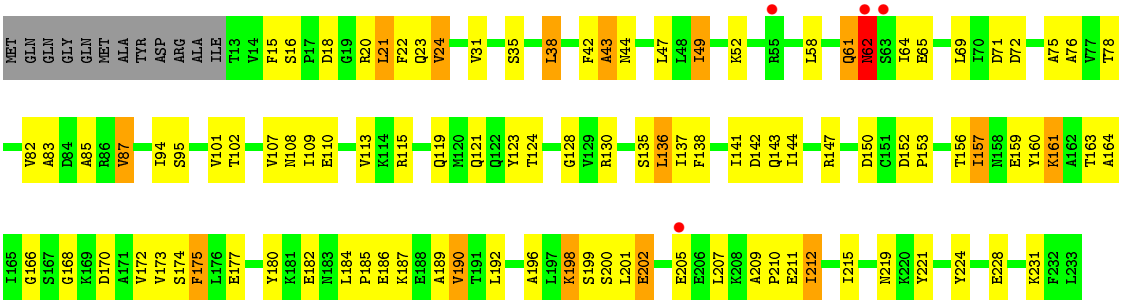
Chain K:





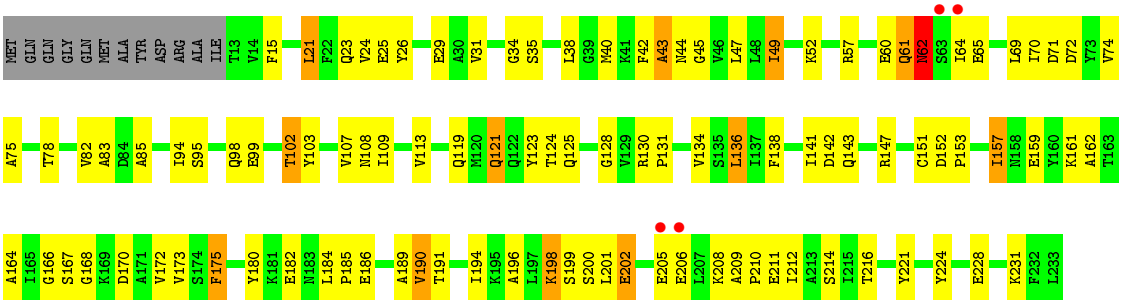
• Molecule 1: PROTEASOME

Chain L:



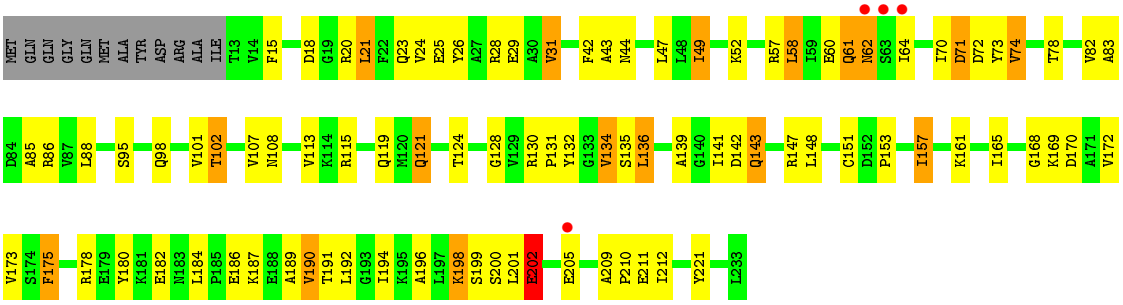
• Molecule 1: PROTEASOME

Chain M:



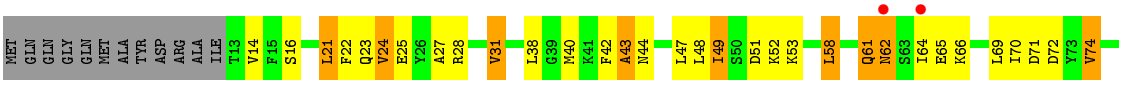
• Molecule 1: PROTEASOME

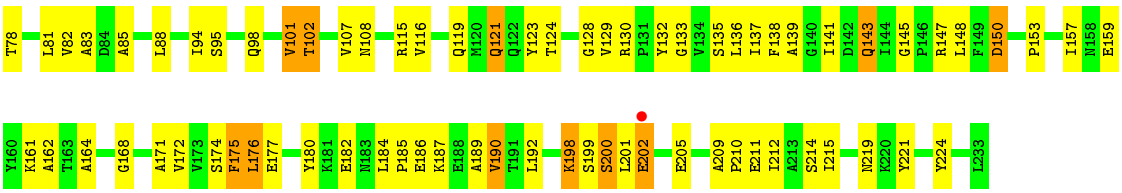
Chain N:



• Molecule 1: PROTEASOME

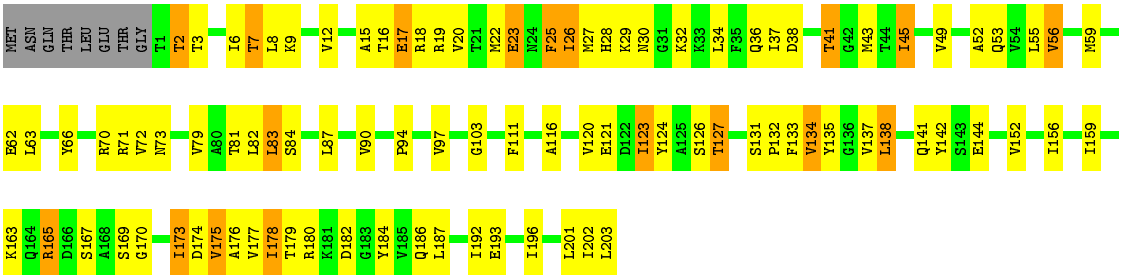
Chain O:





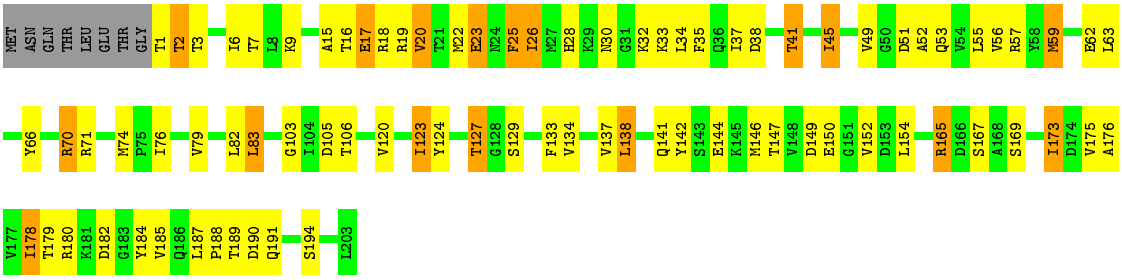
• Molecule 2: PROTEASOME

Chain B:



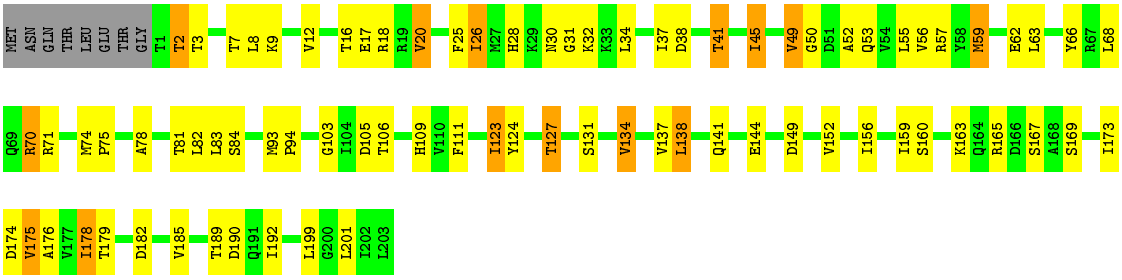
• Molecule 2: PROTEASOME

Chain P:



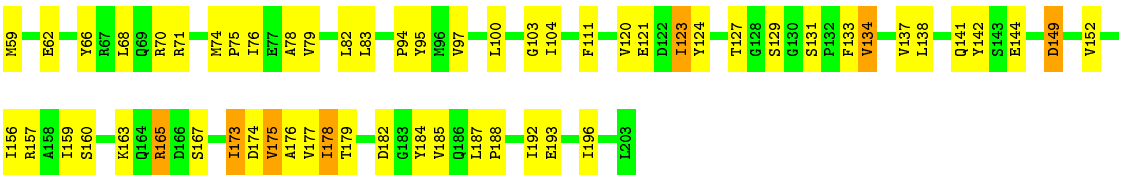
• Molecule 2: PROTEASOME

Chain Q:



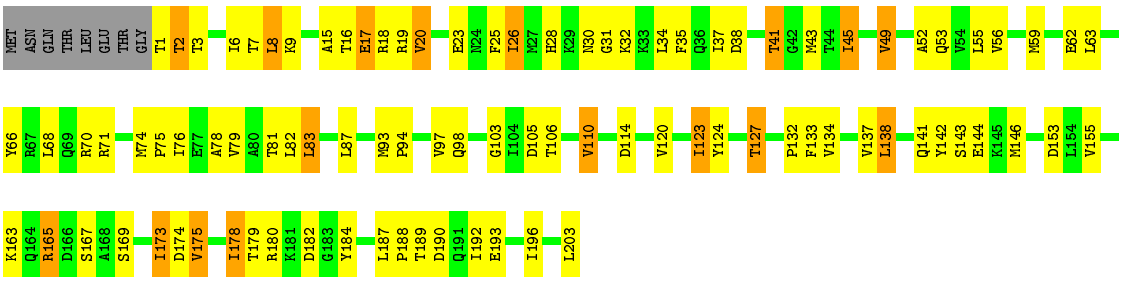
• Molecule 2: PROTEASOME

Chain R:



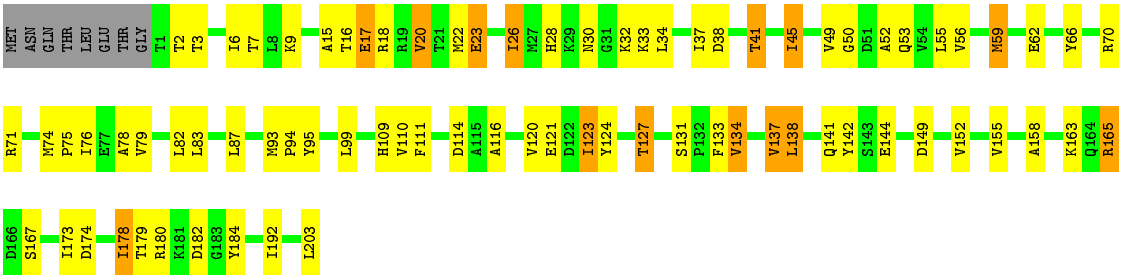
• Molecule 2: PROTEASOME

Chain S:



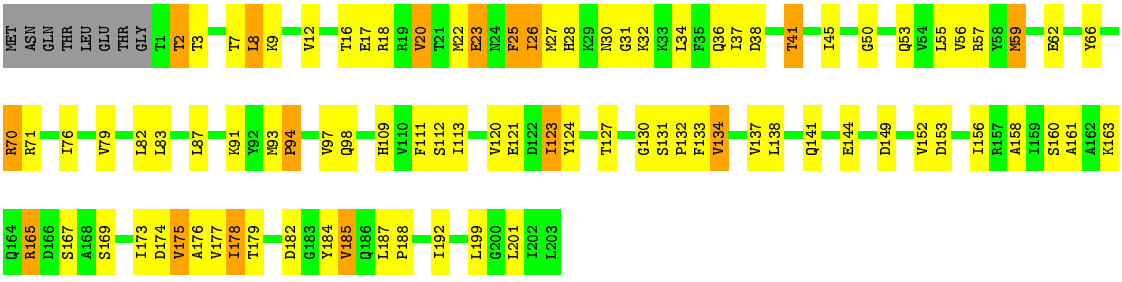
• Molecule 2: PROTEASOME

Chain T:



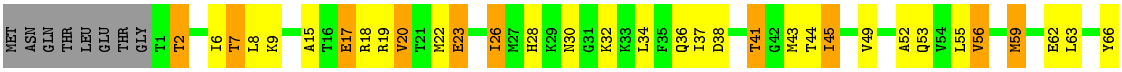
• Molecule 2: PROTEASOME

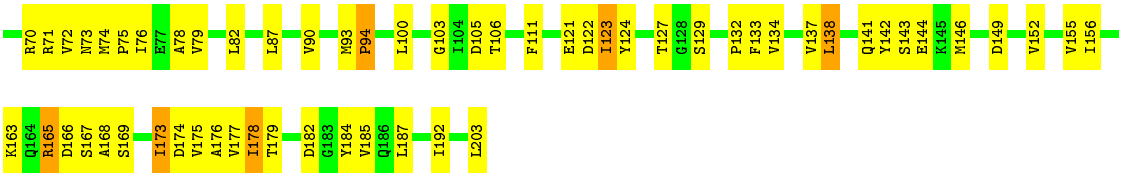
Chain U:



• Molecule 2: PROTEASOME

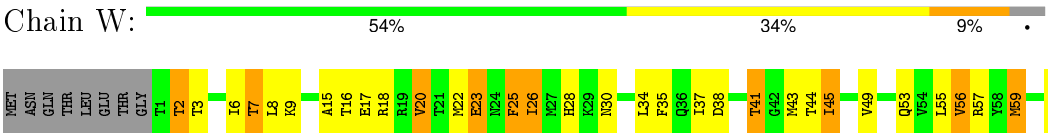
Chain V:





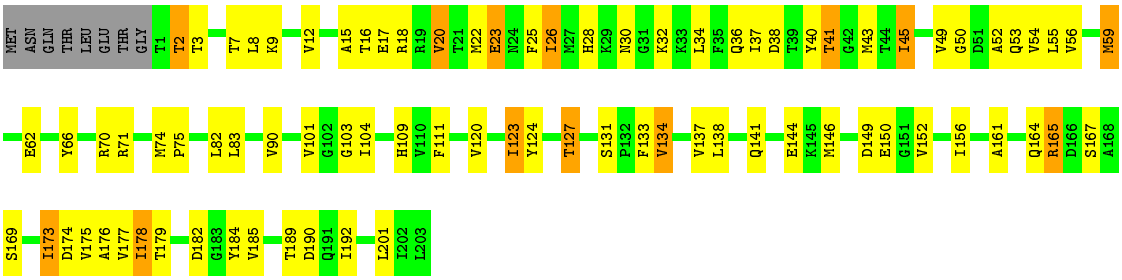
• Molecule 2: PROTEASOME

Chain W:



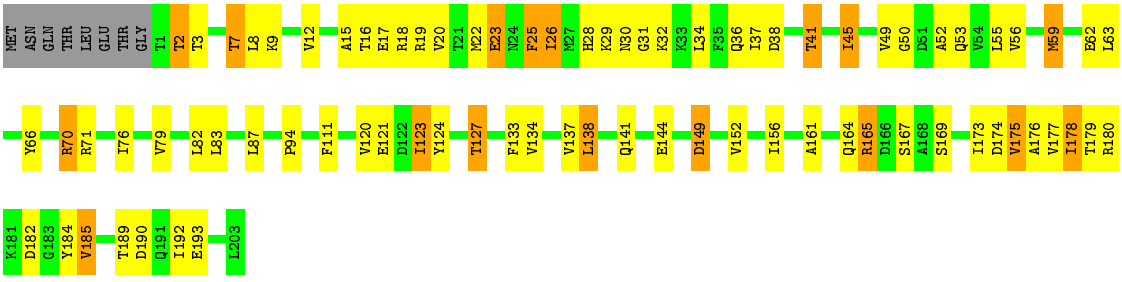
• Molecule 2: PROTEASOME

Chain X:



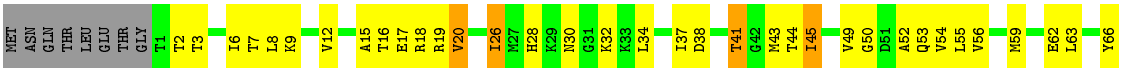
• Molecule 2: PROTEASOME

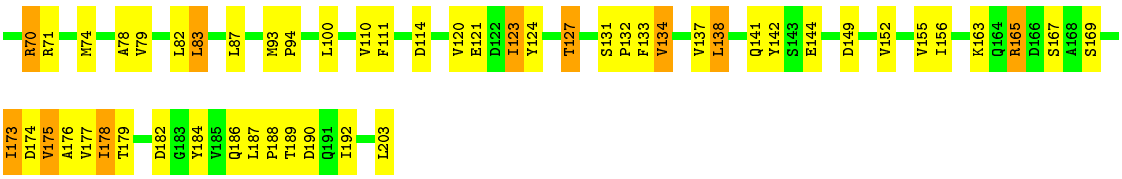
Chain Y:



• Molecule 2: PROTEASOME

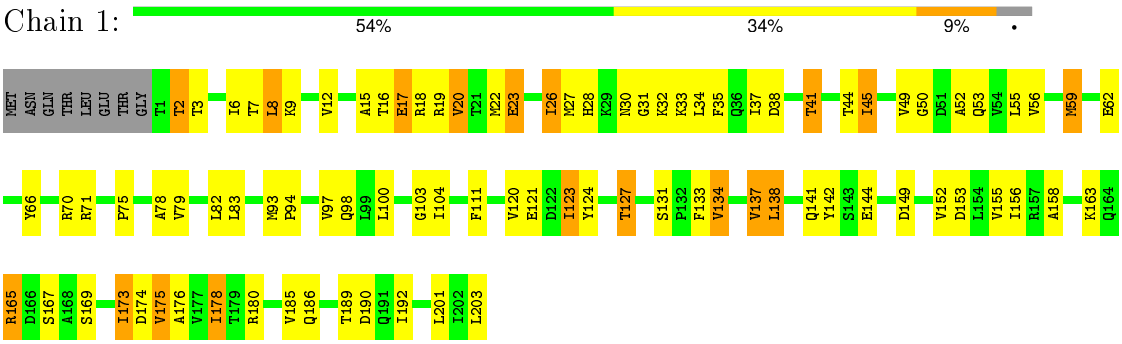
Chain Z:





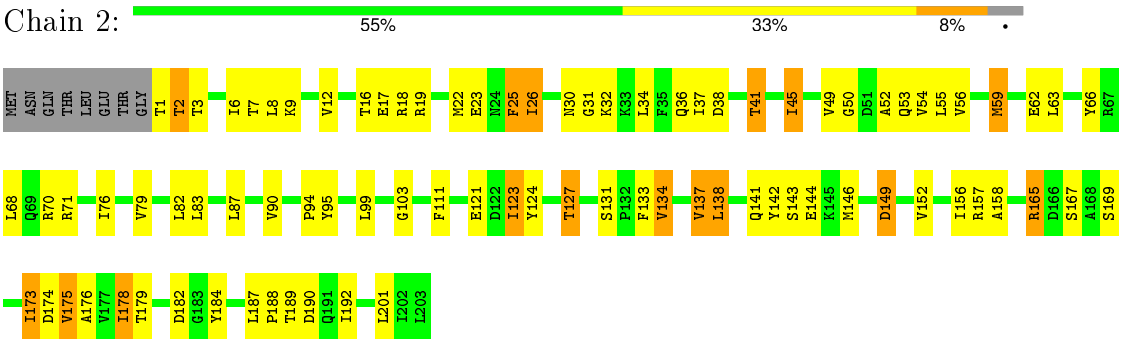
- Molecule 2: PROTEASOME

Chain 1:



- Molecule 2: PROTEASOME

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	311.90Å 209.70Å 117.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.40 20.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	85.7 (10.00-3.40) 85.0 (20.97-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 3.37Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , (Not available) 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 131.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 90045 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	56294	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/1743	0.71	1/2348 (0.0%)
1	C	0.51	0/1743	0.71	0/2348
1	D	0.52	0/1743	0.70	1/2348 (0.0%)
1	E	0.55	0/1743	0.72	0/2348
1	F	0.52	0/1743	0.70	0/2348
1	G	0.54	0/1743	0.69	0/2348
1	H	0.53	0/1743	0.70	0/2348
1	I	0.50	0/1743	0.70	0/2348
1	J	0.51	0/1743	0.69	0/2348
1	K	0.51	0/1743	0.69	1/2348 (0.0%)
1	L	0.53	0/1743	0.70	0/2348
1	M	0.51	0/1743	0.70	0/2348
1	N	0.54	0/1743	0.70	0/2348
1	O	0.52	0/1743	0.71	0/2348
2	1	0.55	0/1577	0.74	1/2129 (0.0%)
2	2	0.53	0/1577	0.75	1/2129 (0.0%)
2	B	0.56	0/1577	0.76	0/2129
2	P	0.57	0/1577	0.76	0/2129
2	Q	0.54	0/1577	0.75	0/2129
2	R	0.55	0/1577	0.77	2/2129 (0.1%)
2	S	0.57	0/1577	0.77	0/2129
2	T	0.55	0/1577	0.75	1/2129 (0.0%)
2	U	0.54	0/1577	0.74	0/2129
2	V	0.56	0/1577	0.77	0/2129
2	W	0.57	0/1577	0.75	1/2129 (0.0%)
2	X	0.54	0/1577	0.73	0/2129
2	Y	0.52	0/1577	0.74	0/2129
2	Z	0.54	0/1577	0.75	0/2129
All	All	0.53	0/46480	0.72	9/62678 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	95	TYR	N-CA-C	-5.91	95.06	111.00
2	1	8	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	128	GLY	N-CA-C	5.36	126.49	113.10
2	W	8	LEU	CA-CB-CG	5.32	127.54	115.30
1	K	128	GLY	N-CA-C	5.31	126.39	113.10
1	A	128	GLY	N-CA-C	5.07	125.78	113.10
2	2	95	TYR	N-CA-C	-5.05	97.37	111.00
2	T	95	TYR	N-CA-C	-5.03	97.41	111.00
2	R	8	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	393	1753	76	0
1	C	1720	393	1753	75	0
1	D	1720	393	1753	76	1
1	E	1720	393	1753	78	0
1	F	1720	393	1753	83	0
1	G	1720	393	1753	97	0
1	H	1720	393	1753	81	0
1	I	1720	393	1753	80	0
1	J	1720	393	1753	74	0
1	K	1720	393	1753	71	0
1	L	1720	393	1753	79	0
1	M	1720	393	1753	74	0
1	N	1720	393	1753	67	1
1	O	1720	393	1753	75	0
2	1	1558	350	1609	76	0
2	2	1558	350	1609	62	0
2	B	1558	350	1609	82	0
2	P	1558	350	1609	64	0
2	Q	1558	350	1609	56	0
2	R	1558	350	1609	68	0
2	S	1558	350	1609	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	1558	350	1609	61	0
2	U	1558	350	1609	69	0
2	V	1558	350	1609	74	0
2	W	1558	350	1609	68	0
2	X	1558	350	1609	63	0
2	Y	1558	350	1609	66	0
2	Z	1558	350	1609	69	0
All	All	45892	10402	47068	1857	1

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 20.

