



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:12 am BST

PDB ID : 5IRO
Title : Crystal structure of a complex between the Human adenovirus type 4 E3-19K protein and MHC class molecule HLA-A2/TAX
Authors : Li, L.; Bouvier, M.
Deposited on : 2016-03-14
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

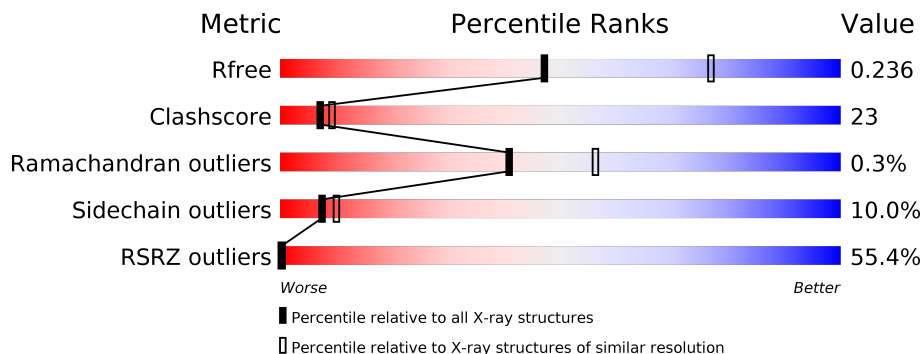
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div style="display: flex; justify-content: space-between;"> <div style="width: 43%;">■ 43%</div> <div style="width: 44%;">■ 46%</div> <div style="width: 6%;">■ 44%</div> <div style="width: 6%;">■ 6%</div> <div style="width: 3%;">■ .</div> </div>
1	E	275	<div style="display: flex; justify-content: space-between;"> <div style="width: 48%;">■ 48%</div> <div style="width: 51%;">■ 51%</div> <div style="width: 41%;">■ 41%</div> <div style="width: 5%;">■ 5%</div> <div style="width: 3%;">■ .</div> </div>
1	I	275	<div style="display: flex; justify-content: space-between;"> <div style="width: 38%;">■ 38%</div> <div style="width: 52%;">■ 52%</div> <div style="width: 35%;">■ 35%</div> <div style="width: 5%;">■ 5%</div> <div style="width: 8%;">■ 8%</div> </div>
1	M	275	<div style="display: flex; justify-content: space-between;"> <div style="width: 48%;">■ 48%</div> <div style="width: 46%;">■ 46%</div> <div style="width: 44%;">■ 44%</div> <div style="width: 6%;">■ 6%</div> <div style="width: 3%;">■ .</div> </div>
1	Q	275	<div style="display: flex; justify-content: space-between;"> <div style="width: 76%;">■ 76%</div> <div style="width: 44%;">■ 44%</div> <div style="width: 43%;">■ 43%</div> <div style="width: 7%;">■ 7%</div> <div style="width: 6%;">■ 6%</div> </div>
1	U	275	<div style="display: flex; justify-content: space-between;"> <div style="width: 72%;">■ 72%</div> <div style="width: 46%;">■ 46%</div> <div style="width: 37%;">■ 37%</div> <div style="width: 6%;">■ 6%</div> <div style="width: 11%;">■ 11%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	9	
2	F	9	
2	J	9	
2	N	9	
2	R	9	
2	V	9	
3	C	100	
3	G	100	
3	K	100	
3	O	100	
3	S	100	
3	W	100	
4	D	108	
4	H	108	
4	L	108	
4	P	108	
4	T	108	
4	X	108	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23039 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	Total 2144	C 1338	N 389	O 408	S 9	0	0	0
1	E	268	Total 2183	C 1363	N 398	O 413	S 9	0	0	0
1	I	252	Total 2053	C 1282	N 376	O 386	S 9	0	0	0
1	M	265	Total 2160	C 1351	N 392	O 408	S 9	0	0	0
1	Q	259	Total 2111	C 1315	N 385	O 402	S 9	0	0	0
1	U	246	Total 2007	C 1259	N 363	O 376	S 9	0	0	0

- Molecule 2 is a protein called TAX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	Total 76	C 56	N 9	O 11	0	0	0
2	F	9	Total 76	C 56	N 9	O 11	0	0	0
2	J	9	Total 76	C 56	N 9	O 11	0	0	0
2	N	9	Total 76	C 56	N 9	O 11	0	0	0
2	R	9	Total 76	C 56	N 9	O 11	0	0	0
2	V	9	Total 76	C 56	N 9	O 11	0	0	0

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			802	513	136	150	3			
3	G	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	K	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	O	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	S	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	W	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
O	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769
W	0	MET	-	initiating methionine	UNP P61769

- Molecule 4 is a protein called E3 19 kDa protein.

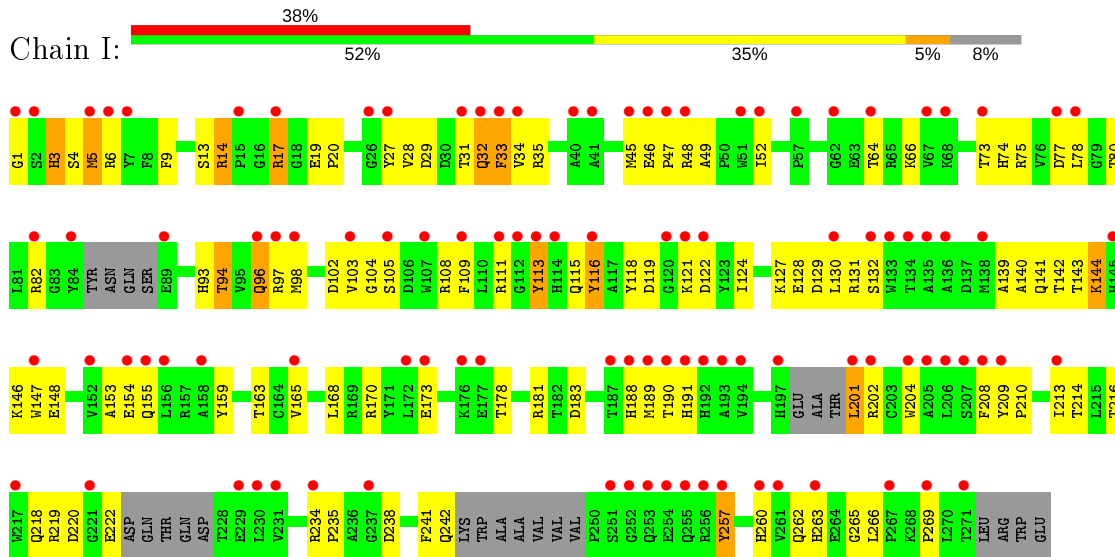
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			823	520	144	149	10			
4	H	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	L	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	P	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	T	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	X	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			

- Molecule 5 is water.

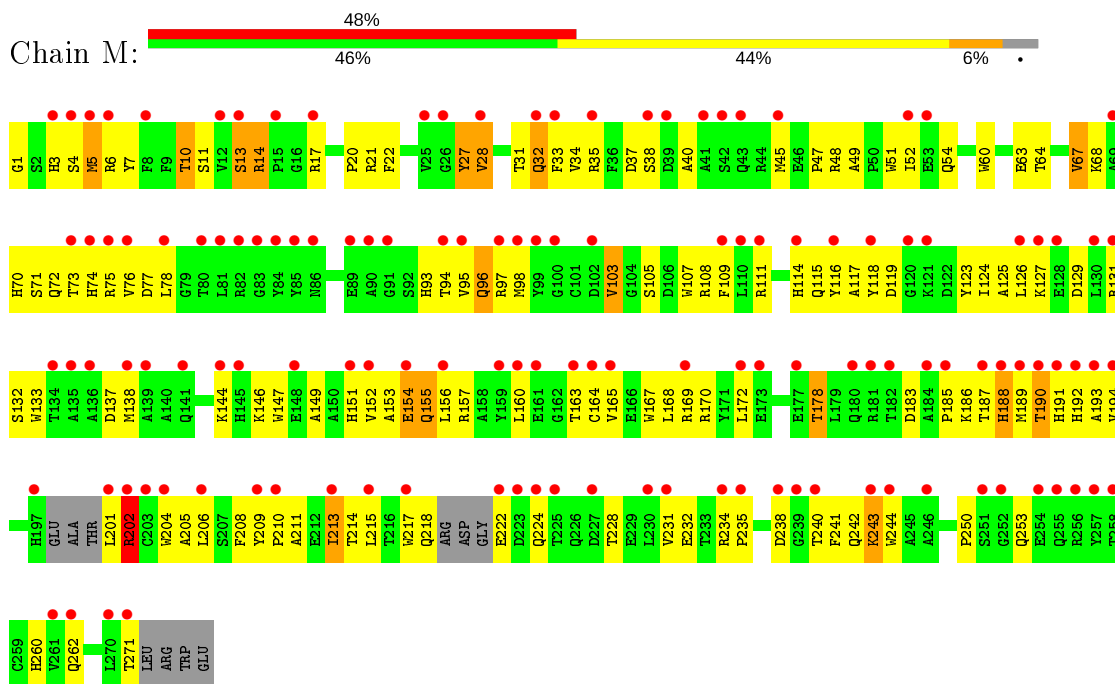
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	D	2	Total O 2 2	0	0
5	E	3	Total O 3 3	0	0
5	G	1	Total O 1 1	0	0
5	I	5	Total O 5 5	0	0
5	J	1	Total O 1 1	0	0
5	K	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	M	4	Total O 4 4	0	0
5	O	2	Total O 2 2	0	0
5	P	3	Total O 3 3	0	0
5	Q	3	Total O 3 3	0	0
5	S	3	Total O 3 3	0	0
5	T	3	Total O 3 3	0	0
5	U	3	Total O 3 3	0	0
5	W	1	Total O 1 1	0	0



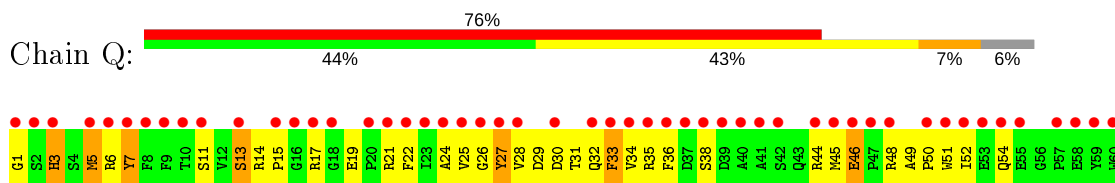
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

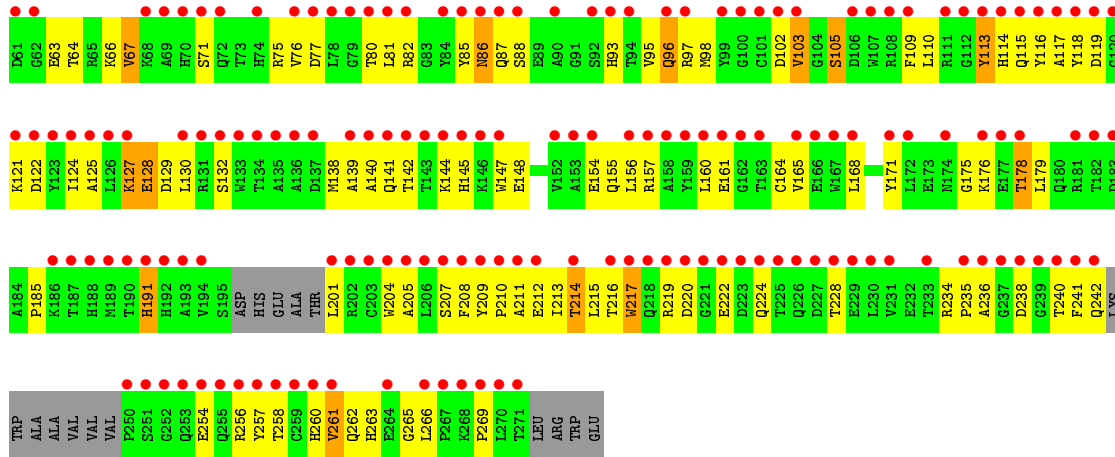


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

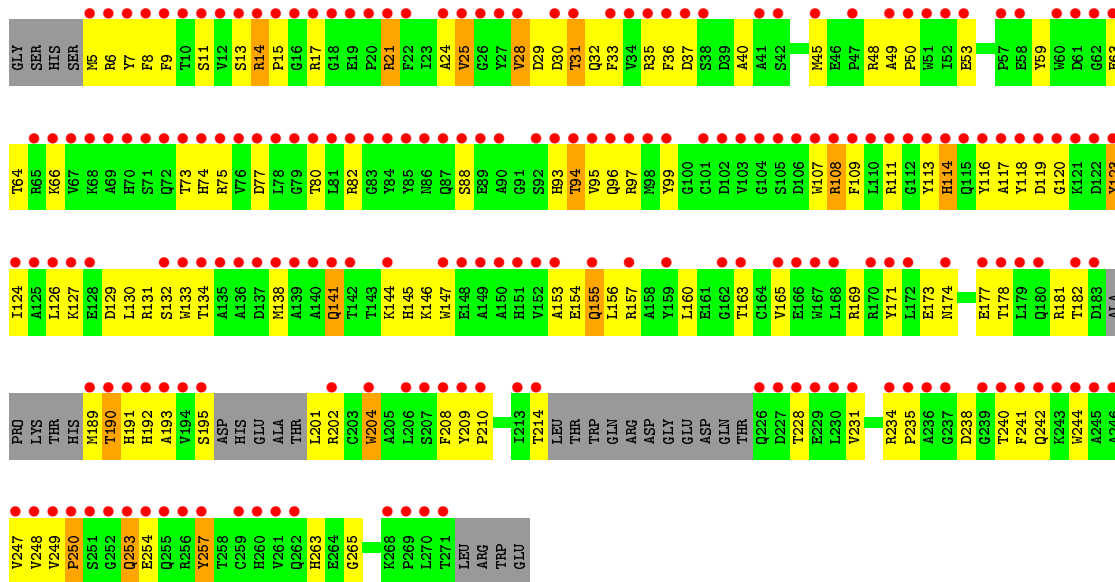
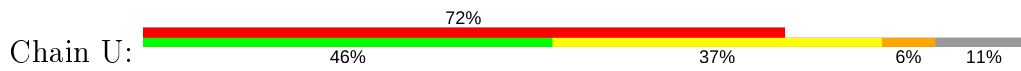


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain





• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



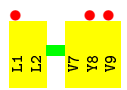
• Molecule 2: TAX protein



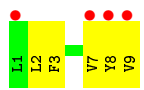
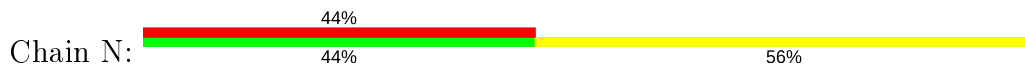
• Molecule 2: TAX protein



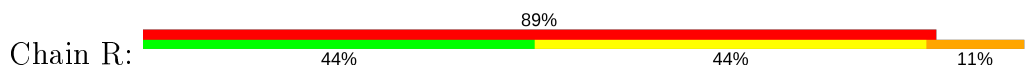
• Molecule 2: TAX protein



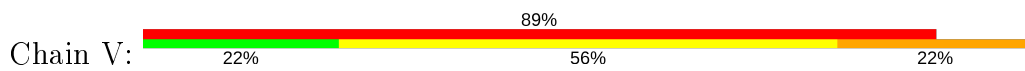
• Molecule 2: TAX protein



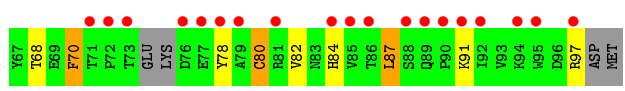
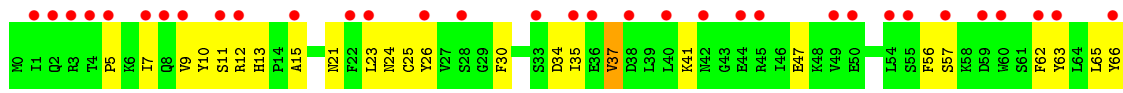
• Molecule 2: TAX protein



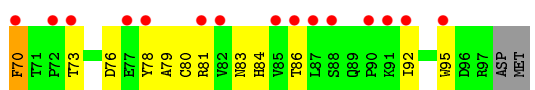
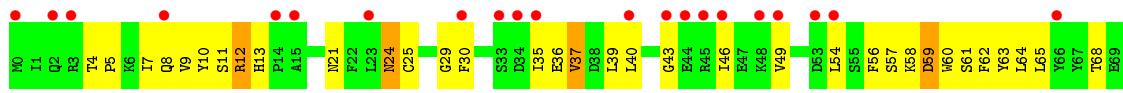
• Molecule 2: TAX protein



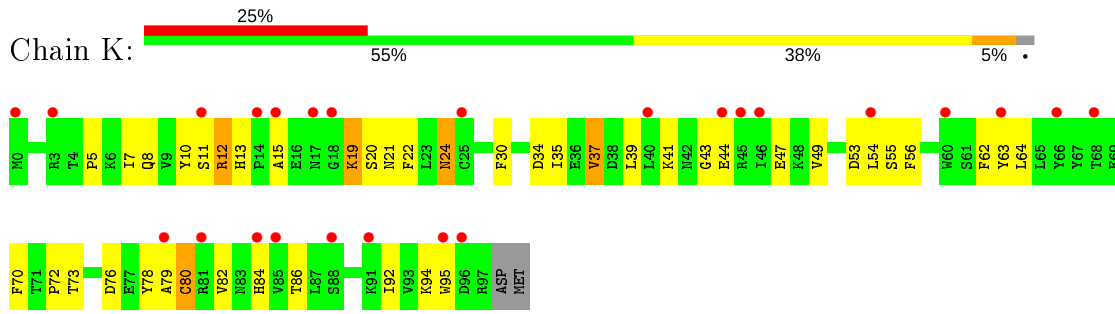
• Molecule 3: Beta-2-microglobulin



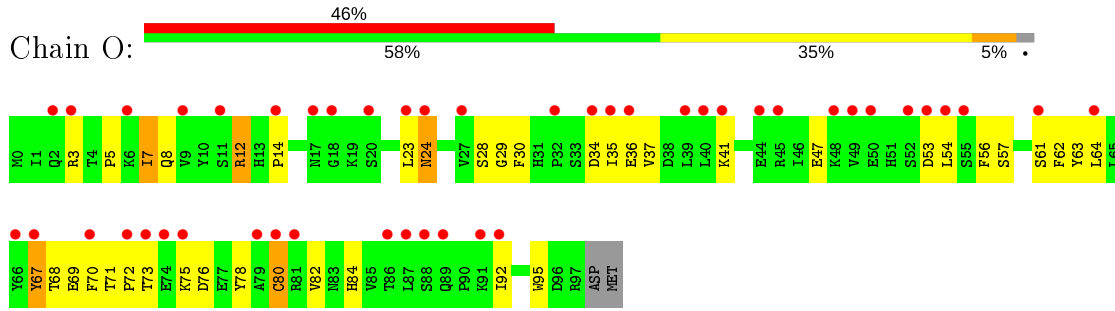
• Molecule 3: Beta-2-microglobulin



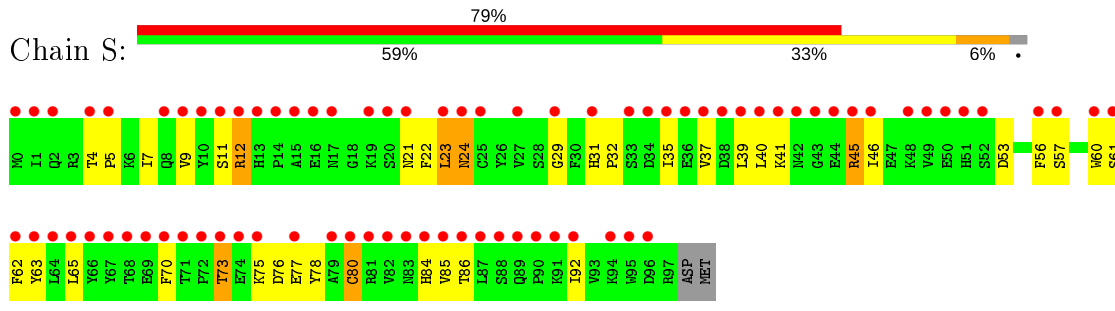
• Molecule 3: Beta-2-microglobulin



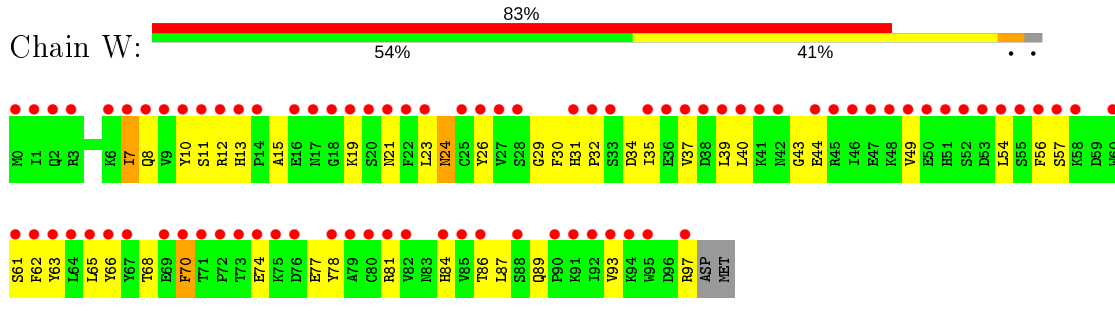
• Molecule 3: Beta-2-microglobulin



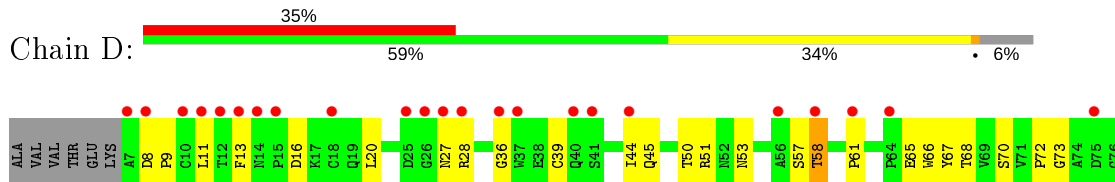
• Molecule 3: Beta-2-microglobulin

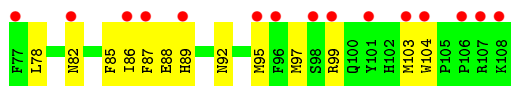


• Molecule 3: Beta-2-microglobulin



• Molecule 4: E3 19 kDa protein

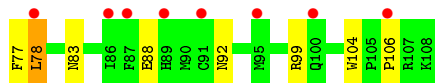
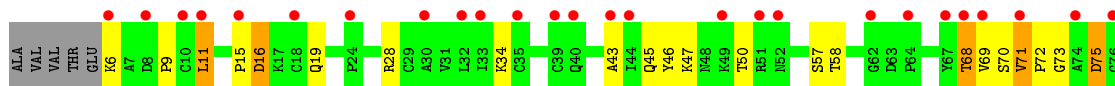




