



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2014 – 05:55 PM BST

PDB ID : 4V5I
Title : STRUCTURE OF THE PHAGE P2 BASEPLATE IN ITS ACTIVATED CONFORMATION WITH CA
Authors : Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; vanHeel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on : 2010-02-05
Resolution : 5.46 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

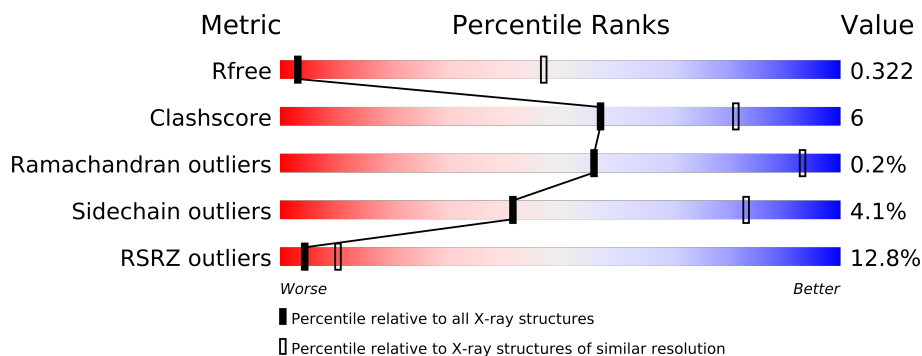
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 5.46 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}	66092	1077 (7.40-3.50)
Clashscore	79885	1008 (7.40-3.52)
Ramachandran outliers	78287	1269 (7.40-3.50)
Sidechain outliers	78261	1246 (7.40-3.50)
RSRZ outliers	66119	1076 (7.40-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A0	372	
1	AY	372	
1	AZ	372	
1	B0	372	
1	BY	372	
1	BZ	372	
2	AA	263	
2	AB	263	
2	AC	263	
2	AD	263	
2	AE	263	
2	AF	263	
2	AG	263	
2	AH	263	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	AI	263	
2	AJ	263	
2	AK	263	
2	AL	263	
2	AM	263	
2	AN	263	
2	AO	263	
2	AP	263	
2	AQ	263	
2	AR	263	
2	BA	263	
2	BB	263	
2	BC	263	
2	BD	263	
2	BE	263	
2	BF	263	
2	BG	263	
2	BH	263	
2	BI	263	
2	BJ	263	
2	BK	263	
2	BL	263	
2	BM	263	
2	BN	263	
2	BO	263	
2	BP	263	
2	BQ	263	
2	BR	263	
3	AS	298	
3	AT	298	
3	AU	298	
3	AV	298	
3	AW	298	
3	AX	298	
3	BS	298	
3	BT	298	
3	BU	298	
3	BV	298	
3	BW	298	
3	BX	298	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 119484 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	B0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AB	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AC	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AD	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AE	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AF	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AG	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AH	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AI	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AJ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AK	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AL	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AM	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AN	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AO	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AP	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AQ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	AR	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BA	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BB	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BC	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BD	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BE	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BF	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BG	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BH	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BI	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BJ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BK	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BL	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BM	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BN	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BO	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BP	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BQ	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	BR	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AT	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AU	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AV	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AW	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	AX	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BS	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BT	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BU	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BV	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BW	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0
3	BX	298	Total 2432	C 1565	N 392	O 469	S 6	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

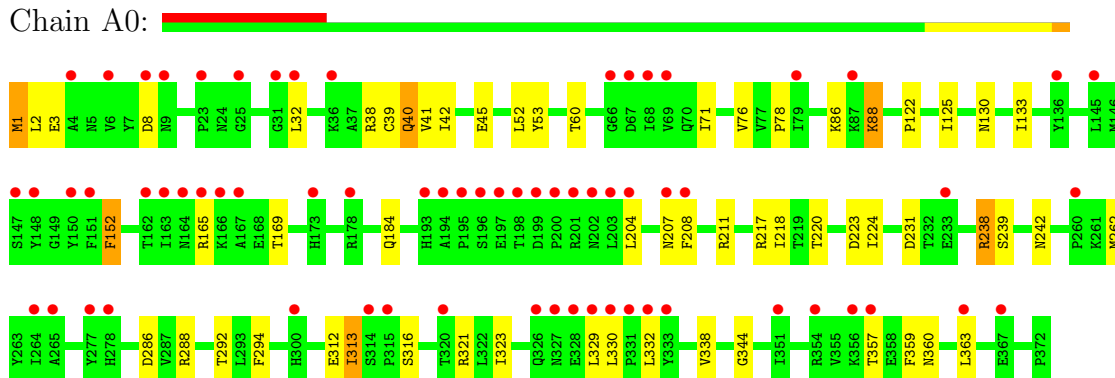
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BU	1	Total	Ca	0	0
			1	1		
4	BT	1	Total	Ca	0	0
			1	1		
4	AV	1	Total	Ca	0	0
			1	1		
4	BV	1	Total	Ca	0	0
			1	1		
4	AW	1	Total	Ca	0	0
			1	1		
4	AT	1	Total	Ca	0	0
			1	1		
4	BS	1	Total	Ca	0	0
			1	1		
4	AU	1	Total	Ca	0	0
			1	1		
4	AX	1	Total	Ca	0	0
			1	1		
4	BW	1	Total	Ca	0	0
			1	1		
4	BX	1	Total	Ca	0	0
			1	1		
4	AS	1	Total	Ca	0	0
			1	1		

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 ($\text{RSRZ} > 2$). 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.

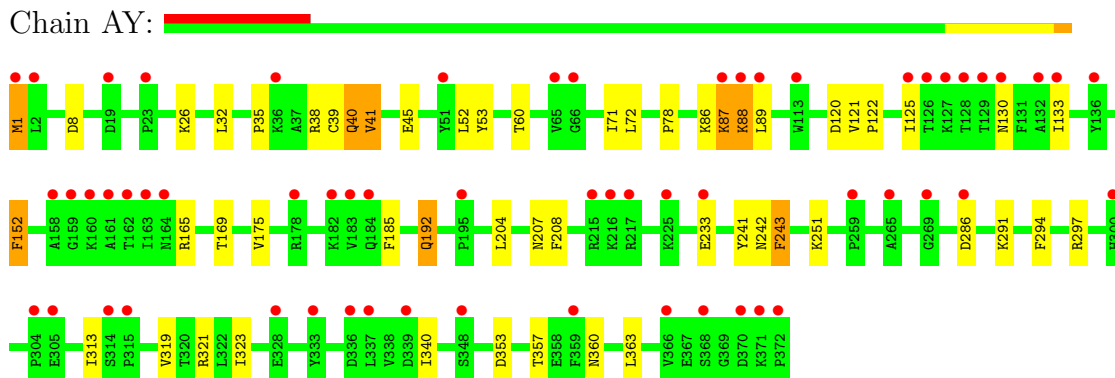
• Molecule 1: ORF16

Chain A0:



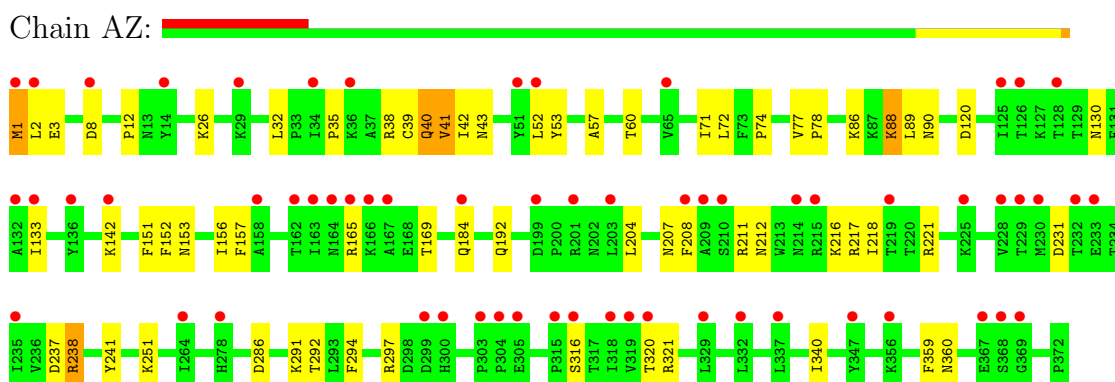
• Molecule 1: ORF16

Chain AY:



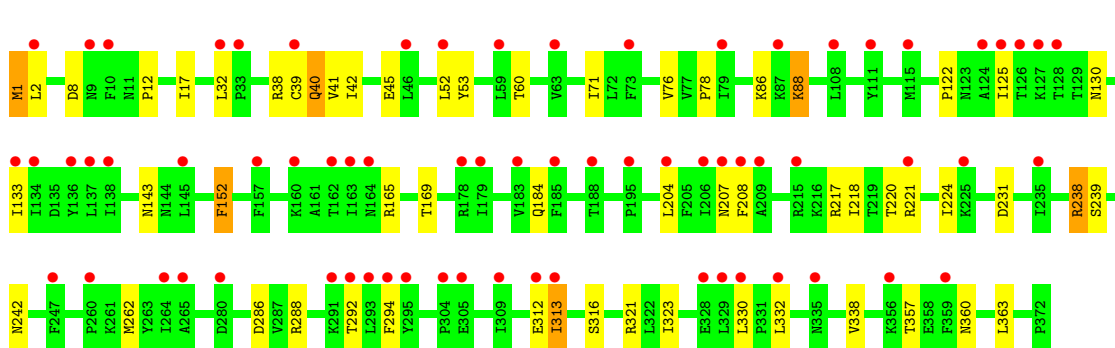
• Molecule 1: ORF16

Chain AZ:



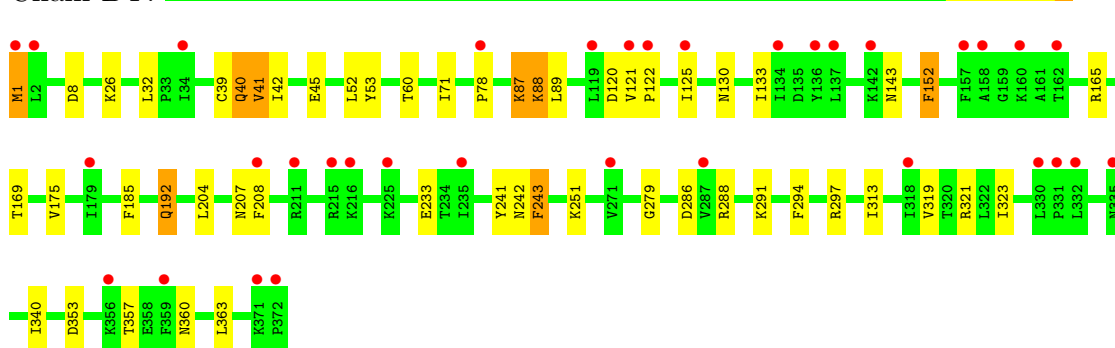
- Molecule 1: ORF16

Chain B0:



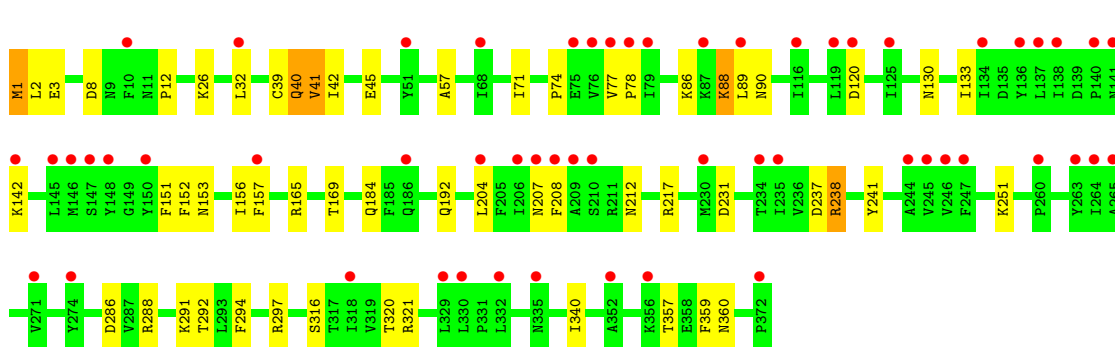
- Molecule 1: ORF16

Chain BY:



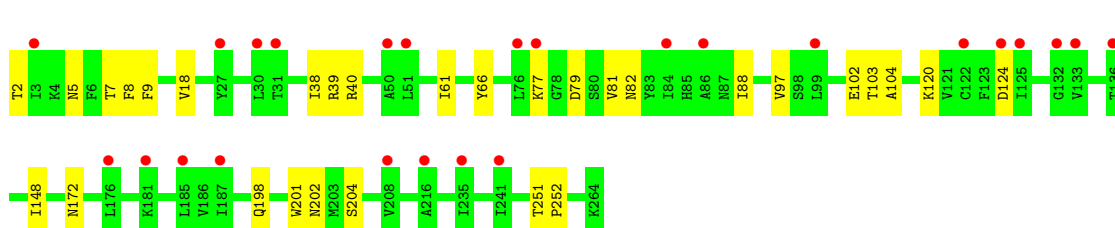
- Molecule 1: ORF16

Chain BZ:



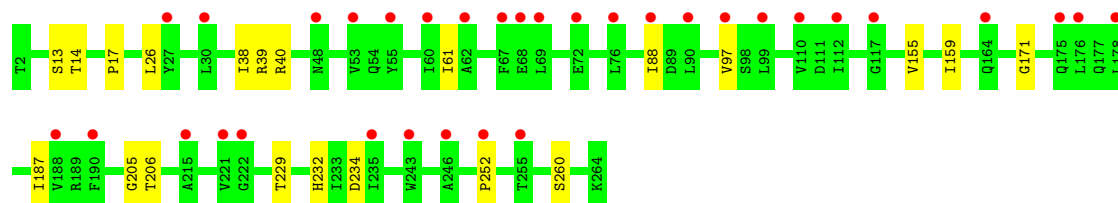
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AA:



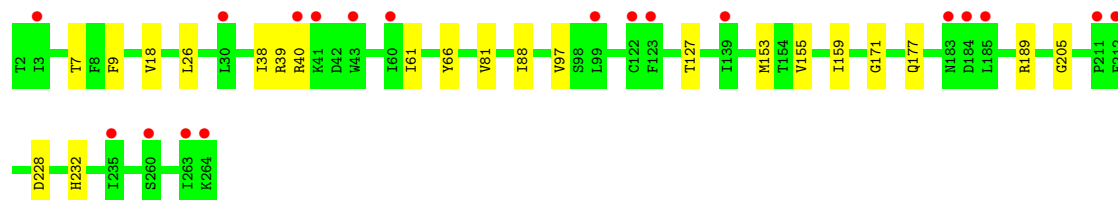
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AB: 



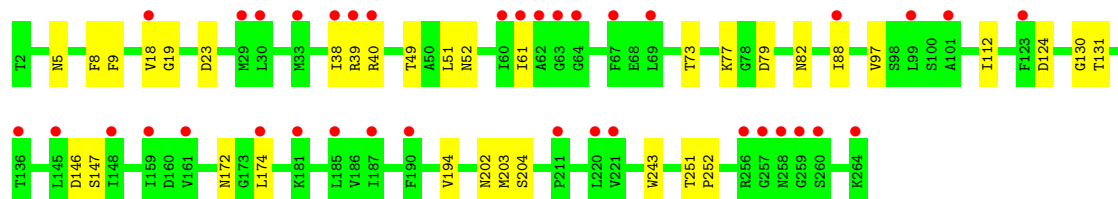
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AC: 



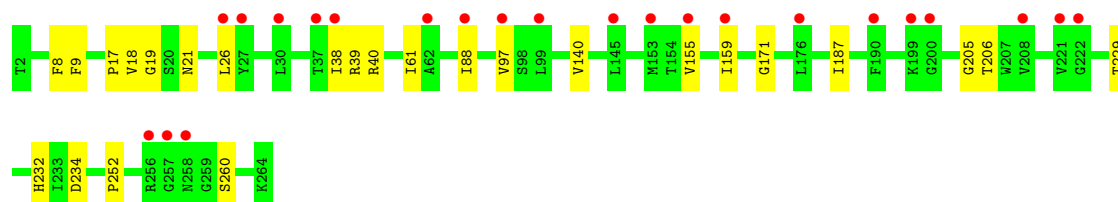
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AD: 



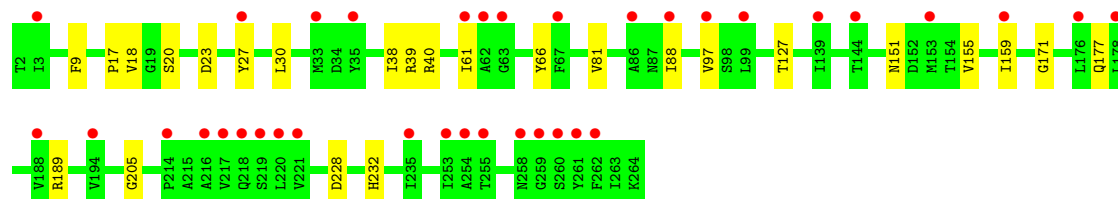
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AE: 



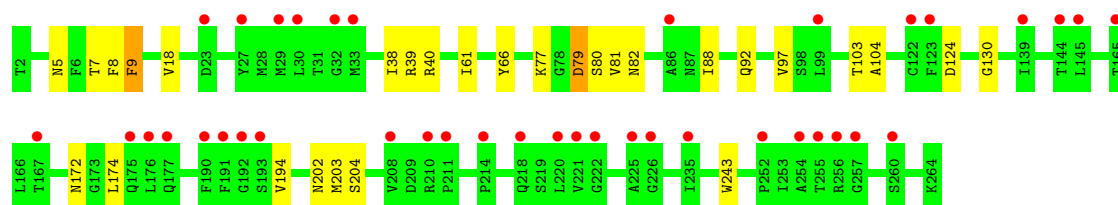
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AF: 



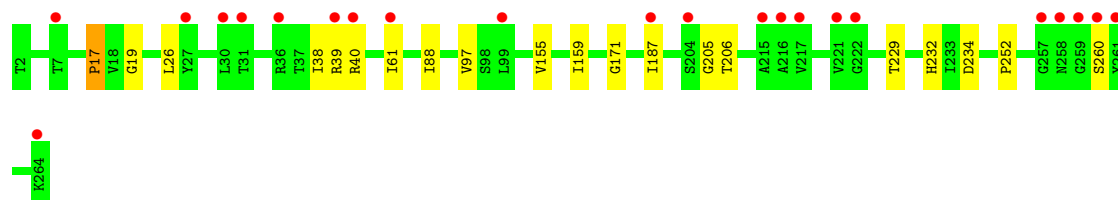
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AG: 



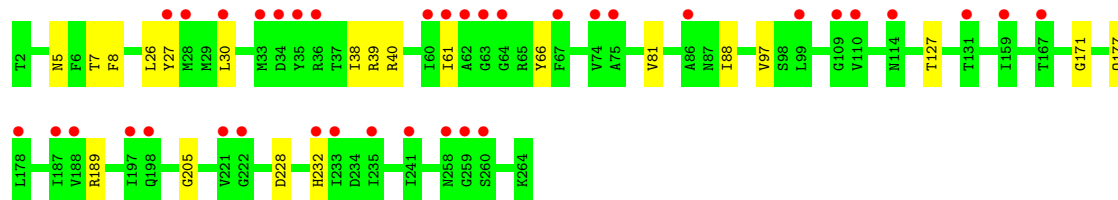
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AH:



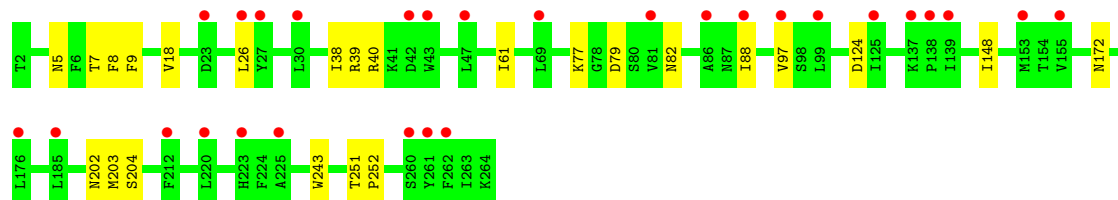
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AI:



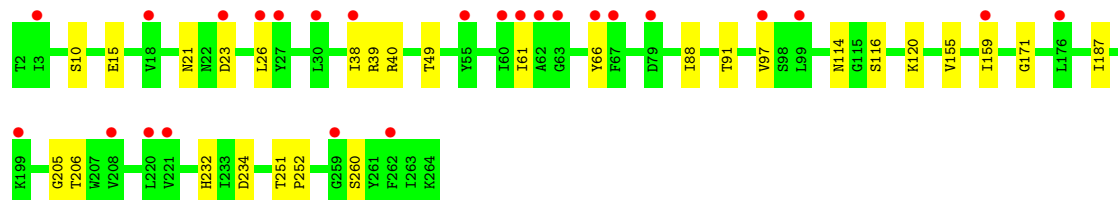
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AJ:



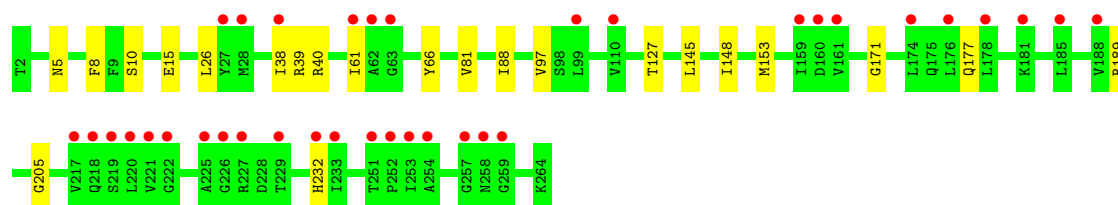
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AK:



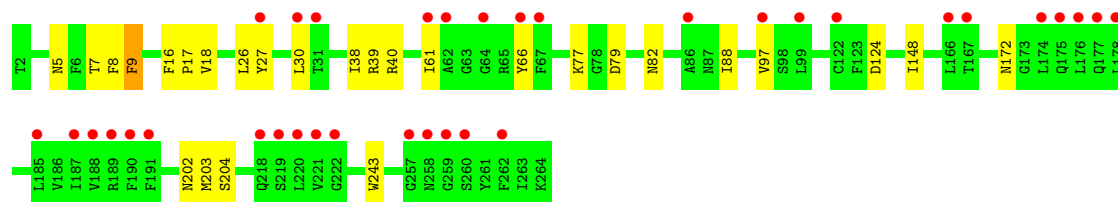
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AL:



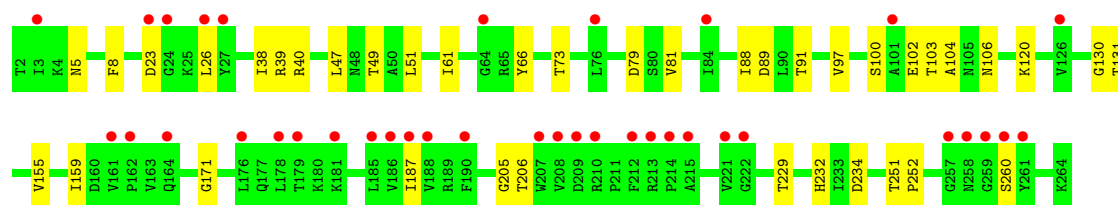
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AM:



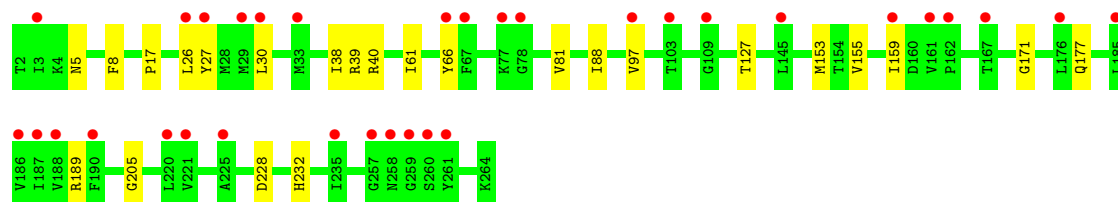
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AN:



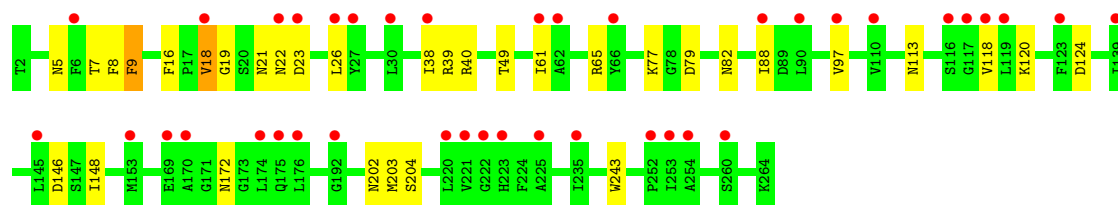
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AO:



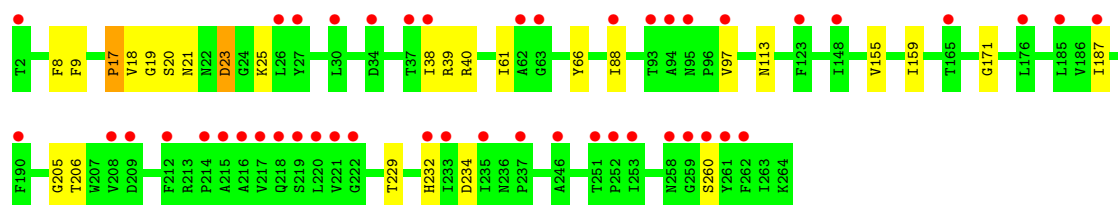
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AP:



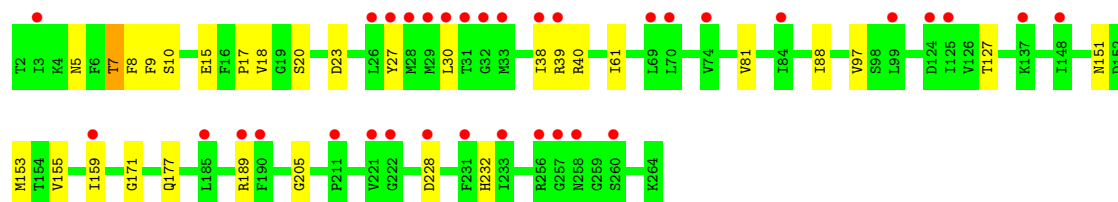
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AQ:



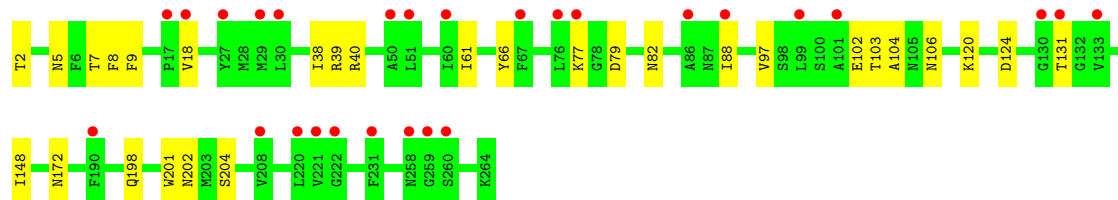
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AR:



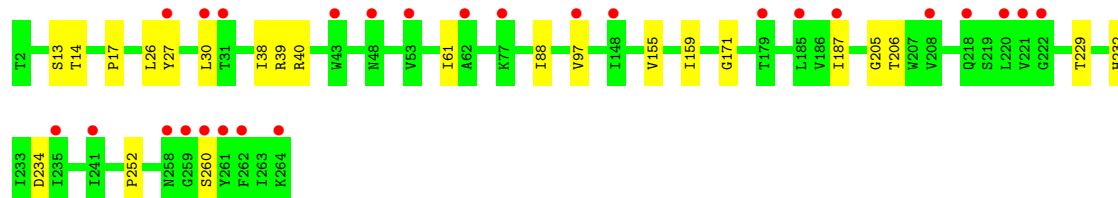
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BA:



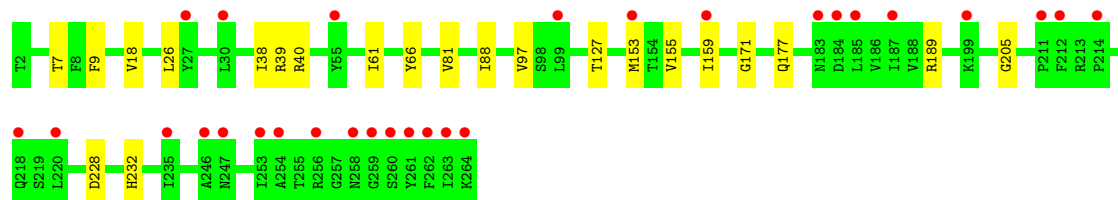
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BB:



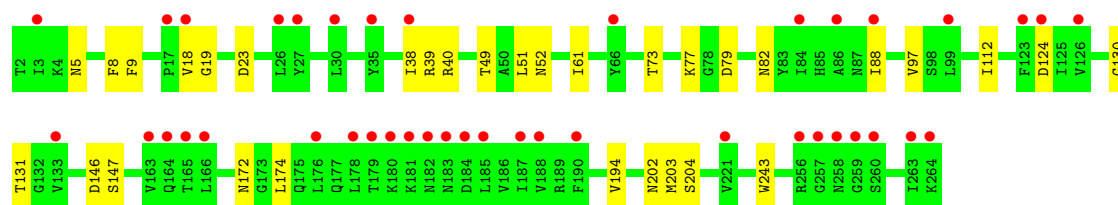
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BC:



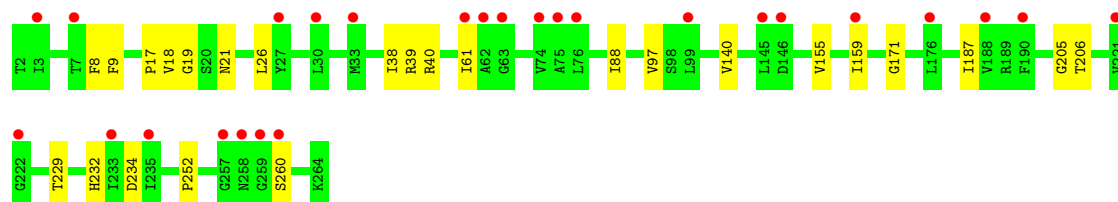
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BD:



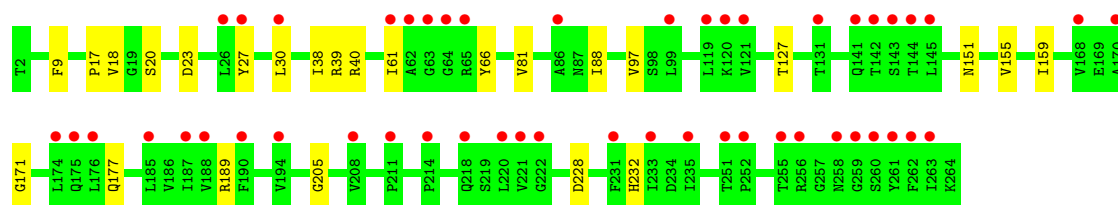
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BE:



