



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:24 AM GMT

PDB ID : 3LK4  
Title : Crystal structure of CapZ bound to the uncapping motif from CD2AP  
Authors : Hernandez-Valladares, M.; Kim, T.; Kannan, B.; Tung, A.; Cooper, J.A.; Robinson, R.C.  
Deposited on : 2010-01-27  
Resolution : 1.99 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

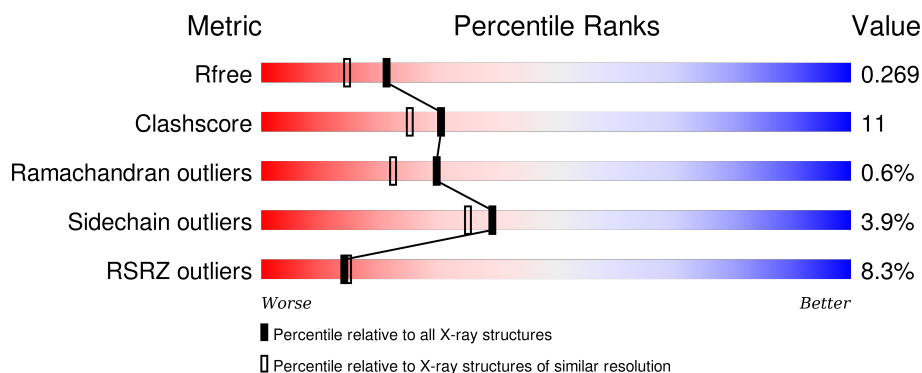
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1	286	<div> <div>9%</div> <div>73% 18% 6%</div> </div>
1	4	286	<div> <div>9%</div> <div>73% 19% 6%</div> </div>
1	7	286	<div> <div>5%</div> <div>73% 18% 6%</div> </div>
1	A	286	<div> <div>9%</div> <div>73% 19% 6%</div> </div>
1	D	286	<div> <div>6%</div> <div>74% 18% 6%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	286	
1	J	286	
1	M	286	
1	P	286	
1	S	286	
1	V	286	
1	Y	286	
2	2	277	
2	5	277	
2	8	277	
2	B	277	
2	E	277	
2	H	277	
2	K	277	
2	N	277	
2	Q	277	
2	T	277	
2	W	277	
2	Z	277	
3	0	29	
3	3	29	
3	6	29	
3	9	29	
3	C	29	
3	F	29	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	29	<div><div></div><div>24%</div><div>59%</div><div>38%</div><div></div></div>
3	L	29	<div><div></div><div>24%</div><div>59%</div><div>38%</div><div></div></div>
3	O	29	<div><div></div><div>28%</div><div>55%</div><div>41%</div><div></div></div>
3	R	29	<div><div></div><div>24%</div><div>55%</div><div>41%</div><div></div></div>
3	U	29	<div><div></div><div>28%</div><div>55%</div><div>41%</div><div></div></div>
3	X	29	<div><div></div><div>21%</div><div>59%</div><div>34%</div><div>7%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54370 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 F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	D	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	G	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	J	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	M	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	P	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	S	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	V	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	Y	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	1	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	4	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	7	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	E	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	K	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	N	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	Q	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	T	237	Total	C	N	O	S	0	0	0
			1870	1171	322	367	10			
2	W	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	Z	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	2	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	5	237	Total	C	N	O	S	0	0	0
			1870	1171	322	367	10			
2	8	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			

- Molecule 3 is a protein called CD2-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	F	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	I	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	L	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	O	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	R	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	U	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	X	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	0	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	6	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	9	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	90	Total	O	0	0
			90	90		
4	C	14	Total	O	0	0
			14	14		
4	D	131	Total	O	0	0
			131	131		
4	E	103	Total	O	0	0
			103	103		
4	F	13	Total	O	0	0
			13	13		
4	G	126	Total	O	0	0
			126	126		
4	H	155	Total	O	0	0
			155	155		
4	I	10	Total	O	0	0
			10	10		
4	J	135	Total	O	0	0
			135	135		
4	K	103	Total	O	0	0
			103	103		
4	L	14	Total	O	0	0
			14	14		
4	M	123	Total	O	0	0
			123	123		
4	N	138	Total	O	0	0
			138	138		
4	O	10	Total	O	0	0
			10	10		
4	P	93	Total	O	0	0
			93	93		

*Continued on next page...*

*Continued from previous page...*

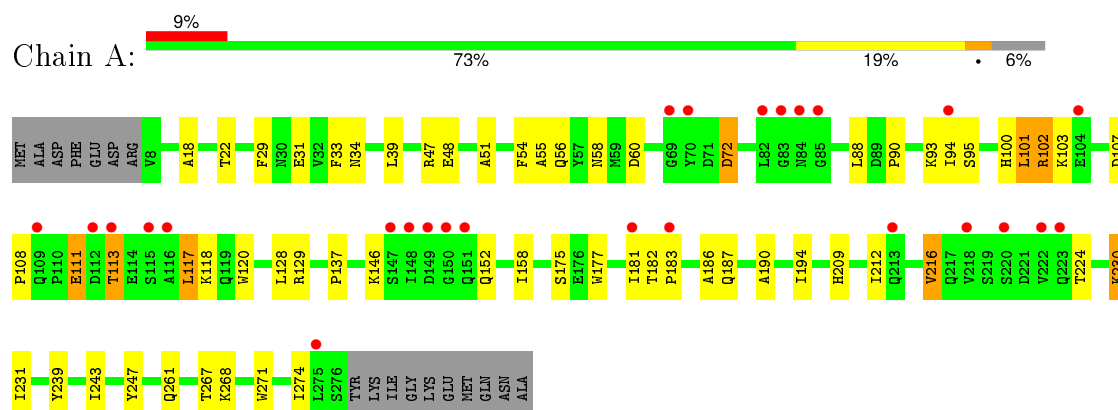
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	76	Total 76	O 76	0	0
4	R	17	Total 17	O 17	0	0
4	S	115	Total 115	O 115	0	0
4	T	110	Total 110	O 110	0	0
4	U	12	Total 12	O 12	0	0
4	V	137	Total 137	O 137	0	0
4	W	134	Total 134	O 134	0	0
4	X	14	Total 14	O 14	0	0
4	Y	91	Total 91	O 91	0	0
4	Z	80	Total 80	O 80	0	0
4	0	13	Total 13	O 13	0	0
4	1	90	Total 90	O 90	0	0
4	2	91	Total 91	O 91	0	0
4	3	14	Total 14	O 14	0	0
4	4	114	Total 114	O 114	0	0
4	5	119	Total 119	O 119	0	0
4	6	10	Total 10	O 10	0	0
4	7	138	Total 138	O 138	0	0
4	8	148	Total 148	O 148	0	0
4	9	11	Total 11	O 11	0	0



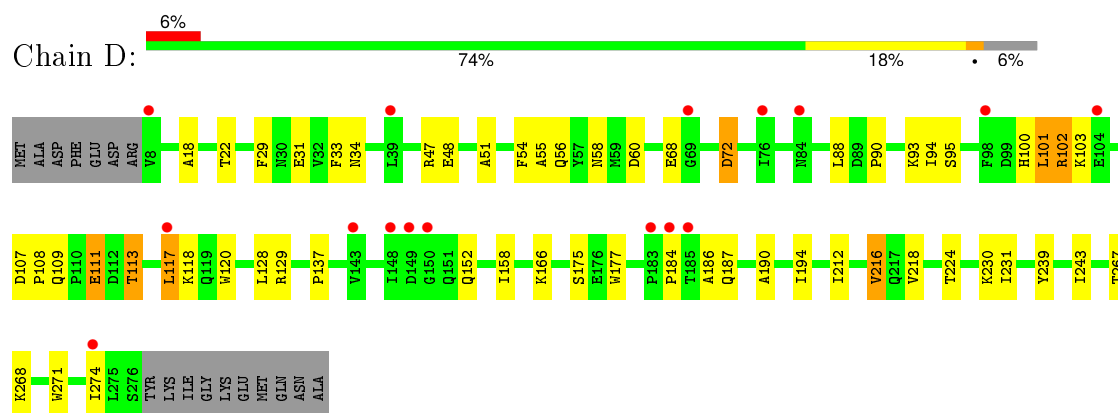
### 3 Residue-property plots

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

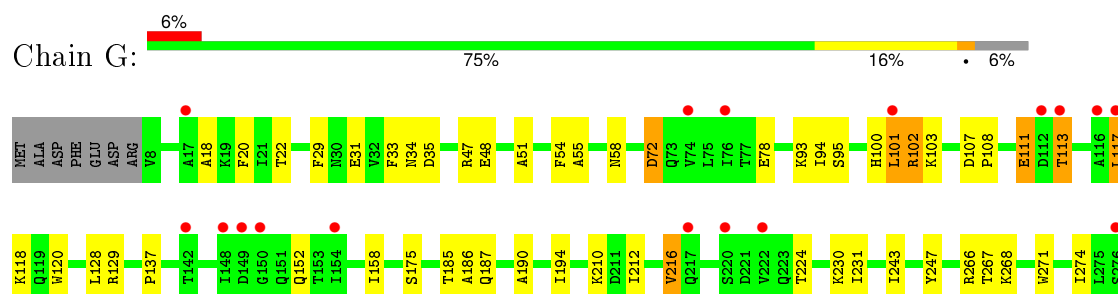
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 1: F-actin-capping protein subunit alpha-1




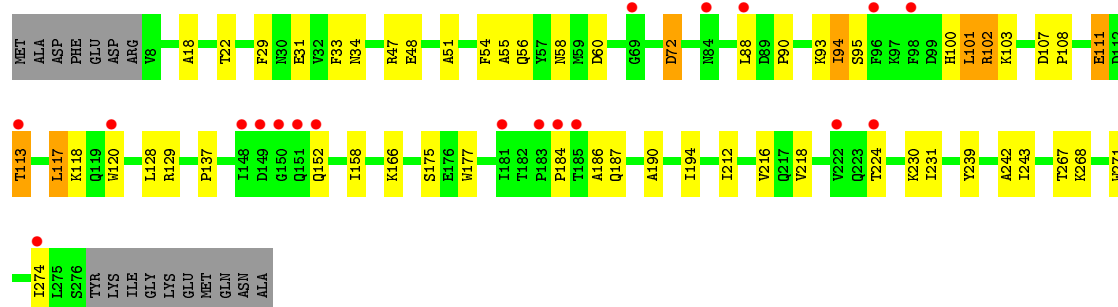
- Molecule 1: F-actin-capping protein subunit alpha-1



TYR  
LYS  
ILE  
GLY  
LYS  
GLU  
MET  
GLN  
ALA

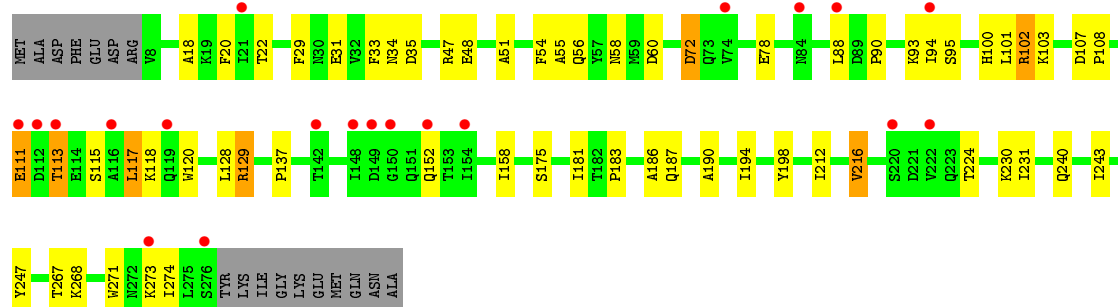
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain J: 



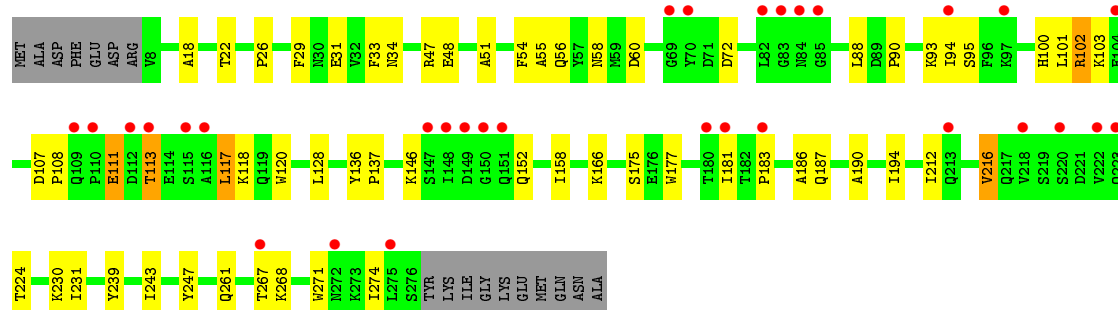
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain M: 



- Molecule 1: F-actin-capping protein subunit alpha-1

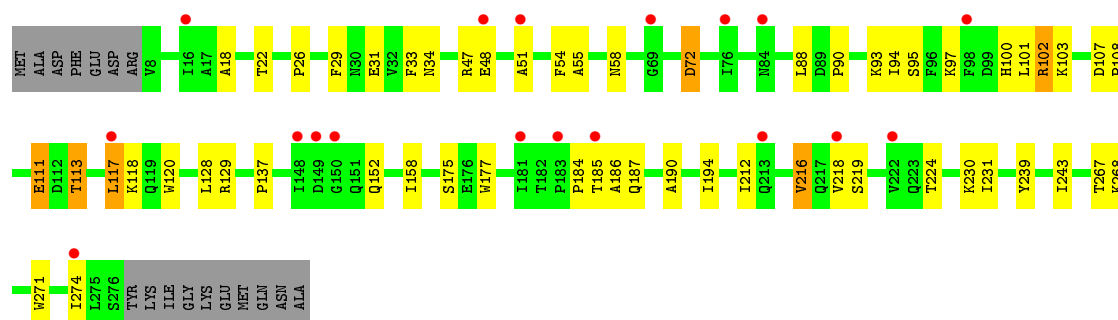
Chain P: 



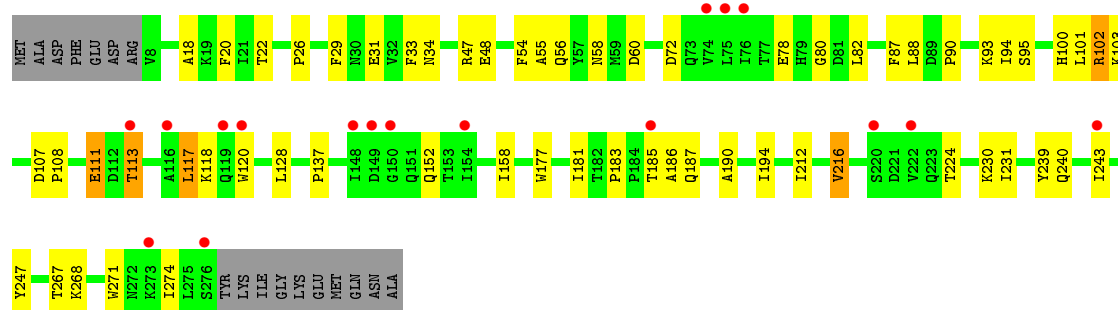
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain S: 

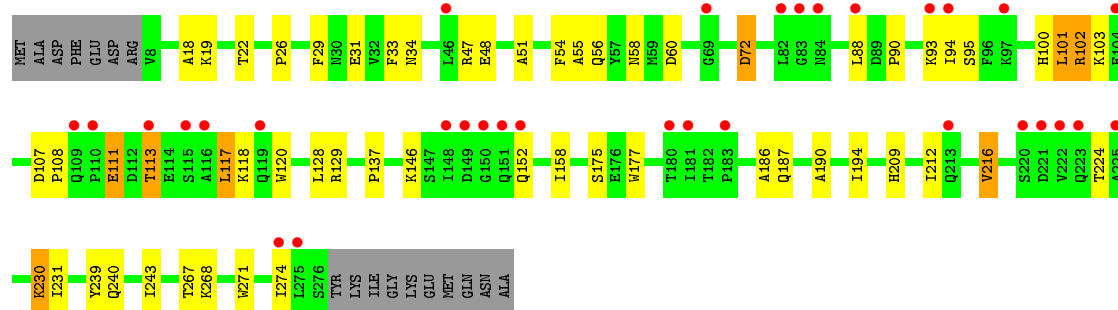
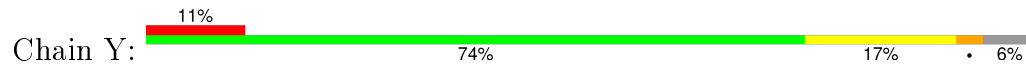




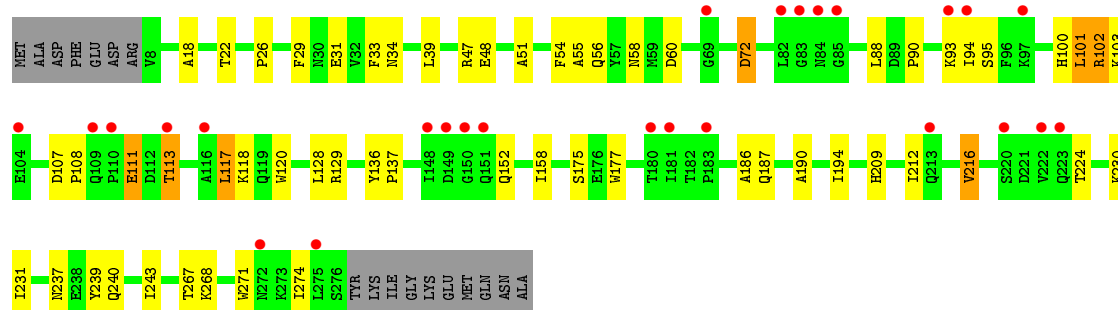
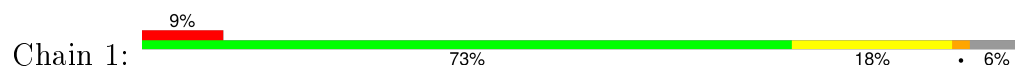
- Molecule 1: F-actin-capping protein subunit alpha-1



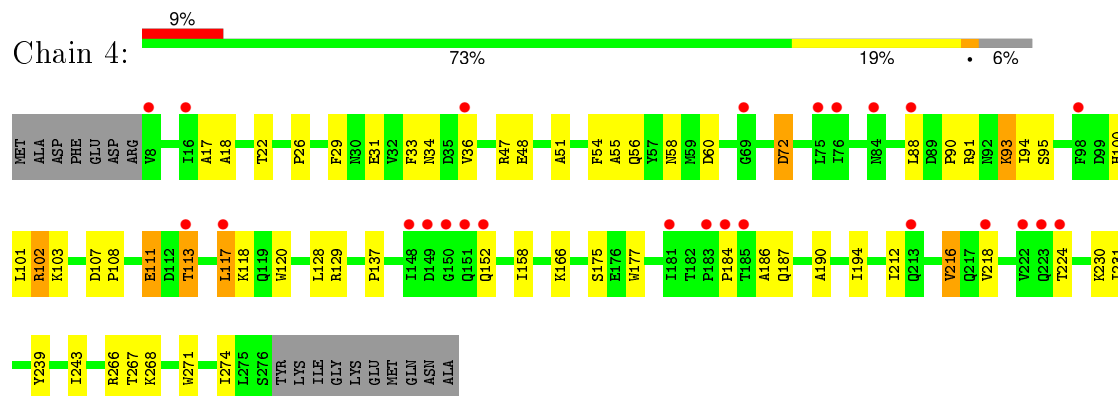
- Molecule 1: F-actin-capping protein subunit alpha-1



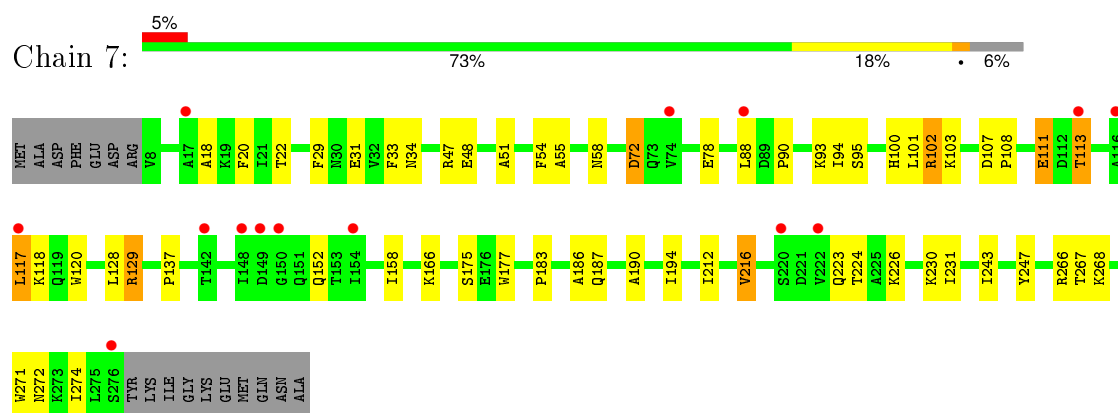
- Molecule 1: F-actin-capping protein subunit alpha-1



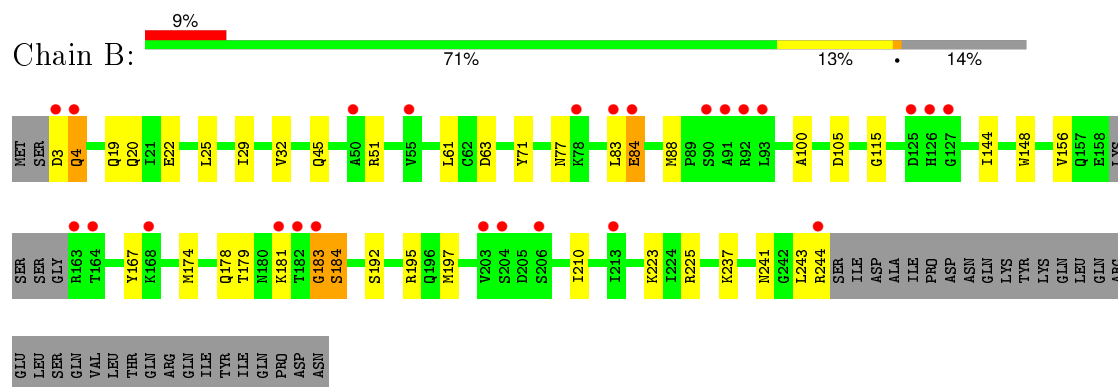
- Molecule 1: F-actin-capping protein subunit alpha-1