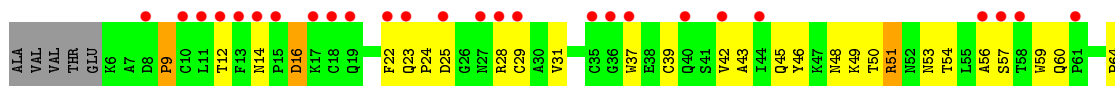
• Molecule 4: E3 19 kDa protein



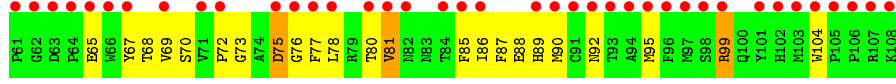
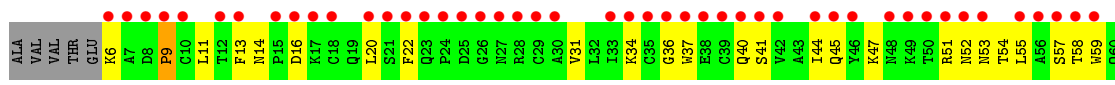
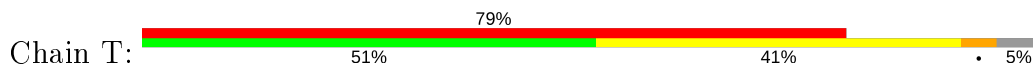
• Molecule 4: E3 19 kDa protein



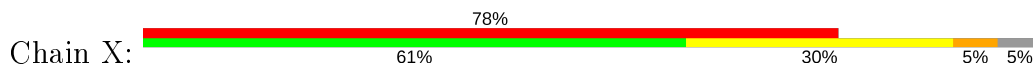
• Molecule 4: E3 19 kDa protein

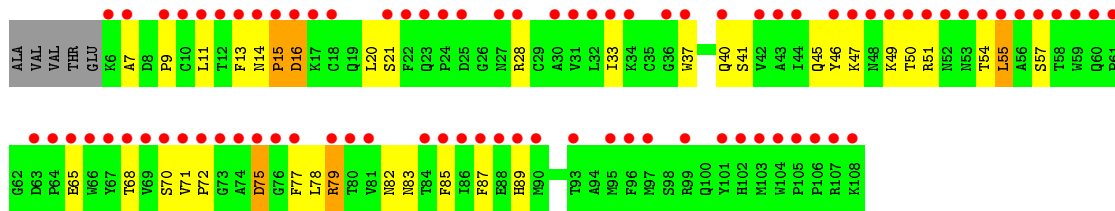


• Molecule 4: E3 19 kDa protein



• Molecule 4: E3 19 kDa protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	165.73Å 165.73Å 122.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 2.64 49.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.62-2.64) 99.3 (49.62-2.64)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.257 , 0.288 0.217 , 0.236	Depositor DCC
R_{free} test set	1983 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.359 for -h,-k,l 0.390 for h,-h-k,-l 0.337 for -k,-h,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 110879 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.38	1/2202 (0.0%)	0.60	0/2983
1	E	0.32	0/2245	0.59	0/3045
1	I	0.29	0/2109	0.57	0/2852
1	M	0.39	0/2221	0.75	3/3012 (0.1%)
1	Q	0.36	0/2169	0.69	1/2937 (0.0%)
1	U	0.34	0/2061	0.62	0/2791
2	B	0.46	0/79	0.66	0/108
2	F	0.48	0/79	0.79	0/108
2	J	0.32	0/79	0.47	0/108
2	N	0.37	0/79	0.45	0/108
2	R	0.33	0/79	0.48	0/108
2	V	0.47	0/79	0.89	1/108 (0.9%)
3	C	0.31	0/824	0.57	0/1115
3	G	0.28	0/843	0.57	0/1141
3	K	0.28	0/843	0.52	0/1141
3	O	0.28	0/843	0.54	0/1141
3	S	0.28	0/843	0.56	0/1141
3	W	0.30	0/843	0.59	0/1141
4	D	0.28	0/849	0.56	0/1154
4	H	0.34	0/858	0.63	0/1165
4	L	0.27	0/858	0.58	0/1165
4	P	0.31	0/858	0.57	0/1165
4	T	0.28	0/858	0.55	0/1165
4	X	0.29	0/858	0.64	1/1165 (0.1%)
All	All	0.33	1/23659 (0.0%)	0.61	6/32067 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	SER	CB-OG	-7.13	1.32	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	202	ARG	NE-CZ-NH2	-17.95	111.33	120.30
1	M	202	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	V	2	LEU	CA-CB-CG	-5.83	101.89	115.30
1	Q	27	TYR	CA-CB-CG	5.74	124.31	113.40
1	M	190	THR	OG1-CB-CG2	-5.69	96.91	110.00
4	X	55	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	189	MET	Peptide

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	2144	0	1999	131	1
1	E	2183	0	2037	105	0
1	I	2053	0	1916	103	0
1	M	2160	0	2016	150	0
1	Q	2111	0	1966	114	0
1	U	2007	0	1881	112	0
2	B	76	0	79	12	0
2	F	76	0	79	9	0
2	J	76	0	79	6	0
2	N	76	0	79	10	0
2	R	76	0	79	8	0
2	V	76	0	79	8	0
3	C	802	0	770	27	0
3	G	820	0	790	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	820	0	790	29	0
3	O	820	0	790	32	0
3	S	820	0	790	36	0
3	W	820	0	790	41	0
4	D	823	0	773	27	0
4	H	832	0	786	16	0
4	L	832	0	786	22	0
4	P	832	0	786	26	0
4	T	832	0	786	39	0
4	X	832	0	786	29	0
5	A	3	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	I	5	0	0	0	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	0	0
5	O	2	0	0	1	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
5	U	3	0	0	0	0
5	W	1	0	0	0	0
All	All	23039	0	21712	1015	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 23.