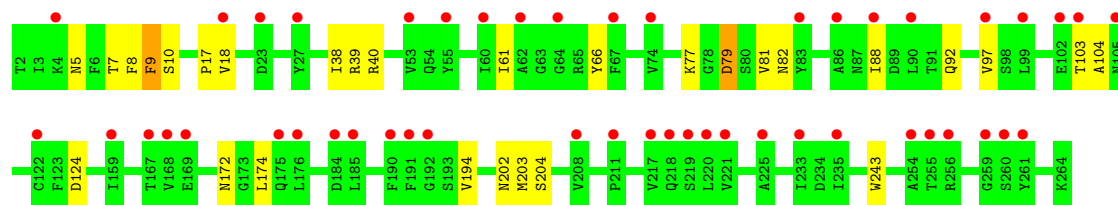
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BF:



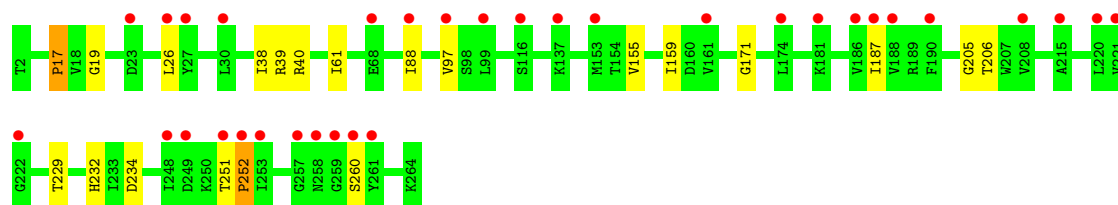
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BG:



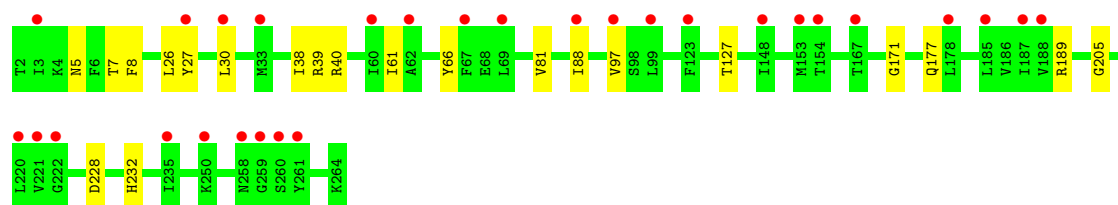
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BH:



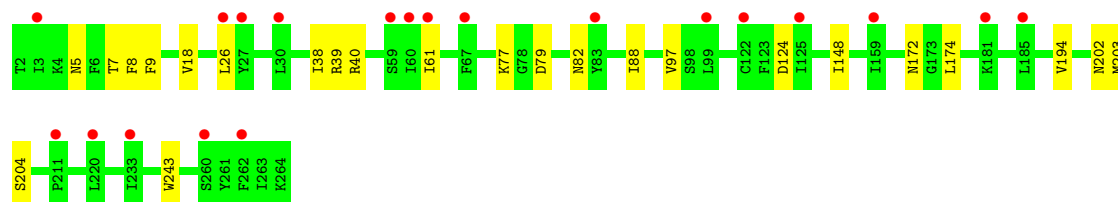
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BI:



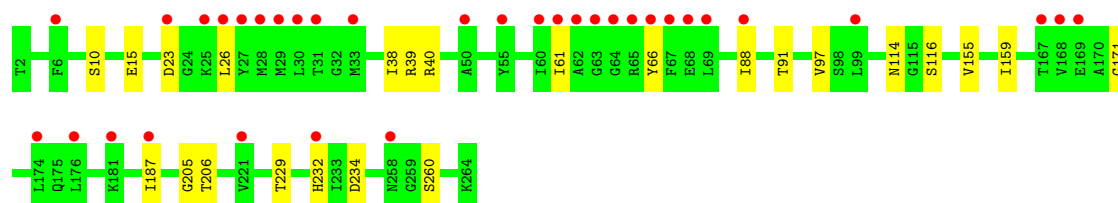
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BJ:



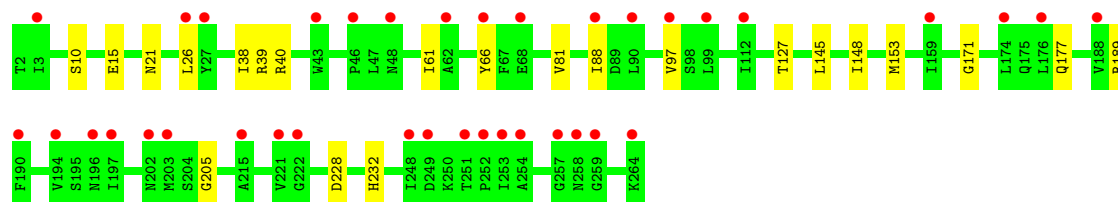
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BK:



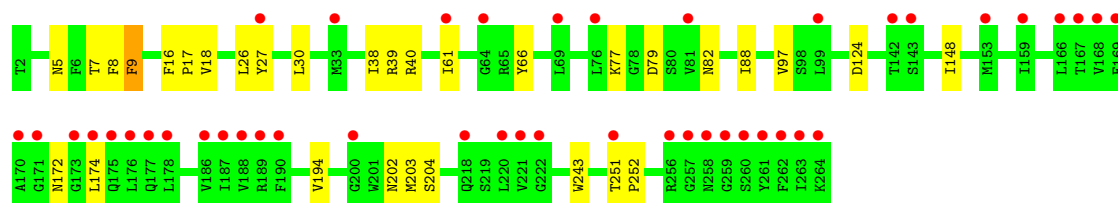
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BL:



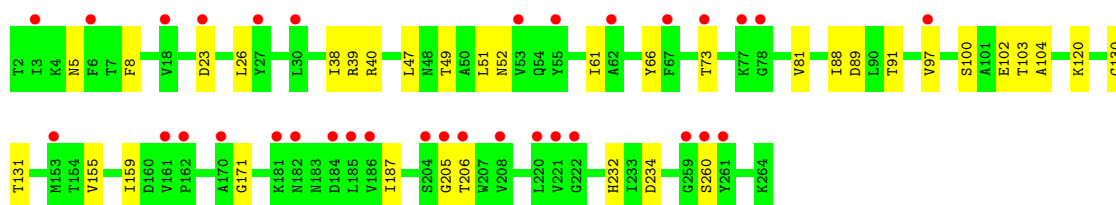
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BM:



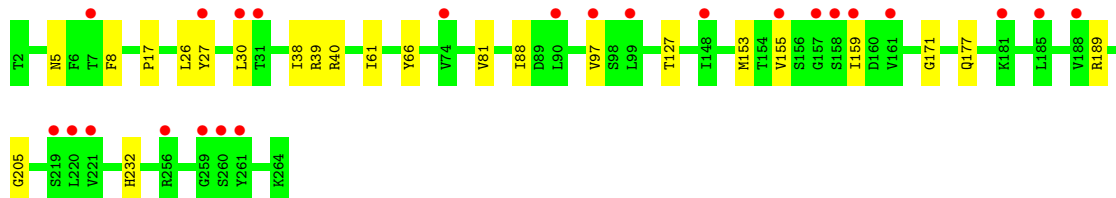
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BN:



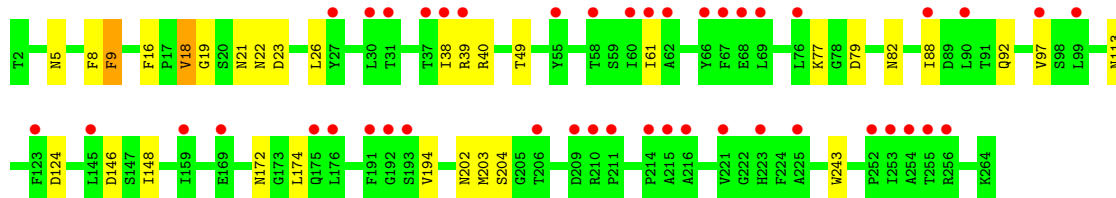
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BO:



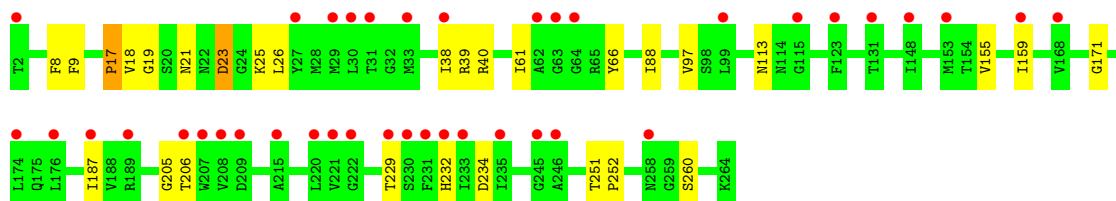
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BP:



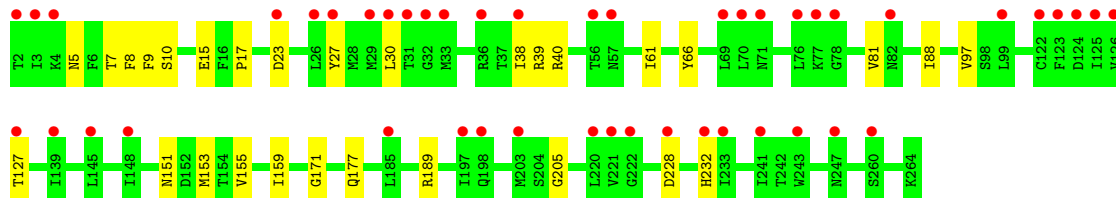
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BQ:



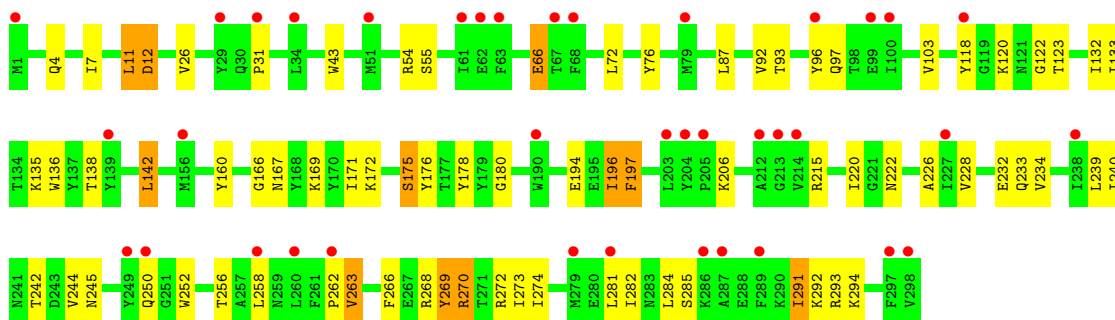
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BR:



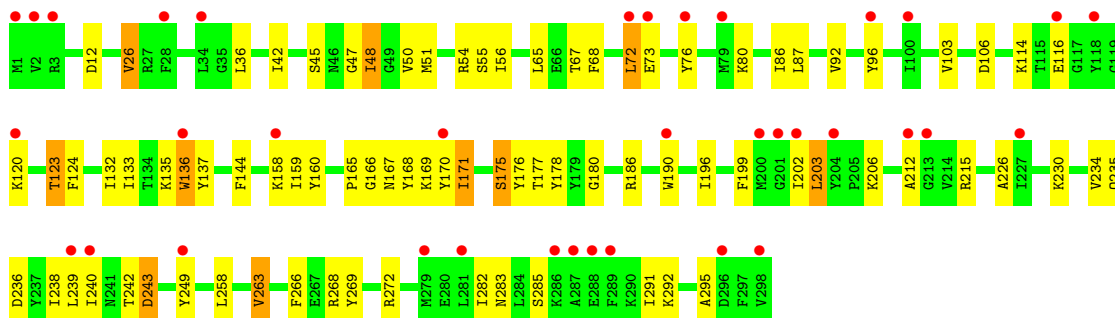
• Molecule 3: ORF15

Chain AS:



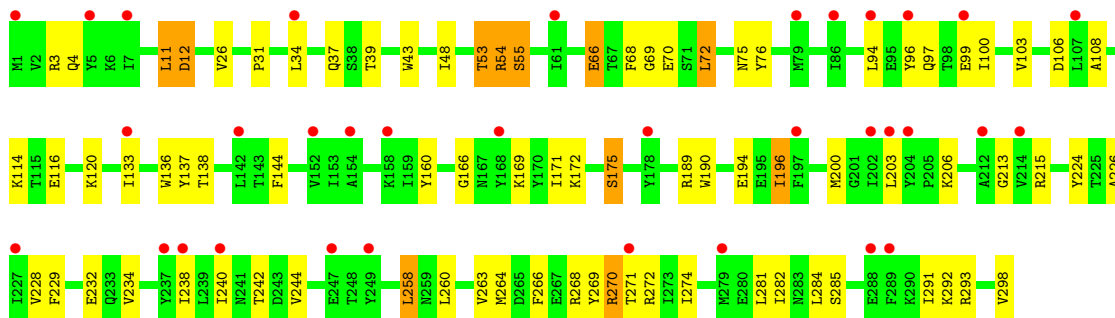
• Molecule 3: ORF15

Chain AT:



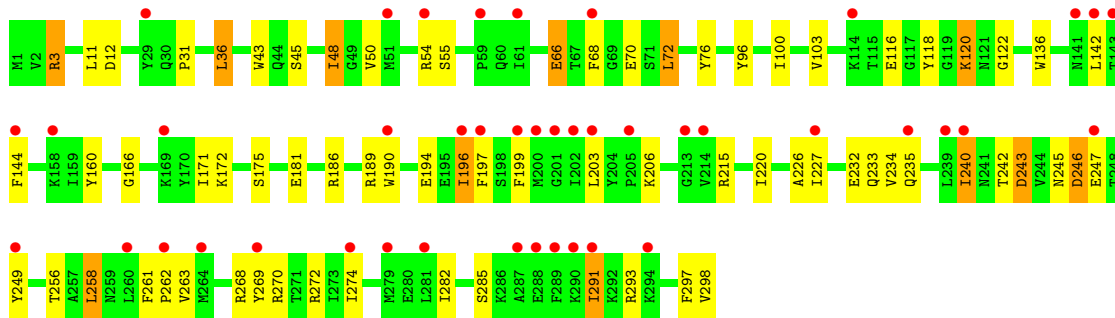
• Molecule 3: ORF15

Chain AU:



• Molecule 3: ORF15

Chain AV:



• Molecule 3: ORF15



Age Group	Very bad	Bad
18-24	10%	10%
25-34	10%	10%
35-44	10%	10%
45-54	10%	10%
55-64	10%	10%
65-74	10%	10%
75+	10%	10%



Age Group	Percentage
18-24	10%
25-34	75%
35-44	10%
45-54	3%
55-64	1%
65-74	1%
75-84	1%
85+	1%

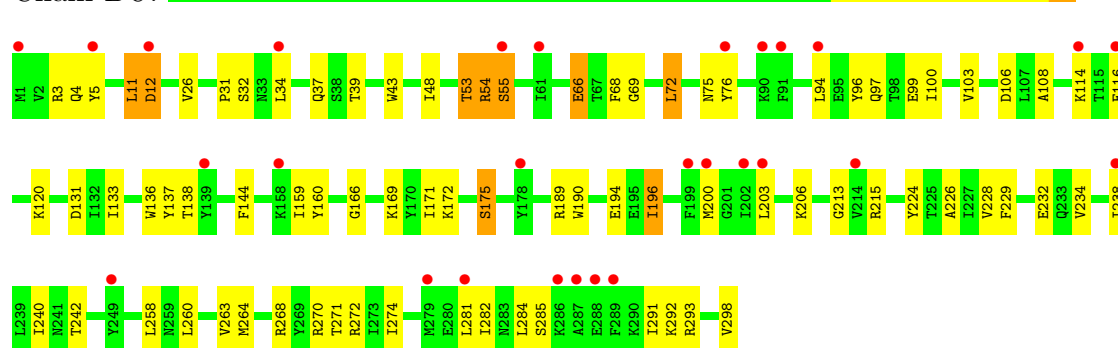


Age Group	Percentage
18-24	10%
25-34	70%
35-44	15%
45-54	3%
55-64	1%
65-74	1%
75-84	1%
85+	1%



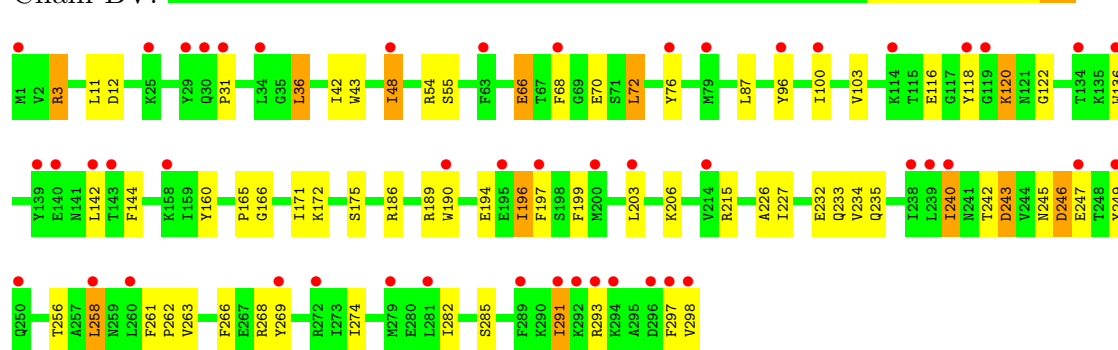
- Molecule 3: ORF15

Chain BU:



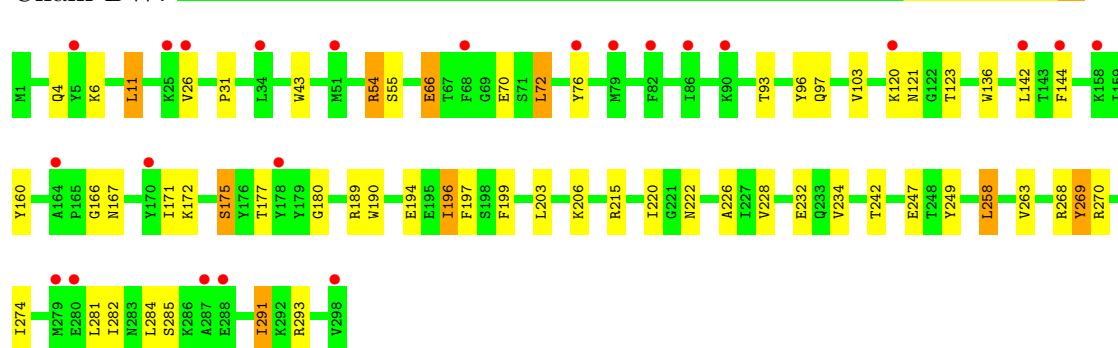
- Molecule 3: ORF15

Chain BV:



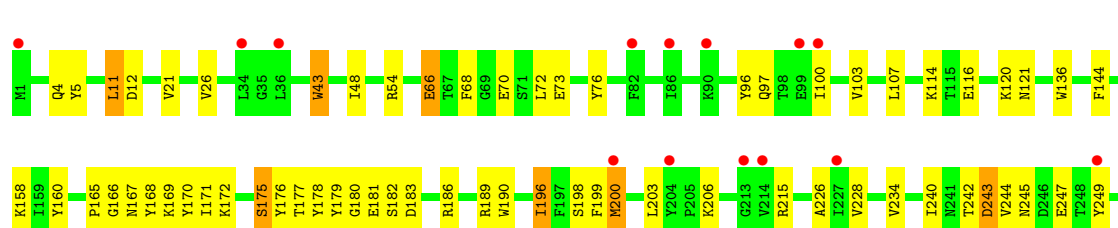
- Molecule 3: ORF15

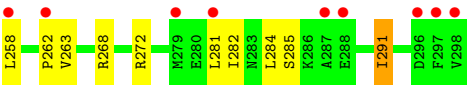
Chain BW:



- Molecule 3: ORF15

Chain BX:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	219.52Å 219.34Å 392.43Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	44.56 – 5.46 44.56 – 5.46	Depositor EDS
% Data completeness (in resolution range)	91.0 (44.56-5.46) 91.0 (44.56-5.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 5.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.291 , 0.297 0.327 , 0.322	Depositor DCC
R_{free} test set	5621 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	205.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 401.9	EDS
Estimated twinning fraction	0.409 for k,h,-l 0.399 for -k,-h,-l 0.408 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	3 of 112350 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	119484	wwPDB-VP
Average B, all atoms (Å ²)	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	A0	0.38	0/3069	0.64	0/4175
1	AY	0.38	0/3069	0.65	0/4175
1	AZ	0.37	0/3069	0.63	0/4175
1	B0	0.38	0/3069	0.64	0/4175
1	BY	0.38	0/3069	0.65	0/4175
1	BZ	0.37	0/3069	0.63	0/4175
2	AA	0.32	0/2048	0.63	0/2791
2	AB	0.36	0/2048	0.58	0/2791
2	AC	0.35	0/2048	0.59	0/2791
2	AD	0.32	0/2048	0.61	0/2791
2	AE	0.36	0/2048	0.58	0/2791
2	AF	0.36	0/2048	0.58	0/2791
2	AG	0.32	0/2048	0.62	0/2791
2	AH	0.37	0/2048	0.58	0/2791
2	AI	0.37	0/2048	0.58	0/2791
2	AJ	0.34	0/2048	0.63	0/2791
2	AK	0.36	0/2048	0.59	0/2791
2	AL	0.36	0/2048	0.58	0/2791
2	AM	0.34	0/2048	0.63	0/2791
2	AN	0.36	0/2048	0.58	0/2791
2	AO	0.36	0/2048	0.58	0/2791
2	AP	0.34	0/2048	0.63	0/2791
2	AQ	0.37	0/2048	0.58	0/2791
2	AR	0.37	0/2048	0.59	0/2791
2	BA	0.32	0/2048	0.63	0/2791
2	BB	0.36	0/2048	0.58	0/2791
2	BC	0.35	0/2048	0.59	0/2791
2	BD	0.32	0/2048	0.61	0/2791
2	BE	0.36	0/2048	0.58	0/2791
2	BF	0.36	0/2048	0.58	0/2791
2	BG	0.32	0/2048	0.62	0/2791
2	BH	0.37	0/2048	0.58	0/2791

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BI	0.37	0/2048	0.58	0/2791
2	BJ	0.34	0/2048	0.63	0/2791
2	BK	0.35	0/2048	0.59	0/2791
2	BL	0.36	0/2048	0.58	0/2791
2	BM	0.34	0/2048	0.63	0/2791
2	BN	0.36	0/2048	0.58	0/2791
2	BO	0.36	0/2048	0.58	0/2791
2	BP	0.34	0/2048	0.63	0/2791
2	BQ	0.37	0/2048	0.58	0/2791
2	BR	0.37	0/2048	0.59	0/2791
3	AS	0.36	0/2485	0.69	0/3356
3	AT	0.36	0/2485	0.69	0/3356
3	AU	0.35	0/2485	0.67	0/3356
3	AV	0.36	0/2485	0.67	0/3356
3	AW	0.35	0/2485	0.66	0/3356
3	AX	0.36	0/2485	0.67	0/3356
3	BS	0.36	0/2485	0.69	0/3356
3	BT	0.36	0/2485	0.69	0/3356
3	BU	0.35	0/2485	0.67	0/3356
3	BV	0.36	0/2485	0.67	0/3356
3	BW	0.35	0/2485	0.66	0/3356
3	BX	0.36	0/2485	0.67	0/3356
All	All	0.36	0/121962	0.62	0/165798