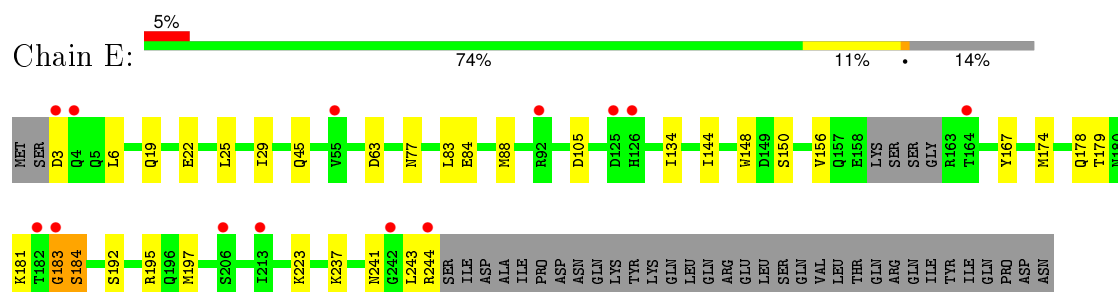
- Molecule 1: F-actin-capping protein subunit alpha-1



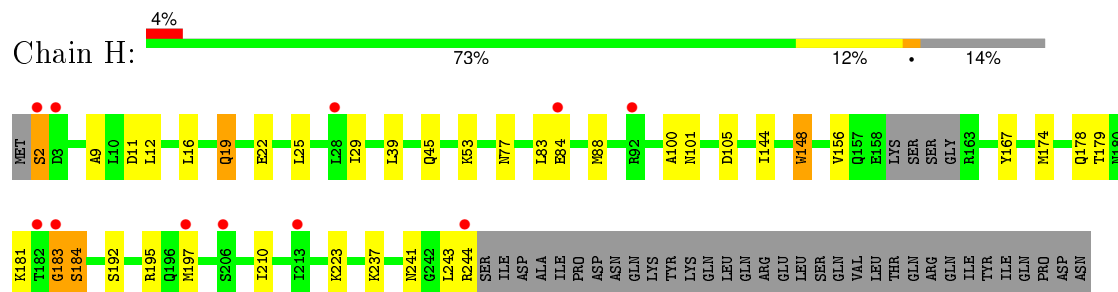
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



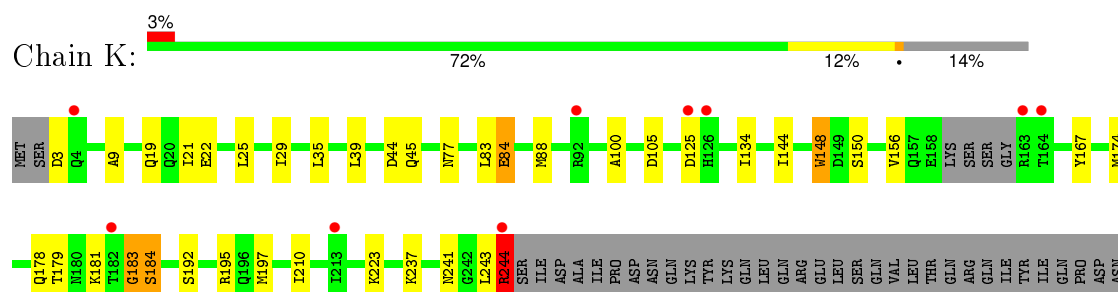
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



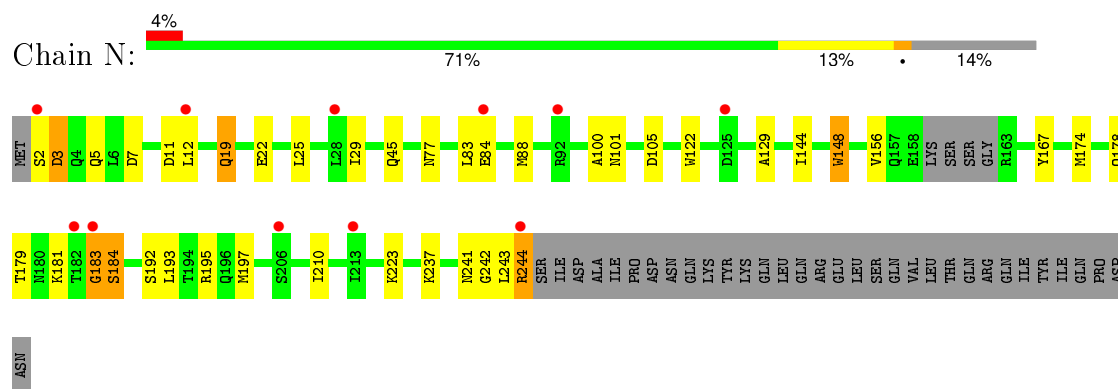
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



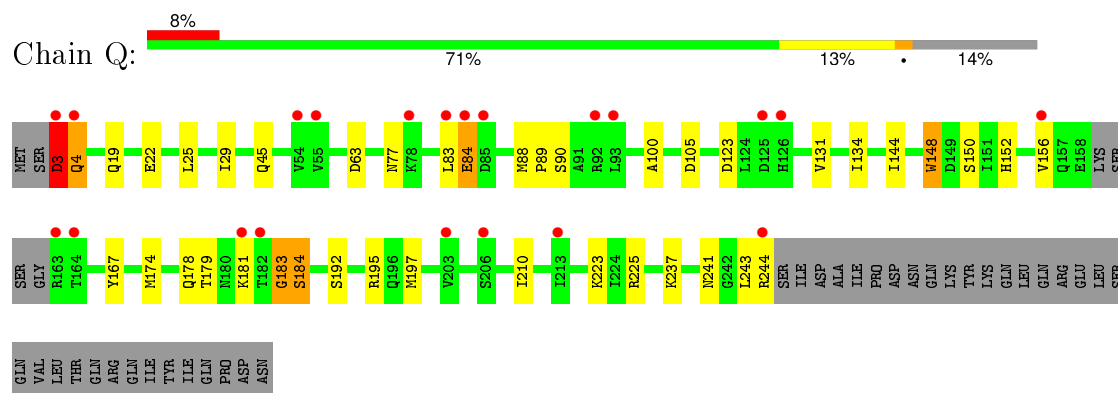
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



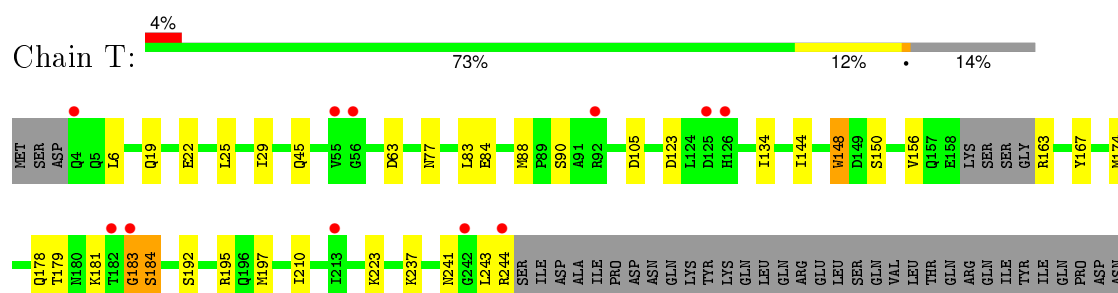
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



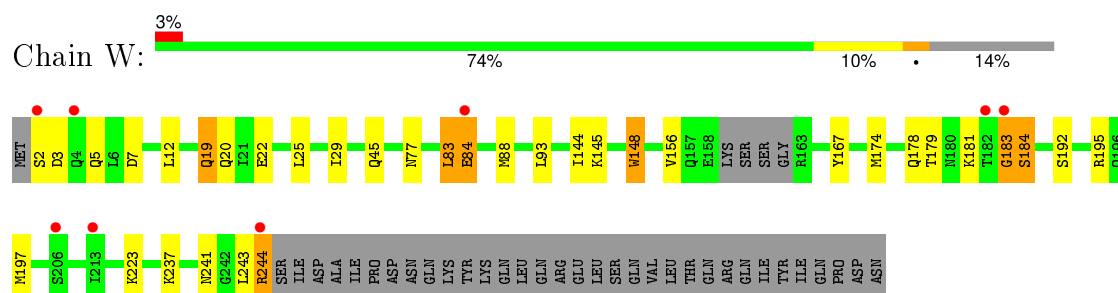
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



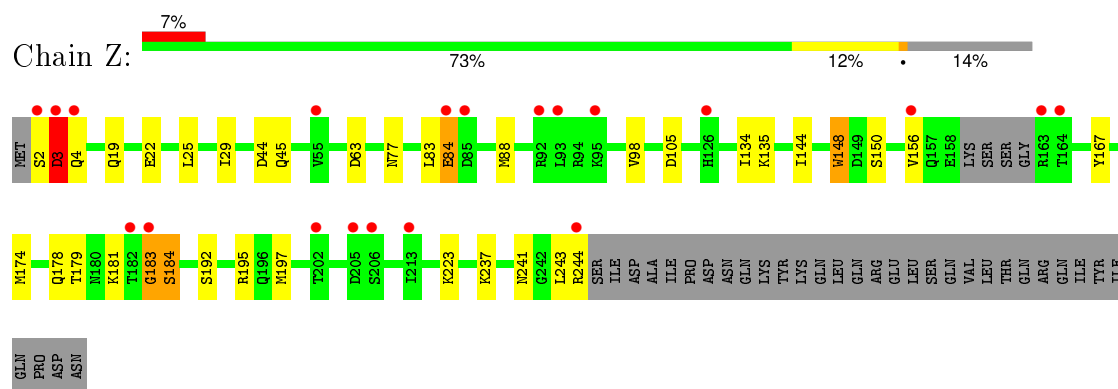
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



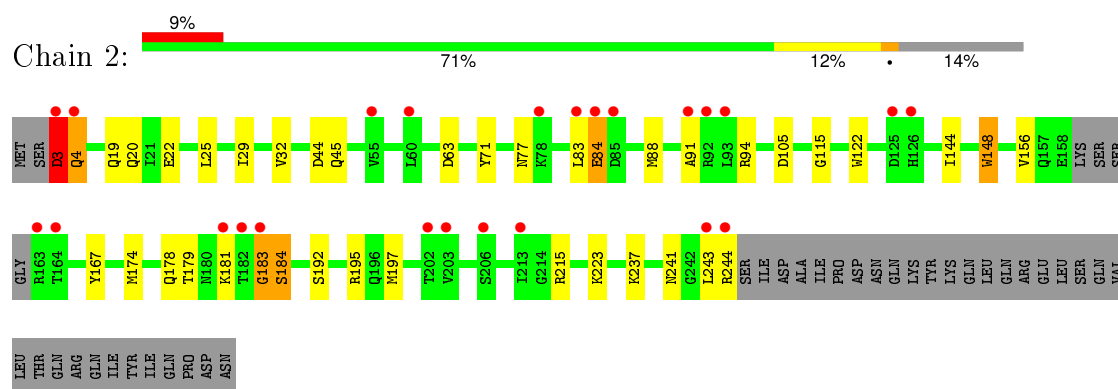
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

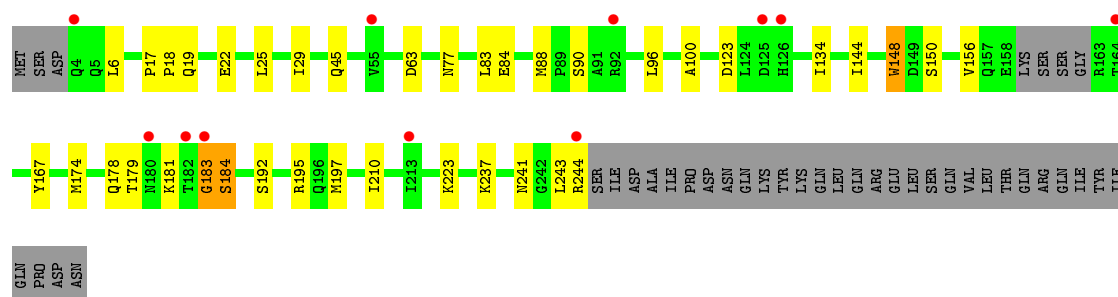


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

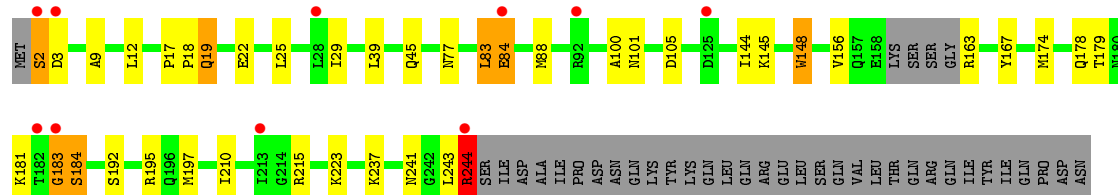


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2





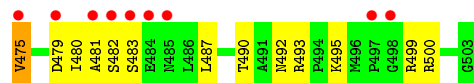
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: CD2-associated protein



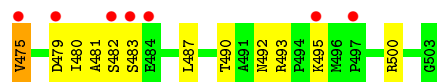
- Molecule 3: CD2-associated protein



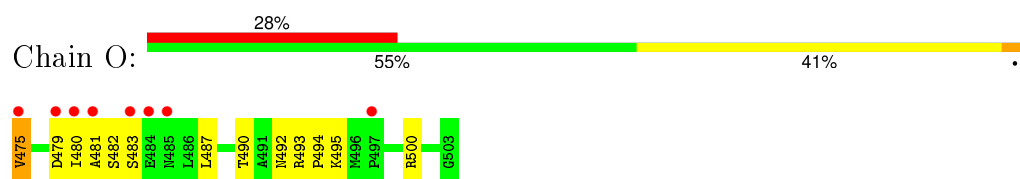
- Molecule 3: CD2-associated protein



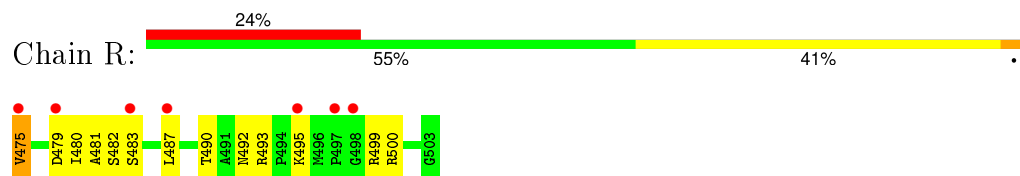
- Molecule 3: CD2-associated protein



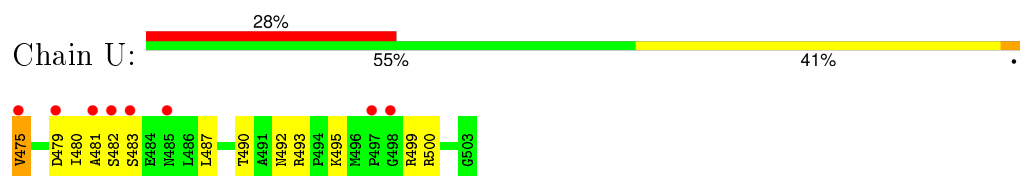
- Molecule 3: CD2-associated protein



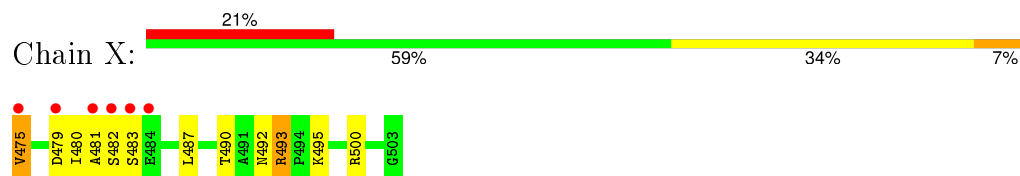
- Molecule 3: CD2-associated protein



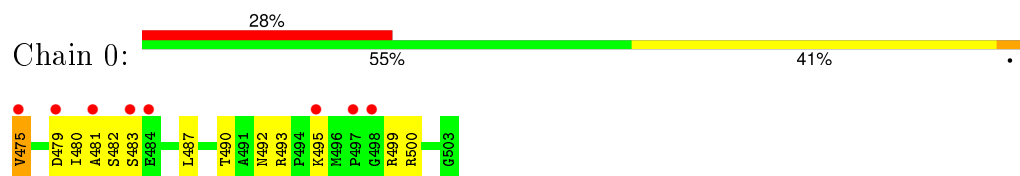
- Molecule 3: CD2-associated protein



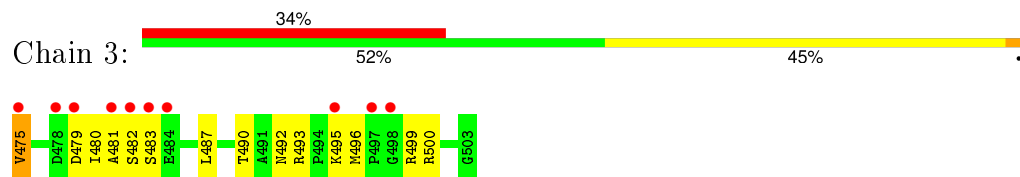
- Molecule 3: CD2-associated protein



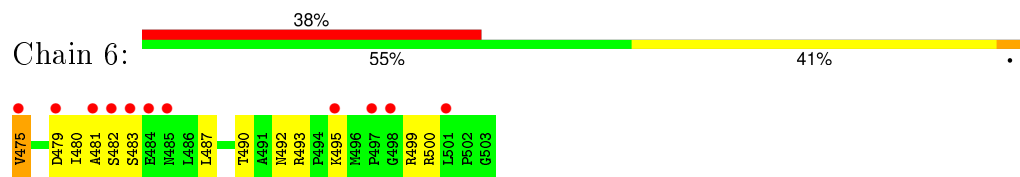
- Molecule 3: CD2-associated protein



- Molecule 3: CD2-associated protein

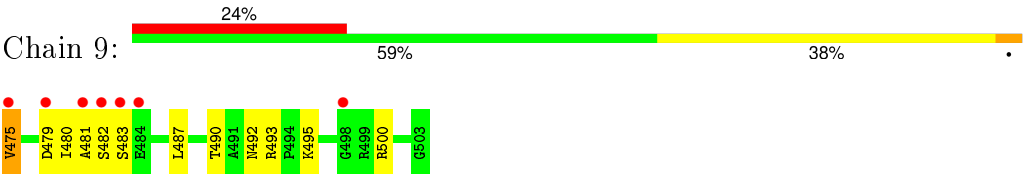


- Molecule 3: CD2-associated protein



- Molecule 3: CD2-associated protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.73 Å 142.34 Å 193.00 Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	19.98 – 1.99 19.98 – 1.99	Depositor EDS
% Data completeness (in resolution range)	82.2 (19.98-1.99) 82.5 (19.98-1.99)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 1.99 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.225 , 0.272 0.222 , 0.269	Depositor DCC
$R_{free}$ test set	17972 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.6	EDS
Estimated twinning fraction	0.470 for h,-k,-l 0.478 for -h,k,-l 0.487 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 359377 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	54370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.4815e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.36	0/2236	0.50	0/3032
1	4	0.36	0/2236	0.51	0/3032
1	7	0.39	0/2236	0.52	0/3032
1	A	0.37	0/2236	0.51	0/3032
1	D	0.37	0/2236	0.51	0/3032
1	G	0.38	0/2236	0.51	0/3032
1	J	0.37	0/2236	0.52	0/3032
1	M	0.37	0/2236	0.51	0/3032
1	P	0.37	0/2236	0.51	0/3032
1	S	0.36	0/2236	0.51	0/3032
1	V	0.40	0/2236	0.52	0/3032
1	Y	0.36	0/2236	0.50	0/3032
2	2	0.39	0/1910	0.54	0/2580
2	5	0.39	0/1902	0.53	0/2569
2	8	0.44	0/1916	0.57	1/2588 (0.0%)
2	B	0.40	0/1910	0.53	0/2580
2	E	0.40	0/1910	0.53	0/2580
2	H	0.42	0/1916	0.56	0/2588
2	K	0.41	0/1910	0.54	1/2580 (0.0%)
2	N	0.43	0/1916	0.57	1/2588 (0.0%)
2	Q	0.40	0/1910	0.55	0/2580
2	T	0.39	0/1902	0.53	0/2569
2	W	0.45	0/1916	0.57	1/2588 (0.0%)
2	Z	0.39	0/1916	0.53	0/2588
3	0	0.37	0/229	0.63	0/309
3	3	0.36	0/229	0.64	0/309
3	6	0.36	0/229	0.67	0/309
3	9	0.38	0/229	0.67	0/309
3	C	0.37	0/229	0.63	0/309
3	F	0.36	0/229	0.64	0/309
3	I	0.38	0/229	0.67	0/309
3	L	0.35	0/229	0.66	0/309
3	O	0.36	0/229	0.64	0/309
3	R	0.35	0/229	0.64	0/309