All (1015) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLN:HB2	1:I:48:ARG:HH12	1.24	1.01
1:M:205:ALA:HB3	1:M:243:LYS:HE2	1.45	0.99
1:Q:5:MET:HG3	1:Q:6:ARG:HG3	1.47	0.96
1:U:250:PRO:O	1:U:253:GLN:NE2	2.01	0.93
1:E:59:TYR:HH	1:E:171:TYR:HH	1.12	0.91
3:W:15:ALA:HB3	3:W:97:ARG:HH12	1.33	0.89
1:E:77:ASP:OD2	1:E:97:ARG:NH2	2.07	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HG2	1:A:6:ARG:HG2	1.58	0.86
1:A:14:ARG:HB3	1:A:17:ARG:HB3	1.58	0.85
1:U:82:ARG:NH2	1:U:88:SER:O	2.10	0.85
3:C:12:ARG:NH2	4:D:97:MET:SD	2.49	0.84
1:A:224:GLN:HE22	1:A:228:THR:H	1.23	0.84
1:Q:77:ASP:OD2	1:Q:97:ARG:NH2	2.10	0.83
1:M:77:ASP:OD2	1:M:97:ARG:NH2	2.13	0.82
1:Q:217:TRP:HD1	1:Q:217:TRP:H	1.25	0.82
4:T:44:ILE:HD13	4:T:55:LEU:HB2	1.60	0.82
1:U:93:HIS:ND1	1:U:119:ASP:OD2	2.12	0.81
1:M:21:ARG:NH1	1:M:22:PHE:H	1.77	0.81
1:Q:141:GLN:OE1	1:Q:144:LYS:NZ	2.14	0.80
3:C:47:GLU:O	3:W:89:GLN:NE2	2.14	0.80
1:E:223:ASP:OD1	1:E:223:ASP:N	2.13	0.80
1:U:173:GLU:O	4:X:51:ARG:NH2	2.14	0.80
1:M:190:THR:O	1:M:202:ARG:HG2	1.82	0.80
1:A:17:ARG:HD3	3:W:44:GLU:HB2	1.63	0.80
1:A:127:LYS:NZ	1:A:132:SER:OG	2.11	0.80
3:G:35:ILE:HD11	3:G:84:HIS:CD2	2.17	0.80
3:C:37:VAL:HB	3:C:82:VAL:HG22	1.61	0.79
1:A:177:GLU:O	4:D:28:ARG:NH1	2.15	0.79
1:I:32:GLN:HB2	1:I:48:ARG:NH1	1.96	0.79
1:A:99:TYR:HB3	1:A:114:HIS:HD2	1.48	0.79
1:M:205:ALA:CB	1:M:243:LYS:HE2	2.13	0.79
1:M:188:HIS:HB2	1:M:204:TRP:HZ2	1.49	0.78
4:T:70:SER:HB3	4:T:78:LEU:HD21	1.66	0.78
1:E:201:LEU:N	1:E:247:VAL:O	2.17	0.78
3:G:39:LEU:HB2	3:G:49:VAL:HG11	1.66	0.77
4:T:92:ASN:HA	4:T:99:ARG:NH2	1.99	0.77
1:M:6:ARG:HH22	1:M:115:GLN:HG3	1.50	0.77
1:Q:262:GLN:HE22	1:Q:269:PRO:HB3	1.50	0.76
3:G:54:LEU:HG	3:G:64:LEU:HD11	1.66	0.76
4:X:77:PHE:O	4:X:79:ARG:NH1	2.18	0.76
1:I:6:ARG:NH1	1:I:98:MET:SD	2.58	0.76
1:Q:21:ARG:NH1	1:Q:38:SER:OG	2.18	0.76
1:A:9:PHE:HB2	1:A:97:ARG:HB2	1.67	0.76
3:K:56:PHE:HA	3:K:62:PHE:HA	1.68	0.76
1:I:77:ASP:OD2	1:I:97:ARG:NH2	2.18	0.76
1:U:77:ASP:OD2	1:U:97:ARG:NH2	2.20	0.75
1:M:147:TRP:NE1	2:N:8:TYR:O	2.19	0.75
1:U:14:ARG:HG2	1:U:17:ARG:HB2	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:PHE:HA	3:C:62:PHE:HA	1.69	0.74
4:T:69:VAL:HG23	4:T:81:VAL:HG13	1.70	0.74
1:M:21:ARG:NH2	1:M:37:ASP:HA	2.01	0.74
1:Q:219:ARG:HB2	1:Q:257:TYR:CZ	2.23	0.74
3:S:31:HIS:HD2	3:S:32:PRO:HA	1.51	0.74
4:T:72:PRO:HA	4:T:78:LEU:HA	1.70	0.74
1:Q:5:MET:HG2	1:Q:27:TYR:HE2	1.52	0.74
3:S:56:PHE:HA	3:S:62:PHE:HA	1.69	0.74
4:L:16:ASP:O	4:L:83:ASN:ND2	2.22	0.73
1:Q:238:ASP:OD2	3:S:12:ARG:NH1	2.20	0.73
3:S:73:THR:OG1	3:S:75:LYS:HG2	1.89	0.73
3:G:81:ARG:HG2	3:G:92:ILE:HG12	1.69	0.73
1:I:218:GLN:HB3	1:I:260:HIS:HD2	1.54	0.73
4:T:92:ASN:HA	4:T:99:ARG:HH22	1.54	0.72
3:W:56:PHE:HA	3:W:62:PHE:HA	1.69	0.72
1:E:209:TYR:H	1:E:209:TYR:HD2	1.36	0.72
3:K:54:LEU:HG	3:K:64:LEU:HD11	1.72	0.72
1:Q:14:ARG:HB3	1:Q:17:ARG:HB2	1.70	0.72
1:M:231:VAL:HG21	1:M:244:TRP:HE3	1.55	0.72
3:G:84:HIS:ND1	3:G:86:THR:HG23	2.05	0.71
1:M:97:ARG:HG2	1:M:116:TYR:HD1	1.55	0.71
1:M:250:PRO:O	1:M:253:GLN:NE2	2.23	0.71
3:G:43:GLY:HA2	1:Q:17:ARG:HH11	1.55	0.71
1:U:109:PHE:O	1:U:111:ARG:NH2	2.22	0.71
1:A:4:SER:HB3	1:A:103:VAL:HG22	1.71	0.71
1:A:8:PHE:HB2	1:A:25:VAL:HG13	1.72	0.71
1:A:73:THR:HG23	1:A:97:ARG:HH22	1.55	0.71
1:E:250:PRO:O	1:E:253:GLN:NE2	2.23	0.71
1:E:21:ARG:NH1	1:E:38:SER:OG	2.20	0.70
1:U:120:GLY:N	1:U:123:TYR:OH	2.24	0.70
1:U:9:PHE:HB3	1:U:74:HIS:HE1	1.55	0.70
1:A:223:ASP:OD1	1:A:223:ASP:N	2.24	0.70
3:C:11:SER:OG	3:C:21:ASN:ND2	2.23	0.70
1:A:13:SER:HB3	1:A:93:HIS:H	1.56	0.70
1:I:235:PRO:O	3:K:10:TYR:OH	2.07	0.70
1:Q:35:ARG:HG3	1:Q:46:GLU:HG3	1.74	0.70
3:W:44:GLU:OE2	3:W:81:ARG:NH2	2.22	0.70
1:M:109:PHE:O	1:M:111:ARG:NH2	2.24	0.70
3:K:24:ASN:OD1	3:K:24:ASN:N	2.24	0.70
3:K:19:LYS:HE2	3:K:20:SER:H	1.57	0.69
1:E:45:MET:H	1:E:64:THR:HG22	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:13:PHE:HE1	4:T:73:GLY:HA2	1.57	0.69
1:U:13:SER:HB3	1:U:93:HIS:H	1.56	0.69
1:I:27:TYR:HA	1:I:32:GLN:HA	1.75	0.69
1:I:147:TRP:NE1	2:J:8:TYR:O	2.23	0.69
1:I:73:THR:OG1	2:J:7:VAL:O	2.11	0.69
3:S:84:HIS:ND1	3:S:86:THR:HG23	2.07	0.69
1:A:45:MET:H	1:A:64:THR:HG22	1.57	0.69
1:I:124:ILE:HD11	1:I:140:ALA:HA	1.75	0.69
4:H:72:PRO:HA	4:H:78:LEU:HA	1.74	0.68
1:A:124:ILE:HG21	1:A:147:TRP:HZ3	1.58	0.68
1:I:219:ARG:N	1:I:222:GLU:OE2	2.25	0.68
1:M:45:MET:H	1:M:64:THR:HG22	1.57	0.68
1:Q:28:VAL:O	1:Q:31:THR:OG1	2.09	0.68
4:X:70:SER:HB3	4:X:78:LEU:HD21	1.73	0.68
1:M:232:GLU:OE1	3:O:28:SER:OG	2.09	0.68
1:A:201:LEU:N	1:A:247:VAL:O	2.27	0.68
3:G:24:ASN:OD1	3:G:24:ASN:N	2.26	0.68
1:M:37:ASP:HB3	1:M:40:ALA:HB2	1.76	0.68
3:C:5:PRO:HB3	3:C:30:PHE:HB3	1.76	0.68
1:E:109:PHE:O	1:E:111:ARG:NH2	2.26	0.68
1:I:218:GLN:NE2	1:I:220:ASP:O	2.25	0.68
1:I:4:SER:HB3	1:I:168:LEU:HD21	1.74	0.68
1:M:13:SER:HA	1:M:20:PRO:HB3	1.76	0.68
1:A:162:GLY:H	1:A:165:VAL:HG22	1.58	0.67
1:U:24:ALA:HB3	1:U:36:PHE:HB3	1.75	0.67
1:E:24:ALA:HB3	1:E:36:PHE:HB3	1.76	0.67
3:G:56:PHE:HA	3:G:62:PHE:HA	1.75	0.67
1:E:235:PRO:HB2	3:G:65:LEU:HD22	1.77	0.67
1:Q:5:MET:HG2	1:Q:27:TYR:CE2	2.29	0.67
3:O:24:ASN:N	3:O:24:ASN:OD1	2.27	0.67
3:O:56:PHE:HA	3:O:62:PHE:HA	1.75	0.67
1:I:4:SER:OG	1:I:102:ASP:OD1	2.12	0.67
4:H:89:HIS:NE2	4:L:19:GLN:OE1	2.27	0.67
1:M:108:ARG:HA	1:M:169:ARG:HH21	1.60	0.67
1:Q:3:HIS:O	1:Q:3:HIS:ND1	2.27	0.67
1:M:6:ARG:NH1	1:M:98:MET:SD	2.68	0.67
4:X:50:THR:O	4:X:51:ARG:HD3	1.95	0.67
1:U:124:ILE:HD11	1:U:133:TRP:HB3	1.75	0.66
4:T:36:GLY:O	4:T:53:ASN:ND2	2.26	0.66
3:G:13:HIS:H	3:G:21:ASN:HD21	1.44	0.66
1:U:189:MET:HG3	1:U:201:LEU:HD23	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:ARG:NH1	1:M:38:SER:OG	2.29	0.66
1:U:13:SER:OG	1:U:82:ARG:NH1	2.27	0.66
1:U:131:ARG:HD3	1:U:153:ALA:HB3	1.76	0.66
1:A:24:ALA:HB3	1:A:36:PHE:HB3	1.77	0.66
1:U:181:ARG:HH21	4:X:28:ARG:HH11	1.44	0.66
3:W:26:TYR:HB2	3:W:65:LEU:HD13	1.78	0.65
1:Q:217:TRP:CD1	1:Q:217:TRP:N	2.64	0.65
3:G:40:LEU:HD11	3:G:79:ALA:HB3	1.78	0.65
1:A:54:GLN:O	4:D:51:ARG:NH2	2.30	0.65
4:L:43:ALA:HB3	4:L:70:SER:HB2	1.77	0.65
1:I:238:ASP:OD2	3:K:12:ARG:NH1	2.29	0.65
1:M:20:PRO:HG2	1:M:75:ARG:HD3	1.78	0.65
1:A:66:LYS:HE3	2:B:2:LEU:HB3	1.77	0.65
3:W:24:ASN:OD1	3:W:24:ASN:N	2.30	0.65
1:Q:147:TRP:NE1	2:R:8:TYR:O	2.30	0.64
3:O:54:LEU:HG	3:O:64:LEU:HD11	1.78	0.64
1:A:213:ILE:HG12	1:A:263:HIS:HD2	1.62	0.64
1:U:45:MET:H	1:U:64:THR:HG22	1.62	0.64
1:E:211:ALA:HB1	1:E:233:THR:HG21	1.79	0.64
1:A:13:SER:OG	1:A:82:ARG:NH1	2.30	0.64
4:P:88:GLU:O	4:P:92:ASN:ND2	2.31	0.64
1:Q:263:HIS:CD2	1:Q:265:GLY:H	2.16	0.64
1:A:93:HIS:ND1	1:A:119:ASP:OD2	2.31	0.64
3:K:30:PHE:CE1	3:K:62:PHE:HB2	2.33	0.64
1:M:231:VAL:HG21	1:M:244:TRP:CE3	2.33	0.64
1:A:157:ARG:HA	1:A:160:LEU:HD12	1.80	0.63
4:P:16:ASP:O	4:P:83:ASN:ND2	2.31	0.63
1:Q:82:ARG:NH2	1:Q:88:SER:O	2.31	0.63
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.11	0.63
1:E:129:ASP:HB2	1:E:132:SER:OG	1.98	0.63
1:Q:157:ARG:HA	1:Q:160:LEU:HD12	1.79	0.63
3:W:13:HIS:H	3:W:21:ASN:HD21	1.43	0.63
1:M:191:HIS:HE1	1:M:193:ALA:HB2	1.62	0.63
1:E:124:ILE:HG23	1:E:133:TRP:CH2	2.34	0.63
3:G:5:PRO:HB3	3:G:30:PHE:HB3	1.81	0.63
2:R:1:LEU:HD23	2:R:2:LEU:HD12	1.81	0.62
3:S:24:ASN:OD1	3:S:24:ASN:N	2.32	0.62
1:M:54:GLN:O	4:P:51:ARG:NH2	2.32	0.62
1:U:191:HIS:CD2	1:U:201:LEU:HD12	2.34	0.62
4:D:28:ARG:NH2	4:D:58:THR:OG1	2.32	0.62
1:M:95:VAL:HG13	1:M:116:TYR:CE1	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:234:ARG:HE	1:U:242:GLN:HB2	1.63	0.62
1:U:73:THR:OG1	2:V:7:VAL:O	2.15	0.62
4:X:16:ASP:O	4:X:83:ASN:ND2	2.32	0.62
4:P:43:ALA:HB3	4:P:70:SER:HB2	1.81	0.62
1:U:37:ASP:HB3	1:U:40:ALA:HB2	1.82	0.62
1:A:82:ARG:HD2	1:A:93:HIS:HB2	1.82	0.62
4:P:42:VAL:HG22	4:P:71:VAL:HG12	1.81	0.62
1:I:13:SER:HA	1:I:20:PRO:HB3	1.81	0.61
1:M:35:ARG:HD2	3:O:53:ASP:HB2	1.80	0.61
3:K:79:ALA:HB2	3:K:94:LYS:HG2	1.82	0.61
1:E:234:ARG:HD3	3:G:8:GLN:NE2	2.16	0.61
4:T:92:ASN:O	4:T:99:ARG:NH1	2.33	0.61
1:A:188:HIS:HB3	1:A:204:TRP:HZ2	1.64	0.61
1:I:9:PHE:HB3	1:I:74:HIS:HE1	1.65	0.61
1:U:14:ARG:NH1	1:U:21:ARG:HB2	2.16	0.61
1:A:188:HIS:CD2	1:A:189:MET:H	2.19	0.61
1:A:235:PRO:O	3:C:10:TYR:OH	2.17	0.61
1:A:99:TYR:HB3	1:A:114:HIS:CD2	2.32	0.61
3:S:11:SER:OG	3:S:21:ASN:ND2	2.34	0.61
1:I:131:ARG:NH2	1:I:154:GLU:OE1	2.34	0.61
1:E:102:ASP:OD2	1:E:113:TYR:OH	2.16	0.60
3:G:36:GLU:HB3	3:G:83:ASN:ND2	2.16	0.60
1:I:45:MET:H	1:I:64:THR:HG22	1.65	0.60
3:S:29:GLY:HA2	3:S:61:SER:HB2	1.83	0.60
1:U:174:ASN:OD1	4:X:51:ARG:NH1	2.34	0.60
1:I:131:ARG:HD3	1:I:153:ALA:HB3	1.83	0.60
1:U:202:ARG:HG3	1:U:204:TRP:CZ3	2.37	0.60
3:O:73:THR:OG1	3:O:75:LYS:HG2	2.01	0.60
4:P:72:PRO:HA	4:P:78:LEU:HA	1.83	0.60
1:A:141:GLN:N	1:A:141:GLN:OE1	2.33	0.60
1:A:98:MET:HB3	1:A:115:GLN:HG3	1.82	0.60
1:E:112:GLY:HA3	1:E:160:LEU:HD11	1.83	0.60
1:M:71:SER:O	1:M:75:ARG:HG2	2.01	0.60
1:Q:144:LYS:HA	1:Q:147:TRP:CE3	2.37	0.60
4:T:34:LYS:HA	4:T:54:THR:HG22	1.82	0.60
1:Q:124:ILE:HD11	1:Q:140:ALA:HA	1.83	0.60
1:E:116:TYR:N	1:E:124:ILE:O	2.18	0.59
1:M:28:VAL:O	1:M:31:THR:OG1	2.18	0.59
4:D:72:PRO:HA	4:D:78:LEU:HA	1.82	0.59
3:O:7:ILE:HD11	3:O:80:CYS:HB3	1.84	0.59
1:U:249:VAL:HG12	1:U:253:GLN:NE2	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:15:PRO:HG2	4:H:71:VAL:HG11	1.83	0.59
1:M:191:HIS:HB2	1:M:201:LEU:HG	1.84	0.59
1:E:21:ARG:CZ	1:E:39:ASP:HB2	2.33	0.59
3:G:36:GLU:HB3	3:G:83:ASN:HD21	1.67	0.59
4:P:49:LYS:NZ	4:P:56:ALA:O	2.29	0.59
4:X:72:PRO:HA	4:X:78:LEU:HA	1.84	0.59
1:I:262:GLN:HG2	1:I:269:PRO:HB3	1.83	0.59
1:M:21:ARG:NH2	1:M:22:PHE:O	2.36	0.59
1:A:82:ARG:HH21	1:A:87:GLN:HG3	1.66	0.59
1:M:137:ASP:OD1	1:M:138:MET:N	2.28	0.59
1:Q:212:GLU:N	1:Q:212:GLU:OE1	2.36	0.59
1:I:27:TYR:HH	3:K:63:TYR:HH	1.43	0.59
1:Q:35:ARG:HE	1:Q:48:ARG:HD3	1.68	0.59
3:C:24:ASN:HB3	3:C:65:LEU:HD11	1.83	0.59
1:E:182:THR:HA	1:E:209:TYR:CZ	2.38	0.59
4:L:72:PRO:HA	4:L:78:LEU:HA	1.85	0.59
3:K:19:LYS:HE2	3:K:20:SER:N	2.18	0.59
1:Q:44:ARG:HA	1:Q:64:THR:HG23	1.85	0.59
1:I:181:ARG:HH21	4:L:28:ARG:HH11	1.50	0.58
1:A:201:LEU:HD22	1:A:257:TYR:OH	2.04	0.58
1:M:157:ARG:HA	1:M:160:LEU:HD12	1.84	0.58
1:M:235:PRO:HA	1:M:241:PHE:HD1	1.69	0.58
1:Q:154:GLU:HA	1:Q:157:ARG:HB3	1.85	0.58
4:T:75:ASP:N	4:T:75:ASP:OD1	2.35	0.58
1:U:5:MET:HG2	1:U:6:ARG:HG2	1.86	0.58
1:A:208:PHE:CE1	1:A:241:PHE:HB2	2.38	0.58
3:O:72:PRO:HB3	3:O:95:TRP:HH2	1.67	0.58
1:Q:154:GLU:HG3	1:Q:157:ARG:HD3	1.84	0.58
1:A:63:GLU:OE1	2:B:2:LEU:HB2	2.04	0.58
1:E:159:TYR:OH	2:F:1:LEU:O	2.14	0.58
3:G:29:GLY:HA2	3:G:61:SER:HB2	1.84	0.58
3:G:59:ASP:N	3:G:59:ASP:OD1	2.37	0.58
1:M:22:PHE:HB2	1:M:75:ARG:HH12	1.68	0.57
1:M:73:THR:HG23	1:M:97:ARG:HH12	1.69	0.57
1:A:191:HIS:CE1	1:A:201:LEU:HD21	2.38	0.57
4:D:70:SER:HB3	4:D:78:LEU:HD21	1.86	0.57
1:E:209:TYR:CD1	1:E:210:PRO:HD3	2.39	0.57
1:M:204:TRP:HZ3	1:M:206:LEU:HB2	1.69	0.57
1:M:4:SER:OG	1:M:103:VAL:N	2.35	0.57
1:A:3:HIS:ND1	1:A:3:HIS:O	2.32	0.57
1:E:13:SER:HA	1:E:20:PRO:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:213:ILE:HD12	1:Q:263:HIS:HB2	1.87	0.57
1:Q:235:PRO:HB2	3:S:65:LEU:HD22	1.86	0.57
1:U:253:GLN:NE2	1:U:253:GLN:H	2.02	0.57
1:U:77:ASP:O	1:U:80:THR:OG1	2.18	0.57
3:G:35:ILE:HG22	3:G:37:VAL:HG12	1.86	0.57
1:I:213:ILE:HB	1:I:263:HIS:HD2	1.70	0.57
1:Q:116:TYR:HE1	1:Q:147:TRP:CH2	2.23	0.57
4:D:92:ASN:HA	4:D:99:ARG:NH2	2.20	0.57
1:E:133:TRP:CD1	1:E:144:LYS:HD3	2.40	0.57
1:M:107:TRP:O	1:M:169:ARG:NE	2.32	0.57
1:M:1:GLY:O	1:M:3:HIS:ND1	2.38	0.57
1:M:250:PRO:HB2	1:M:253:GLN:HE22	1.70	0.57
1:Q:102:ASP:OD2	1:Q:113:TYR:OH	2.22	0.57
1:E:114:HIS:HD1	1:E:126:LEU:HB2	1.70	0.56
4:T:37:TRP:HZ2	4:T:54:THR:HG1	1.53	0.56
1:A:99:TYR:HA	1:A:114:HIS:HA	1.87	0.56
1:M:213:ILE:HB	1:M:243:LYS:HZ2	1.69	0.56
1:E:76:VAL:HG23	2:F:8:TYR:HE1	1.69	0.56
1:Q:185:PRO:HB3	1:Q:208:PHE:CZ	2.40	0.56
1:U:177:GLU:OE1	4:X:49:LYS:NZ	2.39	0.56
1:I:98:MET:HE2	3:K:56:PHE:HE1	1.71	0.56
1:M:124:ILE:HG21	1:M:147:TRP:HZ3	1.70	0.56
1:Q:205:ALA:HB1	1:Q:208:PHE:CE2	2.40	0.56
1:U:174:ASN:HA	4:X:51:ARG:HH12	1.69	0.56
1:M:21:ARG:HH22	1:M:37:ASP:HA	1.70	0.56
1:M:95:VAL:HG13	1:M:116:TYR:HE1	1.69	0.56
1:M:190:THR:HB	1:M:202:ARG:HE	1.71	0.56
1:U:238:ASP:OD2	3:W:12:ARG:NH1	2.38	0.56
1:A:20:PRO:HG3	1:A:78:LEU:HD21	1.86	0.56
1:E:147:TRP:NE1	2:F:8:TYR:O	2.38	0.56
4:P:28:ARG:NH1	4:P:59:TRP:O	2.37	0.56
1:Q:219:ARG:HG3	1:Q:222:GLU:HB2	1.88	0.56
1:U:201:LEU:N	1:U:247:VAL:O	2.39	0.56
1:A:54:GLN:NE2	1:A:174:ASN:O	2.39	0.56
4:D:27:ASN:ND2	4:D:103:MET:HG2	2.21	0.56
1:E:3:HIS:ND1	1:E:3:HIS:O	2.39	0.56
1:E:156:LEU:HA	2:F:3:PHE:CE1	2.40	0.56
1:I:111:ARG:NH1	1:I:111:ARG:HB2	2.20	0.56
4:D:61:PRO:HD3	4:D:104:TRP:CH2	2.41	0.56
1:M:131:ARG:HH22	1:M:151:HIS:CD2	2.24	0.56
3:W:11:SER:OG	3:W:21:ASN:ND2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:54:LEU:HD11	3:W:62:PHE:CD1	2.41	0.56
3:G:40:LEU:HB2	3:G:43:GLY:O	2.06	0.55
1:M:146:LYS:HZ1	2:N:8:TYR:HB3	1.71	0.55
3:S:45:ARG:NH1	3:S:46:ILE:HG22	2.21	0.55
3:W:31:HIS:HD2	3:W:32:PRO:HA	1.71	0.55
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.39	0.55
1:I:3:HIS:ND1	1:I:3:HIS:O	2.39	0.55
4:L:11:LEU:HD12	4:L:11:LEU:H	1.70	0.55
1:Q:86:ASN:N	1:Q:86:ASN:OD1	2.37	0.55
1:E:70:HIS:O	1:E:74:HIS:ND1	2.38	0.55
1:A:177:GLU:HG3	4:D:57:SER:HA	1.89	0.55
1:E:20:PRO:HG3	1:E:78:LEU:HD21	1.88	0.55
1:Q:30:ASP:OD2	1:Q:211:ALA:N	2.31	0.55
4:X:75:ASP:N	4:X:75:ASP:OD1	2.40	0.55
1:E:94:THR:OG1	1:E:96:GLN:OE1	2.24	0.55
3:K:13:HIS:H	3:K:21:ASN:HD21	1.55	0.55
1:A:107:TRP:O	1:A:169:ARG:NE	2.35	0.55
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.39	0.55
3:C:11:SER:OG	3:C:13:HIS:O	2.23	0.55
4:H:70:SER:HB3	4:H:78:LEU:HD21	1.88	0.55
3:O:69:GLU:OE2	3:W:19:LYS:NZ	2.29	0.55
1:U:154:GLU:HG2	1:U:157:ARG:HD3	1.89	0.55
1:A:188:HIS:CG	1:A:189:MET:H	2.25	0.55
3:K:35:ILE:HG22	3:K:37:VAL:HG12	1.89	0.55
1:E:144:LYS:O	1:E:148:GLU:HG3	2.05	0.55
1:I:147:TRP:HZ2	2:J:9:VAL:HG12	1.72	0.55
1:U:181:ARG:HH21	4:X:28:ARG:NH1	2.04	0.55
4:X:37:TRP:HE1	4:X:54:THR:HG1	1.52	0.55
1:A:224:GLN:HE22	1:A:228:THR:N	1.97	0.55
1:I:218:GLN:HB3	1:I:260:HIS:CD2	2.38	0.55
4:X:37:TRP:NE1	4:X:54:THR:OG1	2.37	0.54
1:A:263:HIS:HB3	1:A:266:LEU:HB2	1.90	0.54
1:I:13:SER:HB3	1:I:93:HIS:H	1.73	0.54
4:T:45:GLN:NE2	4:T:47:LYS:O	2.40	0.54
1:U:6:ARG:HD2	1:U:8:PHE:CE2	2.41	0.54
1:A:147:TRP:HZ2	2:B:9:VAL:HG12	1.71	0.54
1:E:33:PHE:CE2	1:E:52:ILE:HB	2.42	0.54
1:M:14:ARG:HB3	1:M:17:ARG:HG2	1.88	0.54
3:K:37:VAL:HB	3:K:82:VAL:HG22	1.90	0.54
1:M:115:GLN:HA	1:M:125:ALA:HA	1.90	0.54
1:U:114:HIS:CD2	1:U:156:LEU:HD21	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:201:LEU:HD13	1:U:257:TYR:OH	2.07	0.54
1:I:257:TYR:H	1:I:257:TYR:HD2	1.55	0.54