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	3000	0	2956	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AY	3000	0	2956	37	0
1	AZ	3000	0	2956	72	0
1	B0	3000	0	2956	45	0
1	BY	3000	0	2956	36	0
1	BZ	3000	0	2956	53	0
2	AA	2008	0	1971	22	0
2	AB	2008	0	1971	16	0
2	AC	2008	0	1971	15	0
2	AD	2008	0	1971	55	0
2	AE	2008	0	1971	34	0
2	AF	2008	0	1971	20	0
2	AG	2008	0	1971	34	0
2	AH	2008	0	1971	9	0
2	AI	2008	0	1971	10	0
2	AJ	2008	0	1971	11	0
2	AK	2008	0	1971	15	0
2	AL	2008	0	1971	10	0
2	AM	2008	0	1971	15	0
2	AN	2008	0	1971	38	0
2	AO	2008	0	1971	13	0
2	AP	2008	0	1971	35	0
2	AQ	2008	0	1971	42	0
2	AR	2008	0	1971	32	0
2	BA	2008	0	1971	18	0
2	BB	2008	0	1971	17	0
2	BC	2008	0	1971	15	0
2	BD	2008	0	1971	46	0
2	BE	2008	0	1971	35	0
2	BF	2008	0	1971	21	0
2	BG	2008	0	1971	25	0
2	BH	2008	0	1971	11	0
2	BI	2008	0	1971	10	0
2	BJ	2008	0	1971	10	0
2	BK	2008	0	1971	12	0
2	BL	2008	0	1971	11	0
2	BM	2008	0	1971	16	0
2	BN	2008	0	1971	37	0
2	BO	2008	0	1971	12	0
2	BP	2008	0	1971	23	0
2	BQ	2008	0	1971	31	0
2	BR	2008	0	1971	23	0
3	AS	2432	0	2392	115	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AT	2432	0	2392	107	0
3	AU	2432	0	2392	100	0
3	AV	2432	0	2392	98	0
3	AW	2432	0	2392	74	0
3	AX	2432	0	2392	141	0
3	BS	2432	0	2392	96	0
3	BT	2432	0	2392	102	0
3	BU	2432	0	2392	92	0
3	BV	2432	0	2392	95	0
3	BW	2432	0	2392	74	0
3	BX	2432	0	2392	112	0
4	AS	1	0	0	0	0
4	AT	1	0	0	0	0
4	AU	1	0	0	0	0
4	AV	1	0	0	0	0
4	AW	1	0	0	0	0
4	AX	1	0	0	0	0
4	BS	1	0	0	0	0
4	BT	1	0	0	0	0
4	BU	1	0	0	0	0
4	BV	1	0	0	0	0
4	BW	1	0	0	0	0
4	BX	1	0	0	0	0
All	All	119484	0	117396	1505	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (1505) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AW:120:LYS:HD3	3:BV:68:PHE:CE1	1.26	1.65
3:AV:68:PHE:CD1	3:BW:120:LYS:HD3	1.30	1.61
3:AV:68:PHE:CE1	3:BW:120:LYS:HD3	1.28	1.58
3:AU:68:PHE:CE1	3:BX:120:LYS:HD3	1.37	1.54
3:AW:120:LYS:HD3	3:BV:68:PHE:CD1	1.42	1.54
3:AX:120:LYS:HD3	3:BU:68:PHE:CE1	1.40	1.51
2:AD:52:ASN:CG	3:AS:258:LEU:HD22	1.30	1.47
3:AV:68:PHE:CE1	3:BW:120:LYS:CD	2.01	1.43
2:AD:52:ASN:ND2	3:AS:258:LEU:HD22	1.28	1.43
1:A0:42:ILE:HB	3:AX:43:TRP:CZ2	1.51	1.41
3:AW:120:LYS:CD	3:BV:68:PHE:CE1	2.04	1.39
3:AV:68:PHE:CD1	3:BW:120:LYS:CD	2.08	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AG:103:THR:CB	1:AZ:78:PRO:HG3	1.53	1.36
3:AV:120:LYS:HZ2	3:BW:66:GLU:CG	1.42	1.32
1:B0:42:ILE:HB	3:BX:43:TRP:CZ2	1.66	1.30
2:AG:103:THR:HB	1:AZ:78:PRO:CG	1.62	1.30
2:BD:52:ASN:CG	3:BS:258:LEU:HD22	1.51	1.28
3:AV:120:LYS:NZ	3:BW:66:GLU:CG	1.99	1.24
2:AD:73:THR:CB	3:AS:256:THR:HG21	1.68	1.22
2:AD:131:THR:HG22	3:AS:262:PRO:O	1.38	1.21
2:BD:52:ASN:ND2	3:BS:258:LEU:HD22	1.54	1.21
1:A0:42:ILE:CB	3:AX:43:TRP:HZ2	1.55	1.20
2:BD:52:ASN:CG	3:BS:258:LEU:CD2	2.10	1.20
3:AW:66:GLU:CG	3:BV:120:LYS:HZ2	1.54	1.20
3:AW:120:LYS:CD	3:BV:68:PHE:CD1	2.21	1.19
2:BD:130:GLY:O	3:BS:262:PRO:HB3	1.39	1.19
3:AU:68:PHE:CE1	3:BX:120:LYS:CD	2.25	1.19
2:BD:131:THR:HG22	3:BS:262:PRO:O	1.42	1.18
2:AB:13:SER:O	3:AS:169:LYS:HD2	1.44	1.16
2:BD:130:GLY:O	3:BS:262:PRO:CB	1.93	1.15
2:BB:13:SER:O	3:BS:169:LYS:HD2	1.46	1.15
3:AW:66:GLU:CG	3:BV:120:LYS:NZ	2.10	1.15
2:AD:130:GLY:O	3:AS:262:PRO:HB3	1.34	1.15
1:A0:88:LYS:NZ	2:AN:104:ALA:HB3	1.62	1.14
3:AX:120:LYS:CD	3:BU:68:PHE:CE1	2.29	1.12
2:AD:130:GLY:O	3:AS:262:PRO:HB2	1.42	1.12
2:AD:52:ASN:ND2	3:AS:258:LEU:CD2	2.03	1.11
2:BD:73:THR:CB	3:BS:256:THR:HG21	1.81	1.10
2:AQ:18:VAL:HG12	3:AX:168:TYR:O	1.50	1.10
2:AQ:17:PRO:HB3	3:AX:167:ASN:HD22	1.11	1.09
3:AV:68:PHE:CE1	3:BW:120:LYS:CG	2.35	1.08
2:AQ:17:PRO:HB3	3:AX:169:LYS:HE3	1.35	1.08
2:BG:103:THR:CB	1:BZ:78:PRO:HG3	1.83	1.07
2:BN:131:THR:HG22	3:BV:262:PRO:O	1.52	1.07
2:BB:13:SER:C	3:BS:169:LYS:HD2	1.74	1.07
3:AV:120:LYS:NZ	3:BW:66:GLU:HG3	1.69	1.06
3:AW:66:GLU:HG2	3:BV:120:LYS:HZ2	1.09	1.06
2:BB:13:SER:O	3:BS:169:LYS:CD	2.04	1.06
2:BB:13:SER:O	3:BS:169:LYS:CE	2.03	1.06
2:AD:52:ASN:CB	3:AS:258:LEU:HD22	1.86	1.05
2:AB:13:SER:O	3:AS:169:LYS:CD	2.03	1.05
1:A0:86:LYS:NZ	2:AN:81:VAL:HB	1.70	1.05
2:AB:13:SER:O	3:AS:169:LYS:CE	2.05	1.04
2:AQ:18:VAL:O	3:AX:167:ASN:HA	1.57	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B0:42:ILE:CB	3:BX:43:TRP:HZ2	1.71	1.03
2:AB:13:SER:C	3:AS:169:LYS:HD2	1.78	1.03
3:AS:197:PHE:CD1	3:AT:48:ILE:HG22	1.93	1.03
2:AD:52:ASN:CG	3:AS:258:LEU:HD23	1.72	1.02
2:BG:103:THR:HB	1:BZ:78:PRO:HG3	1.03	1.02
2:BN:130:GLY:O	3:BV:262:PRO:HB3	1.60	1.02
3:BS:242:THR:CG2	3:BS:272:ARG:HG3	1.90	1.02
3:AV:120:LYS:HZ2	3:BW:66:GLU:HG2	0.85	1.01
3:AS:242:THR:CG2	3:AS:272:ARG:HG3	1.90	1.01
2:AD:52:ASN:CB	3:AS:258:LEU:CD2	2.38	1.00
3:AU:120:LYS:HZ1	3:BX:66:GLU:HG3	1.22	1.00
3:AW:120:LYS:CG	3:BV:68:PHE:CE1	2.44	0.99
3:AW:120:LYS:CD	3:BV:68:PHE:HE1	1.59	0.99
2:BG:103:THR:HB	1:BZ:78:PRO:CG	1.91	0.99
3:AW:120:LYS:CG	3:BV:68:PHE:HE1	1.75	0.98
2:AD:73:THR:HB	3:AS:256:THR:CG2	1.94	0.97
3:AS:66:GLU:HG3	3:BT:120:LYS:NZ	1.78	0.97
2:AQ:19:GLY:HA2	3:AX:166:GLY:O	1.65	0.97
3:AV:68:PHE:HE1	3:BW:120:LYS:CG	1.71	0.97
2:AD:73:THR:HB	3:AS:256:THR:HG21	1.47	0.97
1:B0:42:ILE:HB	3:BX:43:TRP:HZ2	0.80	0.96
3:AU:53:THR:CG2	1:AZ:359:PHE:HB3	1.95	0.96
2:BQ:17:PRO:HB3	3:BX:167:ASN:HD22	1.29	0.96
3:BT:116:GLU:HB2	3:BU:31:PRO:HD2	1.48	0.96
1:BY:169:THR:HG21	1:BZ:294:PHE:CE2	2.00	0.96
3:AX:66:GLU:HG3	3:BU:120:LYS:HZ1	1.31	0.95
2:BN:51:LEU:HD12	3:BV:262:PRO:HG2	1.46	0.95
2:BA:103:THR:HB	1:BY:78:PRO:HG3	1.46	0.95
3:AV:68:PHE:CD1	3:BW:120:LYS:HB3	2.03	0.94
3:AV:68:PHE:HE1	3:BW:120:LYS:HG2	1.30	0.94
2:AN:131:THR:HG22	3:AV:262:PRO:O	1.65	0.94
2:BE:17:PRO:CB	3:BT:167:ASN:HD22	1.79	0.94
3:AV:68:PHE:HE1	3:BW:120:LYS:CD	1.64	0.93
2:BB:13:SER:O	3:BS:169:LYS:NZ	2.02	0.93
2:AD:73:THR:CG2	3:AS:256:THR:HG21	1.99	0.92
2:AP:18:VAL:HG13	3:AX:158:LYS:O	1.70	0.92
2:BD:52:ASN:CB	3:BS:258:LEU:HD22	2.01	0.91
3:AW:66:GLU:HG3	3:BV:120:LYS:NZ	1.83	0.91
3:AV:68:PHE:CE1	3:BW:120:LYS:HG2	2.02	0.91
2:AD:52:ASN:OD1	3:AS:258:LEU:HD23	1.70	0.91
2:AE:17:PRO:CB	3:AT:167:ASN:HD22	1.81	0.91
2:BE:17:PRO:HB3	3:BT:167:ASN:HD22	1.36	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AV:68:PHE:HD1	3:BW:120:LYS:CD	1.77	0.90
3:AV:43:TRP:CD1	1:AZ:42:ILE:HD13	2.07	0.90
2:AE:17:PRO:HB3	3:AT:167:ASN:HD22	1.37	0.89
3:AT:116:GLU:HB2	3:AU:31:PRO:HD2	1.53	0.89
2:BD:73:THR:HB	3:BS:256:THR:HG21	1.52	0.89
2:AA:103:THR:HB	1:AY:78:PRO:HG3	1.53	0.89
2:AG:103:THR:CG2	1:AZ:78:PRO:HG3	2.01	0.89
3:AW:120:LYS:HB3	3:BV:68:PHE:CD1	2.08	0.88
3:AV:120:LYS:NZ	3:BW:66:GLU:HG2	1.72	0.88
2:AQ:17:PRO:HG3	3:AX:169:LYS:HE2	1.55	0.88
2:AQ:19:GLY:CA	3:AX:166:GLY:O	2.21	0.88
3:AU:68:PHE:CD1	3:BX:120:LYS:HD3	2.09	0.87
1:A0:88:LYS:HZ1	2:AN:104:ALA:HB3	1.36	0.87
2:BD:130:GLY:O	3:BS:262:PRO:HB2	1.75	0.86
2:BE:18:VAL:HG12	3:BT:168:TYR:O	1.75	0.85
2:AQ:17:PRO:HB3	3:AX:167:ASN:ND2	1.91	0.85
2:BD:73:THR:HB	3:BS:256:THR:CG2	2.05	0.85
2:BD:52:ASN:ND2	3:BS:258:LEU:CD2	2.33	0.85
3:AW:66:GLU:HG2	3:BV:120:LYS:NZ	1.80	0.85
3:AU:53:THR:HG21	1:AZ:359:PHE:HB3	1.58	0.85
1:A0:86:LYS:HZ2	2:AN:81:VAL:HB	1.40	0.85
2:AA:104:ALA:HB2	1:AY:88:LYS:NZ	1.91	0.85
2:BQ:17:PRO:HB3	3:BX:169:LYS:HE3	1.59	0.85
3:AS:133:ILE:HA	3:AT:42:ILE:HG21	1.59	0.85
2:AQ:17:PRO:CB	3:AX:167:ASN:HD22	1.89	0.84
2:BE:19:GLY:HA2	3:BT:166:GLY:O	1.76	0.84
3:AW:120:LYS:HG2	3:BV:68:PHE:HE1	1.41	0.84
2:AE:17:PRO:CB	3:AT:167:ASN:HB2	2.08	0.84
2:BN:73:THR:OG1	3:BV:256:THR:HG21	1.76	0.84
3:AU:68:PHE:CZ	3:BX:120:LYS:HD3	2.11	0.84
2:AB:13:SER:O	3:AS:169:LYS:NZ	2.10	0.84
3:AU:66:GLU:HG2	3:BX:120:LYS:HE2	1.60	0.83
3:AX:120:LYS:HD3	3:BU:68:PHE:CD1	2.13	0.83
2:AQ:18:VAL:CG1	3:AX:168:TYR:O	2.25	0.83
3:AU:120:LYS:NZ	3:BX:66:GLU:HG3	1.92	0.83
1:A0:86:LYS:HZ1	2:AN:81:VAL:HB	1.42	0.83
3:AS:197:PHE:CD1	3:AT:48:ILE:CG2	2.61	0.83
1:A0:294:PHE:CE2	1:AZ:169:THR:HG21	2.13	0.83
2:AQ:21:ASN:OD1	3:AX:165:PRO:HG2	1.78	0.82
2:AN:51:LEU:HD12	3:AV:262:PRO:HG2	1.59	0.82
3:AU:120:LYS:NZ	3:BX:66:GLU:CG	2.42	0.82
2:BE:17:PRO:CB	3:BT:167:ASN:HB2	2.10	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AE:18:VAL:HG12	3:AT:168:TYR:O	1.79	0.82
2:BE:9:PHE:HA	3:BT:170:TYR:O	1.79	0.82
2:AE:19:GLY:HA2	3:AT:166:GLY:O	1.80	0.81
3:AW:120:LYS:NZ	3:BV:66:GLU:HG3	1.94	0.81
3:AU:120:LYS:HZ1	3:BX:66:GLU:CG	1.93	0.81
3:AX:120:LYS:HE2	3:BU:66:GLU:HG2	1.63	0.81
2:AE:17:PRO:HB2	3:AT:167:ASN:HB2	1.62	0.81
2:AE:9:PHE:HA	3:AT:170:TYR:O	1.80	0.81
3:AW:120:LYS:HE2	3:BV:66:GLU:HG2	1.61	0.81
2:BQ:18:VAL:HG12	3:BX:168:TYR:O	1.79	0.81
2:AD:73:THR:CB	3:AS:256:THR:CG2	2.49	0.81
2:AD:52:ASN:HD22	3:AS:258:LEU:HD22	1.46	0.81
1:B0:239:SER:HB2	1:B0:312:GLU:O	1.81	0.81
2:BE:17:PRO:HB3	3:BT:167:ASN:ND2	1.96	0.80
2:AG:103:THR:HB	1:AZ:78:PRO:HG3	0.82	0.80
3:AT:73:GLU:HG3	3:AU:100:ILE:HG23	1.61	0.80
2:AG:79:ASP:O	1:AZ:212:ASN:ND2	2.14	0.80
2:BE:17:PRO:HB2	3:BT:167:ASN:HB2	1.64	0.80
3:BS:242:THR:HG22	3:BS:272:ARG:HG3	1.64	0.80
2:AC:9:PHE:HA	3:AS:178:TYR:HB2	1.62	0.80
2:BE:17:PRO:HB3	3:BT:169:LYS:HE3	1.64	0.79
3:AW:120:LYS:HG2	3:BV:68:PHE:CE1	2.15	0.79
1:A0:239:SER:HB2	1:A0:312:GLU:O	1.81	0.79
3:AV:68:PHE:CD1	3:BW:120:LYS:CG	2.62	0.79
2:BQ:18:VAL:O	3:BX:167:ASN:HA	1.81	0.79
1:A0:42:ILE:HD13	3:AX:43:TRP:NE1	1.97	0.79
2:BD:52:ASN:CG	3:BS:258:LEU:HD23	2.01	0.79
2:AE:17:PRO:HB3	3:AT:167:ASN:ND2	1.97	0.79
3:AV:66:GLU:HG2	3:BW:120:LYS:HE2	1.65	0.79
2:AN:130:GLY:O	3:AV:262:PRO:HB3	1.81	0.79
2:BB:14:THR:HA	3:BS:169:LYS:HE2	1.63	0.79
3:AW:120:LYS:CD	3:BV:68:PHE:HD1	1.91	0.79
3:AS:66:GLU:HG3	3:BT:120:LYS:HZ1	1.42	0.78
2:AF:17:PRO:HA	3:AT:177:THR:HG22	1.65	0.78
3:AS:142:LEU:HD12	3:AS:291:ILE:HD12	1.65	0.78
3:AS:273:ILE:HD11	3:AT:48:ILE:HD12	1.65	0.78
3:AS:66:GLU:CG	3:BT:120:LYS:NZ	2.45	0.78
2:BF:17:PRO:HA	3:BT:177:THR:HG22	1.66	0.78
1:AY:169:THR:HG21	1:AZ:294:PHE:CE2	2.19	0.78
3:BS:142:LEU:HD12	3:BS:291:ILE:HD12	1.65	0.78
2:AN:49:THR:HB	3:AV:258:LEU:HD21	1.64	0.78
1:A0:330:LEU:HB2	3:AV:261:PHE:CE2	2.19	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AW:120:LYS:HZ1	3:BV:66:GLU:HG3	1.46	0.77
3:AX:120:LYS:HD3	3:BU:68:PHE:CZ	2.16	0.77
3:AT:120:LYS:NZ	3:BS:66:GLU:HG3	1.98	0.77
2:AN:73:THR:OG1	3:AV:256:THR:HG21	1.85	0.77
2:BE:21:ASN:OD1	3:BT:165:PRO:HG2	1.84	0.77
3:AS:242:THR:HG22	3:AS:272:ARG:HG3	1.64	0.77
2:BN:49:THR:O	3:BV:258:LEU:HD21	1.85	0.77
2:AD:73:THR:HG21	3:AS:256:THR:HG21	1.65	0.77
2:BD:52:ASN:CB	3:BS:258:LEU:CD2	2.61	0.77
3:AX:66:GLU:HG3	3:BU:120:LYS:NZ	2.00	0.76
2:AG:79:ASP:C	1:AZ:212:ASN:HD21	1.89	0.76
3:AV:68:PHE:HD1	3:BW:120:LYS:HB3	1.45	0.76
2:AQ:19:GLY:HA2	3:AX:166:GLY:C	2.05	0.76
3:BU:242:THR:CG2	3:BU:272:ARG:HG3	2.16	0.76
3:AU:242:THR:CG2	3:AU:272:ARG:HG3	2.16	0.76
2:BQ:19:GLY:HA2	3:BX:166:GLY:O	1.85	0.76
3:AW:66:GLU:CB	3:BV:120:LYS:HZ2	1.98	0.76
3:AX:120:LYS:HD3	3:BU:68:PHE:HE1	1.37	0.75
3:AS:66:GLU:HG2	3:BT:120:LYS:HE2	1.69	0.75
3:AX:66:GLU:CG	3:BU:120:LYS:NZ	2.49	0.75
2:BR:9:PHE:CE2	3:BX:181:GLU:HG3	2.21	0.75
2:AD:73:THR:OG1	3:AS:256:THR:HG21	1.86	0.75
1:B0:88:LYS:NZ	2:BN:104:ALA:HB3	2.01	0.75
2:AE:17:PRO:HB3	3:AT:169:LYS:HE3	1.68	0.75
2:AE:21:ASN:OD1	3:AT:165:PRO:HG2	1.87	0.75
3:AU:53:THR:HG23	1:AZ:359:PHE:HB3	1.69	0.74
2:AP:65:ARG:NH2	3:AX:181:GLU:OE2	2.19	0.74
2:BC:9:PHE:HA	3:BS:178:TYR:HB2	1.68	0.74
3:AW:120:LYS:NZ	3:BV:66:GLU:CG	2.50	0.74
3:AV:68:PHE:CD1	3:BW:120:LYS:CB	2.70	0.74
3:BU:53:THR:CG2	1:BZ:359:PHE:HB3	2.17	0.74
3:BS:197:PHE:CD1	3:BT:48:ILE:HG22	2.22	0.74
2:AQ:18:VAL:C	3:AX:167:ASN:HA	2.06	0.74
2:BR:9:PHE:CZ	3:BX:181:GLU:HG3	2.23	0.74
2:BD:73:THR:OG1	3:BS:256:THR:HG21	1.88	0.74
2:AC:9:PHE:CD1	3:AS:180:GLY:HA2	2.23	0.73
3:AW:120:LYS:HB3	3:BV:68:PHE:HD1	1.52	0.73
2:AR:23:ASP:OD2	3:AX:176:TYR:OH	2.06	0.73
1:A0:38:ARG:NH2	3:AW:269:TYR:O	2.21	0.73
2:AR:9:PHE:CE1	3:AX:180:GLY:CA	2.72	0.73
3:BS:31:PRO:HD2	3:BX:116:GLU:HB2	1.70	0.73
2:AD:131:THR:HB	3:AS:263:VAL:HG23	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AD:131:THR:CG2	3:AS:262:PRO:O	2.31	0.72
3:AV:66:GLU:HG3	3:BW:120:LYS:NZ	2.04	0.72
1:A0:1:MET:SD	3:AX:48:ILE:HD13	2.30	0.72
3:AS:66:GLU:HG3	3:BT:120:LYS:HZ3	1.53	0.72
3:AV:48:ILE:HD13	1:AZ:1:MET:SD	2.30	0.72
2:AG:81:VAL:HB	1:AZ:86:LYS:NZ	2.05	0.72
3:AU:68:PHE:HE1	3:BX:120:LYS:HD3	1.40	0.71
3:AS:244:VAL:HG21	3:AT:50:VAL:HG22	1.72	0.71
1:B0:294:PHE:CE2	1:BZ:169:THR:HG21	2.25	0.71
2:AC:18:VAL:HG13	3:AS:176:TYR:CZ	2.26	0.71
2:AQ:17:PRO:CB	3:AX:169:LYS:HE3	2.17	0.71
2:AQ:9:PHE:HA	3:AX:170:TYR:O	1.91	0.71
2:AR:9:PHE:CE1	3:AX:180:GLY:HA2	2.26	0.71
1:B0:42:ILE:HD13	3:BX:43:TRP:NE1	2.06	0.70
2:AA:104:ALA:HB2	1:AY:88:LYS:HZ3	1.56	0.70
2:BC:9:PHE:CD1	3:BS:180:GLY:HA2	2.27	0.70
1:A0:211:ARG:NH2	2:AN:79:ASP:HB2	2.06	0.70
3:AU:68:PHE:HE1	3:BX:120:LYS:CG	2.05	0.70
2:AP:113:ASN:O	3:AX:186:ARG:NH2	2.24	0.70
3:AX:66:GLU:CG	3:BU:120:LYS:HZ1	2.00	0.70
2:AQ:18:VAL:O	3:AX:167:ASN:CA	2.38	0.70
2:AA:77:LYS:H	2:AA:82:ASN:HD21	1.39	0.70
2:AD:73:THR:HB	3:AS:256:THR:HG23	1.72	0.70
2:BE:17:PRO:HG3	3:BT:169:LYS:HE2	1.74	0.70
3:AW:121:ASN:HD21	3:BV:68:PHE:HB3	1.57	0.69
3:AS:242:THR:HG22	3:AS:272:ARG:CG	2.21	0.69
2:AP:22:ASN:HD21	3:AX:182:SER:CB	2.04	0.69
3:BT:80:LYS:HE3	3:BU:298:VAL:HG22	1.74	0.69
2:BP:18:VAL:HG13	3:BX:158:LYS:O	1.91	0.69
2:AB:14:THR:HA	3:AS:169:LYS:HE2	1.73	0.69
3:BS:242:THR:HG22	3:BS:272:ARG:CG	2.22	0.69
2:BE:18:VAL:O	3:BT:167:ASN:HA	1.93	0.69
3:AV:120:LYS:NZ	3:BW:66:GLU:CB	2.55	0.69
2:BE:19:GLY:CA	3:BT:166:GLY:O	2.40	0.69
3:AS:120:LYS:HG2	3:BT:68:PHE:CE1	2.28	0.69
3:AS:197:PHE:HD1	3:AT:48:ILE:CG2	2.06	0.69
1:A0:294:PHE:HE2	1:AZ:169:THR:HG21	1.57	0.69
3:AV:70:GLU:HG2	3:BW:70:GLU:HG2	1.74	0.69
2:BA:77:LYS:H	2:BA:82:ASN:HD21	1.39	0.69
3:BT:45:SER:OG	1:BY:1:MET:HB3	1.94	0.68
2:AD:73:THR:HG21	3:AS:256:THR:CG2	2.23	0.68
1:B0:88:LYS:HZ1	2:BN:104:ALA:HB3	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AS:250:GLN:HE21	3:AS:252:TRP:HE1	1.42	0.68
3:AW:120:LYS:CE	3:BV:66:GLU:HG2	2.23	0.68
2:AD:52:ASN:HB2	3:AS:258:LEU:HD22	1.71	0.68
3:BS:250:GLN:HE21	3:BS:252:TRP:HE1	1.42	0.68
2:AR:17:PRO:HA	3:AX:177:THR:HG22	1.74	0.68
3:AU:68:PHE:CD1	3:BX:120:LYS:CD	2.72	0.68
2:AD:77:LYS:H	2:AD:82:ASN:HD21	1.42	0.68
3:AU:66:GLU:HB3	3:BX:120:LYS:HZ3	1.58	0.68
3:BV:43:TRP:CD1	1:BZ:42:ILE:HD13	2.28	0.68
3:AT:80:LYS:HE3	3:AU:298:VAL:HG22	1.75	0.68
2:AP:77:LYS:H	2:AP:82:ASN:HD21	1.41	0.68
2:BP:77:LYS:H	2:BP:82:ASN:HD21	1.41	0.68
3:AV:120:LYS:HZ1	3:BW:66:GLU:CG	2.05	0.67
2:AQ:23:ASP:OD2	3:AX:168:TYR:HE2	1.78	0.67
2:AM:77:LYS:H	2:AM:82:ASN:HD21	1.42	0.67
2:AD:73:THR:CG2	3:AS:256:THR:CG2	2.72	0.67
3:AS:31:PRO:HD2	3:AX:116:GLU:HB2	1.75	0.67
2:AF:18:VAL:O	3:AT:175:SER:OG	2.10	0.67
2:AG:103:THR:HB	1:AZ:78:PRO:CB	2.25	0.67
3:BW:142:LEU:HG	3:BW:291:ILE:HD12	1.77	0.67
3:AT:120:LYS:HZ3	3:BS:66:GLU:HG3	1.59	0.67
2:AP:19:GLY:HA3	3:AX:180:GLY:O	1.95	0.67
3:AU:68:PHE:CE1	3:BX:120:LYS:CG	2.77	0.67
2:BN:130:GLY:O	3:BV:262:PRO:CB	2.41	0.66
3:AW:70:GLU:HG2	3:BV:70:GLU:HG2	1.75	0.66
2:BJ:77:LYS:H	2:BJ:82:ASN:HD21	1.41	0.66
3:AX:120:LYS:HZ3	3:BU:66:GLU:HB3	1.59	0.66
2:BN:49:THR:HG21	3:BV:235:GLN:NE2	2.10	0.66
2:BN:49:THR:HB	3:BV:258:LEU:HD21	1.75	0.66
2:BD:23:ASP:OD2	3:BT:178:TYR:HE1	1.77	0.66
2:BD:77:LYS:H	2:BD:82:ASN:HD21	1.42	0.66
2:AJ:77:LYS:H	2:AJ:82:ASN:HD21	1.41	0.66
3:AS:66:GLU:CG	3:BT:120:LYS:HZ3	2.07	0.66
2:BM:77:LYS:H	2:BM:82:ASN:HD21	1.42	0.66
3:AU:271:THR:HA	1:AZ:3:GLU:HG3	1.76	0.66
3:AV:120:LYS:HZ3	3:BW:66:GLU:HG3	1.61	0.66
2:BC:18:VAL:HG13	3:BS:176:TYR:CZ	2.31	0.66
2:AD:52:ASN:ND2	3:AS:258:LEU:HB3	2.10	0.66
1:BZ:238:ARG:HG3	1:BZ:316:SER:HA	1.78	0.66
3:BT:73:GLU:HG3	3:BU:100:ILE:HG23	1.77	0.66
3:AS:133:ILE:HG13	3:AT:42:ILE:HD13	1.78	0.66
3:AU:269:TYR:O	1:AZ:38:ARG:NH2	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AG:77:LYS:H	2:AG:82:ASN:HD21	1.42	0.66
2:BG:77:LYS:H	2:BG:82:ASN:HD21	1.42	0.66
2:BQ:17:PRO:HG3	3:BX:169:LYS:HE2	1.78	0.66
2:AE:18:VAL:O	3:AT:167:ASN:HA	1.96	0.66
3:AW:142:LEU:HG	3:AW:291:ILE:HD12	1.77	0.66
3:AW:120:LYS:CB	3:BV:68:PHE:CD1	2.80	0.65
2:AE:17:PRO:HB2	3:AT:167:ASN:CB	2.25	0.65
2:AA:104:ALA:HB2	1:AY:88:LYS:HZ2	1.60	0.65
2:AD:51:LEU:CD1	3:AS:262:PRO:HG2	2.26	0.65
2:AP:22:ASN:ND2	3:AX:182:SER:OG	2.30	0.65
3:BU:76:TYR:HB3	3:BV:100:ILE:HD11	1.78	0.65
2:BD:52:ASN:OD1	3:BS:258:LEU:HD23	1.95	0.65
2:AN:49:THR:HB	3:AV:258:LEU:CD2	2.26	0.65
3:AS:244:VAL:CG2	3:AT:50:VAL:HG22	2.27	0.65
1:AZ:238:ARG:HG3	1:AZ:316:SER:HA	1.78	0.65
1:BZ:89:LEU:HD22	1:BZ:192:GLN:HG3	1.79	0.65
3:AV:120:LYS:HZ1	3:BW:66:GLU:CB	2.09	0.65
3:AW:66:GLU:CB	3:BV:120:LYS:NZ	2.58	0.65
2:AE:17:PRO:HG3	3:AT:169:LYS:HE2	1.77	0.65
2:BN:49:THR:HG21	3:BV:235:GLN:HE22	1.62	0.65
3:BU:53:THR:HG21	1:BZ:359:PHE:HB3	1.79	0.65
2:BD:131:THR:HA	3:BS:262:PRO:HB2	1.78	0.65
2:BA:120:LYS:HE2	3:BS:222:ASN:ND2	2.12	0.64
1:AY:152:PHE:HB2	1:AY:208:PHE:HB2	1.80	0.64
1:AY:243:PHE:HA	1:AY:313:ILE:HD11	1.79	0.64
3:AX:120:LYS:CG	3:BU:68:PHE:HE1	2.11	0.64
3:BS:250:GLN:NE2	3:BS:252:TRP:HE1	1.96	0.64
2:AQ:23:ASP:OD2	3:AX:168:TYR:CE2	2.50	0.64
2:AQ:17:PRO:HB3	3:AX:169:LYS:CE	2.20	0.64
3:AX:120:LYS:HZ3	3:BU:66:GLU:CB	2.10	0.64
1:AZ:89:LEU:HD22	1:AZ:192:GLN:HG3	1.79	0.64
3:AU:68:PHE:CD1	3:BX:120:LYS:HB3	2.33	0.64
3:AS:250:GLN:NE2	3:AS:252:TRP:HE1	1.96	0.64
2:AE:19:GLY:CA	3:AT:166:GLY:O	2.44	0.64
2:AG:79:ASP:CA	1:AZ:212:ASN:HD21	2.11	0.63
1:BY:152:PHE:HB2	1:BY:208:PHE:HB2	1.80	0.63
3:AV:66:GLU:CG	3:BW:120:LYS:NZ	2.62	0.63
3:BV:116:GLU:HB2	3:BW:31:PRO:HD2	1.79	0.63
2:BD:73:THR:CG2	3:BS:256:THR:HG21	2.28	0.63
2:BE:17:PRO:HB2	3:BT:167:ASN:CB	2.26	0.63
2:AD:23:ASP:OD2	3:AT:178:TYR:HE1	1.82	0.63
3:BV:247:GLU:OE1	3:BV:249:TYR:HE2	1.82	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AU:68:PHE:HD1	3:BX:120:LYS:HB3	1.63	0.63
3:AV:247:GLU:OE1	3:AV:249:TYR:HE2	1.82	0.63
2:AD:51:LEU:HD11	3:AS:262:PRO:HG2	1.81	0.63
3:AX:11:LEU:HD23	3:AX:12:ASP:H	1.64	0.63
3:AW:66:GLU:HG3	3:BV:120:LYS:HZ3	1.64	0.63
3:AT:120:LYS:HE2	3:BS:66:GLU:HG2	1.80	0.63
1:BY:243:PHE:HA	1:BY:313:ILE:HD11	1.79	0.63
3:BX:11:LEU:HD23	3:BX:12:ASP:H	1.63	0.63
2:AQ:17:PRO:HG3	3:AX:169:LYS:CE	2.27	0.62
1:A0:152:PHE:HB2	1:A0:208:PHE:HB2	1.81	0.62
3:AU:224:TYR:HB2	1:AZ:74:PRO:HB2	1.81	0.62
2:AD:52:ASN:CB	3:AS:258:LEU:HD21	2.27	0.62
3:AV:45:SER:CB	1:AZ:42:ILE:HG22	2.29	0.62
3:AV:66:GLU:HG3	3:BW:120:LYS:HZ1	1.63	0.62
2:BD:73:THR:CB	3:BS:256:THR:CG2	2.63	0.62
1:A0:330:LEU:HB2	3:AV:261:PHE:HE2	1.64	0.62
1:BY:241:TYR:HB2	1:BY:291:LYS:HD2	1.81	0.62
2:AP:9:PHE:HA	3:AX:160:TYR:O	1.99	0.62
2:BR:23:ASP:OD2	3:BX:176:TYR:OH	2.17	0.62
2:BB:17:PRO:HB3	3:BS:167:ASN:HB2	1.81	0.62
3:AX:120:LYS:CD	3:BU:68:PHE:CD1	2.77	0.62
1:A0:88:LYS:HE2	2:AN:106:ASN:OD1	1.99	0.62
3:AU:271:THR:HA	1:AZ:3:GLU:CG	2.30	0.62
3:AV:68:PHE:HD1	3:BW:120:LYS:CB	2.09	0.62
2:AF:23:ASP:OD2	3:AT:176:TYR:OH	2.17	0.62
3:AU:120:LYS:HE2	3:BX:66:GLU:HG2	1.82	0.62
1:B0:152:PHE:HB2	1:B0:208:PHE:HB2	1.81	0.61
3:AS:245:ASN:OD1	3:AT:51:MET:N	2.26	0.61
3:AV:66:GLU:HG2	3:BW:120:LYS:CE	2.30	0.61
1:A0:88:LYS:HZ2	2:AN:104:ALA:HB3	1.62	0.61
3:AU:66:GLU:CB	3:BX:120:LYS:HZ3	2.13	0.61
3:BX:199:PHE:N	3:BX:242:THR:OG1	2.33	0.61
3:AW:215:ARG:HB3	3:AW:282:ILE:HD11	1.83	0.61
1:A0:88:LYS:NZ	2:AN:104:ALA:CB	2.52	0.61
3:BW:215:ARG:HB3	3:BW:282:ILE:HD11	1.83	0.61
3:AS:215:ARG:HB3	3:AS:282:ILE:HD11	1.82	0.61
3:AX:247:GLU:OE1	3:AX:249:TYR:HE2	1.83	0.61
1:A0:3:GLU:HG3	3:AW:271:THR:HA	1.83	0.61
2:AQ:19:GLY:HA3	3:AX:166:GLY:O	2.01	0.61
3:AT:120:LYS:HZ3	3:BS:66:GLU:CG	2.14	0.61
1:BZ:90:ASN:HD22	1:BZ:192:GLN:NE2	1.99	0.61
1:AY:241:TYR:HB2	1:AY:291:LYS:HD2	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AD:131:THR:O	3:AS:263:VAL:HG23	2.01	0.60
2:BD:51:LEU:CD1	3:BS:262:PRO:HG2	2.31	0.60
3:AS:269:TYR:O	1:AY:38:ARG:NH2	2.29	0.60
2:AA:104:ALA:CB	1:AY:88:LYS:NZ	2.63	0.60
3:BU:53:THR:HG23	1:BZ:359:PHE:HB3	1.84	0.60
1:B0:294:PHE:HE2	1:BZ:169:THR:HG21	1.66	0.60
1:AZ:90:ASN:HD22	1:AZ:192:GLN:NE2	1.99	0.60
3:BT:235:GLN:HE22	3:BT:258:LEU:HD12	1.66	0.60
2:BG:81:VAL:HB	1:BZ:86:LYS:NZ	2.16	0.60
3:AT:235:GLN:HE22	3:AT:258:LEU:HD12	1.66	0.60
3:BX:247:GLU:OE1	3:BX:249:TYR:HE2	1.83	0.60
3:AV:68:PHE:CE1	3:BW:120:LYS:CE	2.83	0.60
3:AX:120:LYS:CG	3:BU:68:PHE:CE1	2.84	0.60
3:AU:53:THR:HG21	1:AZ:359:PHE:CB	2.29	0.60
2:AE:17:PRO:CB	3:AT:167:ASN:ND2	2.58	0.60
2:AA:104:ALA:HB3	1:AY:88:LYS:HD2	1.84	0.60
3:AV:50:VAL:HG11	1:AZ:60:THR:HG22	1.84	0.60
3:BU:137:TYR:HD1	3:BU:292:LYS:HB2	1.66	0.60
2:AP:23:ASP:OD2	3:AX:178:TYR:HE1	1.85	0.60
3:AW:121:ASN:ND2	3:BV:68:PHE:HB3	2.16	0.60
3:AU:66:GLU:CG	3:BX:120:LYS:NZ	2.64	0.60
2:BE:17:PRO:CB	3:BT:167:ASN:ND2	2.56	0.60
3:BX:12:ASP:HB2	3:BX:200:MET:HG3	1.84	0.60
3:BX:199:PHE:CE1	3:BX:242:THR:HG21	2.37	0.60
3:AS:206:LYS:HG3	3:AS:285:SER:HB3	1.84	0.60
3:BS:215:ARG:HB3	3:BS:282:ILE:HD11	1.82	0.60
1:A0:42:ILE:HD13	3:AX:43:TRP:HE1	1.65	0.60
2:AR:18:VAL:HG12	3:AX:176:TYR:O	2.02	0.60
2:BF:23:ASP:OD2	3:BT:176:TYR:OH	2.18	0.60
2:BD:52:ASN:HB2	3:BS:258:LEU:HD22	1.82	0.59
2:AR:9:PHE:CZ	3:AX:181:GLU:HG3	2.37	0.59
3:AX:12:ASP:HB2	3:AX:200:MET:HG3	1.84	0.59
2:AG:92:GLN:NE2	3:AU:189:ARG:CZ	2.65	0.59
3:AU:66:GLU:HG3	3:BX:120:LYS:HZ1	1.66	0.59
3:AV:171:ILE:HG22	3:AV:172:LYS:H	1.68	0.59
2:AD:49:THR:CG2	3:AS:233:GLN:HB2	2.32	0.59
3:BS:206:LYS:HG3	3:BS:285:SER:HB3	1.84	0.59
2:AG:79:ASP:O	1:AZ:212:ASN:CG	2.40	0.59
2:BN:49:THR:HB	3:BV:258:LEU:CD2	2.32	0.59
3:BX:215:ARG:HB3	3:BX:282:ILE:HD11	1.84	0.59
3:AX:199:PHE:CE1	3:AX:242:THR:HG21	2.37	0.59
3:AU:137:TYR:HD1	3:AU:292:LYS:HB2	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AV:68:PHE:HB3	3:BW:121:ASN:HD21	1.66	0.59
2:BA:104:ALA:HB2	1:BY:88:LYS:NZ	2.17	0.59
3:AX:199:PHE:N	3:AX:242:THR:OG1	2.33	0.59
3:BU:215:ARG:HB3	3:BU:282:ILE:HD11	1.83	0.59
3:AU:120:LYS:CE	3:BX:66:GLU:HG2	2.33	0.59
2:BQ:19:GLY:CA	3:BX:166:GLY:O	2.49	0.59
3:AU:215:ARG:HB3	3:AU:282:ILE:HD11	1.83	0.59
2:AD:131:THR:HA	3:AS:262:PRO:HB2	1.84	0.59
3:BV:247:GLU:OE1	3:BV:249:TYR:CE2	2.56	0.59
3:BS:273:ILE:HD11	3:BT:48:ILE:HD12	1.83	0.58
3:AX:215:ARG:HB3	3:AX:282:ILE:HD11	1.84	0.58
3:AT:73:GLU:CG	3:AU:100:ILE:HG23	2.31	0.58
1:BZ:41:VAL:HG23	1:BZ:57:ALA:HB1	1.85	0.58
2:BG:79:ASP:O	1:BZ:212:ASN:ND2	2.37	0.58
2:AP:21:ASN:HB3	3:AX:181:GLU:CD	2.23	0.58
1:AZ:41:VAL:HG23	1:AZ:57:ALA:HB1	1.85	0.58
3:AX:120:LYS:NZ	3:BU:66:GLU:CG	2.66	0.58
2:AN:51:LEU:HD12	3:AV:262:PRO:CG	2.33	0.58
3:AU:238:ILE:HG22	3:AU:240:ILE:HG23	1.85	0.58
3:AV:226:ALA:HB3	3:AV:268:ARG:HB3	1.85	0.58
2:AN:120:LYS:HE2	3:AW:222:ASN:ND2	2.18	0.58
2:AR:88:ILE:HG12	2:AR:97:VAL:HG22	1.85	0.58
3:AV:116:GLU:HB2	3:AW:31:PRO:HD2	1.84	0.58
2:AR:9:PHE:CE2	3:AX:181:GLU:HG3	2.38	0.58
3:AT:45:SER:OG	1:AY:1:MET:HB3	2.04	0.58
2:AF:88:ILE:HG12	2:AF:97:VAL:HG22	1.86	0.58
3:BU:238:ILE:HG22	3:BU:240:ILE:HG23	1.85	0.58
1:BZ:153:ASN:HB3	1:BZ:156:ILE:HG12	1.85	0.58
2:AC:88:ILE:HG12	2:AC:97:VAL:HG22	1.85	0.58
3:BS:196:ILE:HG13	3:BS:274:ILE:HB	1.85	0.58
2:BQ:21:ASN:OD1	3:BX:165:PRO:HG2	2.03	0.58
2:BO:88:ILE:HG12	2:BO:97:VAL:HG22	1.85	0.58
3:BV:171:ILE:HG22	3:BV:172:LYS:H	1.68	0.58
3:AU:68:PHE:HB3	3:BX:121:ASN:HD21	1.68	0.57
2:AE:18:VAL:HG13	3:AT:168:TYR:CD2	2.38	0.57
3:AV:247:GLU:OE1	3:AV:249:TYR:CE2	2.56	0.57
2:AD:49:THR:HG22	3:AS:233:GLN:HB2	1.85	0.57
3:AW:120:LYS:CG	3:BV:68:PHE:CD1	2.78	0.57
1:A0:330:LEU:HB2	3:AV:261:PHE:CD2	2.39	0.57
2:AI:88:ILE:HG12	2:AI:97:VAL:HG22	1.85	0.57
1:AZ:153:ASN:HB3	1:AZ:156:ILE:HG12	1.85	0.57
3:AU:66:GLU:HG2	3:BX:120:LYS:CE	2.30	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AS:66:GLU:HG2	3:BT:120:LYS:CE	2.34	0.57
2:AG:81:VAL:HB	1:AZ:86:LYS:HZ1	1.69	0.57
3:BV:226:ALA:HB3	3:BV:268:ARG:HB3	1.85	0.57
3:AX:206:LYS:HG3	3:AX:285:SER:HB3	1.86	0.57
2:AO:88:ILE:HG12	2:AO:97:VAL:HG22	1.85	0.57
3:BU:114:LYS:NZ	3:BV:298:VAL:O	2.37	0.57
2:BN:51:LEU:HD12	3:BV:262:PRO:CG	2.26	0.57
2:BE:18:VAL:HG13	3:BT:168:TYR:CD2	2.39	0.57
2:BF:18:VAL:O	3:BT:175:SER:OG	2.07	0.57
2:BF:88:ILE:HG12	2:BF:97:VAL:HG22	1.86	0.57
2:AQ:21:ASN:CG	3:AX:165:PRO:HG2	2.24	0.57
2:AR:20:SER:HA	3:AX:170:TYR:CD1	2.40	0.57
2:BR:9:PHE:CE1	3:BX:180:GLY:CA	2.87	0.57
3:AS:196:ILE:HG13	3:AS:274:ILE:HB	1.85	0.57