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	U	0.36	0/229	0.65	0/309
3	X	0.40	0/229	0.69	1/309 (0.3%)
All	All	0.39	0/52514	0.54	5/71070 (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
2	2	0	1
2	Q	0	1
2	Z	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	244	ARG	NE-CZ-NH1	-5.57	117.52	120.30
2	N	244	ARG	NE-CZ-NH1	-5.33	117.64	120.30
2	K	244	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	8	244	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	X	493	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	3	ASP	Peptide
2	Q	3	ASP	Peptide
2	Z	3	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2185	0	2104	57	0
1	4	2185	0	2104	56	0
1	7	2185	0	2104	55	0
1	A	2185	0	2104	61	0
1	D	2185	0	2104	52	0
1	G	2185	0	2104	58	0
1	J	2185	0	2104	54	0
1	M	2185	0	2104	57	0
1	P	2185	0	2104	53	0
1	S	2185	0	2104	58	0
1	V	2185	0	2104	60	0
1	Y	2185	0	2104	50	0
2	2	1878	0	1852	52	0
2	5	1870	0	1848	39	0
2	8	1884	0	1857	43	0
2	B	1878	0	1852	49	0
2	E	1878	0	1852	39	0
2	H	1884	0	1857	48	0
2	K	1878	0	1852	42	0
2	N	1884	0	1857	49	0
2	Q	1878	0	1852	42	0
2	T	1870	0	1848	39	0
2	W	1884	0	1857	50	0
2	Z	1884	0	1857	33	0
3	0	225	0	226	16	0
3	3	225	0	226	16	0
3	6	225	0	226	16	0
3	9	225	0	226	14	0
3	C	225	0	226	16	0
3	F	225	0	226	14	0
3	I	225	0	226	14	0
3	L	225	0	226	14	0
3	O	225	0	226	16	0
3	R	225	0	226	15	0
3	U	225	0	226	15	0
3	X	225	0	226	14	0
4	0	13	0	0	0	0
4	1	90	0	0	5	0
4	2	91	0	0	8	0
4	3	14	0	0	0	0
4	4	114	0	0	4	0
4	5	119	0	0	5	0
4	6	10	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7	138	0	0	7	0
4	8	148	0	0	4	0
4	9	11	0	0	0	0
4	A	108	0	0	5	0
4	B	90	0	0	3	0
4	C	14	0	0	1	0
4	D	131	0	0	4	0
4	E	103	0	0	0	0
4	F	13	0	0	0	0
4	G	126	0	0	6	0
4	H	155	0	0	3	0
4	I	10	0	0	1	0
4	J	135	0	0	2	0
4	K	103	0	0	4	0
4	L	14	0	0	0	0
4	M	123	0	0	9	0
4	N	138	0	0	3	0
4	O	10	0	0	0	0
4	P	93	0	0	3	0
4	Q	76	0	0	5	0
4	R	17	0	0	0	0
4	S	115	0	0	5	0
4	T	110	0	0	5	0
4	U	12	0	0	0	0
4	V	137	0	0	11	0
4	W	134	0	0	7	0
4	X	14	0	0	0	0
4	Y	91	0	0	9	0
4	Z	80	0	0	2	0
All	All	54370	0	50201	1122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1122) 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)
1:1:137:PRO:HD3	2:2:244:ARG:NH1	1.50	1.26
2:B:3:ASP:HA	2:B:4:GLN:CB	1.77	1.14
1:1:137:PRO:CD	2:2:244:ARG:NH1	2.10	1.14
1:G:137:PRO:HD3	2:H:244:ARG:HG3	1.12	1.11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PRO:HD3	2:B:244:ARG:HG3	1.22	1.10
1:V:87:PHE:HA	4:V:2723:HOH:O	1.51	1.10
2:B:3:ASP:HA	2:B:4:GLN:HB3	1.22	1.10
1:G:137:PRO:CD	2:H:244:ARG:HG3	1.82	1.09
1:1:137:PRO:CD	2:2:244:ARG:HH11	1.67	1.07
1:1:137:PRO:HD3	2:2:244:ARG:HH11	1.12	1.01
2:B:3:ASP:CA	2:B:4:GLN:HB3	1.88	1.01
1:M:137:PRO:HD3	2:N:244:ARG:HG3	1.42	1.00
1:A:101:LEU:HG	3:C:480:ILE:HD11	1.40	1.00
1:1:101:LEU:HG	3:3:480:ILE:HD11	1.39	1.00
1:D:101:LEU:HG	3:F:480:ILE:HD11	1.44	1.00
1:J:101:LEU:HG	3:L:480:ILE:HD11	1.44	0.99
2:2:244:ARG:HH11	2:2:244:ARG:HG3	1.27	0.99
1:M:137:PRO:CD	2:N:244:ARG:HG3	1.92	0.99
1:Y:101:LEU:HG	3:O:480:ILE:HD11	1.44	0.97
2:5:183:GLY:HA3	2:5:184:SER:CB	1.95	0.96
1:S:137:PRO:HD3	2:T:244:ARG:HG3	1.43	0.96
2:T:183:GLY:HA3	2:T:184:SER:CB	1.96	0.96
2:Z:183:GLY:HA3	2:Z:184:SER:CB	1.96	0.96
2:2:183:GLY:HA3	2:2:184:SER:CB	1.96	0.96
1:G:101:LEU:HG	3:I:480:ILE:HD11	1.47	0.94
2:8:183:GLY:HA3	2:8:184:SER:CB	1.98	0.93
2:E:183:GLY:HA3	2:E:184:SER:CB	1.96	0.93
2:K:183:GLY:HA3	2:K:184:SER:CB	1.96	0.93
1:A:137:PRO:CD	2:B:244:ARG:HG3	1.97	0.93
2:Q:183:GLY:HA3	2:Q:184:SER:CB	1.96	0.93
2:E:183:GLY:HA3	2:E:184:SER:HB3	1.51	0.93
2:K:183:GLY:HA3	2:K:184:SER:HB3	1.51	0.93
2:B:183:GLY:HA3	2:B:184:SER:CB	1.97	0.93
1:P:137:PRO:HD3	2:Q:244:ARG:HG3	1.51	0.92
1:D:137:PRO:HD3	2:E:244:ARG:HG3	1.50	0.92
2:Q:183:GLY:HA3	2:Q:184:SER:HB3	1.52	0.92
2:W:183:GLY:HA3	2:W:184:SER:CB	2.00	0.92
3:X:481:ALA:HB1	3:X:482:SER:HB2	1.51	0.92
2:N:183:GLY:HA3	2:N:184:SER:CB	1.98	0.91
2:H:183:GLY:HA3	2:H:184:SER:CB	1.99	0.91
1:A:137:PRO:CD	2:B:244:ARG:HH11	1.82	0.91
2:5:183:GLY:HA3	2:5:184:SER:HB3	1.51	0.91
2:T:183:GLY:HA3	2:T:184:SER:HB3	1.52	0.91
3:O:481:ALA:HB1	3:O:482:SER:HB2	1.52	0.91
2:B:183:GLY:HA3	2:B:184:SER:HB3	1.53	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:2209:HOH:O	2:H:16:LEU:HD22	1.70	0.91
2:Z:183:GLY:HA3	2:Z:184:SER:HB3	1.53	0.90
1:V:137:PRO:HD3	2:W:244:ARG:HG3	1.53	0.90
1:G:95:SER:HB3	1:G:111:GLU:HG3	1.53	0.90
3:U:481:ALA:HB1	3:U:482:SER:HB2	1.52	0.90
3:O:481:ALA:HB1	3:O:482:SER:HB2	1.51	0.90
2:2:183:GLY:HA3	2:2:184:SER:HB3	1.53	0.89
3:6:481:ALA:HB1	3:6:482:SER:HB2	1.52	0.89
1:M:95:SER:HB3	1:M:111:GLU:HG3	1.54	0.89
3:9:481:ALA:HB1	3:9:482:SER:HB2	1.53	0.89
3:I:481:ALA:HB1	3:I:482:SER:HB2	1.52	0.89
2:N:183:GLY:HA3	2:N:184:SER:HB3	1.55	0.88
3:3:481:ALA:HB1	3:3:482:SER:HB2	1.54	0.88
1:P:137:PRO:CD	2:Q:244:ARG:HG3	2.03	0.88
3:R:481:ALA:HB1	3:R:482:SER:HB2	1.52	0.88
3:C:481:ALA:HB1	3:C:482:SER:HB2	1.53	0.88
1:A:95:SER:HB3	1:A:111:GLU:HG3	1.55	0.88
3:L:481:ALA:HB1	3:L:482:SER:HB2	1.53	0.88
2:K:241:ASN:O	2:K:244:ARG:HG3	1.73	0.88
1:J:95:SER:HB3	1:J:111:GLU:HG3	1.55	0.87
1:D:95:SER:HB3	1:D:111:GLU:HG3	1.56	0.87
1:4:137:PRO:HD3	2:5:244:ARG:HG3	1.55	0.87
3:F:481:ALA:HB1	3:F:482:SER:HB2	1.54	0.87
2:H:183:GLY:HA3	2:H:184:SER:HB3	1.57	0.87
2:Q:3:ASP:HB2	2:Q:4:GLN:HB3	1.56	0.87
1:1:137:PRO:HD3	2:2:244:ARG:HG3	1.57	0.86
1:V:95:SER:HB3	1:V:111:GLU:HG3	1.54	0.86
2:8:183:GLY:HA3	2:8:184:SER:HB3	1.57	0.86
2:Z:243:LEU:N	2:Z:244:ARG:HA	1.89	0.86
1:M:137:PRO:CG	2:N:244:ARG:HG3	2.06	0.86
1:4:95:SER:HB3	1:4:111:GLU:HG3	1.55	0.86
2:W:183:GLY:HA3	2:W:184:SER:HB3	1.57	0.85
1:J:137:PRO:HD3	2:K:244:ARG:HH11	1.40	0.85
2:E:183:GLY:CA	2:E:184:SER:HB3	2.07	0.85
2:K:183:GLY:CA	2:K:184:SER:HB3	2.07	0.85
2:Q:183:GLY:CA	2:Q:184:SER:HB3	2.07	0.85
1:7:95:SER:HB3	1:7:111:GLU:HG3	1.57	0.85
1:S:137:PRO:HD3	2:T:244:ARG:HH11	1.41	0.85
1:S:137:PRO:HD3	2:T:244:ARG:NH1	1.92	0.85
1:P:95:SER:HB3	1:P:111:GLU:HG3	1.59	0.84
1:4:137:PRO:HD3	2:5:244:ARG:HH11	1.42	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:183:GLY:CA	2:T:184:SER:HB3	2.07	0.84
2:5:183:GLY:CA	2:5:184:SER:HB3	2.07	0.84
1:S:95:SER:HB3	1:S:111:GLU:HG3	1.56	0.84
1:J:137:PRO:CD	2:K:244:ARG:HH11	1.90	0.84
2:Z:183:GLY:CA	2:Z:184:SER:HB3	2.07	0.83
2:B:183:GLY:CA	2:B:184:SER:HB3	2.09	0.83
2:2:3:ASP:HB2	2:2:4:GLN:HB3	1.61	0.83
1:1:137:PRO:CG	2:2:244:ARG:HH11	1.91	0.83
2:2:183:GLY:CA	2:2:184:SER:HB3	2.08	0.83
1:1:95:SER:HB3	1:1:111:GLU:HG3	1.58	0.82
1:1:31:GLU:HA	3:3:483:SER:HB2	1.60	0.82
1:A:137:PRO:HD3	2:B:244:ARG:HH11	1.44	0.82
2:N:183:GLY:CA	2:N:184:SER:HB3	2.10	0.82
1:V:82:LEU:HG	4:V:2723:HOH:O	1.80	0.81
1:A:31:GLU:HA	3:C:483:SER:HB2	1.62	0.81
1:4:31:GLU:HA	3:6:483:SER:HB2	1.61	0.81
2:T:243:LEU:N	2:T:244:ARG:HA	1.96	0.81
2:H:183:GLY:CA	2:H:184:SER:HB3	2.11	0.81
2:K:241:ASN:O	2:K:244:ARG:CG	2.27	0.81
1:Y:95:SER:HB3	1:Y:111:GLU:HG3	1.61	0.81
2:5:243:LEU:N	2:5:244:ARG:HA	1.96	0.80
1:Y:31:GLU:HA	3:0:483:SER:HB2	1.62	0.80
2:8:183:GLY:CA	2:8:184:SER:HB3	2.11	0.80
2:Q:243:LEU:N	2:Q:244:ARG:HA	1.96	0.80
1:M:58:ASN:HD22	1:M:100:HIS:HD2	1.30	0.80
1:S:137:PRO:CD	2:T:244:ARG:HH11	1.93	0.80
1:P:58:ASN:HD22	1:P:100:HIS:HD2	1.30	0.80
1:D:31:GLU:HA	3:F:483:SER:HB2	1.64	0.80
1:D:137:PRO:HD3	2:E:244:ARG:HH11	1.44	0.80
1:P:137:PRO:CD	2:Q:244:ARG:HH11	1.95	0.80
2:W:183:GLY:CA	2:W:184:SER:HB3	2.11	0.80
1:V:137:PRO:CD	2:W:244:ARG:HG3	2.11	0.80
1:J:137:PRO:HD3	2:K:244:ARG:NH1	1.97	0.79
1:M:198:TYR:HE2	4:M:720:HOH:O	1.65	0.79
1:G:137:PRO:HD3	2:H:244:ARG:HH11	1.47	0.79
1:G:58:ASN:HD22	1:G:100:HIS:HD2	1.31	0.79
2:2:243:LEU:N	2:2:244:ARG:HA	1.98	0.79
1:7:137:PRO:HG3	2:8:244:ARG:HD3	1.65	0.79
1:P:31:GLU:HA	3:R:483:SER:HB2	1.65	0.78
1:J:31:GLU:HA	3:L:483:SER:HB2	1.66	0.78
1:S:137:PRO:CD	2:T:244:ARG:HG3	2.13	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:HD22	1:A:100:HIS:HD2	1.32	0.78
1:4:137:PRO:CD	2:5:244:ARG:HG3	2.12	0.78
1:7:58:ASN:HD22	1:7:100:HIS:HD2	1.30	0.78
1:4:102:ARG:HD2	4:4:2737:HOH:O	1.82	0.78
1:M:31:GLU:HA	3:O:483:SER:HB2	1.65	0.78
1:V:58:ASN:HD22	1:V:100:HIS:HD2	1.31	0.78
1:S:31:GLU:HA	3:U:483:SER:HB2	1.65	0.77
2:K:243:LEU:N	2:K:244:ARG:HA	2.00	0.77
1:D:137:PRO:CD	2:E:244:ARG:HG3	2.15	0.77
1:4:58:ASN:HD22	1:4:100:HIS:HD2	1.32	0.77
1:D:137:PRO:HD3	2:E:244:ARG:NH1	2.00	0.77
1:D:58:ASN:HD22	1:D:100:HIS:HD2	1.33	0.77
1:S:58:ASN:HD22	1:S:100:HIS:HD2	1.32	0.77
1:G:31:GLU:HA	3:I:483:SER:HB2	1.67	0.77
1:7:31:GLU:HA	3:9:483:SER:HB2	1.66	0.77
1:V:31:GLU:HA	3:X:483:SER:HB2	1.67	0.76
1:A:137:PRO:HD3	2:B:244:ARG:NH1	1.99	0.76
1:1:58:ASN:HD22	1:1:100:HIS:HD2	1.32	0.76
1:J:58:ASN:HD22	1:J:100:HIS:HD2	1.34	0.76
1:Y:58:ASN:HD22	1:Y:100:HIS:HD2	1.33	0.76
1:4:101:LEU:HD22	3:6:480:ILE:HD11	1.67	0.76
4:7:2719:HOH:O	2:8:215:ARG:NH2	2.19	0.76
1:A:137:PRO:CD	2:B:244:ARG:NH1	2.49	0.75
1:G:137:PRO:CD	2:H:244:ARG:HH11	1.98	0.75
1:M:137:PRO:HD3	2:N:244:ARG:NH1	2.00	0.75
1:V:80:GLY:O	4:V:2723:HOH:O	2.03	0.75
1:4:137:PRO:HD3	2:5:244:ARG:NH1	2.01	0.74
1:M:137:PRO:CD	2:N:244:ARG:HH11	2.01	0.74
1:7:58:ASN:HD22	1:7:100:HIS:CD2	2.04	0.74
2:8:241:ASN:O	2:8:244:ARG:HG2	1.88	0.74
1:4:137:PRO:CD	2:5:244:ARG:HH11	2.01	0.74
2:H:244:ARG:HG3	2:H:244:ARG:HH11	1.52	0.74
2:B:3:ASP:HA	2:B:4:GLN:HB2	1.68	0.73
1:M:58:ASN:HD22	1:M:100:HIS:CD2	2.05	0.73
2:N:243:LEU:N	2:N:244:ARG:HA	2.03	0.73
1:M:137:PRO:HD3	2:N:244:ARG:HH11	1.53	0.73
3:X:481:ALA:CB	3:X:482:SER:HB2	2.18	0.73
2:H:243:LEU:N	2:H:244:ARG:HA	2.01	0.73
2:K:183:GLY:CA	2:K:184:SER:CB	2.66	0.73
2:E:183:GLY:CA	2:E:184:SER:CB	2.66	0.72
2:5:183:GLY:CA	2:5:184:SER:CB	2.65	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:137:PRO:CD	2:2:244:ARG:HH12	2.02	0.72
2:T:183:GLY:CA	2:T:184:SER:CB	2.65	0.72
3:0:481:ALA:CB	3:0:482:SER:HB2	2.19	0.72
3:C:495:LYS:HB3	4:C:2809:HOH:O	1.89	0.72
2:Z:183:GLY:CA	2:Z:184:SER:CB	2.65	0.72
2:W:244:ARG:HH11	2:W:244:ARG:HG3	1.53	0.72
1:V:58:ASN:HD22	1:V:100:HIS:CD2	2.07	0.72
2:Q:183:GLY:CA	2:Q:184:SER:CB	2.66	0.72
1:P:137:PRO:HD3	2:Q:244:ARG:NH1	2.05	0.72
1:P:58:ASN:HD22	1:P:100:HIS:CD2	2.06	0.72
2:2:183:GLY:CA	2:2:184:SER:CB	2.66	0.72
3:O:481:ALA:CB	3:O:482:SER:HB2	2.18	0.72
2:H:2:SER:HB2	4:H:288:HOH:O	1.90	0.72
2:B:183:GLY:CA	2:B:184:SER:CB	2.66	0.71
1:G:58:ASN:HD22	1:G:100:HIS:CD2	2.07	0.71
3:6:481:ALA:CB	3:6:482:SER:HB2	2.19	0.71
1:V:185:THR:HG22	4:V:1547:HOH:O	1.89	0.71
3:U:481:ALA:CB	3:U:482:SER:HB2	2.19	0.71
3:I:481:ALA:CB	3:I:482:SER:HB2	2.19	0.71
3:9:481:ALA:CB	3:9:482:SER:HB2	2.20	0.71
1:S:58:ASN:HD22	1:S:100:HIS:CD2	2.08	0.71
3:C:481:ALA:CB	3:C:482:SER:HB2	2.19	0.71
1:4:58:ASN:HD22	1:4:100:HIS:CD2	2.08	0.71
1:1:58:ASN:HD22	1:1:100:HIS:CD2	2.08	0.71
3:R:481:ALA:CB	3:R:482:SER:HB2	2.19	0.71
3:3:481:ALA:CB	3:3:482:SER:HB2	2.20	0.71
1:7:137:PRO:CD	2:8:244:ARG:HH11	2.04	0.71
2:8:183:GLY:CA	2:8:184:SER:CB	2.67	0.70
2:2:94:ARG:HG3	4:2:2894:HOH:O	1.91	0.70
3:L:481:ALA:CB	3:L:482:SER:HB2	2.20	0.70
1:A:58:ASN:HD22	1:A:100:HIS:CD2	2.08	0.70
1:1:137:PRO:CD	2:2:244:ARG:HG3	2.21	0.70
2:H:183:GLY:CA	2:H:184:SER:CB	2.68	0.70
1:P:137:PRO:HD3	2:Q:244:ARG:HH11	1.56	0.70
2:N:183:GLY:CA	2:N:184:SER:CB	2.68	0.70
1:Y:58:ASN:HD22	1:Y:100:HIS:CD2	2.09	0.70
1:S:184:PRO:HG3	2:W:7:ASP:CG	2.12	0.70
3:F:481:ALA:CB	3:F:482:SER:HB2	2.20	0.70
2:8:2:SER:HA	4:8:289:HOH:O	1.92	0.70
1:J:184:PRO:HG3	2:N:7:ASP:CG	2.12	0.70
1:A:137:PRO:CG	2:B:244:ARG:HH11	2.03	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:55:ALA:HA	1:7:100:HIS:CD2	2.27	0.69
1:D:58:ASN:HD22	1:D:100:HIS:CD2	2.09	0.69
2:B:3:ASP:CB	2:B:4:GLN:HB3	2.23	0.69
1:J:58:ASN:HD22	1:J:100:HIS:CD2	2.09	0.69
1:V:101:LEU:HD22	3:X:480:ILE:HD11	1.72	0.69
1:M:101:LEU:HD22	3:O:480:ILE:HD11	1.73	0.69
1:D:137:PRO:CD	2:E:244:ARG:HH11	2.04	0.69
1:V:137:PRO:CG	2:W:244:ARG:HG3	2.23	0.69
2:8:163:ARG:N	4:8:2519:HOH:O	2.26	0.69
1:S:101:LEU:HD22	3:U:480:ILE:HD11	1.74	0.69
2:5:174:MET:HG2	2:5:192:SER:HB3	1.75	0.69
1:G:137:PRO:HD3	2:H:244:ARG:NH1	2.07	0.69
2:W:183:GLY:CA	2:W:184:SER:CB	2.69	0.69
2:8:243:LEU:N	2:8:244:ARG:HA	2.07	0.69
1:1:137:PRO:N	2:2:244:ARG:HH12	1.91	0.68
3:3:490:THR:O	3:3:493:ARG:HD2	1.93	0.68
2:B:243:LEU:N	2:B:244:ARG:HA	2.08	0.68
1:7:137:PRO:HD3	2:8:244:ARG:HH11	1.56	0.68
1:7:101:LEU:HD22	3:9:480:ILE:HD11	1.72	0.68
2:2:244:ARG:HG3	2:2:244:ARG:NH1	1.98	0.68
1:P:137:PRO:CD	2:Q:244:ARG:NH1	2.57	0.68
2:E:243:LEU:N	2:E:244:ARG:HA	2.09	0.68
1:G:137:PRO:CG	2:H:244:ARG:HG3	2.23	0.68
2:W:243:LEU:N	2:W:244:ARG:HA	2.08	0.67
1:4:271:TRP:O	1:4:274:ILE:HG22	1.94	0.67
1:S:55:ALA:HA	1:S:100:HIS:CD2	2.30	0.67
1:1:55:ALA:HA	1:1:100:HIS:CD2	2.30	0.67
1:G:185:THR:HG22	4:G:1863:HOH:O	1.94	0.67
1:4:55:ALA:HA	1:4:100:HIS:CD2	2.30	0.67
1:Y:55:ALA:HA	1:Y:100:HIS:CD2	2.30	0.67
3:C:490:THR:O	3:C:493:ARG:HD2	1.95	0.67
1:S:102:ARG:HD2	4:S:2192:HOH:O	1.93	0.67
2:Q:123:ASP:OD1	4:Q:551:HOH:O	2.13	0.67
1:1:137:PRO:CG	2:2:244:ARG:NH1	2.53	0.66
1:D:55:ALA:HA	1:D:100:HIS:CD2	2.30	0.66
1:1:137:PRO:HG3	2:2:244:ARG:HH11	1.59	0.66
2:8:241:ASN:O	2:8:244:ARG:CG	2.44	0.66
3:R:490:THR:O	3:R:493:ARG:HD2	1.96	0.66
2:5:84:GLU:HG2	4:5:2679:HOH:O	1.94	0.66
1:G:55:ALA:HA	1:G:100:HIS:CD2	2.30	0.66
4:Y:1908:HOH:O	3:0:483:SER:HB3	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:55:ALA:HA	1:M:100:HIS:CD2	2.30	0.66
1:J:137:PRO:CD	2:K:244:ARG:NH1	2.57	0.66
1:7:272:ASN:OD1	4:7:2719:HOH:O	2.14	0.66
1:7:271:TRP:O	1:7:274:ILE:HG22	1.96	0.66
1:V:55:ALA:HA	1:V:100:HIS:CD2	2.31	0.66
1:S:137:PRO:CD	2:T:244:ARG:NH1	2.54	0.65
1:7:137:PRO:HD3	2:8:244:ARG:NH1	2.10	0.65
2:2:183:GLY:HA3	2:2:184:SER:HB2	1.76	0.65
1:J:55:ALA:HA	1:J:100:HIS:CD2	2.31	0.65
1:V:271:TRP:O	1:V:274:ILE:HG22	1.97	0.65
1:P:101:LEU:HD22	3:R:480:ILE:HD11	1.76	0.65
1:S:271:TRP:O	1:S:274:ILE:HG22	1.97	0.65
3:0:490:THR:O	3:0:493:ARG:HD2	1.97	0.65
1:M:271:TRP:O	1:M:274:ILE:HG22	1.96	0.65
1:P:55:ALA:HA	1:P:100:HIS:CD2	2.31	0.65
1:Y:103:LYS:HD3	4:Y:2669:HOH:O	1.96	0.65
1:Y:271:TRP:O	1:Y:274:ILE:HG22	1.97	0.65
2:T:174:MET:HG2	2:T:192:SER:HB3	1.79	0.65
1:P:271:TRP:O	1:P:274:ILE:HG22	1.96	0.65
1:G:271:TRP:O	1:G:274:ILE:HG22	1.96	0.65
1:D:271:TRP:O	1:D:274:ILE:HG22	1.96	0.65
1:P:137:PRO:CG	2:Q:244:ARG:HG3	2.26	0.65
2:T:22:GLU:HA	2:T:45:GLN:HE22	1.62	0.65
1:1:271:TRP:O	1:1:274:ILE:HG22	1.97	0.65
2:8:183:GLY:HA3	2:8:184:SER:HB2	1.77	0.65
2:T:6:LEU:HB3	4:Y:290:HOH:O	1.97	0.65
1:Y:230:LYS:HE3	4:Y:2663:HOH:O	1.97	0.65
1:A:137:PRO:HG3	2:B:244:ARG:HH11	1.62	0.64
1:G:137:PRO:CD	2:H:244:ARG:CG	2.68	0.64
1:V:82:LEU:N	4:V:2723:HOH:O	2.30	0.64
3:U:490:THR:O	3:U:493:ARG:HD2	1.98	0.64
3:F:490:THR:O	3:F:493:ARG:HD2	1.97	0.64
1:1:137:PRO:HG3	2:2:244:ARG:NH1	2.13	0.64
1:J:271:TRP:O	1:J:274:ILE:HG22	1.96	0.64
1:A:55:ALA:HA	1:A:100:HIS:CD2	2.32	0.64
1:G:137:PRO:CG	2:H:244:ARG:CG	2.76	0.64
2:T:183:GLY:HA3	2:T:184:SER:HB2	1.77	0.64
2:Z:183:GLY:HA3	2:Z:184:SER:HB2	1.77	0.64
1:P:137:PRO:CG	2:Q:244:ARG:HH11	2.10	0.64
1:A:271:TRP:O	1:A:274:ILE:HG22	1.97	0.64
1:P:137:PRO:HG3	2:Q:244:ARG:HH11	1.63	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:490:THR:O	3:L:493:ARG:HD2	1.98	0.64
2:2:174:MET:HG2	2:2:192:SER:HB3	1.80	0.64
3:6:490:THR:O	3:6:493:ARG:HD2	1.99	0.63
2:5:183:GLY:HA3	2:5:184:SER:HB2	1.77	0.63
1:V:18:ALA:O	1:V:22:THR:HG23	1.98	0.63
1:G:137:PRO:HD3	2:H:244:ARG:CG	2.08	0.63
2:Z:22:GLU:HA	2:Z:45:GLN:HE22	1.64	0.63
2:N:174:MET:HG2	2:N:192:SER:HB3	1.79	0.63
2:E:174:MET:HG2	2:E:192:SER:HB3	1.81	0.63
1:M:137:PRO:CD	2:N:244:ARG:NH1	2.61	0.63
1:J:18:ALA:O	1:J:22:THR:HG23	1.99	0.63
2:K:183:GLY:HA3	2:K:184:SER:HB2	1.78	0.63
2:K:22:GLU:HA	2:K:45:GLN:HE22	1.63	0.62
2:B:183:GLY:HA3	2:B:184:SER:HB2	1.78	0.62
2:H:183:GLY:HA3	2:H:184:SER:HB2	1.77	0.62
2:Q:183:GLY:HA3	2:Q:184:SER:HB2	1.78	0.62
1:M:18:ALA:O	1:M:22:THR:HG23	2.00	0.62
1:V:137:PRO:HD3	2:W:244:ARG:NH1	2.14	0.62
2:Z:174:MET:HG2	2:Z:192:SER:HB3	1.82	0.62
1:M:137:PRO:CG	2:N:244:ARG:HH11	2.13	0.62
2:E:183:GLY:HA3	2:E:184:SER:HB2	1.78	0.62
2:W:183:GLY:HA3	2:W:184:SER:HB2	1.79	0.62
2:N:183:GLY:HA3	2:N:184:SER:HB2	1.78	0.62
2:E:3:ASP:HB3	2:E:6:LEU:HB3	1.80	0.62
1:G:102:ARG:HD2	4:G:2352:HOH:O	1.98	0.62
2:H:244:ARG:NH1	2:H:244:ARG:HG3	2.15	0.62
4:M:720:HOH:O	2:N:193:LEU:HD22	1.99	0.61
2:W:2:SER:HA	4:W:284:HOH:O	1.98	0.61
2:2:19:GLN:H	2:2:19:GLN:NE2	1.98	0.61
2:Z:19:GLN:NE2	2:Z:19:GLN:H	1.98	0.61
2:2:3:ASP:O	1:7:183:PRO:HD2	2.00	0.61
2:5:84:GLU:CD	2:5:84:GLU:H	2.04	0.61
2:W:174:MET:HG2	2:W:192:SER:HB3	1.83	0.61
1:M:137:PRO:HG3	2:N:244:ARG:HH11	1.63	0.61
2:E:22:GLU:HA	2:E:45:GLN:HE22	1.64	0.61
1:Y:102:ARG:NH2	3:0:479:ASP:OD1	2.34	0.61
4:1:289:HOH:O	2:5:6:LEU:HB3	2.01	0.61
1:A:183:PRO:O	2:E:3:ASP:C	2.39	0.61
2:5:22:GLU:HA	2:5:45:GLN:HE22	1.66	0.61
2:B:20:GLN:NE2	4:B:2406:HOH:O	2.28	0.61
1:G:18:ALA:O	1:G:22:THR:HG23	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ALA:O	1:A:22:THR:HG23	2.01	0.61
1:D:18:ALA:O	1:D:22:THR:HG23	2.01	0.61
1:P:18:ALA:O	1:P:22:THR:HG23	2.01	0.61
2:K:174:MET:HG2	2:K:192:SER:HB3	1.83	0.61
1:1:18:ALA:O	1:1:22:THR:HG23	2.01	0.60
2:2:84:GLU:H	2:2:84:GLU:CD	2.05	0.60
2:W:22:GLU:HA	2:W:45:GLN:HE22	1.67	0.60
2:T:19:GLN:NE2	2:T:19:GLN:H	1.99	0.60
1:V:137:PRO:HG3	2:W:244:ARG:HH11	1.65	0.60
2:K:241:ASN:O	2:K:244:ARG:HG2	2.01	0.60
3:X:490:THR:O	3:X:493:ARG:HD2	2.02	0.60
2:B:84:GLU:CD	2:B:84:GLU:H	2.05	0.60
2:K:84:GLU:H	2:K:84:GLU:CD	2.04	0.60
1:S:137:PRO:CG	2:T:244:ARG:HH11	2.14	0.60
1:Y:137:PRO:HG3	2:Z:244:ARG:HD2	1.81	0.60
2:8:22:GLU:HA	2:8:45:GLN:HE22	1.67	0.60
1:Y:18:ALA:O	1:Y:22:THR:HG23	2.02	0.60
2:T:84:GLU:H	2:T:84:GLU:CD	2.05	0.60
1:J:137:PRO:HG3	2:K:244:ARG:HD3	1.82	0.60
2:K:3:ASP:C	1:P:183:PRO:O	2.40	0.59
2:H:22:GLU:HA	2:H:45:GLN:HE22	1.66	0.59
1:J:137:PRO:CG	2:K:244:ARG:HD3	2.31	0.59
3:O:490:THR:O	3:O:493:ARG:HD2	2.02	0.59
2:2:22:GLU:HA	2:2:45:GLN:HE22	1.68	0.59