1:U:202:ARG:HG3	1:U:204:TRP:CE3	2.42	0.54
1:E:118:TYR:H	1:E:118:TYR:HD2	1.56	0.54
1:M:78:LEU:HB3	1:M:95:VAL:HG21	1.88	0.54
1:Q:208:PHE:O	1:Q:240:THR:HA	2.07	0.54
1:Q:13:SER:HB2	1:Q:93:HIS:H	1.72	0.54
1:E:115:GLN:HA	1:E:125:ALA:HA	1.89	0.54
1:E:185:PRO:HG3	1:E:208:PHE:HB3	1.88	0.54
1:I:77:ASP:O	1:I:80:THR:OG1	2.19	0.54
1:Q:216:THR:O	1:Q:260:HIS:N	2.40	0.54
1:M:28:VAL:HG11	1:M:51:TRP:HH2	1.73	0.54
1:E:28:VAL:O	1:E:31:THR:OG1	2.23	0.53
1:E:238:ASP:OD2	3:G:12:ARG:NH1	2.41	0.53
1:M:108:ARG:NH1	1:M:169:ARG:HH22	2.06	0.53
1:M:217:TRP:CZ2	1:M:224:GLN:HB2	2.43	0.53
1:E:261:VAL:HG13	1:E:270:LEU:HB2	1.89	0.53
3:W:23:LEU:HG	3:W:70:PHE:CG	2.44	0.53
4:P:75:ASP:OD1	4:P:75:ASP:N	2.41	0.53
3:W:30:PHE:HB2	3:W:84:HIS:NE2	2.24	0.53
1:M:103:VAL:HG13	1:M:107:TRP:HA	1.91	0.53
1:M:94:THR:OG1	1:M:96:GLN:OE1	2.25	0.53
1:Q:127:LYS:HG3	1:Q:128:GLU:N	2.23	0.53
3:G:56:PHE:HB3	3:G:62:PHE:CD1	2.43	0.53
1:M:238:ASP:OD1	1:M:240:THR:OG1	2.23	0.53
1:M:33:PHE:HD1	1:M:34:VAL:HG23	1.74	0.53
1:Q:139:ALA:HA	1:Q:142:THR:HG22	1.90	0.53
4:D:45:GLN:HB3	4:D:68:THR:OG1	2.08	0.53
1:Q:121:LYS:HG3	1:Q:122:ASP:H	1.72	0.53
1:U:11:SER:HA	1:U:21:ARG:O	2.09	0.53
1:U:7:TYR:C	1:U:8:PHE:HD2	2.12	0.53
1:A:73:THR:OG1	2:B:7:VAL:O	2.21	0.53
3:C:21:ASN:HB3	3:C:70:PHE:CE2	2.43	0.53
4:H:95:MET:HE1	4:H:104:TRP:CG	2.44	0.53
1:I:48:ARG:HG2	1:I:48:ARG:HH21	1.74	0.53
3:O:12:ARG:HH21	4:P:97:MET:HB3	1.74	0.53
4:P:28:ARG:NH2	4:P:60:GLN:HB3	2.24	0.53
1:A:17:ARG:C	3:W:44:GLU:HB3	2.29	0.53
1:I:19:GLU:OE1	1:I:20:PRO:HD2	2.09	0.53
1:M:1:GLY:HA2	1:M:105:SER:HA	1.90	0.53
4:X:45:GLN:HB3	4:X:68:THR:OG1	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:TRP:CZ2	2:J:9:VAL:HG12	2.44	0.52
1:M:208:PHE:CE1	1:M:241:PHE:HB2	2.44	0.52
1:M:74:HIS:NE2	1:M:97:ARG:HG3	2.24	0.52
4:H:46:TYR:CE2	4:H:47:LYS:HE3	2.44	0.52
1:M:14:ARG:HD2	1:M:21:ARG:HB2	1.90	0.52
1:Q:219:ARG:HB2	1:Q:257:TYR:CE1	2.45	0.52
1:U:204:TRP:HZ2	1:U:244:TRP:CD2	2.27	0.52
1:A:66:LYS:HD2	2:B:4:GLY:HA2	1.91	0.52
1:E:124:ILE:HG23	1:E:133:TRP:CZ2	2.44	0.52
1:Q:216:THR:N	1:Q:260:HIS:O	2.42	0.52
3:S:56:PHE:HB3	3:S:62:PHE:CD1	2.44	0.52
3:W:31:HIS:CD2	3:W:32:PRO:HA	2.43	0.52
1:E:73:THR:OG1	2:F:7:VAL:O	2.24	0.52
3:O:30:PHE:CE1	3:O:62:PHE:HB2	2.45	0.52
1:Q:14:ARG:NE	1:Q:19:GLU:O	2.42	0.52
4:X:20:LEU:HD11	4:X:85:PHE:CD1	2.44	0.52
3:S:35:ILE:CD1	3:S:84:HIS:HD2	2.23	0.52
4:T:65:GLU:HA	4:T:87:PHE:CD2	2.45	0.52
1:U:235:PRO:O	3:W:10:TYR:OH	2.22	0.52
1:E:141:GLN:HA	1:E:144:LYS:HG2	1.91	0.52
3:S:31:HIS:CD2	3:S:32:PRO:HA	2.38	0.52
1:U:191:HIS:HE1	1:U:193:ALA:HB2	1.74	0.52
1:U:263:HIS:CD2	1:U:265:GLY:H	2.28	0.52
3:C:30:PHE:HB2	3:C:84:HIS:HE2	1.74	0.52
3:K:39:LEU:HB2	3:K:49:VAL:HG11	1.90	0.52
1:Q:209:TYR:HB3	1:Q:210:PRO:HD3	1.90	0.52
1:Q:22:PHE:CE2	1:Q:24:ALA:HB2	2.45	0.52
3:S:41:LYS:HB2	3:S:45:ARG:CZ	2.39	0.52
3:W:40:LEU:HG	3:W:43:GLY:O	2.10	0.52
1:Q:63:GLU:OE1	2:R:2:LEU:HD13	2.10	0.52
3:C:11:SER:HG	3:C:21:ASN:HD21	1.57	0.52
1:M:14:ARG:CZ	1:M:17:ARG:HH21	2.22	0.52
3:W:7:ILE:HD11	3:W:93:VAL:HB	1.91	0.52
4:X:49:LYS:HE3	4:X:51:ARG:CZ	2.39	0.52
1:U:250:PRO:C	1:U:253:GLN:HE22	2.06	0.51
3:G:57:SER:OG	3:G:58:LYS:N	2.43	0.51
1:M:93:HIS:ND1	1:M:119:ASP:OD2	2.35	0.51
3:O:29:GLY:HA2	3:O:61:SER:HB2	1.91	0.51
4:P:39:CYS:O	4:P:53:ASN:ND2	2.29	0.51
1:A:115:GLN:HA	1:A:125:ALA:HA	1.92	0.51
4:H:49:LYS:HE3	4:H:51:ARG:HH21	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:PRO:O	3:G:10:TYR:OH	2.17	0.51
1:I:14:ARG:HG2	1:I:17:ARG:HB3	1.93	0.51
1:M:215:LEU:HD21	1:M:243:LYS:HE3	1.92	0.51
1:A:230:LEU:H	1:A:230:LEU:HD23	1.74	0.51
1:E:234:ARG:HE	1:E:242:GLN:HB2	1.75	0.51
1:I:121:LYS:HG3	1:I:122:ASP:H	1.75	0.51
1:U:129:ASP:CG	1:U:130:LEU:H	2.14	0.51
1:A:6:ARG:HG3	1:A:8:PHE:CE2	2.46	0.51
1:I:109:PHE:CZ	1:I:111:ARG:HA	2.46	0.51
1:Q:171:TYR:HE1	2:R:1:LEU:HD13	1.75	0.51
1:A:121:LYS:HG3	1:A:122:ASP:H	1.76	0.51
1:A:137:ASP:O	1:A:141:GLN:NE2	2.43	0.51
1:I:218:GLN:NE2	1:I:222:GLU:H	2.07	0.51
4:T:22:PHE:CD2	4:T:90:MET:HB3	2.46	0.51
1:M:73:THR:OG1	2:N:7:VAL:O	2.28	0.51
4:X:33:ILE:HB	4:X:55:LEU:HG	1.93	0.51
1:A:82:ARG:NH2	1:A:88:SER:O	2.43	0.51
3:G:35:ILE:HD11	3:G:84:HIS:HD2	1.71	0.51
1:A:1:GLY:HA2	1:A:105:SER:HA	1.92	0.51
1:A:177:GLU:HG2	4:D:28:ARG:HH22	1.76	0.51
1:E:27:TYR:OH	1:E:32:GLN:NE2	2.44	0.51
1:I:93:HIS:ND1	1:I:119:ASP:OD2	2.33	0.51
3:S:84:HIS:CE1	3:S:86:THR:HG23	2.46	0.51
4:H:14:ASN:O	4:H:16:ASP:N	2.42	0.50
1:I:109:PHE:CE2	1:I:111:ARG:HA	2.46	0.50
1:I:127:LYS:HD3	1:I:128:GLU:N	2.27	0.50
3:K:84:HIS:ND1	3:K:86:THR:OG1	2.33	0.50
1:Q:164:CYS:O	1:Q:168:LEU:HB2	2.11	0.50
1:Q:11:SER:OG	1:Q:95:VAL:O	2.26	0.50
1:A:108:ARG:HA	1:A:169:ARG:HH21	1.74	0.50
3:G:21:ASN:HB3	3:G:70:PHE:CE2	2.47	0.50
1:I:97:ARG:HD3	1:I:116:TYR:CD2	2.46	0.50
1:Q:145:HIS:ND1	1:Q:148:GLU:OE1	2.30	0.50
1:Q:33:PHE:CE2	1:Q:52:ILE:HB	2.46	0.50
4:L:73:GLY:N	4:L:77:PHE:O	2.41	0.50
1:M:124:ILE:HG21	1:M:147:TRP:CZ3	2.45	0.50
1:M:97:ARG:HG2	1:M:116:TYR:CD1	2.42	0.50
1:Q:109:PHE:CD1	1:Q:161:GLU:HG2	2.46	0.50
1:Q:1:GLY:H2	1:Q:105:SER:HA	1.76	0.50
1:U:108:ARG:HA	1:U:169:ARG:HH21	1.76	0.50
1:A:171:TYR:CE1	2:B:1:LEU:HD22	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:ILE:HG23	4:D:89:HIS:HB2	1.93	0.50
1:E:209:TYR:CG	1:E:210:PRO:CD	2.95	0.50
1:U:35:ARG:HD2	1:U:48:ARG:HG3	1.92	0.50
1:U:94:THR:OG1	1:U:96:GLN:OE1	2.27	0.50
1:I:170:ARG:O	1:I:173:GLU:HG2	2.12	0.50
1:I:234:ARG:HD3	3:K:8:GLN:NE2	2.27	0.50
3:K:5:PRO:HB3	3:K:30:PHE:HB3	1.92	0.50
1:M:116:TYR:CE2	1:M:123:TYR:HD2	2.29	0.50
1:Q:262:GLN:HA	1:Q:266:LEU:HD11	1.93	0.50
1:Q:262:GLN:NE2	1:Q:269:PRO:HB3	2.22	0.50
1:U:97:ARG:HD3	1:U:116:TYR:HD1	1.75	0.50
1:M:191:HIS:ND1	1:M:192:HIS:N	2.59	0.50
1:M:209:TYR:HB3	1:M:210:PRO:HD3	1.93	0.50
1:M:72:GLN:O	1:M:76:VAL:HG22	2.10	0.50
4:D:68:THR:HG22	4:D:82:ASN:OD1	2.11	0.50
1:E:231:VAL:HG11	1:E:244:TRP:CB	2.41	0.50
1:U:177:GLU:HG3	4:X:57:SER:HA	1.94	0.50
3:C:30:PHE:HB2	3:C:84:HIS:NE2	2.27	0.50
1:M:260:HIS:HE1	1:M:271:THR:HG22	1.76	0.50
4:T:73:GLY:N	4:T:77:PHE:O	2.40	0.50
1:U:254:GLU:HB3	1:U:257:TYR:OH	2.12	0.50
3:K:34:ASP:C	3:K:35:ILE:HD12	2.32	0.50
1:Q:93:HIS:ND1	1:Q:119:ASP:OD2	2.45	0.50
1:U:126:LEU:HG	1:U:127:LYS:O	2.11	0.50
3:W:56:PHE:HB3	3:W:62:PHE:CD1	2.47	0.50
1:A:224:GLN:NE2	1:A:228:THR:H	2.01	0.49
1:E:164:CYS:O	1:E:168:LEU:HB2	2.11	0.49
1:E:28:VAL:HG11	1:E:51:TRP:HH2	1.77	0.49
2:V:3:PHE:CE2	2:V:5:TYR:HB2	2.47	0.49
3:S:12:ARG:HB3	3:S:22:PHE:HB2	1.94	0.49
1:M:47:PRO:HB3	1:M:60:TRP:CH2	2.47	0.49
1:U:208:PHE:HB2	1:U:263:HIS:CE1	2.47	0.49
3:C:30:PHE:CE1	3:C:62:PHE:HB2	2.47	0.49
1:M:218:GLN:NE2	1:M:222:GLU:O	2.34	0.49
1:M:250:PRO:C	1:M:253:GLN:HE22	2.13	0.49
4:D:57:SER:OG	4:D:58:THR:N	2.44	0.49
1:E:177:GLU:HG3	4:H:57:SER:HA	1.93	0.49
1:I:139:ALA:HA	1:I:142:THR:HG22	1.93	0.49
1:Q:7:TYR:CZ	1:Q:26:GLY:HA3	2.47	0.49
1:A:33:PHE:HE1	1:A:171:TYR:CD1	2.31	0.49
4:T:14:ASN:O	4:T:16:ASP:N	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:8:PHE:HB2	1:U:25:VAL:HG12	1.93	0.49
1:U:73:THR:HG23	1:U:97:ARG:HH12	1.77	0.49
1:A:152:VAL:HG13	2:B:5:TYR:OH	2.13	0.49
4:D:44:ILE:HD11	4:D:67:TYR:HD1	1.77	0.49
1:I:111:ARG:NH2	1:I:128:GLU:OE2	2.45	0.49
1:M:114:HIS:O	1:M:126:LEU:N	2.41	0.49
1:M:35:ARG:NH1	3:O:53:ASP:OD2	2.40	0.49
1:Q:77:ASP:O	1:Q:80:THR:OG1	2.22	0.49
4:T:95:MET:O	4:T:99:ARG:NH1	2.45	0.49
1:U:21:ARG:NH1	1:U:37:ASP:OD1	2.46	0.49
1:A:146:LYS:HE2	2:B:8:TYR:HE2	1.78	0.49
4:D:88:GLU:O	4:D:92:ASN:ND2	2.46	0.49
1:I:159:TYR:OH	2:J:1:LEU:O	2.25	0.49
1:M:146:LYS:NZ	2:N:8:TYR:HB3	2.27	0.49
1:M:5:MET:HB2	1:M:6:ARG:H	1.46	0.49
4:L:78:LEU:N	4:P:48:ASN:OD1	2.34	0.49
1:E:250:PRO:C	1:E:253:GLN:HE22	2.14	0.49
1:I:127:LYS:C	1:I:129:ASP:H	2.16	0.49
4:L:45:GLN:HB3	4:L:68:THR:OG1	2.13	0.49
1:M:147:TRP:HZ2	2:N:9:VAL:HG12	1.77	0.49
1:M:49:ALA:O	1:M:52:ILE:HG22	2.13	0.49
1:Q:76:VAL:HG13	4:X:7:ALA:O	2.12	0.49
1:I:4:SER:CB	1:I:168:LEU:HD21	2.41	0.48
1:M:116:TYR:CG	1:M:117:ALA:N	2.81	0.48
4:T:22:PHE:CE2	4:T:90:MET:HB3	2.48	0.48
4:L:15:PRO:HG2	4:L:71:VAL:HG11	1.93	0.48
1:M:98:MET:HE2	3:O:56:PHE:HE1	1.78	0.48
1:Q:118:TYR:CG	1:Q:119:ASP:N	2.79	0.48
1:E:27:TYR:HH	3:G:63:TYR:HH	1.60	0.48
1:E:28:VAL:HG11	1:E:51:TRP:CH2	2.48	0.48
1:I:201:LEU:HD13	1:I:257:TYR:OH	2.13	0.48
1:U:114:HIS:O	1:U:114:HIS:ND1	2.46	0.48
3:G:9:VAL:HG22	3:G:25:CYS:SG	2.54	0.48
1:I:234:ARG:HE	1:I:242:GLN:HB2	1.77	0.48
1:M:190:THR:HB	1:M:202:ARG:NE	2.26	0.48
1:M:183:ASP:HB2	1:M:209:TYR:N	2.27	0.48
3:O:41:LYS:HG3	3:O:78:TYR:CE1	2.49	0.48
3:O:37:VAL:HG12	3:O:82:VAL:HG22	1.94	0.48
1:Q:234:ARG:HE	1:Q:242:GLN:HB2	1.78	0.48
4:X:65:GLU:HA	4:X:87:PHE:CD2	2.49	0.48
1:A:232:GLU:O	1:A:234:ARG:HD2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.96	0.48
1:Q:103:VAL:HA	1:Q:110:LEU:H	1.77	0.48
3:S:35:ILE:HD11	3:S:84:HIS:HD2	1.78	0.48
4:H:91:CYS:O	4:H:95:MET:HG3	2.14	0.48
1:I:129:ASP:HB2	1:I:132:SER:OG	2.14	0.48
1:I:32:GLN:N	1:I:32:GLN:OE1	2.40	0.48
4:T:40:GLN:O	4:T:41:SER:OG	2.29	0.48
1:U:127:LYS:C	1:U:129:ASP:H	2.16	0.48
1:A:82:ARG:NH2	1:A:87:GLN:HG3	2.29	0.48
1:A:171:TYR:HE1	2:B:1:LEU:HD22	1.79	0.48
1:Q:85:TYR:HB2	1:Q:87:GLN:HE22	1.79	0.48
1:U:114:HIS:NE2	1:U:126:LEU:HB2	2.29	0.48
1:U:28:VAL:O	1:U:31:THR:HG23	2.14	0.48
3:K:30:PHE:HB2	3:K:84:HIS:NE2	2.29	0.48
1:M:250:PRO:HB2	1:M:253:GLN:NE2	2.28	0.48
1:U:171:TYR:CE1	2:V:1:LEU:HD22	2.48	0.48
1:U:191:HIS:HD2	1:U:201:LEU:HD12	1.79	0.48
3:G:43:GLY:HA3	1:Q:17:ARG:HG2	1.94	0.48
1:U:231:VAL:HG11	1:U:244:TRP:HB3	1.95	0.48
1:E:27:TYR:CZ	1:E:32:GLN:HG3	2.48	0.48
3:K:43:GLY:O	3:K:44:GLU:HG3	2.14	0.48
1:U:96:GLN:HG2	1:U:117:ALA:HB3	1.95	0.48
1:A:154:GLU:HA	1:A:157:ARG:HB3	1.94	0.47
3:G:73:THR:OG1	3:G:76:ASP:HB2	2.14	0.47
1:M:191:HIS:CD2	1:M:201:LEU:HD12	2.49	0.47
1:Q:235:PRO:HA	1:Q:241:PHE:CD1	2.49	0.47
1:A:124:ILE:HG21	1:A:147:TRP:CZ3	2.43	0.47
1:E:14:ARG:HG3	1:E:20:PRO:HA	1.96	0.47
1:M:108:ARG:HD2	1:M:169:ARG:NH2	2.30	0.47
1:A:111:ARG:HD2	1:A:128:GLU:O	2.14	0.47
1:A:185:PRO:HD2	1:A:266:LEU:HD23	1.96	0.47
1:E:66:LYS:HD2	2:F:4:GLY:HA2	1.96	0.47
4:H:72:PRO:HA	4:H:77:PHE:O	2.14	0.47
1:I:209:TYR:HB3	1:I:210:PRO:HD3	1.96	0.47
1:I:94:THR:OG1	1:I:96:GLN:OE1	2.32	0.47
1:M:156:LEU:HA	2:N:3:PHE:CE1	2.50	0.47
4:P:28:ARG:HH22	4:P:59:TRP:C	2.16	0.47
1:U:234:ARG:HH22	1:U:244:TRP:HZ3	1.60	0.47
1:A:17:ARG:HA	3:W:44:GLU:N	2.29	0.47
1:E:35:ARG:HE	1:E:48:ARG:HD3	1.79	0.47
1:E:35:ARG:HG3	1:E:46:GLU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:19:LYS:O	3:K:72:PRO:HD2	2.13	0.47
1:M:234:ARG:HD3	3:O:8:GLN:NE2	2.28	0.47
4:T:44:ILE:HD11	4:T:51:ARG:O	2.15	0.47
4:T:57:SER:OG	4:T:58:THR:N	2.47	0.47
1:U:249:VAL:HG12	1:U:253:GLN:HE21	1.79	0.47
4:D:36:GLY:O	4:D:53:ASN:ND2	2.41	0.47
1:E:231:VAL:HG11	1:E:244:TRP:HB2	1.96	0.47
1:I:208:PHE:CE1	1:I:241:PHE:HB2	2.49	0.47
3:K:15:ALA:HB2	3:K:95:TRP:HZ2	1.79	0.47
1:A:17:ARG:CZ	3:W:40:LEU:HD11	2.44	0.47
4:D:95:MET:O	4:D:99:ARG:NE	2.47	0.47
1:E:21:ARG:HD2	1:E:37:ASP:OD1	2.15	0.47
1:Q:213:ILE:HD11	1:Q:261:VAL:HG23	1.97	0.47
4:T:22:PHE:HE1	4:T:31:VAL:HG13	1.78	0.47
3:W:57:SER:H	3:W:63:TYR:HE2	1.62	0.47
1:A:14:ARG:O	1:A:16:GLY:N	2.45	0.47
1:E:209:TYR:CD2	1:E:210:PRO:HD2	2.49	0.47
1:M:214:THR:CG2	1:M:262:GLN:HB2	2.45	0.47
1:M:34:VAL:HG11	1:M:45:MET:HE1	1.96	0.47
1:A:188:HIS:HD2	1:A:190:THR:HG23	1.79	0.47
1:I:190:THR:O	1:I:201:LEU:HG	2.15	0.47
1:M:27:TYR:H	1:M:33:PHE:HE2	1.62	0.47
3:O:80:CYS:O	3:O:92:ILE:HA	2.15	0.47
1:Q:34:VAL:HG21	1:Q:45:MET:SD	2.54	0.47
1:U:118:TYR:CG	1:U:119:ASP:N	2.75	0.47
1:U:238:ASP:OD1	1:U:240:THR:OG1	2.26	0.47
1:M:164:CYS:O	1:M:168:LEU:HB2	2.15	0.47
1:M:188:HIS:HB2	1:M:204:TRP:CZ2	2.38	0.47
1:Q:24:ALA:HB3	1:Q:36:PHE:HB3	1.95	0.47
1:U:204:TRP:HZ2	1:U:244:TRP:CE2	2.33	0.47
1:A:147:TRP:CZ2	2:B:9:VAL:HG12	2.50	0.47
1:E:51:TRP:CD1	1:E:178:THR:HG21	2.50	0.47
3:O:5:PRO:HB3	3:O:30:PHE:HB3	1.96	0.47
4:P:46:TYR:OH	4:P:59:TRP:HD1	1.98	0.47
1:U:29:ASP:CG	1:U:30:ASP:H	2.18	0.47
1:E:256:ARG:HG3	1:E:257:TYR:HD1	1.80	0.46
1:I:188:HIS:CD2	1:I:189:MET:H	2.34	0.46
1:I:1:GLY:HA2	1:I:105:SER:HA	1.96	0.46
1:M:116:TYR:N	1:M:124:ILE:O	2.40	0.46
4:X:40:GLN:O	4:X:41:SER:OG	2.30	0.46
1:A:127:LYS:C	1:A:129:ASP:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB3	1:A:168:LEU:HD21	1.96	0.46
1:M:154:GLU:HA	1:M:157:ARG:HB3	1.97	0.46
1:M:51:TRP:HE1	1:M:178:THR:HG1	1.63	0.46
4:D:20:LEU:HD11	4:D:85:PHE:CD1	2.50	0.46
3:G:78:TYR:O	3:G:95:TRP:N	2.44	0.46
1:I:109:PHE:HD1	1:I:165:VAL:HG21	1.80	0.46
1:I:118:TYR:CG	1:I:119:ASP:N	2.81	0.46
1:I:33:PHE:CE2	1:I:52:ILE:HB	2.50	0.46
1:M:5:MET:HG3	1:M:27:TYR:HB3	1.97	0.46
1:M:6:ARG:HH22	1:M:115:GLN:CG	2.25	0.46
3:W:24:ASN:CB	3:W:65:LEU:HD11	2.45	0.46
1:I:257:TYR:N	1:I:257:TYR:CD2	2.84	0.46
3:O:73:THR:HG23	3:O:76:ASP:H	1.79	0.46
1:Q:205:ALA:HB1	1:Q:208:PHE:HE2	1.80	0.46
1:M:108:ARG:HA	1:M:108:ARG:HD2	1.64	0.46
1:M:224:GLN:OE1	1:M:228:THR:OG1	2.24	0.46
1:M:235:PRO:HA	1:M:241:PHE:CD1	2.48	0.46
1:M:54:GLN:HB3	4:P:51:ARG:NH2	2.31	0.46
4:X:49:LYS:HE3	4:X:51:ARG:NH2	2.31	0.46
1:A:100:GLY:O	1:A:113:TYR:N	2.36	0.46
1:Q:129:ASP:HB2	1:Q:132:SER:OG	2.15	0.46
1:Q:109:PHE:HD1	1:Q:165:VAL:HG21	1.80	0.46
1:Q:235:PRO:HA	1:Q:241:PHE:HD1	1.79	0.46
1:M:206:LEU:HD11	3:O:14:PRO:HD3	1.96	0.46
1:M:20:PRO:HG2	1:M:75:ARG:CD	2.44	0.46
1:Q:256:ARG:HG3	1:Q:257:TYR:CD1	2.51	0.46
3:S:80:CYS:O	3:S:92:ILE:HA	2.15	0.46
1:A:127:LYS:HG2	1:A:132:SER:OG	2.15	0.46
1:A:154:GLU:HG2	1:A:157:ARG:HD3	1.98	0.46
1:A:164:CYS:O	1:A:168:LEU:HB2	2.16	0.46
3:C:9:VAL:HG22	3:C:25:CYS:SG	2.55	0.46
3:C:87:LEU:HD11	3:C:91:LYS:HE3	1.98	0.46
3:K:73:THR:OG1	3:K:76:ASP:HB2	2.15	0.46
1:Q:44:ARG:HG3	1:Q:64:THR:OG1	2.15	0.46
4:X:14:ASN:OD1	4:X:15:PRO:HD3	2.15	0.46
1:E:14:ARG:HH11	1:E:21:ARG:HB2	1.81	0.46
4:L:99:ARG:HD2	4:L:104:TRP:O	2.16	0.46
1:M:21:ARG:NH2	1:M:37:ASP:OD1	2.48	0.46
3:S:56:PHE:HD1	3:S:60:TRP:HA	1.81	0.46
1:M:76:VAL:HG23	2:N:8:TYR:HE1	1.81	0.45
1:Q:178:THR:O	1:Q:209:TYR:OH	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:31:HIS:HD2	3:S:32:PRO:CA	2.26	0.45
3:K:13:HIS:O	3:K:21:ASN:ND2	2.49	0.45
1:M:127:LYS:HB3	1:M:132:SER:OG	2.16	0.45
1:E:249:VAL:HG21	1:E:257:TYR:HE2	1.81	0.45
1:I:257:TYR:N	1:I:257:TYR:HD2	2.15	0.45
1:I:5:MET:HB3	1:I:6:ARG:H	1.56	0.45
1:Q:214:THR:HG23	1:Q:262:GLN:HB2	1.97	0.45
1:U:123:TYR:CD2	1:U:123:TYR:N	2.83	0.45
1:A:108:ARG:HH11	1:A:169:ARG:HH22	1.65	0.45
1:I:141:GLN:OE1	1:I:144:LYS:NZ	2.41	0.45
4:L:70:SER:HB3	4:L:78:LEU:HD11	1.98	0.45
3:S:23:LEU:HD23	3:S:39:LEU:HD22	1.99	0.45
1:U:114:HIS:CD2	1:U:126:LEU:HB2	2.51	0.45
1:U:155:GLN:O	1:U:155:GLN:HG2	2.15	0.45
3:G:46:ILE:O	3:G:49:VAL:HG13	2.16	0.45