1:B0:86:LYS:NZ	2:BN:81:VAL:HB	2.19	0.57
2:BR:88:ILE:HG12	2:BR:97:VAL:HG22	1.85	0.57
2:AR:9:PHE:CZ	3:AX:180:GLY:C	2.78	0.57
2:AA:120:LYS:HE2	3:AS:222:ASN:ND2	2.19	0.57
2:AP:21:ASN:CB	3:AX:181:GLU:HG2	2.35	0.57
1:A0:78:PRO:HG3	2:AN:103:THR:HB	1.87	0.57
3:AU:196:ILE:HG22	3:AU:293:ARG:HD3	1.87	0.57
2:BI:88:ILE:HG12	2:BI:97:VAL:HG22	1.85	0.57
3:AV:68:PHE:HB3	3:BW:121:ASN:ND2	2.20	0.56
3:BT:73:GLU:HB2	3:BU:99:GLU:CD	2.25	0.56
2:BC:88:ILE:HG12	2:BC:97:VAL:HG22	1.85	0.56
2:BR:17:PRO:HA	3:BX:177:THR:HG22	1.87	0.56
2:AD:131:THR:HG22	3:AS:262:PRO:C	2.18	0.56
3:BU:240:ILE:HD12	3:BU:240:ILE:O	2.05	0.56
3:AW:206:LYS:HG3	3:AW:285:SER:HB3	1.87	0.56
3:AV:206:LYS:HG3	3:AV:285:SER:HB3	1.87	0.56
3:AT:266:PHE:CD1	1:AZ:221:ARG:HB2	2.40	0.56
3:AT:240:ILE:HD12	3:AT:240:ILE:O	2.06	0.56
2:AR:23:ASP:OD2	3:AX:176:TYR:CE2	2.58	0.56
3:BX:206:LYS:HG3	3:BX:285:SER:HB3	1.86	0.56
2:AL:88:ILE:HG12	2:AL:97:VAL:HG22	1.86	0.56
3:BW:206:LYS:HG3	3:BW:285:SER:HB3	1.87	0.56
1:A0:41:VAL:HG11	1:A0:71:ILE:HG12	1.87	0.56
2:BD:19:GLY:HA2	3:BT:180:GLY:O	2.05	0.56
2:AM:26:LEU:HD13	2:AN:66:TYR:HB2	1.88	0.56
3:AU:76:TYR:HB3	3:AV:100:ILE:HD11	1.86	0.56
2:AC:18:VAL:HG13	3:AS:176:TYR:CE2	2.41	0.56
2:AE:187:ILE:HG12	2:AE:260:SER:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AK:10:SER:HA	2:AK:15:GLU:HB2	1.88	0.56
3:BW:76:TYR:HB3	3:BX:100:ILE:HD11	1.87	0.56
3:AS:270:ARG:NH1	1:AY:72:LEU:HD22	2.21	0.56
2:AN:187:ILE:HG12	2:AN:260:SER:HB3	1.88	0.56
3:AX:120:LYS:CD	3:BU:68:PHE:HE1	2.01	0.56
2:BQ:18:VAL:CG1	3:BX:168:TYR:O	2.52	0.56
2:BN:51:LEU:CD1	3:BV:262:PRO:HG2	2.28	0.56
2:BL:88:ILE:HG12	2:BL:97:VAL:HG22	1.86	0.56
2:AB:17:PRO:HB3	3:AS:167:ASN:HB2	1.88	0.56
3:BU:196:ILE:HG22	3:BU:293:ARG:HD3	1.87	0.56
2:BE:187:ILE:HG12	2:BE:260:SER:HB3	1.88	0.56
3:AX:120:LYS:HB3	3:BU:68:PHE:HD1	1.71	0.55
3:AX:247:GLU:OE1	3:AX:249:TYR:CE2	2.59	0.55
2:BN:120:LYS:NZ	3:BW:220:ILE:O	2.34	0.55
2:BB:88:ILE:HG12	2:BB:97:VAL:HG22	1.88	0.55
2:BM:26:LEU:HD13	2:BN:66:TYR:HB2	1.88	0.55
3:BU:224:TYR:HB2	1:BZ:74:PRO:HB2	1.88	0.55
3:BV:206:LYS:HG3	3:BV:285:SER:HB3	1.87	0.55
3:BX:247:GLU:OE1	3:BX:249:TYR:CE2	2.59	0.55
3:BX:240:ILE:O	3:BX:240:ILE:HD12	2.07	0.55
3:AU:66:GLU:HG3	3:BX:120:LYS:NZ	2.22	0.55
3:AX:120:LYS:CE	3:BU:66:GLU:HG2	2.33	0.55
1:B0:42:ILE:HD13	3:BX:43:TRP:HE1	1.69	0.55
2:AQ:18:VAL:O	3:AX:168:TYR:N	2.39	0.55
3:AS:197:PHE:HB2	3:AT:48:ILE:HG21	1.88	0.55
1:A0:88:LYS:CE	2:AN:106:ASN:OD1	2.54	0.55
2:BG:103:THR:CG2	1:BZ:78:PRO:HG3	2.35	0.55
3:AT:120:LYS:NZ	3:BS:66:GLU:CG	2.66	0.55
2:AB:155:VAL:HG21	2:AB:159:ILE:HD11	1.88	0.55
3:BT:240:ILE:HD12	3:BT:240:ILE:O	2.06	0.55
3:AX:120:LYS:HB3	3:BU:68:PHE:CD1	2.41	0.55
3:BT:160:TYR:HB3	3:BT:166:GLY:HA3	1.89	0.55
2:AN:47:LEU:HD22	3:AV:233:GLN:CD	2.26	0.55
3:AU:120:LYS:NZ	3:BX:66:GLU:HG2	2.22	0.55
1:AZ:41:VAL:HG11	1:AZ:71:ILE:HG12	1.88	0.55
3:AU:240:ILE:O	3:AU:240:ILE:HD12	2.05	0.55
3:AU:108:ALA:HB2	3:AU:133:ILE:HD11	1.89	0.55
2:AD:131:THR:HB	3:AS:263:VAL:CG2	2.37	0.55
2:BF:23:ASP:OD2	3:BT:176:TYR:CE2	2.60	0.55
2:BN:187:ILE:HG12	2:BN:260:SER:HB3	1.88	0.55
2:BH:187:ILE:HG12	2:BH:260:SER:HB3	1.88	0.55
3:AX:240:ILE:O	3:AX:240:ILE:HD12	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AQ:187:ILE:HG12	2:AQ:260:SER:HB3	1.88	0.55
3:BU:160:TYR:HB3	3:BU:166:GLY:HA3	1.89	0.55
2:AK:88:ILE:HG12	2:AK:97:VAL:HG22	1.89	0.55
2:AD:52:ASN:ND2	3:AS:258:LEU:CB	2.70	0.55
3:AS:87:LEU:O	3:AT:54:ARG:NH1	2.40	0.55
1:B0:41:VAL:HG11	1:B0:71:ILE:HG12	1.88	0.55
2:AG:92:GLN:HE21	3:AU:189:ARG:NE	2.05	0.54
2:AB:88:ILE:HG12	2:AB:97:VAL:HG22	1.88	0.54
2:AN:89:ASP:OD2	3:AW:189:ARG:NH1	2.33	0.54
3:AT:123:THR:HG21	3:BS:120:LYS:HD2	1.89	0.54
3:AX:120:LYS:NZ	3:BU:66:GLU:HG3	2.23	0.54
1:BY:243:PHE:CD1	1:BY:243:PHE:C	2.80	0.54
2:BK:10:SER:HA	2:BK:15:GLU:HB2	1.87	0.54
2:BK:187:ILE:HG12	2:BK:260:SER:HB3	1.88	0.54
2:AG:80:SER:OG	1:AZ:211:ARG:HD2	2.07	0.54
2:BQ:187:ILE:HG12	2:BQ:260:SER:HB3	1.88	0.54
2:AB:187:ILE:HG12	2:AB:260:SER:HB3	1.88	0.54
3:AX:66:GLU:HG2	3:BU:120:LYS:HE2	1.89	0.54
2:AC:18:VAL:CG1	3:AS:176:TYR:CZ	2.90	0.54
1:AY:243:PHE:C	1:AY:243:PHE:CD1	2.80	0.54
3:BT:106:ASP:O	3:BT:133:ILE:HB	2.07	0.54
2:AP:5:ASN:HB3	2:AP:8:PHE:CD1	2.42	0.54
2:AE:88:ILE:HG12	2:AE:97:VAL:HG22	1.89	0.54
3:AU:160:TYR:HB3	3:AU:166:GLY:HA3	1.89	0.54
2:AK:187:ILE:HG12	2:AK:260:SER:HB3	1.88	0.54
2:AH:88:ILE:HG12	2:AH:97:VAL:HG22	1.89	0.54
2:AH:187:ILE:HG12	2:AH:260:SER:HB3	1.88	0.54
3:AS:160:TYR:HB3	3:AS:166:GLY:HA3	1.89	0.54
3:BT:215:ARG:HB3	3:BT:282:ILE:HD11	1.89	0.54
2:BQ:88:ILE:HG12	2:BQ:97:VAL:HG22	1.89	0.54
2:BD:73:THR:HB	3:BS:256:THR:HG23	1.87	0.54
1:BZ:41:VAL:HG11	1:BZ:71:ILE:HG12	1.88	0.54
2:BQ:17:PRO:HB3	3:BX:167:ASN:ND2	2.12	0.54
3:BX:167:ASN:ND2	3:BX:169:LYS:HE3	2.23	0.54
2:BA:104:ALA:HB2	1:BY:88:LYS:HZ2	1.72	0.54
2:AM:88:ILE:HG12	2:AM:97:VAL:HG22	1.90	0.54
3:AX:226:ALA:HB3	3:AX:268:ARG:HB3	1.89	0.54
3:AT:160:TYR:HB3	3:AT:166:GLY:HA3	1.89	0.54
2:AN:49:THR:O	3:AV:258:LEU:HD21	2.08	0.54
2:BP:5:ASN:HB3	2:BP:8:PHE:CD1	2.42	0.54
3:AT:215:ARG:HB3	3:AT:282:ILE:HD11	1.89	0.54
2:BK:88:ILE:HG12	2:BK:97:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A0:294:PHE:CE2	1:AZ:169:THR:CG2	2.88	0.53
3:BU:242:THR:HG23	3:BU:272:ARG:HG3	1.87	0.53
3:AU:242:THR:HG23	3:AU:272:ARG:HG3	1.87	0.53
3:BU:55:SER:HB3	1:BZ:359:PHE:CE1	2.44	0.53
2:AQ:8:PHE:O	3:AX:170:TYR:HB2	2.07	0.53
2:AQ:88:ILE:HG12	2:AQ:97:VAL:HG22	1.89	0.53
1:A0:344:GLY:HA3	3:AV:270:ARG:HH11	1.73	0.53
2:BB:187:ILE:HG12	2:BB:260:SER:HB3	1.88	0.53
3:BS:160:TYR:HB3	3:BS:166:GLY:HA3	1.89	0.53
3:AT:106:ASP:O	3:AT:133:ILE:HB	2.08	0.53
2:BN:131:THR:CG2	3:BV:262:PRO:O	2.42	0.53
2:BF:17:PRO:HA	3:BT:177:THR:CG2	2.37	0.53
2:AP:21:ASN:H	3:AX:181:GLU:HG2	1.73	0.53
2:AN:47:LEU:HD22	3:AV:233:GLN:NE2	2.23	0.53
2:BB:155:VAL:HG21	2:BB:159:ILE:HD11	1.88	0.53
3:AW:120:LYS:HZ3	3:BV:66:GLU:CG	2.21	0.53
3:AX:121:ASN:HD21	3:BU:68:PHE:HB3	1.73	0.53
1:B0:238:ARG:HG3	1:B0:316:SER:HA	1.89	0.53
1:B0:169:THR:HG21	1:BY:294:PHE:CE2	2.42	0.53
3:BT:114:LYS:HB3	3:BU:34:LEU:HB2	1.90	0.53
3:AX:167:ASN:ND2	3:AX:169:LYS:HE3	2.23	0.53
2:BE:88:ILE:HG12	2:BE:97:VAL:HG22	1.89	0.53
2:AD:19:GLY:HA2	3:AT:180:GLY:O	2.08	0.53
2:AN:47:LEU:HB3	3:AV:233:GLN:OE1	2.09	0.53
1:A0:45:GLU:HA	1:A0:357:THR:HG22	1.91	0.53
2:AG:88:ILE:HG12	2:AG:97:VAL:HG22	1.90	0.53
2:AJ:88:ILE:HG12	2:AJ:97:VAL:HG22	1.90	0.53
2:BH:88:ILE:HG12	2:BH:97:VAL:HG22	1.89	0.53
3:BU:108:ALA:HB2	3:BU:133:ILE:HD11	1.89	0.53
3:BS:133:ILE:HA	3:BT:42:ILE:HG21	1.91	0.53
2:AN:88:ILE:HG12	2:AN:97:VAL:HG22	1.89	0.53
2:AA:5:ASN:HB3	2:AA:8:PHE:CD1	2.44	0.53
2:BN:47:LEU:HB3	3:BV:233:GLN:OE1	2.09	0.53
2:AP:26:LEU:HD13	2:AQ:66:TYR:HB2	1.91	0.53
2:BA:120:LYS:HE2	3:BS:222:ASN:HD21	1.74	0.53
3:BX:226:ALA:HB3	3:BX:268:ARG:HB3	1.89	0.53
3:AT:206:LYS:HG3	3:AT:285:SER:HB3	1.91	0.53
2:BF:18:VAL:HG12	3:BT:176:TYR:O	2.10	0.53
3:AW:68:PHE:CE1	3:BV:120:LYS:HD2	2.44	0.52
3:AX:160:TYR:HB3	3:AX:166:GLY:HA3	1.91	0.52
2:BD:5:ASN:HB3	2:BD:8:PHE:CD1	2.44	0.52
2:BP:88:ILE:HG12	2:BP:97:VAL:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A0:238:ARG:HG3	1:A0:316:SER:HA	1.90	0.52
3:AX:183:ASP:O	3:AX:186:ARG:HG3	2.09	0.52
3:AW:196:ILE:HG13	3:AW:274:ILE:HB	1.90	0.52
1:B0:45:GLU:HA	1:B0:357:THR:HG22	1.91	0.52
2:AD:5:ASN:HB3	2:AD:8:PHE:CD1	2.44	0.52
3:AW:66:GLU:HB3	3:BV:120:LYS:NZ	2.24	0.52
2:AF:17:PRO:CA	3:AT:177:THR:HG22	2.36	0.52
3:BU:55:SER:HB3	1:BZ:359:PHE:HE1	1.74	0.52
2:BQ:25:LYS:HE2	2:BQ:113:ASN:HB3	1.91	0.52
2:BN:88:ILE:HG12	2:BN:97:VAL:HG22	1.89	0.52
2:AP:88:ILE:HG12	2:AP:97:VAL:HG22	1.91	0.52
3:BT:206:LYS:HG3	3:BT:285:SER:HB3	1.91	0.52
2:BP:26:LEU:HD13	2:BQ:66:TYR:HB2	1.91	0.52
2:BA:5:ASN:HB3	2:BA:8:PHE:CD1	2.44	0.52
2:BJ:88:ILE:HG12	2:BJ:97:VAL:HG22	1.91	0.52
2:BR:9:PHE:CE1	3:BX:180:GLY:HA2	2.44	0.52
2:AP:21:ASN:HB3	3:AX:181:GLU:HG2	1.92	0.52
1:AZ:241:TYR:HB2	1:AZ:291:LYS:HD2	1.91	0.52
2:BG:88:ILE:HG12	2:BG:97:VAL:HG22	1.90	0.52
2:AF:23:ASP:OD2	3:AT:176:TYR:CE2	2.63	0.52
3:BW:196:ILE:HG13	3:BW:274:ILE:HB	1.90	0.52
3:AT:230:LYS:HG3	3:AT:263:VAL:HG22	1.91	0.52
3:BX:183:ASP:O	3:BX:186:ARG:HG3	2.09	0.52
3:AV:142:LEU:HG	3:AV:291:ILE:HD12	1.90	0.52
3:AW:66:GLU:HB3	3:BV:120:LYS:HZ2	1.70	0.52
3:AU:116:GLU:HB2	3:AV:31:PRO:HD2	1.91	0.52
2:BE:17:PRO:HB2	3:BT:167:ASN:HD22	1.72	0.52
3:BV:142:LEU:HG	3:BV:291:ILE:HD12	1.90	0.52
1:BY:89:LEU:HD22	1:BY:192:GLN:HG3	1.92	0.52
2:AA:148:ILE:HB	2:AC:153:MET:HG3	1.92	0.52
3:AW:66:GLU:CG	3:BV:120:LYS:HZ3	2.15	0.52
2:AQ:18:VAL:HG13	3:AX:168:TYR:CD2	2.45	0.52
2:AQ:20:SER:OG	3:AX:165:PRO:O	2.18	0.52
3:AV:43:TRP:CZ2	1:AZ:43:ASN:HB2	2.45	0.52
1:B0:12:PRO:HB2	1:BY:288:ARG:NH2	2.25	0.52
3:BT:230:LYS:HG3	3:BT:263:VAL:HG22	1.91	0.52
2:BL:145:LEU:HD13	2:BL:148:ILE:HD11	1.91	0.52
3:AW:160:TYR:HB3	3:AW:166:GLY:HA3	1.92	0.52
3:AU:281:LEU:HB3	3:AU:284:LEU:HD12	1.92	0.52
1:BZ:241:TYR:HB2	1:BZ:291:LYS:HD2	1.91	0.52
2:BR:9:PHE:HE2	3:BX:181:GLU:HG3	1.72	0.51
3:BT:132:ILE:HD13	3:BT:135:LYS:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BW:226:ALA:HB3	3:BW:268:ARG:HB3	1.92	0.51
2:BP:5:ASN:O	2:BP:16:PHE:HB3	2.10	0.51
2:AA:88:ILE:HG12	2:AA:97:VAL:HG22	1.92	0.51
1:A0:42:ILE:HD13	3:AX:43:TRP:CE2	2.44	0.51
3:BS:242:THR:HG23	3:BS:272:ARG:HG3	1.89	0.51
3:BX:160:TYR:HB3	3:BX:166:GLY:HA3	1.91	0.51
2:AP:5:ASN:O	2:AP:16:PHE:HB3	2.11	0.51
1:BY:32:LEU:HD11	1:BY:204:LEU:HB2	1.92	0.51
2:AQ:25:LYS:HE2	2:AQ:113:ASN:HB3	1.92	0.51
2:BM:88:ILE:HG12	2:BM:97:VAL:HG22	1.90	0.51
2:AD:52:ASN:HD21	3:AS:258:LEU:HB3	1.75	0.51
3:AS:266:PHE:CG	1:AY:35:PRO:HD2	2.46	0.51
3:AT:87:LEU:HA	3:AU:54:ARG:NH1	2.25	0.51
2:BA:88:ILE:HG12	2:BA:97:VAL:HG22	1.92	0.51
3:AT:132:ILE:HD13	3:AT:135:LYS:HG3	1.92	0.51
2:AN:100:SER:HB3	3:AW:220:ILE:HG21	1.92	0.51
2:AI:177:GLN:HB3	2:AI:189:ARG:HB2	1.93	0.51
2:BA:148:ILE:HB	2:BC:153:MET:HG3	1.92	0.51
3:AT:199:PHE:N	3:AT:242:THR:OG1	2.39	0.51
2:AQ:17:PRO:CB	3:AX:169:LYS:CE	2.84	0.51
2:BI:177:GLN:HB3	2:BI:189:ARG:HB2	1.93	0.51
3:BW:160:TYR:HB3	3:BW:166:GLY:HA3	1.92	0.51
3:AS:270:ARG:HG3	1:AY:72:LEU:HB3	1.93	0.51
3:BX:144:PHE:HB3	3:BX:190:TRP:CE2	2.45	0.51
2:AL:145:LEU:HD13	2:AL:148:ILE:HD11	1.91	0.51
2:AC:177:GLN:HB3	2:AC:189:ARG:HB2	1.93	0.51
2:BF:177:GLN:HB3	2:BF:189:ARG:HB2	1.93	0.51
2:BO:177:GLN:HB3	2:BO:189:ARG:HB2	1.93	0.51
3:AX:167:ASN:HD22	3:AX:169:LYS:HE3	1.76	0.51
3:BX:167:ASN:HD22	3:BX:169:LYS:HE3	1.76	0.51
3:AX:66:GLU:HG2	3:BU:120:LYS:NZ	2.26	0.51
2:BG:10:SER:N	3:BU:160:TYR:O	2.30	0.51
1:AZ:157:PHE:HE2	1:AZ:208:PHE:HB3	1.76	0.51
1:AY:89:LEU:HD22	1:AY:192:GLN:HG3	1.92	0.51
2:BC:177:GLN:HB3	2:BC:189:ARG:HB2	1.93	0.51
2:BQ:9:PHE:HA	3:BX:170:TYR:O	2.11	0.51
3:AW:120:LYS:CB	3:BV:68:PHE:HD1	2.21	0.50
2:AB:13:SER:O	3:AS:169:LYS:HE2	2.05	0.50
3:AS:244:VAL:HG21	3:AT:50:VAL:CG2	2.40	0.50
1:AY:32:LEU:HD11	1:AY:204:LEU:HB2	1.92	0.50
3:BS:171:ILE:HG22	3:BS:172:LYS:H	1.76	0.50
2:BN:89:ASP:OD2	3:BW:189:ARG:NH1	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BY:120:ASP:HB2	1:BZ:292:THR:HB	1.93	0.50
3:AX:66:GLU:HG2	3:BU:120:LYS:CE	2.40	0.50
3:AT:73:GLU:HB2	3:AU:99:GLU:CD	2.30	0.50
2:BN:102:GLU:OE1	3:BW:222:ASN:ND2	2.40	0.50
1:A0:32:LEU:HD11	1:A0:204:LEU:HB2	1.93	0.50
2:AO:177:GLN:HB3	2:AO:189:ARG:HB2	1.93	0.50
3:AX:144:PHE:HB3	3:AX:190:TRP:CE2	2.45	0.50
1:A0:42:ILE:HB	3:AX:43:TRP:HZ2	0.61	0.50
2:AQ:20:SER:HA	3:AX:160:TYR:CD1	2.46	0.50
2:AF:17:PRO:HA	3:AT:177:THR:CG2	2.38	0.50
3:BS:197:PHE:HD1	3:BT:48:ILE:HG22	1.76	0.50
3:AV:45:SER:HB2	1:AZ:42:ILE:HG22	1.92	0.50
3:BU:138:THR:O	3:BU:292:LYS:HA	2.11	0.50
3:BT:238:ILE:HG22	3:BT:240:ILE:HG23	1.94	0.50
3:AT:124:PHE:O	3:BS:120:LYS:NZ	2.43	0.50
2:BP:113:ASN:O	3:BX:186:ARG:NH2	2.44	0.50
2:AP:120:LYS:NZ	3:AX:220:ILE:O	2.37	0.50
1:BZ:157:PHE:HE2	1:BZ:208:PHE:HB3	1.76	0.50
3:AV:120:LYS:HZ1	3:BW:66:GLU:HB3	1.75	0.50
3:AU:116:GLU:OE2	3:AV:3:ARG:HG3	2.11	0.50
2:AD:88:ILE:HG12	2:AD:97:VAL:HG22	1.93	0.50
1:B0:122:PRO:HD2	1:B0:125:ILE:HD12	1.94	0.50
3:BU:281:LEU:HB3	3:BU:284:LEU:HD12	1.92	0.50
3:BT:87:LEU:HA	3:BU:54:ARG:NH1	2.26	0.50
2:BM:9:PHE:HB2	3:BW:180:GLY:HA2	1.92	0.50
3:BT:243:ASP:OD1	3:BT:243:ASP:C	2.50	0.50
3:BU:196:ILE:HG13	3:BU:274:ILE:HB	1.94	0.50
2:BA:102:GLU:OE2	3:BS:220:ILE:HD12	2.12	0.50
1:A0:288:ARG:NH2	1:AZ:12:PRO:HB2	2.27	0.50
2:BB:13:SER:C	3:BS:169:LYS:CD	2.59	0.50
3:AU:266:PHE:CG	1:AZ:35:PRO:HD2	2.47	0.50
3:AS:4:GLN:HB2	3:AS:97:GLN:HB3	1.93	0.50
1:B0:32:LEU:HD11	1:B0:204:LEU:HB2	1.93	0.50
3:AW:226:ALA:HB3	3:AW:268:ARG:HB3	1.92	0.50
2:AA:81:VAL:HB	1:AY:86:LYS:NZ	2.27	0.50
2:AP:21:ASN:HB3	3:AX:181:GLU:CG	2.42	0.50
3:AV:196:ILE:HG13	3:AV:274:ILE:HB	1.94	0.50
2:AO:171:GLY:HA3	2:AO:205:GLY:H	1.77	0.50
2:BD:88:ILE:HG12	2:BD:97:VAL:HG22	1.93	0.50
3:AT:36:LEU:HD22	3:AT:56:ILE:HD11	1.93	0.50
2:BL:177:GLN:HB3	2:BL:189:ARG:HB2	1.93	0.50
1:AY:39:CYS:HB2	1:AY:60:THR:OG1	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AJ:5:ASN:HB3	2:AJ:8:PHE:CD1	2.47	0.50
3:BV:240:ILE:C	3:BV:240:ILE:HD12	2.32	0.50
3:BV:96:TYR:HB3	3:BV:103:VAL:HG23	1.94	0.50
2:BK:116:SER:OG	3:BV:186:ARG:O	2.29	0.50
3:AU:68:PHE:HE1	3:BX:120:LYS:HG2	1.76	0.49
1:B0:76:VAL:HG11	1:B0:88:LYS:HD2	1.94	0.49
2:AR:9:PHE:CE1	3:AX:180:GLY:N	2.80	0.49
2:AR:177:GLN:HB3	2:AR:189:ARG:HB2	1.93	0.49
2:BR:177:GLN:HB3	2:BR:189:ARG:HB2	1.93	0.49
3:BV:48:ILE:HG21	1:BZ:1:MET:HE1	1.92	0.49
2:BO:171:GLY:HA3	2:BO:205:GLY:H	1.77	0.49
3:AU:171:ILE:HG22	3:AU:172:LYS:H	1.77	0.49
2:AL:177:GLN:HB3	2:AL:189:ARG:HB2	1.93	0.49
2:AA:172:ASN:HD21	2:AA:204:SER:H	1.60	0.49
2:BA:172:ASN:HD21	2:BA:204:SER:H	1.60	0.49
2:BF:17:PRO:CA	3:BT:177:THR:HG22	2.37	0.49
2:AP:22:ASN:HD21	3:AX:182:SER:HB3	1.77	0.49
3:AX:199:PHE:CZ	3:AX:242:THR:HG21	2.47	0.49
1:B0:86:LYS:HZ2	2:BN:81:VAL:HB	1.75	0.49
2:BN:120:LYS:HE2	3:BW:222:ASN:ND2	2.27	0.49
3:AT:199:PHE:H	3:AT:242:THR:HG1	1.57	0.49
1:A0:218:ILE:HB	1:A0:338:VAL:HG12	1.95	0.49
3:AS:171:ILE:HG22	3:AS:172:LYS:H	1.76	0.49
3:BS:4:GLN:HB2	3:BS:97:GLN:HB3	1.93	0.49
2:AF:177:GLN:HB3	2:AF:189:ARG:HB2	1.93	0.49
3:AV:43:TRP:HE1	1:AZ:42:ILE:HB	1.77	0.49
3:BX:199:PHE:CZ	3:BX:242:THR:HG21	2.47	0.49
3:AU:138:THR:O	3:AU:292:LYS:HA	2.11	0.49
1:AZ:152:PHE:CB	1:AZ:208:PHE:HB2	2.42	0.49
3:AW:120:LYS:CE	3:BV:68:PHE:CE1	2.90	0.49
3:AX:120:LYS:HZ1	3:BU:66:GLU:HG3	1.77	0.49
3:BS:197:PHE:CD1	3:BT:48:ILE:CG2	2.94	0.49
2:AQ:39:ARG:HB2	2:AQ:61:ILE:HB	1.94	0.49
3:AW:76:TYR:HB3	3:AX:100:ILE:HD11	1.94	0.49
3:BS:11:LEU:O	3:BS:12:ASP:CG	2.51	0.49
3:BW:4:GLN:HB2	3:BW:97:GLN:HB3	1.94	0.49
1:A0:122:PRO:HD2	1:A0:125:ILE:HD12	1.94	0.49
1:A0:242:ASN:O	1:A0:313:ILE:HD12	2.12	0.49
3:BS:196:ILE:HG22	3:BS:293:ARG:HD3	1.95	0.49
3:BX:171:ILE:HG22	3:BX:172:LYS:H	1.77	0.49
1:BY:45:GLU:HA	1:BY:357:THR:HG22	1.95	0.49
3:AU:270:ARG:NH1	1:AZ:72:LEU:HD22	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AI:171:GLY:HA3	2:AI:205:GLY:H	1.77	0.49
3:AX:171:ILE:HG22	3:AX:172:LYS:H	1.77	0.49
3:BT:36:LEU:HD22	3:BT:56:ILE:HD11	1.93	0.49
3:AT:243:ASP:C	3:AT:243:ASP:OD1	2.50	0.49
2:AR:7:THR:HA	3:AX:178:TYR:CE2	2.47	0.49
3:BV:196:ILE:HG13	3:BV:274:ILE:HB	1.94	0.49
1:BZ:152:PHE:CB	1:BZ:208:PHE:HB2	2.42	0.49
2:AK:39:ARG:HB2	2:AK:61:ILE:HB	1.94	0.49
2:AN:39:ARG:HB2	2:AN:61:ILE:HB	1.94	0.49
3:AW:4:GLN:HB2	3:AW:97:GLN:HB3	1.94	0.49
1:A0:76:VAL:HG11	1:A0:88:LYS:HD2	1.94	0.49
2:AF:18:VAL:HG12	3:AT:176:TYR:O	2.12	0.49
2:BC:18:VAL:HG13	3:BS:176:TYR:CE2	2.47	0.49
3:AU:196:ILE:HG13	3:AU:274:ILE:HB	1.94	0.49
2:AF:171:GLY:HA3	2:AF:205:GLY:H	1.77	0.49
2:AP:118:VAL:HG23	3:AX:278:GLN:NE2	2.27	0.49
2:BQ:39:ARG:HB2	2:BQ:61:ILE:HB	1.94	0.49
3:BU:171:ILE:HG22	3:BU:172:LYS:H	1.77	0.49
2:AD:52:ASN:HB2	3:AS:258:LEU:CD2	2.30	0.49
3:AU:53:THR:HG21	1:AZ:359:PHE:CA	2.43	0.49
2:AG:79:ASP:CB	1:AZ:212:ASN:HD21	2.25	0.49
2:BC:18:VAL:CG1	3:BS:176:TYR:CZ	2.96	0.49
2:BG:79:ASP:C	1:BZ:212:ASN:HD21	2.16	0.49
2:BN:100:SER:HB3	3:BW:220:ILE:HG21	1.95	0.49
3:AS:11:LEU:O	3:AS:12:ASP:CG	2.51	0.49
1:B0:218:ILE:HB	1:B0:338:VAL:HG12	1.95	0.49
2:BF:171:GLY:HA3	2:BF:205:GLY:H	1.77	0.49
2:BM:17:PRO:HA	3:BW:177:THR:HG22	1.95	0.49
2:AK:91:THR:HG21	3:AV:189:ARG:HB2	1.93	0.49
2:BP:22:ASN:HD21	3:BX:182:SER:CB	2.25	0.49
1:BY:169:THR:HG21	1:BZ:294:PHE:CZ	2.47	0.49
3:AS:133:ILE:HA	3:AT:42:ILE:CG2	2.39	0.49
1:BY:39:CYS:HB2	1:BY:60:THR:OG1	2.12	0.49
2:AJ:26:LEU:HD13	2:AK:66:TYR:HB2	1.94	0.49
3:AV:240:ILE:C	3:AV:240:ILE:HD12	2.32	0.49
2:BJ:26:LEU:HD13	2:BK:66:TYR:HB2	1.94	0.49
2:BC:171:GLY:HA3	2:BC:205:GLY:H	1.77	0.49
2:AR:171:GLY:HA3	2:AR:205:GLY:H	1.77	0.49
1:AY:233:GLU:HB2	1:AY:321:ARG:HH21	1.78	0.49
3:BU:229:PHE:CD1	3:BU:264:MET:HB3	2.48	0.49
2:BJ:5:ASN:HB3	2:BJ:8:PHE:CD1	2.47	0.49
3:BT:199:PHE:CE1	3:BT:242:THR:HG21	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AU:229:PHE:CD1	3:AU:264:MET:HB3	2.48	0.49
3:AT:199:PHE:CE1	3:AT:242:THR:HG21	2.48	0.49
2:BG:92:GLN:HE21	3:BU:189:ARG:NE	2.11	0.49
2:BH:19:GLY:HA2	3:BU:166:GLY:O	2.13	0.48
2:BQ:8:PHE:O	3:BX:170:TYR:HB2	2.12	0.48
3:BT:199:PHE:N	3:BT:242:THR:OG1	2.39	0.48
2:BN:39:ARG:HB2	2:BN:61:ILE:HB	1.93	0.48
1:B0:242:ASN:O	1:B0:313:ILE:HD12	2.12	0.48
3:BV:87:LEU:HA	3:BW:54:ARG:NH1	2.28	0.48
2:BL:171:GLY:HA3	2:BL:205:GLY:H	1.77	0.48
2:BH:39:ARG:HB2	2:BH:61:ILE:HB	1.95	0.48
3:BX:242:THR:O	3:BX:272:ARG:HD3	2.13	0.48
3:AT:238:ILE:HG22	3:AT:240:ILE:HG23	1.94	0.48
2:BI:171:GLY:HA3	2:BI:205:GLY:H	1.77	0.48
1:BY:233:GLU:HB2	1:BY:321:ARG:HH21	1.77	0.48
1:A0:184:GLN:HE22	1:A0:217:ARG:HH22	1.61	0.48
3:BT:76:TYR:HE1	3:BU:96:TYR:OH	1.96	0.48
2:BQ:17:PRO:HB3	3:BX:169:LYS:CE	2.38	0.48
2:AR:17:PRO:HA	3:AX:177:THR:CG2	2.43	0.48
3:BV:215:ARG:HB3	3:BV:282:ILE:HD11	1.95	0.48
3:AT:212:ALA:HB2	3:AT:283:ASN:HD22	1.79	0.48
2:AE:39:ARG:HB2	2:AE:61:ILE:HB	1.94	0.48
3:AU:114:LYS:NZ	3:AV:298:VAL:O	2.45	0.48
2:BH:17:PRO:HB3	3:BU:169:LYS:HE3	1.94	0.48
2:AH:39:ARG:HB2	2:AH:61:ILE:HB	1.94	0.48
3:BV:36:LEU:HD21	3:BV:297:PHE:HB2	1.96	0.48
1:B0:288:ARG:NH2	1:BZ:12:PRO:HB2	2.28	0.48
2:BD:52:ASN:ND2	3:BS:258:LEU:HB3	2.29	0.48
3:AU:272:ARG:NH1	1:AZ:40:GLN:OE1	2.46	0.48
2:BR:9:PHE:CZ	3:BX:180:GLY:C	2.87	0.48
1:B0:294:PHE:CE2	1:BZ:169:THR:CG2	2.96	0.48
2:BG:104:ALA:HB3	1:BZ:88:LYS:HD2	1.94	0.48
2:BE:39:ARG:HB2	2:BE:61:ILE:HB	1.95	0.48
1:B0:184:GLN:HE22	1:B0:217:ARG:HH22	1.61	0.48
2:AN:49:THR:HG21	3:AV:235:GLN:NE2	2.29	0.48
3:AT:120:LYS:HZ1	3:BS:66:GLU:HG3	1.75	0.48
3:AS:196:ILE:HG22	3:AS:293:ARG:HD3	1.95	0.48
3:BX:281:LEU:HB3	3:BX:284:LEU:HD12	1.96	0.48
3:AV:243:ASP:OD1	3:AV:243:ASP:C	2.52	0.48
1:A0:231:ASP:OD2	1:A0:321:ARG:NH1	2.47	0.48
2:AC:171:GLY:HA3	2:AC:205:GLY:H	1.77	0.48
1:AY:45:GLU:HA	1:AY:357:THR:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BS:96:TYR:HH	3:BX:76:TYR:HE1	1.62	0.48
2:BE:18:VAL:CG1	3:BT:168:TYR:O	2.54	0.48
2:BR:9:PHE:HZ	3:BX:181:GLU:HG3	1.76	0.48
2:BD:23:ASP:OD2	3:BT:178:TYR:CE1	2.62	0.48
1:AZ:237:ASP:C	1:AZ:238:ARG:HG2	2.33	0.48
2:BN:47:LEU:HD22	3:BV:233:GLN:CD	2.34	0.48
2:BG:92:GLN:NE2	3:BU:189:ARG:CZ	2.77	0.48
2:AR:10:SER:HA	2:AR:15:GLU:HB2	1.96	0.48
1:BY:122:PRO:HD2	1:BY:125:ILE:HD12	1.96	0.48
2:BK:39:ARG:HB2	2:BK:61:ILE:HB	1.94	0.48
3:AV:36:LEU:HD21	3:AV:297:PHE:HB2	1.96	0.48
3:BV:144:PHE:HB3	3:BV:190:TRP:CE2	2.49	0.48
3:AS:242:THR:O	3:AS:272:ARG:HD3	2.14	0.48
1:B0:231:ASP:OD2	1:B0:321:ARG:NH1	2.47	0.48
2:BR:10:SER:HA	2:BR:15:GLU:HB2	1.96	0.48
3:AT:26:VAL:HG23	3:AT:67:THR:HG22	1.96	0.48
3:BT:26:VAL:HG23	3:BT:67:THR:HG22	1.96	0.48
3:AS:239:LEU:C	3:AS:239:LEU:HD23	2.34	0.48
2:AR:9:PHE:CZ	3:AX:181:GLU:N	2.82	0.48
1:BZ:237:ASP:C	1:BZ:238:ARG:HG2	2.33	0.48
3:BS:239:LEU:HD23	3:BS:239:LEU:C	2.35	0.48
2:BR:171:GLY:HA3	2:BR:205:GLY:H	1.77	0.48
1:AY:122:PRO:HD2	1:AY:125:ILE:HD12	1.96	0.48
2:BD:131:THR:O	3:BS:263:VAL:HG23	2.13	0.48
3:BS:242:THR:O	3:BS:272:ARG:HD3	2.14	0.48
3:AX:68:PHE:CE1	3:BU:120:LYS:HD3	2.48	0.48
3:AU:106:ASP:O	3:AU:133:ILE:HB	2.14	0.48
3:BU:116:GLU:HB2	3:BV:31:PRO:HD2	1.95	0.48
3:BW:11:LEU:HD12	3:BW:93:THR:HG21	1.96	0.48
2:AK:116:SER:OG	3:AV:186:ARG:O	2.32	0.48
2:BB:39:ARG:HB2	2:BB:61:ILE:HB	1.95	0.48
2:BP:9:PHE:HA	3:BX:160:TYR:O	2.13	0.47
3:AU:194:GLU:HB2	3:AU:293:ARG:HD2	1.96	0.47
3:BT:226:ALA:HB3	3:BT:268:ARG:HB3	1.95	0.47
2:BR:27:TYR:HA	2:BR:30:LEU:HD12	1.96	0.47
2:BI:27:TYR:HA	2:BI:30:LEU:HD12	1.96	0.47
3:AV:96:TYR:HB3	3:AV:103:VAL:HG23	1.94	0.47
3:AU:120:LYS:HD3	3:BX:68:PHE:CE1	2.49	0.47
2:AP:19:GLY:CA	3:AX:180:GLY:O	2.62	0.47
2:AR:23:ASP:OD2	3:AX:176:TYR:CZ	2.67	0.47
3:AX:242:THR:O	3:AX:272:ARG:HD3	2.13	0.47
1:A0:169:THR:HG21	1:AY:294:PHE:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BT:212:ALA:HB2	3:BT:283:ASN:HD22	1.79	0.47
3:BV:243:ASP:C	3:BV:243:ASP:OD1	2.52	0.47
3:AW:11:LEU:HD12	3:AW:93:THR:HG21	1.96	0.47
2:AP:148:ILE:HB	2:AR:153:MET:HG3	1.96	0.47
3:AW:171:ILE:HG22	3:AW:172:LYS:H	1.79	0.47
3:AV:215:ARG:HB3	3:AV:282:ILE:HD11	1.95	0.47
3:AU:66:GLU:CG	3:BX:120:LYS:CE	2.92	0.47
2:AQ:17:PRO:CG	3:AX:169:LYS:CE	2.93	0.47
3:BT:199:PHE:H	3:BT:242:THR:HG1	1.57	0.47
2:AR:27:TYR:HA	2:AR:30:LEU:HD12	1.96	0.47
2:AB:39:ARG:HB2	2:AB:61:ILE:HB	1.95	0.47
1:BZ:231:ASP:OD2	1:BZ:321:ARG:NH1	2.47	0.47
3:AT:226:ALA:HB3	3:AT:268:ARG:HB3	1.95	0.47
2:BN:73:THR:CB	3:BV:256:THR:HG21	2.44	0.47
3:BW:171:ILE:HG22	3:BW:172:LYS:H	1.79	0.47
2:AB:13:SER:C	3:AS:169:LYS:CD	2.62	0.47
2:BD:73:THR:HG21	3:BS:256:THR:HG21	1.94	0.47
3:BU:194:GLU:HB2	3:BU:293:ARG:HD2	1.96	0.47
3:BU:106:ASP:O	3:BU:133:ILE:HB	2.14	0.47
3:AU:11:LEU:O	3:AU:12:ASP:CG	2.52	0.47
3:AS:281:LEU:HB3	3:AS:284:LEU:HD12	1.96	0.47
2:AL:171:GLY:HA3	2:AL:205:GLY:H	1.77	0.47
3:AX:281:LEU:HB3	3:AX:284:LEU:HD12	1.96	0.47
3:AV:66:GLU:CG	3:BW:120:LYS:HZ3	2.26	0.47
2:AD:77:LYS:H	2:AD:82:ASN:ND2	2.12	0.47
3:AV:144:PHE:HB3	3:AV:190:TRP:CE2	2.49	0.47
3:AV:160:TYR:HB3	3:AV:166:GLY:HA3	1.95	0.47
3:BU:11:LEU:O	3:BU:12:ASP:CG	2.52	0.47
3:BV:160:TYR:HB3	3:BV:166:GLY:HA3	1.95	0.47
1:AZ:231:ASP:OD2	1:AZ:321:ARG:NH1	2.47	0.47
2:BD:51:LEU:HD12	3:BS:262:PRO:HG2	1.95	0.47
2:BE:18:VAL:C	3:BT:167:ASN:HA	2.35	0.47
3:AU:244:VAL:HG11	1:AZ:1:MET:HE1	1.96	0.47
2:AD:23:ASP:OD2	3:AT:178:TYR:CE1	2.67	0.47
3:BS:281:LEU:HB3	3:BS:284:LEU:HD12	1.96	0.47
3:BX:4:GLN:HB2	3:BX:97:GLN:HB3	1.96	0.47
3:BS:72:LEU:HD22	3:BS:76:TYR:CE2	2.50	0.47
1:A0:359:PHE:O	3:AW:53:THR:HG21	2.14	0.47
2:BF:23:ASP:OD2	3:BT:176:TYR:HE2	1.97	0.47
3:AV:196:ILE:HD13	3:AV:291:ILE:HG12	1.97	0.47
2:AI:27:TYR:HA	2:AI:30:LEU:HD12	1.96	0.47
2:BD:19:GLY:CA	3:BT:180:GLY:O	2.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BV:196:ILE:HD13	3:BV:291:ILE:HG12	1.97	0.47
2:AP:172:ASN:HD21	2:AP:204:SER:H	1.63	0.47
3:AX:196:ILE:HD13	3:AX:291:ILE:HG13	1.97	0.47
3:BX:72:LEU:HD22	3:BX:76:TYR:CE2	2.50	0.47
3:BV:243:ASP:OD1	3:BV:245:ASN:N	2.48	0.47
3:AV:43:TRP:NE1	1:AZ:42:ILE:HB	2.30	0.46
2:BE:9:PHE:HD2	3:BT:170:TYR:C	2.18	0.46
2:BG:172:ASN:HD21	2:BG:204:SER:H	1.63	0.46
2:BP:148:ILE:HB	2:BR:153:MET:HG3	1.96	0.46
2:AM:5:ASN:HB3	2:AM:8:PHE:CD1	2.50	0.46
2:AH:17:PRO:HB3	3:AU:169:LYS:HE3	1.97	0.46
3:BX:196:ILE:HD13	3:BX:291:ILE:HG13	1.97	0.46
3:BW:72:LEU:HD22	3:BW:76:TYR:CE2	2.50	0.46
2:BM:5:ASN:HB3	2:BM:8:PHE:CD1	2.51	0.46
2:BP:172:ASN:HD21	2:BP:204:SER:H	1.63	0.46
2:AA:102:GLU:OE2	3:AS:220:ILE:HD12	2.15	0.46
2:AG:79:ASP:O	1:AZ:212:ASN:OD1	2.32	0.46
2:AG:172:ASN:HD21	2:AG:204:SER:H	1.63	0.46
3:BU:72:LEU:HD22	3:BU:76:TYR:CE2	2.51	0.46
3:AS:194:GLU:HB2	3:AS:293:ARG:HD2	1.97	0.46
3:BV:196:ILE:HG22	3:BV:293:ARG:HD3	1.98	0.46
3:BT:242:THR:O	3:BT:272:ARG:HD3	2.16	0.46
3:AX:96:TYR:HB3	3:AX:103:VAL:HG23	1.98	0.46
3:AS:72:LEU:HD22	3:AS:76:TYR:CE2	2.50	0.46
2:AQ:17:PRO:CA	3:AX:169:LYS:HD3	2.46	0.46
2:BA:77:LYS:H	2:BA:82:ASN:ND2	2.11	0.46
2:BG:81:VAL:HB	1:BZ:86:LYS:HZ1	1.79	0.46
3:AT:242:THR:O	3:AT:272:ARG:HD3	2.16	0.46
1:A0:292:THR:HB	1:AZ:120:ASP:HB2	1.97	0.46
3:AV:68:PHE:HD1	3:BW:120:LYS:HD2	1.72	0.46
2:BQ:17:PRO:CB	3:BX:167:ASN:HD22	2.13	0.46
2:BE:19:GLY:HA2	3:BT:166:GLY:C	2.35	0.46
2:AE:9:PHE:HD2	3:AT:170:TYR:C	2.18	0.46
2:BQ:19:GLY:HA2	3:BX:166:GLY:C	2.35	0.46