1:M:102:ARG:HD2	4:M:2170:HOH:O	2.00	0.59
1:G:34:ASN:ND2	3:I:482:SER:HA	2.17	0.59
2:H:174:MET:HG2	2:H:192:SER:HB3	1.84	0.59
2:Z:84:GLU:H	2:Z:84:GLU:CD	2.06	0.59
2:E:84:GLU:H	2:E:84:GLU:CD	2.06	0.59
1:D:190:ALA:HB3	1:D:212:ILE:HB	1.84	0.59
2:Q:22:GLU:HA	2:Q:45:GLN:HE22	1.66	0.59
3:9:490:THR:O	3:9:493:ARG:HD2	2.02	0.59
1:4:113:THR:HG22	1:4:118:LYS:HE2	1.85	0.59
2:B:19:GLN:H	2:B:19:GLN:NE2	2.00	0.59
1:M:273:LYS:HD2	4:M:2424:HOH:O	2.01	0.59
1:S:113:THR:HG22	1:S:118:LYS:HE2	1.85	0.59
2:N:5:GLN:HB2	4:N:288:HOH:O	2.03	0.59
2:W:84:GLU:H	2:W:84:GLU:CD	2.06	0.59
3:I:490:THR:O	3:I:493:ARG:HD2	2.03	0.59
2:Q:84:GLU:H	2:Q:84:GLU:CD	2.06	0.59
1:M:100:HIS:HE1	4:M:2843:HOH:O	1.86	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:18:ALA:O	1:7:22:THR:HG23	2.03	0.59
2:Q:174:MET:HG2	2:Q:192:SER:HB3	1.84	0.59
1:7:34:ASN:ND2	3:9:482:SER:HA	2.18	0.59
2:E:19:GLN:NE2	2:E:19:GLN:H	2.01	0.59
2:N:244:ARG:HH11	2:N:244:ARG:HG3	1.68	0.58
1:S:190:ALA:HB3	1:S:212:ILE:HB	1.84	0.58
1:1:113:THR:HG22	1:1:118:LYS:HE2	1.85	0.58
1:J:113:THR:HG22	1:J:118:LYS:HE2	1.85	0.58
2:Z:98:VAL:HA	4:Z:2845:HOH:O	2.04	0.58
1:4:190:ALA:HB3	1:4:212:ILE:HB	1.84	0.58
1:Y:113:THR:HG22	1:Y:118:LYS:HE2	1.85	0.58
2:8:84:GLU:H	2:8:84:GLU:CD	2.07	0.58
1:M:34:ASN:ND2	3:O:482:SER:HA	2.19	0.58
2:N:22:GLU:HA	2:N:45:GLN:HE22	1.68	0.58
1:M:137:PRO:CG	2:N:244:ARG:CG	2.81	0.58
2:W:19:GLN:H	2:W:19:GLN:NE2	2.02	0.58
2:H:84:GLU:CD	2:H:84:GLU:H	2.06	0.58
2:H:144:ILE:HD13	2:H:179:THR:HB	1.86	0.58
2:B:22:GLU:HA	2:B:45:GLN:HE22	1.68	0.58
2:N:84:GLU:H	2:N:84:GLU:CD	2.07	0.58
2:5:90:SER:OG	4:5:2547:HOH:O	2.17	0.57
2:N:144:ILE:HD13	2:N:179:THR:HB	1.86	0.57
2:W:83:LEU:HG	4:W:2526:HOH:O	2.03	0.57
2:B:174:MET:HG2	2:B:192:SER:HB3	1.86	0.57
1:A:113:THR:HG22	1:A:118:LYS:HE2	1.85	0.57
2:H:19:GLN:NE2	2:H:19:GLN:H	2.02	0.57
1:P:113:THR:HG22	1:P:118:LYS:HE2	1.85	0.57
1:D:113:THR:HG22	1:D:118:LYS:HE2	1.86	0.57
2:8:144:ILE:HD13	2:8:179:THR:HB	1.85	0.57
1:M:113:THR:HG22	1:M:118:LYS:HE2	1.86	0.57
1:J:137:PRO:CG	2:K:244:ARG:HH11	2.17	0.57
1:S:18:ALA:O	1:S:22:THR:HG23	2.04	0.57
1:V:113:THR:HG22	1:V:118:LYS:HE2	1.87	0.57
1:P:166:LYS:HD3	4:P:1705:HOH:O	2.04	0.57
1:P:190:ALA:HB3	1:P:212:ILE:HB	1.86	0.57
2:5:19:GLN:H	2:5:19:GLN:NE2	2.03	0.57
2:Z:144:ILE:HD13	2:Z:179:THR:HB	1.86	0.57
1:D:111:GLU:HG2	4:D:2065:HOH:O	2.05	0.57
2:Z:241:ASN:O	2:Z:244:ARG:HG2	2.05	0.56
2:B:144:ILE:HD13	2:B:179:THR:HB	1.87	0.56
2:8:83:LEU:HG	4:8:2530:HOH:O	2.04	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:190:ALA:HB3	1:J:212:ILE:HB	1.86	0.56
1:4:137:PRO:CG	2:5:244:ARG:HG3	2.35	0.56
1:G:113:THR:HG22	1:G:118:LYS:HE2	1.87	0.56
2:Q:144:ILE:HD13	2:Q:179:THR:HB	1.87	0.56
1:P:47:ARG:NH1	3:R:475:VAL:HG13	2.21	0.56
1:S:137:PRO:HG3	2:T:244:ARG:HH11	1.69	0.56
1:V:34:ASN:ND2	3:X:482:SER:HA	2.21	0.56
2:K:19:GLN:H	2:K:19:GLN:NE2	2.03	0.56
2:W:144:ILE:HD13	2:W:179:THR:HB	1.87	0.56
2:Q:19:GLN:H	2:Q:19:GLN:NE2	2.03	0.56
1:1:102:ARG:NH2	3:3:479:ASP:OD1	2.39	0.56
2:8:174:MET:HG2	2:8:192:SER:HB3	1.88	0.56
2:N:19:GLN:H	2:N:19:GLN:NE2	2.03	0.56
1:7:137:PRO:CG	2:8:244:ARG:HD3	2.34	0.56
2:K:144:ILE:HD13	2:K:179:THR:HB	1.87	0.56
1:7:113:THR:HG22	1:7:118:LYS:HE2	1.88	0.56
2:T:183:GLY:N	2:T:184:SER:HB3	2.21	0.56
2:T:6:LEU:HB2	4:T:2681:HOH:O	2.06	0.56
1:G:190:ALA:HB3	1:G:212:ILE:HB	1.87	0.56
2:W:77:ASN:O	2:W:88:MET:HE1	2.06	0.56
2:8:19:GLN:NE2	2:8:19:GLN:H	2.04	0.56
2:Z:183:GLY:N	2:Z:184:SER:HB3	2.21	0.55
1:7:102:ARG:HD2	4:7:1507:HOH:O	2.05	0.55
1:P:102:ARG:NH2	3:R:479:ASP:OD1	2.39	0.55
1:4:18:ALA:O	1:4:22:THR:HG23	2.06	0.55
1:Y:47:ARG:NH1	3:0:475:VAL:HG13	2.21	0.55
2:5:183:GLY:N	2:5:184:SER:HB3	2.21	0.55
2:T:244:ARG:HG3	2:T:244:ARG:HH11	1.71	0.55
2:Q:210:ILE:HG12	4:Q:2031:HOH:O	2.05	0.55
2:2:144:ILE:HD13	2:2:179:THR:HB	1.87	0.55
1:7:47:ARG:NH1	3:9:475:VAL:HG13	2.22	0.55
1:1:47:ARG:NH1	3:3:475:VAL:HG13	2.21	0.55
2:K:21:ILE:HD11	4:K:2177:HOH:O	2.06	0.55
2:B:25:LEU:O	2:B:29:ILE:HG12	2.07	0.55
1:A:190:ALA:HB3	1:A:212:ILE:HB	1.88	0.55
1:4:34:ASN:ND2	3:6:482:SER:HA	2.22	0.55
1:J:102:ARG:NH2	3:L:479:ASP:OD1	2.39	0.55
1:S:102:ARG:NH2	3:U:479:ASP:OD1	2.40	0.55
2:K:25:LEU:O	2:K:29:ILE:HG12	2.07	0.55
1:J:166:LYS:HD3	4:J:1694:HOH:O	2.06	0.55
2:2:183:GLY:N	2:2:184:SER:HB3	2.22	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:100:HIS:O	1:4:103:LYS:HD2	2.06	0.55
1:J:100:HIS:O	1:J:103:LYS:HD2	2.07	0.55
1:D:100:HIS:O	1:D:103:LYS:HD2	2.07	0.55
1:G:186:ALA:HB3	1:G:216:VAL:HG23	1.89	0.55
2:H:77:ASN:O	2:H:88:MET:HE1	2.06	0.55
1:S:100:HIS:O	1:S:103:LYS:HD2	2.06	0.54
2:H:195:ARG:HH22	2:H:223:LYS:HE2	1.72	0.54
1:A:102:ARG:NH2	3:C:479:ASP:OD1	2.39	0.54
1:7:226:LYS:HG3	4:7:1511:HOH:O	2.06	0.54
2:5:77:ASN:O	2:5:88:MET:HE1	2.07	0.54
1:G:47:ARG:NH1	3:I:475:VAL:HG13	2.23	0.54
1:7:190:ALA:HB3	1:7:212:ILE:HB	1.88	0.54
1:1:190:ALA:HB3	1:1:212:ILE:HB	1.88	0.54
1:M:216:VAL:HG11	1:M:231:ILE:HG13	1.88	0.54
1:Y:190:ALA:HB3	1:Y:212:ILE:HB	1.89	0.54
1:A:47:ARG:NH1	3:C:475:VAL:HG13	2.23	0.54
2:N:195:ARG:HH22	2:N:223:LYS:HE2	1.72	0.54
1:A:209:HIS:HD2	4:A:1787:HOH:O	1.90	0.54
1:G:137:PRO:CD	2:H:244:ARG:NH1	2.68	0.54
1:D:34:ASN:ND2	3:F:482:SER:HA	2.22	0.54
1:7:137:PRO:CD	2:8:244:ARG:NH1	2.70	0.54
1:1:216:VAL:HG11	1:1:231:ILE:HG13	1.89	0.54
1:J:184:PRO:HD3	2:N:3:ASP:O	2.07	0.54
1:M:186:ALA:HB3	1:M:216:VAL:HG23	1.90	0.54
1:G:266:ARG:HH12	2:N:244:ARG:NH2	2.04	0.54
2:K:183:GLY:N	2:K:184:SER:HB3	2.21	0.54
1:D:137:PRO:CD	2:E:244:ARG:NH1	2.69	0.54
1:P:100:HIS:O	1:P:103:LYS:HD2	2.08	0.54
3:9:495:LYS:HD2	3:9:495:LYS:N	2.23	0.54
2:8:183:GLY:N	2:8:184:SER:HB3	2.23	0.54
1:Y:31:GLU:HG3	3:0:483:SER:HA	1.90	0.54
2:H:210:ILE:HG12	4:H:2767:HOH:O	2.08	0.54
2:E:144:ILE:HD13	2:E:179:THR:HB	1.90	0.53
1:7:216:VAL:HG11	1:7:231:ILE:HG13	1.89	0.53
1:V:216:VAL:HG11	1:V:231:ILE:HG13	1.89	0.53
2:5:144:ILE:HD13	2:5:179:THR:HB	1.89	0.53
2:E:183:GLY:N	2:E:184:SER:HB3	2.22	0.53
1:1:107:ASP:N	1:1:108:PRO:HD3	2.23	0.53
1:P:216:VAL:HG11	1:P:231:ILE:HG13	1.89	0.53
2:Q:183:GLY:N	2:Q:184:SER:HB3	2.22	0.53
1:1:100:HIS:O	1:1:103:LYS:HD2	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:195:ARG:HH22	2:K:223:LYS:HE2	1.73	0.53
3:X:495:LYS:HD2	3:X:495:LYS:N	2.24	0.53
1:1:31:GLU:HG3	3:3:483:SER:HA	1.91	0.53
1:P:107:ASP:N	1:P:108:PRO:HD3	2.24	0.53
1:S:47:ARG:NH1	3:U:475:VAL:HG13	2.23	0.53
2:W:195:ARG:HH22	2:W:223:LYS:HE2	1.73	0.53
1:V:47:ARG:NH1	3:X:475:VAL:HG13	2.24	0.53
2:T:144:ILE:HD13	2:T:179:THR:HB	1.89	0.53
1:A:107:ASP:N	1:A:108:PRO:HD3	2.24	0.53
1:J:34:ASN:ND2	3:L:482:SER:HA	2.24	0.53
1:4:31:GLU:HG3	3:6:483:SER:HA	1.91	0.53
1:P:146:LYS:NZ	4:P:1651:HOH:O	2.41	0.53
2:W:244:ARG:HG3	2:W:244:ARG:NH1	2.19	0.53
1:G:216:VAL:HG11	1:G:231:ILE:HG13	1.90	0.53
1:V:137:PRO:HD3	2:W:244:ARG:HH11	1.73	0.53
3:O:481:ALA:CA	3:O:482:SER:HB2	2.39	0.53
1:G:100:HIS:O	1:G:103:LYS:HD2	2.09	0.53
1:Y:100:HIS:O	1:Y:103:LYS:HD2	2.08	0.53
2:N:2:SER:HA	4:N:288:HOH:O	2.08	0.53
2:E:244:ARG:HH11	2:E:244:ARG:HG3	1.74	0.52
3:X:481:ALA:CA	3:X:482:SER:HB2	2.39	0.52
3:C:481:ALA:CA	3:C:482:SER:HB2	2.39	0.52
1:V:186:ALA:HB3	1:V:216:VAL:HG23	1.90	0.52
1:A:230:LYS:HE3	4:A:1902:HOH:O	2.07	0.52
2:8:195:ARG:HH22	2:8:223:LYS:HE2	1.73	0.52
1:J:216:VAL:HG11	1:J:231:ILE:HG13	1.89	0.52
3:R:481:ALA:CA	3:R:482:SER:HB2	2.39	0.52
3:L:481:ALA:CA	3:L:482:SER:HB2	2.40	0.52
1:Y:267:THR:HG23	1:Y:268:LYS:O	2.09	0.52
1:V:137:PRO:CD	2:W:244:ARG:HH11	2.22	0.52
1:7:186:ALA:HB3	1:7:216:VAL:HG23	1.91	0.52
2:E:195:ARG:HH22	2:E:223:LYS:HE2	1.74	0.52
2:2:77:ASN:O	2:2:88:MET:HE1	2.10	0.52
1:Y:107:ASP:N	1:Y:108:PRO:HD3	2.24	0.52
3:I:481:ALA:CA	3:I:482:SER:HB2	2.40	0.52
1:4:102:ARG:NH2	3:6:479:ASP:OD1	2.43	0.52
1:V:78:GLU:HG2	4:V:2279:HOH:O	2.10	0.52
1:D:102:ARG:NH2	3:F:479:ASP:OD1	2.42	0.52
2:B:195:ARG:HH22	2:B:223:LYS:HE2	1.74	0.52
1:V:190:ALA:HB3	1:V:212:ILE:HB	1.90	0.52
3:O:495:LYS:HD2	3:O:495:LYS:N	2.24	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:100:HIS:O	1:7:103:LYS:HD2	2.09	0.52
1:A:182:THR:O	2:E:3:ASP:N	2.42	0.52
1:A:216:VAL:HG11	1:A:231:ILE:HG13	1.90	0.52
2:W:183:GLY:N	2:W:184:SER:HB3	2.24	0.52
1:A:100:HIS:O	1:A:103:LYS:HD2	2.10	0.52
1:7:216:VAL:CG1	1:7:231:ILE:HG13	2.40	0.52
2:T:195:ARG:HH22	2:T:223:LYS:HE2	1.74	0.52
2:2:25:LEU:O	2:2:29:ILE:HG12	2.09	0.52
2:T:77:ASN:O	2:T:88:MET:HE1	2.10	0.52
2:Q:25:LEU:O	2:Q:29:ILE:HG12	2.10	0.52
1:G:137:PRO:HG3	2:H:244:ARG:HD3	1.92	0.52
3:0:481:ALA:CA	3:0:482:SER:HB2	2.40	0.52
2:8:77:ASN:O	2:8:88:MET:HE1	2.10	0.52
2:T:148:TRP:CD1	2:T:148:TRP:C	2.83	0.52
1:G:137:PRO:CG	2:H:244:ARG:HH11	2.23	0.52
2:B:183:GLY:N	2:B:184:SER:HB3	2.23	0.52
3:6:481:ALA:CA	3:6:482:SER:HB2	2.40	0.52
2:Q:195:ARG:HH22	2:Q:223:LYS:HE2	1.75	0.52
2:Z:195:ARG:HH22	2:Z:223:LYS:HE2	1.74	0.52
2:N:183:GLY:N	2:N:184:SER:HB3	2.23	0.52
1:J:137:PRO:HG3	2:K:244:ARG:HH11	1.75	0.52
1:Y:216:VAL:HG11	1:Y:231:ILE:HG13	1.91	0.52
1:M:107:ASP:N	1:M:108:PRO:HD3	2.25	0.52
3:U:481:ALA:CA	3:U:482:SER:HB2	2.40	0.52
3:9:481:ALA:CA	3:9:482:SER:HB2	2.40	0.52
1:P:31:GLU:HG3	3:R:483:SER:HA	1.92	0.52
1:S:216:VAL:HG11	1:S:231:ILE:HG13	1.91	0.52
1:V:33:PHE:CE2	3:X:480:ILE:HD12	2.44	0.51
2:B:77:ASN:O	2:B:88:MET:HE1	2.10	0.51
1:P:34:ASN:ND2	3:R:482:SER:HA	2.26	0.51
3:F:481:ALA:CA	3:F:482:SER:HB2	2.40	0.51
1:G:187:GLN:CD	4:G:1863:HOH:O	2.48	0.51
2:W:2:SER:N	4:W:2469:HOH:O	2.43	0.51
1:V:216:VAL:CG1	1:V:231:ILE:HG13	2.40	0.51
2:H:183:GLY:N	2:H:184:SER:HB3	2.24	0.51
2:E:25:LEU:O	2:E:29:ILE:HG12	2.11	0.51
2:T:25:LEU:O	2:T:29:ILE:HG12	2.10	0.51
1:G:107:ASP:N	1:G:108:PRO:HD3	2.26	0.51
1:J:216:VAL:CG1	1:J:231:ILE:HG13	2.40	0.51
1:J:107:ASP:N	1:J:108:PRO:HD3	2.26	0.51
3:I:495:LYS:N	3:I:495:LYS:HD2	2.24	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:ND2	3:C:482:SER:HA	2.26	0.51
1:Y:186:ALA:HB3	1:Y:216:VAL:HG23	1.92	0.51
1:4:216:VAL:HG11	1:4:231:ILE:HG13	1.92	0.51
2:5:195:ARG:HH22	2:5:223:LYS:HE2	1.75	0.51
3:U:495:LYS:HD2	3:U:495:LYS:N	2.26	0.51
2:B:3:ASP:HB2	2:B:4:GLN:HB3	1.92	0.51
3:3:481:ALA:CA	3:3:482:SER:HB2	2.41	0.51
2:W:5:GLN:HB2	4:W:284:HOH:O	2.10	0.51
3:6:495:LYS:HD2	3:6:495:LYS:N	2.26	0.51
1:G:33:PHE:CE2	3:I:480:ILE:HD12	2.45	0.51
1:D:31:GLU:HG3	3:F:483:SER:HA	1.93	0.51
1:S:31:GLU:HG3	3:U:483:SER:HA	1.93	0.51
1:M:216:VAL:CG1	1:M:231:ILE:HG13	2.40	0.51
1:A:186:ALA:HB3	1:A:216:VAL:HG23	1.93	0.51
1:4:47:ARG:NH1	3:6:475:VAL:HG13	2.26	0.51
1:M:47:ARG:NH1	3:O:475:VAL:HG13	2.26	0.51
2:5:148:TRP:C	2:5:148:TRP:CD1	2.85	0.51
2:T:210:ILE:HG12	4:T:2291:HOH:O	2.10	0.51
1:4:107:ASP:N	1:4:108:PRO:HD3	2.25	0.50
2:K:148:TRP:C	2:K:148:TRP:CD1	2.83	0.50
2:B:115:GLY:O	4:B:560:HOH:O	2.19	0.50
1:S:97:LYS:HE2	4:S:1958:HOH:O	2.10	0.50
1:Y:29:PHE:HZ	1:Y:54:PHE:HD1	1.59	0.50
1:1:186:ALA:HB3	1:1:216:VAL:HG23	1.93	0.50
2:W:20:GLN:NE2	4:W:2111:HOH:O	2.26	0.50
3:3:495:LYS:N	3:3:495:LYS:HD2	2.26	0.50
2:Z:77:ASN:O	2:Z:88:MET:HE1	2.12	0.50
1:V:137:PRO:CG	2:W:244:ARG:HH11	2.24	0.50
1:Y:216:VAL:CG1	1:Y:231:ILE:HG13	2.41	0.50
1:D:107:ASP:N	1:D:108:PRO:HD3	2.27	0.50
2:N:25:LEU:O	2:N:29:ILE:HG12	2.12	0.50
2:2:195:ARG:HH22	2:2:223:LYS:HE2	1.76	0.50
3:0:495:LYS:N	3:0:495:LYS:HD2	2.27	0.50
1:D:216:VAL:CG1	1:D:231:ILE:HG13	2.41	0.50
1:7:29:PHE:HZ	1:7:54:PHE:HD1	1.59	0.50
1:1:216:VAL:CG1	1:1:231:ILE:HG13	2.41	0.50
1:M:100:HIS:O	1:M:103:LYS:HD2	2.12	0.50
1:D:186:ALA:HB3	1:D:216:VAL:HG23	1.94	0.50
2:5:25:LEU:O	2:5:29:ILE:HG12	2.11	0.50
1:4:216:VAL:CG1	1:4:231:ILE:HG13	2.41	0.50
2:E:77:ASN:O	2:E:88:MET:HE1	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:2:SER:N	4:N:2182:HOH:O	2.43	0.50
1:P:216:VAL:CG1	1:P:231:ILE:HG13	2.40	0.50
2:Q:77:ASN:O	2:Q:88:MET:HE1	2.11	0.50
1:S:107:ASP:N	1:S:108:PRO:HD3	2.26	0.50
3:L:495:LYS:HD2	3:L:495:LYS:N	2.26	0.50
1:S:34:ASN:ND2	3:U:482:SER:HA	2.27	0.50
2:2:94:ARG:CG	4:2:2894:HOH:O	2.54	0.50
1:D:68:GLU:OE2	4:D:1969:HOH:O	2.19	0.50
2:Z:148:TRP:CD1	2:Z:148:TRP:C	2.85	0.50
1:1:34:ASN:ND2	3:3:482:SER:HA	2.27	0.50
1:P:186:ALA:HB3	1:P:216:VAL:HG23	1.94	0.50
1:D:216:VAL:HG11	1:D:231:ILE:HG13	1.93	0.50
1:G:216:VAL:CG1	1:G:231:ILE:HG13	2.41	0.49
1:S:186:ALA:HB3	1:S:216:VAL:HG23	1.93	0.49
1:S:216:VAL:CG1	1:S:231:ILE:HG13	2.41	0.49
1:D:47:ARG:NH1	3:F:475:VAL:HG13	2.27	0.49
2:T:90:SER:OG	4:T:2887:HOH:O	2.19	0.49
2:2:20:GLN:NE2	4:2:2026:HOH:O	2.40	0.49
3:F:495:LYS:HD2	3:F:495:LYS:N	2.26	0.49
2:Z:244:ARG:NH1	2:Z:244:ARG:HG2	2.26	0.49
1:J:186:ALA:HB3	1:J:216:VAL:HG23	1.94	0.49
1:4:267:THR:HG23	1:4:268:LYS:O	2.12	0.49
2:W:145:LYS:HD3	4:W:2594:HOH:O	2.11	0.49
1:V:100:HIS:O	1:V:103:LYS:HD2	2.12	0.49
1:7:107:ASP:N	1:7:108:PRO:HD3	2.26	0.49
1:4:166:LYS:HD3	4:4:1606:HOH:O	2.12	0.49
3:R:495:LYS:N	3:R:495:LYS:HD2	2.26	0.49
2:2:148:TRP:CD1	2:2:148:TRP:C	2.86	0.49
1:A:31:GLU:HG3	3:C:483:SER:HA	1.95	0.49
1:1:128:LEU:HD11	1:1:158:ILE:HD11	1.94	0.49
1:D:166:LYS:HD3	4:D:1720:HOH:O	2.11	0.49
1:A:137:PRO:N	2:B:244:ARG:NH1	2.60	0.49
1:J:31:GLU:HG3	3:L:483:SER:HA	1.94	0.49
1:7:33:PHE:CE2	3:9:480:ILE:HD12	2.48	0.49
1:J:47:ARG:NH1	3:L:475:VAL:HG13	2.28	0.49
3:C:495:LYS:HD2	3:C:495:LYS:N	2.27	0.49
1:7:54:PHE:CE1	1:7:101:LEU:HD21	2.48	0.49
1:7:223:GLN:NE2	4:7:1345:HOH:O	2.45	0.49
1:A:29:PHE:HZ	1:A:54:PHE:HD1	1.60	0.49
1:V:137:PRO:CD	2:W:244:ARG:NH1	2.75	0.49
1:4:186:ALA:HB3	1:4:216:VAL:HG23	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:240:GLN:OE1	4:1:2448:HOH:O	2.20	0.49
2:Q:181:LYS:C	2:Q:183:GLY:H	2.16	0.49
2:8:195:ARG:NH2	2:8:223:LYS:NZ	2.61	0.49
1:4:128:LEU:HD11	1:4:158:ILE:HD11	1.95	0.49
1:S:267:THR:HG23	1:S:268:LYS:O	2.13	0.49
1:Y:146:LYS:NZ	4:Y:1416:HOH:O	2.45	0.49
1:S:184:PRO:HD3	2:W:3:ASP:O	2.13	0.49
1:S:88:LEU:HD13	1:S:90:PRO:HD3	1.95	0.49
2:K:77:ASN:O	2:K:88:MET:HE1	2.13	0.49
2:K:125:ASP:N	4:K:1875:HOH:O	2.41	0.49
1:M:115:SER:HB2	4:M:2558:HOH:O	2.12	0.48
1:1:267:THR:HG23	1:1:268:LYS:O	2.13	0.48
2:E:148:TRP:CD1	2:E:148:TRP:C	2.85	0.48
1:7:137:PRO:HG3	2:8:244:ARG:HH11	1.78	0.48
1:7:137:PRO:CG	2:8:244:ARG:HH11	2.26	0.48
1:4:101:LEU:HD22	3:6:480:ILE:CD1	2.39	0.48
1:G:78:GLU:HG2	4:G:300:HOH:O	2.13	0.48
1:V:107:ASP:N	1:V:108:PRO:HD3	2.27	0.48
1:P:29:PHE:HZ	1:P:54:PHE:HD1	1.60	0.48
1:A:216:VAL:CG1	1:A:231:ILE:HG13	2.42	0.48
2:H:156:VAL:HG22	2:H:167:TYR:CD2	2.48	0.48
2:Q:148:TRP:C	2:Q:148:TRP:CD1	2.85	0.48
1:1:137:PRO:CG	2:2:244:ARG:HG3	2.43	0.48
2:Q:89:PRO:HA	4:Q:551:HOH:O	2.13	0.48
1:V:102:ARG:NH2	3:X:479:ASP:OD1	2.46	0.48
1:1:136:TYR:C	2:2:244:ARG:HH12	2.17	0.48
2:K:237:LYS:HE2	2:K:241:ASN:OD1	2.13	0.48
1:1:137:PRO:N	2:2:244:ARG:NH1	2.52	0.48
2:5:181:LYS:C	2:5:183:GLY:H	2.16	0.48
2:2:181:LYS:C	2:2:183:GLY:H	2.16	0.48
1:A:267:THR:HG23	1:A:268:LYS:O	2.13	0.48
1:7:267:THR:HG23	1:7:268:LYS:O	2.14	0.48
1:V:82:LEU:CB	4:V:2723:HOH:O	2.61	0.48
2:B:148:TRP:C	2:B:148:TRP:CD1	2.86	0.48
2:E:181:LYS:C	2:E:183:GLY:H	2.16	0.48
2:K:181:LYS:C	2:K:183:GLY:H	2.16	0.48
1:S:29:PHE:HZ	1:S:54:PHE:HD1	1.61	0.48
2:Q:195:ARG:NH2	2:Q:223:LYS:NZ	2.61	0.48
2:Z:25:LEU:O	2:Z:29:ILE:HG12	2.13	0.48
1:1:29:PHE:HZ	1:1:54:PHE:HD1	1.61	0.48
2:B:181:LYS:C	2:B:183:GLY:H	2.17	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:117:LEU:HD22	1:P:152:GLN:OE1	2.13	0.48
1:A:137:PRO:CD	2:B:244:ARG:CG	2.81	0.48
1:D:33:PHE:CE2	3:F:480:ILE:HD12	2.49	0.48
1:V:29:PHE:HZ	1:V:54:PHE:HD1	1.61	0.48
1:S:128:LEU:HD11	1:S:158:ILE:HD11	1.96	0.48
1:J:117:LEU:HD22	1:J:152:GLN:OE1	2.14	0.48
2:E:237:LYS:HE2	2:E:241:ASN:OD1	2.14	0.48
1:G:137:PRO:HG3	2:H:244:ARG:HH11	1.79	0.47
1:M:102:ARG:NH2	3:O:479:ASP:OD1	2.47	0.47
1:Y:113:THR:CG2	1:Y:118:LYS:HE2	2.43	0.47
1:G:267:THR:HG23	1:G:268:LYS:O	2.14	0.47
1:4:137:PRO:CD	2:5:244:ARG:NH1	2.68	0.47
2:K:3:ASP:OD2	2:K:35:LEU:HD21	2.14	0.47
1:J:33:PHE:CE2	3:L:480:ILE:HD12	2.49	0.47
1:M:29:PHE:HZ	1:M:54:PHE:HD1	1.61	0.47
2:E:3:ASP:HB3	2:E:6:LEU:CB	2.44	0.47
1:A:113:THR:CG2	1:A:118:LYS:HE2	2.44	0.47
1:V:102:ARG:HD2	4:V:2143:HOH:O	2.13	0.47
1:M:190:ALA:HB3	1:M:212:ILE:HB	1.95	0.47
1:4:88:LEU:HD13	1:4:90:PRO:HD3	1.96	0.47
2:H:195:ARG:NH2	2:H:223:LYS:NZ	2.62	0.47
1:1:88:LEU:HD13	1:1:90:PRO:HD3	1.96	0.47
1:V:267:THR:HG23	1:V:268:LYS:O	2.14	0.47
2:W:156:VAL:HG22	2:W:167:TYR:CD2	2.50	0.47
2:Z:181:LYS:C	2:Z:183:GLY:H	2.16	0.47
2:N:181:LYS:C	2:N:183:GLY:H	2.17	0.47
2:H:181:LYS:C	2:H:183:GLY:H	2.17	0.47
1:A:182:THR:HB	2:E:3:ASP:N	2.28	0.47
2:Z:195:ARG:NH2	2:Z:223:LYS:NZ	2.62	0.47
1:Y:128:LEU:HD11	1:Y:158:ILE:HD11	1.96	0.47
2:T:163:ARG:N	4:T:1822:HOH:O	2.47	0.47
1:D:128:LEU:HD11	1:D:158:ILE:HD11	1.97	0.47
2:W:237:LYS:HE2	2:W:241:ASN:OD1	2.13	0.47
1:P:113:THR:CG2	1:P:118:LYS:HE2	2.44	0.47
2:K:195:ARG:NH2	2:K:223:LYS:NZ	2.62	0.47
1:P:128:LEU:HD11	1:P:158:ILE:HD11	1.97	0.47
2:8:148:TRP:CD1	2:8:148:TRP:C	2.88	0.47
4:M:720:HOH:O	2:N:193:LEU:CD2	2.60	0.47
1:G:187:GLN:HA	1:G:187:GLN:OE1	2.14	0.47
2:5:123:ASP:OD2	4:5:2547:HOH:O	2.19	0.47
2:N:195:ARG:NH2	2:N:223:LYS:NZ	2.62	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:195:ARG:NH2	2:5:223:LYS:NZ	2.63	0.47
2:2:223:LYS:HG3	4:2:2022:HOH:O	2.14	0.47
1:G:268:LYS:HD3	4:M:2089:HOH:O	2.13	0.47
1:D:267:THR:HG23	1:D:268:LYS:O	2.14	0.47
1:D:187:GLN:OE1	1:D:187:GLN:HA	2.15	0.47
1:S:117:LEU:HD22	1:S:152:GLN:OE1	2.15	0.47
1:Y:117:LEU:HD22	1:Y:152:GLN:OE1	2.15	0.47
1:Y:230:LYS:CE	4:Y:2663:HOH:O	2.58	0.47
2:2:237:LYS:HE2	2:2:241:ASN:OD1	2.14	0.47
1:G:29:PHE:HZ	1:G:54:PHE:HD1	1.62	0.47
2:8:181:LYS:C	2:8:183:GLY:H	2.17	0.47
1:M:33:PHE:CE2	3:O:480:ILE:HD12	2.49	0.47
2:K:174:MET:HE2	4:K:2177:HOH:O	2.13	0.47
1:D:117:LEU:HD22	1:D:152:GLN:OE1	2.15	0.47
1:A:54:PHE:CE1	1:A:101:LEU:HD11	2.50	0.47
2:W:195:ARG:NH2	2:W:223:LYS:NZ	2.63	0.47
2:E:195:ARG:NH2	2:E:223:LYS:NZ	2.62	0.47
2:5:223:LYS:HE2	4:5:2443:HOH:O	2.15	0.47
1:4:117:LEU:HD22	1:4:152:GLN:OE1	2.15	0.47
2:2:63:ASP:O	3:3:499:ARG:NH2	2.48	0.47