All (1857) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ASP:HB3	2:B:41:THR:HG23	1.38	1.03
2:T:38:ASP:HB3	2:T:41:THR:HG23	1.44	1.00
2:Q:45:ILE:HG12	2:Q:52:ALA:HB1	1.44	0.99
2:Q:38:ASP:HB3	2:Q:41:THR:HG23	1.46	0.98
2:R:38:ASP:HB3	2:R:41:THR:HG23	1.45	0.98
2:B:66:TYR:OH	1:H:107:VAL:HG11	1.62	0.97
2:T:45:ILE:HG12	2:T:52:ALA:HB1	1.46	0.96
1:M:107:VAL:HG11	2:1:66:TYR:OH	1.65	0.96
2:U:38:ASP:HB3	2:U:41:THR:HG23	1.47	0.95
2:2:38:ASP:HB3	2:2:41:THR:HG23	1.47	0.95
2:Y:38:ASP:HB3	2:Y:41:THR:HG23	1.48	0.95
2:W:38:ASP:HB3	2:W:41:THR:HG23	1.45	0.95
2:P:38:ASP:HB3	2:P:41:THR:HG23	1.49	0.94
1:K:107:VAL:HG11	2:Y:66:TYR:OH	1.68	0.94
2:1:38:ASP:HB3	2:1:41:THR:HG23	1.50	0.93
1:I:107:VAL:HG11	2:W:66:TYR:OH	1.68	0.93
2:Z:38:ASP:HB3	2:Z:41:THR:HG23	1.50	0.93
1:A:107:VAL:HG11	2:P:66:TYR:OH	1.69	0.93
1:L:107:VAL:HG11	2:Z:66:TYR:OH	1.69	0.92
1:D:107:VAL:HG11	2:R:66:TYR:OH	1.70	0.91
1:N:107:VAL:HG11	2:2:66:TYR:OH	1.69	0.91
2:X:45:ILE:HG12	2:X:52:ALA:HB1	1.53	0.91
1:F:107:VAL:HG11	2:T:66:TYR:OH	1.71	0.90
2:1:37:ILE:HD11	2:1:59:MET:HB3	1.54	0.90
2:X:38:ASP:HB3	2:X:41:THR:HG23	1.54	0.89
1:E:107:VAL:HG11	2:S:66:TYR:OH	1.73	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:53:GLN:O	2:X:56:VAL:HG12	1.73	0.88
2:Z:59:MET:HE2	2:Z:79:VAL:HG23	1.54	0.88
2:T:37:ILE:HD11	2:T:59:MET:HB3	1.56	0.87
1:J:107:VAL:HG11	2:X:66:TYR:OH	1.75	0.85
1:L:124:THR:HG22	1:M:130:ARG:HH21	1.42	0.85
1:D:108:ASN:HB3	2:R:70:ARG:HG2	1.57	0.85
2:S:38:ASP:HB3	2:S:41:THR:HG23	1.59	0.85
1:I:130:ARG:HH21	1:O:124:THR:HG22	1.41	0.84
1:K:124:THR:HG22	1:L:130:ARG:HH21	1.43	0.84
2:V:38:ASP:HB3	2:V:41:THR:HG23	1.57	0.84
1:O:107:VAL:HG11	2:V:66:TYR:OH	1.78	0.84
1:M:168:GLY:O	1:M:172:VAL:HG12	1.77	0.83
2:U:53:GLN:O	2:U:56:VAL:HG12	1.78	0.83
2:P:123:ILE:HG12	2:P:124:TYR:HD1	1.44	0.83
2:Q:37:ILE:HD11	2:Q:59:MET:HB3	1.61	0.82
1:G:124:THR:HG22	1:H:130:ARG:HH21	1.44	0.81
1:C:107:VAL:HG11	2:Q:66:TYR:OH	1.79	0.81
2:Z:123:ILE:HG12	2:Z:124:TYR:HD1	1.44	0.81
2:T:20:VAL:HG13	2:T:28:HIS:HB2	1.62	0.81
1:A:52:LYS:NZ	1:A:62:ASN:HA	1.96	0.81
2:W:123:ILE:HG12	2:W:124:TYR:HD1	1.46	0.80
1:I:108:ASN:HB3	2:W:70:ARG:HG2	1.62	0.80
1:F:124:THR:HG22	1:G:130:ARG:HH21	1.45	0.80
1:G:107:VAL:HG11	2:U:66:TYR:OH	1.83	0.79
2:R:123:ILE:HG12	2:R:124:TYR:HD1	1.48	0.78
2:B:123:ILE:HG12	2:B:124:TYR:HD1	1.48	0.78
2:1:123:ILE:HD13	2:1:123:ILE:H	1.47	0.78
2:B:70:ARG:HG2	1:H:108:ASN:HB3	1.65	0.78
2:P:53:GLN:O	2:P:56:VAL:HG12	1.83	0.78
2:Q:123:ILE:H	2:Q:123:ILE:HD13	1.49	0.78
1:A:186:GLU:O	1:A:190:VAL:HG12	1.84	0.78
1:K:52:LYS:NZ	1:K:62:ASN:HA	2.00	0.77
1:M:107:VAL:HG11	2:1:66:TYR:HH	1.49	0.76
2:W:53:GLN:O	2:W:56:VAL:HG12	1.86	0.76
2:2:53:GLN:O	2:2:56:VAL:HG12	1.86	0.76
1:H:168:GLY:O	1:H:172:VAL:HG12	1.85	0.76
1:C:18:ASP:OD2	1:C:20:ARG:HD3	1.85	0.76
1:K:108:ASN:HB3	2:Y:70:ARG:HG2	1.66	0.76
1:I:198:LYS:O	1:I:202:GLU:HB2	1.85	0.76
1:A:124:THR:HG22	1:C:130:ARG:HH21	1.50	0.76
2:V:123:ILE:HG12	2:V:124:TYR:HD1	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:32:LYS:HE2	2:U:34:LEU:O	1.85	0.75
1:K:78:THR:HG21	1:K:85:ALA:HB1	1.67	0.75
1:F:21:LEU:HD11	1:G:130:ARG:HD2	1.68	0.75
2:S:53:GLN:O	2:S:56:VAL:HG12	1.87	0.75
2:1:3:THR:OG1	2:1:127:THR:HG22	1.86	0.75
2:1:53:GLN:O	2:1:56:VAL:HG12	1.86	0.74
2:Y:53:GLN:O	2:Y:56:VAL:HG12	1.87	0.74
1:G:21:LEU:O	1:G:24:VAL:HG12	1.87	0.73
2:S:2:THR:HG22	2:S:169:SER:OG	1.89	0.73
1:E:135:SER:OG	1:E:153:PRO:HD3	1.88	0.73
1:M:78:THR:HG21	1:M:85:ALA:HB1	1.71	0.73
2:T:18:ARG:HE	2:T:30:ASN:HD22	1.37	0.73
2:2:37:ILE:HD11	2:2:59:MET:HB3	1.71	0.73
1:A:78:THR:HG21	1:A:85:ALA:HB1	1.70	0.73
1:I:130:ARG:HD2	1:O:21:LEU:HD11	1.69	0.73
2:V:123:ILE:H	2:V:123:ILE:HD13	1.53	0.73
2:P:38:ASP:HB3	2:P:41:THR:CG2	2.19	0.73
2:P:103:GLY:HA2	2:P:178:ILE:HD11	1.71	0.73
2:U:62:GLU:HG2	2:U:82:LEU:HD21	1.70	0.72
2:U:123:ILE:H	2:U:123:ILE:HD13	1.52	0.72
1:M:198:LYS:O	1:M:202:GLU:HB2	1.89	0.72
1:L:198:LYS:O	1:L:202:GLU:HB2	1.90	0.72
1:I:78:THR:HG21	1:I:85:ALA:HB1	1.71	0.72
1:D:52:LYS:NZ	1:D:62:ASN:HA	2.04	0.72
2:X:123:ILE:HG12	2:X:124:TYR:HD1	1.54	0.72
1:A:168:GLY:O	1:A:172:VAL:HG12	1.89	0.72
1:J:184:LEU:HD23	1:J:189:ALA:HA	1.71	0.72
1:J:78:THR:HG21	1:J:85:ALA:HB1	1.70	0.72
2:B:53:GLN:O	2:B:56:VAL:HG12	1.89	0.72
2:T:123:ILE:HG12	2:T:124:TYR:HD1	1.53	0.72
1:J:198:LYS:O	1:J:202:GLU:HB2	1.89	0.71
2:B:32:LYS:HE2	2:B:34:LEU:O	1.89	0.71
1:K:168:GLY:O	1:K:172:VAL:HG12	1.89	0.71
2:S:7:THR:HB	2:S:123:ILE:O	1.90	0.71
2:2:18:ARG:HB2	2:2:31:GLY:O	1.91	0.71
2:B:43:MET:HE1	2:B:56:VAL:HG23	1.72	0.71
2:S:20:VAL:HG13	2:S:28:HIS:HB2	1.71	0.71
2:R:167:SER:HB2	2:V:167:SER:HB2	1.73	0.71
1:K:184:LEU:HD23	1:K:189:ALA:HA	1.73	0.71
1:F:52:LYS:NZ	1:F:62:ASN:HA	2.06	0.71
1:K:21:LEU:O	1:K:24:VAL:HG12	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:186:GLU:O	1:M:190:VAL:HG12	1.90	0.70
2:B:59:MET:HE2	2:B:79:VAL:HG23	1.73	0.70
1:D:98:GLN:O	1:D:102:THR:HG22	1.91	0.70
2:V:149:ASP:O	2:V:152:VAL:HG12	1.91	0.70
2:U:37:ILE:HD11	2:U:59:MET:HB3	1.73	0.70
2:P:103:GLY:HA2	2:P:178:ILE:CD1	2.22	0.70
2:2:55:LEU:HD23	2:2:99:LEU:HD11	1.74	0.70
2:X:3:THR:OG1	2:X:127:THR:HG22	1.92	0.70
2:1:62:GLU:HG2	2:1:82:LEU:HD21	1.73	0.69
1:H:21:LEU:O	1:H:24:VAL:HG12	1.92	0.69
2:Z:53:GLN:O	2:Z:56:VAL:HG12	1.92	0.69
2:Q:45:ILE:CG1	2:Q:52:ALA:HB1	2.22	0.69
1:J:42:PHE:HB2	1:J:184:LEU:O	1.91	0.69
2:B:45:ILE:HG12	2:B:52:ALA:HB1	1.74	0.69
2:W:38:ASP:HB3	2:W:41:THR:CG2	2.19	0.69
1:G:198:LYS:O	1:G:202:GLU:HB2	1.92	0.69
2:V:124:TYR:CD2	2:V:138:LEU:HD23	2.28	0.69
2:W:18:ARG:HE	2:W:30:ASN:HD22	1.37	0.69
2:P:62:GLU:HG2	2:P:82:LEU:HD21	1.74	0.69
1:G:52:LYS:NZ	1:G:62:ASN:HA	2.06	0.69
2:Y:45:ILE:HG12	2:Y:52:ALA:HB1	1.74	0.69
2:S:193:GLU:HA	2:S:196:ILE:HD12	1.74	0.69
1:A:184:LEU:HD23	1:A:189:ALA:HA	1.75	0.69
2:X:32:LYS:HE2	2:X:34:LEU:O	1.92	0.69
2:B:167:SER:HB2	2:Y:167:SER:HB2	1.75	0.69
2:R:12:VAL:HG13	2:R:178:ILE:HG23	1.74	0.69
1:C:42:PHE:HB2	1:C:184:LEU:O	1.92	0.69
2:Q:53:GLN:O	2:Q:56:VAL:HG12	1.91	0.69
1:D:135:SER:OG	1:D:153:PRO:HD3	1.92	0.69
2:Z:15:ALA:HB2	2:Z:175:VAL:HB	1.74	0.68
2:Z:18:ARG:HE	2:Z:30:ASN:HD22	1.39	0.68
2:Y:32:LYS:HE2	2:Y:34:LEU:O	1.93	0.68
2:1:32:LYS:HE2	2:1:34:LEU:O	1.93	0.68
2:T:53:GLN:O	2:T:56:VAL:HG12	1.93	0.68
2:W:43:MET:HE1	2:W:56:VAL:HG23	1.74	0.68
2:T:3:THR:OG1	2:T:127:THR:HG22	1.93	0.68
2:X:37:ILE:HD11	2:X:59:MET:HB3	1.75	0.68
1:K:52:LYS:HZ1	1:K:62:ASN:HA	1.57	0.68
1:G:52:LYS:HE3	1:G:64:ILE:HG23	1.75	0.68
1:D:198:LYS:O	1:D:202:GLU:HB2	1.94	0.68
1:O:198:LYS:O	1:O:202:GLU:HB2	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:149:ASP:O	2:Q:152:VAL:HG12	1.94	0.68
1:C:78:THR:HG21	1:C:85:ALA:HB1	1.74	0.68
1:O:52:LYS:NZ	1:O:62:ASN:HA	2.09	0.68
1:E:124:THR:HG22	1:F:130:ARG:HH21	1.58	0.68
1:M:109:ILE:CG2	1:M:147:ARG:HD3	2.24	0.68
1:M:184:LEU:HD23	1:M:189:ALA:HA	1.76	0.68
1:J:186:GLU:O	1:J:190:VAL:HG12	1.94	0.68
1:I:52:LYS:NZ	1:I:62:ASN:HA	2.08	0.68
2:U:38:ASP:HB3	2:U:41:THR:CG2	2.21	0.67
1:L:168:GLY:O	1:L:172:VAL:HG12	1.94	0.67
2:R:7:THR:HB	2:R:123:ILE:O	1.93	0.67
1:N:78:THR:HG21	1:N:85:ALA:HB1	1.75	0.67
1:H:95:SER:OG	1:H:115:ARG:HD3	1.94	0.67
2:T:123:ILE:H	2:T:123:ILE:HD13	1.60	0.67
2:V:53:GLN:O	2:V:56:VAL:HG12	1.95	0.67
1:E:198:LYS:O	1:E:202:GLU:HB2	1.95	0.67
2:P:133:PHE:CZ	2:P:165:ARG:HB3	2.30	0.67
1:H:198:LYS:O	1:H:202:GLU:HB2	1.95	0.67
2:B:59:MET:SD	2:B:83:LEU:HD13	2.35	0.67
1:E:78:THR:HG21	1:E:85:ALA:HB1	1.75	0.67
1:K:198:LYS:O	1:K:202:GLU:HB2	1.95	0.67
1:C:168:GLY:O	1:C:172:VAL:HG12	1.95	0.67
1:I:23:GLN:OE1	1:O:14:VAL:HB	1.95	0.67
1:M:69:LEU:HD23	1:M:75:ALA:HB2	1.75	0.67
1:G:21:LEU:HD11	1:H:130:ARG:HD2	1.76	0.66
2:Z:111:PHE:CE2	2:Z:121:GLU:HB2	2.29	0.66
1:G:184:LEU:HD23	1:G:189:ALA:HA	1.77	0.66
2:V:6:ILE:HD11	2:V:142:TYR:CD1	2.31	0.66
1:G:186:GLU:O	1:G:190:VAL:HG12	1.95	0.66
2:W:124:TYR:CD2	2:W:138:LEU:HD23	2.31	0.66
2:R:28:HIS:CD2	2:S:120:VAL:HG11	2.31	0.66
1:C:108:ASN:HB3	2:Q:70:ARG:HG2	1.78	0.66
1:D:21:LEU:O	1:D:25:GLU:HG2	1.95	0.66
2:P:7:THR:HB	2:P:123:ILE:O	1.96	0.66
2:Q:2:THR:HG22	2:Q:169:SER:OG	1.96	0.66
1:D:108:ASN:CB	2:R:70:ARG:HG2	2.25	0.66
2:R:123:ILE:HG12	2:R:124:TYR:CD1	2.31	0.66
1:G:78:THR:HG21	1:G:85:ALA:HB1	1.76	0.66
2:Q:75:PRO:O	2:Q:78:ALA:HB3	1.96	0.66
1:F:168:GLY:O	1:F:172:VAL:HG12	1.96	0.66
2:2:45:ILE:HG12	2:2:52:ALA:HB1	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LYS:O	1:A:202:GLU:HB2	1.96	0.66
2:V:7:THR:HB	2:V:123:ILE:O	1.96	0.65
1:L:49:ILE:HD11	1:L:210:PRO:HB3	1.78	0.65
2:V:45:ILE:HG12	2:V:52:ALA:HB1	1.78	0.65
1:F:69:LEU:HD23	1:F:75:ALA:HB2	1.79	0.65
2:Q:18:ARG:HE	2:Q:30:ASN:HD22	1.41	0.65
1:I:43:ALA:HB2	1:I:185:PRO:HA	1.79	0.65
1:O:98:GLN:O	1:O:102:THR:HG22	1.96	0.65
1:F:186:GLU:O	1:F:190:VAL:HG12	1.96	0.65
2:S:37:ILE:HD11	2:S:59:MET:HB3	1.79	0.65
1:D:15:PHE:HD2	1:E:23:GLN:HE22	1.45	0.65
2:S:59:MET:SD	2:S:83:LEU:HD13	2.36	0.65
1:I:21:LEU:HD11	1:J:130:ARG:HD2	1.79	0.65
2:2:32:LYS:HE2	2:2:34:LEU:O	1.97	0.65
1:A:159:GLU:HG2	1:C:60:GLU:HG3	1.79	0.65
1:E:52:LYS:NZ	1:E:62:ASN:HA	2.10	0.65
1:L:52:LYS:NZ	1:L:62:ASN:HA	2.11	0.65
2:B:38:ASP:HB3	2:B:41:THR:CG2	2.20	0.65
2:T:45:ILE:CG1	2:T:52:ALA:HB1	2.26	0.65
1:L:170:ASP:O	1:L:173:VAL:HG12	1.96	0.65
1:N:98:GLN:O	1:N:102:THR:HG22	1.97	0.65
2:P:123:ILE:HD13	2:P:123:ILE:H	1.62	0.65
2:S:123:ILE:HG12	2:S:124:TYR:HD1	1.61	0.65
1:F:198:LYS:O	1:F:202:GLU:HB2	1.97	0.65
1:M:21:LEU:O	1:M:24:VAL:HG12	1.97	0.65
1:N:198:LYS:O	1:N:202:GLU:HB2	1.96	0.65
1:F:21:LEU:O	1:F:24:VAL:HG12	1.98	0.64
2:X:18:ARG:HE	2:X:30:ASN:HD22	1.42	0.64
2:P:45:ILE:HG12	2:P:52:ALA:HB1	1.79	0.64
1:J:124:THR:HG22	1:K:130:ARG:HH21	1.62	0.64
1:H:61:GLN:O	1:H:64:ILE:HG22	1.96	0.64
2:1:59:MET:SD	2:1:83:LEU:HD13	2.37	0.64
1:A:52:LYS:HZ1	1:A:62:ASN:HA	1.59	0.64
1:A:61:GLN:O	1:A:64:ILE:HG22	1.95	0.64
1:A:21:LEU:HD11	1:C:130:ARG:HD2	1.79	0.64
2:T:124:TYR:CD2	2:T:138:LEU:HD23	2.31	0.64
1:N:21:LEU:O	1:N:24:VAL:HG12	1.97	0.64
2:Y:37:ILE:HD11	2:Y:59:MET:HB3	1.79	0.64
2:P:20:VAL:HG13	2:P:28:HIS:HB2	1.79	0.64
2:U:123:ILE:HG12	2:U:124:TYR:HD2	1.61	0.64
2:X:20:VAL:HG13	2:X:28:HIS:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:GLN:O	1:G:124:THR:HB	1.96	0.64
2:B:123:ILE:HD13	2:B:123:ILE:H	1.62	0.64
2:Z:149:ASP:O	2:Z:152:VAL:HG12	1.97	0.64
2:Y:124:TYR:CD1	2:Y:138:LEU:HD23	2.32	0.64
1:L:108:ASN:HB3	2:Z:70:ARG:HG2	1.80	0.64
2:P:124:TYR:CD2	2:P:138:LEU:HD23	2.32	0.64
1:N:52:LYS:NZ	1:N:62:ASN:HA	2.13	0.64
1:L:144:ILE:HD12	1:L:147:ARG:NH1	2.13	0.64
2:W:3:THR:OG1	2:W:127:THR:HG22	1.97	0.64
1:M:109:ILE:HG22	1:M:142:ASP:OD1	1.98	0.64
1:G:137:ILE:HG22	1:G:150:ASP:HB2	1.78	0.64
2:V:103:GLY:HA2	2:V:178:ILE:CD1	2.28	0.64
2:Z:123:ILE:HD13	2:Z:123:ILE:H	1.64	0.63
2:S:124:TYR:CD2	2:S:138:LEU:HD23	2.33	0.63
1:G:135:SER:OG	1:G:153:PRO:HD3	1.98	0.63
2:S:18:ARG:HB2	2:S:31:GLY:O	1.98	0.63
2:R:123:ILE:H	2:R:123:ILE:HD13	1.63	0.63
1:J:21:LEU:O	1:J:24:VAL:HG12	1.98	0.63
2:Y:7:THR:HB	2:Y:123:ILE:O	1.98	0.63
2:V:76:ILE:O	2:V:79:VAL:HG12	1.98	0.63
2:T:49:VAL:HG23	2:T:50:GLY:H	1.62	0.63
1:E:52:LYS:HZ3	1:E:62:ASN:HA	1.63	0.63
1:H:52:LYS:NZ	1:H:62:ASN:HA	2.14	0.63
1:J:108:ASN:HB3	2:X:70:ARG:HG2	1.79	0.63
1:M:52:LYS:NZ	1:M:62:ASN:HA	2.12	0.63
2:U:179:THR:HG23	2:U:182:ASP:H	1.63	0.63
2:1:123:ILE:HG12	2:1:124:TYR:CD1	2.34	0.63
2:1:123:ILE:HG12	2:1:124:TYR:HD1	1.63	0.63
2:Y:59:MET:HE2	2:Y:79:VAL:HG23	1.79	0.63
2:2:2:THR:HG22	2:2:169:SER:OG	1.98	0.63
2:V:32:LYS:HE2	2:V:34:LEU:O	1.98	0.63
1:F:180:TYR:HA	1:F:192:LEU:HD21	1.80	0.63
1:F:108:ASN:HB3	2:T:70:ARG:HG2	1.78	0.63
2:W:3:THR:HB	2:W:16:THR:HG22	1.80	0.63
1:J:52:LYS:NZ	1:J:62:ASN:HA	2.14	0.63
2:Q:103:GLY:HA2	2:Q:178:ILE:HD13	1.81	0.63
1:C:52:LYS:HE3	1:C:64:ILE:HG23	1.81	0.63
1:I:137:ILE:HG22	1:I:150:ASP:HB2	1.81	0.63
1:G:168:GLY:O	1:G:172:VAL:HG12	1.99	0.63
1:N:168:GLY:O	1:N:172:VAL:HG12	1.97	0.63
1:J:168:GLY:O	1:J:172:VAL:HG12	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:TYR:CD2	2:B:138:LEU:HD23	2.33	0.63
2:B:123:ILE:HG12	2:B:124:TYR:CD1	2.33	0.63
1:D:49:ILE:HD11	1:D:210:PRO:HB3	1.80	0.63
2:R:59:MET:HE3	2:R:82:LEU:HD23	1.81	0.63
2:R:193:GLU:HA	2:R:196:ILE:HD12	1.81	0.63
1:D:61:GLN:O	1:D:64:ILE:HG22	1.98	0.62
2:P:167:SER:HB2	2:X:167:SER:HB2	1.81	0.62
2:U:167:SER:HB2	2:Z:167:SER:HB2	1.81	0.62
1:E:108:ASN:HB3	2:S:70:ARG:HG2	1.81	0.62
2:S:15:ALA:HB2	2:S:175:VAL:HB	1.81	0.62
1:C:94:ILE:HG13	1:C:95:SER:N	2.14	0.62
1:N:184:LEU:HD23	1:N:189:ALA:HA	1.82	0.62
2:R:3:THR:HB	2:R:16:THR:HG22	1.80	0.62
2:V:124:TYR:HD2	2:V:138:LEU:HD23	1.61	0.62
2:U:133:PHE:CZ	2:U:165:ARG:HB3	2.34	0.62
2:B:55:LEU:HD21	2:B:87:LEU:HD11	1.80	0.62
1:D:21:LEU:O	1:D:24:VAL:HG12	2.00	0.62
1:O:108:ASN:HB3	2:V:70:ARG:HG2	1.81	0.62
2:P:76:ILE:O	2:P:79:VAL:HG12	2.00	0.62
2:Z:38:ASP:HB3	2:Z:41:THR:CG2	2.27	0.62
2:2:123:ILE:HD13	2:2:123:ILE:H	1.63	0.62
2:Q:103:GLY:HA2	2:Q:178:ILE:CD1	2.29	0.62
2:Z:19:ARG:NE	2:Z:26:ILE:HG13	2.15	0.62
2:1:18:ARG:HB2	2:1:31:GLY:O	2.00	0.62
1:H:78:THR:HG21	1:H:85:ALA:HB1	1.82	0.62
1:I:168:GLY:O	1:I:172:VAL:HG12	1.99	0.62
2:P:37:ILE:HD11	2:P:59:MET:HB3	1.82	0.62
1:O:61:GLN:O	1:O:64:ILE:HG22	2.00	0.62
2:R:141:GLN:NE2	2:W:141:GLN:HE21	1.98	0.62
2:X:124:TYR:CD2	2:X:138:LEU:HD23	2.35	0.62
1:F:52:LYS:HE3	1:F:64:ILE:HG23	1.82	0.62
1:M:21:LEU:O	1:M:25:GLU:HG2	1.99	0.62
2:Y:62:GLU:HG2	2:Y:82:LEU:HD21	1.82	0.62
1:N:70:ILE:HD12	1:N:74:VAL:HG22	1.81	0.62
1:G:18:ASP:OD2	1:G:20:ARG:HD3	2.00	0.62
2:T:123:ILE:HG12	2:T:124:TYR:CD1	2.33	0.61
2:T:149:ASP:O	2:T:152:VAL:HG12	1.99	0.61
1:C:186:GLU:O	1:C:190:VAL:HG12	1.99	0.61
1:F:70:ILE:HD12	1:F:74:VAL:HG22	1.82	0.61
1:F:78:THR:HG21	1:F:85:ALA:HB1	1.81	0.61
1:F:170:ASP:O	1:F:173:VAL:HG12	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:141:GLN:NE2	2:W:141:GLN:NE2	2.48	0.61
2:Y:174:ASP:HA	2:Y:192:ILE:HD13	1.83	0.61
1:M:175:PHE:CD2	1:M:196:ALA:HA	2.36	0.61
2:B:2:THR:HG22	2:B:169:SER:OG	2.00	0.61
1:J:170:ASP:O	1:J:173:VAL:HG12	2.01	0.61
2:B:43:MET:CE	2:B:56:VAL:HG23	2.29	0.61
1:N:124:THR:HG22	1:O:130:ARG:HH21	1.65	0.61
2:B:37:ILE:HD11	2:B:59:MET:HB3	1.82	0.61
2:U:76:ILE:O	2:U:79:VAL:HG12	2.00	0.61
2:Z:44:THR:OG1	2:Z:100:LEU:HB3	2.00	0.61
1:L:124:THR:HG22	1:M:130:ARG:NH2	2.13	0.61
1:L:184:LEU:HD23	1:L:189:ALA:HA	1.82	0.61
2:Y:18:ARG:HE	2:Y:30:ASN:HD22	1.47	0.61
1:A:61:GLN:OE1	1:A:62:ASN:HB3	2.01	0.61
1:K:21:LEU:O	1:K:25:GLU:HG2	2.01	0.61
2:Y:123:ILE:HG12	2:Y:124:TYR:HD2	1.66	0.61
1:O:137:ILE:HG22	1:O:150:ASP:HB2	1.83	0.61
1:A:121:GLN:O	1:A:124:THR:HB	2.00	0.60
1:E:61:GLN:O	1:E:64:ILE:HG22	2.00	0.60
1:A:88:LEU:HD21	1:A:120:MET:SD	2.41	0.60
1:K:18:ASP:OD2	1:K:20:ARG:HD3	2.01	0.60
1:D:186:GLU:O	1:D:190:VAL:HG12	2.01	0.60
1:L:21:LEU:O	1:L:24:VAL:HG12	2.02	0.60
1:K:52:LYS:HE3	1:K:64:ILE:HG23	1.83	0.60
1:L:43:ALA:HB2	1:L:185:PRO:HA	1.84	0.60
1:L:156:THR:HG23	1:M:82:VAL:HG11	1.82	0.60
2:S:38:ASP:HB3	2:S:41:THR:CG2	2.32	0.60
2:X:62:GLU:HG2	2:X:82:LEU:HD21	1.82	0.60
1:H:170:ASP:O	1:H:173:VAL:HG12	2.01	0.60
1:K:21:LEU:HD11	1:L:130:ARG:HD2	1.83	0.60
1:C:43:ALA:HB2	1:C:185:PRO:HA	1.82	0.60
2:W:178:ILE:HB	2:W:184:TYR:HA	1.83	0.60
1:D:168:GLY:O	1:D:172:VAL:HG12	2.02	0.60
1:I:135:SER:OG	1:I:153:PRO:HD3	2.01	0.60
1:J:18:ASP:OD2	1:J:20:ARG:HD3	2.00	0.60
2:1:38:ASP:HB3	2:1:41:THR:CG2	2.29	0.60
1:E:24:VAL:O	1:E:27:ALA:HB3	2.02	0.60
1:F:52:LYS:HZ3	1:F:62:ASN:HA	1.64	0.60
1:C:198:LYS:O	1:C:202:GLU:HB2	2.01	0.60
1:H:98:GLN:O	1:H:102:THR:HG22	2.01	0.60
1:N:135:SER:OG	1:N:153:PRO:HD3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:111:PHE:CE2	2:V:121:GLU:HB2	2.37	0.60
1:A:49:ILE:HD12	1:A:211:GLU:O	2.01	0.60
1:G:61:GLN:O	1:G:64:ILE:HG22	2.01	0.60
2:Q:38:ASP:HB2	2:Q:63:LEU:HD23	1.84	0.60
1:A:28:ARG:O	1:A:31:VAL:HG22	2.02	0.60
1:A:42:PHE:HD1	1:A:43:ALA:N	2.00	0.60
1:C:198:LYS:HG2	1:C:202:GLU:HG2	1.82	0.60
1:K:88:LEU:HD13	1:K:132:TYR:CD2	2.36	0.60
1:I:49:ILE:HD12	1:I:211:GLU:O	2.01	0.60
2:S:3:THR:HB	2:S:16:THR:HG22	1.83	0.60
1:D:52:LYS:HZ3	1:D:62:ASN:HA	1.66	0.60
1:O:98:GLN:O	1:O:101:VAL:HG12	2.02	0.60
1:N:52:LYS:HB3	1:N:209:ALA:O	2.01	0.60
1:N:61:GLN:O	1:N:64:ILE:HG22	2.02	0.60
1:C:84:ASP:O	1:C:87:VAL:HG12	2.02	0.60
2:S:32:LYS:HE2	2:S:34:LEU:O	2.01	0.60
2:X:43:MET:HE1	2:X:56:VAL:HA	1.83	0.60
1:D:52:LYS:HA	1:D:66:LYS:NZ	2.17	0.60
1:O:52:LYS:HE3	1:O:64:ILE:HG23	1.83	0.60
2:X:2:THR:HG22	2:X:169:SER:OG	2.02	0.60
1:K:186:GLU:O	1:K:190:VAL:HG12	2.01	0.59
2:V:62:GLU:HG2	2:V:82:LEU:HD21	1.82	0.59
2:Y:133:PHE:CZ	2:Y:165:ARG:HB3	2.37	0.59
1:N:170:ASP:O	1:N:173:VAL:HG12	2.02	0.59
2:1:20:VAL:HG13	2:1:28:HIS:HB2	1.83	0.59
2:2:179:THR:HG23	2:2:182:ASP:H	1.68	0.59
1:I:186:GLU:O	1:I:190:VAL:HG12	2.03	0.59
2:T:133:PHE:CZ	2:T:165:ARG:HB3	2.36	0.59
2:U:178:ILE:HB	2:U:184:TYR:HA	1.84	0.59
2:Z:12:VAL:HG13	2:Z:178:ILE:HG23	1.82	0.59
2:Y:111:PHE:CE2	2:Y:121:GLU:HB2	2.37	0.59
2:R:152:VAL:O	2:R:156:ILE:HG13	2.03	0.59
2:Z:37:ILE:HD11	2:Z:59:MET:HB3	1.84	0.59
2:W:124:TYR:HD2	2:W:138:LEU:HD23	1.67	0.59
1:M:52:LYS:HB3	1:M:209:ALA:O	2.01	0.59
1:J:61:GLN:O	1:J:64:ILE:HG22	2.00	0.59
1:O:49:ILE:HD12	1:O:211:GLU:O	2.01	0.59
2:Y:2:THR:HG22	2:Y:169:SER:OG	2.02	0.59
2:X:179:THR:HG23	2:X:182:ASP:H	1.66	0.59
1:K:98:GLN:O	1:K:102:THR:HG22	2.03	0.59
2:T:38:ASP:HB3	2:T:41:THR:CG2	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:66:TYR:CZ	2:1:70:ARG:HD2	2.37	0.59
1:O:49:ILE:HD11	1:O:210:PRO:HB3	1.83	0.59
1:M:94:ILE:HG13	1:M:95:SER:N	2.17	0.59
2:R:38:ASP:HB3	2:R:41:THR:CG2	2.26	0.59
1:A:49:ILE:HD11	1:A:210:PRO:HB3	1.85	0.59
2:R:159:ILE:O	2:R:163:LYS:HG3	2.02	0.59
2:R:32:LYS:HE2	2:R:34:LEU:O	2.02	0.59
2:U:3:THR:HB	2:U:16:THR:HG22	1.83	0.59
1:F:121:GLN:O	1:F:124:THR:HB	2.03	0.59
2:R:124:TYR:CD2	2:R:138:LEU:HD23	2.37	0.59
1:G:95:SER:OG	1:G:115:ARG:HD3	2.03	0.59
2:2:36:GLN:HB2	2:2:184:TYR:CE1	2.37	0.59
1:G:148:LEU:O	1:G:159:GLU:HG3	2.03	0.59
2:B:8:LEU:O	2:B:8:LEU:HD12	2.03	0.59
1:M:136:LEU:HD13	1:M:138:PHE:CE2	2.37	0.59
1:F:95:SER:OG	1:F:115:ARG:HD3	2.03	0.59
2:Q:7:THR:HB	2:Q:123:ILE:O	2.03	0.58
2:S:123:ILE:H	2:S:123:ILE:HD13	1.67	0.58
1:I:42:PHE:HB2	1:I:184:LEU:O	2.03	0.58
1:E:176:LEU:HB3	1:F:58:LEU:HD21	1.85	0.58
1:I:34:GLY:O	1:I:167:SER:HB2	2.03	0.58
1:E:21:LEU:HD11	1:F:130:ARG:HD2	1.85	0.58
1:L:52:LYS:HZ3	1:L:62:ASN:HA	1.67	0.58
2:2:3:THR:OG1	2:2:127:THR:HG22	2.02	0.58
1:L:18:ASP:OD2	1:L:20:ARG:HD3	2.03	0.58
2:P:123:ILE:HG12	2:P:124:TYR:CD1	2.32	0.58
1:I:184:LEU:HD23	1:I:189:ALA:HA	1.86	0.58
1:L:61:GLN:O	1:L:64:ILE:HG22	2.04	0.58
1:K:121:GLN:O	1:K:124:THR:HB	2.04	0.58
1:O:81:LEU:HD23	1:O:133:GLY:HA3	1.84	0.58
2:P:149:ASP:O	2:P:152:VAL:HG12	2.03	0.58
1:A:52:LYS:HZ3	1:A:62:ASN:HA	1.66	0.58
2:2:76:ILE:HG22	2:2:111:PHE:CE2	2.38	0.58
1:G:42:PHE:HB2	1:G:184:LEU:O	2.03	0.58
1:G:49:ILE:HD11	1:G:210:PRO:HB3	1.86	0.58
2:W:133:PHE:CZ	2:W:165:ARG:HB3	2.39	0.58
1:D:78:THR:HG21	1:D:85:ALA:HB1	1.85	0.58
2:R:131:SER:O	2:R:134:VAL:HG13	2.04	0.58
1:G:108:ASN:HB3	2:U:70:ARG:HG2	1.86	0.58
2:S:28:HIS:CD2	2:T:120:VAL:HG11	2.39	0.58
1:F:124:THR:HG22	1:G:130:ARG:NH2	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:LEU:O	1:N:25:GLU:HG2	2.03	0.58
2:Z:133:PHE:CZ	2:Z:165:ARG:HB3	2.39	0.58
2:V:28:HIS:CD2	2:W:120:VAL:HG11	2.39	0.58
1:M:42:PHE:HB2	1:M:184:LEU:O	2.03	0.57
1:D:101:VAL:HG23	2:Q:57:ARG:HB3	1.85	0.57
2:B:152:VAL:O	2:B:156:ILE:HG13	2.04	0.57
2:2:149:ASP:O	2:2:152:VAL:HG12	2.04	0.57
1:L:121:GLN:O	1:L:124:THR:HB	2.04	0.57
2:2:18:ARG:HE	2:2:30:ASN:HD22	1.51	0.57
1:G:52:LYS:HZ3	1:G:62:ASN:HA	1.68	0.57
2:R:20:VAL:HG22	2:R:28:HIS:HB2	1.86	0.57
1:L:186:GLU:O	1:L:190:VAL:HG12	2.05	0.57
1:I:95:SER:OG	1:I:115:ARG:HD3	2.04	0.57
2:Z:59:MET:CE	2:Z:82:LEU:HD23	2.34	0.57
1:O:70:ILE:HD12	1:O:74:VAL:HG22	1.86	0.57
2:Y:12:VAL:HG13	2:Y:178:ILE:HG23	1.85	0.57
1:G:98:GLN:O	1:G:102:THR:HG22	2.04	0.57
1:F:61:GLN:O	1:F:64:ILE:HG22	2.05	0.57
2:P:51:ASP:O	2:P:55:LEU:HB2	2.04	0.57
1:A:135:SER:OG	1:A:153:PRO:HD3	2.04	0.57
2:S:179:THR:HG23	2:S:182:ASP:H	1.70	0.57
1:J:42:PHE:HD1	1:J:43:ALA:N	2.02	0.57
1:I:49:ILE:HD11	1:I:210:PRO:HB3	1.86	0.57
1:J:49:ILE:HD11	1:J:210:PRO:HB3	1.85	0.57
1:O:135:SER:OG	1:O:153:PRO:HD3	2.04	0.57
1:H:180:TYR:HA	1:H:192:LEU:HD21	1.85	0.57
1:L:78:THR:HG21	1:L:85:ALA:HB1	1.86	0.57
2:T:75:PRO:O	2:T:78:ALA:HB3	2.04	0.57
1:G:124:THR:HG22	1:H:130:ARG:NH2	2.16	0.57
2:V:20:VAL:HG13	2:V:28:HIS:HB2	1.85	0.57
1:C:159:GLU:HG2	1:D:60:GLU:HG3	1.85	0.57
1:F:144:ILE:HD12	1:F:147:ARG:NH1	2.19	0.57
2:W:55:LEU:HD21	2:W:87:LEU:HD11	1.87	0.57
2:Q:199:LEU:HB3	2:Q:201:LEU:HD13	1.85	0.57
1:K:81:LEU:HD23	1:K:133:GLY:HA3	1.85	0.57
2:W:20:VAL:HG13	2:W:28:HIS:HB2	1.87	0.57
2:T:28:HIS:CD2	2:U:120:VAL:HG11	2.39	0.57
2:Q:160:SER:O	2:Q:163:LYS:HB2	2.04	0.57
1:L:35:SER:O	1:L:166:GLY:HA3	2.05	0.57
1:E:49:ILE:HD13	1:E:212:ILE:HB	1.87	0.57
2:W:43:MET:CE	2:W:56:VAL:HG23	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:7:THR:HB	2:2:123:ILE:O	2.05	0.57
1:H:76:ALA:HB2	1:H:138:PHE:CD1	2.40	0.57
1:A:35:SER:O	1:A:166:GLY:HA3	2.03	0.57
2:R:45:ILE:HG12	2:R:52:ALA:HB1	1.87	0.57
1:G:42:PHE:HD1	1:G:43:ALA:N	2.03	0.57
1:I:69:LEU:HD23	1:I:75:ALA:HB2	1.87	0.57
1:E:94:ILE:HG13	1:E:95:SER:N	2.20	0.57
2:S:43:MET:CE	2:S:56:VAL:HG23	2.35	0.56
2:B:37:ILE:HD11	2:B:59:MET:CG	2.35	0.56
2:Z:178:ILE:HB	2:Z:184:TYR:HA	1.86	0.56
2:Q:3:THR:OG1	2:Q:127:THR:HG22	2.05	0.56
1:C:165:ILE:HG13	1:C:166:GLY:H	1.70	0.56
2:U:174:ASP:HA	2:U:192:ILE:HD13	1.87	0.56
1:A:143:GLN:HE21	1:A:143:GLN:HA	1.70	0.56
1:I:21:LEU:O	1:I:24:VAL:HG12	2.05	0.56
2:Z:152:VAL:O	2:Z:156:ILE:HG13	2.05	0.56
2:R:141:GLN:HE21	2:W:141:GLN:NE2	2.03	0.56
2:U:124:TYR:CD1	2:U:138:LEU:HD23	2.39	0.56
2:V:6:ILE:HD11	2:V:142:TYR:HD1	1.68	0.56
2:R:59:MET:HE2	2:R:79:VAL:HG23	1.88	0.56
2:Z:19:ARG:HE	2:Z:26:ILE:HG13	1.71	0.56
1:J:88:LEU:HD13	1:J:132:TYR:CD2	2.39	0.56
2:X:133:PHE:CZ	2:X:165:ARG:HB3	2.40	0.56
2:U:152:VAL:O	2:U:156:ILE:HG13	2.05	0.56
2:1:75:PRO:O	2:1:78:ALA:HB3	2.06	0.56
1:F:175:PHE:CD2	1:F:196:ALA:HA	2.39	0.56
2:T:178:ILE:HB	2:T:184:TYR:HA	1.87	0.56
1:O:184:LEU:HD23	1:O:189:ALA:HA	1.87	0.56
2:2:62:GLU:HG2	2:2:82:LEU:HD21	1.86	0.56
1:A:43:ALA:HB2	1:A:185:PRO:HA	1.88	0.56
2:R:18:ARG:HE	2:R:30:ASN:HD22	1.51	0.56
1:E:81:LEU:HD23	1:E:133:GLY:HA3	1.85	0.56
1:L:76:ALA:HB2	1:L:138:PHE:CD2	2.41	0.56
1:I:108:ASN:CB	2:W:70:ARG:HG2	2.33	0.56
1:H:52:LYS:HB3	1:H:209:ALA:O	2.05	0.56
1:A:23:GLN:HE22	1:H:15:PHE:HB2	1.71	0.56
2:X:26:ILE:HD13	2:X:26:ILE:C	2.26	0.56
2:Q:123:ILE:HG12	2:Q:124:TYR:HD1	1.69	0.56
1:I:38:LEU:HG	1:I:49:ILE:HG23	1.86	0.56
2:B:174:ASP:HA	2:B:192:ILE:HD13	1.88	0.56
2:T:32:LYS:HE2	2:T:34:LEU:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HG11	2:U:28:HIS:CD2	2.41	0.56
2:B:70:ARG:HG2	1:H:108:ASN:CB	2.36	0.56
1:I:124:THR:HG22	1:J:130:ARG:HH21	1.71	0.56
1:E:49:ILE:HD12	1:E:211:GLU:O	2.05	0.56
1:I:198:LYS:HG2	1:I:202:GLU:HG2	1.88	0.56
2:Q:167:SER:HB2	2:W:167:SER:HB2	1.88	0.56
2:1:174:ASP:HA	2:1:192:ILE:HD13	1.87	0.56
1:K:61:GLN:O	1:K:64:ILE:HG22	2.06	0.56
1:H:137:ILE:HG22	1:H:150:ASP:HB2	1.86	0.56
2:X:149:ASP:O	2:X:152:VAL:HG12	2.06	0.56
2:V:152:VAL:O	2:V:156:ILE:HG13	2.06	0.55
1:L:49:ILE:HD12	1:L:211:GLU:O	2.06	0.55
1:J:21:LEU:HD11	1:K:130:ARG:HD2	1.88	0.55
1:I:61:GLN:O	1:I:64:ILE:HG22	2.06	0.55
1:N:108:ASN:HB3	2:2:70:ARG:HG2	1.88	0.55
1:L:38:LEU:HA	1:L:164:ALA:HA	1.87	0.55
2:U:26:ILE:HD13	2:U:26:ILE:C	2.27	0.55
1:G:85:ALA:O	1:G:89:VAL:HG23	2.06	0.55
1:H:42:PHE:HD1	1:H:43:ALA:N	2.04	0.55
1:H:186:GLU:O	1:H:190:VAL:HG12	2.06	0.55
2:Z:6:ILE:HD11	2:Z:142:TYR:CD1	2.41	0.55
1:G:70:ILE:HD12	1:G:74:VAL:HG22	1.88	0.55
2:X:37:ILE:HD11	2:X:59:MET:CG	2.36	0.55
1:L:175:PHE:CD2	1:L:196:ALA:HA	2.41	0.55
1:O:186:GLU:O	1:O:190:VAL:HG12	2.06	0.55
2:Z:59:MET:HE3	2:Z:82:LEU:HD23	1.88	0.55
2:T:76:ILE:HG21	2:T:109:HIS:HB2	1.87	0.55
2:B:179:THR:HG23	2:B:182:ASP:H	1.71	0.55
2:P:17:GLU:O	2:P:33:LYS:HD2	2.07	0.55
2:T:37:ILE:HD11	2:T:59:MET:CB	2.35	0.55
2:Z:124:TYR:CD2	2:Z:138:LEU:HD23	2.41	0.55
1:K:108:ASN:CB	2:Y:70:ARG:HG2	2.37	0.55
2:X:28:HIS:CD2	2:Y:120:VAL:HG11	2.42	0.55
1:I:130:ARG:NH2	1:O:124:THR:HG22	2.15	0.55
1:H:42:PHE:HB2	1:H:184:LEU:O	2.06	0.55
1:E:170:ASP:O	1:E:173:VAL:HG12	2.07	0.55
1:G:156:THR:HG23	1:H:82:VAL:HG11	1.88	0.55
2:U:66:TYR:CZ	2:U:70:ARG:HD2	2.41	0.55
2:X:123:ILE:H	2:X:123:ILE:HD13	1.71	0.55
2:Y:123:ILE:HD13	2:Y:123:ILE:H	1.71	0.55
1:O:48:LEU:HD13	1:O:139:ALA:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LEU:HG	1:F:49:ILE:HG23	1.89	0.55
2:1:131:SER:O	2:1:134:VAL:HG13	2.07	0.55
1:C:121:GLN:O	1:C:124:THR:HB	2.06	0.55
1:G:175:PHE:CD2	1:G:196:ALA:HA	2.41	0.55
1:L:137:ILE:HG22	1:L:150:ASP:HB2	1.89	0.55
2:W:123:ILE:H	2:W:123:ILE:HD13	1.72	0.55
1:A:70:ILE:HD12	1:A:74:VAL:HG22	1.88	0.55
1:D:26:TYR:O	1:D:29:GLU:HB2	2.06	0.55
1:A:95:SER:OG	1:A:115:ARG:HD3	2.07	0.55
1:E:184:LEU:HD23	1:E:189:ALA:HA	1.87	0.54
1:M:49:ILE:HD11	1:M:210:PRO:HB3	1.88	0.54
1:H:21:LEU:O	1:H:25:GLU:HG2	2.08	0.54
1:I:42:PHE:HD1	1:I:43:ALA:N	2.05	0.54
1:E:107:VAL:HG11	2:S:66:TYR:HH	1.72	0.54
1:K:52:LYS:HA	1:K:66:LYS:NZ	2.23	0.54
2:B:62:GLU:HG2	2:B:82:LEU:HD21	1.87	0.54
1:O:78:THR:HG21	1:O:85:ALA:HB1	1.88	0.54
2:2:26:ILE:C	2:2:26:ILE:HD13	2.27	0.54
1:C:38:LEU:HA	1:C:164:ALA:HA	1.89	0.54
2:Z:124:TYR:HD2	2:Z:138:LEU:HD23	1.73	0.54
2:1:7:THR:HB	2:1:123:ILE:O	2.08	0.54
1:K:198:LYS:HG2	1:K:202:GLU:HG2	1.89	0.54
2:B:159:ILE:O	2:B:163:LYS:HG3	2.08	0.54
2:S:132:PRO:HA	2:V:133:PHE:HE1	1.72	0.54
1:A:124:THR:HG22	1:C:130:ARG:NH2	2.23	0.54
1:C:109:ILE:CG2	1:C:147:ARG:HD3	2.37	0.54
1:C:61:GLN:O	1:C:64:ILE:HG22	2.08	0.54
1:I:109:ILE:CG2	1:I:147:ARG:HD3	2.37	0.54
1:H:174:SER:O	1:H:177:GLU:HB3	2.08	0.54
2:Z:45:ILE:HG12	2:Z:52:ALA:HB1	1.90	0.54
1:D:38:LEU:HA	1:D:164:ALA:HA	1.89	0.54
1:M:61:GLN:OE1	1:M:62:ASN:HB3	2.07	0.54
2:R:62:GLU:HG2	2:R:82:LEU:HD21	1.90	0.54
2:W:193:GLU:O	2:W:196:ILE:HB	2.08	0.54
1:J:69:LEU:HD23	1:J:75:ALA:HB2	1.89	0.54
1:L:94:ILE:HG13	1:L:95:SER:N	2.23	0.54
2:Z:62:GLU:HG2	2:Z:82:LEU:HD21	1.89	0.54
1:F:187:LYS:O	1:F:190:VAL:HG13	2.08	0.54
2:Q:131:SER:O	2:Q:134:VAL:HG13	2.08	0.54
1:A:130:ARG:HH21	1:H:124:THR:HG22	1.73	0.54
2:W:59:MET:SD	2:W:83:LEU:HD13	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:137:ILE:HG22	1:K:150:ASP:HB2	1.89	0.54
2:V:15:ALA:HB2	2:V:175:VAL:HB	1.89	0.54
1:K:143:GLN:HA	1:K:143:GLN:HE21	1.73	0.54
1:A:42:PHE:HB2	1:A:184:LEU:O	2.08	0.54
1:A:198:LYS:HG2	1:A:202:GLU:HG2	1.88	0.54
2:B:6:ILE:HD11	2:B:142:TYR:CD1	2.42	0.54
1:I:174:SER:O	1:I:177:GLU:HB3	2.08	0.54
2:X:131:SER:O	2:X:134:VAL:HG13	2.08	0.54
1:O:51:ASP:HB3	1:O:53:LYS:NZ	2.23	0.54
1:I:31:VAL:HA	1:I:80:GLY:HA2	1.90	0.54
1:C:95:SER:OG	1:C:115:ARG:HD3	2.08	0.53
1:I:144:ILE:HD12	1:I:147:ARG:NH1	2.22	0.53
2:U:199:LEU:HB3	2:U:201:LEU:HD13	1.90	0.53
2:S:45:ILE:HG12	2:S:52:ALA:HB1	1.90	0.53
1:O:168:GLY:O	1:O:172:VAL:HG12	2.09	0.53