3:AW:72:LEU:HD22	3:AW:76:TYR:CE2	2.50	0.46
2:BA:131:THR:HG22	3:BX:262:PRO:O	2.16	0.46
1:A0:130:ASN:HA	1:A0:133:ILE:HD12	1.98	0.46
2:AM:172:ASN:HD21	2:AM:204:SER:H	1.62	0.46
2:BB:13:SER:O	3:BS:169:LYS:HE2	2.07	0.46
2:AR:9:PHE:CD1	3:AX:180:GLY:HA2	2.51	0.46
3:BV:72:LEU:HD22	3:BV:76:TYR:CE2	2.50	0.46
1:AZ:130:ASN:HA	1:AZ:133:ILE:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BE:171:GLY:HA3	2:BE:205:GLY:H	1.81	0.46
2:AD:112:ILE:O	3:AT:186:ARG:NH1	2.46	0.46
2:BP:77:LYS:H	2:BP:82:ASN:ND2	2.12	0.46
2:AA:81:VAL:HB	1:AY:86:LYS:HZ1	1.81	0.46
3:AV:243:ASP:OD1	3:AV:245:ASN:N	2.48	0.46
2:BD:172:ASN:HD21	2:BD:204:SER:H	1.64	0.46
3:BU:69:GLY:H	3:BU:75:ASN:HD21	1.64	0.46
3:AT:96:TYR:HB3	3:AT:103:VAL:HG23	1.98	0.46
2:BM:148:ILE:HB	2:BO:153:MET:HG3	1.98	0.46
3:AU:206:LYS:HG3	3:AU:285:SER:HB3	1.98	0.46
3:AV:196:ILE:HG22	3:AV:293:ARG:HD3	1.98	0.46
3:BS:194:GLU:HB2	3:BS:293:ARG:HD2	1.97	0.46
3:BT:76:TYR:CE1	3:BU:96:TYR:OH	2.68	0.46
2:AE:26:LEU:HD13	2:AF:66:TYR:HB2	1.98	0.46
3:AX:72:LEU:HD22	3:AX:76:TYR:CE2	2.51	0.46
3:AV:72:LEU:HD22	3:AV:76:TYR:CE2	2.50	0.46
2:AR:5:ASN:HB3	2:AR:8:PHE:CD1	2.51	0.46
2:BK:171:GLY:HA3	2:BK:205:GLY:H	1.81	0.46
2:BH:171:GLY:HA3	2:BH:205:GLY:H	1.81	0.46
3:BT:96:TYR:HB3	3:BT:103:VAL:HG23	1.98	0.46
2:AE:171:GLY:HA3	2:AE:205:GLY:H	1.81	0.46
3:AU:72:LEU:HD22	3:AU:76:TYR:CE2	2.51	0.45
3:BU:229:PHE:CD1	3:BU:260:LEU:HB3	2.52	0.45
2:BE:26:LEU:HD13	2:BF:66:TYR:HB2	1.98	0.45
3:BW:144:PHE:HB3	3:BW:190:TRP:CE2	2.52	0.45
1:B0:130:ASN:HA	1:B0:133:ILE:HD12	1.98	0.45
2:BQ:17:PRO:HG3	3:BX:169:LYS:CE	2.45	0.45
2:AE:18:VAL:HG13	3:AT:168:TYR:CE2	2.51	0.45
3:BU:242:THR:CG2	3:BU:272:ARG:CG	2.93	0.45
3:AU:229:PHE:CD1	3:AU:260:LEU:HB3	2.52	0.45
1:AY:251:LYS:HG2	1:AY:297:ARG:HD3	1.97	0.45
1:AY:130:ASN:HA	1:AY:133:ILE:HD12	1.99	0.45
2:BR:5:ASN:HB3	2:BR:8:PHE:CD1	2.51	0.45
1:BZ:130:ASN:HA	1:BZ:133:ILE:HD12	1.98	0.45
2:BG:17:PRO:HA	3:BU:159:ILE:HG22	1.98	0.45
3:AX:4:GLN:HB2	3:AX:97:GLN:HB3	1.96	0.45
1:A0:42:ILE:CB	3:AX:43:TRP:CZ2	2.47	0.45
2:AE:8:PHE:O	3:AT:170:TYR:HB2	2.15	0.45
2:BG:77:LYS:H	2:BG:82:ASN:ND2	2.12	0.45
2:BO:17:PRO:CB	3:BW:167:ASN:HB2	2.47	0.45
3:BU:206:LYS:HG3	3:BU:285:SER:HB3	1.97	0.45
2:AD:172:ASN:HD21	2:AD:204:SER:H	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AW:120:LYS:CE	3:BV:66:GLU:CG	2.92	0.45
1:BY:169:THR:HG21	1:BZ:294:PHE:HE2	1.71	0.45
2:BE:8:PHE:O	3:BT:170:TYR:HB2	2.16	0.45
2:AP:113:ASN:C	3:AX:186:ARG:NH2	2.68	0.45
2:AJ:172:ASN:HD21	2:AJ:204:SER:H	1.63	0.45
2:AB:26:LEU:HD13	2:AC:66:TYR:HB2	1.98	0.45
3:BX:96:TYR:HB3	3:BX:103:VAL:HG23	1.98	0.45
3:AT:72:LEU:HD22	3:AT:76:TYR:CE2	2.51	0.45
3:AU:96:TYR:HB3	3:AU:103:VAL:HG23	1.99	0.45
3:BU:4:GLN:HB2	3:BU:97:GLN:HB3	1.97	0.45
3:AV:120:LYS:NZ	3:BW:66:GLU:HB3	2.28	0.45
1:A0:329:LEU:HB3	3:AV:261:PHE:CG	2.52	0.45
3:AU:229:PHE:CE1	3:AU:264:MET:HB3	2.52	0.45
2:BJ:148:ILE:HB	2:BL:153:MET:HG3	1.99	0.45
3:AU:4:GLN:HB2	3:AU:97:GLN:HB3	1.97	0.45
1:B0:1:MET:SD	3:BX:48:ILE:HD13	2.57	0.45
1:B0:78:PRO:HG3	2:BN:103:THR:HB	1.98	0.45
3:BT:144:PHE:HB3	3:BT:190:TRP:CE2	2.52	0.45
2:BJ:172:ASN:HD21	2:BJ:204:SER:H	1.63	0.45
3:AU:69:GLY:H	3:AU:75:ASN:HD21	1.64	0.45
2:BN:52:ASN:ND2	3:BV:258:LEU:HG	2.32	0.45
3:AT:240:ILE:HG22	3:AT:249:TYR:HD1	1.82	0.45
3:BS:11:LEU:HD12	3:BS:93:THR:HG21	1.99	0.45
3:BT:72:LEU:HD22	3:BT:76:TYR:CE2	2.51	0.45
2:BQ:171:GLY:HA3	2:BQ:205:GLY:H	1.81	0.45
2:AP:39:ARG:HB2	2:AP:61:ILE:HB	1.99	0.45
2:AM:27:TYR:HA	2:AM:30:LEU:HD12	1.99	0.45
1:BY:130:ASN:HA	1:BY:133:ILE:HD12	1.99	0.45
2:AG:77:LYS:H	2:AG:82:ASN:ND2	2.12	0.45
2:BA:106:ASN:OD1	1:BY:88:LYS:HD2	2.17	0.45
2:BM:27:TYR:HA	2:BM:30:LEU:HD12	1.99	0.45
3:BU:144:PHE:HB3	3:BU:190:TRP:CE2	2.52	0.45
2:AJ:148:ILE:HB	2:AL:153:MET:HG3	1.99	0.45
2:BP:22:ASN:ND2	3:BX:182:SER:OG	2.43	0.45
3:AW:144:PHE:HB3	3:AW:190:TRP:CE2	2.52	0.45
2:AM:17:PRO:HA	3:AW:177:THR:HG22	1.98	0.45
2:BD:77:LYS:H	2:BD:82:ASN:ND2	2.12	0.45
2:AG:9:PHE:HA	3:AU:160:TYR:HB2	1.98	0.45
3:BU:116:GLU:OE2	3:BV:3:ARG:HG3	2.16	0.45
3:AT:76:TYR:HE1	3:AU:96:TYR:OH	2.00	0.45
3:AU:144:PHE:HB3	3:AU:190:TRP:CE2	2.52	0.45
2:AD:146:ASP:O	2:AF:151:ASN:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BY:251:LYS:HG2	1:BY:297:ARG:HD3	1.97	0.45
2:AR:81:VAL:HG22	2:AR:127:THR:HG23	1.99	0.45
2:BM:172:ASN:HD21	2:BM:204:SER:H	1.62	0.45
2:BD:51:LEU:HD11	3:BS:262:PRO:HG2	1.97	0.45
3:AT:136:TRP:HB2	3:AT:295:ALA:O	2.17	0.45
2:AB:171:GLY:HA3	2:AB:205:GLY:H	1.81	0.45
2:BR:81:VAL:HG22	2:BR:127:THR:HG23	1.99	0.45
2:BB:171:GLY:HA3	2:BB:205:GLY:H	1.81	0.45
2:BP:19:GLY:HA3	3:BX:180:GLY:O	2.17	0.44
2:AR:23:ASP:OD2	3:AX:176:TYR:HE2	1.99	0.44
3:AU:266:PHE:CD2	1:AZ:35:PRO:HD2	2.52	0.44
3:BW:194:GLU:HB2	3:BW:293:ARG:HD2	1.99	0.44
2:BC:81:VAL:HG22	2:BC:127:THR:HG23	1.99	0.44
2:BN:171:GLY:HA3	2:BN:205:GLY:H	1.81	0.44
2:AJ:39:ARG:HB2	2:AJ:61:ILE:HB	1.99	0.44
2:AH:171:GLY:HA3	2:AH:205:GLY:H	1.81	0.44
2:AA:77:LYS:H	2:AA:82:ASN:ND2	2.11	0.44
2:AM:148:ILE:HB	2:AO:153:MET:HG3	1.98	0.44
2:AQ:171:GLY:HA3	2:AQ:205:GLY:H	1.81	0.44
2:BD:146:ASP:O	2:BF:151:ASN:HB2	2.17	0.44
2:BP:39:ARG:HB2	2:BP:61:ILE:HB	1.99	0.44
2:BQ:251:THR:HA	2:BQ:252:PRO:HD3	1.86	0.44
3:BS:197:PHE:HD1	3:BT:48:ILE:CG2	2.30	0.44
3:BT:240:ILE:HG22	3:BT:249:TYR:HD1	1.82	0.44
3:AS:239:LEU:HD23	3:AS:240:ILE:N	2.32	0.44
2:AG:104:ALA:HB3	1:AZ:88:LYS:HD2	1.98	0.44
1:A0:220:THR:HG21	1:A0:332:LEU:HD21	2.00	0.44
1:BY:1:MET:HG3	1:BY:40:GLN:HB2	2.00	0.44
3:BU:96:TYR:HB3	3:BU:103:VAL:HG23	1.99	0.44
2:AO:81:VAL:HG22	2:AO:127:THR:HG23	1.99	0.44
2:AA:39:ARG:HB2	2:AA:61:ILE:HB	2.00	0.44
2:AC:81:VAL:HG22	2:AC:127:THR:HG23	1.99	0.44
2:BH:26:LEU:HD13	2:BI:66:TYR:HB2	1.99	0.44
3:AT:144:PHE:HB3	3:AT:190:TRP:CE2	2.52	0.44
3:AX:120:LYS:CE	3:BU:66:GLU:CG	2.96	0.44
3:BU:271:THR:HA	1:BZ:3:GLU:HG3	1.99	0.44
2:AA:172:ASN:ND2	2:AA:204:SER:H	2.16	0.44
3:BU:229:PHE:CE1	3:BU:264:MET:HB3	2.52	0.44
3:BV:76:TYR:HE1	3:BW:96:TYR:HH	1.63	0.44
3:AW:247:GLU:OE1	3:AW:249:TYR:HE2	2.01	0.44
1:AZ:184:GLN:HE22	1:AZ:217:ARG:HH22	1.66	0.44
3:AU:70:GLU:HG2	3:BX:70:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AU:55:SER:HB3	1:AZ:359:PHE:CE1	2.53	0.44
2:BF:20:SER:HA	3:BT:170:TYR:CD1	2.53	0.44
3:AU:242:THR:CG2	3:AU:272:ARG:CG	2.93	0.44
3:AV:194:GLU:HB2	3:AV:293:ARG:HD2	1.99	0.44
3:AS:11:LEU:HD12	3:AS:93:THR:HG21	1.99	0.44
3:BS:239:LEU:HD23	3:BS:240:ILE:N	2.33	0.44
1:B0:220:THR:HG21	1:B0:332:LEU:HD21	2.00	0.44
2:AF:81:VAL:HG22	2:AF:127:THR:HG23	1.99	0.44
2:BG:39:ARG:HB2	2:BG:61:ILE:HB	2.00	0.44
1:BZ:251:LYS:HG2	1:BZ:297:ARG:HD3	1.98	0.44
2:BK:26:LEU:HD13	2:BL:66:TYR:HB2	2.00	0.44
2:BB:26:LEU:HD13	2:BC:66:TYR:HB2	1.99	0.44
2:AN:171:GLY:HA3	2:AN:205:GLY:H	1.81	0.44
2:AK:171:GLY:HA3	2:AK:205:GLY:H	1.81	0.44
2:BA:39:ARG:HB2	2:BA:61:ILE:HB	2.00	0.44
2:BI:81:VAL:HG22	2:BI:127:THR:HG23	1.99	0.44
3:AS:138:THR:O	3:AS:292:LYS:HA	2.17	0.44
1:B0:262:MET:SD	1:BZ:142:LYS:HG2	2.57	0.44
3:AX:5:TYR:HB3	3:AX:21:VAL:HG23	2.00	0.44
2:BG:9:PHE:HA	3:BU:160:TYR:HB2	1.98	0.44
3:BT:136:TRP:HB2	3:BT:295:ALA:O	2.17	0.44
2:BQ:18:VAL:C	3:BX:167:ASN:HA	2.36	0.44
3:AT:76:TYR:CE1	3:AU:96:TYR:OH	2.70	0.44
1:AZ:251:LYS:HG2	1:AZ:297:ARG:HD3	1.98	0.44
2:BL:39:ARG:HB2	2:BL:61:ILE:HB	2.00	0.44
2:AL:39:ARG:HB2	2:AL:61:ILE:HB	2.00	0.44
2:BM:66:TYR:HB2	2:BO:26:LEU:HD13	1.99	0.44
2:AG:39:ARG:HB2	2:AG:61:ILE:HB	2.00	0.44
2:AG:81:VAL:HB	1:AZ:86:LYS:HZ2	1.82	0.44
2:BH:17:PRO:HB3	3:BU:169:LYS:CE	2.48	0.44
2:BC:39:ARG:HB2	2:BC:61:ILE:HB	2.00	0.44
2:BD:112:ILE:O	3:BT:186:ARG:NH1	2.45	0.44
1:BZ:32:LEU:HD11	1:BZ:204:LEU:HB2	1.99	0.44
1:B0:39:CYS:HB2	1:B0:60:THR:OG1	2.18	0.44
3:BS:138:THR:O	3:BS:292:LYS:HA	2.17	0.44
3:AW:194:GLU:HB2	3:AW:293:ARG:HD2	1.99	0.44
1:AZ:1:MET:HG3	1:AZ:40:GLN:HB2	2.00	0.43
2:AR:9:PHE:CZ	3:AX:180:GLY:HA2	2.53	0.43
1:A0:1:MET:HG3	1:A0:40:GLN:HB2	2.00	0.43
1:B0:1:MET:HG3	1:B0:40:GLN:HB2	2.00	0.43
2:BL:81:VAL:HG22	2:BL:127:THR:HG23	2.00	0.43
2:AH:26:LEU:HD13	2:AI:66:TYR:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BO:81:VAL:HG22	2:BO:127:THR:HG23	1.99	0.43
2:AM:39:ARG:HB2	2:AM:61:ILE:HB	2.00	0.43
3:BV:194:GLU:HB2	3:BV:293:ARG:HD2	1.99	0.43
2:AK:114:ASN:O	3:AV:186:ARG:CD	2.66	0.43
1:A0:262:MET:SD	1:AZ:142:LYS:HG2	2.57	0.43
2:BO:39:ARG:HB2	2:BO:61:ILE:HB	2.01	0.43
2:BF:81:VAL:HG22	2:BF:127:THR:HG23	1.99	0.43
2:AK:49:THR:HB	3:AU:258:LEU:HD21	2.00	0.43
1:BY:41:VAL:HG11	1:BY:71:ILE:HG12	2.00	0.43
2:BE:155:VAL:HG21	2:BE:159:ILE:HD11	2.00	0.43
2:AM:66:TYR:HB2	2:AO:26:LEU:HD13	1.99	0.43
2:BO:27:TYR:HA	2:BO:30:LEU:HD12	2.00	0.43
2:BD:39:ARG:HB2	2:BD:61:ILE:HB	2.00	0.43
2:BD:49:THR:CG2	3:BS:233:GLN:HB2	2.49	0.43
2:AD:51:LEU:HD12	3:AS:262:PRO:HG2	2.00	0.43
1:B0:12:PRO:HB2	1:BY:288:ARG:CZ	2.47	0.43
2:AD:39:ARG:HB2	2:AD:61:ILE:HB	2.00	0.43
3:BX:5:TYR:HB3	3:BX:21:VAL:HG23	2.00	0.43
3:AV:66:GLU:CG	3:BW:120:LYS:CE	2.95	0.43
2:AQ:20:SER:HA	3:AX:160:TYR:CE1	2.53	0.43
2:AE:18:VAL:C	3:AT:167:ASN:HA	2.39	0.43
2:AF:9:PHE:CB	3:AT:180:GLY:HA2	2.48	0.43
2:AO:39:ARG:HB2	2:AO:61:ILE:HB	2.00	0.43
2:AL:81:VAL:HG22	2:AL:127:THR:HG23	2.00	0.43
2:AA:66:TYR:HB2	2:AC:26:LEU:HD13	1.99	0.43
1:A0:39:CYS:HB2	1:A0:60:THR:OG1	2.18	0.43
2:AM:9:PHE:HB2	3:AW:180:GLY:HA2	2.01	0.43
2:AH:155:VAL:HG21	2:AH:159:ILE:HD11	2.00	0.43
2:AG:92:GLN:HE21	3:AU:189:ARG:CZ	2.31	0.43
1:AY:1:MET:HG3	1:AY:40:GLN:HB2	1.99	0.43
2:AH:19:GLY:HA2	3:AU:166:GLY:O	2.19	0.43
1:AY:41:VAL:HG11	1:AY:71:ILE:HG12	2.00	0.43
2:BF:155:VAL:HG21	2:BF:159:ILE:HD11	2.01	0.43
2:AQ:155:VAL:HG21	2:AQ:159:ILE:HD11	2.01	0.43
3:BS:96:TYR:HB3	3:BS:103:VAL:HG23	1.99	0.43
1:AZ:32:LEU:HD11	1:AZ:204:LEU:HB2	1.99	0.43
1:B0:17:ILE:HD13	1:BY:279:GLY:O	2.18	0.43
2:BF:39:ARG:HB2	2:BF:61:ILE:HB	2.00	0.43
2:AE:155:VAL:HG21	2:AE:159:ILE:HD11	2.00	0.43
2:AI:81:VAL:HG22	2:AI:127:THR:HG23	1.99	0.43
2:AK:21:ASN:H	3:AV:181:GLU:HG2	1.83	0.43
1:BZ:184:GLN:HE22	1:BZ:217:ARG:HH22	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BJ:39:ARG:HB2	2:BJ:61:ILE:HB	1.99	0.43
2:AP:49:THR:HB	3:AW:258:LEU:HD21	2.00	0.43
2:AG:79:ASP:OD1	1:AZ:216:LYS:HB2	2.18	0.43
3:BU:271:THR:HA	1:BZ:3:GLU:CG	2.49	0.43
3:AT:171:ILE:H	3:AT:175:SER:HA	1.84	0.43
2:BM:77:LYS:H	2:BM:82:ASN:ND2	2.13	0.43
3:AW:196:ILE:HD11	3:AW:199:PHE:HD1	1.83	0.43
3:BV:48:ILE:HD13	1:BZ:1:MET:SD	2.59	0.43
3:BT:43:TRP:HD1	1:BY:42:ILE:HB	1.84	0.43
2:AK:26:LEU:HD13	2:AL:66:TYR:HB2	2.00	0.43
2:BI:39:ARG:HB2	2:BI:61:ILE:HB	2.00	0.43
2:BP:92:GLN:HE21	3:BX:189:ARG:NE	2.17	0.43
2:BA:66:TYR:HB2	2:BC:26:LEU:HD13	1.99	0.43
3:BT:137:TYR:CE1	3:BT:292:LYS:HD2	2.54	0.43
1:BY:121:VAL:HG11	1:BY:175:VAL:HG21	2.01	0.43
3:AS:96:TYR:HB3	3:AS:103:VAL:HG23	1.99	0.43
2:BE:18:VAL:HG13	3:BT:168:TYR:CE2	2.54	0.43
2:AE:17:PRO:CB	3:AT:167:ASN:CB	2.86	0.43
2:AE:17:PRO:HG3	3:AT:169:LYS:CE	2.48	0.43
3:BW:196:ILE:HD11	3:BW:199:PHE:HD1	1.83	0.43
1:B0:143:ASN:O	1:BY:288:ARG:NH1	2.51	0.43
2:BG:172:ASN:ND2	2:BG:204:SER:H	2.17	0.43
2:AI:39:ARG:HB2	2:AI:61:ILE:HB	2.00	0.43
2:BL:21:ASN:OD1	3:BV:165:PRO:HG2	2.19	0.43
3:BW:247:GLU:OE1	3:BW:249:TYR:HE2	2.01	0.43
3:AS:118:TYR:HB3	3:AS:122:GLY:HA2	1.99	0.43
2:AC:39:ARG:HB2	2:AC:61:ILE:HB	2.00	0.43
1:B0:221:ARG:HB2	3:BV:266:PHE:HB3	2.00	0.43
2:AD:52:ASN:ND2	3:AS:258:LEU:CG	2.77	0.43
2:BA:172:ASN:ND2	2:BA:204:SER:H	2.16	0.43
2:AJ:251:THR:HA	2:AJ:252:PRO:HD3	1.87	0.43
2:AO:155:VAL:HG21	2:AO:159:ILE:HD11	2.01	0.43
2:BO:155:VAL:HG21	2:BO:159:ILE:HD11	2.01	0.43
3:AU:66:GLU:CB	3:BX:120:LYS:NZ	2.82	0.43
2:AP:7:THR:HG23	3:AX:160:TYR:CE2	2.54	0.43
3:BX:196:ILE:HD11	3:BX:199:PHE:HD1	1.84	0.43
3:BX:198:SER:HA	3:BX:242:THR:OG1	2.19	0.43
2:AA:120:LYS:HE2	3:AS:222:ASN:HD21	1.84	0.43
2:BN:91:THR:HG21	3:BW:189:ARG:HB2	2.01	0.43
2:AG:172:ASN:ND2	2:AG:204:SER:H	2.17	0.43
2:BR:39:ARG:HB2	2:BR:61:ILE:HB	2.00	0.43
2:AF:23:ASP:OD2	3:AT:176:TYR:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AJ:77:LYS:H	2:AJ:82:ASN:ND2	2.12	0.42
3:BU:203:LEU:HB2	3:BU:238:ILE:HB	2.01	0.42
2:AN:26:LEU:HD13	2:AO:66:TYR:HB2	2.01	0.42
3:BS:118:TYR:HB3	3:BS:122:GLY:HA2	2.00	0.42
2:BK:91:THR:HG21	3:BV:189:ARG:HB2	2.01	0.42
3:BT:171:ILE:H	3:BT:175:SER:HA	1.84	0.42
3:BU:203:LEU:HD13	3:BU:213:GLY:HA2	2.01	0.42
3:BW:96:TYR:HB3	3:BW:103:VAL:HG23	2.01	0.42
3:BX:243:ASP:OD1	3:BX:245:ASN:N	2.52	0.42
2:AO:27:TYR:HA	2:AO:30:LEU:HD12	2.00	0.42
2:AF:27:TYR:HA	2:AF:30:LEU:HD12	2.01	0.42
2:AG:174:LEU:HB2	2:AG:194:VAL:HG22	2.01	0.42
3:AW:96:TYR:HB3	3:AW:103:VAL:HG23	2.01	0.42
2:BO:5:ASN:HB3	2:BO:8:PHE:CD1	2.54	0.42
2:AN:155:VAL:HG21	2:AN:159:ILE:HD11	2.01	0.42
3:AX:243:ASP:OD1	3:AX:245:ASN:N	2.52	0.42
2:BN:155:VAL:HG21	2:BN:159:ILE:HD11	2.01	0.42
2:BH:155:VAL:HG21	2:BH:159:ILE:HD11	2.01	0.42
2:BQ:155:VAL:HG21	2:BQ:159:ILE:HD11	2.00	0.42
2:AO:5:ASN:HB3	2:AO:8:PHE:CD1	2.54	0.42
3:AU:120:LYS:HZ3	3:BX:66:GLU:CG	2.29	0.42
2:AR:9:PHE:CZ	3:AX:180:GLY:CA	3.03	0.42
2:AD:19:GLY:CA	3:AT:180:GLY:O	2.67	0.42
3:BT:43:TRP:CD1	1:BY:42:ILE:HB	2.54	0.42
3:BV:118:TYR:HB3	3:BV:122:GLY:HA2	2.02	0.42
3:BS:34:LEU:HB2	3:BX:114:LYS:HB3	2.00	0.42
2:AG:203:MET:SD	2:AG:243:TRP:HB2	2.59	0.42
3:AS:66:GLU:CG	3:BT:120:LYS:CE	2.96	0.42
2:AG:92:GLN:NE2	3:AU:189:ARG:NE	2.67	0.42
3:AU:203:LEU:HD13	3:AU:213:GLY:HA2	2.01	0.42
2:BQ:9:PHE:CE1	3:BX:172:LYS:HB2	2.54	0.42
3:BW:247:GLU:OE1	3:BW:249:TYR:CE2	2.73	0.42
2:AR:39:ARG:HB2	2:AR:61:ILE:HB	2.00	0.42
3:BU:226:ALA:HB3	3:BU:268:ARG:HB3	2.01	0.42
2:AD:147:SER:HB2	2:AE:140:VAL:HG22	2.02	0.42
2:BG:203:MET:SD	2:BG:243:TRP:HB2	2.59	0.42
2:BR:155:VAL:HG21	2:BR:159:ILE:HD11	2.02	0.42
2:BM:39:ARG:HB2	2:BM:61:ILE:HB	2.00	0.42
2:BQ:18:VAL:HG13	3:BX:168:TYR:CD2	2.54	0.42
2:AF:20:SER:HA	3:AT:170:TYR:CD1	2.54	0.42
2:AM:77:LYS:H	2:AM:82:ASN:ND2	2.13	0.42
3:BW:199:PHE:CE1	3:BW:242:THR:HG21	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BW:196:ILE:HD13	3:BW:291:ILE:HG12	2.02	0.42
1:BZ:1:MET:HG3	1:BZ:40:GLN:HB2	2.00	0.42
3:AV:118:TYR:HB3	3:AV:122:GLY:HA2	2.02	0.42
2:BC:155:VAL:HG21	2:BC:159:ILE:HD11	2.02	0.42
3:AT:137:TYR:CE1	3:AT:292:LYS:HD2	2.54	0.42
2:AF:39:ARG:HB2	2:AF:61:ILE:HB	2.00	0.42
2:BF:27:TYR:HA	2:BF:30:LEU:HD12	2.01	0.42
1:A0:76:VAL:HG21	1:A0:88:LYS:HE3	2.02	0.42
2:BJ:77:LYS:H	2:BJ:82:ASN:ND2	2.12	0.42
3:AW:199:PHE:CE1	3:AW:242:THR:HG21	2.55	0.42
3:AX:196:ILE:HD11	3:AX:199:PHE:HD1	1.84	0.42
1:AZ:241:TYR:CD2	1:AZ:241:TYR:N	2.88	0.42
2:BK:114:ASN:O	3:BV:186:ARG:CD	2.68	0.42
2:AC:155:VAL:HG21	2:AC:159:ILE:HD11	2.02	0.42
2:BN:26:LEU:HD13	2:BO:66:TYR:HB2	2.01	0.42
1:B0:38:ARG:NH2	3:BW:269:TYR:O	2.48	0.42
2:AQ:20:SER:N	3:AX:160:TYR:CD1	2.88	0.42
2:AP:21:ASN:N	3:AX:181:GLU:HG2	2.34	0.42
2:AR:18:VAL:CG1	3:AX:176:TYR:O	2.65	0.42
3:AU:203:LEU:HB2	3:AU:238:ILE:HB	2.01	0.42
2:AN:91:THR:HG21	3:AW:189:ARG:HB2	2.01	0.42
2:AM:5:ASN:O	2:AM:16:PHE:HB3	2.20	0.42
2:AK:155:VAL:HG21	2:AK:159:ILE:HD11	2.02	0.42
3:AT:114:LYS:HB3	3:AU:34:LEU:HB2	2.02	0.42
3:AS:132:ILE:HG21	3:AS:135:LYS:HB2	2.00	0.42
2:BQ:23:ASP:OD2	3:BX:168:TYR:HE2	2.03	0.42
2:BE:17:PRO:CB	3:BT:167:ASN:CB	2.87	0.42
3:AW:196:ILE:HD13	3:AW:291:ILE:HG12	2.02	0.42
1:BZ:77:VAL:O	1:BZ:89:LEU:HB3	2.20	0.42
3:AX:198:SER:HA	3:AX:242:THR:OG1	2.19	0.42
3:AT:86:ILE:HA	3:AT:92:VAL:HG21	2.01	0.42
1:BY:52:LEU:HD23	1:BY:53:TYR:CE2	2.55	0.42
2:AR:155:VAL:HG21	2:AR:159:ILE:HD11	2.02	0.42
2:BP:23:ASP:OD2	3:BX:178:TYR:HE1	2.03	0.42
2:AI:5:ASN:HB3	2:AI:8:PHE:CD1	2.55	0.42
2:BP:49:THR:HB	3:BW:258:LEU:HD21	2.01	0.42
3:BT:86:ILE:HA	3:BT:92:VAL:HG21	2.01	0.42
2:AE:18:VAL:CG1	3:AT:168:TYR:O	2.59	0.41
1:AZ:77:VAL:O	1:AZ:89:LEU:HB3	2.20	0.41
3:AS:266:PHE:CD2	1:AY:35:PRO:HD2	2.55	0.41
3:AV:199:PHE:CZ	3:AV:242:THR:HG21	2.55	0.41
3:BU:131:ASP:HB3	3:BV:42:ILE:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BS:132:ILE:HG21	3:BS:135:LYS:HB2	2.00	0.41
2:BD:147:SER:HB2	2:BE:140:VAL:HG22	2.02	0.41
3:BS:99:GLU:OE2	3:BX:73:GLU:HB2	2.19	0.41
3:AS:294:LYS:HD2	3:AT:47:GLY:O	2.19	0.41
3:AU:53:THR:HG21	1:AZ:359:PHE:C	2.41	0.41
2:BR:9:PHE:CZ	3:BX:181:GLU:N	2.88	0.41
2:AP:77:LYS:H	2:AP:82:ASN:ND2	2.12	0.41
3:BT:87:LEU:HA	3:BU:54:ARG:HH11	1.85	0.41
2:AK:251:THR:HA	2:AK:252:PRO:HD3	1.90	0.41
2:BD:203:MET:SD	2:BD:243:TRP:HB2	2.60	0.41
2:AF:155:VAL:HG21	2:AF:159:ILE:HD11	2.01	0.41
3:BT:202:ILE:HG12	3:BT:239:LEU:HD12	2.01	0.41
2:BD:73:THR:CG2	3:BS:256:THR:CG2	2.98	0.41
3:BV:199:PHE:CZ	3:BV:242:THR:HG21	2.55	0.41
3:AW:247:GLU:OE1	3:AW:249:TYR:CE2	2.73	0.41
2:BG:66:TYR:HB2	2:BI:26:LEU:HD13	2.02	0.41
3:BW:281:LEU:HB3	3:BW:284:LEU:HD12	2.03	0.41
2:BI:5:ASN:HB3	2:BI:8:PHE:CD1	2.55	0.41
2:BE:21:ASN:CG	3:BT:165:PRO:HG2	2.40	0.41
3:BT:199:PHE:HB3	3:BT:291:ILE:HD13	2.02	0.41
2:BK:155:VAL:HG21	2:BK:159:ILE:HD11	2.02	0.41
1:A0:323:ILE:HA	1:A0:363:LEU:O	2.20	0.41
2:BG:5:ASN:HB3	2:BG:8:PHE:CD1	2.56	0.41
1:AY:323:ILE:HA	1:AY:363:LEU:O	2.20	0.41
1:A0:52:LEU:HD23	1:A0:53:TYR:CE2	2.55	0.41
2:AQ:229:THR:HB	2:AR:228:ASP:HB2	2.03	0.41
2:AJ:203:MET:SD	2:AJ:243:TRP:HB2	2.61	0.41
3:AT:202:ILE:HG12	3:AT:239:LEU:HD12	2.00	0.41
1:AY:121:VAL:HG11	1:AY:175:VAL:HG21	2.01	0.41
2:AD:203:MET:SD	2:AD:243:TRP:HB2	2.60	0.41
2:BQ:23:ASP:OD2	3:BX:168:TYR:CE2	2.74	0.41
2:BP:21:ASN:HB3	3:BX:181:GLU:CD	2.41	0.41
1:B0:76:VAL:HG21	1:B0:88:LYS:HE3	2.02	0.41
3:AT:203:LEU:HD21	3:AT:240:ILE:HG13	2.03	0.41
2:BN:100:SER:CB	3:BW:220:ILE:HG21	2.51	0.41
1:B0:288:ARG:CZ	1:BZ:12:PRO:HB2	2.50	0.41
3:BS:99:GLU:CD	3:BX:73:GLU:HB2	2.41	0.41
2:AD:251:THR:HA	2:AD:252:PRO:HD3	1.96	0.41
1:B0:323:ILE:HA	1:B0:363:LEU:O	2.20	0.41
2:BM:251:THR:HA	2:BM:252:PRO:HD3	1.90	0.41
2:BQ:229:THR:HB	2:BR:228:ASP:HB2	2.03	0.41
2:AE:19:GLY:HA2	3:AT:166:GLY:C	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AP:5:ASN:HD21	2:AQ:97:VAL:HB	1.85	0.41
1:BZ:241:TYR:CD2	1:BZ:241:TYR:N	2.88	0.41
2:BD:172:ASN:ND2	2:BD:204:SER:H	2.19	0.41
2:AA:251:THR:HA	2:AA:252:PRO:HD3	1.95	0.41
2:AG:5:ASN:HB3	2:AG:8:PHE:CD1	2.56	0.41
2:BJ:203:MET:SD	2:BJ:243:TRP:HB2	2.60	0.41
1:B0:330:LEU:HB2	3:BV:261:PHE:CE2	2.55	0.41
1:A0:223:ASP:CG	3:AV:272:ARG:HH12	2.24	0.41
2:BG:174:LEU:HB2	2:BG:194:VAL:HG22	2.02	0.41
2:BE:9:PHE:CA	3:BT:170:TYR:O	2.61	0.41
2:AP:21:ASN:CG	3:AX:181:GLU:HG2	2.41	0.41
1:BZ:89:LEU:CD2	1:BZ:192:GLN:HG3	2.49	0.41
3:AT:199:PHE:HB3	3:AT:291:ILE:HD13	2.02	0.41
3:AS:171:ILE:H	3:AS:175:SER:HA	1.86	0.41
3:BU:171:ILE:H	3:BU:175:SER:HA	1.86	0.41
2:BM:5:ASN:O	2:BM:16:PHE:HB3	2.20	0.41
3:AV:76:TYR:HE1	3:AW:96:TYR:HH	1.63	0.41
2:AG:66:TYR:HB2	2:AI:26:LEU:HD13	2.02	0.41
2:AK:120:LYS:NZ	3:AV:220:ILE:O	2.48	0.41
2:BQ:26:LEU:HD13	2:BR:66:TYR:HB2	2.03	0.41
1:AY:52:LEU:HD23	1:AY:53:TYR:CE2	2.55	0.41
3:BT:115:THR:HG22	3:BU:32:SER:O	2.21	0.41
1:BY:323:ILE:HA	1:BY:363:LEU:O	2.20	0.41
3:AS:7:ILE:HG23	3:AS:92:VAL:CG1	2.51	0.41
3:BV:246:ASP:O	3:BV:246:ASP:CG	2.59	0.41
2:BD:73:THR:HG21	3:BS:256:THR:CG2	2.51	0.41
3:BU:272:ARG:NH1	1:BZ:3:GLU:OE1	2.54	0.41
2:AN:102:GLU:OE1	3:AW:222:ASN:ND2	2.46	0.41
2:AP:172:ASN:ND2	2:AP:204:SER:H	2.19	0.41
2:BB:229:THR:HB	2:BC:228:ASP:HB2	2.03	0.41
1:BY:143:ASN:O	1:BZ:288:ARG:NH1	2.53	0.41
1:AY:120:ASP:HB2	1:AZ:292:THR:HB	2.03	0.41
2:BM:203:MET:SD	2:BM:243:TRP:HB2	2.61	0.41
2:BP:174:LEU:HB2	2:BP:194:VAL:HG22	2.03	0.41
3:AU:226:ALA:HB3	3:AU:268:ARG:HB3	2.01	0.41
3:AX:58:GLN:HA	3:AX:59:PRO:HD3	1.99	0.41
2:AE:17:PRO:HB2	3:AT:167:ASN:HD22	1.76	0.41
3:AT:158:LYS:HD2	3:AT:176:TYR:CE1	2.56	0.41
3:AU:271:THR:HA	1:AZ:3:GLU:HG2	2.02	0.41
1:AY:185:PHE:CE2	1:AY:208:PHE:HA	2.56	0.41
2:BF:23:ASP:OD2	3:BT:176:TYR:CZ	2.74	0.41
1:AY:87:LYS:HZ1	1:AY:89:LEU:HD23	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BV:240:ILE:CD1	3:BV:242:THR:HG23	2.51	0.41
1:AZ:52:LEU:HD23	1:AZ:53:TYR:CE2	2.56	0.41
2:AM:203:MET:SD	2:AM:243:TRP:HB2	2.61	0.41
2:AH:229:THR:HB	2:AI:228:ASP:HB2	2.03	0.41
3:AV:246:ASP:O	3:AV:246:ASP:CG	2.59	0.41
2:BP:146:ASP:O	2:BR:151:ASN:HB2	2.21	0.41
2:BH:251:THR:HA	2:BH:252:PRO:HD3	1.89	0.41
3:AW:281:LEU:HB3	3:AW:284:LEU:HD12	2.03	0.41
2:BM:174:LEU:HB2	2:BM:194:VAL:HG22	2.03	0.41
3:AS:242:THR:HG23	3:AS:272:ARG:HG3	1.89	0.41
2:AE:9:PHE:CA	3:AT:170:TYR:O	2.61	0.41
3:BT:158:LYS:HD2	3:BT:176:TYR:CE1	2.56	0.41
3:BT:203:LEU:HD21	3:BT:240:ILE:HG13	2.02	0.41
3:AT:87:LEU:HA	3:AU:54:ARG:HH11	1.84	0.41
3:BS:171:ILE:H	3:BS:175:SER:HA	1.86	0.41
2:BP:172:ASN:ND2	2:BP:204:SER:H	2.19	0.41
2:AJ:172:ASN:ND2	2:AJ:204:SER:H	2.19	0.41
2:AN:229:THR:HB	2:AO:228:ASP:HB2	2.03	0.41
2:AA:198:GLN:HB2	2:AA:201:TRP:CD1	2.56	0.41
2:BL:10:SER:HA	2:BL:15:GLU:HB2	2.03	0.41
2:AN:251:THR:HA	2:AN:252:PRO:HD3	1.90	0.41
2:AB:229:THR:HB	2:AC:228:ASP:HB2	2.03	0.41
3:AT:68:PHE:CE1	3:BS:120:LYS:HG2	2.56	0.40
1:BY:87:LYS:HZ1	1:BY:89:LEU:HD23	1.86	0.40
3:BX:171:ILE:H	3:BX:175:SER:HA	1.86	0.40
2:AM:172:ASN:ND2	2:AM:204:SER:H	2.19	0.40
3:AS:226:ALA:HB3	3:AS:268:ARG:HB3	2.03	0.40
2:AE:229:THR:HB	2:AF:228:ASP:HB2	2.03	0.40
2:AG:130:GLY:HA3	1:AZ:218:ILE:HG23	2.02	0.40
2:BD:174:LEU:HB2	2:BD:194:VAL:HG22	2.03	0.40
2:BA:198:GLN:HB2	2:BA:201:TRP:CD1	2.56	0.40
2:AG:79:ASP:CB	1:AZ:212:ASN:ND2	2.85	0.40
2:AL:10:SER:HA	2:AL:15:GLU:HB2	2.03	0.40
1:BZ:45:GLU:HA	1:BZ:357:THR:HG22	2.03	0.40
2:BJ:174:LEU:HB2	2:BJ:194:VAL:HG22	2.04	0.40
2:BB:27:TYR:HA	2:BB:30:LEU:HD12	2.03	0.40
2:AP:146:ASP:O	2:AR:151:ASN:HB2	2.21	0.40
3:BS:7:ILE:HG23	3:BS:92:VAL:CG1	2.51	0.40
2:AO:17:PRO:CB	3:AW:167:ASN:HB2	2.51	0.40
2:AL:5:ASN:HB3	2:AL:8:PHE:CD1	2.56	0.40
1:B0:52:LEU:HD23	1:B0:53:TYR:CE2	2.56	0.40
2:BE:17:PRO:HG3	3:BT:169:LYS:CE	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A0:3:GLU:CG	3:AW:271:THR:HA	2.51	0.40
3:AV:240:ILE:CD1	3:AV:242:THR:HG23	2.51	0.40
3:AX:118:TYR:HB3	3:AX:122:GLY:HA2	2.04	0.40
3:BS:226:ALA:HB3	3:BS:268:ARG:HB3	2.03	0.40
2:AP:203:MET:SD	2:AP:243:TRP:HB2	2.61	0.40
3:AU:171:ILE:H	3:AU:175:SER:HA	1.86	0.40
2:BE:229:THR:HB	2:BF:228:ASP:HB2	2.03	0.40
2:AD:174:LEU:HB2	2:AD:194:VAL:HG22	2.02	0.40
2:BH:229:THR:HB	2:BI:228:ASP:HB2	2.03	0.40
2:AQ:17:PRO:N	3:AX:169:LYS:HD3	2.36	0.40
3:BT:116:GLU:OE2	3:BU:5:TYR:CE2	2.74	0.40
1:BY:185:PHE:CE2	1:BY:208:PHE:HA	2.56	0.40
2:BF:9:PHE:CB	3:BT:180:GLY:HA2	2.52	0.40
3:AS:270:ARG:CZ	1:AY:72:LEU:HD22	2.51	0.40
2:BG:9:PHE:HB2	3:BU:166:GLY:CA	2.51	0.40
3:AT:132:ILE:HG21	3:AT:135:LYS:HB2	2.04	0.40
3:BW:171:ILE:H	3:BW:175:SER:HA	1.86	0.40
2:BN:5:ASN:HB3	2:BN:8:PHE:CD1	2.57	0.40
2:BK:229:THR:HB	2:BL:228:ASP:HB2	2.03	0.40
2:BP:203:MET:SD	2:BP:243:TRP:HB2	2.61	0.40
1:B0:292:THR:HB	1:BZ:120:ASP:HB2	2.03	0.40
2:AN:5:ASN:HB3	2:AN:8:PHE:CD1	2.57	0.40
3:AW:3:ARG:HD2	3:AW:3:ARG:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	A0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	AY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	AZ	370/372 (100%)	358 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	BY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	BZ	370/372 (100%)	357 (96%)	13 (4%)	0	100	100
2	AA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AG	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AP	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BG	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BP	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
3	AS	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	30	84
3	AT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	30	84
3	AU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	30	84
3	AV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	30	84
3	AW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	30	84
3	AX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	30	84
3	BS	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	30	84
3	BT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	30	84
3	BU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	30	84
3	BV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	30	84
3	BW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	30	84
3	BX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	30	84
All	All	15168/15276 (99%)	14418 (95%)	726 (5%)	24 (0%)	56	93