1:D:29:PHE:HZ	1:D:54:PHE:HD1	1.62	0.46
1:4:29:PHE:HZ	1:4:54:PHE:HD1	1.62	0.46
1:V:54:PHE:CE1	1:V:101:LEU:HD21	2.51	0.46
2:Z:44:ASP:HB3	2:Z:174:MET:HE1	1.95	0.46
2:5:237:LYS:HE2	2:5:241:ASN:OD1	2.15	0.46
1:S:219:SER:N	4:S:2045:HOH:O	2.48	0.46
2:T:244:ARG:HG3	2:T:244:ARG:NH1	2.30	0.46
1:G:54:PHE:CE1	1:G:101:LEU:HD11	2.50	0.46
1:P:267:THR:HG23	1:P:268:LYS:O	2.15	0.46
1:M:31:GLU:HG3	3:O:483:SER:HA	1.97	0.46
1:J:184:PRO:HG3	2:N:7:ASP:CB	2.45	0.46
2:B:195:ARG:NH2	2:B:223:LYS:NZ	2.63	0.46
2:2:195:ARG:NH2	2:2:223:LYS:NZ	2.63	0.46
2:B:63:ASP:O	3:C:499:ARG:NH2	2.48	0.46
2:8:156:VAL:HG22	2:8:167:TYR:CD2	2.51	0.46
2:T:181:LYS:C	2:T:183:GLY:H	2.17	0.46
2:Z:237:LYS:HE2	2:Z:241:ASN:OD1	2.15	0.46
1:V:31:GLU:HG3	3:X:483:SER:HA	1.97	0.46
1:1:209:HIS:HD2	4:1:1935:HOH:O	1.97	0.46
1:A:158:ILE:HB	1:A:175:SER:OG	2.14	0.46
1:J:187:GLN:OE1	1:J:187:GLN:HA	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:148:TRP:C	2:W:148:TRP:CD1	2.89	0.46
1:Y:88:LEU:HD13	1:Y:90:PRO:HD3	1.98	0.46
2:T:195:ARG:NH2	2:T:223:LYS:NZ	2.63	0.46
1:P:88:LEU:HD13	1:P:90:PRO:HD3	1.97	0.46
1:J:184:PRO:HG3	2:N:7:ASP:OD1	2.15	0.46
1:P:33:PHE:CE2	3:R:480:ILE:HD12	2.51	0.46
1:A:117:LEU:HD22	1:A:152:GLN:OE1	2.15	0.46
1:Y:54:PHE:CE1	1:Y:101:LEU:HD11	2.50	0.46
1:A:100:HIS:HE1	4:A:2670:HOH:O	1.99	0.46
2:N:156:VAL:HG22	2:N:167:TYR:CD2	2.50	0.46
1:7:187:GLN:OE1	1:7:187:GLN:HA	2.15	0.46
1:G:31:GLU:HG3	3:I:483:SER:HA	1.97	0.46
2:T:237:LYS:HE2	2:T:241:ASN:OD1	2.15	0.46
2:T:134:ILE:HB	2:T:150:SER:HB2	1.97	0.46
1:J:29:PHE:HZ	1:J:54:PHE:HD1	1.63	0.46
1:M:54:PHE:CE1	1:M:101:LEU:HD21	2.50	0.46
2:T:123:ASP:OD2	4:T:2887:HOH:O	2.21	0.46
1:1:117:LEU:HD22	1:1:152:GLN:OE1	2.16	0.46
2:B:237:LYS:HE2	2:B:241:ASN:OD1	2.15	0.46
2:E:134:ILE:HB	2:E:150:SER:HB2	1.97	0.46
1:J:128:LEU:HD11	1:J:158:ILE:HD11	1.98	0.46
1:M:187:GLN:HA	1:M:187:GLN:OE1	2.16	0.46
1:1:54:PHE:CE1	1:1:101:LEU:HD11	2.51	0.46
2:W:181:LYS:C	2:W:183:GLY:H	2.18	0.46
1:J:184:PRO:HG3	2:N:7:ASP:HB2	1.97	0.46
1:4:26:PRO:HG3	4:4:290:HOH:O	2.15	0.46
1:J:88:LEU:HD13	1:J:90:PRO:HD3	1.98	0.46
1:V:117:LEU:HD22	1:V:152:GLN:OE1	2.16	0.45
1:7:194:ILE:HD12	1:7:243:ILE:CD1	2.47	0.45
2:8:237:LYS:HE2	2:8:241:ASN:OD1	2.15	0.45
1:P:54:PHE:CE1	1:P:101:LEU:HD21	2.51	0.45
1:G:102:ARG:NH2	3:I:479:ASP:OD1	2.49	0.45
1:S:177:TRP:CE3	1:S:190:ALA:HB2	2.51	0.45
2:N:237:LYS:HE2	2:N:241:ASN:OD1	2.16	0.45
1:Y:239:TYR:CZ	1:Y:243:ILE:HD11	2.51	0.45
2:2:91:ALA:HB3	4:2:283:HOH:O	2.15	0.45
1:S:239:TYR:CZ	1:S:243:ILE:HD11	2.52	0.45
2:N:77:ASN:O	2:N:88:MET:HE1	2.16	0.45
1:V:187:GLN:HA	1:V:187:GLN:OE1	2.16	0.45
1:4:187:GLN:OE1	1:4:187:GLN:HA	2.16	0.45
1:4:54:PHE:CE1	1:4:101:LEU:HD21	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:184:PRO:HG3	2:W:7:ASP:CB	2.47	0.45
1:S:184:PRO:HG3	2:W:7:ASP:OD1	2.16	0.45
1:D:177:TRP:CE3	1:D:190:ALA:HB2	2.51	0.45
1:Y:26:PRO:HG3	4:Y:289:HOH:O	2.16	0.45
1:M:267:THR:HG23	1:M:268:LYS:O	2.16	0.45
2:H:25:LEU:O	2:H:29:ILE:HG12	2.16	0.45
1:J:267:THR:HG23	1:J:268:LYS:O	2.16	0.45
1:A:33:PHE:CE2	3:C:480:ILE:HD12	2.51	0.45
1:1:113:THR:CG2	1:1:118:LYS:HE2	2.44	0.45
1:J:113:THR:CG2	1:J:118:LYS:HE2	2.46	0.45
1:7:102:ARG:NH2	3:9:479:ASP:OD1	2.50	0.45
2:T:156:VAL:HG22	2:T:167:TYR:CD2	2.52	0.45
2:8:100:ALA:HB2	2:8:210:ILE:HD12	1.99	0.45
2:8:25:LEU:O	2:8:29:ILE:HG12	2.16	0.45
2:Q:237:LYS:HE2	2:Q:241:ASN:OD1	2.15	0.45
1:Y:209:HIS:HD2	4:Y:2418:HOH:O	2.00	0.45
2:N:148:TRP:C	2:N:148:TRP:CD1	2.89	0.45
2:H:148:TRP:CD1	2:H:148:TRP:C	2.88	0.45
1:S:187:GLN:OE1	1:S:187:GLN:HA	2.16	0.45
1:7:247:TYR:CD1	2:8:237:LYS:HD3	2.52	0.45
1:4:33:PHE:CE2	3:6:480:ILE:HD12	2.51	0.45
1:S:26:PRO:HG3	4:S:288:HOH:O	2.16	0.45
1:V:240:GLN:HE22	1:7:266:ARG:HE	1.65	0.45
1:A:128:LEU:HD11	1:A:158:ILE:HD11	1.99	0.45
1:V:88:LEU:HD13	1:V:90:PRO:HD3	1.99	0.45
1:P:187:GLN:HA	1:P:187:GLN:OE1	2.17	0.45
1:4:239:TYR:CZ	1:4:243:ILE:HD11	2.52	0.45
2:2:44:ASP:HB3	2:2:174:MET:HE1	1.97	0.45
1:1:158:ILE:HB	1:1:175:SER:OG	2.15	0.45
1:G:117:LEU:HD22	1:G:152:GLN:OE1	2.17	0.45
1:V:120:TRP:HZ3	1:V:224:THR:HG21	1.81	0.45
1:D:137:PRO:CG	2:E:244:ARG:HG3	2.48	0.45
1:Y:34:ASN:ND2	3:0:482:SER:HA	2.32	0.45
1:S:184:PRO:HG3	2:W:7:ASP:HB2	1.99	0.45
1:4:177:TRP:CE3	1:4:190:ALA:HB2	2.52	0.45
1:G:129:ARG:NH1	4:G:2403:HOH:O	2.33	0.45
1:D:120:TRP:HZ3	1:D:224:THR:HG21	1.81	0.45
1:S:54:PHE:CE1	1:S:101:LEU:HD21	2.53	0.44
2:W:25:LEU:O	2:W:29:ILE:HG12	2.17	0.44
2:H:243:LEU:HA	2:H:243:LEU:HD23	1.59	0.44
1:D:137:PRO:CG	2:E:244:ARG:HH11	2.30	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:239:TYR:CZ	1:1:243:ILE:HD11	2.52	0.44
2:T:243:LEU:H	2:T:244:ARG:HA	1.78	0.44
1:D:109:GLN:HG2	4:D:2877:HOH:O	2.17	0.44
2:5:156:VAL:HG22	2:5:167:TYR:CD2	2.52	0.44
1:S:120:TRP:HZ3	1:S:224:THR:HG21	1.81	0.44
1:7:117:LEU:HD22	1:7:152:GLN:OE1	2.18	0.44
1:V:194:ILE:HD12	1:V:243:ILE:CD1	2.48	0.44
1:D:239:TYR:CZ	1:D:243:ILE:HD11	2.51	0.44
1:M:117:LEU:HD22	1:M:152:GLN:OE1	2.17	0.44
1:A:187:GLN:OE1	1:A:187:GLN:HA	2.17	0.44
1:D:54:PHE:CE1	1:D:101:LEU:HD11	2.52	0.44
1:J:54:PHE:CE1	1:J:101:LEU:HD11	2.52	0.44
1:S:113:THR:CG2	1:S:118:LYS:HE2	2.46	0.44
1:P:158:ILE:HB	1:P:175:SER:OG	2.17	0.44
1:S:58:ASN:OD1	1:S:103:LYS:HE3	2.17	0.44
1:M:113:THR:CG2	1:M:118:LYS:HE2	2.47	0.44
1:M:88:LEU:HD13	1:M:90:PRO:HD3	1.99	0.44
2:E:63:ASP:O	3:F:499:ARG:NH2	2.51	0.44
1:A:56:GLN:O	1:A:60:ASP:HB2	2.18	0.44
2:W:244:ARG:NH2	1:7:266:ARG:HH12	2.16	0.44
2:8:241:ASN:O	2:8:244:ARG:HG3	2.16	0.44
1:A:177:TRP:CE3	1:A:190:ALA:HB2	2.52	0.44
1:J:47:ARG:O	1:J:51:ALA:HB2	2.18	0.44
1:Y:187:GLN:OE1	1:Y:187:GLN:HA	2.17	0.44
1:Y:158:ILE:HB	1:Y:175:SER:OG	2.16	0.44
2:H:237:LYS:HE2	2:H:241:ASN:OD1	2.17	0.44
2:8:101:ASN:O	2:8:105:ASP:HB2	2.18	0.44
2:2:215:ARG:NH2	4:2:1905:HOH:O	2.50	0.44
3:0:487:LEU:N	3:0:487:LEU:HD22	2.32	0.44
1:P:47:ARG:O	1:P:51:ALA:HB2	2.18	0.44
1:M:47:ARG:O	1:M:51:ALA:HB2	2.18	0.44
1:7:78:GLU:HG2	4:7:1449:HOH:O	2.17	0.44
1:J:239:TYR:CZ	1:J:243:ILE:HD11	2.52	0.44
1:M:78:GLU:HG2	4:M:1076:HOH:O	2.18	0.44
2:E:243:LEU:HD23	2:E:243:LEU:HA	1.83	0.44
2:Q:4:GLN:N	4:Q:2522:HOH:O	2.51	0.44
2:8:243:LEU:HA	2:8:243:LEU:HD23	1.83	0.44
1:Y:194:ILE:HD12	1:Y:243:ILE:CD1	2.48	0.44
1:G:247:TYR:CD1	2:H:237:LYS:HD3	2.52	0.44
2:Z:156:VAL:HG22	2:Z:167:TYR:CD2	2.53	0.44
1:4:137:PRO:CG	2:5:244:ARG:HH11	2.30	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:33:PHE:CE2	3:U:480:ILE:HD12	2.52	0.43
1:7:120:TRP:HZ3	1:7:224:THR:HG21	1.82	0.43
1:7:54:PHE:CD1	1:7:101:LEU:HD21	2.53	0.43
1:J:177:TRP:CE3	1:J:190:ALA:HB2	2.53	0.43
1:1:177:TRP:CE3	1:1:190:ALA:HB2	2.53	0.43
1:4:158:ILE:HB	1:4:175:SER:OG	2.17	0.43
1:V:194:ILE:HD12	1:V:243:ILE:HD13	2.00	0.43
1:G:120:TRP:HZ3	1:G:224:THR:HG21	1.82	0.43
1:4:120:TRP:HZ3	1:4:224:THR:HG21	1.82	0.43
1:A:88:LEU:HD13	1:A:90:PRO:HD3	2.00	0.43
1:A:137:PRO:CG	2:B:244:ARG:CG	2.97	0.43
2:B:243:LEU:HA	2:B:243:LEU:HD23	1.81	0.43
2:Z:244:ARG:HH11	2:Z:244:ARG:HG2	1.82	0.43
1:P:177:TRP:CE3	1:P:190:ALA:HB2	2.53	0.43
1:A:239:TYR:CZ	1:A:243:ILE:HD11	2.52	0.43
1:M:158:ILE:HB	1:M:175:SER:OG	2.18	0.43
2:K:156:VAL:HG22	2:K:167:TYR:CD2	2.53	0.43
1:G:128:LEU:HD11	1:G:158:ILE:HD11	2.01	0.43
1:J:120:TRP:HZ3	1:J:224:THR:HG21	1.83	0.43
1:G:194:ILE:HD12	1:G:243:ILE:CD1	2.49	0.43
1:7:166:LYS:HB2	4:7:1899:HOH:O	2.18	0.43
1:1:187:GLN:HA	1:1:187:GLN:OE1	2.18	0.43
1:V:101:LEU:HD22	3:X:480:ILE:CD1	2.43	0.43
1:1:120:TRP:HZ3	1:1:224:THR:HG21	1.82	0.43
2:E:156:VAL:HG22	2:E:167:TYR:CD2	2.53	0.43
1:S:103:LYS:HD3	4:S:2382:HOH:O	2.17	0.43
1:D:194:ILE:HD12	1:D:243:ILE:CD1	2.49	0.43
1:G:35:ASP:OD1	2:H:11:ASP:OD2	2.37	0.43
1:M:120:TRP:HZ3	1:M:224:THR:HG21	1.82	0.43
2:K:134:ILE:HB	2:K:150:SER:HB2	2.00	0.43
1:P:137:PRO:HG3	2:Q:244:ARG:HD3	1.99	0.43
1:7:177:TRP:CE3	1:7:190:ALA:HB2	2.54	0.43
1:S:158:ILE:HB	1:S:175:SER:OG	2.17	0.43
2:Q:63:ASP:O	3:R:499:ARG:NH2	2.51	0.43
1:Y:137:PRO:CG	2:Z:244:ARG:HG3	2.48	0.43
1:4:113:THR:CG2	1:4:118:LYS:HE2	2.47	0.43
1:V:247:TYR:CD1	2:W:237:LYS:HD3	2.54	0.43
1:1:194:ILE:HD12	1:1:243:ILE:CD1	2.49	0.43
2:5:134:ILE:HB	2:5:150:SER:HB2	2.00	0.43
1:7:31:GLU:HG3	3:9:483:SER:HA	2.01	0.43
2:K:44:ASP:O	4:K:2177:HOH:O	2.22	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:63:ASP:O	3:O:499:ARG:NH2	2.52	0.43
1:M:194:ILE:HD12	1:M:243:ILE:CD1	2.49	0.43
1:A:47:ARG:O	1:A:51:ALA:HB2	2.19	0.43
1:M:20:PHE:CD2	2:N:12:LEU:HD21	2.54	0.43
1:7:128:LEU:HD11	1:7:158:ILE:HD11	2.01	0.43
1:G:113:THR:CG2	1:G:118:LYS:HE2	2.49	0.42
2:5:63:ASP:O	3:6:499:ARG:NH2	2.52	0.42
1:Y:19:LYS:HE2	4:Y:2825:HOH:O	2.18	0.42
1:Y:56:GLN:O	1:Y:60:ASP:HB2	2.19	0.42
1:D:113:THR:CG2	1:D:118:LYS:HE2	2.48	0.42
1:4:47:ARG:O	1:4:51:ALA:HB2	2.18	0.42
1:G:20:PHE:CD2	2:H:12:LEU:HD21	2.54	0.42
1:Y:120:TRP:HZ3	1:Y:224:THR:HG21	1.83	0.42
1:V:26:PRO:HG3	4:V:1172:HOH:O	2.19	0.42
3:C:487:LEU:N	3:C:487:LEU:HD22	2.34	0.42
1:D:158:ILE:HB	1:D:175:SER:OG	2.19	0.42
1:G:158:ILE:HB	1:G:175:SER:OG	2.19	0.42
1:A:120:TRP:HZ3	1:A:224:THR:HG21	1.83	0.42
2:8:145:LYS:HD3	4:8:2373:HOH:O	2.20	0.42
2:Q:156:VAL:HG22	2:Q:167:TYR:CD2	2.54	0.42
1:M:101:LEU:HD22	3:O:480:ILE:CD1	2.44	0.42
1:D:47:ARG:O	1:D:51:ALA:HB2	2.20	0.42
1:J:194:ILE:HD12	1:J:243:ILE:CD1	2.50	0.42
1:G:266:ARG:HE	1:M:240:GLN:HE22	1.65	0.42
1:S:185:THR:HB	2:W:3:ASP:OD2	2.19	0.42
1:1:47:ARG:O	1:1:51:ALA:HB2	2.18	0.42
1:P:26:PRO:HG3	4:P:353:HOH:O	2.19	0.42
3:3:487:LEU:HD22	3:3:487:LEU:N	2.34	0.42
1:G:210:LYS:NZ	2:H:183:GLY:O	2.45	0.42
1:Y:47:ARG:O	1:Y:51:ALA:HB2	2.19	0.42
1:P:120:TRP:HZ3	1:P:224:THR:HG21	1.83	0.42
1:Y:33:PHE:CE2	3:O:480:ILE:HD12	2.54	0.42
1:7:101:LEU:HD22	3:9:480:ILE:CD1	2.44	0.42
1:A:183:PRO:O	2:E:3:ASP:N	2.52	0.42
1:V:113:THR:CG2	1:V:118:LYS:HE2	2.48	0.42
1:S:47:ARG:O	1:S:51:ALA:HB2	2.19	0.42
1:A:247:TYR:CD1	2:B:237:LYS:HD3	2.54	0.42
1:P:56:GLN:O	1:P:60:ASP:HB2	2.20	0.42
1:4:72:ASP:HB2	1:4:129:ARG:HH22	1.84	0.42
3:U:487:LEU:HD22	3:U:487:LEU:N	2.34	0.42
1:A:137:PRO:CG	2:B:244:ARG:HG3	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PRO:HG3	2:E:244:ARG:HH11	1.85	0.42
2:2:3:ASP:O	2:2:4:GLN:HB2	2.19	0.42
1:S:194:ILE:HD12	1:S:243:ILE:CD1	2.50	0.42
1:D:56:GLN:O	1:D:60:ASP:HB2	2.20	0.42
2:N:100:ALA:HB2	2:N:210:ILE:HD12	2.01	0.42
2:B:51:ARG:HD2	4:B:2754:HOH:O	2.19	0.42
2:8:17:PRO:HA	2:8:18:PRO:HD2	1.94	0.42
1:P:239:TYR:CZ	1:P:243:ILE:HD11	2.54	0.42
3:O:481:ALA:HB1	3:O:482:SER:CB	2.36	0.42
1:1:31:GLU:CA	3:3:483:SER:HB2	2.43	0.42
1:D:88:LEU:HD13	1:D:90:PRO:HD3	2.02	0.42
3:I:481:ALA:HB1	3:I:482:SER:CB	2.37	0.41
2:Q:90:SER:N	4:Q:551:HOH:O	2.18	0.41
1:A:230:LYS:CE	4:A:1902:HOH:O	2.68	0.41
1:1:56:GLN:O	1:1:60:ASP:HB2	2.20	0.41
1:Y:240:GLN:HE22	1:4:266:ARG:HE	1.68	0.41
1:J:72:ASP:HB2	1:J:129:ARG:HH22	1.84	0.41
2:B:156:VAL:HG22	2:B:167:TYR:CD2	2.54	0.41
2:Q:131:VAL:HA	2:Q:152:HIS:O	2.20	0.41
1:4:184:PRO:C	1:4:218:VAL:HG12	2.40	0.41
3:O:487:LEU:N	3:O:487:LEU:HD22	2.35	0.41
2:W:243:LEU:HD23	2:W:243:LEU:HA	1.78	0.41
1:M:247:TYR:CD1	2:N:237:LYS:HD3	2.54	0.41
1:Y:72:ASP:HB2	1:Y:129:ARG:HH22	1.85	0.41
1:7:20:PHE:CD2	2:8:12:LEU:HD21	2.55	0.41
3:R:487:LEU:N	3:R:487:LEU:HD22	2.35	0.41
1:S:101:LEU:HD22	3:U:480:ILE:CD1	2.47	0.41
1:7:113:THR:CG2	1:7:118:LYS:HE2	2.49	0.41
1:A:194:ILE:HD12	1:A:243:ILE:CD1	2.50	0.41
2:Z:134:ILE:HB	2:Z:150:SER:HB2	2.01	0.41
2:H:101:ASN:O	2:H:105:ASP:HB2	2.20	0.41
3:9:487:LEU:N	3:9:487:LEU:HD22	2.35	0.41
1:V:82:LEU:CG	4:V:2723:HOH:O	2.52	0.41
1:1:33:PHE:CE2	3:3:480:ILE:HD12	2.55	0.41
2:Z:243:LEU:H	2:Z:244:ARG:HA	1.80	0.41
1:Y:58:ASN:OD1	1:Y:103:LYS:HE3	2.20	0.41
1:S:88:LEU:HD13	1:S:90:PRO:CD	2.51	0.41
1:D:117:LEU:HD13	1:D:117:LEU:HA	1.87	0.41
2:B:237:LYS:HD2	2:B:237:LYS:HA	1.96	0.41
1:G:247:TYR:CG	2:H:237:LYS:HD3	2.56	0.41
1:V:56:GLN:O	1:V:60:ASP:HB2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:ASP:OD1	2:N:11:ASP:OD2	2.38	0.41
3:X:487:LEU:HD22	3:X:487:LEU:N	2.35	0.41
3:C:481:ALA:HB1	3:C:482:SER:CB	2.37	0.41
1:4:194:ILE:HD12	1:4:243:ILE:CD1	2.50	0.41
1:V:239:TYR:CZ	1:V:243:ILE:HD11	2.56	0.41
1:M:128:LEU:HD11	1:M:158:ILE:HD11	2.03	0.41
1:V:181:ILE:HG22	1:V:183:PRO:HD3	2.02	0.41
2:2:115:GLY:O	4:2:1227:HOH:O	2.22	0.41
3:6:487:LEU:HD22	3:6:487:LEU:N	2.35	0.41
1:D:58:ASN:OD1	1:D:103:LYS:HE3	2.21	0.41
1:P:181:ILE:HG22	1:P:183:PRO:HD3	2.02	0.41
2:K:9:ALA:HB1	2:K:39:LEU:HD21	2.03	0.41
1:D:72:ASP:HB2	1:D:129:ARG:HH22	1.85	0.41
1:1:237:ASN:HB2	4:1:2793:HOH:O	2.19	0.41
1:S:72:ASP:HB2	1:S:129:ARG:HH22	1.85	0.41
3:F:487:LEU:HD22	3:F:487:LEU:N	2.36	0.41
1:D:184:PRO:C	1:D:218:VAL:HG12	2.41	0.41
1:Y:31:GLU:CA	3:0:483:SER:HB2	2.42	0.41
3:O:493:ARG:HB3	3:O:494:PRO:HD2	2.01	0.41
1:P:194:ILE:HD12	1:P:243:ILE:CD1	2.51	0.41
1:J:56:GLN:O	1:J:60:ASP:HB2	2.21	0.41
3:L:481:ALA:HB1	3:L:482:SER:CB	2.37	0.41
1:J:184:PRO:C	1:J:218:VAL:HG12	2.41	0.41
2:H:100:ALA:HB2	2:H:210:ILE:HD12	2.01	0.41
1:J:117:LEU:HA	1:J:117:LEU:HD13	1.87	0.41
1:V:20:PHE:CD2	2:W:12:LEU:HD21	2.56	0.41
2:H:53:LYS:HD2	4:H:2202:HOH:O	2.21	0.41
1:V:87:PHE:CA	4:V:2723:HOH:O	2.34	0.41
3:R:481:ALA:HB1	3:R:482:SER:CB	2.37	0.41
2:K:237:LYS:HA	2:K:237:LYS:HD2	1.97	0.41
1:S:184:PRO:C	1:S:218:VAL:HG12	2.41	0.41
1:V:54:PHE:CD1	1:V:101:LEU:HD21	2.56	0.41
1:M:54:PHE:CD1	1:M:101:LEU:HD21	2.56	0.41
1:7:47:ARG:O	1:7:51:ALA:HB2	2.20	0.41
1:G:47:ARG:O	1:G:51:ALA:HB2	2.21	0.41
1:V:177:TRP:CE3	1:V:190:ALA:HB2	2.56	0.41
1:4:88:LEU:HD13	1:4:90:PRO:CD	2.51	0.41
1:G:72:ASP:HB2	1:G:129:ARG:HH22	1.85	0.41
2:Z:135:LYS:NZ	4:Z:282:HOH:O	2.54	0.41
1:V:128:LEU:HD11	1:V:158:ILE:HD11	2.03	0.41
1:4:17:ALA:HB1	1:4:36:VAL:CG1	2.51	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:91:ARG:O	1:4:93:LYS:CE	2.69	0.41
2:5:100:ALA:HB2	2:5:210:ILE:HD12	2.03	0.41
2:B:61:LEU:HD22	2:B:71:TYR:CG	2.55	0.41
2:T:63:ASP:O	3:U:499:ARG:NH2	2.54	0.41
1:A:261:GLN:HG2	2:B:225:ARG:CZ	2.51	0.41
2:2:122:TRP:CD1	3:3:496:MET:HG3	2.56	0.41
2:2:156:VAL:HG22	2:2:167:TYR:CD2	2.56	0.41
2:Q:134:ILE:HB	2:Q:150:SER:HB2	2.02	0.41
2:N:122:TRP:CE2	2:N:129:ALA:HB3	2.56	0.41
1:J:242:ALA:HB1	2:K:184:SER:HB2	2.03	0.41
2:5:244:ARG:HH11	2:5:244:ARG:HG3	1.86	0.41
1:A:181:ILE:HG22	1:A:183:PRO:HD3	2.03	0.41
1:Y:177:TRP:CE3	1:Y:190:ALA:HB2	2.56	0.41
3:I:499:ARG:NH1	4:I:1933:HOH:O	2.54	0.41
1:P:261:GLN:HG2	2:Q:225:ARG:CZ	2.51	0.41
2:W:93:LEU:HD12	2:W:93:LEU:HA	1.95	0.41
1:4:102:ARG:HB2	4:4:2273:HOH:O	2.21	0.40
1:4:58:ASN:OD1	1:4:103:LYS:HE3	2.21	0.40
2:Q:100:ALA:HB2	2:Q:210:ILE:HD12	2.03	0.40
1:J:158:ILE:HB	1:J:175:SER:OG	2.21	0.40
2:N:101:ASN:O	2:N:105:ASP:HB2	2.21	0.40
1:Y:137:PRO:HD3	2:Z:244:ARG:CD	2.51	0.40
1:A:146:LYS:NZ	4:A:800:HOH:O	2.54	0.40
1:7:72:ASP:HB2	1:7:129:ARG:HH22	1.86	0.40
2:K:100:ALA:HB2	2:K:210:ILE:HD12	2.03	0.40
2:5:17:PRO:HA	2:5:18:PRO:HD2	1.96	0.40
2:2:71:TYR:O	4:2:2304:HOH:O	2.22	0.40
1:A:39:LEU:HD22	2:B:32:VAL:HG21	2.03	0.40
1:P:136:TYR:HA	1:P:137:PRO:HD3	1.97	0.40
1:P:247:TYR:CD1	2:Q:237:LYS:HD3	2.56	0.40
2:5:96:LEU:HD13	4:5:2369:HOH:O	2.21	0.40
1:A:72:ASP:HB2	1:A:129:ARG:HH22	1.85	0.40
1:M:181:ILE:HG22	1:M:183:PRO:HD3	2.03	0.40
1:J:94:ILE:HD12	4:J:1634:HOH:O	2.21	0.40
1:M:56:GLN:O	1:M:60:ASP:HB2	2.21	0.40
1:M:72:ASP:HB2	1:M:129:ARG:HH22	1.85	0.40
2:W:244:ARG:NH1	2:W:244:ARG:CG	2.82	0.40
1:1:39:LEU:HD22	2:2:32:VAL:HG21	2.03	0.40
1:1:72:ASP:HB2	1:1:129:ARG:HH22	1.86	0.40
3:L:487:LEU:N	3:L:487:LEU:HD22	2.37	0.40
2:8:9:ALA:HB1	2:8:39:LEU:HD21	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:242:GLY:C	2:N:244:ARG:HG2	2.42	0.40
1:4:31:GLU:CA	3:6:483:SER:HB2	2.42	0.40
2:W:145:LYS:NZ	4:W:2883:HOH:O	2.43	0.40
1:Y:194:ILE:HD12	1:Y:243:ILE:HD13	2.03	0.40
1:7:158:ILE:HB	1:7:175:SER:OG	2.21	0.40
2:B:100:ALA:HB2	2:B:210:ILE:HD12	2.03	0.40
1:7:88:LEU:HD13	1:7:90:PRO:HD3	2.04	0.40
1:4:56:GLN:O	1:4:60:ASP:HB2	2.21	0.40
2:H:9:ALA:HB1	2:H:39:LEU:HD21	2.03	0.40
2:Z:2:SER:HA	2:Z:3:ASP:HA	1.50	0.40
1:1:26:PRO:HG3	4:1:349:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	4	267/286 (93%)	259 (97%)	7 (3%)	1 (0%)	39	33
1	7	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	A	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	D	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	G	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	J	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	M	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	P	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	S	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	V	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
2	2	234/277 (84%)	227 (97%)	4 (2%)	3 (1%)	15	7
2	5	233/277 (84%)	227 (97%)	4 (2%)	2 (1%)	21	13
2	8	235/277 (85%)	228 (97%)	5 (2%)	2 (1%)	21	13
2	B	234/277 (84%)	225 (96%)	6 (3%)	3 (1%)	15	7
2	E	234/277 (84%)	228 (97%)	4 (2%)	2 (1%)	21	13
2	H	235/277 (85%)	230 (98%)	3 (1%)	2 (1%)	21	13
2	K	234/277 (84%)	228 (97%)	4 (2%)	2 (1%)	21	13
2	N	235/277 (85%)	230 (98%)	3 (1%)	2 (1%)	21	13
2	Q	234/277 (84%)	227 (97%)	4 (2%)	3 (1%)	15	7
2	T	233/277 (84%)	228 (98%)	3 (1%)	2 (1%)	21	13
2	W	235/277 (85%)	229 (97%)	4 (2%)	2 (1%)	21	13
2	Z	235/277 (85%)	228 (97%)	4 (2%)	3 (1%)	15	7
3	0	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	3	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	6	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	9	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	C	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	F	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	I	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	L	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	O	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	R	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	U	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
3	X	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	6339/7104 (89%)	6139 (97%)	160 (2%)	40 (1%)	30	22