1:K:174:SER:O	1:K:177:GLU:HB3	2.08	0.53
2:Y:179:THR:HG23	2:Y:182:ASP:H	1.72	0.53
1:E:71:ASP:OD2	1:E:74:VAL:HG12	2.08	0.53
1:M:52:LYS:HZ3	1:M:62:ASN:HA	1.72	0.53
2:V:55:LEU:HD21	2:V:87:LEU:HD11	1.90	0.53
1:N:88:LEU:HD13	1:N:132:TYR:CD2	2.42	0.53
1:H:97:GLN:OE1	1:H:97:GLN:HA	2.07	0.53
1:L:52:LYS:HE3	1:L:64:ILE:HG23	1.89	0.53
1:E:180:TYR:HA	1:E:192:LEU:HD21	1.90	0.53
1:D:88:LEU:HD13	1:D:132:TYR:CD2	2.44	0.53
2:S:62:GLU:HG2	2:S:82:LEU:HD21	1.91	0.53
1:G:61:GLN:OE1	1:G:62:ASN:HB3	2.09	0.53
2:U:149:ASP:O	2:U:152:VAL:HG12	2.08	0.53
1:O:52:LYS:HZ1	1:O:62:ASN:HA	1.74	0.53
1:A:49:ILE:HD13	1:A:212:ILE:HB	1.89	0.53
2:B:26:ILE:HD13	2:B:26:ILE:C	2.28	0.53
2:Q:3:THR:HB	2:Q:16:THR:HG22	1.90	0.53
1:N:15:PHE:HB2	1:O:23:GLN:HE22	1.74	0.53
2:W:26:ILE:HD13	2:W:26:ILE:O	2.08	0.53
1:K:124:THR:HG22	1:L:130:ARG:NH2	2.20	0.53
1:D:52:LYS:HZ1	1:D:62:ASN:HA	1.73	0.53
2:W:37:ILE:HD11	2:W:59:MET:CG	2.39	0.53
2:W:35:PHE:CE2	2:W:45:ILE:HD12	2.43	0.53
2:1:49:VAL:HG23	2:1:50:GLY:H	1.74	0.53
2:Y:26:ILE:HD13	2:Y:26:ILE:C	2.29	0.53
1:N:113:VAL:HG22	1:N:157:ILE:HD12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:THR:HB	2:P:16:THR:HG22	1.90	0.53
2:1:124:TYR:CD2	2:1:138:LEU:HD23	2.44	0.53
1:J:202:GLU:HG3	1:J:205:GLU:O	2.08	0.53
2:B:133:PHE:CZ	2:B:165:ARG:HB3	2.43	0.53
2:Q:32:LYS:HE2	2:Q:34:LEU:O	2.08	0.53
2:Z:174:ASP:HA	2:Z:192:ILE:HD13	1.91	0.53
1:E:109:ILE:CG2	1:E:147:ARG:HD3	2.38	0.53
2:2:103:GLY:HA2	2:2:178:ILE:HD13	1.90	0.53
1:J:43:ALA:HB2	1:J:185:PRO:HA	1.91	0.53
1:C:144:ILE:HD12	1:C:147:ARG:NH1	2.24	0.53
2:1:111:PHE:CE2	2:1:121:GLU:HB2	2.44	0.53
2:S:26:ILE:HD13	2:S:26:ILE:O	2.09	0.53
2:U:18:ARG:HE	2:U:30:ASN:HD22	1.57	0.53
2:Q:26:ILE:C	2:Q:26:ILE:HD13	2.29	0.53
1:J:42:PHE:CD1	1:J:43:ALA:N	2.76	0.53
1:J:198:LYS:HG3	1:J:207:LEU:HD22	1.91	0.53
1:C:165:ILE:HG13	1:C:166:GLY:N	2.24	0.53
2:S:35:PHE:CE2	2:S:45:ILE:HD12	2.43	0.53
1:E:175:PHE:CD2	1:E:196:ALA:HA	2.44	0.53
1:J:95:SER:OG	1:J:115:ARG:HD3	2.09	0.53
2:X:50:GLY:O	2:X:54:VAL:HG12	2.08	0.53
1:F:41:LYS:HE3	1:F:160:TYR:O	2.09	0.53
1:H:184:LEU:HD23	1:H:189:ALA:HA	1.92	0.52
2:S:133:PHE:HE1	2:V:132:PRO:HA	1.74	0.52
2:R:26:ILE:C	2:R:26:ILE:HD13	2.29	0.52
2:V:133:PHE:CZ	2:V:165:ARG:HB3	2.43	0.52
1:F:159:GLU:HG2	1:G:60:GLU:HG3	1.91	0.52
1:K:170:ASP:O	1:K:173:VAL:HG12	2.09	0.52
2:T:6:ILE:HD11	2:T:142:TYR:CD1	2.44	0.52
1:J:52:LYS:HB3	1:J:209:ALA:O	2.10	0.52
2:W:59:MET:HE3	2:W:82:LEU:HD23	1.91	0.52
1:M:35:SER:O	1:M:166:GLY:HA3	2.10	0.52
2:U:131:SER:O	2:U:134:VAL:HG13	2.09	0.52
2:Y:49:VAL:HG23	2:Y:50:GLY:H	1.74	0.52
2:T:55:LEU:HD23	2:T:99:LEU:HD11	1.91	0.52
2:Q:37:ILE:HD11	2:Q:59:MET:CB	2.38	0.52
2:2:76:ILE:HG22	2:2:111:PHE:HE2	1.74	0.52
1:F:198:LYS:HG3	1:F:207:LEU:HD22	1.90	0.52
1:J:24:VAL:O	1:J:28:ARG:HG3	2.09	0.52
2:R:37:ILE:HD11	2:R:59:MET:HB3	1.90	0.52
2:R:173:ILE:C	2:R:173:ILE:HD13	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HD12	1:A:147:ARG:NH1	2.24	0.52
2:Q:28:HIS:CD2	2:R:120:VAL:HG11	2.44	0.52
1:C:180:TYR:HA	1:C:192:LEU:HD21	1.91	0.52
1:L:21:LEU:HD11	1:M:130:ARG:HD2	1.91	0.52
1:A:42:PHE:CD1	1:A:43:ALA:N	2.78	0.52
1:M:42:PHE:HD1	1:M:43:ALA:N	2.08	0.52
1:L:95:SER:OG	1:L:115:ARG:HD3	2.09	0.52
2:B:3:THR:HB	2:B:16:THR:HG22	1.90	0.52
1:E:143:GLN:HE21	1:E:143:GLN:HA	1.75	0.52
1:F:21:LEU:O	1:F:25:GLU:HG2	2.09	0.52
1:G:107:VAL:HG11	2:U:66:TYR:HH	1.73	0.52
2:R:103:GLY:HA2	2:R:178:ILE:HD13	1.91	0.52
1:G:43:ALA:HB2	1:G:185:PRO:HA	1.91	0.52
1:D:24:VAL:O	1:D:28:ARG:HG3	2.09	0.52
2:P:45:ILE:CG1	2:P:52:ALA:HB1	2.39	0.52
1:G:94:ILE:HG13	1:G:95:SER:N	2.24	0.52
1:G:144:ILE:HD12	1:G:147:ARG:NH1	2.24	0.52
2:1:3:THR:HB	2:1:16:THR:HG22	1.91	0.52
1:L:109:ILE:CG2	1:L:147:ARG:HD3	2.39	0.52
1:J:61:GLN:OE1	1:J:62:ASN:HB3	2.07	0.52
1:L:42:PHE:HB2	1:L:184:LEU:O	2.09	0.52
2:R:15:ALA:HB2	2:R:175:VAL:HB	1.92	0.52
2:S:55:LEU:HD21	2:S:87:LEU:HD11	1.92	0.52
1:M:108:ASN:HB3	2:1:70:ARG:HG2	1.91	0.52
1:H:61:GLN:OE1	1:H:62:ASN:HB3	2.09	0.52
1:A:70:ILE:HB	1:A:74:VAL:HG13	1.92	0.52
1:H:214:SER:HG	1:H:224:TYR:HE1	1.56	0.52
1:A:160:TYR:CD2	1:A:163:THR:HB	2.45	0.52
1:H:160:TYR:CD2	1:H:163:THR:HB	2.44	0.52
2:P:18:ARG:HE	2:P:30:ASN:HD22	1.57	0.52
1:G:21:LEU:O	1:G:25:GLU:HG2	2.09	0.52
2:S:141:GLN:NE2	2:V:141:GLN:HE21	2.07	0.52
1:H:135:SER:OG	1:H:153:PRO:HD3	2.10	0.52
2:P:63:LEU:HD11	2:P:74:MET:SD	2.48	0.52
1:G:160:TYR:CD2	1:G:163:THR:HB	2.45	0.52
2:W:137:VAL:HG21	2:W:158:ALA:HA	1.90	0.52
2:R:165:ARG:HA	2:V:26:ILE:HG23	1.92	0.52
2:1:59:MET:HE2	2:1:79:VAL:HG23	1.91	0.52
1:E:175:PHE:C	1:E:175:PHE:HD1	2.14	0.52
2:R:36:GLN:HB2	2:R:184:TYR:CE1	2.43	0.52
2:Q:124:TYR:CD2	2:Q:138:LEU:HD23	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:103:GLY:HA2	2:V:178:ILE:HD11	1.91	0.52
2:W:59:MET:CE	2:W:82:LEU:HD23	2.40	0.52
2:Q:189:THR:HG23	2:Q:190:ASP:N	2.25	0.52
2:S:103:GLY:HA2	2:S:178:ILE:CD1	2.39	0.52
2:R:53:GLN:O	2:R:56:VAL:HG12	2.10	0.52
1:H:49:ILE:HD11	1:H:210:PRO:HB3	1.92	0.52
2:P:179:THR:HG23	2:P:182:ASP:H	1.75	0.52
1:F:108:ASN:CB	2:T:70:ARG:HG2	2.41	0.51
1:M:109:ILE:HG22	1:M:147:ARG:HD3	1.92	0.51
1:I:52:LYS:HZ3	1:I:62:ASN:HA	1.73	0.51
2:W:131:SER:O	2:W:134:VAL:HG13	2.10	0.51
1:M:113:VAL:HG22	1:M:157:ILE:HD12	1.91	0.51
2:U:2:THR:HG22	2:U:169:SER:OG	2.10	0.51
1:J:137:ILE:HG22	1:J:150:ASP:HA	1.91	0.51
2:1:19:ARG:NE	2:1:26:ILE:HG13	2.25	0.51
2:T:20:VAL:CG1	2:T:28:HIS:HB2	2.36	0.51
2:2:111:PHE:CE1	2:2:121:GLU:HB2	2.46	0.51
1:D:15:PHE:HD2	1:E:23:GLN:NE2	2.09	0.51
1:J:21:LEU:O	1:J:25:GLU:HG2	2.10	0.51
2:Y:152:VAL:O	2:Y:156:ILE:HG13	2.10	0.51
1:J:26:TYR:O	1:J:29:GLU:HB2	2.09	0.51
2:1:37:ILE:HD11	2:1:59:MET:CB	2.35	0.51
1:A:85:ALA:O	1:A:89:VAL:HG23	2.11	0.51
1:E:175:PHE:CD1	1:E:175:PHE:C	2.83	0.51
2:Y:28:HIS:CD2	2:Z:120:VAL:HG11	2.45	0.51
1:J:38:LEU:HA	1:J:164:ALA:HA	1.92	0.51
2:W:173:ILE:C	2:W:173:ILE:HD13	2.30	0.51
1:A:21:LEU:O	1:A:24:VAL:HG12	2.10	0.51
1:I:70:ILE:HB	1:I:74:VAL:HG13	1.91	0.51
2:X:174:ASP:HA	2:X:192:ILE:HD13	1.91	0.51
1:K:15:PHE:HB2	1:L:23:GLN:HE22	1.75	0.51
1:L:69:LEU:HD23	1:L:75:ALA:HB2	1.93	0.51
1:I:175:PHE:CD1	1:I:175:PHE:C	2.83	0.51
1:L:135:SER:OG	1:L:153:PRO:HD3	2.11	0.51
1:I:107:VAL:HG11	2:W:66:TYR:HH	1.73	0.51
1:K:165:ILE:HG13	1:K:166:GLY:N	2.25	0.51
1:H:18:ASP:OD2	1:H:20:ARG:HD3	2.11	0.51
1:E:14:VAL:HB	1:F:23:GLN:OE1	2.10	0.51
2:B:116:ALA:O	2:U:50:GLY:HA3	2.11	0.51
2:V:123:ILE:HG12	2:V:124:TYR:CD1	2.37	0.51
2:S:124:TYR:HD2	2:S:138:LEU:HD23	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:LYS:HG2	1:G:202:GLU:HG2	1.91	0.51
1:J:187:LYS:O	1:J:190:VAL:HG13	2.10	0.51
2:1:18:ARG:HE	2:1:30:ASN:HD22	1.57	0.51
1:J:109:ILE:CG2	1:J:147:ARG:HD3	2.40	0.51
1:F:34:GLY:O	1:F:167:SER:HB2	2.11	0.51
1:J:174:SER:O	1:J:177:GLU:HB3	2.10	0.51
2:B:173:ILE:C	2:B:173:ILE:HD13	2.31	0.51
1:H:24:VAL:O	1:H:28:ARG:HG3	2.09	0.51
2:B:45:ILE:CG1	2:B:52:ALA:HB1	2.39	0.51
1:I:52:LYS:HB3	1:I:209:ALA:O	2.11	0.51
2:P:141:GLN:HE21	2:Y:141:GLN:NE2	2.09	0.51
1:C:113:VAL:HG22	1:C:157:ILE:HD12	1.92	0.51
2:R:174:ASP:HA	2:R:192:ILE:HD13	1.92	0.51
2:S:167:SER:HB2	2:2:167:SER:HB2	1.92	0.51
1:G:35:SER:O	1:G:166:GLY:HA3	2.11	0.51
2:R:25:PHE:C	2:R:25:PHE:CD1	2.80	0.51
2:X:123:ILE:HG12	2:X:124:TYR:CD1	2.39	0.51
1:D:198:LYS:HG2	1:D:202:GLU:HG2	1.93	0.51
1:M:159:GLU:HG2	1:N:60:GLU:HG3	1.92	0.51
1:A:156:THR:HG23	1:C:82:VAL:HG11	1.92	0.51
1:F:184:LEU:HD23	1:F:189:ALA:HA	1.92	0.51
1:K:49:ILE:HD11	1:K:210:PRO:HB3	1.92	0.51
2:V:174:ASP:HA	2:V:192:ILE:HD13	1.93	0.51
1:G:137:ILE:HG22	1:G:150:ASP:CB	2.40	0.51
2:T:49:VAL:HG23	2:T:50:GLY:N	2.25	0.51
1:C:52:LYS:NZ	1:C:62:ASN:HA	2.26	0.51
2:2:124:TYR:CD1	2:2:138:LEU:HD23	2.46	0.51
2:U:141:GLN:HE21	2:1:141:GLN:NE2	2.08	0.51
1:E:110:GLU:O	1:E:113:VAL:HG13	2.10	0.51
2:1:6:ILE:HD11	2:1:142:TYR:CD1	2.45	0.51
1:A:191:THR:O	1:A:194:ILE:HG22	2.11	0.51
2:Z:123:ILE:HG12	2:Z:124:TYR:CD1	2.35	0.51
1:O:52:LYS:HZ3	1:O:62:ASN:HA	1.76	0.51
2:Q:160:SER:HA	2:Q:163:LYS:HD3	1.93	0.51
1:N:49:ILE:HD11	1:N:210:PRO:HB3	1.93	0.51
1:F:40:MET:HA	1:F:162:ALA:HA	1.93	0.51
1:F:24:VAL:O	1:F:28:ARG:HG3	2.11	0.50
1:J:52:LYS:HZ1	1:J:62:ASN:HA	1.75	0.50
1:J:52:LYS:HE3	1:J:64:ILE:HG23	1.93	0.50
1:M:49:ILE:HD12	1:M:211:GLU:O	2.11	0.50
2:Y:19:ARG:HE	2:Y:26:ILE:HG13	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:ILE:HG23	1:H:224:TYR:HB2	1.93	0.50
2:Y:3:THR:OG1	2:Y:127:THR:HG22	2.11	0.50
2:Z:28:HIS:CD2	2:1:120:VAL:HG11	2.46	0.50
1:F:123:TYR:CD1	1:F:123:TYR:N	2.78	0.50
2:P:66:TYR:CZ	2:P:70:ARG:HD2	2.46	0.50
2:1:3:THR:CB	2:1:16:THR:HG22	2.42	0.50
1:O:52:LYS:HB3	1:O:209:ALA:O	2.11	0.50
1:I:175:PHE:HD1	1:I:175:PHE:C	2.15	0.50
1:K:38:LEU:HG	1:K:49:ILE:HG23	1.92	0.50
2:B:141:GLN:NE2	2:Z:141:GLN:HE21	2.08	0.50
2:2:50:GLY:O	2:2:54:VAL:HG12	2.10	0.50
1:F:43:ALA:HB2	1:F:185:PRO:HA	1.92	0.50
1:K:69:LEU:HD23	1:K:75:ALA:HB2	1.92	0.50
1:O:180:TYR:HA	1:O:192:LEU:HD21	1.91	0.50
1:M:21:LEU:HD11	1:N:130:ARG:HD2	1.93	0.50
1:H:43:ALA:HB2	1:H:185:PRO:HA	1.94	0.50
2:T:131:SER:O	2:T:134:VAL:HG13	2.10	0.50
1:D:95:SER:OG	1:D:115:ARG:HD3	2.10	0.50
2:B:178:ILE:HB	2:B:184:TYR:HA	1.93	0.50
1:M:98:GLN:O	1:M:102:THR:HG22	2.12	0.50
1:M:180:TYR:HB3	1:N:57:ARG:NH2	2.24	0.50
2:X:37:ILE:HD11	2:X:59:MET:CB	2.39	0.50
1:I:62:ASN:O	1:I:65:GLU:HG2	2.11	0.50
2:U:36:GLN:HB2	2:U:184:TYR:CE1	2.46	0.50
1:E:95:SER:OG	1:E:115:ARG:HD3	2.11	0.50
1:J:175:PHE:HD2	1:J:199:SER:HG	1.60	0.50
2:X:12:VAL:HG13	2:X:178:ILE:HG23	1.93	0.50
1:A:180:TYR:HA	1:A:192:LEU:HD21	1.93	0.50
2:B:176:ALA:HA	2:B:186:GLN:HA	1.92	0.50
2:X:59:MET:CE	2:X:82:LEU:HD23	2.42	0.50
2:S:133:PHE:CZ	2:S:165:ARG:HB3	2.47	0.50
1:O:172:VAL:O	1:O:176:LEU:HD22	2.11	0.50
1:F:137:ILE:HG22	1:F:150:ASP:HB2	1.92	0.50
2:T:62:GLU:HG2	2:T:82:LEU:HD21	1.93	0.50
1:E:98:GLN:O	1:E:102:THR:HG22	2.11	0.50
2:Q:62:GLU:HG2	2:Q:82:LEU:HD21	1.94	0.50
2:W:152:VAL:O	2:W:156:ILE:HG13	2.11	0.50
2:T:26:ILE:HD13	2:T:26:ILE:O	2.11	0.50
1:A:149:PHE:CE1	1:A:159:GLU:HB2	2.46	0.50
2:U:20:VAL:HG13	2:U:28:HIS:HB2	1.93	0.50
2:X:15:ALA:HB2	2:X:175:VAL:HB	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:3:THR:HB	2:Z:16:THR:HG22	1.94	0.50
2:1:123:ILE:CD1	2:1:123:ILE:H	2.22	0.50
2:Q:123:ILE:CD1	2:Q:123:ILE:H	2.22	0.50
2:P:59:MET:CE	2:P:82:LEU:HD23	2.41	0.50
1:M:43:ALA:HB2	1:M:185:PRO:HA	1.94	0.50
2:S:173:ILE:HD13	2:S:173:ILE:C	2.32	0.50
2:Y:189:THR:HG23	2:Y:190:ASP:H	1.76	0.50
1:D:137:ILE:HG22	1:D:150:ASP:HB2	1.93	0.50
1:G:17:PRO:HA	1:H:26:TYR:CD1	2.46	0.50
2:2:133:PHE:CZ	2:2:165:ARG:HB3	2.47	0.50
2:V:43:MET:CE	2:V:56:VAL:HG23	2.41	0.50
2:V:43:MET:HE2	2:V:56:VAL:HG23	1.93	0.50
1:E:61:GLN:OE1	1:E:62:ASN:HB3	2.12	0.50
1:C:70:ILE:HD12	1:C:74:VAL:HG22	1.92	0.50
1:N:121:GLN:O	1:N:124:THR:HB	2.11	0.50
1:M:62:ASN:O	1:M:65:GLU:HG2	2.12	0.50
1:C:198:LYS:CG	1:C:202:GLU:HG2	2.42	0.50
2:W:28:HIS:CD2	2:X:120:VAL:HG11	2.47	0.50
1:E:49:ILE:HD11	1:E:210:PRO:HB3	1.94	0.50
2:U:112:SER:O	2:U:113:ILE:HD13	2.12	0.50
1:A:26:TYR:CD1	1:H:17:PRO:HA	2.45	0.50
2:1:152:VAL:O	2:1:156:ILE:HG13	2.11	0.50
1:D:175:PHE:C	1:D:175:PHE:CD1	2.85	0.50
2:U:123:ILE:HG12	2:U:124:TYR:CD2	2.44	0.49
1:F:52:LYS:HB3	1:F:209:ALA:O	2.12	0.49
1:O:51:ASP:HB3	1:O:53:LYS:HZ3	1.76	0.49
1:K:38:LEU:HA	1:K:164:ALA:HA	1.93	0.49
2:X:161:ALA:O	2:X:164:GLN:HB2	2.12	0.49
2:R:179:THR:HG23	2:R:182:ASP:H	1.77	0.49
1:D:113:VAL:HG22	1:D:157:ILE:HD12	1.94	0.49
1:O:174:SER:O	1:O:177:GLU:HB3	2.11	0.49
1:C:170:ASP:O	1:C:173:VAL:HG12	2.10	0.49
1:O:28:ARG:O	1:O:31:VAL:HG22	2.12	0.49
2:S:43:MET:HE1	2:S:56:VAL:HG23	1.94	0.49
1:H:52:LYS:HZ3	1:H:62:ASN:HA	1.76	0.49
2:2:3:THR:HB	2:2:16:THR:HG22	1.93	0.49
1:A:175:PHE:HD1	1:A:175:PHE:C	2.15	0.49
2:X:38:ASP:HB3	2:X:41:THR:CG2	2.36	0.49
1:O:21:LEU:O	1:O:24:VAL:HG12	2.12	0.49
1:D:62:ASN:O	1:D:65:GLU:HG2	2.11	0.49
1:I:52:LYS:HZ1	1:I:62:ASN:HA	1.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:PHE:O	1:D:25:GLU:HB2	2.12	0.49
2:Y:189:THR:HG23	2:Y:190:ASP:N	2.27	0.49
1:A:175:PHE:CD1	1:A:175:PHE:C	2.84	0.49
2:V:75:PRO:O	2:V:78:ALA:HB3	2.12	0.49
1:O:38:LEU:HA	1:O:164:ALA:HA	1.94	0.49
2:2:174:ASP:HA	2:2:192:ILE:HD13	1.93	0.49
2:Y:76:ILE:O	2:Y:79:VAL:HG12	2.13	0.49
1:I:94:ILE:HG13	1:I:95:SER:N	2.27	0.49
2:1:19:ARG:HE	2:1:26:ILE:HG13	1.77	0.49
2:W:149:ASP:O	2:W:152:VAL:HG12	2.11	0.49
1:A:137:ILE:HG22	1:A:150:ASP:HB2	1.95	0.49
1:H:84:ASP:O	1:H:88:LEU:HB2	2.13	0.49
1:O:95:SER:OG	1:O:115:ARG:HD3	2.12	0.49
1:A:170:ASP:O	1:A:173:VAL:HG12	2.13	0.49
1:G:116:VAL:HG11	1:G:138:PHE:CZ	2.46	0.49
2:W:123:ILE:HG12	2:W:124:TYR:CD1	2.36	0.49
2:T:124:TYR:HD2	2:T:138:LEU:HD23	1.76	0.49
2:S:189:THR:HG23	2:S:190:ASP:N	2.28	0.49
1:N:52:LYS:HZ3	1:N:62:ASN:HA	1.77	0.49
1:E:42:PHE:HB2	1:E:184:LEU:O	2.13	0.49
2:P:3:THR:OG1	2:P:127:THR:HG22	2.12	0.49
2:1:12:VAL:HG13	2:1:178:ILE:HG23	1.95	0.49
1:A:110:GLU:O	1:A:113:VAL:HG12	2.13	0.49
1:I:49:ILE:HD13	1:I:212:ILE:HB	1.95	0.49
1:F:134:VAL:CG2	1:F:135:SER:N	2.76	0.49
1:E:17:PRO:HA	1:F:26:TYR:CD1	2.48	0.49
1:G:128:GLY:O	1:G:129:VAL:HB	2.13	0.49
2:W:25:PHE:CD1	2:W:25:PHE:C	2.84	0.49
1:K:52:LYS:HZ3	1:K:62:ASN:HA	1.75	0.49
1:E:135:SER:OG	1:E:152:ASP:HA	2.12	0.49
2:R:175:VAL:CG2	2:R:176:ALA:N	2.75	0.49
2:V:15:ALA:HB3	2:V:155:VAL:HG11	1.95	0.49
1:A:137:ILE:HG22	1:A:150:ASP:CB	2.43	0.49
1:G:174:SER:O	1:G:177:GLU:HB3	2.12	0.49
1:N:175:PHE:C	1:N:175:PHE:CD1	2.86	0.49
2:2:157:ARG:HA	2:2:201:LEU:HD21	1.95	0.49
1:C:184:LEU:HD23	1:C:189:ALA:HA	1.95	0.49
2:S:18:ARG:HE	2:S:30:ASN:HD22	1.61	0.49
2:1:149:ASP:O	2:1:152:VAL:HG12	2.12	0.49
1:H:88:LEU:HD13	1:H:132:TYR:CD2	2.47	0.49
2:Q:174:ASP:HA	2:Q:192:ILE:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:GLU:O	1:L:113:VAL:HG13	2.13	0.49
2:Z:173:ILE:C	2:Z:173:ILE:HD13	2.34	0.49
1:L:42:PHE:HD1	1:L:43:ALA:N	2.11	0.49
1:D:38:LEU:HB3	1:D:164:ALA:HB2	1.94	0.49
2:Y:25:PHE:CD1	2:Y:25:PHE:C	2.83	0.49
2:V:38:ASP:HB3	2:V:41:THR:CG2	2.38	0.48
1:L:187:LYS:O	1:L:190:VAL:HG13	2.14	0.48
1:H:42:PHE:CD1	1:H:43:ALA:N	2.81	0.48
2:R:133:PHE:CZ	2:R:165:ARG:HB3	2.48	0.48
2:Q:18:ARG:HB2	2:Q:31:GLY:O	2.13	0.48
1:N:21:LEU:HD11	1:O:130:ARG:HD2	1.94	0.48
2:X:152:VAL:O	2:X:156:ILE:HG13	2.13	0.48
1:O:187:LYS:O	1:O:190:VAL:HG13	2.13	0.48
1:F:32:LYS:O	1:F:167:SER:HA	2.14	0.48
1:E:69:LEU:HD23	1:E:75:ALA:HB2	1.96	0.48
1:N:186:GLU:O	1:N:190:VAL:HG12	2.13	0.48
1:I:97:GLN:OE1	1:I:97:GLN:HA	2.13	0.48
1:K:124:THR:CG2	1:L:130:ARG:HH21	2.22	0.48
1:C:187:LYS:O	1:C:190:VAL:HG13	2.14	0.48
1:M:136:LEU:HD12	1:M:151:CYS:HB3	1.94	0.48
1:G:70:ILE:HB	1:G:74:VAL:HG13	1.95	0.48
2:T:76:ILE:O	2:T:79:VAL:HG12	2.14	0.48
2:R:43:MET:HE1	2:R:56:VAL:HG23	1.95	0.48
1:D:148:LEU:O	1:D:159:GLU:HG3	2.13	0.48
2:P:15:ALA:HB2	2:P:175:VAL:HB	1.93	0.48
2:1:189:THR:HG23	2:1:190:ASP:N	2.29	0.48
2:Y:38:ASP:HB3	2:Y:41:THR:CG2	2.32	0.48
1:L:198:LYS:HG2	1:L:202:GLU:HG2	1.95	0.48
2:V:45:ILE:CG1	2:V:52:ALA:HB1	2.42	0.48
1:N:98:GLN:O	1:N:101:VAL:HG12	2.13	0.48
1:C:124:THR:HG22	1:D:130:ARG:HH21	1.79	0.48
2:B:12:VAL:HG13	2:B:178:ILE:HG23	1.96	0.48
2:T:26:ILE:C	2:T:26:ILE:HD13	2.34	0.48
1:A:228:GLU:O	1:A:231:LYS:HB3	2.13	0.48
1:E:35:SER:O	1:E:166:GLY:HA3	2.13	0.48
1:K:34:GLY:O	1:K:167:SER:HB2	2.13	0.48
2:2:131:SER:O	2:2:134:VAL:HG13	2.13	0.48
1:D:180:TYR:HA	1:D:192:LEU:HD21	1.95	0.48
2:B:124:TYR:HD2	2:B:138:LEU:HD23	1.76	0.48
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.43	0.48
1:G:175:PHE:C	1:G:175:PHE:CD1	2.87	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLN:HB2	2:B:184:TYR:CE1	2.48	0.48
2:X:104:ILE:HG22	2:X:178:ILE:HD11	1.94	0.48
1:O:215:ILE:HD11	1:O:219:ASN:O	2.13	0.48
1:J:123:TYR:CE2	1:J:129:VAL:HG21	2.48	0.48
1:C:28:ARG:O	1:C:31:VAL:HG22	2.13	0.48
1:G:69:LEU:HD23	1:G:75:ALA:HB2	1.94	0.48
1:O:175:PHE:C	1:O:175:PHE:CD1	2.87	0.48
1:A:62:ASN:O	1:A:65:GLU:HG2	2.13	0.48
1:F:49:ILE:HD11	1:F:210:PRO:HB3	1.94	0.48
1:J:144:ILE:HD12	1:J:147:ARG:NH1	2.28	0.48
2:Q:109:HIS:HB3	2:Q:111:PHE:HE1	1.79	0.48
1:A:148:LEU:O	1:A:159:GLU:HG3	2.14	0.48
1:E:168:GLY:O	1:E:172:VAL:HG12	2.12	0.48
2:T:179:THR:HG23	2:T:182:ASP:H	1.79	0.48
1:O:61:GLN:CD	1:O:62:ASN:H	2.16	0.48
1:D:121:GLN:O	1:D:124:THR:HB	2.13	0.48
1:N:24:VAL:O	1:N:28:ARG:HG3	2.14	0.48
2:V:111:PHE:CD2	2:V:121:GLU:HB2	2.49	0.48
1:K:98:GLN:O	1:K:101:VAL:HG12	2.14	0.48
1:D:85:ALA:O	1:D:89:VAL:HG23	2.14	0.48
1:E:15:PHE:HD2	1:F:23:GLN:HE22	1.61	0.48
2:B:17:GLU:HB2	2:B:170:GLY:O	2.14	0.48
2:B:141:GLN:NE2	2:Z:141:GLN:NE2	2.61	0.48
2:X:36:GLN:HB2	2:X:184:TYR:CE1	2.48	0.48
2:W:202:ILE:HG12	2:W:203:LEU:N	2.28	0.48
2:1:137:VAL:HG21	2:1:158:ALA:HA	1.95	0.48
1:E:127:GLY:O	1:E:129:VAL:N	2.47	0.48
1:F:76:ALA:HB2	1:F:138:PHE:CD1	2.48	0.48
2:2:55:LEU:HD21	2:2:87:LEU:HD11	1.96	0.48
1:M:42:PHE:CD1	1:M:43:ALA:N	2.81	0.48
1:H:52:LYS:HA	1:H:66:LYS:NZ	2.29	0.48
1:C:125:GLN:HB3	1:D:130:ARG:NH2	2.28	0.48
2:U:141:GLN:NE2	2:1:141:GLN:HE21	2.12	0.48
2:Z:3:THR:OG1	2:Z:127:THR:HG22	2.14	0.48
1:D:147:ARG:HB3	1:D:149:PHE:HE1	1.79	0.48
2:T:167:SER:HB2	2:1:167:SER:HB2	1.95	0.48
2:Q:66:TYR:CD2	2:Q:74:MET:HE2	2.48	0.48
2:Y:34:LEU:HD21	2:Y:176:ALA:HB3	1.95	0.48
2:X:37:ILE:HD11	2:X:59:MET:HG3	1.96	0.48
1:M:61:GLN:O	1:M:64:ILE:HG22	2.12	0.48
1:J:49:ILE:HD12	1:J:211:GLU:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:55:LEU:HD21	2:Y:87:LEU:HD11	1.94	0.48
1:C:175:PHE:CD1	1:C:175:PHE:C	2.88	0.48
2:V:26:ILE:O	2:V:26:ILE:HD13	2.13	0.47
1:F:42:PHE:HB2	1:F:184:LEU:O	2.14	0.47
1:O:94:ILE:HG13	1:O:95:SER:N	2.29	0.47
1:C:24:VAL:O	1:C:28:ARG:HG3	2.14	0.47
1:I:113:VAL:HG22	1:I:157:ILE:HD12	1.96	0.47
1:H:48:LEU:HB3	1:H:67:ILE:HD13	1.96	0.47
2:P:22:MET:O	2:P:23:GLU:HB2	2.14	0.47
2:B:66:TYR:CZ	2:B:70:ARG:HD2	2.49	0.47
1:A:108:ASN:HB3	2:P:70:ARG:HG2	1.95	0.47
2:1:15:ALA:HB2	2:1:175:VAL:HB	1.95	0.47
1:G:42:PHE:CD1	1:G:43:ALA:N	2.81	0.47
2:Q:159:ILE:O	2:Q:163:LYS:HG3	2.14	0.47
1:D:90:ASP:O	1:D:94:ILE:HG23	2.14	0.47
2:V:44:THR:OG1	2:V:100:LEU:HB3	2.14	0.47
2:B:126:SER:HB3	2:B:135:TYR:CE2	2.49	0.47
1:E:191:THR:O	1:E:194:ILE:HG22	2.13	0.47
2:2:6:ILE:HD11	2:2:142:TYR:CD1	2.49	0.47
2:R:44:THR:OG1	2:R:100:LEU:HB3	2.14	0.47
2:1:133:PHE:CZ	2:1:165:ARG:HB3	2.49	0.47
1:E:134:VAL:CG2	1:E:135:SER:N	2.76	0.47
1:D:52:LYS:HA	1:D:66:LYS:HZ2	1.78	0.47
1:G:198:LYS:CG	1:G:202:GLU:HG2	2.44	0.47
2:2:123:ILE:HG12	2:2:124:TYR:CD2	2.49	0.47
2:T:74:MET:HG2	2:T:78:ALA:HB3	1.95	0.47
1:F:38:LEU:CD2	1:F:49:ILE:HG23	2.44	0.47
1:N:187:LYS:O	1:N:190:VAL:HG13	2.14	0.47
2:P:189:THR:HG23	2:P:190:ASP:H	1.79	0.47
2:P:189:THR:HG23	2:P:190:ASP:N	2.28	0.47
2:P:32:LYS:HE2	2:P:34:LEU:O	2.14	0.47
1:C:137:ILE:HG22	1:C:150:ASP:HB2	1.96	0.47
2:R:103:GLY:HA2	2:R:178:ILE:CD1	2.44	0.47
1:E:202:GLU:HG3	1:E:205:GLU:O	2.14	0.47
2:V:103:GLY:HA2	2:V:178:ILE:HD13	1.95	0.47
1:F:49:ILE:HD12	1:F:211:GLU:O	2.14	0.47
2:W:62:GLU:HG2	2:W:82:LEU:HD21	1.96	0.47
1:K:165:ILE:HG13	1:K:166:GLY:H	1.79	0.47
1:D:175:PHE:HD1	1:D:175:PHE:C	2.18	0.47
1:L:113:VAL:HG22	1:L:157:ILE:HD12	1.96	0.47
1:I:81:LEU:HD23	1:I:133:GLY:HA3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:26:TYR:O	1:N:29:GLU:HB2	2.15	0.47
1:N:95:SER:OG	1:N:115:ARG:HD3	2.14	0.47
2:U:175:VAL:CG2	2:U:176:ALA:N	2.78	0.47
1:I:130:ARG:HH21	1:O:124:THR:CG2	2.20	0.47
1:E:130:ARG:HH11	1:E:130:ARG:HG2	1.80	0.47
2:Y:123:ILE:HG12	2:Y:124:TYR:CD2	2.49	0.47
1:N:61:GLN:OE1	1:N:62:ASN:HB3	2.13	0.47
1:M:94:ILE:CG1	1:M:95:SER:N	2.77	0.47
1:L:175:PHE:CD1	1:L:175:PHE:C	2.88	0.47
2:S:132:PRO:HA	2:V:133:PHE:CE1	2.49	0.47
2:U:18:ARG:HB2	2:U:31:GLY:O	2.14	0.47
2:Y:22:MET:O	2:Y:23:GLU:HB2	2.14	0.47
2:U:91:LYS:O	2:U:94:PRO:HD3	2.15	0.47
2:V:143:SER:O	2:V:146:MET:HG3	2.14	0.47
1:I:160:TYR:CD2	1:I:163:THR:HB	2.49	0.47
2:V:17:GLU:HA	2:V:173:ILE:HA	1.96	0.47
2:P:26:ILE:C	2:P:26:ILE:HD13	2.35	0.47
2:T:7:THR:HB	2:T:123:ILE:O	2.14	0.47
1:G:52:LYS:HZ1	1:G:62:ASN:HA	1.76	0.47
2:Z:15:ALA:HB3	2:Z:155:VAL:CG1	2.44	0.47
1:J:62:ASN:O	1:J:65:GLU:HG2	2.14	0.47
1:C:94:ILE:CG1	1:C:95:SER:N	2.78	0.47
2:1:103:GLY:HA2	2:1:178:ILE:HD13	1.97	0.47
1:C:98:GLN:O	1:C:102:THR:HG23	2.15	0.47
1:N:82:VAL:HG13	1:N:83:ALA:N	2.29	0.47
2:1:45:ILE:HG12	2:1:52:ALA:HB1	1.95	0.47
1:M:34:GLY:O	1:M:167:SER:HB2	2.14	0.47
2:1:2:THR:HG22	2:1:169:SER:OG	2.14	0.47
2:U:25:PHE:CD1	2:U:25:PHE:C	2.84	0.47
2:Q:45:ILE:HD11	2:Q:52:ALA:O	2.14	0.47
2:1:59:MET:HE3	2:1:82:LEU:HD23	1.95	0.47
1:K:42:PHE:HB2	1:K:184:LEU:O	2.15	0.47
2:B:83:LEU:HA	2:B:83:LEU:HD12	1.69	0.47
2:X:59:MET:HE3	2:X:82:LEU:HD23	1.97	0.47
2:Q:152:VAL:O	2:Q:156:ILE:HG13	2.14	0.47
1:E:52:LYS:HE3	1:E:64:ILE:HG23	1.96	0.47
2:P:35:PHE:CE2	2:P:45:ILE:HD12	2.50	0.47
1:N:52:LYS:HZ1	1:N:62:ASN:HA	1.79	0.47
1:A:134:VAL:O	1:A:153:PRO:HG3	2.14	0.47
2:B:103:GLY:HA2	2:B:178:ILE:CD1	2.44	0.47
2:1:104:ILE:HG22	2:1:178:ILE:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:VAL:HG13	1:D:230:LYS:N	2.30	0.47
2:S:174:ASP:HA	2:S:192:ILE:HD13	1.96	0.47
1:G:143:GLN:HE21	1:G:143:GLN:HA	1.80	0.47
1:H:45:GLY:HA3	1:H:216:THR:HA	1.96	0.47
1:J:159:GLU:HG2	1:K:60:GLU:HG3	1.96	0.47
2:T:22:MET:O	2:T:23:GLU:HB2	2.15	0.47
2:U:27:MET:HG2	2:U:27:MET:O	2.15	0.47
1:H:16:SER:HB3	1:H:22:PHE:CE2	2.50	0.47
1:L:109:ILE:HG22	1:L:147:ARG:HD3	1.97	0.47
2:R:59:MET:CE	2:R:82:LEU:HD23	2.43	0.47
1:G:38:LEU:HA	1:G:164:ALA:HA	1.95	0.47
1:C:21:LEU:HD11	1:D:130:ARG:HD2	1.97	0.47
2:B:6:ILE:HD11	2:B:142:TYR:HD1	1.80	0.47
2:Q:175:VAL:CG2	2:Q:176:ALA:N	2.78	0.47
1:I:180:TYR:HB3	1:J:57:ARG:NH2	2.30	0.47
2:T:141:GLN:HE21	2:2:141:GLN:NE2	2.12	0.47
1:O:116:VAL:HG11	1:O:138:PHE:CZ	2.50	0.47
1:N:18:ASP:OD2	1:N:20:ARG:HD3	2.15	0.47
2:B:20:VAL:HG22	2:B:28:HIS:HB2	1.96	0.47
1:L:108:ASN:HA	1:L:142:ASP:OD1	2.15	0.47
2:B:37:ILE:HD11	2:B:59:MET:CB	2.45	0.47
1:O:130:ARG:HG2	1:O:130:ARG:NH1	2.30	0.47
1:N:52:LYS:HE3	1:N:64:ILE:HG23	1.97	0.47
2:W:37:ILE:HD11	2:W:59:MET:HG3	1.97	0.47
2:2:189:THR:HG23	2:2:190:ASP:N	2.30	0.47
1:E:159:GLU:HG2	1:F:60:GLU:HG3	1.96	0.47
1:I:35:SER:O	1:I:166:GLY:HA3	2.15	0.47
1:H:114:LYS:O	1:H:117:ALA:HB3	2.15	0.47
1:C:58:LEU:CD1	1:C:58:LEU:N	2.78	0.47
1:K:130:ARG:HH11	1:K:130:ARG:HG2	1.80	0.47
2:Y:59:MET:CE	2:Y:82:LEU:HD23	2.45	0.47
1:G:152:ASP:HB2	1:G:153:PRO:HD2	1.96	0.47
1:I:135:SER:OG	1:I:152:ASP:HA	2.15	0.47
1:I:187:LYS:O	1:I:190:VAL:HG13	2.14	0.47
1:F:38:LEU:HA	1:F:164:ALA:HA	1.97	0.47
2:V:175:VAL:CG2	2:V:176:ALA:N	2.78	0.47
1:C:110:GLU:O	1:C:113:VAL:HG13	2.15	0.47
1:N:142:ASP:OD2	1:N:147:ARG:HD2	2.16	0.47
2:Q:81:THR:O	2:Q:84:SER:HB3	2.15	0.47
2:V:177:VAL:HG12	2:V:187:LEU:HD11	1.96	0.47
1:E:134:VAL:O	1:E:153:PRO:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:124:TYR:HD2	2:X:138:LEU:HD23	1.80	0.46
2:Y:175:VAL:CG2	2:Y:176:ALA:N	2.78	0.46
2:2:123:ILE:HG12	2:2:124:TYR:HD2	1.80	0.46
1:F:135:SER:OG	1:F:153:PRO:HD3	2.15	0.46
2:X:22:MET:O	2:X:23:GLU:HB2	2.16	0.46
2:R:74:MET:HG2	2:R:78:ALA:HB3	1.97	0.46
2:U:123:ILE:N	2:U:123:ILE:HD13	2.26	0.46
2:U:59:MET:HE2	2:U:79:VAL:HG23	1.97	0.46
2:Y:59:MET:HE2	2:Y:79:VAL:CG2	2.44	0.46
1:O:108:ASN:CB	2:V:70:ARG:HG2	2.44	0.46
2:W:131:SER:HB2	2:W:132:PRO:HD3	1.97	0.46
1:L:152:ASP:HB2	1:L:153:PRO:HD2	1.97	0.46
1:A:98:GLN:O	1:A:102:THR:HG23	2.15	0.46
1:F:98:GLN:O	1:F:101:VAL:HG12	2.16	0.46
2:Z:177:VAL:HG12	2:Z:187:LEU:HD11	1.97	0.46
2:W:138:LEU:HD12	2:W:138:LEU:HA	1.73	0.46
1:I:121:GLN:O	1:I:124:THR:HB	2.14	0.46
2:Y:36:GLN:HB2	2:Y:184:TYR:CE1	2.50	0.46
1:I:48:LEU:HB3	1:I:67:ILE:HD13	1.97	0.46
1:I:72:ASP:HB2	1:I:73:TYR:CD1	2.51	0.46
2:W:76:ILE:HA	2:W:79:VAL:HG12	1.96	0.46
1:H:175:PHE:CD1	1:H:175:PHE:C	2.88	0.46
2:B:177:VAL:HG12	2:B:187:LEU:CD1	2.46	0.46
1:K:172:VAL:O	1:K:176:LEU:HD22	2.16	0.46
2:B:59:MET:HE2	2:B:79:VAL:CG2	2.44	0.46
2:Y:34:LEU:HD21	2:Y:176:ALA:CB	2.46	0.46
2:1:15:ALA:HB3	2:1:155:VAL:HG11	1.98	0.46
1:D:21:LEU:HD11	1:E:130:ARG:HD2	1.97	0.46
2:P:20:VAL:CG1	2:P:28:HIS:HB2	2.44	0.46
1:M:175:PHE:C	1:M:175:PHE:CD1	2.89	0.46
1:D:172:VAL:O	1:D:176:LEU:HD22	2.16	0.46
2:Y:178:ILE:HB	2:Y:184:TYR:HA	1.96	0.46
1:J:88:LEU:HD13	1:J:132:TYR:CE2	2.51	0.46
2:B:165:ARG:HA	2:Y:26:ILE:HG23	1.98	0.46
2:V:19:ARG:HE	2:V:26:ILE:HG13	1.80	0.46
1:L:180:TYR:HA	1:L:192:LEU:HD21	1.97	0.46
1:A:60:GLU:HG3	1:H:159:GLU:HG2	1.96	0.46
2:R:50:GLY:O	2:R:54:VAL:HG12	2.14	0.46
1:I:18:ASP:OD2	1:I:20:ARG:HD3	2.16	0.46
1:D:198:LYS:O	1:D:199:SER:C	2.54	0.46
1:M:124:THR:HG22	1:N:130:ARG:HH21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:CD2	1:A:196:ALA:HA	2.50	0.46
2:U:132:PRO:HA	2:1:133:PHE:HE1	1.81	0.46
2:Z:50:GLY:O	2:Z:54:VAL:HG12	2.16	0.46
1:J:165:ILE:HD12	1:J:169:LYS:HD2	1.97	0.46
2:Z:8:LEU:HD12	2:Z:8:LEU:O	2.16	0.46
2:S:43:MET:HE2	2:S:56:VAL:HG23	1.98	0.46
1:L:174:SER:O	1:L:177:GLU:HB3	2.15	0.46
2:S:178:ILE:O	2:S:178:ILE:HG12	2.14	0.46
2:R:48:LEU:HD12	2:R:49:VAL:N	2.31	0.46
2:W:15:ALA:HB2	2:W:175:VAL:HB	1.96	0.46
1:F:228:GLU:O	1:F:231:LYS:HB3	2.15	0.46
1:H:31:VAL:HA	1:H:80:GLY:HA2	1.98	0.46
1:L:161:LYS:HD2	1:M:60:GLU:OE2	2.16	0.46
1:F:81:LEU:HD23	1:F:133:GLY:HA3	1.97	0.46
2:2:25:PHE:C	2:2:25:PHE:CD1	2.89	0.46
2:U:76:ILE:HG21	2:U:109:HIS:HB2	1.96	0.46
1:C:42:PHE:HD1	1:C:43:ALA:N	2.14	0.46
1:O:61:GLN:OE1	1:O:62:ASN:HB3	2.16	0.46
2:R:160:SER:HA	2:R:163:LYS:HD3	1.98	0.46
1:E:70:ILE:HB	1:E:74:VAL:HG13	1.98	0.46
1:H:135:SER:OG	1:H:152:ASP:HA	2.16	0.46
2:X:40:TYR:O	2:X:178:ILE:HD11	2.15	0.46
1:F:152:ASP:HB2	1:F:153:PRO:CD	2.46	0.46
2:U:55:LEU:HD21	2:U:87:LEU:HD11	1.97	0.46
1:O:88:LEU:HD13	1:O:132:TYR:CD2	2.51	0.46
2:V:37:ILE:HD11	2:V:59:MET:HB3	1.97	0.46
2:1:22:MET:O	2:1:23:GLU:HB2	2.15	0.46
2:S:75:PRO:O	2:S:78:ALA:HB3	2.16	0.46
1:E:108:ASN:CB	2:S:70:ARG:HG2	2.43	0.46
2:2:59:MET:HE2	2:2:79:VAL:HG23	1.98	0.46
1:J:198:LYS:HG2	1:J:202:GLU:HG2	1.96	0.46
2:1:15:ALA:HB3	2:1:155:VAL:CG1	2.46	0.46
1:H:52:LYS:HZ1	1:H:62:ASN:HA	1.81	0.46
2:V:26:ILE:C	2:V:26:ILE:HD13	2.36	0.46
2:S:103:GLY:HA2	2:S:178:ILE:HD11	1.98	0.46
2:B:72:VAL:HG22	2:B:73:ASN:N	2.31	0.46
1:K:228:GLU:O	1:K:231:LYS:HB3	2.16	0.46
1:G:130:ARG:HA	1:G:131:PRO:HD3	1.82	0.46
1:L:38:LEU:HG	1:L:49:ILE:HG23	1.98	0.46
1:E:42:PHE:CD1	1:E:43:ALA:N	2.84	0.46
2:P:175:VAL:CG2	2:P:176:ALA:N	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:146:MET:HE2	2:X:150:GLU:HB3	1.97	0.46
2:U:109:HIS:HB3	2:U:111:PHE:HE1	1.81	0.46
1:I:137:ILE:HG22	1:I:150:ASP:CB	2.45	0.46
1:H:187:LYS:O	1:H:190:VAL:HG13	2.16	0.46
1:N:88:LEU:HD13	1:N:132:TYR:CE2	2.51	0.46
2:R:17:GLU:HA	2:R:173:ILE:HA	1.98	0.46
1:G:109:ILE:CG2	1:G:147:ARG:HD3	2.46	0.46
2:R:165:ARG:C	2:V:26:ILE:HG22	2.36	0.46
2:1:26:ILE:HD13	2:1:26:ILE:O	2.16	0.46
1:D:94:ILE:HG13	1:D:95:SER:N	2.29	0.46
1:K:43:ALA:HB2	1:K:185:PRO:HA	1.97	0.46
1:E:77:VAL:CG1	1:E:137:ILE:HG12	2.46	0.46
2:T:174:ASP:HA	2:T:192:ILE:HD13	1.98	0.46
2:B:193:GLU:HA	2:B:196:ILE:HD12	1.98	0.46
1:K:175:PHE:C	1:K:175:PHE:CD1	2.89	0.46
2:R:124:TYR:HD2	2:R:138:LEU:HD23	1.80	0.45
1:E:198:LYS:O	1:E:199:SER:C	2.54	0.45
2:Y:18:ARG:HB2	2:Y:31:GLY:O	2.16	0.45