1:I:219:ARG:HG2	1:I:257:TYR:HB2	1.98	0.45
4:T:6:LYS:HE2	1:U:75:ARG:NH2	2.32	0.45
1:I:6:ARG:HH22	1:I:115:GLN:HG2	1.81	0.45
1:M:108:ARG:HH11	1:M:169:ARG:HH22	1.63	0.45
1:U:190:THR:HG23	1:U:202:ARG:HD3	1.99	0.45
4:X:45:GLN:OE1	4:X:50:THR:HG22	2.16	0.45
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.24	0.45
1:E:224:GLN:NE2	1:E:228:THR:H	2.14	0.45
1:E:49:ALA:O	1:E:52:ILE:HG22	2.16	0.45
1:M:208:PHE:CD1	1:M:213:ILE:HD11	2.51	0.45
1:E:96:GLN:HG3	3:G:60:TRP:HE3	1.82	0.45
4:L:88:GLU:O	4:L:92:ASN:ND2	2.49	0.45
1:M:14:ARG:NE	1:M:17:ARG:HE	2.15	0.45
1:M:215:LEU:HD11	1:M:243:LYS:CD	2.46	0.45
4:T:86:ILE:HD11	4:T:88:GLU:HB3	1.98	0.45
4:T:9:PRO:HD2	2:V:8:TYR:OH	2.15	0.45
4:X:14:ASN:O	4:X:16:ASP:N	2.49	0.45
4:X:50:THR:OG1	4:X:50:THR:O	2.31	0.45
1:A:178:THR:OG1	1:A:178:THR:O	2.33	0.45
3:C:37:VAL:HG13	3:C:66:TYR:CE1	2.51	0.45
1:E:213:ILE:HB	1:E:263:HIS:HD2	1.82	0.45
4:L:77:PHE:CZ	4:P:64:PRO:HD3	2.52	0.45
1:Q:201:LEU:HD13	1:Q:254:GLU:OE1	2.17	0.45
3:S:11:SER:HG	3:S:21:ASN:ND2	2.15	0.45
1:U:99:TYR:HA	1:U:114:HIS:HA	1.98	0.45
1:E:44:ARG:HB3	1:E:64:THR:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ARG:NE	1:I:113:TYR:HD1	2.15	0.45
1:I:66:LYS:HE3	2:J:2:LEU:HB2	1.98	0.45
1:M:118:TYR:HD2	1:M:123:TYR:HB2	1.82	0.45
1:M:21:ARG:CZ	1:M:38:SER:H	2.29	0.45
1:M:147:TRP:CZ2	2:N:9:VAL:HG12	2.51	0.45
1:Q:220:ASP:O	1:Q:222:GLU:N	2.49	0.45
3:W:37:VAL:HG21	3:W:66:TYR:CD1	2.52	0.45
1:E:209:TYR:CG	1:E:210:PRO:HD3	2.52	0.44
1:E:208:PHE:HZ	1:E:243:LYS:HG3	1.82	0.44
4:L:6:LYS:NZ	4:L:6:LYS:HA	2.32	0.44
1:Q:236:ALA:O	3:S:12:ARG:HD2	2.17	0.44
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.53	0.44
3:C:9:VAL:CG2	3:C:80:CYS:HB2	2.47	0.44
1:I:183:ASP:HB2	1:I:209:TYR:N	2.33	0.44
1:M:186:LYS:HA	1:M:186:LYS:HD2	1.79	0.44
1:M:211:ALA:HB2	1:M:241:PHE:CE2	2.52	0.44
3:S:73:THR:HG1	3:S:75:LYS:H	1.64	0.44
1:U:49:ALA:HA	1:U:50:PRO:HD3	1.74	0.44
3:W:23:LEU:HG	3:W:70:PHE:CD2	2.52	0.44
3:W:86:THR:OG1	3:W:87:LEU:N	2.50	0.44
3:C:23:LEU:HB2	3:C:68:THR:HG22	1.99	0.44
4:D:8:ASP:OD1	4:D:11:LEU:HG	2.16	0.44
1:E:178:THR:HG23	1:E:179:LEU:HD12	1.98	0.44
1:M:116:TYR:CD2	1:M:123:TYR:HD2	2.36	0.44
1:U:107:TRP:O	1:U:169:ARG:NH2	2.49	0.44
3:W:34:ASP:C	3:W:35:ILE:HD12	2.38	0.44
1:A:66:LYS:HG2	2:B:2:LEU:HD23	1.99	0.44
1:I:6:ARG:HG3	1:I:113:TYR:HE1	1.82	0.44
1:I:144:LYS:O	1:I:148:GLU:HG3	2.17	0.44
1:M:32:GLN:CD	1:M:32:GLN:H	2.21	0.44
1:M:6:ARG:HD3	1:M:98:MET:HG2	2.00	0.44
1:Q:21:ARG:HH11	1:Q:38:SER:HG	1.62	0.44
1:A:77:ASP:O	1:A:80:THR:OG1	2.21	0.44
3:K:11:SER:OG	3:K:21:ASN:ND2	2.50	0.44
4:L:19:GLN:O	4:L:34:LYS:N	2.49	0.44
1:M:107:TRP:CH2	1:M:172:LEU:HB3	2.53	0.44
1:Q:127:LYS:C	1:Q:129:ASP:H	2.20	0.44
3:S:46:ILE:O	3:S:46:ILE:HG23	2.17	0.44
1:U:154:GLU:HA	1:U:157:ARG:HB3	1.99	0.44
3:W:30:PHE:CE1	3:W:62:PHE:HB2	2.53	0.44
1:E:124:ILE:HG23	1:E:133:TRP:HH2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:THR:O	1:I:202:ARG:HB2	2.17	0.44
1:M:108:ARG:HH11	1:M:169:ARG:NH2	2.15	0.44
1:M:204:TRP:CZ3	1:M:206:LEU:HB2	2.51	0.44
1:Q:127:LYS:NZ	1:Q:129:ASP:OD1	2.38	0.44
1:A:45:MET:SD	1:A:67:VAL:HG21	2.58	0.44
1:A:235:PRO:HB2	3:C:65:LEU:HD22	1.99	0.44
4:H:28:ARG:NH2	4:H:60:GLN:HB3	2.33	0.44
1:M:160:LEU:O	1:M:165:VAL:HG23	2.17	0.44
1:Q:176:LYS:HA	1:Q:179:LEU:HG	2.00	0.44
1:Q:115:GLN:HA	1:Q:125:ALA:HA	1.99	0.44
1:Q:49:ALA:HA	1:Q:50:PRO:HD3	1.84	0.44
1:U:204:TRP:CZ2	1:U:244:TRP:CD2	3.06	0.44
2:B:2:LEU:HD12	2:B:2:LEU:HA	1.89	0.44
1:E:108:ARG:HD2	1:E:108:ARG:HA	1.76	0.44
1:E:138:MET:O	1:E:141:GLN:HG2	2.18	0.44
3:G:30:PHE:CE1	3:G:62:PHE:HB2	2.53	0.44
3:O:3:ARG:NH1	5:O:101:HOH:O	2.50	0.44
1:U:156:LEU:HA	2:V:3:PHE:HE1	1.83	0.44
1:U:234:ARG:HD3	3:W:8:GLN:NE2	2.33	0.44
1:U:50:PRO:O	1:U:53:GLU:HG2	2.17	0.44
1:U:6:ARG:HD2	1:U:8:PHE:CZ	2.53	0.44
3:W:39:LEU:HA	3:W:39:LEU:HD23	1.91	0.44
4:D:65:GLU:HA	4:D:87:PHE:CD2	2.53	0.43
1:E:2:SER:HB2	1:E:264:GLU:OE2	2.18	0.43
1:I:127:LYS:HB3	1:I:132:SER:OG	2.18	0.43
3:O:35:ILE:HG13	3:O:84:HIS:HD2	1.83	0.43
4:P:9:PRO:O	4:P:12:THR:OG1	2.36	0.43
1:A:254:GLU:C	1:A:257:TYR:HE2	2.22	0.43
1:A:68:LYS:O	1:A:72:GLN:HG2	2.19	0.43
1:E:103:VAL:HG13	1:E:107:TRP:HA	1.99	0.43
1:Q:49:ALA:O	1:Q:52:ILE:HG22	2.17	0.43
1:Q:63:GLU:O	1:Q:67:VAL:HG22	2.18	0.43
3:W:35:ILE:HD11	3:W:84:HIS:CD2	2.53	0.43
1:A:18:GLY:N	3:W:44:GLU:HB3	2.33	0.43
3:W:77:GLU:HG2	3:W:78:TYR:N	2.33	0.43
1:M:215:LEU:HD11	1:M:243:LYS:CE	2.49	0.43
3:W:31:HIS:HD2	3:W:32:PRO:CA	2.32	0.43
1:A:4:SER:CB	1:A:168:LEU:HD21	2.48	0.43
1:E:121:LYS:HG3	1:E:122:ASP:H	1.82	0.43
1:I:181:ARG:HH21	4:L:28:ARG:NH1	2.15	0.43
1:I:191:HIS:HB2	1:I:201:LEU:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:75:ASP:HB2	4:L:77:PHE:CD2	2.53	0.43
4:P:28:ARG:HH11	4:P:29:CYS:H	1.66	0.43
4:T:65:GLU:OE2	4:T:88:GLU:HB2	2.19	0.43
1:U:114:HIS:CE1	1:U:126:LEU:HB2	2.53	0.43
1:U:208:PHE:CE1	1:U:241:PHE:HB2	2.53	0.43
3:C:34:ASP:C	3:C:35:ILE:HD12	2.39	0.43
1:E:66:LYS:HE3	2:F:2:LEU:HB2	2.01	0.43
1:I:1:GLY:N	1:I:104:GLY:O	2.46	0.43
1:Q:114:HIS:CG	1:Q:156:LEU:HD21	2.54	0.43
2:R:3:PHE:CE2	2:R:5:TYR:HB2	2.53	0.43
3:S:9:VAL:HG22	3:S:80:CYS:HB2	1.99	0.43
1:Q:54:GLN:HA	4:T:54:THR:OG1	2.19	0.43
1:U:97:ARG:HD3	1:U:116:TYR:CD1	2.52	0.43
1:A:172:LEU:HD22	1:A:179:LEU:HD22	2.00	0.43
3:K:80:CYS:O	3:K:92:ILE:HA	2.18	0.43
3:O:7:ILE:HD12	3:O:82:VAL:HG21	2.00	0.43
1:M:234:ARG:HG3	1:M:242:GLN:HB2	1.99	0.43
1:M:60:TRP:O	1:M:64:THR:HG23	2.18	0.43
3:S:45:ARG:HH11	3:S:45:ARG:HG3	1.84	0.43
4:T:59:TRP:CD1	4:T:87:PHE:HB2	2.53	0.43
1:U:204:TRP:CZ2	1:U:244:TRP:CG	3.07	0.43
1:A:208:PHE:CG	1:A:213:ILE:HD11	2.54	0.43
3:C:23:LEU:HG	3:C:70:PHE:CD2	2.54	0.43
3:C:57:SER:H	3:C:63:TYR:HE2	1.67	0.43
4:D:65:GLU:HA	4:D:87:PHE:CE2	2.54	0.43
1:Q:7:TYR:CE1	2:R:2:LEU:HD11	2.54	0.43
1:U:191:HIS:ND1	1:U:192:HIS:N	2.66	0.43
1:A:234:ARG:HA	1:A:235:PRO:HD3	1.84	0.43
1:A:33:PHE:CE2	1:A:52:ILE:HB	2.54	0.43
1:E:118:TYR:CD2	1:E:123:TYR:HB2	2.53	0.43
1:E:177:GLU:CD	1:E:177:GLU:H	2.22	0.43
1:I:188:HIS:CG	1:I:189:MET:H	2.37	0.43
1:U:141:GLN:HG3	1:U:145:HIS:CE1	2.54	0.43
1:U:209:TYR:HB3	1:U:210:PRO:HD3	2.01	0.43
1:E:133:TRP:CG	1:E:134:THR:N	2.86	0.43
1:E:256:ARG:HG3	1:E:257:TYR:CD1	2.54	0.43
1:E:82:ARG:HD2	1:E:93:HIS:HB2	2.00	0.43
1:M:238:ASP:OD2	3:O:12:ARG:NH1	2.52	0.43
3:O:71:THR:HA	3:O:72:PRO:HD2	1.87	0.43
1:Q:219:ARG:HB2	1:Q:257:TYR:CE2	2.53	0.43
4:T:44:ILE:HG22	4:T:69:VAL:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:114:HIS:CD2	1:U:126:LEU:HD22	2.54	0.43
1:U:96:GLN:HB2	3:W:56:PHE:CE2	2.53	0.43
1:A:87:GLN:CD	1:A:88:SER:H	2.21	0.42
1:M:95:VAL:HG13	1:M:116:TYR:OH	2.19	0.42
1:M:11:SER:HA	1:M:21:ARG:O	2.19	0.42
1:Q:201:LEU:HB2	1:Q:254:GLU:CD	2.40	0.42
4:T:20:LEU:HD11	4:T:85:PHE:CD1	2.54	0.42
3:C:35:ILE:HG22	3:C:37:VAL:HG12	2.01	0.42
1:I:35:ARG:CZ	1:I:48:ARG:HD3	2.49	0.42
1:I:74:HIS:NE2	1:I:97:ARG:HG3	2.34	0.42
3:O:57:SER:H	3:O:63:TYR:HE2	1.66	0.42
1:Q:66:LYS:HD2	2:R:3:PHE:O	2.19	0.42
3:C:26:TYR:HB2	3:C:65:LEU:HD13	2.00	0.42
2:F:1:LEU:HD12	2:F:2:LEU:N	2.33	0.42
3:G:11:SER:OG	3:G:21:ASN:ND2	2.52	0.42
1:M:260:HIS:CE1	1:M:271:THR:HA	2.54	0.42
1:Q:51:TRP:CE3	1:Q:175:GLY:HA3	2.54	0.42
4:T:22:PHE:CZ	4:T:87:PHE:HD1	2.37	0.42
1:A:251:SER:HA	1:A:254:GLU:OE2	2.20	0.42
1:M:127:LYS:C	1:M:129:ASP:H	2.23	0.42
1:M:253:GLN:H	1:M:253:GLN:NE2	2.16	0.42
3:O:34:ASP:C	3:O:35:ILE:HD12	2.40	0.42
4:P:65:GLU:HA	4:P:87:PHE:CD2	2.55	0.42
1:U:6:ARG:HB2	1:U:8:PHE:HE2	1.85	0.42
1:A:63:GLU:O	1:A:67:VAL:HG23	2.20	0.42
1:E:1:GLY:N	1:E:104:GLY:O	2.50	0.42
1:I:49:ALA:O	1:I:52:ILE:HG22	2.20	0.42
1:M:129:ASP:HB2	1:M:132:SER:OG	2.19	0.42
4:P:45:GLN:HB3	4:P:68:THR:OG1	2.19	0.42
1:Q:22:PHE:CD2	1:Q:71:SER:HB2	2.55	0.42
4:T:44:ILE:HG13	4:T:52:ASN:O	2.20	0.42
1:A:204:TRP:N	1:A:204:TRP:CE3	2.87	0.42
1:A:204:TRP:HE3	1:A:204:TRP:N	2.18	0.42
1:M:191:HIS:O	1:M:202:ARG:NH1	2.53	0.42
1:Q:66:LYS:HE3	2:R:2:LEU:HB2	2.01	0.42
3:S:35:ILE:HG22	3:S:37:VAL:HG13	2.01	0.42
3:W:29:GLY:HA2	3:W:61:SER:HB2	2.01	0.42
1:A:177:GLU:HG2	4:D:28:ARG:NH2	2.35	0.42
1:E:181:ARG:HB3	1:E:183:ASP:OD2	2.19	0.42
3:K:41:LYS:HG3	3:K:78:TYR:CE1	2.54	0.42
1:M:149:ALA:O	1:M:151:HIS:ND1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH1	1:A:169:ARG:HH22	2.17	0.42
1:I:108:ARG:HA	1:I:108:ARG:HD2	1.82	0.42
1:I:46:GLU:HA	1:I:47:PRO:HD3	1.71	0.42
1:Q:144:LYS:HE2	1:Q:148:GLU:OE2	2.19	0.42
1:Q:30:ASP:OD2	1:Q:210:PRO:HA	2.20	0.42
1:Q:85:TYR:HB2	1:Q:87:GLN:OE1	2.18	0.42
4:T:45:GLN:O	4:T:67:TYR:HB2	2.20	0.42
1:U:124:ILE:HA	1:U:134:THR:O	2.19	0.42
3:W:23:LEU:HB2	3:W:68:THR:HG22	2.02	0.42
1:A:22:PHE:CD2	1:A:71:SER:HB2	2.54	0.42
1:A:85:TYR:HB3	1:A:86:ASN:H	1.64	0.42
1:Q:191:HIS:HB2	1:Q:201:LEU:HD12	2.02	0.42
4:D:66:TRP:HZ3	4:D:68:THR:HG23	1.84	0.42
1:E:234:ARG:HA	1:E:235:PRO:HD3	1.82	0.42
1:I:3:HIS:HB2	1:I:29:ASP:OD2	2.19	0.42
1:M:191:HIS:HD2	1:M:201:LEU:HD12	1.84	0.42
1:U:141:GLN:HG3	1:U:145:HIS:HE1	1.84	0.42
1:U:171:TYR:OH	2:V:1:LEU:HD22	2.20	0.42
1:A:188:HIS:O	1:A:189:MET:HG2	2.20	0.41
1:M:167:TRP:CE3	1:M:170:ARG:HD3	2.55	0.41
1:M:185:PRO:CB	1:M:205:ALA:HB1	2.49	0.41
4:P:37:TRP:NE1	4:P:54:THR:OG1	2.52	0.41
1:Q:3:HIS:HB2	1:Q:29:ASP:CG	2.41	0.41
3:S:57:SER:H	3:S:63:TYR:HE2	1.68	0.41
4:T:76:GLY:HA2	1:U:146:LYS:HG3	2.01	0.41
1:A:96:GLN:HG2	1:A:117:ALA:HB3	2.02	0.41
1:E:137:ASP:CG	1:E:138:MET:H	2.23	0.41
1:I:111:ARG:NH1	1:I:128:GLU:HG2	2.34	0.41
1:I:31:THR:HG21	1:I:209:TYR:OH	2.19	0.41
4:L:28:ARG:CD	4:L:106:PRO:HG3	2.50	0.41
1:M:70:HIS:CE1	2:N:2:LEU:HD22	2.55	0.41
3:S:40:LEU:HA	3:S:45:ARG:HH12	1.85	0.41
3:S:4:THR:HA	3:S:5:PRO:HD3	1.84	0.41
1:A:135:ALA:HB1	1:A:140:ALA:HB1	2.02	0.41
1:A:131:ARG:HD3	1:A:153:ALA:HB3	2.01	0.41
1:I:33:PHE:HA	1:I:33:PHE:HD2	1.73	0.41
1:I:48:ARG:NH2	1:I:48:ARG:HG2	2.34	0.41
1:M:155:GLN:HG2	1:M:155:GLN:O	2.21	0.41
1:M:63:GLU:O	1:M:67:VAL:HG22	2.19	0.41
4:P:45:GLN:HG3	4:P:46:TYR:N	2.34	0.41
3:W:21:ASN:HB3	3:W:70:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:HA3	3:W:44:GLU:OE1	2.20	0.41
1:E:66:LYS:HE2	1:E:66:LYS:HB2	1.85	0.41
4:H:40:GLN:O	4:H:41:SER:OG	2.33	0.41
1:I:13:SER:OG	1:I:82:ARG:NH1	2.53	0.41
1:A:127:LYS:HZ2	1:A:132:SER:HG	1.53	0.41
1:A:168:LEU:O	1:A:172:LEU:HG	2.21	0.41
1:A:76:VAL:O	1:A:80:THR:HG23	2.21	0.41
3:G:13:HIS:N	3:G:21:ASN:HD21	2.15	0.41
4:H:60:GLN:HG2	4:H:63:ASP:OD2	2.20	0.41
1:Q:25:VAL:HG13	1:Q:48:ARG:NH1	2.35	0.41
1:Q:96:GLN:HG2	1:Q:117:ALA:HB3	2.02	0.41
1:U:156:LEU:HA	2:V:3:PHE:CE1	2.55	0.41
1:A:70:HIS:HA	1:A:73:THR:HG22	2.03	0.41
1:I:4:SER:HB3	1:I:103:VAL:HG22	2.01	0.41
1:Q:15:PRO:HD2	1:Q:17:ARG:HG3	2.03	0.41
1:Q:219:ARG:NH1	1:Q:257:TYR:OH	2.48	0.41
1:A:220:ASP:O	1:A:222:GLU:N	2.54	0.41
1:A:33:PHE:HA	1:A:33:PHE:HD2	1.69	0.41
1:E:101:CYS:HB3	1:E:160:LEU:HD12	2.03	0.41
1:I:127:LYS:HD3	1:I:128:GLU:H	1.85	0.41
1:I:14:ARG:HE	1:I:17:ARG:HD2	1.86	0.41
1:I:181:ARG:NH2	4:L:106:PRO:HB3	2.35	0.41
3:O:41:LYS:HE3	3:O:78:TYR:OH	2.21	0.41
4:P:29:CYS:HB2	4:P:95:MET:HG3	2.02	0.41
3:S:12:ARG:CB	3:S:22:PHE:HB2	2.50	0.41
3:S:77:GLU:HG2	3:S:78:TYR:N	2.36	0.41
1:U:141:GLN:O	1:U:145:HIS:ND1	2.54	0.41
1:E:176:LYS:O	1:E:180:GLN:N	2.54	0.41
4:H:20:LEU:HD11	4:H:85:PHE:CD1	2.56	0.41
1:I:143:THR:O	1:I:146:LYS:HB2	2.21	0.41
3:K:12:ARG:HB3	3:K:22:PHE:HB2	2.02	0.41
1:Q:3:HIS:HB2	1:Q:29:ASP:OD2	2.20	0.41
1:Q:80:THR:OG1	1:Q:81:LEU:N	2.54	0.41
4:T:65:GLU:HA	4:T:87:PHE:HD2	1.85	0.41
1:U:14:ARG:HA	1:U:15:PRO:HD3	1.94	0.41
1:U:59:TYR:O	1:U:63:GLU:HB2	2.21	0.41
1:A:45:MET:H	1:A:64:THR:CG2	2.30	0.41
1:E:206:LEU:HD23	1:E:206:LEU:HA	1.78	0.41
3:G:21:ASN:HB3	3:G:70:PHE:HE2	1.83	0.41
1:I:20:PRO:HG3	1:I:78:LEU:HD21	2.01	0.41
1:M:147:TRP:HB3	1:M:152:VAL:CG1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:201:LEU:HB3	1:M:202:ARG:H	1.52	0.41
4:T:68:THR:HB	4:T:80:THR:CG2	2.50	0.41
1:U:129:ASP:HB3	1:U:132:SER:OG	2.21	0.41
1:A:159:TYR:CD1	1:A:163:THR:HB	2.55	0.41
1:A:6:ARG:CZ	1:A:8:PHE:HZ	2.33	0.41
1:E:250:PRO:HB2	1:E:253:GLN:OE1	2.21	0.41
1:I:189:MET:HG3	1:I:201:LEU:CD2	2.51	0.41
1:I:214:THR:CG2	1:I:262:GLN:HB2	2.51	0.41
1:I:33:PHE:CE1	1:I:52:ILE:HD13	2.55	0.41
1:U:147:TRP:CH2	2:V:9:VAL:HG12	2.56	0.41
1:U:160:LEU:O	1:U:165:VAL:HG23	2.21	0.41
1:U:95:VAL:HA	1:U:117:ALA:O	2.21	0.41
1:A:1:GLY:H2	1:A:105:SER:HA	1.85	0.41
1:A:231:VAL:HG22	1:A:234:ARG:CZ	2.50	0.41
4:D:13:PHE:HE1	4:D:73:GLY:HA2	1.85	0.41
1:E:35:ARG:HG3	1:E:35:ARG:O	2.21	0.41
1:I:201:LEU:HD23	1:I:202:ARG:H	1.86	0.41
1:M:64:THR:O	1:M:68:LYS:HG3	2.21	0.41
4:P:22:PHE:CE1	4:P:31:VAL:HG13	2.56	0.41
3:S:73:THR:HG21	3:S:76:ASP:HB2	2.02	0.41
1:A:266:LEU:HD12	1:A:268:LYS:O	2.22	0.40
1:E:123:TYR:CD2	1:E:124:ILE:HG12	2.56	0.40
1:E:181:ARG:HD3	1:E:181:ARG:HA	1.84	0.40
1:E:99:TYR:HB3	1:E:114:HIS:HD2	1.86	0.40
1:M:10:THR:HG21	3:O:62:PHE:HE1	1.87	0.40
1:Q:266:LEU:HD12	1:Q:266:LEU:O	2.20	0.40
4:D:27:ASN:HD22	4:D:103:MET:HG2	1.87	0.40
4:H:72:PRO:HD3	4:H:78:LEU:HD12	2.02	0.40
3:O:23:LEU:O	3:O:67:TYR:HA	2.21	0.40
4:P:23:GLN:HA	4:P:24:PRO:HD3	1.92	0.40
4:T:99:ARG:HH21	4:T:104:TRP:HE1	1.69	0.40
1:U:9:PHE:HB3	1:U:74:HIS:CE1	2.45	0.40
1:A:139:ALA:O	1:A:142:THR:HG22	2.21	0.40
1:A:188:HIS:HB3	1:A:204:TRP:CZ2	2.52	0.40
3:C:41:LYS:HE3	3:C:78:TYR:OH	2.21	0.40
1:E:250:PRO:HB2	1:E:253:GLN:HE22	1.86	0.40
4:L:57:SER:OG	4:L:58:THR:N	2.51	0.40
1:Q:115:GLN:C	1:Q:116:TYR:HD2	2.25	0.40
1:Q:127:LYS:HG2	1:Q:132:SER:OG	2.21	0.40
1:Q:213:ILE:HD11	1:Q:261:VAL:CG2	2.51	0.40
4:T:22:PHE:HZ	4:T:87:PHE:CD1	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:66:LYS:HE2	1:U:66:LYS:HB2	1.91	0.40
4:X:68:THR:HG22	4:X:82:ASN:OD1	2.21	0.40
1:A:209:TYR:HB3	1:A:210:PRO:HD3	2.02	0.40
1:E:4:SER:HB2	1:E:102:ASP:HA	2.04	0.40
1:E:220:ASP:HB3	1:E:221:GLY:H	1.76	0.40
1:E:249:VAL:HG12	1:E:253:GLN:HE21	1.87	0.40
1:E:27:TYR:OH	3:G:63:TYR:OH	2.33	0.40
4:L:46:TYR:CE2	4:L:47:LYS:HE3	2.56	0.40
1:M:6:ARG:NH2	1:M:115:GLN:HG3	2.28	0.40
1:M:156:LEU:HA	2:N:3:PHE:HE1	1.86	0.40
3:S:84:HIS:CG	3:S:85:VAL:H	2.40	0.40
1:U:118:TYR:N	1:U:123:TYR:CE2	2.87	0.40
1:U:191:HIS:CE1	1:U:193:ALA:HB2	2.55	0.40
4:X:46:TYR:CE2	4:X:47:LYS:HE3	2.57	0.40
1:A:181:ARG:HB3	1:A:183:ASP:OD1	2.20	0.40
3:C:15:ALA:HB3	3:C:97:ARG:NH1	2.37	0.40
1:E:9:PHE:HZ	2:F:2:LEU:HD21	1.85	0.40
1:I:234:ARG:HA	1:I:235:PRO:HD3	1.81	0.40
1:I:263:HIS:CE1	1:I:265:GLY:H	2.39	0.40
1:M:133:TRP:CZ2	1:M:153:ALA:HB2	2.57	0.40
3:O:36:GLU:N	3:O:36:GLU:OE1	2.55	0.40
1:Q:33:PHE:HA	1:Q:33:PHE:HD2	1.72	0.40
3:S:9:VAL:CG2	3:S:80:CYS:HB2	2.51	0.40
1:U:118:TYR:HB3	1:U:123:TYR:CZ	2.56	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:A:105:SER:OG	1:A:129:ASP:OD1[3_555]	2.13	0.07