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	184	SER
2	E	184	SER
2	H	184	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	184	SER
2	N	184	SER
2	Q	4	GLN
2	Q	184	SER
2	T	184	SER
2	W	184	SER
2	Z	4	GLN
2	Z	184	SER
2	2	4	GLN
2	2	184	SER
2	5	184	SER
2	8	184	SER
2	B	4	GLN
2	B	183	GLY
2	E	183	GLY
2	H	183	GLY
2	K	183	GLY
2	N	183	GLY
2	Q	183	GLY
2	T	183	GLY
2	W	183	GLY
2	Z	183	GLY
2	2	183	GLY
2	5	183	GLY
2	8	183	GLY
1	A	72	ASP
1	D	72	ASP
1	J	72	ASP
1	P	72	ASP
1	S	72	ASP
1	Y	72	ASP
1	1	72	ASP
1	4	72	ASP
1	G	72	ASP
1	M	72	ASP
1	V	72	ASP
1	7	72	ASP

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	4	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	7	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	A	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	D	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	G	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	J	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	M	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	P	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	S	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	V	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	Y	238/252 (94%)	228 (96%)	10 (4%)	36	31
2	2	210/248 (85%)	203 (97%)	7 (3%)	45	43
2	5	209/248 (84%)	205 (98%)	4 (2%)	65	67
2	8	211/248 (85%)	202 (96%)	9 (4%)	35	30
2	B	210/248 (85%)	205 (98%)	5 (2%)	57	58
2	E	210/248 (85%)	206 (98%)	4 (2%)	65	67
2	H	211/248 (85%)	205 (97%)	6 (3%)	51	50
2	K	210/248 (85%)	203 (97%)	7 (3%)	45	43
2	N	211/248 (85%)	205 (97%)	6 (3%)	51	50
2	Q	210/248 (85%)	203 (97%)	7 (3%)	45	43
2	T	209/248 (84%)	204 (98%)	5 (2%)	57	58
2	W	211/248 (85%)	205 (97%)	6 (3%)	51	50
2	Z	211/248 (85%)	204 (97%)	7 (3%)	45	43
3	0	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	3	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	6	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	9	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	C	25/25 (100%)	22 (88%)	3 (12%)	6	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	I	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	L	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	O	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	R	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	U	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	X	25/25 (100%)	22 (88%)	3 (12%)	6	3
All	All	5679/6300 (90%)	5455 (96%)	224 (4%)	39	35