1:H:38:LEU:HG	1:H:49:ILE:HG23	1.98	0.45
2:1:189:THR:HG23	2:1:190:ASP:H	1.81	0.45
2:Z:32:LYS:HE2	2:Z:34:LEU:O	2.16	0.45
2:R:111:PHE:CE2	2:R:121:GLU:HB2	2.51	0.45
2:U:187:LEU:HA	2:U:188:PRO:HD3	1.81	0.45
2:R:27:MET:O	2:R:27:MET:HG2	2.16	0.45
1:G:81:LEU:HD23	1:G:133:GLY:HA3	1.97	0.45
1:K:198:LYS:HG3	1:K:207:LEU:HD22	1.98	0.45
1:F:194:ILE:O	1:F:198:LYS:HB2	2.16	0.45
2:W:103:GLY:HA2	2:W:178:ILE:CD1	2.46	0.45
2:R:43:MET:CE	2:R:56:VAL:HG23	2.45	0.45
2:W:189:THR:HG23	2:W:190:ASP:N	2.31	0.45
2:T:15:ALA:HB3	2:T:155:VAL:HG11	1.98	0.45
1:I:148:LEU:O	1:I:159:GLU:HG3	2.16	0.45
1:C:15:PHE:HD2	1:D:23:GLN:HE22	1.64	0.45
2:U:124:TYR:HD1	2:U:138:LEU:HD23	1.81	0.45
2:X:59:MET:SD	2:X:83:LEU:HD13	2.56	0.45
1:H:52:LYS:HE3	1:H:64:ILE:HG23	1.99	0.45
2:B:55:LEU:HA	2:B:55:LEU:HD12	1.50	0.45
2:B:132:PRO:HA	2:Z:133:PHE:HE1	1.81	0.45
2:S:19:ARG:HE	2:S:26:ILE:HG13	1.82	0.45
2:R:75:PRO:O	2:R:78:ALA:HB3	2.16	0.45
2:Q:179:THR:HG23	2:Q:182:ASP:H	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:18:ARG:HE	2:V:30:ASN:HD22	1.65	0.45
1:J:76:ALA:HB2	1:J:138:PHE:CD1	2.52	0.45
2:T:110:VAL:HG13	2:T:110:VAL:O	2.16	0.45
1:J:143:GLN:HA	1:J:143:GLN:HE21	1.82	0.45
1:N:58:LEU:N	1:N:58:LEU:CD1	2.79	0.45
1:A:52:LYS:HE3	1:A:64:ILE:HG23	1.99	0.45
2:B:7:THR:HB	2:B:123:ILE:O	2.16	0.45
1:D:52:LYS:HE3	1:D:64:ILE:HG23	1.98	0.45
1:F:61:GLN:OE1	1:F:62:ASN:HB3	2.16	0.45
2:1:175:VAL:CG2	2:1:176:ALA:N	2.78	0.45
1:C:49:ILE:HD11	1:C:210:PRO:HB3	1.98	0.45
2:W:26:ILE:HD13	2:W:26:ILE:C	2.35	0.45
2:P:105:ASP:OD1	2:P:106:THR:N	2.49	0.45
2:B:111:PHE:CE2	2:B:121:GLU:HB2	2.51	0.45
2:Z:15:ALA:HB3	2:Z:155:VAL:HG11	1.97	0.45
1:I:42:PHE:CD1	1:I:43:ALA:N	2.83	0.45
2:R:149:ASP:O	2:R:152:VAL:HG12	2.17	0.45
1:L:152:ASP:HB2	1:L:153:PRO:CD	2.46	0.45
1:J:175:PHE:C	1:J:175:PHE:CD1	2.90	0.45
2:X:189:THR:HG23	2:X:190:ASP:N	2.31	0.45
2:1:93:MET:N	2:1:94:PRO:CD	2.79	0.45
2:W:147:THR:OG1	2:W:150:GLU:HG3	2.16	0.45
2:2:76:ILE:O	2:2:79:VAL:HG12	2.17	0.45
1:M:198:LYS:HG2	1:M:202:GLU:HG2	1.98	0.45
2:U:130:GLY:O	2:U:134:VAL:HG12	2.17	0.45
2:Q:20:VAL:HG13	2:Q:28:HIS:HB2	1.97	0.45
1:M:180:TYR:HB3	1:N:57:ARG:HH22	1.80	0.45
1:G:51:ASP:HB3	1:G:53:LYS:NZ	2.31	0.45
1:D:18:ASP:OD2	1:D:20:ARG:HD3	2.15	0.45
2:Q:141:GLN:HE21	2:X:141:GLN:NE2	2.14	0.45
2:B:27:MET:HG2	2:B:27:MET:O	2.17	0.45
2:2:66:TYR:CZ	2:2:70:ARG:HD2	2.52	0.45
2:Z:59:MET:SD	2:Z:83:LEU:HD13	2.57	0.45
1:K:52:LYS:CE	1:K:64:ILE:HG23	2.46	0.45
2:U:37:ILE:HD11	2:U:59:MET:CG	2.46	0.45
1:O:198:LYS:O	1:O:199:SER:C	2.55	0.45
1:C:198:LYS:O	1:C:199:SER:C	2.55	0.45
2:T:6:ILE:O	2:T:6:ILE:HG23	2.17	0.45
2:Q:189:THR:HG23	2:Q:190:ASP:H	1.81	0.45
2:X:103:GLY:HA2	2:X:178:ILE:HD13	1.99	0.45
2:Y:190:ASP:HA	2:Y:193:GLU:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:141:GLN:NE2	2:2:141:GLN:HE21	2.14	0.45
1:E:148:LEU:O	1:E:159:GLU:HG3	2.17	0.45
1:I:171:ALA:HB3	1:I:200:SER:OG	2.17	0.45
1:C:69:LEU:HD23	1:C:75:ALA:HB2	1.98	0.45
2:U:97:VAL:HG22	2:U:98:GLN:H	1.81	0.45
1:M:228:GLU:O	1:M:231:LYS:HB3	2.17	0.45
1:J:107:VAL:HG11	2:X:66:TYR:HH	1.80	0.45
1:A:24:VAL:O	1:A:28:ARG:HG3	2.17	0.45
1:E:21:LEU:O	1:E:24:VAL:HG12	2.16	0.45
1:M:175:PHE:C	1:M:175:PHE:HD1	2.20	0.45
1:C:175:PHE:C	1:C:175:PHE:HD1	2.20	0.45
2:U:93:MET:N	2:U:94:PRO:CD	2.78	0.45
1:M:99:GLU:HG3	1:M:103:TYR:HD2	1.81	0.45
1:N:136:LEU:HD12	1:N:151:CYS:HB3	1.97	0.45
2:1:97:VAL:HG22	2:1:98:GLN:H	1.81	0.45
1:H:123:TYR:N	1:H:123:TYR:CD1	2.85	0.45
2:P:173:ILE:C	2:P:173:ILE:HD13	2.37	0.45
2:X:45:ILE:CG1	2:X:52:ALA:HB1	2.34	0.45
1:I:198:LYS:O	1:I:199:SER:C	2.55	0.45
1:A:49:ILE:HD11	1:A:210:PRO:CB	2.47	0.45
2:S:19:ARG:NE	2:S:26:ILE:HG13	2.32	0.45
1:F:149:PHE:CE2	1:F:159:GLU:HB2	2.52	0.45
1:C:134:VAL:CG2	1:C:135:SER:N	2.79	0.45
1:D:228:GLU:O	1:D:231:LYS:HB3	2.17	0.45
2:2:143:SER:O	2:2:146:MET:HG3	2.17	0.45
2:1:55:LEU:HD12	2:1:55:LEU:HA	1.85	0.45
1:D:123:TYR:N	1:D:123:TYR:CD1	2.85	0.45
1:O:121:GLN:O	1:O:124:THR:HB	2.17	0.45
2:2:59:MET:CE	2:2:82:LEU:HD23	2.46	0.45
1:H:22:PHE:O	1:H:25:GLU:HB2	2.17	0.45
1:H:61:GLN:CD	1:H:62:ASN:H	2.20	0.45
1:E:176:LEU:O	1:E:178:ARG:N	2.49	0.45
1:E:186:GLU:O	1:E:190:VAL:HG12	2.17	0.45
2:Q:105:ASP:OD1	2:Q:106:THR:N	2.50	0.45
2:Z:2:THR:HG22	2:Z:169:SER:OG	2.16	0.45
2:P:146:MET:HA	2:P:150:GLU:OE1	2.17	0.45
2:2:22:MET:O	2:2:23:GLU:HB2	2.16	0.45
2:B:180:ARG:HA	2:B:180:ARG:HD2	1.79	0.45
2:Z:111:PHE:CD2	2:Z:121:GLU:HB2	2.53	0.44
2:2:103:GLY:HA2	2:2:178:ILE:CD1	2.47	0.44
1:I:175:PHE:CD2	1:I:196:ALA:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:LYS:HG2	1:I:180:TYR:HE2	1.82	0.44
2:P:6:ILE:HD11	2:P:142:TYR:CD1	2.52	0.44
2:S:6:ILE:HD11	2:S:142:TYR:CD1	2.52	0.44
1:N:180:TYR:HA	1:N:192:LEU:HD21	1.99	0.44
2:X:173:ILE:C	2:X:173:ILE:HD13	2.37	0.44
1:K:24:VAL:O	1:K:28:ARG:HG3	2.17	0.44
2:P:138:LEU:HD12	2:P:154:LEU:HD11	1.98	0.44
1:L:198:LYS:O	1:L:199:SER:C	2.56	0.44
1:C:42:PHE:HD2	1:C:47:LEU:HD23	1.83	0.44
1:M:52:LYS:HZ1	1:M:62:ASN:HA	1.81	0.44
1:M:82:VAL:HG13	1:M:83:ALA:N	2.32	0.44
1:E:15:PHE:HD2	1:F:23:GLN:NE2	2.15	0.44
1:N:49:ILE:HD12	1:N:211:GLU:O	2.17	0.44
2:U:97:VAL:HG22	2:U:98:GLN:N	2.32	0.44
2:Z:93:MET:N	2:Z:94:PRO:CD	2.79	0.44
2:Q:49:VAL:HG23	2:Q:50:GLY:H	1.82	0.44
2:U:160:SER:HA	2:U:163:LYS:HD3	2.00	0.44
1:I:170:ASP:O	1:I:173:VAL:HG12	2.16	0.44
1:L:82:VAL:HG13	1:L:83:ALA:N	2.33	0.44
2:S:110:VAL:O	2:S:110:VAL:HG13	2.16	0.44
1:M:198:LYS:O	1:M:199:SER:C	2.56	0.44
1:N:42:PHE:HB2	1:N:184:LEU:O	2.17	0.44
1:M:159:GLU:O	1:N:60:GLU:HB2	2.17	0.44
2:S:74:MET:HG2	2:S:78:ALA:HB3	2.00	0.44
2:W:75:PRO:O	2:W:78:ALA:HB3	2.18	0.44
2:B:22:MET:O	2:B:23:GLU:HB2	2.17	0.44
1:L:212:ILE:HG23	1:L:224:TYR:HB2	1.99	0.44
1:C:44:ASN:HD22	1:C:44:ASN:HA	1.56	0.44
1:J:58:LEU:N	1:J:58:LEU:CD1	2.81	0.44
1:N:143:GLN:HE21	1:N:143:GLN:HA	1.82	0.44
2:2:90:VAL:O	2:2:90:VAL:HG22	2.17	0.44
2:U:37:ILE:HD11	2:U:59:MET:CB	2.43	0.44
1:G:187:LYS:O	1:G:190:VAL:HG13	2.17	0.44
1:M:125:GLN:HB3	1:N:130:ARG:NH2	2.32	0.44
1:D:49:ILE:HD12	1:D:211:GLU:O	2.17	0.44
1:G:149:PHE:CE2	1:G:159:GLU:HB2	2.53	0.44
1:I:70:ILE:HD12	1:I:74:VAL:HG22	1.99	0.44
2:Z:20:VAL:HG22	2:Z:28:HIS:HB2	1.99	0.44
2:S:17:GLU:HA	2:S:173:ILE:HA	1.99	0.44
2:S:93:MET:N	2:S:94:PRO:CD	2.80	0.44
1:M:170:ASP:O	1:M:173:VAL:HG12	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:OD2	1:A:20:ARG:HD3	2.17	0.44
1:K:148:LEU:O	1:K:159:GLU:HG3	2.17	0.44
2:P:2:THR:HG22	2:P:169:SER:OG	2.17	0.44
2:Y:133:PHE:CE2	2:Y:165:ARG:HB3	2.52	0.44
1:E:174:SER:O	1:E:177:GLU:HB3	2.18	0.44
2:B:29:LYS:NZ	2:Y:164:GLN:NE2	2.64	0.44
1:J:180:TYR:HA	1:J:192:LEU:HD21	1.99	0.44
1:H:44:ASN:HA	1:H:44:ASN:HD22	1.60	0.44
1:L:107:VAL:HG11	2:Z:66:TYR:HH	1.79	0.44
1:L:62:ASN:O	1:L:65:GLU:HG2	2.18	0.44
2:Z:26:ILE:C	2:Z:26:ILE:HD13	2.38	0.44
1:L:83:ALA:O	1:L:87:VAL:HG12	2.18	0.44
1:A:81:LEU:HD23	1:A:133:GLY:HA3	2.00	0.44
1:K:180:TYR:HA	1:K:192:LEU:HD21	2.00	0.44
1:O:123:TYR:CE2	1:O:129:VAL:HG21	2.53	0.44
1:G:28:ARG:O	1:G:31:VAL:HG13	2.18	0.44
1:N:165:ILE:HD12	1:N:169:LYS:HD2	2.00	0.44
1:G:180:TYR:HA	1:G:192:LEU:HD21	2.00	0.44
1:K:135:SER:OG	1:K:153:PRO:HD3	2.17	0.44
1:E:123:TYR:CD1	1:E:123:TYR:N	2.84	0.44
1:A:78:THR:CG2	1:A:85:ALA:HB1	2.45	0.44
2:U:7:THR:HB	2:U:123:ILE:O	2.18	0.44
1:G:52:LYS:HA	1:G:66:LYS:NZ	2.32	0.44
1:N:61:GLN:CD	1:N:62:ASN:H	2.20	0.44
2:B:141:GLN:HE21	2:Z:141:GLN:NE2	2.15	0.44
2:Y:161:ALA:O	2:Y:164:GLN:HB2	2.17	0.44
1:A:32:LYS:O	1:A:167:SER:HA	2.18	0.44
1:G:15:PHE:HD2	1:H:23:GLN:HE22	1.65	0.44
2:Z:74:MET:HG2	2:Z:78:ALA:HB3	2.00	0.44
2:Z:55:LEU:HD21	2:Z:87:LEU:HD11	1.99	0.44
2:R:55:LEU:HD12	2:R:55:LEU:HA	1.79	0.44
2:B:25:PHE:CD1	2:B:25:PHE:C	2.90	0.44
1:C:20:ARG:CZ	1:C:22:PHE:CE1	3.01	0.44
1:I:202:GLU:HG3	1:I:205:GLU:O	2.18	0.44
2:B:165:ARG:CZ	2:Y:29:LYS:HE3	2.48	0.44
1:O:38:LEU:HB3	1:O:164:ALA:HB2	1.99	0.44
1:L:228:GLU:O	1:L:231:LYS:HB3	2.17	0.44
1:N:191:THR:O	1:N:194:ILE:HG22	2.18	0.44
2:U:8:LEU:HD12	2:U:8:LEU:O	2.17	0.44
1:M:107:VAL:HG13	1:M:108:ASN:N	2.32	0.44
2:Q:123:ILE:HG12	2:Q:124:TYR:CD1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:MET:HE3	2:B:82:LEU:HD23	1.98	0.44
2:S:189:THR:HG23	2:S:190:ASP:H	1.83	0.44
1:J:52:LYS:HA	1:J:66:LYS:NZ	2.33	0.44
2:R:76:ILE:O	2:R:79:VAL:HG12	2.17	0.44
2:B:133:PHE:HE1	2:Z:132:PRO:HA	1.83	0.44
1:J:83:ALA:O	1:J:87:VAL:HG12	2.18	0.44
1:D:136:LEU:HD12	1:D:151:CYS:HB3	1.99	0.44
1:D:184:LEU:HD23	1:D:189:ALA:HA	1.99	0.44
2:X:101:VAL:O	2:X:101:VAL:HG13	2.18	0.44
2:Y:59:MET:HE1	2:Y:82:LEU:HD23	2.00	0.43
1:H:175:PHE:HD1	1:H:175:PHE:C	2.22	0.43
1:F:225:ASP:OD1	1:F:228:GLU:HB2	2.18	0.43
1:O:145:GLY:O	1:O:147:ARG:HG3	2.18	0.43
2:S:180:ARG:HA	2:S:180:ARG:HD2	1.71	0.43
2:S:8:LEU:O	2:S:8:LEU:HD12	2.17	0.43
2:P:25:PHE:C	2:P:25:PHE:CD1	2.91	0.43
2:Z:7:THR:HB	2:Z:123:ILE:O	2.19	0.43
1:F:52:LYS:HZ1	1:F:62:ASN:HA	1.83	0.43
1:O:98:GLN:O	1:O:102:THR:CG2	2.66	0.43
1:D:130:ARG:HA	1:D:131:PRO:HD3	1.86	0.43
2:T:141:GLN:NE2	2:2:141:GLN:NE2	2.67	0.43
1:E:137:ILE:HG22	1:E:150:ASP:HB2	2.00	0.43
1:L:16:SER:HB3	1:L:22:PHE:CE2	2.52	0.43
2:W:6:ILE:HD11	2:W:142:TYR:CD1	2.53	0.43
1:A:16:SER:HB3	1:A:22:PHE:CE2	2.53	0.43
1:F:107:VAL:HG13	1:F:108:ASN:N	2.33	0.43
1:F:107:VAL:HG13	1:F:108:ASN:H	1.82	0.43
2:W:7:THR:HB	2:W:123:ILE:O	2.18	0.43
2:U:123:ILE:CD1	2:U:123:ILE:H	2.24	0.43
2:S:20:VAL:CG1	2:S:28:HIS:HB2	2.45	0.43
1:L:52:LYS:HB3	1:L:209:ALA:O	2.18	0.43
1:H:52:LYS:CE	1:H:64:ILE:HG23	2.48	0.43
1:C:52:LYS:HB3	1:C:209:ALA:O	2.18	0.43
1:C:202:GLU:HG3	1:C:205:GLU:O	2.19	0.43
1:J:147:ARG:HB3	1:J:149:PHE:HE1	1.83	0.43
2:V:129:SER:HG	2:V:166:ASP:CG	2.20	0.43
1:M:38:LEU:HA	1:M:164:ALA:HA	1.98	0.43
2:Z:179:THR:HG23	2:Z:182:ASP:H	1.83	0.43
1:K:145:GLY:O	1:K:147:ARG:HG3	2.19	0.43
1:C:32:LYS:O	1:C:167:SER:HA	2.18	0.43
1:G:97:GLN:OE1	1:G:97:GLN:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ILE:HG12	2:B:203:LEU:N	2.34	0.43
1:A:109:ILE:CG2	1:A:147:ARG:HD3	2.48	0.43
1:O:175:PHE:HD1	1:O:175:PHE:C	2.21	0.43
1:L:159:GLU:HG2	1:M:60:GLU:HG3	2.00	0.43
2:T:93:MET:N	2:T:94:PRO:CD	2.81	0.43
1:D:205:GLU:HG3	1:D:206:GLU:N	2.34	0.43
1:E:158:ASN:HB2	1:E:160:TYR:CE1	2.53	0.43
1:I:136:LEU:HD12	1:I:151:CYS:HB3	1.99	0.43
2:S:76:ILE:HA	2:S:79:VAL:HG12	2.00	0.43
1:G:107:VAL:HG13	1:G:108:ASN:N	2.34	0.43
1:J:14:VAL:O	1:J:21:LEU:HD12	2.18	0.43
2:R:34:LEU:HD21	2:R:176:ALA:HB3	2.00	0.43
1:G:175:PHE:C	1:G:175:PHE:HD1	2.21	0.43
2:S:178:ILE:HB	2:S:184:TYR:HA	2.01	0.43
2:P:141:GLN:NE2	2:Y:141:GLN:NE2	2.66	0.43
1:G:113:VAL:HA	1:G:116:VAL:HG12	2.01	0.43
2:W:187:LEU:HA	2:W:188:PRO:HD3	1.67	0.43
2:W:2:THR:HG22	2:W:169:SER:OG	2.18	0.43
2:B:90:VAL:HG22	2:B:90:VAL:O	2.18	0.43
2:Y:180:ARG:HA	2:Y:180:ARG:HD2	1.75	0.43
2:P:124:TYR:HD2	2:P:138:LEU:HD23	1.78	0.43
1:A:52:LYS:HB3	1:A:209:ALA:O	2.19	0.43
2:X:3:THR:HB	2:X:16:THR:HG22	2.01	0.43
2:2:2:THR:HG22	2:2:169:SER:CB	2.49	0.43
1:C:61:GLN:CD	1:C:62:ASN:H	2.21	0.43
2:S:3:THR:OG1	2:S:127:THR:HG22	2.19	0.43
1:A:130:ARG:NH1	1:A:131:PRO:O	2.51	0.43
2:B:17:GLU:HA	2:B:173:ILE:HA	2.01	0.43
2:Q:141:GLN:NE2	2:X:141:GLN:HE21	2.16	0.43
2:1:97:VAL:HG22	2:1:98:GLN:N	2.34	0.43
2:W:179:THR:HG23	2:W:182:ASP:H	1.84	0.43
2:Z:131:SER:O	2:Z:134:VAL:HG13	2.19	0.43
2:X:90:VAL:O	2:X:90:VAL:HG22	2.19	0.43
1:O:24:VAL:O	1:O:28:ARG:HG3	2.18	0.43
2:2:59:MET:SD	2:2:83:LEU:HD13	2.58	0.43
2:T:138:LEU:HD12	2:T:138:LEU:HA	1.86	0.43
2:Z:43:MET:HE1	2:Z:56:VAL:HA	2.01	0.43
1:N:25:GLU:O	1:N:28:ARG:HB2	2.18	0.43
1:L:175:PHE:C	1:L:175:PHE:HD1	2.21	0.43
1:F:160:TYR:CD2	1:F:163:THR:HB	2.53	0.43
1:G:146:PRO:O	1:G:147:ARG:HG2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:149:ASP:O	2:Y:152:VAL:HG12	2.18	0.43
1:M:26:TYR:O	1:M:29:GLU:HB2	2.18	0.43
2:T:87:LEU:HD23	2:T:114:ASP:O	2.19	0.43
2:R:6:ILE:HD11	2:R:142:TYR:CD1	2.53	0.43
2:B:15:ALA:HB2	2:B:175:VAL:HB	1.99	0.43
1:J:208:LYS:HA	1:J:208:LYS:HD2	1.82	0.43
1:A:61:GLN:CD	1:A:62:ASN:H	2.22	0.43
2:U:111:PHE:CE2	2:U:121:GLU:HB2	2.53	0.43
1:H:198:LYS:O	1:H:199:SER:C	2.56	0.43
1:D:124:THR:HG22	1:E:130:ARG:HH21	1.84	0.43
2:V:19:ARG:NE	2:V:26:ILE:HG13	2.34	0.43
1:J:109:ILE:HG22	1:J:147:ARG:HD3	2.01	0.43
2:B:28:HIS:CD2	2:P:120:VAL:HG11	2.54	0.43
1:K:142:ASP:OD2	1:K:147:ARG:HD2	2.18	0.43
2:2:187:LEU:HA	2:2:188:PRO:HD3	1.81	0.43
2:B:131:SER:O	2:B:134:VAL:HG13	2.19	0.43
1:C:71:ASP:O	1:C:73:TYR:N	2.51	0.43
1:O:148:LEU:O	1:O:159:GLU:HG3	2.19	0.43
2:Y:15:ALA:HB2	2:Y:175:VAL:HB	2.01	0.43
2:V:76:ILE:HA	2:V:79:VAL:HG12	2.01	0.43
2:W:34:LEU:HD21	2:W:176:ALA:HB3	1.99	0.43
2:V:93:MET:N	2:V:94:PRO:CD	2.82	0.43
1:E:83:ALA:O	1:E:87:VAL:HG12	2.19	0.43
1:N:107:VAL:HG11	2:2:66:TYR:HH	1.75	0.43
1:G:125:GLN:HB3	1:H:130:ARG:NH2	2.34	0.43
2:S:43:MET:HE1	2:S:56:VAL:HA	2.01	0.43
1:F:198:LYS:HG2	1:F:202:GLU:HG2	2.01	0.43
1:C:21:LEU:O	1:C:25:GLU:HG2	2.19	0.43
2:V:36:GLN:HB2	2:V:184:TYR:CE1	2.53	0.43
1:O:214:SER:HG	1:O:224:TYR:HE1	1.67	0.43
1:F:82:VAL:HG13	1:F:83:ALA:H	1.84	0.43
2:1:66:TYR:C	2:1:66:TYR:CD1	2.92	0.42
1:L:198:LYS:HG3	1:L:207:LEU:HD22	2.01	0.42
2:Z:176:ALA:HB2	2:Z:186:GLN:HG3	2.00	0.42
1:F:130:ARG:HA	1:F:131:PRO:HD3	1.91	0.42
1:K:198:LYS:O	1:K:199:SER:C	2.57	0.42
1:C:62:ASN:O	1:C:65:GLU:HG2	2.18	0.42
2:B:19:ARG:HE	2:B:26:ILE:HG13	1.84	0.42
2:2:152:VAL:O	2:2:156:ILE:HG13	2.19	0.42
1:C:165:ILE:HD12	1:C:169:LYS:HD2	2.01	0.42
2:U:141:GLN:HE21	2:1:141:GLN:HE21	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:PHE:HB2	1:D:184:LEU:O	2.20	0.42
1:F:35:SER:O	1:F:166:GLY:HA3	2.19	0.42
2:V:22:MET:O	2:V:23:GLU:HB2	2.18	0.42
2:2:173:ILE:HD13	2:2:173:ILE:C	2.39	0.42
1:O:24:VAL:O	1:O:27:ALA:HB3	2.19	0.42
2:U:141:GLN:NE2	2:1:141:GLN:NE2	2.66	0.42
2:P:187:LEU:HA	2:P:188:PRO:HD3	1.83	0.42
1:A:58:LEU:CD1	1:A:58:LEU:N	2.83	0.42
1:I:123:TYR:N	1:I:123:TYR:CD1	2.88	0.42
1:L:174:SER:O	1:L:175:PHE:C	2.57	0.42
2:T:109:HIS:HB3	2:T:111:PHE:HE1	1.84	0.42
1:F:159:GLU:O	1:G:60:GLU:HB2	2.19	0.42
2:Z:20:VAL:HG13	2:Z:28:HIS:HB2	2.00	0.42
2:B:103:GLY:HA2	2:B:178:ILE:HD13	2.01	0.42
1:I:149:PHE:CE2	1:I:159:GLU:HB2	2.54	0.42
1:J:15:PHE:HD2	1:K:23:GLN:HE22	1.67	0.42
2:W:174:ASP:HA	2:W:192:ILE:HD13	2.00	0.42
1:M:40:MET:HA	1:M:162:ALA:HA	2.01	0.42
2:S:163:LYS:CE	2:S:203:LEU:HD23	2.50	0.42
1:A:187:LYS:O	1:A:190:VAL:HG13	2.19	0.42
1:K:52:LYS:HA	1:K:66:LYS:HZ2	1.84	0.42
1:G:198:LYS:O	1:G:199:SER:C	2.57	0.42
2:1:34:LEU:HD21	2:1:176:ALA:HB3	2.00	0.42
1:I:21:LEU:O	1:I:25:GLU:HG2	2.18	0.42
2:P:45:ILE:CD1	2:P:52:ALA:HB1	2.49	0.42
2:Y:124:TYR:HD1	2:Y:138:LEU:HD23	1.83	0.42
2:S:15:ALA:HB3	2:S:155:VAL:CG1	2.49	0.42
2:R:157:ARG:O	2:R:160:SER:HB2	2.19	0.42
1:L:136:LEU:HD13	1:L:138:PHE:CE1	2.54	0.42
1:F:49:ILE:HD12	1:F:50:SER:N	2.34	0.42
2:S:165:ARG:HA	2:2:26:ILE:HG23	2.00	0.42
1:D:146:PRO:O	1:D:147:ARG:HG2	2.19	0.42
1:O:88:LEU:HA	1:O:88:LEU:HD12	1.91	0.42
2:T:114:ASP:OD1	2:T:116:ALA:HB3	2.20	0.42
1:A:56:SER:OG	1:A:58:LEU:HB2	2.20	0.42
1:C:100:LYS:O	1:C:104:GLY:CA	2.68	0.42
1:L:160:TYR:CD2	1:L:163:THR:HB	2.55	0.42
2:V:2:THR:HG22	2:V:169:SER:OG	2.19	0.42
2:V:105:ASP:OD1	2:V:106:THR:N	2.53	0.42
1:M:152:ASP:HB2	1:M:153:PRO:CD	2.49	0.42
2:R:187:LEU:HA	2:R:188:PRO:HD3	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:72:VAL:HG22	2:V:73:ASN:N	2.34	0.42
2:2:137:VAL:HG21	2:2:158:ALA:HA	2.01	0.42
1:C:41:LYS:HE3	1:C:160:TYR:O	2.19	0.42
2:S:105:ASP:OD1	2:S:106:THR:N	2.52	0.42
2:R:1:THR:H3	2:R:129:SER:HB3	1.83	0.42
2:V:123:ILE:H	2:V:123:ILE:CD1	2.29	0.42
2:Z:87:LEU:HD23	2:Z:114:ASP:O	2.20	0.42
2:T:137:VAL:HG21	2:T:158:ALA:HA	2.01	0.42
1:N:139:ALA:HB2	1:N:148:LEU:HD13	2.01	0.42
2:U:22:MET:O	2:U:23:GLU:HB2	2.20	0.42
1:D:160:TYR:CD2	1:D:163:THR:HB	2.54	0.42
1:H:51:ASP:HB3	1:H:53:LYS:NZ	2.35	0.42
1:M:70:ILE:HB	1:M:74:VAL:HG13	2.01	0.42
1:O:43:ALA:HB2	1:O:185:PRO:HA	2.00	0.42
1:O:143:GLN:HE21	1:O:143:GLN:HA	1.84	0.42
1:C:97:GLN:HA	1:C:97:GLN:OE1	2.19	0.42
2:1:66:TYR:CE1	2:1:70:ARG:HD2	2.54	0.42
1:C:108:ASN:CB	2:Q:70:ARG:HG2	2.48	0.42
1:J:52:LYS:HZ3	1:J:62:ASN:HA	1.83	0.42
1:C:52:LYS:HA	1:C:66:LYS:NZ	2.34	0.42
1:N:134:VAL:CG2	1:N:135:SER:N	2.83	0.42
1:O:42:PHE:HB2	1:O:184:LEU:O	2.19	0.42
1:H:82:VAL:HG13	1:H:83:ALA:N	2.34	0.42
2:Y:19:ARG:NE	2:Y:26:ILE:HG13	2.35	0.42
2:B:165:ARG:C	2:Y:26:ILE:HG22	2.40	0.42
1:I:161:LYS:HG2	1:I:180:TYR:CE2	2.55	0.42
1:L:180:TYR:HB3	1:M:57:ARG:NH2	2.35	0.42
2:V:129:SER:OG	2:V:168:ALA:HB3	2.18	0.42
1:D:162:ALA:O	1:D:163:THR:HB	2.19	0.42
2:1:44:THR:OG1	2:1:100:LEU:HB3	2.19	0.42
1:C:191:THR:O	1:C:194:ILE:HG22	2.19	0.42
1:O:40:MET:HA	1:O:162:ALA:HA	2.02	0.42
1:N:71:ASP:O	1:N:73:TYR:N	2.53	0.42
1:K:107:VAL:HG11	2:Y:66:TYR:HH	1.77	0.42
1:G:125:GLN:O	1:H:129:VAL:HG23	2.20	0.42
1:D:61:GLN:OE1	1:D:62:ASN:HB3	2.20	0.42
2:S:190:ASP:HA	2:S:193:GLU:HG2	2.02	0.42
2:1:176:ALA:HA	2:1:186:GLN:HA	2.02	0.42
2:S:15:ALA:HB3	2:S:155:VAL:HG11	2.00	0.42
2:T:184:TYR:C	2:T:184:TYR:CD1	2.93	0.42
2:1:173:ILE:O	2:1:192:ILE:HG21	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ARG:HB3	1:E:149:PHE:HE1	1.83	0.42
1:G:79:SER:OG	1:G:166:GLY:HA2	2.20	0.42
1:L:15:PHE:HB2	1:M:23:GLN:HE22	1.84	0.42
2:X:74:MET:HA	2:X:75:PRO:HD3	1.88	0.42
1:E:31:VAL:HA	1:E:80:GLY:HA2	2.01	0.42
1:L:215:ILE:HD11	1:L:219:ASN:O	2.19	0.42
2:V:163:LYS:CE	2:V:203:LEU:HD23	2.49	0.42
1:I:26:TYR:N	1:I:26:TYR:CD1	2.88	0.42
1:M:206:GLU:HG2	1:M:208:LYS:H	1.84	0.42
1:M:123:TYR:CD1	1:M:123:TYR:N	2.87	0.42
2:V:90:VAL:O	2:V:90:VAL:HG22	2.20	0.42
1:I:107:VAL:HG13	1:I:108:ASN:H	1.84	0.42
2:1:34:LEU:HD21	2:1:176:ALA:CB	2.50	0.42
1:E:130:ARG:HG2	1:E:130:ARG:NH1	2.34	0.42
2:S:165:ARG:C	2:2:26:ILE:HG22	2.40	0.42
2:S:55:LEU:HD12	2:S:55:LEU:HA	1.67	0.42
2:Y:20:VAL:HG22	2:Y:28:HIS:HB2	2.02	0.42
2:X:175:VAL:CG2	2:X:176:ALA:N	2.83	0.42
1:H:88:LEU:HD13	1:H:132:TYR:CE2	2.55	0.42
1:N:82:VAL:HG13	1:N:83:ALA:H	1.84	0.42
2:1:35:PHE:CE2	2:1:45:ILE:HD12	2.55	0.42
1:G:215:ILE:HD11	1:G:219:ASN:O	2.19	0.42
1:G:191:THR:HA	1:G:194:ILE:HG22	2.02	0.42
1:K:44:ASN:HA	1:K:44:ASN:HD22	1.58	0.42
2:2:66:TYR:C	2:2:66:TYR:CD1	2.93	0.42
2:P:83:LEU:HA	2:P:83:LEU:HD12	1.88	0.42
2:W:83:LEU:HD12	2:W:83:LEU:HA	1.79	0.42
1:K:144:ILE:HD12	1:K:147:ARG:NH1	2.35	0.42
1:J:98:GLN:O	1:J:101:VAL:HG12	2.20	0.42
1:I:88:LEU:HD21	1:I:120:MET:SD	2.59	0.42
2:T:180:ARG:HA	2:T:180:ARG:HD2	1.77	0.42
2:1:27:MET:HG2	2:1:27:MET:O	2.20	0.42
1:G:22:PHE:O	1:G:25:GLU:HB2	2.20	0.42
1:D:64:ILE:O	1:D:64:ILE:HG23	2.20	0.42
1:J:85:ALA:O	1:J:89:VAL:HG23	2.19	0.42
1:F:198:LYS:O	1:F:199:SER:C	2.58	0.42
1:F:58:LEU:CD1	1:F:58:LEU:N	2.83	0.42
1:G:70:ILE:HD11	1:G:76:ALA:HB2	2.01	0.42
1:O:48:LEU:CD1	1:O:139:ALA:HB3	2.49	0.42
2:2:19:ARG:HE	2:2:26:ILE:HG13	1.85	0.42
2:Q:109:HIS:HB3	2:Q:111:PHE:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:VAL:CG2	1:K:135:SER:N	2.82	0.42
1:A:54:VAL:HG22	1:A:55:ARG:N	2.34	0.42
2:1:17:GLU:O	2:1:33:LYS:HD2	2.20	0.42
1:H:208:LYS:HD2	1:H:208:LYS:HA	1.90	0.42
1:O:58:LEU:CD1	1:O:58:LEU:N	2.82	0.42
2:S:25:PHE:CD1	2:S:25:PHE:C	2.91	0.42
1:G:59:ILE:HD13	1:G:59:ILE:HA	1.92	0.42
1:M:107:VAL:HG13	1:M:108:ASN:H	1.85	0.41
2:T:66:TYR:CZ	2:T:70:ARG:HD2	2.54	0.41
1:G:62:ASN:O	1:G:65:GLU:HG2	2.20	0.41
1:C:121:GLN:HG3	1:D:83:ALA:HB1	2.02	0.41
2:Q:34:LEU:HD21	2:Q:176:ALA:CB	2.50	0.41
2:B:3:THR:OG1	2:B:127:THR:HG22	2.19	0.41
1:G:41:LYS:HE3	1:G:160:TYR:O	2.20	0.41
1:J:58:LEU:N	1:J:58:LEU:HD12	2.35	0.41
1:D:42:PHE:O	1:D:43:ALA:C	2.59	0.41
1:D:170:ASP:O	1:D:173:VAL:HG12	2.20	0.41
2:1:163:LYS:CE	2:1:203:LEU:HD23	2.50	0.41
2:U:138:LEU:HA	2:U:138:LEU:HD12	1.71	0.41
1:G:16:SER:C	1:G:18:ASP:H	2.24	0.41
1:L:94:ILE:CG1	1:L:95:SER:N	2.83	0.41
1:E:102:THR:O	2:S:81:THR:HG22	2.20	0.41
1:H:175:PHE:CD2	1:H:196:ALA:HA	2.56	0.41
2:Q:141:GLN:HE21	2:X:141:GLN:HE21	1.68	0.41
1:K:156:THR:HG23	1:L:82:VAL:HG11	2.02	0.41
1:F:174:SER:O	1:F:177:GLU:HB3	2.20	0.41
2:W:126:SER:HB3	2:W:135:TYR:CE2	2.55	0.41
2:V:124:TYR:CE2	2:V:138:LEU:HB3	2.54	0.41
1:O:130:ARG:HG2	1:O:130:ARG:HH11	1.84	0.41
1:F:160:TYR:C	1:G:60:GLU:HG2	2.40	0.41
1:K:175:PHE:C	1:K:175:PHE:HD1	2.24	0.41
2:W:44:THR:OG1	2:W:100:LEU:HB3	2.19	0.41
2:P:1:THR:H3	2:P:129:SER:HB3	1.85	0.41
2:T:163:LYS:CE	2:T:203:LEU:HD23	2.50	0.41
2:X:109:HIS:HB3	2:X:111:PHE:HE1	1.84	0.41
1:G:88:LEU:HD13	1:G:132:TYR:CD2	2.54	0.41
1:E:97:GLN:OE1	1:E:97:GLN:HA	2.19	0.41
1:O:25:GLU:O	1:O:28:ARG:HB2	2.21	0.41
2:X:7:THR:HB	2:X:123:ILE:O	2.21	0.41
2:U:59:MET:SD	2:U:83:LEU:HD13	2.60	0.41
1:G:52:LYS:CE	1:G:64:ILE:HG23	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:THR:HG22	1:J:130:ARG:NH2	2.35	0.41
1:N:28:ARG:O	1:N:31:VAL:HG22	2.20	0.41
1:G:94:ILE:CG1	1:G:95:SER:N	2.82	0.41
1:G:156:THR:CG2	1:H:82:VAL:HG11	2.50	0.41
2:W:193:GLU:HA	2:W:196:ILE:HD12	2.02	0.41
2:P:191:GLN:O	2:P:194:SER:HB3	2.20	0.41
2:S:143:SER:O	2:S:146:MET:HG3	2.20	0.41
1:E:26:TYR:O	1:E:29:GLU:HB2	2.20	0.41
2:V:179:THR:HG23	2:V:182:ASP:H	1.86	0.41
1:D:71:ASP:OD1	1:D:72:ASP:N	2.53	0.41
2:Z:189:THR:HG23	2:Z:190:ASP:N	2.35	0.41
2:P:180:ARG:HA	2:P:180:ARG:HD2	1.81	0.41
1:L:123:TYR:CD1	1:L:123:TYR:N	2.88	0.41
1:L:52:LYS:HZ1	1:L:62:ASN:HA	1.85	0.41
1:L:42:PHE:CD1	1:L:43:ALA:N	2.89	0.41
2:T:111:PHE:CE2	2:T:121:GLU:HB2	2.55	0.41
1:K:35:SER:O	1:K:166:GLY:HA3	2.20	0.41
2:P:175:VAL:HG22	2:P:176:ALA:N	2.35	0.41
2:P:147:THR:OG1	2:P:150:GLU:HG3	2.21	0.41
1:G:157:ILE:HG12	1:G:158:ASN:N	2.34	0.41
1:M:15:PHE:HD2	1:N:23:GLN:HE22	1.66	0.41
1:M:191:THR:O	1:M:194:ILE:HG22	2.21	0.41
1:H:101:VAL:HG23	2:U:57:ARG:HB3	2.03	0.41
2:B:18:ARG:HE	2:B:30:ASN:HD22	1.67	0.41
1:O:16:SER:HB3	1:O:22:PHE:CE2	2.56	0.41
1:E:228:GLU:O	1:E:231:LYS:HB3	2.20	0.41
2:Z:59:MET:HE1	2:Z:82:LEU:HD23	2.03	0.41
2:1:138:LEU:HA	2:1:138:LEU:HD12	1.83	0.41
2:W:56:VAL:CG1	2:W:57:ARG:N	2.83	0.41
2:Y:59:MET:CE	2:Y:79:VAL:HG23	2.48	0.41
2:P:55:LEU:HD12	2:P:55:LEU:HA	1.90	0.41
2:S:87:LEU:HD23	2:S:114:ASP:O	2.20	0.41
2:V:37:ILE:HD11	2:V:59:MET:CG	2.50	0.41
1:L:16:SER:HB3	1:L:22:PHE:CD2	2.56	0.41
1:I:45:GLY:HA3	1:I:216:THR:HA	2.02	0.41
1:H:144:ILE:HD12	1:H:147:ARG:NH1	2.36	0.41
2:T:17:GLU:O	2:T:33:LYS:HD2	2.20	0.41
1:O:171:ALA:HB3	1:O:200:SER:OG	2.20	0.41
2:2:45:ILE:CG1	2:2:52:ALA:HB1	2.45	0.41
1:A:198:LYS:O	1:A:199:SER:C	2.59	0.41
1:N:130:ARG:HA	1:N:131:PRO:HD3	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:HG23	2:Y:165:ARG:HA	2.01	0.41
1:H:113:VAL:HG23	1:H:138:PHE:CE2	2.56	0.41
1:C:38:LEU:HG	1:C:49:ILE:HG23	2.02	0.41
1:D:38:LEU:HB3	1:D:164:ALA:CB	2.51	0.41
2:S:97:VAL:HG22	2:S:98:GLN:N	2.36	0.41
1:F:18:ASP:OD2	1:F:20:ARG:HD3	2.21	0.41
1:K:41:LYS:HE3	1:K:160:TYR:O	2.20	0.41
2:U:158:ALA:O	2:U:161:ALA:HB3	2.21	0.41
1:M:45:GLY:HA3	1:M:216:THR:HA	2.01	0.41
1:J:152:ASP:HB2	1:J:153:PRO:CD	2.50	0.41
1:G:159:GLU:HG2	1:H:60:GLU:HG3	2.03	0.41
1:J:175:PHE:CD2	1:J:196:ALA:HA	2.56	0.41
2:W:105:ASP:OD1	2:W:106:THR:N	2.54	0.41
2:2:175:VAL:CG2	2:2:176:ALA:N	2.83	0.41
2:1:180:ARG:HD2	2:1:180:ARG:HA	1.85	0.41
2:W:22:MET:O	2:W:23:GLU:HB2	2.21	0.41
1:H:107:VAL:H	1:H:107:VAL:HG12	1.60	0.41
2:P:59:MET:SD	2:P:83:LEU:HD13	2.61	0.41
1:D:134:VAL:CG2	1:D:135:SER:N	2.83	0.41
1:L:38:LEU:HB3	1:L:164:ALA:HB2	2.02	0.41
1:K:130:ARG:HG2	1:K:130:ARG:NH1	2.36	0.41
2:X:20:VAL:HG22	2:X:20:VAL:O	2.20	0.41
1:D:89:VAL:O	1:D:92:ALA:HB3	2.20	0.41
1:L:137:ILE:HG22	1:L:150:ASP:CB	2.50	0.41
2:1:26:ILE:HD13	2:1:26:ILE:C	2.41	0.41
2:V:74:MET:HG2	2:V:78:ALA:HB3	2.02	0.41
1:N:175:PHE:HD1	1:N:175:PHE:C	2.23	0.41
1:F:136:LEU:HD13	1:F:138:PHE:CE2	2.56	0.41
1:I:26:TYR:O	1:I:29:GLU:HB2	2.21	0.41
2:R:22:MET:O	2:R:23:GLU:HB2	2.21	0.41
1:O:82:VAL:HG13	1:O:83:ALA:H	1.86	0.41
1:F:48:LEU:HD13	1:F:139:ALA:HB3	2.02	0.41
2:U:177:VAL:HG13	2:U:185:VAL:HG13	2.03	0.41
2:X:55:LEU:HD12	2:X:55:LEU:HA	1.90	0.41
2:Z:37:ILE:HD11	2:Z:59:MET:CG	2.51	0.41
2:P:56:VAL:CG1	2:P:57:ARG:N	2.84	0.41
2:V:138:LEU:HA	2:V:138:LEU:HD12	1.88	0.41
2:2:55:LEU:HA	2:2:55:LEU:HD12	1.74	0.41
2:V:6:ILE:HD11	2:V:142:TYR:CE1	2.56	0.41
1:K:98:GLN:O	1:K:102:THR:CG2	2.69	0.41
2:Y:3:THR:HB	2:Y:16:THR:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLN:O	1:E:102:THR:CG2	2.69	0.41
1:J:123:TYR:CD1	1:J:123:TYR:N	2.88	0.41
1:J:165:ILE:HG13	1:J:166:GLY:H	1.84	0.41
1:G:191:THR:O	1:G:194:ILE:HG22	2.20	0.41
1:I:127:GLY:O	1:I:129:VAL:N	2.53	0.41
1:E:207:LEU:HD23	1:E:233:LEU:HD12	2.02	0.41
1:H:188:GLU:O	1:H:191:THR:HB	2.20	0.41
1:O:69:LEU:HD23	1:O:69:LEU:HA	1.90	0.41
1:E:88:LEU:HA	1:E:88:LEU:HD12	1.84	0.41
2:S:66:TYR:CZ	2:S:70:ARG:HD2	2.56	0.40
1:K:52:LYS:HB3	1:K:209:ALA:O	2.21	0.40
2:W:103:GLY:HA2	2:W:178:ILE:HD13	2.03	0.40
1:E:42:PHE:HD1	1:E:43:ALA:N	2.19	0.40
1:M:121:GLN:CG	1:N:83:ALA:HB1	2.51	0.40
1:D:226:GLN:O	1:D:229:VAL:HG12	2.20	0.40
2:U:55:LEU:HD12	2:U:55:LEU:HA	1.96	0.40
2:Z:163:LYS:HE2	2:Z:203:LEU:HD23	2.01	0.40
1:E:116:VAL:HG11	1:E:138:PHE:CZ	2.56	0.40
1:M:214:SER:HG	1:M:224:TYR:HE1	1.69	0.40
1:J:107:VAL:HG12	1:J:107:VAL:H	1.67	0.40
1:M:130:ARG:HA	1:M:131:PRO:HD3	1.95	0.40
2:Z:175:VAL:CG2	2:Z:176:ALA:N	2.84	0.40
1:C:108:ASN:OD1	1:C:147:ARG:NH1	2.54	0.40
1:N:198:LYS:O	1:N:199:SER:C	2.59	0.40
1:K:187:LYS:O	1:K:190:VAL:HG13	2.21	0.40
1:G:38:LEU:HG	1:G:49:ILE:HG23	2.03	0.40
1:H:76:ALA:HA	1:H:137:ILE:O	2.21	0.40
1:J:142:ASP:OD2	1:J:147:ARG:HD2	2.21	0.40
2:B:81:THR:O	2:B:84:SER:HB3	2.21	0.40
2:Y:177:VAL:HG13	2:Y:185:VAL:HG13	2.02	0.40
2:Q:93:MET:N	2:Q:94:PRO:CD	2.84	0.40
1:N:86:ARG:HD3	1:N:86:ARG:HH11	1.76	0.40
2:X:25:PHE:C	2:X:25:PHE:CD1	2.92	0.40
1:D:208:LYS:HD2	1:D:208:LYS:HA	1.93	0.40
2:S:20:VAL:HG13	2:S:28:HIS:CB	2.47	0.40
1:O:52:LYS:HA	1:O:66:LYS:NZ	2.36	0.40
2:X:20:VAL:CG1	2:X:28:HIS:HB2	2.50	0.40
2:W:134:VAL:HG23	2:W:158:ALA:HB1	2.04	0.40
1:G:32:LYS:O	1:G:167:SER:HA	2.22	0.40
1:A:165:ILE:HD12	1:A:169:LYS:HD2	2.03	0.40
1:C:152:ASP:HB2	1:C:153:PRO:CD	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:GLU:HG2	1:F:208:LYS:H	1.85	0.40
1:J:171:ALA:HB3	1:J:200:SER:OG	2.22	0.40
1:A:123:TYR:N	1:A:123:TYR:CD1	2.88	0.40
1:G:58:LEU:N	1:G:58:LEU:CD1	2.84	0.40
1:I:130:ARG:HH11	1:I:130:ARG:HG2	1.87	0.40
2:T:3:THR:HB	2:T:16:THR:HG22	2.02	0.40
2:V:15:ALA:HB3	2:V:155:VAL:CG1	2.51	0.40
2:P:19:ARG:NE	2:P:26:ILE:HG13	2.36	0.40
2:P:26:ILE:O	2:P:26:ILE:HD13	2.22	0.40
2:Z:187:LEU:HA	2:Z:188:PRO:HD3	1.87	0.40
1:J:35:SER:O	1:J:166:GLY:HA3	2.21	0.40
2:B:202:ILE:CG1	2:B:203:LEU:N	2.85	0.40
2:S:187:LEU:HA	2:S:188:PRO:HD3	1.76	0.40
2:Z:66:TYR:CZ	2:Z:70:ARG:HD2	2.57	0.40
1:C:107:VAL:HG11	2:Q:66:TYR:HH	1.80	0.40
2:P:178:ILE:HB	2:P:184:TYR:HA	2.03	0.40
1:O:62:ASN:O	1:O:65:GLU:HG2	2.21	0.40
1:D:176:LEU:C	1:D:178:ARG:N	2.74	0.40
2:R:26:ILE:HG23	2:V:165:ARG:HA	2.03	0.40
1:H:222:ARG:NH2	1:H:224:TYR:CZ	2.89	0.40
1:F:123:TYR:HD1	1:F:123:TYR:H	1.70	0.40
1:F:123:TYR:HD1	1:F:123:TYR:N	2.19	0.40
1:N:175:PHE:CD2	1:N:196:ALA:HA	2.57	0.40
1:I:180:TYR:HA	1:I:192:LEU:HD21	2.02	0.40
2:R:49:VAL:HG23	2:R:50:GLY:H	1.86	0.40
1:F:48:LEU:HB3	1:F:67:ILE:CD1	2.51	0.40
1:G:119:GLN:O	1:G:122:GLN:HB2	2.22	0.40