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	256/275 (93%)	229 (90%)	27 (10%)	0	100	100
1	E	264/275 (96%)	233 (88%)	31 (12%)	0	100	100
1	I	242/275 (88%)	216 (89%)	26 (11%)	0	100	100
1	M	259/275 (94%)	230 (89%)	29 (11%)	0	100	100
1	Q	253/275 (92%)	225 (89%)	27 (11%)	1 (0%)	34	48
1	U	238/275 (86%)	214 (90%)	23 (10%)	1 (0%)	34	48
2	B	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	N	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	V	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	C	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
3	G	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
3	K	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
3	O	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	S	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	W	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
4	D	100/108 (93%)	88 (88%)	11 (11%)	1 (1%)	15	22
4	H	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	15	22
4	L	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	15	22
4	P	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	15	22
4	T	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	15	22
4	X	101/108 (94%)	89 (88%)	10 (10%)	2 (2%)	7	10
All	All	2731/2952 (92%)	2424 (89%)	298 (11%)	9 (0%)	41	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	9	PRO
4	P	9	PRO
4	X	9	PRO
4	H	9	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	9	PRO
4	D	9	PRO
1	Q	128	GLU
1	U	250	PRO
4	X	15	PRO

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	222/231 (96%)	199 (90%)	23 (10%)	7	9
1	E	225/231 (97%)	200 (89%)	25 (11%)	6	8
1	I	211/231 (91%)	188 (89%)	23 (11%)	6	8
1	M	223/231 (96%)	200 (90%)	23 (10%)	7	9
1	Q	218/231 (94%)	188 (86%)	30 (14%)	3	3
1	U	206/231 (89%)	179 (87%)	27 (13%)	4	4
2	B	8/8 (100%)	6 (75%)	2 (25%)	0	0
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
2	J	8/8 (100%)	8 (100%)	0	100	100
2	N	8/8 (100%)	8 (100%)	0	100	100
2	R	8/8 (100%)	7 (88%)	1 (12%)	4	5
2	V	8/8 (100%)	6 (75%)	2 (25%)	0	0
3	C	91/95 (96%)	86 (94%)	5 (6%)	21	33
3	G	93/95 (98%)	84 (90%)	9 (10%)	8	11
3	K	93/95 (98%)	83 (89%)	10 (11%)	6	8
3	O	93/95 (98%)	85 (91%)	8 (9%)	10	15
3	S	93/95 (98%)	84 (90%)	9 (10%)	8	11
3	W	93/95 (98%)	88 (95%)	5 (5%)	22	35
4	D	91/96 (95%)	87 (96%)	4 (4%)	28	44
4	H	92/96 (96%)	85 (92%)	7 (8%)	13	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	92/96 (96%)	84 (91%)	8 (9%)	10	14
4	P	92/96 (96%)	83 (90%)	9 (10%)	8	10
4	T	92/96 (96%)	87 (95%)	5 (5%)	22	35
4	X	92/96 (96%)	84 (91%)	8 (9%)	10	14
All	All	2460/2580 (95%)	2214 (90%)	246 (10%)	7	10