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	93	LYS
1	A	94	ILE
1	A	101	LEU
1	A	102	ARG
1	A	111	GLU
1	A	113	THR
1	A	117	LEU
1	A	216	VAL
1	A	230	LYS
2	B	83	LEU
2	B	84	GLU
2	B	105	ASP
2	B	178	GLN
2	B	197	MET
3	C	475	VAL
3	C	492	ASN
3	C	500	ARG
1	D	48	GLU
1	D	93	LYS
1	D	94	ILE
1	D	101	LEU
1	D	102	ARG
1	D	111	GLU
1	D	113	THR
1	D	117	LEU
1	D	216	VAL
1	D	230	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	83	LEU
2	E	105	ASP
2	E	178	GLN
2	E	197	MET
3	F	475	VAL
3	F	492	ASN
3	F	500	ARG
1	G	48	GLU
1	G	93	LYS
1	G	94	ILE
1	G	101	LEU
1	G	102	ARG
1	G	111	GLU
1	G	113	THR
1	G	117	LEU
1	G	216	VAL
1	G	230	LYS
2	H	2	SER
2	H	19	GLN
2	H	83	LEU
2	H	148	TRP
2	H	178	GLN
2	H	197	MET
3	I	475	VAL
3	I	492	ASN
3	I	500	ARG
1	J	48	GLU
1	J	93	LYS
1	J	94	ILE
1	J	101	LEU
1	J	102	ARG
1	J	111	GLU
1	J	113	THR
1	J	117	LEU
1	J	230	LYS
2	K	83	LEU
2	K	84	GLU
2	K	105	ASP
2	K	148	TRP
2	K	178	GLN
2	K	197	MET
2	K	244	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	L	475	VAL
3	L	492	ASN
3	L	500	ARG
1	M	48	GLU
1	M	93	LYS
1	M	94	ILE
1	M	102	ARG
1	M	111	GLU
1	M	113	THR
1	M	117	LEU
1	M	129	ARG
1	M	216	VAL
1	M	230	LYS
2	N	3	ASP
2	N	19	GLN
2	N	83	LEU
2	N	148	TRP
2	N	178	GLN
2	N	197	MET
3	O	475	VAL
3	O	492	ASN
3	O	500	ARG
1	P	48	GLU
1	P	93	LYS
1	P	94	ILE
1	P	102	ARG
1	P	111	GLU
1	P	113	THR
1	P	117	LEU
1	P	216	VAL
1	P	230	LYS
2	Q	3	ASP
2	Q	83	LEU
2	Q	84	GLU
2	Q	105	ASP
2	Q	148	TRP
2	Q	178	GLN
2	Q	197	MET
3	R	475	VAL
3	R	492	ASN
3	R	500	ARG
1	S	48	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	S	93	LYS
1	S	94	ILE
1	S	102	ARG
1	S	111	GLU
1	S	113	THR
1	S	117	LEU
1	S	216	VAL
1	S	230	LYS
2	T	83	LEU
2	T	105	ASP
2	T	148	TRP
2	T	178	GLN
2	T	197	MET
3	U	475	VAL
3	U	492	ASN
3	U	500	ARG
1	V	48	GLU
1	V	93	LYS
1	V	94	ILE
1	V	102	ARG
1	V	111	GLU
1	V	113	THR
1	V	117	LEU
1	V	216	VAL
1	V	230	LYS
2	W	19	GLN
2	W	83	LEU
2	W	84	GLU
2	W	148	TRP
2	W	178	GLN
2	W	197	MET
3	X	475	VAL
3	X	492	ASN
3	X	500	ARG
1	Y	48	GLU
1	Y	93	LYS
1	Y	94	ILE
1	Y	101	LEU
1	Y	102	ARG
1	Y	111	GLU
1	Y	113	THR
1	Y	117	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Y	216	VAL
1	Y	230	LYS
2	Z	3	ASP
2	Z	83	LEU
2	Z	84	GLU
2	Z	105	ASP
2	Z	148	TRP
2	Z	178	GLN
2	Z	197	MET
3	0	475	VAL
3	0	492	ASN
3	0	500	ARG
1	1	48	GLU
1	1	93	LYS
1	1	94	ILE
1	1	101	LEU
1	1	102	ARG
1	1	111	GLU
1	1	113	THR
1	1	117	LEU
1	1	216	VAL
1	1	230	LYS
2	2	3	ASP
2	2	83	LEU
2	2	84	GLU
2	2	105	ASP
2	2	148	TRP
2	2	178	GLN
2	2	197	MET
3	3	475	VAL
3	3	492	ASN
3	3	500	ARG
1	4	48	GLU
1	4	93	LYS
1	4	94	ILE
1	4	102	ARG
1	4	111	GLU
1	4	113	THR
1	4	117	LEU
1	4	216	VAL
1	4	230	LYS
2	5	83	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	5	148	TRP
2	5	178	GLN
2	5	197	MET
3	6	475	VAL
3	6	492	ASN
3	6	500	ARG
1	7	48	GLU
1	7	93	LYS
1	7	94	ILE
1	7	102	ARG
1	7	111	GLU
1	7	113	THR
1	7	117	LEU
1	7	129	ARG
1	7	216	VAL
1	7	230	LYS
2	8	2	SER
2	8	3	ASP
2	8	19	GLN
2	8	83	LEU
2	8	84	GLU
2	8	148	TRP
2	8	178	GLN
2	8	197	MET
2	8	244	ARG
3	9	475	VAL
3	9	492	ASN
3	9	500	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	44	ASN
1	A	73	GLN
1	A	100	HIS
1	A	109	GLN
1	A	151	GLN
1	A	164	GLN
1	A	213	GLN
1	A	248	GLN
2	B	4	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	19	GLN
2	B	45	GLN
2	B	157	GLN
2	B	229	ASN
1	D	34	ASN
1	D	44	ASN
1	D	73	GLN
1	D	100	HIS
1	D	109	GLN
1	D	151	GLN
1	D	164	GLN
1	D	213	GLN
1	D	248	GLN
2	E	4	GLN
2	E	19	GLN
2	E	45	GLN
2	E	157	GLN
2	E	229	ASN
1	G	34	ASN
1	G	44	ASN
1	G	73	GLN
1	G	100	HIS
1	G	109	GLN
1	G	151	GLN
1	G	164	GLN
1	G	213	GLN
1	G	240	GLN
1	G	248	GLN
2	H	4	GLN
2	H	19	GLN
2	H	45	GLN
2	H	157	GLN
2	H	229	ASN
1	J	34	ASN
1	J	44	ASN
1	J	73	GLN
1	J	100	HIS
1	J	109	GLN
1	J	151	GLN
1	J	164	GLN
1	J	213	GLN
1	J	240	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	248	GLN
2	K	4	GLN
2	K	19	GLN
2	K	45	GLN
2	K	157	GLN
2	K	229	ASN
1	M	44	ASN
1	M	73	GLN
1	M	100	HIS
1	M	109	GLN
1	M	151	GLN
1	M	164	GLN
1	M	213	GLN
1	M	240	GLN
1	M	248	GLN
2	N	4	GLN
2	N	19	GLN
2	N	45	GLN
2	N	126	HIS
2	N	157	GLN
2	N	229	ASN
1	P	34	ASN
1	P	44	ASN
1	P	73	GLN
1	P	100	HIS
1	P	109	GLN
1	P	151	GLN
1	P	164	GLN
1	P	213	GLN
1	P	240	GLN
1	P	248	GLN
2	Q	4	GLN
2	Q	19	GLN
2	Q	45	GLN
2	Q	157	GLN
2	Q	229	ASN
1	S	34	ASN
1	S	44	ASN
1	S	73	GLN
1	S	100	HIS
1	S	109	GLN
1	S	151	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	S	164	GLN
1	S	213	GLN
1	S	240	GLN
1	S	248	GLN
2	T	4	GLN
2	T	19	GLN
2	T	45	GLN
2	T	157	GLN
2	T	229	ASN
1	V	44	ASN
1	V	73	GLN
1	V	100	HIS
1	V	109	GLN
1	V	151	GLN
1	V	164	GLN
1	V	213	GLN
1	V	240	GLN
1	V	248	GLN
2	W	4	GLN
2	W	19	GLN
2	W	45	GLN
2	W	126	HIS
2	W	157	GLN
2	W	229	ASN
1	Y	34	ASN
1	Y	44	ASN
1	Y	73	GLN
1	Y	100	HIS
1	Y	109	GLN
1	Y	151	GLN
1	Y	164	GLN
1	Y	213	GLN
1	Y	240	GLN
1	Y	248	GLN
2	Z	4	GLN
2	Z	19	GLN
2	Z	45	GLN
2	Z	157	GLN
2	Z	229	ASN
1	1	34	ASN
1	1	44	ASN
1	1	73	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	100	HIS
1	1	109	GLN
1	1	151	GLN
1	1	164	GLN
1	1	213	GLN
1	1	248	GLN
2	2	4	GLN
2	2	19	GLN
2	2	45	GLN
2	2	157	GLN
2	2	229	ASN
1	4	34	ASN
1	4	44	ASN
1	4	73	GLN
1	4	100	HIS
1	4	109	GLN
1	4	151	GLN
1	4	164	GLN
1	4	213	GLN
1	4	248	GLN
2	5	4	GLN
2	5	19	GLN
2	5	45	GLN
2	5	157	GLN
2	5	229	ASN
1	7	44	ASN
1	7	73	GLN
1	7	100	HIS
1	7	109	GLN
1	7	151	GLN
1	7	164	GLN
1	7	213	GLN
1	7	240	GLN
1	7	248	GLN
2	8	4	GLN
2	8	19	GLN
2	8	45	GLN
2	8	157	GLN
2	8	229	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	269/286 (94%)	0.71	26 (9%)	10 10	23, 48, 94, 120	0
1	4	269/286 (94%)	0.62	25 (9%)	11 11	28, 47, 89, 116	0
1	7	269/286 (94%)	0.54	14 (5%)	31 33	20, 40, 88, 116	0
1	A	269/286 (94%)	0.67	26 (9%)	10 10	20, 48, 94, 119	0
1	D	269/286 (94%)	0.56	16 (5%)	26 27	23, 44, 89, 116	0
1	G	269/286 (94%)	0.56	17 (6%)	23 24	22, 42, 88, 116	0
1	J	269/286 (94%)	0.53	19 (7%)	19 20	24, 44, 87, 115	0
1	M	269/286 (94%)	0.61	20 (7%)	17 18	22, 42, 88, 116	0
1	P	269/286 (94%)	0.69	31 (11%)	6 7	22, 47, 92, 118	0
1	S	269/286 (94%)	0.60	18 (6%)	21 22	27, 46, 89, 116	0
1	V	269/286 (94%)	0.57	17 (6%)	23 24	19, 40, 87, 116	0
1	Y	269/286 (94%)	0.70	32 (11%)	6 6	26, 49, 91, 118	0
2	2	238/277 (85%)	0.59	24 (10%)	9 10	25, 46, 77, 117	0
2	5	237/277 (85%)	0.35	11 (4%)	36 38	28, 42, 69, 114	0
2	8	239/277 (86%)	0.37	10 (4%)	40 41	21, 34, 68, 116	0
2	B	238/277 (85%)	0.52	25 (10%)	8 9	24, 42, 74, 116	0
2	E	238/277 (85%)	0.38	13 (5%)	29 30	26, 40, 70, 113	0
2	H	239/277 (86%)	0.41	11 (4%)	36 38	23, 36, 69, 116	0
2	K	238/277 (85%)	0.29	9 (3%)	44 45	24, 39, 71, 113	0
2	N	239/277 (86%)	0.41	11 (4%)	36 38	23, 36, 68, 116	0
2	Q	238/277 (85%)	0.49	21 (8%)	12 13	23, 44, 74, 117	0
2	T	237/277 (85%)	0.35	11 (4%)	36 38	29, 42, 68, 113	0
2	W	239/277 (86%)	0.33	8 (3%)	50 51	20, 34, 67, 116	0
2	Z	239/277 (86%)	0.61	20 (8%)	14 14	26, 47, 75, 148	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	0	29/29 (100%)	1.78	8 (27%) 1 1	44, 72, 107, 129	0
3	3	29/29 (100%)	1.76	10 (34%) 0 1	42, 71, 107, 129	0
3	6	29/29 (100%)	1.65	11 (37%) 0 1	40, 67, 107, 129	0
3	9	29/29 (100%)	1.29	7 (24%) 1 1	35, 66, 104, 127	0
3	C	29/29 (100%)	1.54	10 (34%) 0 1	39, 68, 106, 128	0
3	F	29/29 (100%)	1.37	9 (31%) 1 1	40, 69, 106, 129	0
3	I	29/29 (100%)	1.57	7 (24%) 1 1	38, 68, 107, 127	0
3	L	29/29 (100%)	1.41	7 (24%) 1 1	38, 66, 106, 128	0
3	O	29/29 (100%)	1.59	8 (27%) 1 1	39, 66, 106, 128	0
3	R	29/29 (100%)	1.59	7 (24%) 1 1	38, 70, 106, 129	0
3	U	29/29 (100%)	1.40	8 (27%) 1 1	39, 68, 107, 128	0
3	X	29/29 (100%)	1.56	6 (20%) 1 1	35, 66, 104, 128	0
All	All	6435/7104 (90%)	0.58	533 (8%) 14 15	19, 44, 89, 148	0