All (1) 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:D:178:ARG:HH22	1:N:178:ARG:HH22[4_457]	1.29	0.31

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	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	3	30
1	C	219/233 (94%)	185 (84%)	25 (11%)	9 (4%)	3	30
1	D	219/233 (94%)	184 (84%)	28 (13%)	7 (3%)	5	38
1	E	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	3	30
1	F	219/233 (94%)	183 (84%)	25 (11%)	11 (5%)	3	24
1	G	219/233 (94%)	186 (85%)	23 (10%)	10 (5%)	3	26
1	H	219/233 (94%)	186 (85%)	25 (11%)	8 (4%)	4	33
1	I	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	3	30
1	J	219/233 (94%)	182 (83%)	26 (12%)	11 (5%)	3	24
1	K	219/233 (94%)	187 (85%)	26 (12%)	6 (3%)	6	41
1	L	219/233 (94%)	186 (85%)	24 (11%)	9 (4%)	3	30
1	M	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	3	30
1	N	219/233 (94%)	187 (85%)	23 (10%)	9 (4%)	3	30
1	O	219/233 (94%)	188 (86%)	23 (10%)	8 (4%)	4	33
2	1	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	19	63
2	2	201/211 (95%)	181 (90%)	19 (10%)	1 (0%)	34	75
2	B	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	19	63
2	P	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	19	63
2	Q	201/211 (95%)	180 (90%)	20 (10%)	1 (0%)	34	75
2	R	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	19	63
2	S	201/211 (95%)	181 (90%)	16 (8%)	4 (2%)	9	48
2	T	201/211 (95%)	176 (88%)	23 (11%)	2 (1%)	19	63
2	U	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	19	63
2	V	201/211 (95%)	179 (89%)	20 (10%)	2 (1%)	19	63
2	W	201/211 (95%)	186 (92%)	13 (6%)	2 (1%)	19	63
2	X	201/211 (95%)	181 (90%)	18 (9%)	2 (1%)	19	63
2	Y	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	19	63
2	Z	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	19	63
All	All	5880/6216 (95%)	5150 (88%)	578 (10%)	152 (3%)	7	42