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AS	175	SER
3	AT	175	SER
3	AU	175	SER
3	AV	175	SER
3	AW	175	SER
3	AX	175	SER
3	BS	175	SER
3	BT	175	SER
3	BU	175	SER
3	BV	175	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BW	175	SER
3	BX	175	SER
3	AS	136	TRP
3	AU	136	TRP
3	AV	136	TRP
3	AW	136	TRP
3	AX	136	TRP
3	BS	136	TRP
3	BU	136	TRP
3	BV	136	TRP
3	BW	136	TRP
3	BX	136	TRP
3	AT	136	TRP
3	BT	136	TRP

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	A0	337/337 (100%)	324 (96%)	13 (4%)	43	84
1	AY	337/337 (100%)	319 (95%)	18 (5%)	32	77
1	AZ	337/337 (100%)	321 (95%)	16 (5%)	36	80
1	B0	337/337 (100%)	324 (96%)	13 (4%)	43	84
1	BY	337/337 (100%)	319 (95%)	18 (5%)	32	77
1	BZ	337/337 (100%)	321 (95%)	16 (5%)	36	80
2	AA	227/227 (100%)	218 (96%)	9 (4%)	42	83
2	AB	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	AC	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	AD	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	AE	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	AF	227/227 (100%)	224 (99%)	3 (1%)	80	95
2	AG	227/227 (100%)	219 (96%)	8 (4%)	48	87
2	AH	227/227 (100%)	220 (97%)	7 (3%)	52	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AI	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	AJ	227/227 (100%)	219 (96%)	8 (4%)	48	87
2	AK	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	AL	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	AM	227/227 (100%)	219 (96%)	8 (4%)	48	87
2	AN	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	AO	227/227 (100%)	224 (99%)	3 (1%)	80	95
2	AP	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	AQ	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	AR	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	BA	227/227 (100%)	218 (96%)	9 (4%)	42	83
2	BB	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	BC	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	BD	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	BE	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	BF	227/227 (100%)	224 (99%)	3 (1%)	80	95
2	BG	227/227 (100%)	219 (96%)	8 (4%)	48	87
2	BH	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	BI	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	BJ	227/227 (100%)	219 (96%)	8 (4%)	48	87
2	BK	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	BL	227/227 (100%)	223 (98%)	4 (2%)	71	93
2	BM	227/227 (100%)	219 (96%)	8 (4%)	48	87
2	BN	227/227 (100%)	221 (97%)	6 (3%)	59	89
2	BO	227/227 (100%)	224 (99%)	3 (1%)	80	95
2	BP	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	BQ	227/227 (100%)	220 (97%)	7 (3%)	52	88
2	BR	227/227 (100%)	223 (98%)	4 (2%)	71	93
3	AS	264/265 (100%)	246 (93%)	18 (7%)	22	69
3	AT	264/265 (100%)	248 (94%)	16 (6%)	26	73
3	AU	264/265 (100%)	241 (91%)	23 (9%)	15	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AV	264/265 (100%)	241 (91%)	23 (9%)	15	58
3	AW	264/265 (100%)	244 (92%)	20 (8%)	19	65
3	AX	264/265 (100%)	247 (94%)	17 (6%)	25	71
3	BS	264/265 (100%)	245 (93%)	19 (7%)	21	67
3	BT	264/265 (100%)	247 (94%)	17 (6%)	25	71
3	BU	264/265 (100%)	241 (91%)	23 (9%)	15	58
3	BV	264/265 (100%)	241 (91%)	23 (9%)	15	58
3	BW	264/265 (100%)	244 (92%)	20 (8%)	19	65
3	BX	264/265 (100%)	247 (94%)	17 (6%)	25	71
All	All	13362/13374 (100%)	12818 (96%)	544 (4%)	41	83