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	7	TYR
1	A	25	VAL
1	A	31	THR
1	A	32	GLN
1	A	33	PHE
1	A	74	HIS
1	A	87	GLN
1	A	96	GLN
1	A	113	TYR
1	A	127	LYS
1	A	134	THR
1	A	143	THR
1	A	144	LYS
1	A	163	THR
1	A	178	THR
1	A	179	LEU
1	A	204	TRP
1	A	214	THR
1	A	223	ASP
1	A	224	GLN
1	A	230	LEU
1	A	266	LEU
2	B	5	TYR
2	B	8	TYR
3	C	7	ILE
3	C	37	VAL
3	C	70	PHE
3	C	80	CYS
3	C	87	LEU
4	D	16	ASP
4	D	39	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	50	THR
4	D	58	THR
1	E	3	HIS
1	E	7	TYR
1	E	12	VAL
1	E	28	VAL
1	E	32	GLN
1	E	33	PHE
1	E	34	VAL
1	E	81	LEU
1	E	94	THR
1	E	103	VAL
1	E	113	TYR
1	E	116	TYR
1	E	118	TYR
1	E	119	ASP
1	E	142	THR
1	E	178	THR
1	E	188	HIS
1	E	192	HIS
1	E	202	ARG
1	E	204	TRP
1	E	209	TYR
1	E	223	ASP
1	E	224	GLN
1	E	244	TRP
1	E	261	VAL
2	F	1	LEU
2	F	7	VAL
2	F	9	VAL
3	G	4	THR
3	G	7	ILE
3	G	12	ARG
3	G	24	ASN
3	G	37	VAL
3	G	59	ASP
3	G	68	THR
3	G	70	PHE
3	G	80	CYS
4	H	14	ASN
4	H	19	GLN
4	H	68	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	69	VAL
4	H	75	ASP
4	H	77	PHE
4	H	95	MET
1	I	3	HIS
1	I	5	MET
1	I	14	ARG
1	I	17	ARG
1	I	28	VAL
1	I	32	GLN
1	I	33	PHE
1	I	34	VAL
1	I	75	ARG
1	I	94	THR
1	I	96	GLN
1	I	113	TYR
1	I	116	TYR
1	I	130	LEU
1	I	144	LYS
1	I	155	GLN
1	I	163	THR
1	I	178	THR
1	I	201	LEU
1	I	204	TRP
1	I	216	THR
1	I	257	TYR
1	I	266	LEU
3	K	7	ILE
3	K	12	ARG
3	K	19	LYS
3	K	24	ASN
3	K	37	VAL
3	K	47	GLU
3	K	53	ASP
3	K	55	SER
3	K	70	PHE
3	K	80	CYS
4	L	11	LEU
4	L	16	ASP
4	L	50	THR
4	L	68	THR
4	L	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	71	VAL
4	L	75	ASP
4	L	78	LEU
1	M	5	MET
1	M	7	TYR
1	M	10	THR
1	M	13	SER
1	M	14	ARG
1	M	27	TYR
1	M	28	VAL
1	M	32	GLN
1	M	48	ARG
1	M	67	VAL
1	M	96	GLN
1	M	103	VAL
1	M	144	LYS
1	M	154	GLU
1	M	155	GLN
1	M	163	THR
1	M	178	THR
1	M	187	THR
1	M	188	HIS
1	M	194	VAL
1	M	202	ARG
1	M	213	ILE
1	M	243	LYS
3	O	7	ILE
3	O	12	ARG
3	O	24	ASN
3	O	47	GLU
3	O	67	TYR
3	O	68	THR
3	O	70	PHE
3	O	80	CYS
4	P	14	ASN
4	P	16	ASP
4	P	25	ASP
4	P	50	THR
4	P	51	ARG
4	P	57	SER
4	P	69	VAL
4	P	75	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	P	89	HIS
1	Q	3	HIS
1	Q	5	MET
1	Q	7	TYR
1	Q	13	SER
1	Q	32	GLN
1	Q	33	PHE
1	Q	46	GLU
1	Q	67	VAL
1	Q	75	ARG
1	Q	86	ASN
1	Q	96	GLN
1	Q	98	MET
1	Q	103	VAL
1	Q	105	SER
1	Q	113	TYR
1	Q	127	LYS
1	Q	130	LEU
1	Q	138	MET
1	Q	155	GLN
1	Q	178	THR
1	Q	191	HIS
1	Q	204	TRP
1	Q	207	SER
1	Q	214	THR
1	Q	215	LEU
1	Q	217	TRP
1	Q	224	GLN
1	Q	228	THR
1	Q	258	THR
1	Q	261	VAL
2	R	1	LEU
3	S	7	ILE
3	S	12	ARG
3	S	23	LEU
3	S	24	ASN
3	S	45	ARG
3	S	53	ASP
3	S	70	PHE
3	S	73	THR
3	S	80	CYS
4	T	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	75	ASP
4	T	81	VAL
4	T	89	HIS
4	T	99	ARG
1	U	14	ARG
1	U	21	ARG
1	U	25	VAL
1	U	28	VAL
1	U	31	THR
1	U	32	GLN
1	U	33	PHE
1	U	94	THR
1	U	108	ARG
1	U	113	TYR
1	U	114	HIS
1	U	123	TYR
1	U	138	MET
1	U	141	GLN
1	U	144	LYS
1	U	155	GLN
1	U	163	THR
1	U	178	THR
1	U	182	THR
1	U	190	THR
1	U	195	SER
1	U	204	TRP
1	U	214	THR
1	U	228	THR
1	U	248	VAL
1	U	253	GLN
1	U	257	TYR
2	V	2	LEU
2	V	7	VAL
3	W	7	ILE
3	W	24	ASN
3	W	49	VAL
3	W	70	PHE
3	W	74	GLU
4	X	11	LEU
4	X	13	PHE
4	X	16	ASP
4	X	21	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	X	71	VAL
4	X	75	ASP
4	X	79	ARG
4	X	89	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	188	HIS
1	A	224	GLN
4	D	27	ASN
1	E	115	GLN
1	E	253	GLN
1	I	54	GLN
1	I	114	HIS
1	I	188	HIS
1	I	260	HIS
4	L	92	ASN
1	M	96	GLN
1	M	253	GLN
3	O	8	GLN
4	P	92	ASN
1	Q	224	GLN
1	Q	260	HIS
1	Q	262	GLN
1	Q	263	HIS
3	S	31	HIS
4	T	92	ASN
1	U	114	HIS
1	U	253	GLN
3	W	31	HIS
4	X	19	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/275 (96%)	2.18	118 (44%) 0 0	20, 49, 98, 218	0
1	E	268/275 (97%)	2.51	133 (49%) 0 0	18, 49, 126, 173	0
1	I	252/275 (91%)	2.06	104 (41%) 0 0	14, 41, 85, 176	0
1	M	265/275 (96%)	2.55	132 (49%) 0 0	18, 51, 117, 161	0
1	Q	259/275 (94%)	4.73	210 (81%) 0 0	22, 61, 134, 238	0
1	U	246/275 (89%)	4.96	199 (80%) 0 0	27, 59, 131, 224	0
2	B	9/9 (100%)	2.16	2 (22%) 0 0	29, 33, 52, 58	0
2	F	9/9 (100%)	2.20	4 (44%) 0 0	34, 53, 82, 85	0
2	J	9/9 (100%)	2.06	3 (33%) 0 0	22, 33, 49, 83	0
2	N	9/9 (100%)	2.16	4 (44%) 0 0	20, 39, 61, 77	0
2	R	9/9 (100%)	4.52	8 (88%) 0 0	33, 41, 70, 75	0
2	V	9/9 (100%)	4.30	8 (88%) 0 0	41, 51, 77, 80	0
3	C	96/100 (96%)	2.31	52 (54%) 0 0	30, 54, 130, 166	0
3	G	98/100 (98%)	1.97	36 (36%) 0 0	16, 42, 73, 218	0
3	K	98/100 (98%)	1.62	25 (25%) 0 0	15, 40, 74, 180	0
3	O	98/100 (98%)	2.28	46 (46%) 0 0	26, 48, 121, 147	0
3	S	98/100 (98%)	5.06	79 (80%) 0 0	23, 57, 142, 203	0
3	W	98/100 (98%)	4.93	83 (84%) 0 0	20, 57, 115, 187	0
4	D	102/108 (94%)	1.87	38 (37%) 0 0	15, 42, 79, 193	0
4	H	103/108 (95%)	1.95	35 (33%) 0 0	22, 38, 76, 132	0
4	L	103/108 (95%)	1.77	34 (33%) 0 0	17, 36, 81, 129	0
4	P	103/108 (95%)	2.00	36 (34%) 0 0	16, 44, 115, 147	0
4	T	103/108 (95%)	4.49	85 (82%) 0 0	19, 54, 114, 160	0
4	X	103/108 (95%)	3.98	84 (81%) 0 0	18, 49, 92, 186	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2811/2952 (95%)	3.01	1558 (55%) 0 0	14, 49, 118, 238	0