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	A	182	GLU
1	A	200	SER
1	C	128	GLY
1	C	200	SER
1	D	128	GLY
1	D	182	GLU
1	D	200	SER
1	E	128	GLY
1	E	182	GLU
1	E	200	SER
1	F	128	GLY
1	F	182	GLU
1	F	200	SER
1	G	128	GLY
1	G	200	SER
1	H	128	GLY
1	H	182	GLU
1	H	200	SER
1	I	128	GLY
1	I	182	GLU
1	I	200	SER
1	I	205	GLU
1	J	128	GLY
1	J	182	GLU
1	J	200	SER
1	K	128	GLY
1	K	182	GLU
1	K	200	SER
1	L	128	GLY
1	L	182	GLU
1	L	200	SER
1	M	43	ALA
1	M	128	GLY
1	M	182	GLU
1	M	200	SER
1	N	128	GLY
1	N	182	GLU
1	N	200	SER
1	O	182	GLU
1	O	200	SER
2	P	9	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	9	LYS
2	T	9	LYS
2	V	9	LYS
2	Y	9	LYS
1	A	43	ALA
1	A	72	ASP
1	A	205	GLU
2	B	9	LYS
1	C	43	ALA
1	C	72	ASP
1	C	182	GLU
1	C	205	GLU
1	D	43	ALA
1	D	205	GLU
1	E	43	ALA
1	E	205	GLU
1	F	72	ASP
1	G	43	ALA
1	G	129	VAL
1	G	182	GLU
1	G	205	GLU
1	H	43	ALA
1	J	43	ALA
1	J	72	ASP
1	J	205	GLU
1	K	43	ALA
1	K	205	GLU
1	L	43	ALA
1	L	205	GLU
1	M	62	ASN
1	M	72	ASP
1	M	205	GLU
1	N	72	ASP
1	N	205	GLU
1	O	43	ALA
1	O	128	GLY
1	O	205	GLU
2	Q	9	LYS
2	R	9	LYS
2	U	9	LYS
2	W	9	LYS
2	X	9	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Z	9	LYS
2	1	9	LYS
2	2	9	LYS
2	B	23	GLU
1	E	72	ASP
1	E	177	GLU
1	F	43	ALA
1	F	61	GLN
1	F	198	LYS
1	F	205	GLU
1	G	61	GLN
1	G	62	ASN
1	H	61	GLN
1	H	62	ASN
1	H	198	LYS
1	H	205	GLU
1	I	43	ALA
1	J	186	GLU
1	L	72	ASP
1	M	61	GLN
1	M	198	LYS
1	N	43	ALA
1	N	202	GLU
1	O	61	GLN
1	O	72	ASP
1	O	198	LYS
2	R	23	GLU
2	Y	23	GLU
1	C	61	GLN
1	D	198	LYS
1	E	61	GLN
1	F	62	ASN
1	I	61	GLN
1	I	62	ASN
1	I	72	ASP
1	I	198	LYS
1	K	198	LYS
1	L	62	ASN
1	N	198	LYS
2	T	23	GLU
2	V	23	GLU
2	X	23	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	198	LYS
1	A	202	GLU
1	C	198	LYS
1	G	72	ASP
1	J	61	GLN
1	J	198	LYS
1	J	202	GLU
1	L	198	LYS
1	N	61	GLN
2	S	23	GLU
2	U	23	GLU
2	W	23	GLU
2	1	23	GLU
1	C	62	ASN
1	D	61	GLN
1	E	198	LYS
1	F	129	VAL
1	F	167	SER
1	G	198	LYS
1	L	61	GLN
2	P	23	GLU
2	S	49	VAL
2	Z	110	VAL
1	J	129	VAL
2	S	110	VAL
1	A	129	VAL