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	1	MET
1	A0	2	LEU
1	A0	8	ASP
1	A0	40	GLN
1	A0	88	LYS
1	A0	152	PHE
1	A0	165	ARG
1	A0	207	ASN
1	A0	224	ILE
1	A0	238	ARG
1	A0	286	ASP
1	A0	313	ILE
1	A0	360	ASN
2	AA	2	THR
2	AA	7	THR
2	AA	9	PHE
2	AA	18	VAL
2	AA	38	ILE
2	AA	40	ARG
2	AA	79	ASP
2	AA	124	ASP
2	AA	202	ASN
2	AB	38	ILE
2	AB	40	ARG
2	AB	206	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	232	HIS
2	AB	234	ASP
2	AB	252	PRO
2	AC	7	THR
2	AC	38	ILE
2	AC	40	ARG
2	AC	232	HIS
2	AD	9	PHE
2	AD	18	VAL
2	AD	38	ILE
2	AD	40	ARG
2	AD	79	ASP
2	AD	124	ASP
2	AD	202	ASN
2	AE	38	ILE
2	AE	40	ARG
2	AE	206	THR
2	AE	232	HIS
2	AE	234	ASP
2	AE	252	PRO
2	AF	38	ILE
2	AF	40	ARG
2	AF	232	HIS
2	AG	7	THR
2	AG	9	PHE
2	AG	18	VAL
2	AG	38	ILE
2	AG	40	ARG
2	AG	79	ASP
2	AG	124	ASP
2	AG	202	ASN
2	AH	17	PRO
2	AH	38	ILE
2	AH	40	ARG
2	AH	206	THR
2	AH	232	HIS
2	AH	234	ASP
2	AH	252	PRO
2	AI	7	THR
2	AI	38	ILE
2	AI	40	ARG
2	AI	232	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AJ	7	THR
2	AJ	9	PHE
2	AJ	18	VAL
2	AJ	38	ILE
2	AJ	40	ARG
2	AJ	79	ASP
2	AJ	124	ASP
2	AJ	202	ASN
2	AK	23	ASP
2	AK	38	ILE
2	AK	40	ARG
2	AK	206	THR
2	AK	232	HIS
2	AK	234	ASP
2	AL	26	LEU
2	AL	38	ILE
2	AL	40	ARG
2	AL	232	HIS
2	AM	7	THR
2	AM	9	PHE
2	AM	18	VAL
2	AM	38	ILE
2	AM	40	ARG
2	AM	79	ASP
2	AM	124	ASP
2	AM	202	ASN
2	AN	23	ASP
2	AN	38	ILE
2	AN	40	ARG
2	AN	206	THR
2	AN	232	HIS
2	AN	234	ASP
2	AO	38	ILE
2	AO	40	ARG
2	AO	232	HIS
2	AP	9	PHE
2	AP	18	VAL
2	AP	38	ILE
2	AP	40	ARG
2	AP	79	ASP
2	AP	124	ASP
2	AP	202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AQ	17	PRO
2	AQ	23	ASP
2	AQ	38	ILE
2	AQ	40	ARG
2	AQ	206	THR
2	AQ	232	HIS
2	AQ	234	ASP
2	AR	7	THR
2	AR	38	ILE
2	AR	40	ARG
2	AR	232	HIS
3	AS	11	LEU
3	AS	12	ASP
3	AS	26	VAL
3	AS	43	TRP
3	AS	54	ARG
3	AS	55	SER
3	AS	66	GLU
3	AS	123	THR
3	AS	142	LEU
3	AS	196	ILE
3	AS	197	PHE
3	AS	228	VAL
3	AS	232	GLU
3	AS	234	VAL
3	AS	263	VAL
3	AS	269	TYR
3	AS	270	ARG
3	AS	291	ILE
3	AT	12	ASP
3	AT	26	VAL
3	AT	48	ILE
3	AT	55	SER
3	AT	65	LEU
3	AT	72	LEU
3	AT	123	THR
3	AT	159	ILE
3	AT	171	ILE
3	AT	196	ILE
3	AT	203	LEU
3	AT	234	VAL
3	AT	236	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AT	243	ASP
3	AT	263	VAL
3	AT	269	TYR
3	AU	3	ARG
3	AU	11	LEU
3	AU	12	ASP
3	AU	26	VAL
3	AU	37	GLN
3	AU	39	THR
3	AU	43	TRP
3	AU	48	ILE
3	AU	53	THR
3	AU	54	ARG
3	AU	55	SER
3	AU	66	GLU
3	AU	72	LEU
3	AU	94	LEU
3	AU	196	ILE
3	AU	200	MET
3	AU	228	VAL
3	AU	232	GLU
3	AU	234	VAL
3	AU	258	LEU
3	AU	263	VAL
3	AU	270	ARG
3	AU	291	ILE
3	AV	3	ARG
3	AV	11	LEU
3	AV	12	ASP
3	AV	36	LEU
3	AV	48	ILE
3	AV	54	ARG
3	AV	55	SER
3	AV	66	GLU
3	AV	72	LEU
3	AV	120	LYS
3	AV	196	ILE
3	AV	197	PHE
3	AV	203	LEU
3	AV	227	ILE
3	AV	232	GLU
3	AV	234	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AV	240	ILE
3	AV	243	ASP
3	AV	246	ASP
3	AV	258	LEU
3	AV	263	VAL
3	AV	269	TYR
3	AV	291	ILE
3	AW	6	LYS
3	AW	11	LEU
3	AW	26	VAL
3	AW	43	TRP
3	AW	54	ARG
3	AW	55	SER
3	AW	66	GLU
3	AW	72	LEU
3	AW	123	THR
3	AW	196	ILE
3	AW	197	PHE
3	AW	203	LEU
3	AW	228	VAL
3	AW	232	GLU
3	AW	234	VAL
3	AW	258	LEU
3	AW	263	VAL
3	AW	269	TYR
3	AW	270	ARG
3	AW	291	ILE
3	AX	11	LEU
3	AX	26	VAL
3	AX	43	TRP
3	AX	54	ARG
3	AX	66	GLU
3	AX	107	LEU
3	AX	179	TYR
3	AX	196	ILE
3	AX	200	MET
3	AX	203	LEU
3	AX	228	VAL
3	AX	234	VAL
3	AX	243	ASP
3	AX	244	VAL
3	AX	258	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AX	263	VAL
3	AX	291	ILE
1	AY	1	MET
1	AY	8	ASP
1	AY	26	LYS
1	AY	40	GLN
1	AY	41	VAL
1	AY	87	LYS
1	AY	88	LYS
1	AY	152	PHE
1	AY	165	ARG
1	AY	192	GLN
1	AY	207	ASN
1	AY	242	ASN
1	AY	243	PHE
1	AY	286	ASP
1	AY	319	VAL
1	AY	340	ILE
1	AY	353	ASP
1	AY	360	ASN
1	AZ	1	MET
1	AZ	2	LEU
1	AZ	8	ASP
1	AZ	26	LYS
1	AZ	39	CYS
1	AZ	40	GLN
1	AZ	41	VAL
1	AZ	88	LYS
1	AZ	151	PHE
1	AZ	165	ARG
1	AZ	207	ASN
1	AZ	238	ARG
1	AZ	286	ASP
1	AZ	320	THR
1	AZ	340	ILE
1	AZ	360	ASN
1	B0	1	MET
1	B0	2	LEU
1	B0	8	ASP
1	B0	40	GLN
1	B0	88	LYS
1	B0	152	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B0	165	ARG
1	B0	207	ASN
1	B0	224	ILE
1	B0	238	ARG
1	B0	286	ASP
1	B0	313	ILE
1	B0	360	ASN
2	BA	2	THR
2	BA	7	THR
2	BA	9	PHE
2	BA	18	VAL
2	BA	38	ILE
2	BA	40	ARG
2	BA	79	ASP
2	BA	124	ASP
2	BA	202	ASN
2	BB	38	ILE
2	BB	40	ARG
2	BB	206	THR
2	BB	232	HIS
2	BB	234	ASP
2	BB	252	PRO
2	BC	7	THR
2	BC	38	ILE
2	BC	40	ARG
2	BC	232	HIS
2	BD	9	PHE
2	BD	18	VAL
2	BD	38	ILE
2	BD	40	ARG
2	BD	79	ASP
2	BD	124	ASP
2	BD	202	ASN
2	BE	38	ILE
2	BE	40	ARG
2	BE	206	THR
2	BE	232	HIS
2	BE	234	ASP
2	BE	252	PRO
2	BF	38	ILE
2	BF	40	ARG
2	BF	232	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	BG	7	THR
2	BG	9	PHE
2	BG	18	VAL
2	BG	38	ILE
2	BG	40	ARG
2	BG	79	ASP
2	BG	124	ASP
2	BG	202	ASN
2	BH	17	PRO
2	BH	38	ILE
2	BH	40	ARG
2	BH	206	THR
2	BH	232	HIS
2	BH	234	ASP
2	BH	252	PRO
2	BI	7	THR
2	BI	38	ILE
2	BI	40	ARG
2	BI	232	HIS
2	BJ	7	THR
2	BJ	9	PHE
2	BJ	18	VAL
2	BJ	38	ILE
2	BJ	40	ARG
2	BJ	79	ASP
2	BJ	124	ASP
2	BJ	202	ASN
2	BK	23	ASP
2	BK	38	ILE
2	BK	40	ARG
2	BK	206	THR
2	BK	232	HIS
2	BK	234	ASP
2	BL	26	LEU
2	BL	38	ILE
2	BL	40	ARG
2	BL	232	HIS
2	BM	7	THR
2	BM	9	PHE
2	BM	18	VAL
2	BM	38	ILE
2	BM	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	BM	79	ASP
2	BM	124	ASP
2	BM	202	ASN
2	BN	23	ASP
2	BN	38	ILE
2	BN	40	ARG
2	BN	206	THR
2	BN	232	HIS
2	BN	234	ASP
2	BO	38	ILE
2	BO	40	ARG
2	BO	232	HIS
2	BP	9	PHE
2	BP	18	VAL
2	BP	38	ILE
2	BP	40	ARG
2	BP	79	ASP
2	BP	124	ASP
2	BP	202	ASN
2	BQ	17	PRO
2	BQ	23	ASP
2	BQ	38	ILE
2	BQ	40	ARG
2	BQ	206	THR
2	BQ	232	HIS
2	BQ	234	ASP
2	BR	7	THR
2	BR	38	ILE
2	BR	40	ARG
2	BR	232	HIS
3	BS	11	LEU
3	BS	12	ASP
3	BS	26	VAL
3	BS	43	TRP
3	BS	54	ARG
3	BS	55	SER
3	BS	66	GLU
3	BS	72	LEU
3	BS	123	THR
3	BS	142	LEU
3	BS	196	ILE
3	BS	197	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BS	228	VAL
3	BS	232	GLU
3	BS	234	VAL
3	BS	263	VAL
3	BS	269	TYR
3	BS	270	ARG
3	BS	291	ILE
3	BT	12	ASP
3	BT	26	VAL
3	BT	48	ILE
3	BT	55	SER
3	BT	65	LEU
3	BT	72	LEU
3	BT	123	THR
3	BT	135	LYS
3	BT	159	ILE
3	BT	171	ILE
3	BT	196	ILE
3	BT	203	LEU
3	BT	234	VAL
3	BT	236	ASP
3	BT	243	ASP
3	BT	263	VAL
3	BT	269	TYR
3	BU	3	ARG
3	BU	11	LEU
3	BU	12	ASP
3	BU	26	VAL
3	BU	37	GLN
3	BU	39	THR
3	BU	43	TRP
3	BU	48	ILE
3	BU	53	THR
3	BU	54	ARG
3	BU	55	SER
3	BU	66	GLU
3	BU	72	LEU
3	BU	94	LEU
3	BU	196	ILE
3	BU	200	MET
3	BU	228	VAL
3	BU	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BU	234	VAL
3	BU	258	LEU
3	BU	263	VAL
3	BU	270	ARG
3	BU	291	ILE
3	BV	3	ARG
3	BV	11	LEU
3	BV	12	ASP
3	BV	36	LEU
3	BV	48	ILE
3	BV	54	ARG
3	BV	55	SER
3	BV	66	GLU
3	BV	72	LEU
3	BV	120	LYS
3	BV	196	ILE
3	BV	197	PHE
3	BV	203	LEU
3	BV	227	ILE
3	BV	232	GLU
3	BV	234	VAL
3	BV	240	ILE
3	BV	243	ASP
3	BV	246	ASP
3	BV	258	LEU
3	BV	263	VAL
3	BV	269	TYR
3	BV	291	ILE
3	BW	6	LYS
3	BW	11	LEU
3	BW	26	VAL
3	BW	43	TRP
3	BW	54	ARG
3	BW	55	SER
3	BW	66	GLU
3	BW	72	LEU
3	BW	123	THR
3	BW	196	ILE
3	BW	197	PHE
3	BW	203	LEU
3	BW	228	VAL
3	BW	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BW	234	VAL
3	BW	258	LEU
3	BW	263	VAL
3	BW	269	TYR
3	BW	270	ARG
3	BW	291	ILE
3	BX	11	LEU
3	BX	26	VAL
3	BX	43	TRP
3	BX	54	ARG
3	BX	66	GLU
3	BX	107	LEU
3	BX	179	TYR
3	BX	196	ILE
3	BX	200	MET
3	BX	203	LEU
3	BX	228	VAL
3	BX	234	VAL
3	BX	243	ASP
3	BX	244	VAL
3	BX	258	LEU
3	BX	263	VAL
3	BX	291	ILE
1	BY	1	MET
1	BY	8	ASP
1	BY	26	LYS
1	BY	40	GLN
1	BY	41	VAL
1	BY	87	LYS
1	BY	88	LYS
1	BY	152	PHE
1	BY	165	ARG
1	BY	192	GLN
1	BY	207	ASN
1	BY	242	ASN
1	BY	243	PHE
1	BY	286	ASP
1	BY	319	VAL
1	BY	340	ILE
1	BY	353	ASP
1	BY	360	ASN
1	BZ	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BZ	2	LEU
1	BZ	8	ASP
1	BZ	26	LYS
1	BZ	39	CYS
1	BZ	40	GLN
1	BZ	41	VAL
1	BZ	88	LYS
1	BZ	151	PHE
1	BZ	165	ARG
1	BZ	207	ASN
1	BZ	238	ARG
1	BZ	286	ASP
1	BZ	320	THR
1	BZ	340	ILE
1	BZ	360	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	184	GLN
1	A0	267	ASN
2	AA	5	ASN
2	AA	71	ASN
2	AA	82	ASN
2	AA	172	ASN
2	AA	175	GLN
2	AB	71	ASN
2	AC	172	ASN
2	AD	5	ASN
2	AD	52	ASN
2	AD	71	ASN
2	AD	82	ASN
2	AD	92	GLN
2	AD	172	ASN
2	AD	175	GLN
2	AD	196	ASN
2	AE	54	GLN
2	AE	71	ASN
2	AF	172	ASN
2	AG	71	ASN
2	AG	82	ASN
2	AG	92	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AG	172	ASN
2	AG	175	GLN
2	AG	196	ASN
2	AH	71	ASN
2	AI	151	ASN
2	AI	172	ASN
2	AJ	71	ASN
2	AJ	82	ASN
2	AJ	172	ASN
2	AJ	175	GLN
2	AJ	196	ASN
2	AK	54	GLN
2	AK	71	ASN
2	AL	151	ASN
2	AL	172	ASN
2	AM	71	ASN
2	AM	82	ASN
2	AM	172	ASN
2	AM	175	GLN
2	AM	196	ASN
2	AN	54	GLN
2	AN	71	ASN
2	AO	172	ASN
2	AP	5	ASN
2	AP	22	ASN
2	AP	71	ASN
2	AP	82	ASN
2	AP	92	GLN
2	AP	172	ASN
2	AP	175	GLN
2	AP	196	ASN
2	AQ	71	ASN
2	AR	151	ASN
2	AR	172	ASN
3	AS	102	GLN
3	AS	222	ASN
3	AS	250	GLN
3	AT	102	GLN
3	AT	167	ASN
3	AT	235	GLN
3	AU	23	ASN
3	AU	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AU	250	GLN
3	AV	23	ASN
3	AV	102	GLN
3	AV	121	ASN
3	AV	235	GLN
3	AV	250	GLN
3	AW	102	GLN
3	AW	121	ASN
3	AX	102	GLN
3	AX	121	ASN
3	AX	167	ASN
3	AX	250	GLN
3	AX	278	GLN
1	AY	11	ASN
1	AY	90	ASN
1	AY	143	ASN
1	AZ	143	ASN
1	AZ	184	GLN
1	AZ	192	GLN
1	AZ	212	ASN
1	B0	184	GLN
1	B0	267	ASN
2	BA	5	ASN
2	BA	71	ASN
2	BA	82	ASN
2	BA	172	ASN
2	BA	175	GLN
2	BB	71	ASN
2	BC	172	ASN
2	BD	5	ASN
2	BD	52	ASN
2	BD	71	ASN
2	BD	82	ASN
2	BD	92	GLN
2	BD	172	ASN
2	BD	175	GLN
2	BD	196	ASN
2	BE	54	GLN
2	BE	71	ASN
2	BF	172	ASN
2	BG	71	ASN
2	BG	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	BG	92	GLN
2	BG	172	ASN
2	BG	175	GLN
2	BG	196	ASN
2	BH	71	ASN
2	BI	151	ASN
2	BI	172	ASN
2	BJ	71	ASN
2	BJ	82	ASN
2	BJ	172	ASN
2	BJ	175	GLN
2	BJ	196	ASN
2	BK	71	ASN
2	BL	151	ASN
2	BL	172	ASN
2	BM	71	ASN
2	BM	82	ASN
2	BM	172	ASN
2	BM	175	GLN
2	BM	196	ASN
2	BN	54	GLN
2	BN	71	ASN
2	BO	172	ASN
2	BP	5	ASN
2	BP	22	ASN
2	BP	71	ASN
2	BP	82	ASN
2	BP	92	GLN
2	BP	172	ASN
2	BP	175	GLN
2	BP	196	ASN
2	BQ	54	GLN
2	BQ	71	ASN
2	BR	151	ASN
2	BR	172	ASN
3	BS	102	GLN
3	BS	222	ASN
3	BS	250	GLN
3	BT	102	GLN
3	BT	167	ASN
3	BT	222	ASN
3	BT	235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BU	23	ASN
3	BU	75	ASN
3	BU	250	GLN
3	BV	23	ASN
3	BV	102	GLN
3	BV	121	ASN
3	BV	235	GLN
3	BV	250	GLN
3	BW	102	GLN
3	BW	121	ASN
3	BX	102	GLN
3	BX	121	ASN
3	BX	167	ASN
3	BX	250	GLN
1	BY	90	ASN
1	BY	143	ASN
1	BZ	143	ASN
1	BZ	184	GLN
1	BZ	192	GLN
1	BZ	212	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A0	372/372 (100%)	1.12	67 (18%)	2 6	351, 388, 435, 523	0
1	AY	372/372 (100%)	0.94	59 (15%)	3 7	359, 396, 449, 555	0
1	AZ	372/372 (100%)	0.99	61 (16%)	2 7	364, 394, 445, 557	0
1	B0	372/372 (100%)	1.09	69 (18%)	2 6	337, 377, 425, 485	0
1	BY	372/372 (100%)	0.79	34 (9%)	9 17	331, 361, 429, 557	0
1	BZ	372/372 (100%)	1.02	56 (15%)	3 8	332, 360, 422, 502	0
2	AA	263/263 (100%)	0.66	25 (9%)	8 16	248, 312, 407, 435	0
2	AB	263/263 (100%)	0.75	33 (12%)	5 11	284, 350, 440, 481	0
2	AC	263/263 (100%)	0.44	19 (7%)	15 21	257, 345, 417, 473	0
2	AD	263/263 (100%)	0.86	37 (14%)	3 9	258, 320, 441, 485	0
2	AE	263/263 (100%)	0.56	23 (8%)	10 17	277, 344, 466, 480	0
2	AF	263/263 (100%)	0.72	36 (13%)	4 9	265, 367, 471, 497	0
2	AG	263/263 (100%)	0.88	39 (14%)	3 8	265, 348, 500, 556	0
2	AH	263/263 (100%)	0.45	22 (8%)	11 18	315, 402, 524, 572	0
2	AI	263/263 (100%)	0.74	37 (14%)	3 9	282, 416, 532, 576	0
2	AJ	263/263 (100%)	0.60	28 (10%)	7 13	264, 342, 429, 539	0
2	AK	263/263 (100%)	0.61	25 (9%)	8 16	255, 301, 456, 521	0
2	AL	263/263 (100%)	0.78	36 (13%)	4 9	277, 345, 485, 575	0
2	AM	263/263 (100%)	0.76	35 (13%)	4 9	266, 358, 425, 467	0
2	AN	263/263 (100%)	0.81	37 (14%)	3 9	252, 313, 386, 420	0
2	AO	263/263 (100%)	0.74	33 (12%)	5 11	276, 347, 419, 449	0
2	AP	263/263 (100%)	0.80	39 (14%)	3 8	267, 341, 556, 576	0
2	AQ	263/263 (100%)	0.94	46 (17%)	2 6	295, 397, 566, 605	0
2	AR	263/263 (100%)	0.76	34 (12%)	4 10	298, 417, 541, 571	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	BA	263/263 (100%)	0.72	27 (10%) 7 14	259, 312, 430, 466	0
2	BB	263/263 (100%)	0.64	26 (9%) 8 15	282, 346, 455, 506	0
2	BC	263/263 (100%)	0.57	29 (11%) 6 13	273, 344, 419, 481	0
2	BD	263/263 (100%)	0.85	41 (15%) 3 8	252, 316, 445, 484	0
2	BE	263/263 (100%)	0.60	26 (9%) 8 15	274, 342, 448, 477	0
2	BF	263/263 (100%)	1.02	49 (18%) 2 6	258, 361, 457, 487	0
2	BG	263/263 (100%)	0.95	48 (18%) 2 6	252, 346, 496, 557	0
2	BH	263/263 (100%)	0.76	33 (12%) 5 11	314, 408, 514, 559	0
2	BI	263/263 (100%)	0.63	29 (11%) 6 13	276, 420, 541, 584	0
2	BJ	263/263 (100%)	0.44	20 (7%) 14 20	268, 345, 419, 521	0
2	BK	263/263 (100%)	0.80	34 (12%) 4 10	256, 305, 435, 496	0
2	BL	263/263 (100%)	0.76	37 (14%) 3 9	283, 341, 452, 534	0
2	BM	263/263 (100%)	1.07	44 (16%) 2 7	264, 357, 438, 484	0
2	BN	263/263 (100%)	0.82	33 (12%) 5 11	255, 316, 388, 433	0
2	BO	263/263 (100%)	0.65	24 (9%) 9 17	276, 348, 418, 453	0
2	BP	263/263 (100%)	1.02	44 (16%) 2 7	261, 365, 541, 549	0
2	BQ	263/263 (100%)	0.84	39 (14%) 3 8	312, 413, 547, 559	0
2	BR	263/263 (100%)	0.95	46 (17%) 2 6	308, 418, 537, 556	0
3	AS	298/298 (100%)	0.94	38 (12%) 4 10	219, 262, 346, 379	0
3	AT	298/298 (100%)	0.90	36 (12%) 5 11	230, 260, 318, 344	0
3	AU	298/298 (100%)	0.80	34 (11%) 6 12	228, 269, 334, 364	0
3	AV	298/298 (100%)	0.86	43 (14%) 3 8	229, 264, 317, 332	0
3	AW	298/298 (100%)	0.82	27 (9%) 9 17	213, 254, 317, 347	0
3	AX	298/298 (100%)	0.74	26 (8%) 10 17	216, 255, 347, 401	0
3	BS	298/298 (100%)	0.86	36 (12%) 5 11	222, 256, 339, 388	0
3	BT	298/298 (100%)	0.86	34 (11%) 6 12	218, 265, 316, 343	0
3	BU	298/298 (100%)	0.77	28 (9%) 9 16	228, 262, 338, 382	0
3	BV	298/298 (100%)	0.97	49 (16%) 2 7	218, 260, 305, 324	0
3	BW	298/298 (100%)	0.73	23 (7%) 13 20	215, 256, 341, 403	0
3	BX	298/298 (100%)	0.73	23 (7%) 13 20	228, 272, 370, 407	0
All	All	15276/15276 (100%)	0.80	1956 (12%) 4 10	213, 344, 468, 605	0