All (533) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	3	ASP	9.5
1	1	150	GLY	9.3
1	1	148	ILE	9.2
1	D	150	GLY	9.2
1	P	148	ILE	8.3
3	0	483	SER	8.3
3	X	483	SER	7.9
3	X	475	VAL	7.8
1	A	150	GLY	7.7
1	A	148	ILE	7.6
3	O	475	VAL	7.2
1	4	150	GLY	7.1
1	Y	148	ILE	7.0
1	P	150	GLY	6.9
3	I	475	VAL	6.7
2	2	182	THR	6.4
3	R	475	VAL	6.3
3	L	475	VAL	6.1
3	U	483	SER	6.1
3	0	475	VAL	6.0
1	Y	150	GLY	6.0

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	S	150	GLY	6.0
3	6	475	VAL	5.9
2	5	182	THR	5.8
3	3	483	SER	5.8
2	Z	182	THR	5.8
2	E	182	THR	5.7
1	J	150	GLY	5.7
2	T	182	THR	5.7
1	M	148	ILE	5.6
1	P	69	GLY	5.6
2	2	92	ARG	5.6
1	M	116	ALA	5.5
3	C	483	SER	5.5
2	B	182	THR	5.5
1	7	148	ILE	5.5
1	V	116	ALA	5.4
1	Y	69	GLY	5.4
3	3	479	ASP	5.3
3	9	475	VAL	5.3
3	6	483	SER	5.2
3	9	483	SER	5.1
2	Q	182	THR	5.1
1	1	149	ASP	5.0
1	V	148	ILE	5.0
3	O	483	SER	4.9
3	F	483	SER	4.9
3	L	483	SER	4.9
1	7	116	ALA	4.9
2	W	182	THR	4.9
3	I	483	SER	4.9
2	8	182	THR	4.9
2	Q	163	ARG	4.8
3	3	498	GLY	4.8
1	J	84	ASN	4.8
3	R	483	SER	4.8
2	W	244	ARG	4.8
2	Z	2	SER	4.7
1	A	222	VAL	4.6
3	R	498	GLY	4.6
1	Y	222	VAL	4.5
3	U	475	VAL	4.5
3	C	498	GLY	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	Z	244	ARG	4.5
3	F	475	VAL	4.5
1	7	113	THR	4.4
1	M	113	THR	4.4
2	H	182	THR	4.4
1	Y	149	ASP	4.3
2	N	182	THR	4.3
1	G	222	VAL	4.3
3	I	484	GLU	4.3
1	A	149	ASP	4.3
2	K	182	THR	4.2
3	6	479	ASP	4.2
1	P	222	VAL	4.2
1	G	148	ILE	4.2
2	Z	163	ARG	4.2
1	A	69	GLY	4.1
1	P	151	GLN	4.1
1	P	149	ASP	4.1
3	3	495	LYS	4.1
3	0	479	ASP	4.0
2	N	244	ARG	4.0
1	V	74	VAL	4.0
1	M	150	GLY	4.0
2	B	92	ARG	4.0
1	4	148	ILE	4.0
1	D	69	GLY	4.0
2	B	244	ARG	3.9
1	1	151	GLN	3.9
3	F	479	ASP	3.9
1	M	74	VAL	3.9
2	2	163	ARG	3.9
1	1	222	VAL	3.8
2	H	244	ARG	3.8
1	D	185	THR	3.8
3	3	475	VAL	3.8
1	4	84	ASN	3.8
2	2	93	LEU	3.7
1	G	150	GLY	3.7
1	P	84	ASN	3.7
1	V	222	VAL	3.7
3	L	479	ASP	3.7
1	7	222	VAL	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	82	LEU	3.7
2	B	93	LEU	3.7
1	J	148	ILE	3.6
1	1	183	PRO	3.6
2	2	55	VAL	3.6
3	3	497	PRO	3.6
3	6	498	GLY	3.6
2	T	244	ARG	3.6
1	S	69	GLY	3.6
1	7	74	VAL	3.6
1	D	148	ILE	3.6
2	B	163	ARG	3.5
1	1	223	GLN	3.5
3	C	479	ASP	3.5
2	N	183	GLY	3.5
3	0	498	GLY	3.5
1	S	84	ASN	3.5
1	Y	84	ASN	3.5
1	V	113	THR	3.5
2	H	206	SER	3.5
3	R	479	ASP	3.5
1	M	222	VAL	3.5
2	K	125	ASP	3.5
1	G	116	ALA	3.5
3	C	481	ALA	3.5
1	P	181	ILE	3.4
2	Q	92	ARG	3.4
2	8	244	ARG	3.4
2	E	125	ASP	3.4
2	H	2	SER	3.4
1	G	74	VAL	3.4
2	Q	55	VAL	3.4
2	B	206	SER	3.4
1	4	183	PRO	3.4
3	C	497	PRO	3.4
1	S	148	ILE	3.4
1	Y	220	SER	3.4
2	E	126	HIS	3.4
2	Z	93	LEU	3.4
2	2	244	ARG	3.4
1	D	183	PRO	3.4
2	Z	213	ILE	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	4	185	THR	3.4
2	Q	244	ARG	3.3
2	2	126	HIS	3.3
1	S	274	ILE	3.3
1	1	213	GLN	3.3
2	N	213	ILE	3.3
2	N	2	SER	3.3
1	A	104	GLU	3.3
1	M	149	ASP	3.3
1	A	84	ASN	3.3
2	2	3	ASP	3.3
2	5	126	HIS	3.3
1	Y	116	ALA	3.2
3	U	479	ASP	3.2
1	7	220	SER	3.2
1	S	185	THR	3.2
2	Z	202	THR	3.2
2	Q	93	LEU	3.2
1	1	110	PRO	3.2
3	0	495	LYS	3.2
1	1	69	GLY	3.2
1	Y	275	LEU	3.2
2	2	83	LEU	3.2
1	S	222	VAL	3.1
1	A	223	GLN	3.1
2	5	125	ASP	3.1
2	Z	206	SER	3.1
1	Y	109	GLN	3.1
1	7	149	ASP	3.1
3	O	479	ASP	3.1
3	6	481	ALA	3.1
1	V	119	GLN	3.1
2	W	2	SER	3.1
1	A	85	GLY	3.1
1	J	69	GLY	3.1
2	H	213	ILE	3.0
3	O	481	ALA	3.0
1	7	150	GLY	3.0
1	P	83	GLY	3.0
2	W	84	GLU	3.0
1	G	113	THR	3.0
1	A	183	PRO	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	I	497	PRO	3.0
2	N	28	LEU	3.0
2	2	84	GLU	3.0
3	F	484	GLU	3.0
1	P	110	PRO	3.0
3	U	498	GLY	3.0
1	A	82	LEU	3.0
1	Y	82	LEU	3.0
1	V	276	SER	3.0
2	8	2	SER	3.0
2	B	126	HIS	3.0
1	D	184	PRO	2.9
2	8	84	GLU	2.9
2	K	4	GLN	2.9
2	T	4	GLN	2.9
2	K	126	HIS	2.9
2	H	92	ARG	2.9
1	4	8	VAL	2.9
1	P	116	ALA	2.9
1	1	84	ASN	2.9
2	K	213	ILE	2.9
1	V	150	GLY	2.9
2	K	244	ARG	2.9
3	3	484	GLU	2.8
1	P	147	SER	2.8
2	B	90	SER	2.8
1	4	184	PRO	2.8
1	A	94	ILE	2.8
1	4	149	ASP	2.8
2	T	126	HIS	2.8
3	0	497	PRO	2.8
1	A	181	ILE	2.8
2	2	183	GLY	2.8
2	2	85	ASP	2.8
1	Y	151	GLN	2.8
1	4	117	LEU	2.8
2	2	213	ILE	2.8
2	E	3	ASP	2.8
1	Y	213	GLN	2.8
2	Q	126	HIS	2.7
2	5	244	ARG	2.7
2	8	125	ASP	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Y	274	ILE	2.7
2	8	213	ILE	2.7
1	Y	223	GLN	2.7
1	P	183	PRO	2.7
1	A	220	SER	2.7
2	E	244	ARG	2.7
2	E	213	ILE	2.7
2	T	213	ILE	2.7
1	V	220	SER	2.7
2	Z	4	GLN	2.7
1	A	115	SER	2.7
1	G	220	SER	2.7
2	5	213	ILE	2.7
3	F	482	SER	2.7
1	P	113	THR	2.7
2	Q	78	LYS	2.7
1	P	223	GLN	2.7
2	2	91	ALA	2.7
3	F	481	ALA	2.7
2	K	163	ARG	2.7
2	Q	213	ILE	2.6
3	U	485	ASN	2.6
1	4	151	GLN	2.6
1	P	115	SER	2.6
2	E	206	SER	2.6
1	A	83	GLY	2.6
2	B	183	GLY	2.6
2	E	183	GLY	2.6
3	6	485	ASN	2.6
2	Q	164	THR	2.6
2	2	203	VAL	2.6
3	6	482	SER	2.6
2	Z	92	ARG	2.6
1	4	69	GLY	2.6
2	H	183	GLY	2.6
1	1	82	LEU	2.6
2	B	213	ILE	2.6
1	M	112	ASP	2.6
1	P	112	ASP	2.6
2	Q	3	ASP	2.6
2	Z	205	ASP	2.6
3	F	498	GLY	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	185	THR	2.6
2	Q	181	LYS	2.6
3	C	482	SER	2.6
3	6	497	PRO	2.6
2	2	78	LYS	2.6
1	J	151	GLN	2.6
1	1	220	SER	2.6
2	Q	206	SER	2.6
3	F	485	ASN	2.5
3	6	484	GLU	2.5
1	G	149	ASP	2.5
1	1	109	GLN	2.5
2	Z	55	VAL	2.5
2	Q	125	ASP	2.5
3	L	495	LYS	2.5
3	R	495	LYS	2.5
2	T	92	ARG	2.5
3	R	497	PRO	2.5
1	S	51	ALA	2.5
1	D	117	LEU	2.5
1	P	275	LEU	2.5
1	7	88	LEU	2.5
2	H	28	LEU	2.5
2	T	125	ASP	2.5
3	9	484	GLU	2.5
1	P	220	SER	2.5
1	1	181	ILE	2.5
2	2	164	THR	2.5
1	J	183	PRO	2.5
1	V	149	ASP	2.5
1	7	117	LEU	2.5
1	4	224	THR	2.5
2	E	164	THR	2.5
1	G	76	ILE	2.5
2	E	92	ARG	2.5
1	G	276	SER	2.5
1	S	117	LEU	2.5
2	H	84	GLU	2.5
3	O	484	GLU	2.5
1	M	142	THR	2.5
1	P	85	GLY	2.5
2	E	4	GLN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	112	ASP	2.5
2	8	3	ASP	2.5
1	S	218	VAL	2.5
3	C	475	VAL	2.5
2	W	213	ILE	2.5
1	Y	104	GLU	2.5
1	M	273	LYS	2.5
2	T	183	GLY	2.5
3	6	501	LEU	2.5
1	A	218	VAL	2.4
2	N	84	GLU	2.4
2	Q	203	VAL	2.4
2	N	206	SER	2.4
1	M	119	GLN	2.4
1	V	76	ILE	2.4
1	Y	119	GLN	2.4
1	Y	225	ALA	2.4
3	I	481	ALA	2.4
1	Y	83	GLY	2.4
2	N	92	ARG	2.4
2	B	78	LYS	2.4
1	A	151	GLN	2.4
2	B	203	VAL	2.4
1	G	112	ASP	2.4
1	S	181	ILE	2.4
2	K	92	ARG	2.4
3	L	484	GLU	2.4
3	O	480	ILE	2.4
1	A	213	GLN	2.4
3	L	482	SER	2.4
3	R	487	LEU	2.4
2	B	3	ASP	2.4
2	E	242	GLY	2.4
2	Q	54	VAL	2.4
3	O	485	ASN	2.4
1	4	181	ILE	2.4
1	J	224	THR	2.4
2	W	183	GLY	2.4
1	P	180	THR	2.4
2	Q	85	ASP	2.4
3	X	479	ASP	2.4
1	M	154	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	4	152	GLN	2.4
2	Z	164	THR	2.4
1	D	84	ASN	2.3
1	1	83	GLY	2.3
2	N	125	ASP	2.3
2	8	28	LEU	2.3
1	G	142	THR	2.3
2	5	183	GLY	2.3
3	9	498	GLY	2.3
1	4	16	ILE	2.3
2	B	125	ASP	2.3
2	5	4	GLN	2.3
1	Y	93	LYS	2.3
1	7	142	THR	2.3
3	6	495	LYS	2.3
1	4	36	VAL	2.3
2	5	55	VAL	2.3
3	I	479	ASP	2.3
2	Z	84	GLU	2.3
3	X	484	GLU	2.3
1	P	94	ILE	2.3
2	W	206	SER	2.3
3	C	495	LYS	2.3
1	G	117	LEU	2.3
1	Y	113	THR	2.3
1	J	149	ASP	2.3
1	1	85	GLY	2.3
2	8	183	GLY	2.3
2	B	168	LYS	2.3
3	3	482	SER	2.3
1	V	154	ILE	2.3
1	V	120	TRP	2.3
3	I	485	ASN	2.3
2	Q	84	GLU	2.3
1	J	98	PHE	2.3
1	J	274	ILE	2.3
1	S	16	ILE	2.3
2	Q	4	GLN	2.3
2	2	202	THR	2.3
3	3	481	ALA	2.3
1	A	70	TYR	2.3
1	1	275	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	83	LEU	2.2
2	Q	83	LEU	2.2
1	D	149	ASP	2.2
1	J	184	PRO	2.2
2	2	206	SER	2.2
1	P	218	VAL	2.2
1	V	185	THR	2.2
1	1	180	THR	2.2
2	B	84	GLU	2.2
3	U	481	ALA	2.2
3	X	481	ALA	2.2
3	9	479	ASP	2.2
1	D	39	LEU	2.2
1	J	88	LEU	2.2
1	1	97	LYS	2.2
3	9	482	SER	2.2
1	P	213	GLN	2.2
1	4	213	GLN	2.2
2	B	127	GLY	2.2
1	Y	180	THR	2.2
1	1	113	THR	2.2
1	A	116	ALA	2.2
3	9	481	ALA	2.2
1	J	152	GLN	2.2
2	2	4	GLN	2.2
1	Y	110	PRO	2.2
3	C	484	GLU	2.2
1	A	275	LEU	2.2
1	D	8	VAL	2.2
1	Y	221	ASP	2.2
1	A	147	SER	2.2
1	Y	94	ILE	2.2
1	Y	183	PRO	2.2
1	1	94	ILE	2.2
1	7	154	ILE	2.2
1	V	273	LYS	2.2
1	G	101	LEU	2.2
1	4	75	LEU	2.2
2	2	125	ASP	2.2
2	2	243	LEU	2.2
1	M	152	GLN	2.2
2	W	4	GLN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	55	VAL	2.2
1	1	116	ALA	2.2
1	7	17	ALA	2.2
2	B	50	ALA	2.2
3	F	497	PRO	2.2
1	D	98	PHE	2.2
1	D	76	ILE	2.2
1	V	75	LEU	2.2
2	B	164	THR	2.2
2	8	92	ARG	2.2
1	G	17	ALA	2.1
3	0	481	ALA	2.1
3	L	497	PRO	2.1
2	T	56	GLY	2.1
1	P	109	GLN	2.1
1	J	96	PHE	2.1
1	Y	181	ILE	2.1
1	Y	97	LYS	2.1
2	B	181	LYS	2.1
1	M	88	LEU	2.1
1	M	111	GLU	2.1
1	M	84	ASN	2.1
2	H	197	MET	2.1
3	3	478	ASP	2.1
1	D	143	VAL	2.1
1	Y	152	GLN	2.1
1	4	218	VAL	2.1
2	E	55	VAL	2.1
2	Z	95	LYS	2.1
1	P	104	GLU	2.1
1	M	21	ILE	2.1
2	5	180	ASN	2.1
1	A	109	GLN	2.1
2	B	4	GLN	2.1
1	4	88	LEU	2.1
1	J	222	VAL	2.1
2	T	55	VAL	2.1
1	S	213	GLN	2.1
1	7	276	SER	2.1
2	H	3	ASP	2.1
2	K	164	THR	2.1
2	5	164	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	274	ILE	2.1
1	S	76	ILE	2.1
3	O	497	PRO	2.1
1	1	93	LYS	2.1
3	U	482	SER	2.1
1	A	113	THR	2.1
1	4	113	THR	2.1
3	0	484	GLU	2.1
2	T	242	GLY	2.1
1	S	98	PHE	2.1
1	G	154	ILE	2.1
1	Y	46	LEU	2.1
1	4	223	GLN	2.1
2	B	91	ALA	2.1
1	Y	115	SER	2.1
3	X	482	SER	2.1
2	Z	183	GLY	2.1
1	S	183	PRO	2.1
1	S	149	ASP	2.1
1	1	104	GLU	2.0
1	J	181	ILE	2.0
1	M	94	ILE	2.0
1	V	243	ILE	2.0
1	4	98	PHE	2.0
2	5	92	ARG	2.0
1	J	120	TRP	2.0
1	P	70	TYR	2.0
1	Y	88	LEU	2.0
2	B	204	SER	2.0
1	J	113	THR	2.0
1	D	104	GLU	2.0
1	G	217	GLN	2.0
1	P	97	LYS	2.0
2	Z	85	ASP	2.0
3	U	497	PRO	2.0
1	1	272	ASN	2.0
1	M	220	SER	2.0
1	4	76	ILE	2.0
1	S	48	GLU	2.0
2	N	12	LEU	2.0
2	2	60	LEU	2.0
2	2	181	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	487	LEU	2.0
1	P	267	THR	2.0
1	P	272	ASN	2.0
1	4	222	VAL	2.0
2	Q	156	VAL	2.0
2	Z	156	VAL	2.0
1	M	276	SER	2.0
2	Z	126	HIS	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.