5.3.2 Protein sidechains (i)

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	184/193 (95%)	163 (89%)	21 (11%)	7 31
1	C	184/193 (95%)	160 (87%)	24 (13%)	5 25
1	D	184/193 (95%)	159 (86%)	25 (14%)	5 24
1	E	184/193 (95%)	159 (86%)	25 (14%)	5 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	184/193 (95%)	158 (86%)	26 (14%)	4	22
1	G	184/193 (95%)	162 (88%)	22 (12%)	6	29
1	H	184/193 (95%)	164 (89%)	20 (11%)	8	34
1	I	184/193 (95%)	162 (88%)	22 (12%)	6	29
1	J	184/193 (95%)	162 (88%)	22 (12%)	6	29
1	K	184/193 (95%)	160 (87%)	24 (13%)	5	25
1	L	184/193 (95%)	159 (86%)	25 (14%)	5	24
1	M	184/193 (95%)	162 (88%)	22 (12%)	6	29
1	N	184/193 (95%)	160 (87%)	24 (13%)	5	25
1	O	184/193 (95%)	157 (85%)	27 (15%)	4	20
2	1	170/177 (96%)	148 (87%)	22 (13%)	5	26
2	2	170/177 (96%)	144 (85%)	26 (15%)	3	19
2	B	170/177 (96%)	145 (85%)	25 (15%)	4	20
2	P	170/177 (96%)	148 (87%)	22 (13%)	5	26
2	Q	170/177 (96%)	143 (84%)	27 (16%)	3	17
2	R	170/177 (96%)	143 (84%)	27 (16%)	3	17
2	S	170/177 (96%)	146 (86%)	24 (14%)	4	22
2	T	170/177 (96%)	152 (89%)	18 (11%)	8	36
2	U	170/177 (96%)	146 (86%)	24 (14%)	4	22
2	V	170/177 (96%)	145 (85%)	25 (15%)	4	20
2	W	170/177 (96%)	145 (85%)	25 (15%)	4	20
2	X	170/177 (96%)	149 (88%)	21 (12%)	6	27
2	Y	170/177 (96%)	144 (85%)	26 (15%)	3	19
2	Z	170/177 (96%)	150 (88%)	20 (12%)	6	29
All	All	4956/5180 (96%)	4295 (87%)	661 (13%)	5	24