All (1558) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	33	PHE	22.1
1	E	227	ASP	22.0
3	W	9	VAL	21.8
3	W	93	VAL	21.0
3	S	9	VAL	20.0
1	U	83	GLY	20.0
1	M	189	MET	19.7
1	U	112	GLY	18.7
4	X	7	ALA	17.7
1	Q	190	THR	17.7
1	Q	172	LEU	17.4
1	Q	188	HIS	17.3
4	T	97	MET	16.8
1	Q	16	GLY	16.2
1	U	61	ASP	16.1
1	Q	239	GLY	16.1
3	S	42	ASN	15.4
3	W	1	ILE	15.4
3	S	15	ALA	15.3
1	U	136	ALA	14.9
4	X	74	ALA	14.6
3	O	44	GLU	14.1
4	T	103	MET	14.1
1	U	150	ALA	13.9
1	U	152	VAL	13.8
1	Q	8	PHE	13.7
1	A	190	THR	13.7
1	E	135	ALA	13.7
1	Q	256	ARG	13.6
1	Q	111	ARG	13.4
1	U	269	PRO	13.3
1	Q	18	GLY	13.3
3	S	90	PRO	13.3
1	U	194	VAL	13.2
3	S	8	GLN	13.0
4	T	52	ASN	12.8
3	S	10	TYR	12.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	230	LEU	12.5
1	M	193	ALA	12.4
1	U	25	VAL	12.3
1	Q	183	ASP	12.2
1	Q	93	HIS	12.2
4	T	21	SER	12.1
1	U	178	THR	12.0
3	S	40	LEU	11.9
1	Q	118	TYR	11.8
4	T	15	PRO	11.8
1	U	261	VAL	11.8
3	S	39	LEU	11.8
1	E	15	PRO	11.8
1	U	107	TRP	11.8
3	W	84	HIS	11.7
1	Q	27	TYR	11.7
1	U	208	PHE	11.6
4	T	35	CYS	11.6
1	U	111	ARG	11.6
4	P	11	LEU	11.3
1	U	15	PRO	11.2
1	U	74	HIS	11.2
3	W	78	TYR	11.1
1	U	18	GLY	11.0
1	Q	116	TYR	10.9
1	E	190	THR	10.8
3	S	1	ILE	10.8
1	U	271	THR	10.7
1	E	193	ALA	10.6
1	Q	177	GLU	10.6
3	G	44	GLU	10.6
1	U	127	LYS	10.3
1	U	9	PHE	10.3
1	U	119	ASP	10.3
1	M	188	HIS	10.3
4	X	31	VAL	10.2
1	E	223	ASP	10.2
1	Q	192	HIS	10.1
4	T	98	SER	10.1
1	Q	41	ALA	10.0
1	Q	226	GLN	9.9
1	Q	71	SER	9.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	V	5	TYR	9.8
1	E	182	THR	9.8
3	W	35	ILE	9.7
1	M	90	ALA	9.7
1	Q	133	TRP	9.7
4	T	16	ASP	9.7
1	Q	254	GLU	9.6
1	Q	143	THR	9.6
4	X	13	PHE	9.5
4	L	8	ASP	9.5
1	A	188	HIS	9.5
3	S	66	TYR	9.5
4	T	80	THR	9.3
1	U	93	HIS	9.3
4	T	18	CYS	9.3
1	U	204	TRP	9.2
1	U	248	VAL	9.2
1	U	24	ALA	9.1
1	Q	194	VAL	9.1
3	W	2	GLN	9.1
1	U	151	HIS	9.0
1	M	251	SER	8.9
4	X	33	ILE	8.9
1	Q	15	PRO	8.9
1	Q	109	PHE	8.8
1	U	6	ARG	8.8
1	U	190	THR	8.8
1	M	252	GLY	8.8
1	Q	62	GLY	8.8
1	M	217	TRP	8.8
3	G	88	SER	8.8
1	U	247	VAL	8.7
4	X	71	VAL	8.7
1	U	90	ALA	8.7
4	X	77	PHE	8.7
1	U	270	LEU	8.7
1	Q	70	HIS	8.7
1	U	47	PRO	8.6
4	T	7	ALA	8.6
3	S	89	GLN	8.6
4	T	9	PRO	8.5
1	Q	139	ALA	8.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	P	18	CYS	8.5
4	X	57	SER	8.5
3	S	60	TRP	8.5
1	I	221	GLY	8.4
1	Q	236	ALA	8.4
4	X	56	ALA	8.4
1	A	223	ASP	8.3
2	R	9	VAL	8.3
4	T	89	HIS	8.3
1	U	192	HIS	8.3
1	Q	233	THR	8.3
1	U	241	PHE	8.3
3	W	32	PRO	8.3
4	X	24	PRO	8.2
3	S	25	CYS	8.2
1	U	67	VAL	8.2
1	M	111	ARG	8.2
1	Q	227	ASP	8.2
1	E	131	ARG	8.2
3	S	84	HIS	8.2
1	Q	9	PHE	8.2
3	W	47	GLU	8.2
4	T	58	THR	8.2
1	U	239	GLY	8.1
1	Q	229	GLU	8.1
1	A	180	GLN	8.1
3	S	69	GLU	8.1
3	S	21	ASN	8.1
3	W	67	TYR	8.1
3	S	14	PRO	8.1
1	Q	142	THR	8.1
4	X	16	ASP	8.1
3	W	57	SER	8.1
1	Q	42	SER	8.1
1	Q	208	PHE	8.0
4	H	13	PHE	8.0
3	W	63	TYR	8.0
1	U	249	VAL	8.0
1	Q	126	LEU	8.0
4	X	85	PHE	8.0
1	Q	60	TRP	7.9
1	U	259	CYS	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	160	LEU	7.9
1	M	192	HIS	7.8
1	U	214	THR	7.8
1	Q	235	PRO	7.8
4	T	85	PHE	7.8
1	Q	161	GLU	7.8
1	Q	88	SER	7.8
1	Q	132	SER	7.8
3	W	10	TYR	7.8
1	U	115	GLN	7.7
1	E	18	GLY	7.7
3	S	73	THR	7.7
3	S	41	LYS	7.7
3	W	20	SER	7.7
1	Q	103	VAL	7.6
1	Q	250	PRO	7.6
1	I	197	HIS	7.6
1	I	194	VAL	7.6
1	U	12	VAL	7.6
1	U	257	TYR	7.5
1	Q	228	THR	7.5
1	Q	61	ASP	7.5
1	Q	231	VAL	7.5
3	S	85	VAL	7.5
4	H	15	PRO	7.5
1	U	250	PRO	7.5
1	U	101	CYS	7.4
3	W	37	VAL	7.4
1	U	94	THR	7.4
3	O	49	VAL	7.4
3	G	35	ILE	7.4
3	S	63	TYR	7.4
1	E	133	TRP	7.4
3	W	72	PRO	7.4
1	M	194	VAL	7.3
1	U	105	SER	7.3
1	U	117	ALA	7.3
1	E	194	VAL	7.3
3	S	64	LEU	7.3
1	Q	259	CYS	7.3
3	S	43	GLY	7.3
3	S	65	LEU	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	X	69	VAL	7.2
1	U	231	VAL	7.2
1	M	15	PRO	7.2
1	A	189	MET	7.2
4	T	24	PRO	7.1
1	E	160	LEU	7.1
3	W	49	VAL	7.1
1	I	192	HIS	7.1
3	W	80	CYS	7.1
1	Q	222	GLU	7.1
1	U	195	SER	7.1
1	M	225	THR	7.1
1	Q	225	THR	7.0
1	Q	33	PHE	7.0
3	W	51	HIS	7.0
1	U	135	ALA	7.0
3	W	38	ASP	7.0
4	T	105	PRO	7.0
1	M	3	HIS	7.0
1	U	244	TRP	7.0
1	U	26	GLY	7.0
1	U	163	THR	6.9
1	U	109	PHE	6.9
1	I	201	LEU	6.9
3	S	52	SER	6.9
4	T	26	GLY	6.9
1	U	69	ALA	6.9
3	S	34	ASP	6.9
1	I	138	MET	6.9
3	W	54	LEU	6.9
1	U	230	LEU	6.9
1	U	116	TYR	6.8
1	U	124	ILE	6.8
1	Q	84	TYR	6.8
1	Q	258	THR	6.8
4	H	86	ILE	6.8
3	C	9	VAL	6.8
4	T	12	THR	6.8
3	W	31	HIS	6.8
1	Q	30	ASP	6.8
1	U	210	PRO	6.7
3	W	79	ALA	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	254	GLU	6.7
1	E	257	TYR	6.7
3	S	72	PRO	6.7
3	S	20	SER	6.7
1	Q	261	VAL	6.7
1	U	140	ALA	6.7
3	S	81	ARG	6.7
1	Q	39	ASP	6.7
1	M	209	TYR	6.6
1	I	193	ALA	6.6
1	U	22	PHE	6.6
1	Q	219	ARG	6.6
1	U	180	GLN	6.6
1	Q	217	TRP	6.6
2	R	4	GLY	6.6
3	O	88	SER	6.6
3	C	72	PRO	6.5
1	U	31	THR	6.5
1	U	177	GLU	6.5
4	H	11	LEU	6.5
1	A	217	TRP	6.5
4	T	93	THR	6.5
1	Q	187	THR	6.5
1	Q	253	GLN	6.4
1	I	98	MET	6.4
1	I	47	PRO	6.4
2	V	9	VAL	6.4
4	T	102	HIS	6.4
3	W	56	PHE	6.4
1	M	17	ARG	6.4
1	M	256	ARG	6.4
1	U	114	HIS	6.4
4	X	96	PHE	6.4
1	Q	125	ALA	6.4
1	E	252	GLY	6.4
1	U	254	GLU	6.4
1	U	75	ARG	6.4
3	O	74	GLU	6.3
4	X	55	LEU	6.3
1	E	247	VAL	6.3
1	U	193	ALA	6.3
1	M	206	LEU	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	P	28	ARG	6.3
3	O	72	PRO	6.3
1	E	230	LEU	6.3
1	Q	76	VAL	6.3
1	U	174	ASN	6.3
1	A	193	ALA	6.3
1	U	82	ARG	6.3
3	O	45	ARG	6.3
1	U	227	ASP	6.3
4	T	42	VAL	6.3
1	Q	214	THR	6.3
4	X	15	PRO	6.2
1	U	17	ARG	6.2
3	K	54	LEU	6.2
1	A	90	ALA	6.2
1	U	260	HIS	6.2
1	I	15	PRO	6.2
1	U	179	LEU	6.2
4	X	75	ASP	6.2
3	W	91	LYS	6.2
1	U	191	HIS	6.2
3	W	65	LEU	6.2
1	M	224	GLN	6.2
4	T	17	LYS	6.2
4	X	52	ASN	6.2
1	Q	6	ARG	6.2
3	S	46	ILE	6.2
1	U	27	TYR	6.2
1	Q	36	PHE	6.2
1	Q	45	MET	6.2
1	E	205	ALA	6.2
1	Q	124	ILE	6.1
1	M	83	GLY	6.1
1	I	217	TRP	6.1
1	E	181	ARG	6.1
1	U	182	THR	6.1
1	U	255	GLN	6.1
1	Q	162	GLY	6.1
4	X	89	HIS	6.1
3	W	73	THR	6.1
3	W	85	VAL	6.1
4	T	107	ARG	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	W	16	GLU	6.0
1	Q	48	ARG	6.0
3	S	74	GLU	6.0
1	M	271	THR	6.0
4	T	78	LEU	6.0
3	S	91	LYS	6.0
3	S	31	HIS	6.0
3	W	45	ARG	6.0
4	H	41	SER	6.0
3	S	49	VAL	6.0
1	Q	174	ASN	6.0
3	S	35	ILE	6.0
1	A	122	ASP	5.9
1	M	172	LEU	5.9
1	Q	117	ALA	5.9
4	T	50	THR	5.9
3	K	88	SER	5.9
1	Q	241	PHE	5.9
1	U	106	ASP	5.9
3	W	52	SER	5.9
4	X	106	PRO	5.9
1	Q	7	TYR	5.9
1	M	89	GLU	5.9
1	A	248	VAL	5.9
1	U	240	THR	5.9
1	I	116	TYR	5.9
3	W	41	LYS	5.9
1	I	254	GLU	5.8
4	X	84	THR	5.8
1	E	127	LYS	5.8
3	W	11	SER	5.8
1	U	16	GLY	5.8
1	U	65	ARG	5.8
1	E	116	TYR	5.8
4	T	30	ALA	5.8
4	T	56	ALA	5.8
1	U	8	PHE	5.8
1	U	243	LYS	5.8
4	T	37	TRP	5.8
4	X	37	TRP	5.8
1	M	187	THR	5.7
1	U	36	PHE	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	X	103	MET	5.7
3	S	95	TRP	5.7
1	Q	120	GLY	5.6
1	M	136	ALA	5.6
2	F	8	TYR	5.6
4	T	55	LEU	5.6
1	Q	140	ALA	5.6
1	A	210	PRO	5.6
1	M	197	HIS	5.6
1	Q	17	ARG	5.6
1	U	120	GLY	5.6
3	W	86	THR	5.6
1	U	148	GLU	5.6
1	Q	223	ASP	5.6
4	T	99	ARG	5.6
1	E	187	THR	5.6
1	U	137	ASP	5.5
3	S	82	VAL	5.5
3	W	17	ASN	5.5
1	A	247	VAL	5.5
1	M	231	VAL	5.5
1	U	113	TYR	5.5
1	Q	165	VAL	5.5
1	M	120	GLY	5.5
4	T	27	ASN	5.5
4	X	48	ASN	5.5
2	B	5	TYR	5.5
1	Q	85	TYR	5.5
4	P	106	PRO	5.5
1	U	133	TRP	5.4
1	Q	189	MET	5.4
1	U	76	VAL	5.4
1	U	7	TYR	5.4
1	U	142	THR	5.4
1	M	223	ASP	5.4
1	Q	112	GLY	5.4
3	W	69	GLU	5.4
3	S	23	LEU	5.4
1	U	34	VAL	5.4
1	Q	136	ALA	5.3
4	X	30	ALA	5.3
3	S	67	TYR	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	165	VAL	5.3
1	E	118	TYR	5.3
3	C	86	THR	5.3
1	E	189	MET	5.3
1	Q	13	SER	5.3
1	A	234	ARG	5.3
1	I	136	ALA	5.3
1	Q	28	VAL	5.3
1	M	227	ASP	5.3
4	L	11	LEU	5.3
1	Q	47	PRO	5.2
1	Q	269	PRO	5.2
3	S	79	ALA	5.2
1	U	86	ASN	5.2
2	B	8	TYR	5.2
1	A	267	PRO	5.2
1	E	204	TRP	5.2
3	W	3	ARG	5.2
1	Q	242	GLN	5.2
3	G	0	MET	5.1
1	U	141	GLN	5.1
4	H	75	ASP	5.1
1	E	41	ALA	5.1
1	U	11	SER	5.1
3	S	50	GLU	5.1
3	S	83	ASN	5.1
3	W	42	ASN	5.1
1	Q	266	LEU	5.1
3	O	92	ILE	5.1
1	A	206	LEU	5.1
1	U	126	LEU	5.1
4	X	46	TYR	5.1
1	I	78	LEU	5.1
1	Q	50	PRO	5.1
3	C	35	ILE	5.1
3	K	14	PRO	5.1
4	X	12	THR	5.0
3	S	62	PHE	5.0
1	Q	193	ALA	5.0
4	T	71	VAL	5.0
4	T	96	PHE	5.0
1	M	262	GLN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	260	HIS	5.0
4	T	94	ALA	5.0
1	A	6	ARG	5.0
1	U	228	THR	5.0
1	E	221	GLY	5.0
2	R	5	TYR	5.0
1	Q	90	ALA	5.0
1	U	35	ARG	5.0
1	U	62	GLY	5.0
1	Q	78	LEU	5.0
3	C	66	TYR	5.0
1	U	229	GLU	5.0
1	A	162	GLY	5.0
1	M	243	LYS	5.0
3	W	60	TRP	5.0
1	Q	237	GLY	4.9
4	X	108	LYS	4.9
1	I	46	GLU	4.9
1	I	209	TYR	4.9
1	Q	182	THR	4.9
1	U	167	TRP	4.9
4	D	108	LYS	4.9
4	T	39	CYS	4.9
1	M	13	SER	4.9
4	H	6	LYS	4.9
1	Q	25	VAL	4.9
4	D	10	CYS	4.9
3	W	74	GLU	4.8
3	G	40	LEU	4.8
2	N	8	TYR	4.8
4	T	41	SER	4.8
4	X	93	THR	4.8
4	T	25	ASP	4.8
1	Q	79	GLY	4.8
1	U	42	SER	4.8
3	W	81	ARG	4.8
3	W	50	GLU	4.8
1	Q	212	GLU	4.8
3	S	77	GLU	4.8
1	I	251	SER	4.8
1	Q	152	VAL	4.8
4	X	42	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	207	SER	4.8
3	S	38	ASP	4.8
3	W	94	LYS	4.8
1	M	82	ARG	4.8
1	U	71	SER	4.8
1	Q	176	LYS	4.7
4	T	36	GLY	4.7
4	T	101	TYR	4.7
3	K	45	ARG	4.7
1	Q	178	THR	4.7
1	Q	141	GLN	4.7
4	D	103	MET	4.7
4	D	11	LEU	4.7
1	Q	2	SER	4.7
1	Q	257	TYR	4.7
1	U	53	GLU	4.7
1	U	84	TYR	4.7
1	Q	119	ASP	4.7
1	A	222	GLU	4.7
1	A	213	ILE	4.7
1	I	256	ARG	4.7
1	U	226	GLN	4.7
4	T	86	ILE	4.7
3	W	25	CYS	4.7
1	U	21	ARG	4.7
3	S	70	PHE	4.7
3	K	46	ILE	4.7
1	Q	210	PRO	4.7
1	Q	127	LYS	4.7
1	A	106	ASP	4.7
4	H	42	VAL	4.6
1	E	84	TYR	4.6
4	P	15	PRO	4.6
3	W	0	MET	4.6
1	Q	206	LEU	4.6
1	U	37	ASP	4.6
3	W	27	VAL	4.6
1	Q	74	HIS	4.6
1	U	19	GLU	4.6
3	O	36	GLU	4.6
3	S	37	VAL	4.6
1	I	206	LEU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	1	LEU	4.6
4	X	67	TYR	4.6
1	U	110	LEU	4.6
4	T	22	PHE	4.6
4	X	43	ALA	4.6
1	M	201	LEU	4.6
1	A	262	GLN	4.6
1	E	192	HIS	4.6
1	U	237	GLY	4.6
1	U	132	SER	4.6
1	U	68	LYS	4.6
3	K	17	ASN	4.6
4	D	86	ILE	4.5
1	Q	156	LEU	4.5
3	W	6	LYS	4.5
4	H	74	ALA	4.5
4	L	100	GLN	4.5
1	I	205	ALA	4.5
1	Q	38	SER	4.5
1	Q	240	THR	4.5
3	W	40	LEU	4.5
1	U	95	VAL	4.5
3	K	81	ARG	4.5
1	U	123	TYR	4.5
3	O	87	LEU	4.5
4	H	80	THR	4.5
4	P	13	PHE	4.5
1	I	252	GLY	4.5
1	E	229	GLU	4.5
1	Q	137	ASP	4.5
3	C	78	TYR	4.5
3	S	4	THR	4.5
2	R	8	TYR	4.5
1	M	257	TYR	4.4
1	Q	186	LYS	4.4
1	U	81	LEU	4.4
3	S	92	ILE	4.4
4	L	40	GLN	4.4
4	T	46	TYR	4.4
4	H	77	PHE	4.4
1	E	217	TRP	4.4
1	Q	271	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	W	62	PHE	4.4
3	S	17	ASN	4.4
4	L	78	LEU	4.4
3	O	86	THR	4.4
1	U	28	VAL	4.3
3	O	3	ARG	4.3
1	U	85	TYR	4.3
1	U	209	TYR	4.3
4	D	96	PHE	4.3
1	M	53	GLU	4.3
3	W	36	GLU	4.3
1	E	244	TRP	4.3
1	E	82	ARG	4.3
3	W	88	SER	4.3
4	X	70	SER	4.3
3	W	64	LEU	4.3
1	A	212	GLU	4.3
1	M	204	TRP	4.3
1	I	189	MET	4.3
4	T	81	VAL	4.3
1	A	225	THR	4.3
2	V	7	VAL	4.3
1	I	31	THR	4.3
1	A	243	LYS	4.3
3	S	96	ASP	4.3
4	D	25	ASP	4.3
1	M	185	PRO	4.3
3	C	90	PRO	4.3
4	T	61	PRO	4.3
3	G	73	THR	4.3
4	D	89	HIS	4.3
1	U	256	ARG	4.3
1	M	118	TYR	4.3
1	Q	106	ASP	4.3
4	X	105	PRO	4.2
3	G	53	ASP	4.2
1	A	194	VAL	4.2
4	P	69	VAL	4.2
1	Q	121	LYS	4.2
1	M	128	GLU	4.2
1	M	244	TRP	4.2
2	V	4	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	30	ASP	4.2
3	C	54	LEU	4.2
3	C	3	ARG	4.2
1	U	149	ALA	4.2
1	Q	20	PRO	4.2
3	W	53	ASP	4.2
1	U	97	ARG	4.2
1	U	41	ALA	4.2
1	E	130	LEU	4.2
4	X	22	PHE	4.2
1	E	17	ARG	4.1
1	E	220	ASP	4.1
1	M	116	TYR	4.1
4	P	27	ASN	4.1
4	D	28	ARG	4.1
1	Q	22	PHE	4.1
3	O	40	LEU	4.1
3	G	90	PRO	4.1
1	Q	92	SER	4.1
3	W	33	SER	4.1
3	S	88	SER	4.1
1	I	84	TYR	4.1
1	U	170	ARG	4.1
4	X	99	ARG	4.1
1	I	1	GLY	4.1
1	E	128	GLU	4.1
1	E	61	ASP	4.1
1	M	130	LEU	4.1
1	U	168	LEU	4.1
1	E	267	PRO	4.1
1	E	146	LYS	4.1
2	R	3	PHE	4.1
1	Q	221	GLY	4.0
1	U	207	SER	4.0
3	C	49	VAL	4.0
1	U	172	LEU	4.0
3	O	39	LEU	4.0
4	X	10	CYS	4.0
1	A	136	ALA	4.0
4	X	28	ARG	4.0
1	U	73	THR	4.0
1	A	86	ASN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	6	ARG	4.0
1	E	117	ALA	4.0
1	Q	268	LYS	4.0
1	M	141	GLN	4.0
1	Q	52	ILE	4.0
1	A	22	PHE	4.0
1	A	51	TRP	4.0
1	E	162	GLY	4.0
3	C	5	PRO	4.0
1	E	165	VAL	4.0
1	U	246	ALA	4.0
3	W	66	TYR	4.0
1	Q	163	THR	4.0
3	C	73	THR	4.0
1	Q	267	PRO	4.0
1	U	50	PRO	4.0
3	O	27	VAL	4.0
4	X	23	GLN	4.0
1	E	98	MET	4.0
1	U	96	GLN	4.0
1	M	239	GLY	3.9
1	I	260	HIS	3.9
1	Q	216	THR	3.9
4	P	10	CYS	3.9
1	U	213	ILE	3.9
1	Q	35	ARG	3.9
1	I	187	THR	3.9
1	U	118	TYR	3.9
4	T	106	PRO	3.9
3	C	85	VAL	3.9
1	M	191	HIS	3.9
1	U	122	ASP	3.9
1	U	72	GLN	3.9
1	Q	1	GLY	3.9
1	E	211	ALA	3.9
4	H	89	HIS	3.9
3	G	48	LYS	3.9
1	Q	115	GLN	3.9
4	L	71	VAL	3.9
1	A	271	THR	3.9
4	X	17	LYS	3.9
1	E	154	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	44	ILE	3.9
4	D	82	ASN	3.9
1	Q	224	GLN	3.9
1	I	120	GLY	3.9
4	T	92	ASN	3.9
1	M	4	SER	3.8
3	S	27	VAL	3.8
1	E	159	TYR	3.8
4	T	104	TRP	3.8
1	M	121	LYS	3.8
4	X	51	ARG	3.8
1	A	160	LEU	3.8
1	U	63	GLU	3.8
1	I	271	THR	3.8
1	E	109	PHE	3.8
1	Q	58	GLU	3.8
1	A	257	TYR	3.8
1	Q	97	ARG	3.8
1	Q	202	ARG	3.8
3	C	15	ALA	3.8
1	U	102	ASP	3.8
1	U	234	ARG	3.8
4	T	48	ASN	3.8
1	A	205	ALA	3.8
1	I	176	LYS	3.8
1	I	230	LEU	3.8
1	U	251	SER	3.8
1	Q	21	ARG	3.8
4	T	10	CYS	3.8
3	W	39	LEU	3.8
4	P	74	ALA	3.8
3	W	21	ASN	3.8
4	X	61	PRO	3.8
1	E	87	GLN	3.8
4	H	40	GLN	3.8
1	E	111	ARG	3.7
1	Q	99	TYR	3.7
1	Q	204	TRP	3.7
1	E	191	HIS	3.7
1	Q	144	LYS	3.7
1	A	249	VAL	3.7
4	X	73	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	22	PHE	3.7
1	E	3	HIS	3.7
3	K	79	ALA	3.7
4	P	102	HIS	3.7
3	S	80	CYS	3.7
1	I	40	ALA	3.7
1	A	5	MET	3.7
1	M	26	GLY	3.7
1	Q	102	ASP	3.7
4	P	25	ASP	3.7
3	K	44	GLU	3.7
4	P	44	ILE	3.7
1	I	257	TYR	3.7
4	L	52	ASN	3.7
1	U	45	MET	3.7
3	W	7	ILE	3.6
1	U	77	ASP	3.6
1	Q	100	GLY	3.6
3	C	7	ILE	3.6
1	E	222	GLU	3.6
1	M	84	TYR	3.6
3	O	89	GLN	3.6
1	A	227	ASP	3.6
4	P	42	VAL	3.6
1	I	105	SER	3.6
1	E	78	LEU	3.6
3	G	49	VAL	3.6
3	G	72	PRO	3.6
3	G	78	TYR	3.6
4	H	12	THR	3.6
4	X	87	PHE	3.6
1	M	75	ARG	3.6
1	Q	181	ARG	3.6
1	U	60	TRP	3.6
4	X	9	PRO	3.6
1	M	94	THR	3.6
1	U	58	GLU	3.6
1	E	86	ASN	3.6
4	D	95	MET	3.6
1	Q	191	HIS	3.6
1	U	10	THR	3.6
4	P	12	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	171	TYR	3.6
1	A	201	LEU	3.6
1	U	162	GLY	3.6
1	M	109	PHE	3.6
4	X	107	ARG	3.6
1	Q	80	THR	3.6
3	S	56	PHE	3.5
1	I	191	HIS	3.5
1	U	92	SER	3.5
2	R	7	VAL	3.5
3	K	11	SER	3.5
3	S	94	LYS	3.5
3	G	23	LEU	3.5
1	A	192	HIS	3.5
4	D	8	ASP	3.5
1	A	233	THR	3.5
1	Q	81	LEU	3.5
1	Q	159	TYR	3.5
2	V	2	LEU	3.5
3	W	23	LEU	3.5
4	T	67	TYR	3.5
1	Q	264	GLU	3.5
3	C	77	GLU	3.5
1	M	45	MET	3.5
1	A	43	GLN	3.5
1	M	28	VAL	3.5
4	P	36	GLY	3.5
4	X	40	GLN	3.5
1	Q	157	ARG	3.5
3	C	60	TRP	3.5
4	T	13	PHE	3.5
1	M	165	VAL	3.5
1	U	103	VAL	3.5
1	A	156	LEU	3.5
2	J	8	TYR	3.5
3	G	91	LYS	3.5
1	U	157	ARG	3.5
4	X	32	LEU	3.5
1	A	121	LYS	3.4
1	M	98	MET	3.4
3	C	38	ASP	3.4
3	S	87	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	204	TRP	3.4
1	A	265	GLY	3.4
1	E	209	TYR	3.4
3	K	0	MET	3.4
3	C	97	ARG	3.4
1	E	231	VAL	3.4
1	M	33	PHE	3.4
4	D	26	GLY	3.4
1	E	113	TYR	3.4
1	Q	211	ALA	3.4
4	X	90	MET	3.4
1	E	225	THR	3.4
3	C	71	THR	3.4
4	T	69	VAL	3.4
3	C	91	LYS	3.4
1	A	135	ALA	3.4
3	S	0	MET	3.4
4	L	33	ILE	3.4
1	E	60	TRP	3.4
3	C	33	SER	3.4
3	C	81	ARG	3.4
2	V	1	LEU	3.4
3	G	86	THR	3.4
1	M	52	ILE	3.4
1	Q	203	CYS	3.4
1	U	206	LEU	3.4
1	E	228	THR	3.4
1	Q	54	GLN	3.4
1	U	253	GLN	3.4
4	L	51	ARG	3.4
4	T	38	GLU	3.4
1	Q	87	GLN	3.4
1	U	242	GLN	3.4
1	I	190	THR	3.3
1	A	8	PHE	3.3
3	G	33	SER	3.3
1	Q	26	GLY	3.3
4	D	40	GLN	3.3
1	E	124	ILE	3.3
4	D	75	ASP	3.3
1	E	89	GLU	3.3
3	C	63	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	68	THR	3.3
3	W	82	VAL	3.3
1	E	19	GLU	3.3
1	U	128	GLU	3.3
3	C	44	GLU	3.3
1	Q	255	GLN	3.3
4	D	99	ARG	3.3
1	E	250	PRO	3.3
3	O	61	SER	3.3
1	M	164	CYS	3.3
3	K	95	TRP	3.3
1	Q	5	MET	3.3
1	Q	59	TYR	3.3
4	X	50	THR	3.3
1	A	250	PRO	3.3
1	Q	77	ASP	3.3
3	G	34	ASP	3.3
1	A	207	SER	3.3
4	X	101	TYR	3.3
4	H	62	GLY	3.3
1	M	156	LEU	3.3
1	E	13	SER	3.3
1	A	107	TRP	3.3
1	E	224	GLN	3.3
1	I	45	MET	3.3
3	O	2	GLN	3.3
1	M	86	ASN	3.2
1	U	159	TYR	3.2
4	T	84	THR	3.2
1	E	122	ASP	3.2
1	U	20	PRO	3.2
1	M	135	ALA	3.2
1	Q	130	LEU	3.2
1	M	42	SER	3.2
3	S	19	LYS	3.2
3	S	61	SER	3.2
4	X	34	LYS	3.2
1	Q	114	HIS	3.2
4	H	36	GLY	3.2
4	P	29	CYS	3.2
1	M	131	ARG	3.2
1	Q	32	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	7	ALA	3.2
1	I	51	TRP	3.2
4	X	104	TRP	3.2
1	I	173	GLU	3.2
4	X	14	ASN	3.2
3	S	86	THR	3.2
3	O	54	LEU	3.2
1	E	197	HIS	3.2
3	W	22	PHE	3.2
4	D	41	SER	3.2
4	X	97	MET	3.2
4	H	99	ARG	3.2
1	Q	69	ALA	3.2
3	K	25	CYS	3.2
3	K	40	LEU	3.2
3	C	45	ARG	3.2
3	O	48	LYS	3.2
1	I	64	THR	3.2
1	Q	10	THR	3.2
3	O	73	THR	3.2
1	M	69	ALA	3.2
3	O	79	ALA	3.2
4	X	44	ILE	3.2
1	A	215	LEU	3.2
1	Q	168	LEU	3.2
1	U	87	GLN	3.2
3	W	8	GLN	3.2
4	P	19	GLN	3.2
1	U	189	MET	3.1
4	L	95	MET	3.1
4	T	59	TRP	3.1
1	I	134	THR	3.1
1	A	221	GLY	3.1
3	W	26	TYR	3.1
4	D	107	ARG	3.1
1	M	180	GLN	3.1
1	M	246	ALA	3.1
1	I	269	PRO	3.1
1	M	182	THR	3.1
3	S	71	THR	3.1
1	A	72	GLN	3.1
1	Q	113	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	88	SER	3.1
1	E	45	MET	3.1
3	C	95	TRP	3.1
1	E	143	THR	3.1
1	I	111	ARG	3.1
1	M	255	GLN	3.1
4	X	79	ARG	3.1
1	U	52	ILE	3.1
1	U	125	ALA	3.1
1	E	50	PRO	3.1
1	Q	209	TYR	3.1
2	V	6	PRO	3.1
1	M	39	ASP	3.1
1	Q	145	HIS	3.1
1	Q	107	TRP	3.1
4	X	59	TRP	3.1
4	T	44	ILE	3.1
1	Q	123	TYR	3.1
1	I	48	ARG	3.1
3	G	77	GLU	3.1
3	W	19	LYS	3.1
1	E	207	SER	3.1
4	X	86	ILE	3.1
1	Q	238	ASP	3.1
4	X	95	MET	3.1
1	I	156	LEU	3.1
1	Q	40	ALA	3.1
1	Q	251	SER	3.1
2	R	6	PRO	3.1
3	C	4	THR	3.0
4	P	14	ASN	3.0
4	X	21	SER	3.0
1	E	268	LYS	3.0
1	U	236	ALA	3.0
1	U	245	ALA	3.0
3	S	16	GLU	3.0
4	P	108	LYS	3.0
4	T	91	CYS	3.0
1	E	216	THR	3.0
1	M	25	VAL	3.0
4	D	27	ASN	3.0
1	Q	270	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	P	56	ALA	3.0
1	A	74	HIS	3.0
4	H	91	CYS	3.0
1	A	131	ARG	3.0
1	U	38	SER	3.0
1	I	172	LEU	3.0
1	U	183	ASP	3.0
4	X	25	ASP	3.0
2	F	6	PRO	3.0
1	E	256	ARG	3.0
1	E	12	VAL	3.0
1	E	29	ASP	3.0
4	T	57	SER	3.0
1	M	160	LEU	3.0
1	A	211	ALA	3.0
3	S	13	HIS	3.0
2	N	1	LEU	3.0
3	W	58	LYS	3.0
4	T	49	LYS	3.0
3	W	18	GLY	3.0
1	A	197	HIS	3.0
4	T	82	ASN	3.0
1	E	7	TYR	3.0
1	U	98	MET	3.0
4	T	66	TRP	3.0
1	M	169	ARG	3.0
1	A	27	TYR	3.0
1	A	159	TYR	3.0
1	E	123	TYR	3.0
1	Q	153	ALA	3.0
1	A	115	GLN	2.9
4	D	87	PHE	2.9
1	E	25	VAL	2.9
4	D	104	TRP	2.9
1	E	218	GLN	2.9
1	A	33	PHE	2.9
1	A	166	GLU	2.9
4	D	13	PHE	2.9
1	A	134	THR	2.9
1	M	78	LEU	2.9
1	Q	134	THR	2.9
3	C	40	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	P	95	MET	2.9
1	M	43	GLN	2.9
3	G	2	GLN	2.9
4	T	64	PRO	2.9
1	A	52	ILE	2.9
3	W	92	ILE	2.9
4	H	8	ASP	2.9
3	O	18	GLY	2.9
1	M	230	LEU	2.9
4	D	12	THR	2.9
1	Q	34	VAL	2.9
2	F	7	VAL	2.9
4	H	81	VAL	2.9
4	P	8	ASP	2.9
4	X	63	ASP	2.9
1	M	202	ARG	2.9
1	A	78	LEU	2.9
2	J	1	LEU	2.9
4	L	69	VAL	2.9
1	E	125	ALA	2.9
1	I	130	LEU	2.9
1	I	229	GLU	2.9
2	J	9	VAL	2.9
1	U	51	TRP	2.9
3	W	95	TRP	2.9
4	T	72	PRO	2.9
1	A	35	ARG	2.9
3	C	1	ILE	2.9
3	C	28	SER	2.9
1	U	49	ALA	2.9
3	K	63	TYR	2.9
3	C	11	SER	2.9
1	A	173	GLU	2.9
4	P	58	THR	2.9
1	E	202	ARG	2.9
1	E	27	TYR	2.9
1	I	267	PRO	2.9
1	M	145	HIS	2.8
3	W	13	HIS	2.8
3	W	61	SER	2.8
4	T	6	LYS	2.8
4	T	33	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	81	ARG	2.8
4	X	58	THR	2.8
3	W	76	ASP	2.8
2	N	9	VAL	2.8
1	U	104	GLY	2.8
4	X	102	HIS	2.8
4	P	96	PHE	2.8
3	W	12	ARG	2.8
1	E	141	GLN	2.8
1	E	251	SER	2.8
3	C	92	ILE	2.8
3	C	55	SER	2.8
3	W	55	SER	2.8
3	S	36	GLU	2.8
4	T	8	ASP	2.8
1	E	83	GLY	2.8
4	X	36	GLY	2.8
1	A	138	MET	2.8
1	I	158	ALA	2.8
1	A	132	SER	2.8
1	M	114	HIS	2.8
1	E	186	LYS	2.8
4	P	37	TRP	2.8
1	E	72	GLN	2.8
1	U	262	GLN	2.8
1	A	39	ASP	2.8
1	E	179	LEU	2.8
4	T	77	PHE	2.8
1	E	149	ALA	2.8
4	H	79	ARG	2.8
3	K	84	HIS	2.8
3	O	55	SER	2.8
1	A	155	GLN	2.8
1	I	177	GLU	2.8
4	X	27	ASN	2.8
1	M	12	VAL	2.8
4	D	61	PRO	2.8
4	H	10	CYS	2.8
1	I	152	VAL	2.7
1	U	89	GLU	2.7
3	C	36	GLU	2.7
4	D	56	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	45	GLN	2.7
4	X	65	GLU	2.7
1	A	253	GLN	2.7
1	E	101	CYS	2.7
1	E	210	PRO	2.7
3	S	5	PRO	2.7
3	S	57	SER	2.7
4	T	95	MET	2.7
3	S	75	LYS	2.7
4	T	63	ASP	2.7
4	T	108	LYS	2.7
1	A	120	GLY	2.7
3	K	66	TYR	2.7
1	I	6	ARG	2.7
1	I	202	ARG	2.7
1	Q	108	ARG	2.7
4	T	28	ARG	2.7
1	I	89	GLU	2.7
4	X	64	PRO	2.7
1	M	5	MET	2.7
1	Q	122	ASP	2.7
1	M	126	LEU	2.7
3	S	45	ARG	2.7
1	Q	72	GLN	2.7
3	G	92	ILE	2.7
1	M	41	ALA	2.7
4	L	24	PRO	2.7
1	I	122	ASP	2.7
4	T	75	ASP	2.7
1	E	63	GLU	2.7
1	U	171	TYR	2.7
1	U	80	THR	2.7
1	A	191	HIS	2.7
4	H	107	ARG	2.7
1	I	96	GLN	2.7
4	L	35	CYS	2.7
1	Q	86	ASN	2.7
1	M	99	TYR	2.7
1	E	236	ALA	2.7
1	I	261	VAL	2.7
1	M	81	LEU	2.7
3	C	12	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	X	72	PRO	2.7
3	C	84	HIS	2.7
1	Q	46	GLU	2.7
1	Q	51	TRP	2.7
4	L	91	CYS	2.7
4	P	40	GLN	2.6
1	I	188	HIS	2.6
1	Q	3	HIS	2.6
3	K	85	VAL	2.6
1	E	5	MET	2.6
4	T	90	MET	2.6
3	G	45	ARG	2.6
4	T	51	ARG	2.6
4	L	10	CYS	2.6
4	P	23	GLN	2.6
4	T	40	GLN	2.6
3	S	48	LYS	2.6
1	I	52	ILE	2.6
1	I	133	TRP	2.6
1	I	213	ILE	2.6
1	A	203	CYS	2.6
1	M	139	ALA	2.6
1	U	66	LYS	2.6
1	A	226	GLN	2.6
3	S	2	GLN	2.6
2	F	5	TYR	2.6
3	W	14	PRO	2.6
1	I	145	HIS	2.6
1	A	181	ARG	2.6
1	I	17	ARG	2.6
1	I	231	VAL	2.6
1	M	215	LEU	2.6
3	G	54	LEU	2.6
4	X	88	GLU	2.6
1	I	113	TYR	2.6
1	M	85	TYR	2.6
3	C	8	GLN	2.6
3	C	59	ASP	2.6
1	E	66	LYS	2.6
4	L	87	PHE	2.6
1	A	88	SER	2.6
3	S	44	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	147	TRP	2.6
3	G	3	ARG	2.6
4	L	15	PRO	2.6
4	L	86	ILE	2.6
3	C	79	ALA	2.6
4	L	89	HIS	2.6
2	N	7	VAL	2.6
3	C	2	GLN	2.6
1	I	62	GLY	2.6
4	T	62	GLY	2.6
4	L	68	THR	2.6
1	A	41	ALA	2.6
3	S	51	HIS	2.6
4	P	71	VAL	2.6
1	E	215	LEU	2.6
3	G	87	LEU	2.6
1	E	239	GLY	2.6
3	W	28	SER	2.6
1	Q	218	GLN	2.5
3	C	89	GLN	2.5
3	W	71	THR	2.5
1	A	61	ASP	2.5
1	M	91	GLY	2.5
3	C	94	LYS	2.5
1	U	70	HIS	2.5
1	A	179	LEU	2.5
1	I	237	GLY	2.5
1	I	82	ARG	2.5
1	U	202	ARG	2.5
1	A	98	MET	2.5
1	E	33	PHE	2.5
1	M	144	LYS	2.5
1	M	203	CYS	2.5
4	X	68	THR	2.5
3	G	82	VAL	2.5
4	H	71	VAL	2.5
4	L	76	GLY	2.5
1	I	33	PHE	2.5
1	M	138	MET	2.5
3	O	20	SER	2.5
1	M	210	PRO	2.5
1	U	134	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	80	CYS	2.5
1	U	14	ARG	2.5
1	E	81	LEU	2.5
3	S	33	SER	2.5
4	H	70	SER	2.5
1	I	121	LYS	2.5
1	I	263	HIS	2.5
1	M	97	ARG	2.5
1	Q	131	ARG	2.5
1	U	57	PRO	2.5
1	U	166	GLU	2.5
3	C	26	TYR	2.5
4	D	15	PRO	2.5
1	A	24	ALA	2.5
1	I	41	ALA	2.5
4	L	32	LEU	2.5
1	A	84	TYR	2.5
1	E	59	TYR	2.5
4	L	6	LYS	2.5
3	S	12	ARG	2.5
1	M	235	PRO	2.5
1	Q	57	PRO	2.5
1	M	270	LEU	2.5
3	C	23	LEU	2.5
4	T	20	LEU	2.5
1	E	107	TRP	2.5
4	H	87	PHE	2.5
1	M	35	ARG	2.5
1	A	216	THR	2.4
1	E	31	THR	2.4
1	I	114	HIS	2.4
1	U	153	ALA	2.4
3	O	91	LYS	2.4
3	W	48	LYS	2.4
1	E	8	PHE	2.4
3	G	81	ARG	2.4
4	L	18	CYS	2.4
4	T	29	CYS	2.4
3	W	46	ILE	2.4
4	H	32	LEU	2.4
1	E	38	SER	2.4
4	X	81	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	96	ASP	2.4
4	D	77	PHE	2.4
1	A	87	GLN	2.4
1	I	109	PHE	2.4
1	M	238	ASP	2.4
4	D	14	ASN	2.4
1	I	7	TYR	2.4
1	A	3	HIS	2.4
1	A	31	THR	2.4
3	W	97	ARG	2.4
1	E	148	GLU	2.4
3	O	23	LEU	2.4
4	P	57	SER	2.4
1	Q	37	ASP	2.4
1	Q	167	TRP	2.4
4	H	25	ASP	2.4
4	P	22	PHE	2.4
1	I	27	TYR	2.4
1	U	99	TYR	2.4
1	E	161	GLU	2.4
1	Q	146	LYS	2.4
1	U	139	ALA	2.4
1	I	77	ASP	2.4
1	E	36	PHE	2.4
3	K	60	TRP	2.4
1	Q	158	ALA	2.4
4	D	18	CYS	2.4
4	P	35	CYS	2.4
4	H	14	ASN	2.4
4	L	44	ILE	2.4
3	K	18	GLY	2.4
1	E	248	VAL	2.4
1	M	173	GLU	2.4
1	U	108	ARG	2.4
3	C	50	GLU	2.4
3	O	50	GLU	2.4
1	I	32	GLN	2.4
4	T	23	GLN	2.4
1	M	213	ILE	2.4
1	U	79	GLY	2.4
4	D	36	GLY	2.4
1	U	144	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	34	LYS	2.4
1	E	169	ARG	2.4
1	M	8	PHE	2.4
1	M	76	VAL	2.4
3	C	62	PHE	2.4
1	U	147	TRP	2.4
1	A	171	TYR	2.3
1	E	253	GLN	2.3
1	E	184	ALA	2.3
1	Q	220	ASP	2.3
4	D	58	THR	2.3
4	H	94	ALA	2.3
4	X	11	LEU	2.3
4	X	54	THR	2.3
1	A	174	ASN	2.3
4	X	18	CYS	2.3
1	A	99	TYR	2.3
1	M	181	ARG	2.3
3	S	24	ASN	2.3
1	E	115	GLN	2.3
3	G	95	TRP	2.3
3	O	66	TYR	2.3
1	E	79	GLY	2.3
3	S	29	GLY	2.3
4	X	76	GLY	2.3
1	A	187	THR	2.3
1	E	240	THR	2.3
1	Q	96	GLN	2.3
1	M	73	THR	2.3
3	O	17	ASN	2.3
4	P	68	THR	2.3
1	E	212	GLU	2.3
1	I	147	TRP	2.3
4	T	65	GLU	2.3
1	U	88	SER	2.3
1	Q	68	LYS	2.3
1	A	34	VAL	2.3
1	M	95	VAL	2.3
3	O	9	VAL	2.3
4	L	49	LYS	2.3
4	L	64	PRO	2.3
4	L	106	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	123	TYR	2.3
1	E	99	TYR	2.3
3	G	66	TYR	2.3
3	K	15	ALA	2.3
4	L	67	TYR	2.3
1	I	67	VAL	2.3
1	M	110	LEU	2.3
3	W	90	PRO	2.3
4	D	106	PRO	2.3
4	D	7	ALA	2.3
4	L	74	ALA	2.3
1	Q	94	THR	2.3
1	M	6	ARG	2.3
4	X	6	LYS	2.3
1	I	253	GLN	2.2
1	A	45	MET	2.2
1	I	135	ALA	2.2
4	L	43	ALA	2.2
1	M	134	THR	2.2
1	A	7	TYR	2.2
1	I	103	VAL	2.2
3	G	8	GLN	2.2
1	A	114	HIS	2.2
1	E	47	PRO	2.2
1	I	154	GLU	2.2
1	E	110	LEU	2.2
4	T	53	ASN	2.2
1	A	125	ALA	2.2
1	I	208	PHE	2.2
3	O	35	ILE	2.2
1	I	2	SER	2.2
1	I	68	LYS	2.2
1	U	78	LEU	2.2
3	O	6	LYS	2.2
1	M	234	ARG	2.2
4	D	37	TRP	2.2
3	C	76	ASP	2.2
1	A	76	VAL	2.2
4	P	17	LYS	2.2
4	X	47	LYS	2.2
1	I	57	PRO	2.2
1	Q	44	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	103	MET	2.2
4	X	80	THR	2.2
4	X	60	GLN	2.2
1	E	85	TYR	2.2
1	E	121	LYS	2.2
1	I	34	VAL	2.2
1	M	261	VAL	2.2
1	Q	82	ARG	2.2
1	Q	201	LEU	2.2
4	L	39	CYS	2.2
1	E	136	ALA	2.2
1	I	5	MET	2.2
1	I	255	GLN	2.2
1	Q	135	ALA	2.2
1	A	83	GLY	2.2
1	M	240	THR	2.2
1	Q	166	GLU	2.2
3	K	91	LYS	2.2
3	O	41	LYS	2.2
1	A	126	LEU	2.2
1	U	235	PRO	2.2
3	W	75	LYS	2.2
1	A	16	GLY	2.2
1	Q	205	ALA	2.2
1	E	163	THR	2.2
1	Q	252	GLY	2.2
3	O	34	ASP	2.2
3	G	46	ILE	2.2
1	A	130	LEU	2.2
3	O	75	LYS	2.2
1	M	32	GLN	2.2
1	U	155	GLN	2.2
4	P	61	PRO	2.2
1	A	214	THR	2.2
3	K	3	ARG	2.2
1	A	4	SER	2.1
4	X	53	ASN	2.1
1	A	67	VAL	2.1
1	Q	55	GLU	2.1
3	O	64	LEU	2.1
1	E	100	GLY	2.1
1	U	138	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	203	CYS	2.1
3	W	44	GLU	2.1
1	M	74	HIS	2.1
3	G	14	PRO	2.1
4	H	28	ARG	2.1
1	A	144	LYS	2.1
3	G	15	ALA	2.1
1	M	258	THR	2.1
4	X	66	TRP	2.1
1	Q	53	GLU	2.1
1	M	152	VAL	2.1
1	Q	23	ILE	2.1
1	A	50	PRO	2.1
1	E	170	ARG	2.1
1	U	252	GLY	2.1
4	D	64	PRO	2.1
4	T	76	GLY	2.1
1	M	222	GLU	2.1
4	L	30	ALA	2.1
3	C	57	SER	2.1
1	I	165	VAL	2.1
1	E	114	HIS	2.1
1	M	151	HIS	2.1
3	O	14	PRO	2.1
1	I	73	THR	2.1
1	M	190	THR	2.1
1	Q	11	SER	2.1
2	V	3	PHE	2.1
4	H	73	GLY	2.1
4	L	62	GLY	2.1
1	M	154	GLU	2.1
3	O	67	TYR	2.1
4	D	101	TYR	2.1
1	A	184	ALA	2.1
1	I	107	TRP	2.1
1	M	163	THR	2.1
3	O	24	ASN	2.1
3	S	68	THR	2.1
1	A	202	ARG	2.1
1	U	13	SER	2.1
3	O	52	SER	2.1
3	S	11	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	154	GLU	2.1
3	G	85	VAL	2.1
4	X	49	LYS	2.1
1	A	143	THR	2.1
1	E	112	GLY	2.1
1	M	102	ASP	2.1
3	O	70	PHE	2.1
1	A	103	VAL	2.1
1	A	68	LYS	2.1
3	C	42	ASN	2.1
1	M	161	GLU	2.1
1	U	5	MET	2.1
3	O	11	SER	2.1
4	P	65	GLU	2.1
1	I	112	GLY	2.1
3	G	43	GLY	2.1
3	W	70	PHE	2.1
1	M	127	LYS	2.0
1	I	97	ARG	2.0
1	M	148	GLU	2.0
1	E	39	ASP	2.0
1	I	207	SER	2.0
1	U	268	LYS	2.0
3	G	30	PHE	2.0
3	G	70	PHE	2.0
1	A	47	PRO	2.0
1	E	249	VAL	2.0
1	A	85	TYR	2.0
1	E	232	GLU	2.0
1	M	177	GLU	2.0
1	M	184	ALA	2.0
1	Q	24	ALA	2.0
1	A	196	ASP	2.0
1	I	26	GLY	2.0
1	I	132	SER	2.0
1	M	38	SER	2.0
1	M	80	THR	2.0
1	M	100	GLY	2.0
3	O	53	ASP	2.0
4	D	98	SER	2.0
1	I	155	GLN	2.0
1	A	53	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	159	TYR	2.0
1	U	121	LYS	2.0
1	A	142	THR	2.0
1	Q	101	CYS	2.0
1	A	151	HIS	2.0
1	I	234	ARG	2.0
1	A	12	VAL	2.0
3	O	32	PRO	2.0
4	H	24	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.