All (661) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	38	LEU
1	A	44	ASN
1	A	47	LEU
1	A	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	71	ASP
1	A	102	THR
1	A	119	GLN
1	A	134	VAL
1	A	136	LEU
1	A	141	ILE
1	A	143	GLN
1	A	157	ILE
1	A	161	LYS
1	A	175	PHE
1	A	176	LEU
1	A	190	VAL
1	A	201	LEU
1	A	202	GLU
1	A	212	ILE
1	A	221	TYR
2	B	2	THR
2	B	7	THR
2	B	17	GLU
2	B	25	PHE
2	B	26	ILE
2	B	41	THR
2	B	45	ILE
2	B	49	VAL
2	B	56	VAL
2	B	63	LEU
2	B	71	ARG
2	B	83	LEU
2	B	94	PRO
2	B	97	VAL
2	B	123	ILE
2	B	127	THR
2	B	134	VAL
2	B	137	VAL
2	B	138	LEU
2	B	144	GLU
2	B	165	ARG
2	B	173	ILE
2	B	175	VAL
2	B	178	ILE
2	B	201	LEU
1	C	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	24	VAL
1	C	31	VAL
1	C	38	LEU
1	C	44	ASN
1	C	47	LEU
1	C	49	ILE
1	C	62	ASN
1	C	71	ASP
1	C	102	THR
1	C	119	GLN
1	C	121	GLN
1	C	134	VAL
1	C	136	LEU
1	C	141	ILE
1	C	143	GLN
1	C	157	ILE
1	C	161	LYS
1	C	175	PHE
1	C	190	VAL
1	C	201	LEU
1	C	202	GLU
1	C	212	ILE
1	C	221	TYR
1	D	21	LEU
1	D	31	VAL
1	D	44	ASN
1	D	47	LEU
1	D	48	LEU
1	D	49	ILE
1	D	58	LEU
1	D	62	ASN
1	D	71	ASP
1	D	87	VAL
1	D	102	THR
1	D	116	VAL
1	D	119	GLN
1	D	136	LEU
1	D	141	ILE
1	D	143	GLN
1	D	157	ILE
1	D	161	LYS
1	D	175	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	176	LEU
1	D	190	VAL
1	D	201	LEU
1	D	202	GLU
1	D	212	ILE
1	D	221	TYR
1	E	21	LEU
1	E	24	VAL
1	E	31	VAL
1	E	44	ASN
1	E	47	LEU
1	E	49	ILE
1	E	58	LEU
1	E	62	ASN
1	E	71	ASP
1	E	101	VAL
1	E	102	THR
1	E	119	GLN
1	E	134	VAL
1	E	136	LEU
1	E	141	ILE
1	E	143	GLN
1	E	150	ASP
1	E	161	LYS
1	E	175	PHE
1	E	176	LEU
1	E	190	VAL
1	E	201	LEU
1	E	202	GLU
1	E	212	ILE
1	E	221	TYR
1	F	21	LEU
1	F	24	VAL
1	F	31	VAL
1	F	38	LEU
1	F	44	ASN
1	F	47	LEU
1	F	48	LEU
1	F	62	ASN
1	F	71	ASP
1	F	101	VAL
1	F	102	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	119	GLN
1	F	121	GLN
1	F	134	VAL
1	F	136	LEU
1	F	141	ILE
1	F	143	GLN
1	F	150	ASP
1	F	157	ILE
1	F	161	LYS
1	F	175	PHE
1	F	176	LEU
1	F	190	VAL
1	F	201	LEU
1	F	202	GLU
1	F	221	TYR
1	G	21	LEU
1	G	31	VAL
1	G	38	LEU
1	G	44	ASN
1	G	47	LEU
1	G	62	ASN
1	G	71	ASP
1	G	101	VAL
1	G	102	THR
1	G	119	GLN
1	G	136	LEU
1	G	141	ILE
1	G	143	GLN
1	G	150	ASP
1	G	157	ILE
1	G	161	LYS
1	G	175	PHE
1	G	190	VAL
1	G	201	LEU
1	G	202	GLU
1	G	212	ILE
1	G	221	TYR
1	H	21	LEU
1	H	31	VAL
1	H	44	ASN
1	H	47	LEU
1	H	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	71	ASP
1	H	102	THR
1	H	107	VAL
1	H	119	GLN
1	H	134	VAL
1	H	136	LEU
1	H	141	ILE
1	H	143	GLN
1	H	157	ILE
1	H	161	LYS
1	H	175	PHE
1	H	190	VAL
1	H	201	LEU
1	H	202	GLU
1	H	221	TYR
1	I	21	LEU
1	I	38	LEU
1	I	44	ASN
1	I	47	LEU
1	I	62	ASN
1	I	71	ASP
1	I	102	THR
1	I	119	GLN
1	I	121	GLN
1	I	123	TYR
1	I	134	VAL
1	I	136	LEU
1	I	141	ILE
1	I	143	GLN
1	I	150	ASP
1	I	161	LYS
1	I	175	PHE
1	I	190	VAL
1	I	201	LEU
1	I	202	GLU
1	I	212	ILE
1	I	221	TYR
1	J	21	LEU
1	J	24	VAL
1	J	31	VAL
1	J	44	ASN
1	J	47	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	49	ILE
1	J	62	ASN
1	J	71	ASP
1	J	102	THR
1	J	119	GLN
1	J	134	VAL
1	J	136	LEU
1	J	141	ILE
1	J	143	GLN
1	J	150	ASP
1	J	157	ILE
1	J	161	LYS
1	J	175	PHE
1	J	190	VAL
1	J	201	LEU
1	J	202	GLU
1	J	221	TYR
1	K	21	LEU
1	K	31	VAL
1	K	38	LEU
1	K	44	ASN
1	K	47	LEU
1	K	48	LEU
1	K	49	ILE
1	K	58	LEU
1	K	62	ASN
1	K	71	ASP
1	K	102	THR
1	K	119	GLN
1	K	134	VAL
1	K	136	LEU
1	K	141	ILE
1	K	143	GLN
1	K	161	LYS
1	K	175	PHE
1	K	176	LEU
1	K	190	VAL
1	K	201	LEU
1	K	202	GLU
1	K	212	ILE
1	K	221	TYR
1	L	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	24	VAL
1	L	31	VAL
1	L	38	LEU
1	L	44	ASN
1	L	47	LEU
1	L	49	ILE
1	L	58	LEU
1	L	62	ASN
1	L	71	ASP
1	L	87	VAL
1	L	101	VAL
1	L	102	THR
1	L	119	GLN
1	L	136	LEU
1	L	141	ILE
1	L	143	GLN
1	L	157	ILE
1	L	161	LYS
1	L	175	PHE
1	L	190	VAL
1	L	201	LEU
1	L	202	GLU
1	L	212	ILE
1	L	221	TYR
1	M	21	LEU
1	M	31	VAL
1	M	44	ASN
1	M	47	LEU
1	M	49	ILE
1	M	62	ASN
1	M	71	ASP
1	M	102	THR
1	M	119	GLN
1	M	121	GLN
1	M	134	VAL
1	M	136	LEU
1	M	141	ILE
1	M	143	GLN
1	M	157	ILE
1	M	161	LYS
1	M	175	PHE
1	M	190	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	201	LEU
1	M	202	GLU
1	M	212	ILE
1	M	221	TYR
1	N	21	LEU
1	N	31	VAL
1	N	44	ASN
1	N	47	LEU
1	N	49	ILE
1	N	58	LEU
1	N	62	ASN
1	N	71	ASP
1	N	74	VAL
1	N	102	THR
1	N	119	GLN
1	N	121	GLN
1	N	134	VAL
1	N	136	LEU
1	N	141	ILE
1	N	143	GLN
1	N	157	ILE
1	N	161	LYS
1	N	175	PHE
1	N	190	VAL
1	N	201	LEU
1	N	202	GLU
1	N	212	ILE
1	N	221	TYR
1	O	21	LEU
1	O	24	VAL
1	O	31	VAL
1	O	44	ASN
1	O	47	LEU
1	O	49	ILE
1	O	58	LEU
1	O	62	ASN
1	O	71	ASP
1	O	74	VAL
1	O	101	VAL
1	O	102	THR
1	O	119	GLN
1	O	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	136	LEU
1	O	141	ILE
1	O	143	GLN
1	O	150	ASP
1	O	157	ILE
1	O	161	LYS
1	O	175	PHE
1	O	176	LEU
1	O	190	VAL
1	O	201	LEU
1	O	202	GLU
1	O	212	ILE
1	O	221	TYR
2	P	2	THR
2	P	17	GLU
2	P	20	VAL
2	P	25	PHE
2	P	26	ILE
2	P	41	THR
2	P	45	ILE
2	P	49	VAL
2	P	59	MET
2	P	70	ARG
2	P	71	ARG
2	P	83	LEU
2	P	123	ILE
2	P	127	THR
2	P	134	VAL
2	P	137	VAL
2	P	138	LEU
2	P	144	GLU
2	P	165	ARG
2	P	173	ILE
2	P	178	ILE
2	P	185	VAL
2	Q	2	THR
2	Q	8	LEU
2	Q	12	VAL
2	Q	17	GLU
2	Q	20	VAL
2	Q	25	PHE
2	Q	26	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	41	THR
2	Q	45	ILE
2	Q	49	VAL
2	Q	55	LEU
2	Q	59	MET
2	Q	68	LEU
2	Q	70	ARG
2	Q	71	ARG
2	Q	83	LEU
2	Q	123	ILE
2	Q	127	THR
2	Q	134	VAL
2	Q	137	VAL
2	Q	138	LEU
2	Q	144	GLU
2	Q	165	ARG
2	Q	173	ILE
2	Q	175	VAL
2	Q	178	ILE
2	Q	185	VAL
2	R	2	THR
2	R	7	THR
2	R	17	GLU
2	R	25	PHE
2	R	26	ILE
2	R	41	THR
2	R	45	ILE
2	R	49	VAL
2	R	56	VAL
2	R	68	LEU
2	R	71	ARG
2	R	83	LEU
2	R	94	PRO
2	R	97	VAL
2	R	104	ILE
2	R	123	ILE
2	R	127	THR
2	R	134	VAL
2	R	137	VAL
2	R	144	GLU
2	R	149	ASP
2	R	165	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	173	ILE
2	R	175	VAL
2	R	177	VAL
2	R	178	ILE
2	R	185	VAL
2	S	1	THR
2	S	2	THR
2	S	8	LEU
2	S	17	GLU
2	S	20	VAL
2	S	26	ILE
2	S	41	THR
2	S	45	ILE
2	S	49	VAL
2	S	63	LEU
2	S	68	LEU
2	S	71	ARG
2	S	83	LEU
2	S	123	ILE
2	S	127	THR
2	S	134	VAL
2	S	137	VAL
2	S	138	LEU
2	S	144	GLU
2	S	153	ASP
2	S	165	ARG
2	S	173	ILE
2	S	175	VAL
2	S	178	ILE
2	T	2	THR
2	T	17	GLU
2	T	20	VAL
2	T	26	ILE
2	T	41	THR
2	T	45	ILE
2	T	59	MET
2	T	71	ARG
2	T	83	LEU
2	T	123	ILE
2	T	127	THR
2	T	134	VAL
2	T	137	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	138	LEU
2	T	144	GLU
2	T	165	ARG
2	T	173	ILE
2	T	178	ILE
2	U	2	THR
2	U	8	LEU
2	U	12	VAL
2	U	17	GLU
2	U	20	VAL
2	U	25	PHE
2	U	26	ILE
2	U	41	THR
2	U	45	ILE
2	U	59	MET
2	U	70	ARG
2	U	71	ARG
2	U	94	PRO
2	U	123	ILE
2	U	127	THR
2	U	134	VAL
2	U	137	VAL
2	U	144	GLU
2	U	153	ASP
2	U	165	ARG
2	U	173	ILE
2	U	175	VAL
2	U	178	ILE
2	U	185	VAL
2	V	2	THR
2	V	7	THR
2	V	8	LEU
2	V	17	GLU
2	V	20	VAL
2	V	26	ILE
2	V	41	THR
2	V	45	ILE
2	V	49	VAL
2	V	56	VAL
2	V	59	MET
2	V	63	LEU
2	V	71	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	94	PRO
2	V	122	ASP
2	V	123	ILE
2	V	127	THR
2	V	134	VAL
2	V	137	VAL
2	V	138	LEU
2	V	144	GLU
2	V	165	ARG
2	V	173	ILE
2	V	178	ILE
2	V	185	VAL
2	W	2	THR
2	W	7	THR
2	W	17	GLU
2	W	20	VAL
2	W	25	PHE
2	W	26	ILE
2	W	41	THR
2	W	45	ILE
2	W	49	VAL
2	W	56	VAL
2	W	59	MET
2	W	71	ARG
2	W	94	PRO
2	W	97	VAL
2	W	123	ILE
2	W	127	THR
2	W	134	VAL
2	W	137	VAL
2	W	138	LEU
2	W	144	GLU
2	W	165	ARG
2	W	173	ILE
2	W	175	VAL
2	W	178	ILE
2	W	185	VAL
2	X	2	THR
2	X	8	LEU
2	X	17	GLU
2	X	20	VAL
2	X	26	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	41	THR
2	X	45	ILE
2	X	49	VAL
2	X	59	MET
2	X	71	ARG
2	X	123	ILE
2	X	127	THR
2	X	134	VAL
2	X	137	VAL
2	X	144	GLU
2	X	165	ARG
2	X	173	ILE
2	X	177	VAL
2	X	178	ILE
2	X	185	VAL
2	X	201	LEU
2	Y	2	THR
2	Y	7	THR
2	Y	8	LEU
2	Y	17	GLU
2	Y	25	PHE
2	Y	26	ILE
2	Y	41	THR
2	Y	45	ILE
2	Y	59	MET
2	Y	63	LEU
2	Y	70	ARG
2	Y	71	ARG
2	Y	83	LEU
2	Y	94	PRO
2	Y	123	ILE
2	Y	127	THR
2	Y	134	VAL
2	Y	137	VAL
2	Y	138	LEU
2	Y	144	GLU
2	Y	149	ASP
2	Y	165	ARG
2	Y	173	ILE
2	Y	175	VAL
2	Y	178	ILE
2	Y	185	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Z	17	GLU
2	Z	20	VAL
2	Z	26	ILE
2	Z	41	THR
2	Z	45	ILE
2	Z	49	VAL
2	Z	63	LEU
2	Z	70	ARG
2	Z	71	ARG
2	Z	83	LEU
2	Z	123	ILE
2	Z	127	THR
2	Z	134	VAL
2	Z	137	VAL
2	Z	138	LEU
2	Z	144	GLU
2	Z	165	ARG
2	Z	173	ILE
2	Z	175	VAL
2	Z	178	ILE
2	1	2	THR
2	1	8	LEU
2	1	17	GLU
2	1	20	VAL
2	1	26	ILE
2	1	41	THR
2	1	45	ILE
2	1	59	MET
2	1	71	ARG
2	1	123	ILE
2	1	127	THR
2	1	134	VAL
2	1	137	VAL
2	1	138	LEU
2	1	144	GLU
2	1	153	ASP
2	1	165	ARG
2	1	173	ILE
2	1	175	VAL
2	1	178	ILE
2	1	185	VAL
2	1	201	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1	THR
2	2	2	THR
2	2	8	LEU
2	2	12	VAL
2	2	17	GLU
2	2	25	PHE
2	2	26	ILE
2	2	41	THR
2	2	45	ILE
2	2	49	VAL
2	2	59	MET
2	2	63	LEU
2	2	68	LEU
2	2	71	ARG
2	2	94	PRO
2	2	123	ILE
2	2	127	THR
2	2	134	VAL
2	2	137	VAL
2	2	138	LEU
2	2	144	GLU
2	2	149	ASP
2	2	165	ARG
2	2	173	ILE
2	2	175	VAL
2	2	178	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	44	ASN
1	A	98	GLN
1	A	121	GLN
1	A	125	GLN
1	A	143	GLN
2	B	30	ASN
2	B	36	GLN
2	B	164	GLN
1	C	44	ASN
1	C	98	GLN
1	C	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	125	GLN
1	C	143	GLN
1	D	23	GLN
1	D	44	ASN
1	D	98	GLN
1	D	121	GLN
1	D	125	GLN
1	D	143	GLN
1	E	44	ASN
1	E	98	GLN
1	E	121	GLN
1	E	125	GLN
1	E	143	GLN
1	F	44	ASN
1	F	98	GLN
1	F	119	GLN
1	F	121	GLN
1	F	125	GLN
1	F	143	GLN
1	G	44	ASN
1	G	98	GLN
1	G	121	GLN
1	G	125	GLN
1	G	143	GLN
1	H	44	ASN
1	H	98	GLN
1	H	121	GLN
1	H	125	GLN
1	H	143	GLN
1	I	44	ASN
1	I	98	GLN
1	I	121	GLN
1	I	125	GLN
1	I	143	GLN
1	J	44	ASN
1	J	98	GLN
1	J	121	GLN
1	J	125	GLN
1	J	143	GLN
1	K	44	ASN
1	K	98	GLN
1	K	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	125	GLN
1	K	143	GLN
1	L	23	GLN
1	L	44	ASN
1	L	98	GLN
1	L	121	GLN
1	L	125	GLN
1	L	143	GLN
1	M	44	ASN
1	M	98	GLN
1	M	121	GLN
1	M	125	GLN
1	M	143	GLN
1	N	23	GLN
1	N	44	ASN
1	N	98	GLN
1	N	121	GLN
1	N	125	GLN
1	N	143	GLN
1	O	23	GLN
1	O	44	ASN
1	O	98	GLN
1	O	121	GLN
1	O	125	GLN
1	O	143	GLN
2	P	30	ASN
2	P	36	GLN
2	P	73	ASN
2	P	164	GLN
2	Q	30	ASN
2	Q	36	GLN
2	Q	141	GLN
2	Q	164	GLN
2	R	28	HIS
2	R	30	ASN
2	R	85	ASN
2	R	141	GLN
2	R	164	GLN
2	S	30	ASN
2	S	36	GLN
2	S	141	GLN
2	S	164	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	30	ASN
2	T	141	GLN
2	T	164	GLN
2	U	30	ASN
2	U	164	GLN
2	V	28	HIS
2	V	30	ASN
2	V	85	ASN
2	V	164	GLN
2	W	30	ASN
2	W	36	GLN
2	W	73	ASN
2	W	164	GLN
2	X	28	HIS
2	X	30	ASN
2	X	36	GLN
2	X	164	GLN
2	Y	30	ASN
2	Y	141	GLN
2	Y	164	GLN
2	Z	28	HIS
2	Z	30	ASN
2	Z	141	GLN
2	Z	164	GLN
2	1	28	HIS
2	1	30	ASN
2	1	141	GLN
2	1	164	GLN
2	2	30	ASN
2	2	164	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	221/233 (94%)	-0.13	5 (2%)	64	58	17, 56, 117, 155	0
1	C	221/233 (94%)	-0.18	2 (0%)	85	81	13, 53, 115, 154	0
1	D	221/233 (94%)	-0.23	6 (2%)	58	53	21, 53, 116, 153	0
1	E	221/233 (94%)	-0.20	4 (1%)	71	65	17, 52, 115, 155	0
1	F	221/233 (94%)	-0.11	4 (1%)	71	65	16, 57, 116, 153	0
1	G	221/233 (94%)	-0.08	6 (2%)	58	53	20, 56, 118, 155	0
1	H	221/233 (94%)	-0.12	5 (2%)	64	58	21, 57, 116, 154	0
1	I	221/233 (94%)	-0.11	8 (3%)	46	41	17, 55, 116, 155	0
1	J	221/233 (94%)	-0.12	8 (3%)	46	41	21, 55, 116, 156	0
1	K	221/233 (94%)	-0.23	5 (2%)	64	58	20, 55, 116, 153	0
1	L	221/233 (94%)	-0.22	4 (1%)	71	65	13, 53, 116, 153	0
1	M	221/233 (94%)	-0.20	4 (1%)	71	65	17, 53, 117, 153	0
1	N	221/233 (94%)	-0.22	4 (1%)	71	65	19, 52, 116, 156	0
1	O	221/233 (94%)	-0.22	3 (1%)	78	73	18, 51, 116, 152	0
2	1	203/211 (96%)	-0.55	0	100	100	9, 33, 69, 85	0
2	2	203/211 (96%)	-0.60	0	100	100	6, 33, 69, 88	0
2	B	203/211 (96%)	-0.54	0	100	100	11, 34, 69, 90	0
2	P	203/211 (96%)	-0.53	0	100	100	8, 35, 69, 89	0
2	Q	203/211 (96%)	-0.64	0	100	100	8, 33, 71, 90	0
2	R	203/211 (96%)	-0.69	0	100	100	6, 32, 68, 86	0
2	S	203/211 (96%)	-0.63	0	100	100	7, 33, 68, 91	0
2	T	203/211 (96%)	-0.60	0	100	100	10, 35, 73, 90	0
2	U	203/211 (96%)	-0.58	0	100	100	14, 34, 70, 92	0
2	V	203/211 (96%)	-0.59	0	100	100	11, 32, 69, 89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	W	203/211 (96%)	-0.61	0	100	100	11, 34, 69, 85	0
2	X	203/211 (96%)	-0.65	0	100	100	8, 32, 70, 90	0
2	Y	203/211 (96%)	-0.65	0	100	100	10, 32, 68, 92	0
2	Z	203/211 (96%)	-0.70	0	100	100	9, 32, 69, 91	0
All	All	5936/6216 (95%)	-0.38	68 (1%)	82	77	6, 43, 107, 156	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	205	GLU	4.3
1	L	55	ARG	4.1
1	I	64	ILE	4.0
1	D	63	SER	3.9
1	I	205	GLU	3.8
1	D	64	ILE	3.8
1	N	205	GLU	3.7
1	G	201	LEU	3.6
1	E	62	ASN	3.4
1	E	64	ILE	3.4
1	J	205	GLU	3.4
1	J	201	LEU	3.4
1	F	64	ILE	3.3
1	L	205	GLU	3.2
1	O	64	ILE	3.2
1	O	202	GLU	3.2
1	I	202	GLU	3.2
1	G	203	GLU	3.1
1	A	202	GLU	3.1
1	J	202	GLU	3.1
1	N	63	SER	3.0
1	D	62	ASN	2.9
1	H	205	GLU	2.9
1	N	64	ILE	2.8
1	H	64	ILE	2.8
1	F	44	ASN	2.8
1	E	202	GLU	2.7
1	N	62	ASN	2.7
1	C	64	ILE	2.7
1	M	63	SER	2.7
1	A	226	GLN	2.6
1	I	52	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	206	GLU	2.5
1	H	62	ASN	2.5
1	G	230	LYS	2.4
1	K	62	ASN	2.4
1	A	181	LYS	2.4
1	H	230	LYS	2.4
1	D	61	GLN	2.3
1	I	230	LYS	2.3
1	M	64	ILE	2.3
1	M	205	GLU	2.3
1	G	202	GLU	2.3
1	J	206	GLU	2.3
1	J	39	GLY	2.2
1	J	63	SER	2.2
1	O	62	ASN	2.2
1	F	39	GLY	2.2
1	L	62	ASN	2.2
1	K	205	GLU	2.2
1	J	181	LYS	2.2
1	H	202	GLU	2.2
1	F	206	GLU	2.2
1	E	63	SER	2.2
1	A	217	VAL	2.2
1	C	205	GLU	2.1
1	K	32	LYS	2.1
1	I	206	GLU	2.1
1	J	203	GLU	2.1
1	M	206	GLU	2.1
1	K	227	GLU	2.1
1	K	63	SER	2.1
1	L	63	SER	2.1
1	G	178	ARG	2.1
1	I	45	GLY	2.1
1	I	161	LYS	2.0
1	A	216	THR	2.0
1	D	205	GLU	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.