All (1956) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AQ	220	LEU	20.9
2	AQ	221	VAL	17.8
2	BR	30	LEU	11.6
1	BY	1	MET	11.6
2	AM	176	LEU	11.3
2	BM	174	LEU	10.5
1	A0	32	LEU	10.4
1	BZ	209	ALA	10.4
2	BH	259	GLY	10.3
2	BM	259	GLY	9.9
2	BG	254	ALA	9.9
1	A0	198	THR	9.6
2	BR	221	VAL	9.5
2	BO	259	GLY	8.9
2	BI	259	GLY	8.9
2	BP	192	GLY	8.7
1	A0	195	PRO	8.6
2	BQ	221	VAL	8.4
2	BB	260	SER	8.1
3	AS	298	VAL	8.1
2	AL	221	VAL	8.0
2	BR	3	ILE	8.0
2	BA	221	VAL	8.0
2	AO	259	GLY	7.9
2	BF	259	GLY	7.9
2	BN	260	SER	7.9
2	AR	221	VAL	7.8
2	BB	221	VAL	7.8
2	BO	260	SER	7.8
2	AR	222	GLY	7.8
2	BQ	233	ILE	7.8
2	BG	221	VAL	7.8
2	BH	261	TYR	7.7
2	BM	176	LEU	7.7
1	AZ	367	GLU	7.7
2	BM	257	GLY	7.7
1	AZ	1	MET	7.6
2	AF	62	ALA	7.6
1	AZ	215	ARG	7.6
2	AM	221	VAL	7.5
2	BL	252	PRO	7.5
2	BQ	222	GLY	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BY	215	ARG	7.3
2	AM	174	LEU	7.3
2	AQ	222	GLY	7.3
2	BA	222	GLY	7.3
2	BF	221	VAL	7.2
2	AP	117	GLY	7.2
2	BF	260	SER	7.2
2	BD	264	LYS	7.2
2	AM	175	GLN	7.1
2	BC	260	SER	7.1
1	BZ	208	PHE	7.0
3	BX	298	VAL	7.0
1	AY	1	MET	7.0
2	BF	174	LEU	6.9
2	BO	157	GLY	6.9
2	BM	167	THR	6.9
2	BM	258	ASN	6.9
2	BQ	231	PHE	6.9
1	A0	332	LEU	6.8
2	BK	30	LEU	6.8
2	BR	31	THR	6.8
2	BH	260	SER	6.8
1	A0	356	LYS	6.7
2	AF	259	GLY	6.7
2	AI	35	TYR	6.7
2	AI	36	ARG	6.7
2	BP	193	SER	6.6
2	AG	225	ALA	6.6
1	B0	195	PRO	6.6
1	AY	217	ARG	6.6
2	AO	260	SER	6.6
2	BM	188	VAL	6.6
2	AG	192	GLY	6.6
2	BN	259	GLY	6.6
2	BF	63	GLY	6.6
1	A0	197	GLU	6.5
2	BN	185	LEU	6.5
2	AF	260	SER	6.5
2	AP	222	GLY	6.5
1	A0	68	ILE	6.5
2	AE	221	VAL	6.4
1	B0	164	ASN	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AD	38	ILE	6.3
2	BP	211	PRO	6.3
2	AD	258	ASN	6.3
2	BK	27	TYR	6.3
1	AY	128	THR	6.3
2	BM	261	TYR	6.3
2	BG	220	LEU	6.2
2	BK	168	VAL	6.2
2	AG	211	PRO	6.2
2	BP	176	LEU	6.2
2	BE	258	ASN	6.2
2	BR	29	MET	6.2
2	AJ	26	LEU	6.2
2	BM	168	VAL	6.2
2	BM	153	MET	6.2
2	AO	221	VAL	6.1
2	BF	220	LEU	6.1
2	AK	221	VAL	6.1
2	AR	31	THR	6.1
1	B0	162	THR	6.1
2	BP	61	ILE	6.1
1	A0	164	ASN	6.1
3	BU	1	MET	6.1
2	AD	221	VAL	6.0
2	BP	38	ILE	6.0
1	AZ	164	ASN	5.9
2	AR	258	ASN	5.9
2	BM	166	LEU	5.9
3	BT	247	GLU	5.8
2	AQ	27	TYR	5.8
3	AX	200	MET	5.8
2	BD	181	LYS	5.8
2	AR	99	LEU	5.8
1	A0	326	GLN	5.7
2	AQ	63	GLY	5.7
3	BS	212	ALA	5.7
2	BB	261	TYR	5.7
2	AQ	253	ILE	5.7
2	AG	27	TYR	5.6
2	BQ	2	THR	5.6
2	BH	252	PRO	5.6
2	BH	222	GLY	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AQ	94	ALA	5.6
3	AT	298	VAL	5.6
2	AP	254	ALA	5.6
2	AF	220	LEU	5.6
2	BQ	230	SER	5.6
2	BB	222	GLY	5.6
3	BX	99	GLU	5.6
2	BH	99	LEU	5.6
2	BR	126	VAL	5.6
2	BA	130	GLY	5.6
2	BH	221	VAL	5.5
1	AY	129	THR	5.5
2	AG	254	ALA	5.5
1	B0	209	ALA	5.5
2	BP	253	ILE	5.5
2	BO	159	ILE	5.5
3	BV	298	VAL	5.5
3	BV	249	TYR	5.5
2	BQ	38	ILE	5.5
2	AJ	261	TYR	5.5
2	AQ	219	SER	5.5
2	AL	62	ALA	5.4
2	BN	261	TYR	5.4
2	AQ	30	LEU	5.4
2	BI	188	VAL	5.4
2	AM	62	ALA	5.4
2	BQ	220	LEU	5.4
1	BZ	264	ILE	5.4
3	BS	249	TYR	5.4
2	AA	30	LEU	5.4
2	AR	30	LEU	5.4
2	BM	260	SER	5.3
1	AZ	233	GLU	5.3
2	BK	64	GLY	5.3
2	AM	27	TYR	5.3
2	BQ	215	ALA	5.3
2	BI	260	SER	5.3
2	BQ	62	ALA	5.3
2	BO	30	LEU	5.3
3	BV	296	ASP	5.3
2	AE	257	GLY	5.3
2	BK	69	LEU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AD	99	LEU	5.3
1	A0	200	PRO	5.3
3	AT	1	MET	5.3
3	BS	34	LEU	5.3
3	BW	279	MET	5.3
2	AI	188	VAL	5.3
3	AT	240	ILE	5.2
2	BF	99	LEU	5.2
3	AT	34	LEU	5.2
1	B0	125	ILE	5.2
2	AG	221	VAL	5.2
3	BV	139	TYR	5.2
2	AD	161	VAL	5.2
3	AT	287	ALA	5.2
2	BP	175	GLN	5.2
2	AP	223	HIS	5.2
2	AJ	27	TYR	5.2
2	BG	175	GLN	5.2
2	BR	220	LEU	5.2
2	AL	220	LEU	5.1
2	AO	220	LEU	5.1
2	BG	176	LEU	5.1
2	BB	259	GLY	5.1
2	BM	190	PHE	5.1
2	AP	30	LEU	5.1
2	BD	27	TYR	5.1
1	AY	164	ASN	5.1
2	AL	63	GLY	5.1
2	BG	27	TYR	5.1
2	BF	176	LEU	5.1
2	BH	258	ASN	5.1
3	AW	281	LEU	5.0
2	BE	221	VAL	5.0
1	BZ	142	LYS	5.0
2	AB	69	LEU	5.0
2	BA	220	LEU	5.0
2	BG	99	LEU	5.0
2	AM	260	SER	5.0
2	AN	27	TYR	5.0
1	BY	372	PRO	5.0
3	BV	247	GLU	5.0
2	BN	186	VAL	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AN	259	GLY	5.0
2	BB	30	LEU	5.0
3	AU	203	LEU	5.0
2	AM	177	GLN	5.0
1	AY	158	ALA	4.9
2	BP	62	ALA	4.9
1	BZ	356	LYS	4.9
3	AX	187	LEU	4.9
2	BR	197	ILE	4.9
1	A0	202	ASN	4.9
1	B0	328	GLU	4.9
2	BB	220	LEU	4.9
2	BP	254	ALA	4.9
2	BP	252	PRO	4.9
2	BK	26	LEU	4.9
2	AG	256	ARG	4.9
2	BF	261	TYR	4.9
2	AQ	62	ALA	4.9
2	AA	31	THR	4.9
3	AT	72	LEU	4.9
2	BC	218	GLN	4.8
2	BN	153	MET	4.8
1	AY	315	PRO	4.8
2	BH	257	GLY	4.8
2	AN	221	VAL	4.8
2	AD	211	PRO	4.8
2	BP	223	HIS	4.8
1	AY	162	THR	4.8
2	AD	220	LEU	4.8
2	AK	27	TYR	4.8
2	BR	233	ILE	4.8
2	AM	61	ILE	4.8
1	B0	292	THR	4.8
1	BY	162	THR	4.8
2	BF	64	GLY	4.8
3	AS	204	TYR	4.8
2	AO	27	TYR	4.8
2	AG	190	PHE	4.8
2	BF	144	THR	4.7
2	AL	254	ALA	4.7
2	AQ	259	GLY	4.7
3	AV	200	MET	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BD	257	GLY	4.7
2	AG	220	LEU	4.7
2	BP	66	TYR	4.7
3	BU	203	LEU	4.7
3	BX	100	ILE	4.7
2	BI	221	VAL	4.7
1	A0	196	SER	4.7
2	AL	222	GLY	4.7
2	BM	220	LEU	4.7
2	BG	235	ILE	4.7
2	BN	221	VAL	4.7
1	AZ	136	TYR	4.7
2	AI	75	ALA	4.7
3	AT	202	ILE	4.7
2	BQ	99	LEU	4.6
3	BX	1	MET	4.6
1	AZ	52	LEU	4.6
1	A0	327	ASN	4.6
1	BY	332	LEU	4.6
2	BI	27	TYR	4.6
2	BA	260	SER	4.6
2	BP	216	ALA	4.6
1	BZ	207	ASN	4.6
2	BJ	185	LEU	4.6
2	BF	62	ALA	4.6
2	AG	167	THR	4.6
1	BZ	263	TYR	4.6
2	BF	262	PHE	4.6
1	BY	271	VAL	4.6
1	AY	233	GLU	4.6
2	BL	197	ILE	4.6
3	BU	287	ALA	4.6
2	BJ	260	SER	4.6
1	AZ	299	ASP	4.6
3	AS	287	ALA	4.6
3	AW	1	MET	4.6
1	BZ	76	VAL	4.6
3	AV	287	ALA	4.6
2	AN	213	ARG	4.6
3	AT	2	VAL	4.6
2	AQ	260	SER	4.6
1	B0	280	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BK	99	LEU	4.6
2	BH	253	ILE	4.5
3	AU	158	LYS	4.5
2	AP	221	VAL	4.5
2	AP	26	LEU	4.5
2	BL	188	VAL	4.5
2	AG	175	GLN	4.5
1	B0	329	LEU	4.5
2	BF	222	GLY	4.5
2	BG	185	LEU	4.5
2	AM	30	LEU	4.5
2	BH	251	THR	4.5
2	BE	257	GLY	4.5
2	AM	188	VAL	4.5
2	AN	187	ILE	4.4
2	AP	145	LEU	4.4
2	AN	258	ASN	4.4
3	AT	288	GLU	4.4
2	BR	232	HIS	4.4
1	AY	184	GLN	4.4
2	BL	43	TRP	4.4
2	BD	99	LEU	4.4
2	AQ	233	ILE	4.4
2	AK	62	ALA	4.4
3	AT	212	ALA	4.4
2	AL	188	VAL	4.4
2	BL	176	LEU	4.4
2	AI	259	GLY	4.4
1	BZ	244	ALA	4.4
2	BL	66	TYR	4.4
2	BD	221	VAL	4.4
2	AG	30	LEU	4.4
3	AX	272	ARG	4.4
2	AG	191	PHE	4.4
2	BE	99	LEU	4.4
2	BB	27	TYR	4.3
3	AV	269	TYR	4.3
2	AQ	97	VAL	4.3
1	AZ	230	MET	4.3
2	BI	69	LEU	4.3
1	AZ	166	LYS	4.3
1	AZ	201	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BK	176	LEU	4.3
2	BM	189	ARG	4.3
2	AO	185	LEU	4.3
3	AV	289	PHE	4.3
2	BR	4	LYS	4.3
1	AZ	300	HIS	4.3
2	BP	30	LEU	4.3
2	BA	30	LEU	4.3
2	BO	221	VAL	4.3
2	AI	27	TYR	4.3
3	BT	158	LYS	4.3
1	BZ	119	LEU	4.3
3	AX	1	MET	4.3
2	AQ	237	PRO	4.3
1	BZ	318	ILE	4.3
2	AD	18	VAL	4.3
2	BK	62	ALA	4.3
2	BR	222	GLY	4.3
2	AB	27	TYR	4.3
2	BC	261	TYR	4.3
2	BL	221	VAL	4.3
2	AN	23	ASP	4.3
2	AL	227	ARG	4.3
2	AN	181	LYS	4.3
2	BM	221	VAL	4.3
3	BX	281	LEU	4.3
1	AY	36	LYS	4.3
2	AF	63	GLY	4.3
1	A0	199	ASP	4.2
2	AG	226	GLY	4.2
2	BQ	232	HIS	4.2
1	BZ	148	TYR	4.2
2	BD	184	ASP	4.2
2	AH	99	LEU	4.2
1	A0	151	PHE	4.2
2	BR	228	ASP	4.2
2	BG	192	GLY	4.2
2	BH	188	VAL	4.2
2	BK	31	THR	4.2
2	AF	99	LEU	4.2
1	BZ	116	ILE	4.2
2	BP	31	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BO	27	TYR	4.2
2	BM	263	ILE	4.2
2	BA	76	LEU	4.2
3	AX	118	TYR	4.2
1	A0	194	ALA	4.1
2	AR	27	TYR	4.1
1	AZ	232	THR	4.1
2	AB	176	LEU	4.1
2	BK	169	GLU	4.1
1	B0	235	ILE	4.1
2	AH	260	SER	4.1
3	AV	190	TRP	4.1
1	AY	372	PRO	4.1
2	AM	259	GLY	4.1
2	AC	184	ASP	4.1
1	AY	337	LEU	4.1
2	BP	169	GLU	4.1
2	BQ	208	VAL	4.1
1	AZ	209	ALA	4.1
2	BM	142	THR	4.1
2	BH	26	LEU	4.1
2	AQ	95	ASN	4.1
2	BC	185	LEU	4.1
2	AE	222	GLY	4.1
2	AP	90	LEU	4.0
3	BU	158	LYS	4.0
2	AN	208	VAL	4.0
2	BO	97	VAL	4.0
2	BP	215	ALA	4.0
2	BG	167	THR	4.0
2	BM	69	LEU	4.0
1	A0	265	ALA	4.0
1	AZ	278	HIS	4.0
2	AB	88	ILE	4.0
2	BL	253	ILE	4.0
2	BO	220	LEU	4.0
1	B0	136	TYR	4.0
1	A0	333	TYR	4.0
1	AZ	14	TYR	4.0
2	AQ	215	ALA	4.0
2	BO	188	VAL	4.0
2	AF	262	PHE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AZ	210	SER	4.0
2	AC	183	ASN	4.0
2	AG	23	ASP	4.0
2	AM	258	ASN	4.0
2	BC	247	ASN	4.0
2	BP	67	PHE	4.0
2	BD	182	ASN	4.0
2	AD	61	ILE	3.9
2	BK	67	PHE	3.9
1	AY	126	THR	3.9
2	AE	145	LEU	3.9
2	BL	194	VAL	3.9
2	AC	30	LEU	3.9
2	AB	222	GLY	3.9
2	BE	259	GLY	3.9
2	BP	39	ARG	3.9
3	BU	200	MET	3.9
1	BY	78	PRO	3.9
2	BH	27	TYR	3.9
2	AC	185	LEU	3.9
2	BG	159	ILE	3.9
3	AV	249	TYR	3.9
1	AZ	368	SER	3.9
1	BZ	247	PHE	3.9
2	BK	29	MET	3.9
2	BO	158	SER	3.9
2	BK	187	ILE	3.9
3	AU	238	ILE	3.9
3	AS	203	LEU	3.9
2	AI	64	GLY	3.9
2	BN	206	THR	3.9
2	AL	27	TYR	3.9
2	AI	99	LEU	3.9
1	B0	163	ILE	3.8
1	B0	127	LYS	3.8
1	AY	87	LYS	3.8
2	AN	185	LEU	3.8
2	BJ	60	ILE	3.8
2	BD	185	LEU	3.8
2	BP	60	ILE	3.8
2	BN	78	GLY	3.8
1	BY	330	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BN	97	VAL	3.8
3	BW	68	PHE	3.8
2	BO	219	SER	3.8
3	BX	296	ASP	3.8
2	BM	169	GLU	3.8
2	BA	259	GLY	3.8
3	BV	142	LEU	3.8
3	BS	114	LYS	3.8
2	BD	179	THR	3.8
2	BC	262	PHE	3.8
2	BR	185	LEU	3.8
2	BI	261	TYR	3.8
2	AR	26	LEU	3.8
1	B0	124	ALA	3.8
1	BZ	137	LEU	3.8
2	BP	221	VAL	3.8
2	BD	86	ALA	3.7
2	AG	176	LEU	3.7
3	AS	212	ALA	3.7
2	BQ	206	THR	3.7
3	AT	296	ASP	3.7
1	BY	331	PRO	3.7
2	AL	258	ASN	3.7
2	AR	33	MET	3.7
3	BV	200	MET	3.7
1	BY	235	ILE	3.7
2	BL	248	ILE	3.7
2	AL	161	VAL	3.7
2	BO	261	TYR	3.7
1	AY	182	LYS	3.7
3	AS	286	LYS	3.7
1	B0	183	VAL	3.7
2	AF	176	LEU	3.7
3	AV	142	LEU	3.7
3	BT	142	LEU	3.7
2	BI	167	THR	3.7
2	AF	218	GLN	3.7
2	AG	235	ILE	3.7
3	BW	158	LYS	3.7
2	AK	67	PHE	3.7
2	BD	123	PHE	3.7
2	BP	27	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AY	159	GLY	3.7
2	AD	62	ALA	3.7
3	AS	249	TYR	3.7
2	AC	264	LYS	3.7
2	BB	185	LEU	3.7
3	AS	61	ILE	3.7
2	AM	220	LEU	3.7
1	A0	163	ILE	3.7
2	BR	77	LYS	3.7
1	AY	2	LEU	3.7
2	BC	254	ALA	3.7
1	BZ	32	LEU	3.7
2	AG	214	PRO	3.7
2	AJ	212	PHE	3.7
2	BF	185	LEU	3.7
2	AR	257	GLY	3.7
2	BR	70	LEU	3.7
2	AE	256	ARG	3.7
1	A0	331	PRO	3.6
2	AQ	218	GLN	3.6
2	BK	63	GLY	3.6
2	AO	103	THR	3.6
2	AD	30	LEU	3.6
2	AI	30	LEU	3.6
2	AR	69	LEU	3.6
2	BD	178	LEU	3.6
2	AO	261	TYR	3.6
1	A0	31	GLY	3.6
2	AB	178	LEU	3.6
1	AZ	304	PRO	3.6
2	AF	216	ALA	3.6
2	AK	60	ILE	3.6
1	B0	356	LYS	3.6
2	AD	101	ALA	3.6
2	AK	97	VAL	3.6
2	BD	260	SER	3.6
2	BC	258	ASN	3.6
2	AM	99	LEU	3.6
2	AI	33	MET	3.6
3	AW	34	LEU	3.6
2	AN	176	LEU	3.6
1	BZ	372	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AC	99	LEU	3.6
2	AN	260	SER	3.6
2	BA	27	TYR	3.6
2	BL	251	THR	3.6
2	AR	29	MET	3.6
2	BG	260	SER	3.6
1	A0	203	LEU	3.6
1	B0	138	ILE	3.6
2	BQ	246	ALA	3.6
2	BR	26	LEU	3.6
2	AE	258	ASN	3.6
2	BK	25	LYS	3.6
2	BR	125	ILE	3.6
2	BN	205	GLY	3.6
3	AX	76	TYR	3.6
1	AY	132	ALA	3.6
3	AT	76	TYR	3.6
2	BK	221	VAL	3.5
1	A0	9	ASN	3.5
2	BJ	262	PHE	3.5
3	BT	248	THR	3.5
2	AA	3	ILE	3.5
2	BJ	3	ILE	3.5
2	BM	178	LEU	3.5
2	BP	99	LEU	3.5
3	AX	290	LYS	3.5
2	AP	27	TYR	3.5
2	BN	27	TYR	3.5
2	BR	27	TYR	3.5
3	BV	260	LEU	3.5
1	AZ	315	PRO	3.5
2	BM	187	ILE	3.5
2	AI	187	ILE	3.5
3	AU	289	PHE	3.5
2	BE	27	TYR	3.5
2	BJ	30	LEU	3.5
2	BP	256	ARG	3.5
3	AT	279	MET	3.5
3	AU	279	MET	3.5
3	BV	294	LYS	3.5
2	AH	222	GLY	3.5
1	AZ	126	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BF	175	GLN	3.5
2	AF	254	ALA	3.5
3	AX	280	GLU	3.5
2	BG	103	THR	3.5
3	AV	202	ILE	3.5
2	AM	86	ALA	3.5
2	BL	190	PHE	3.5
2	BP	69	LEU	3.5
2	BA	18	VAL	3.5
1	BY	125	ILE	3.5
3	BU	178	TYR	3.5
1	BY	137	LEU	3.5
2	BC	259	GLY	3.5
2	AH	261	TYR	3.5
2	AQ	235	ILE	3.5
2	AO	162	PRO	3.5
2	AE	38	ILE	3.5
2	BM	264	LYS	3.5
2	BD	166	LEU	3.5
3	AS	281	LEU	3.5
2	BQ	168	VAL	3.5
1	A0	162	THR	3.5
2	BK	55	TYR	3.5
2	BQ	176	LEU	3.5
1	AY	160	LYS	3.5
2	AC	122	CYS	3.4
2	AK	220	LEU	3.4
3	AS	156	MET	3.4
2	BF	27	TYR	3.4
2	BR	139	ILE	3.4
1	A0	315	PRO	3.4
2	AL	219	SER	3.4
2	BE	222	GLY	3.4
1	A0	148	TYR	3.4
2	AD	260	SER	3.4
2	BL	222	GLY	3.4
2	AK	61	ILE	3.4
2	BQ	174	LEU	3.4
3	BS	227	ILE	3.4
1	B0	208	PHE	3.4
2	AQ	216	ALA	3.4
2	BG	102	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BH	30	LEU	3.4
3	AV	61	ILE	3.4
3	AU	154	ALA	3.4
1	B0	160	LYS	3.4
2	BE	62	ALA	3.4
2	AB	99	LEU	3.4
2	BA	231	PHE	3.4
1	B0	295	TYR	3.4
2	AC	263	ILE	3.4
2	BL	112	ILE	3.4
2	BR	241	ILE	3.4
3	AV	240	ILE	3.4
3	AW	107	LEU	3.4
3	BV	272	ARG	3.4
2	AI	63	GLY	3.4
2	BA	131	THR	3.4
3	BX	258	LEU	3.4
2	AK	199	LYS	3.4
2	BR	260	SER	3.4
3	AW	279	MET	3.4
2	BG	218	GLN	3.4
1	AZ	163	ILE	3.4
3	BS	61	ILE	3.4
2	BI	153	MET	3.4
2	AB	188	VAL	3.4
1	BZ	138	ILE	3.4
1	BY	371	LYS	3.4
2	BH	220	LEU	3.4
2	AK	159	ILE	3.4
2	AA	27	TYR	3.4
2	AA	77	LYS	3.4
2	BN	208	VAL	3.4
1	AY	333	TYR	3.4
2	AB	190	PHE	3.4
2	BC	187	ILE	3.4
1	A0	357	THR	3.4
2	BB	97	VAL	3.4
2	BP	88	ILE	3.4
2	BO	185	LEU	3.4
3	AW	158	LYS	3.4
1	AZ	305	GLU	3.4
2	AL	253	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AP	220	LEU	3.3
3	AV	59	PRO	3.3
2	BQ	63	GLY	3.3
2	BO	99	LEU	3.3
2	BH	116	SER	3.3
1	A0	87	LYS	3.3
2	BH	68	GLU	3.3
3	BT	118	TYR	3.3
2	AL	181	LYS	3.3
2	BE	159	ILE	3.3
1	A0	36	LYS	3.3
1	BY	160	LYS	3.3
2	AB	68	GLU	3.3
3	BT	281	LEU	3.3
1	B0	137	LEU	3.3
2	AJ	220	LEU	3.3
1	B0	221	ARG	3.3
2	BB	48	ASN	3.3
3	AT	3	ARG	3.3
3	BS	213	GLY	3.3
1	BZ	204	LEU	3.3
2	AC	211	PRO	3.3
2	AP	116	SER	3.3
2	BE	145	LEU	3.3
1	B0	178	ARG	3.3
2	AJ	223	HIS	3.3
2	BB	53	VAL	3.3
3	AT	79	MET	3.3
2	AL	159	ILE	3.3
2	AM	31	THR	3.3
1	AY	328	GLU	3.3
1	A0	145	LEU	3.3
2	AF	188	VAL	3.3
2	AP	176	LEU	3.3
3	BU	12	ASP	3.3
2	BL	259	GLY	3.3
2	AP	97	VAL	3.3
3	BW	25	LYS	3.3
3	BV	291	ILE	3.3
2	BD	176	LEU	3.3
3	AS	238	ILE	3.3
2	AH	215	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AN	188	VAL	3.2
2	AR	190	PHE	3.2
2	BE	75	ALA	3.2
3	AV	144	PHE	3.2
3	AW	212	ALA	3.2
1	AY	371	LYS	3.2
2	AD	60	ILE	3.2
2	AJ	138	PRO	3.2
2	AR	125	ILE	3.2
3	BS	279	MET	3.2
2	AD	259	GLY	3.2
2	AO	257	GLY	3.2
3	BV	119	GLY	3.2
2	AB	90	LEU	3.2
2	BF	168	VAL	3.2
2	BI	148	ILE	3.2
2	AI	109	GLY	3.2
2	BD	164	GLN	3.2
1	BZ	125	ILE	3.2
2	BP	210	ARG	3.2
3	BV	30	GLN	3.2
2	AB	110	VAL	3.2
2	AF	221	VAL	3.2
3	BT	143	THR	3.2
2	AJ	262	PHE	3.2
1	AY	88	LYS	3.2
2	BI	220	LEU	3.2
1	A0	66	GLY	3.2
1	BZ	79	ILE	3.2
2	BI	99	LEU	3.2
2	BF	214	PRO	3.2
2	BL	203	MET	3.2
2	AJ	81	VAL	3.2
3	BS	250	GLN	3.2
3	BV	34	LEU	3.2
1	A0	320	THR	3.2
2	BF	143	SER	3.2
2	AF	253	ILE	3.2
3	AW	118	TYR	3.2
2	AI	28	MET	3.2
2	BQ	153	MET	3.2
1	BZ	271	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BN	18	VAL	3.2
2	AL	160	ASP	3.2
2	AJ	30	LEU	3.2
2	AP	253	ILE	3.2
2	AC	40	ARG	3.2
2	BG	67	PHE	3.2
3	AT	118	TYR	3.2
2	BD	187	ILE	3.2
3	AX	289	PHE	3.2
2	AD	185	LEU	3.2
3	BU	90	LYS	3.2
2	AP	225	ALA	3.2
2	AD	33	MET	3.2
1	A0	165	ARG	3.2
2	BI	178	LEU	3.2
2	BQ	131	THR	3.2
1	B0	126	THR	3.2
2	AE	37	THR	3.2
2	AE	62	ALA	3.2
2	AJ	69	LEU	3.2
3	BW	120	LYS	3.2
2	AQ	261	TYR	3.2
2	BN	53	VAL	3.1
1	BY	335	ASN	3.1
3	AW	122	GLY	3.1
2	BC	99	LEU	3.1
2	BR	33	MET	3.1
2	AA	235	ILE	3.1
2	BB	258	ASN	3.1
1	AZ	162	THR	3.1
2	AH	258	ASN	3.1
1	B0	87	LYS	3.1
2	AA	124	ASP	3.1
1	B0	9	ASN	3.1
2	AR	231	PHE	3.1
3	AV	201	GLY	3.1
3	BV	289	PHE	3.1
2	AO	161	VAL	3.1
1	AY	136	TYR	3.1
2	BF	256	ARG	3.1
2	BJ	27	TYR	3.1
1	BZ	186	GLN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BZ	134	ILE	3.1
2	AQ	187	ILE	3.1
2	AJ	185	LEU	3.1
2	BL	202	ASN	3.1
2	BP	255	THR	3.1
3	AW	114	LYS	3.1
1	BZ	136	TYR	3.1
2	AB	55	TYR	3.1
2	AO	258	ASN	3.1
2	BO	90	LEU	3.1
1	BY	359	PHE	3.1
2	BK	174	LEU	3.1
2	AH	221	VAL	3.1
2	BF	65	ARG	3.1
2	BJ	122	CYS	3.1
3	BX	200	MET	3.1
1	BZ	245	VAL	3.1
2	BI	3	ILE	3.1
3	AS	1	MET	3.1
1	BY	136	TYR	3.1
2	BG	86	ALA	3.1
2	AB	60	ILE	3.1
2	AL	232	HIS	3.1
1	AZ	167	ALA	3.1
2	AI	260	SER	3.1
2	BH	187	ILE	3.1
2	BM	170	ALA	3.1
3	BW	5	TYR	3.1
1	AY	215	ARG	3.1
1	AZ	225	LYS	3.1
2	AA	99	LEU	3.1
2	AE	88	ILE	3.1
2	AR	185	LEU	3.1
2	BM	200	GLY	3.1
1	AZ	319	VAL	3.1
1	AZ	165	ARG	3.1
3	BU	279	MET	3.1
2	BG	105	ASN	3.1
2	BI	222	GLY	3.1
2	AQ	93	THR	3.1
3	BV	239	LEU	3.0
3	AW	211	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	BX	288	GLU	3.0
1	A0	363	LEU	3.0
3	BS	118	TYR	3.0
2	BK	61	ILE	3.0
2	AO	188	VAL	3.0
1	B0	309	ILE	3.0
3	AX	90	LYS	3.0
1	AY	314	SER	3.0
1	BZ	274	TYR	3.0
2	AF	219	SER	3.0
2	AL	176	LEU	3.0
2	BG	60	ILE	3.0
2	BR	198	GLN	3.0
2	AJ	99	LEU	3.0
2	BE	76	LEU	3.0
3	BT	152	VAL	3.0
1	AY	366	VAL	3.0
2	BH	88	ILE	3.0
3	AW	79	MET	3.0
1	A0	367	GLU	3.0
2	BL	90	LEU	3.0
2	BN	30	LEU	3.0
3	AU	142	LEU	3.0
1	AY	216	LYS	3.0
2	BC	253	ILE	3.0
3	BW	288	GLU	3.0
2	BM	177	GLN	3.0
2	BF	142	THR	3.0
2	AG	144	THR	3.0
2	BB	262	PHE	3.0
2	BH	215	ALA	3.0
2	BM	175	GLN	3.0
1	BZ	246	VAL	3.0
2	AG	99	LEU	3.0
2	AI	131	THR	3.0
2	BF	255	THR	3.0
2	BP	123	PHE	3.0
3	AW	280	GLU	3.0
2	AP	88	ILE	3.0
2	AC	123	PHE	3.0
2	AN	178	LEU	3.0
2	AR	70	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BK	28	MET	3.0
3	BS	199	PHE	3.0
2	AN	257	GLY	3.0
2	BP	68	GLU	3.0
3	BS	59	PRO	3.0
1	AY	65	VAL	3.0
2	BD	163	VAL	3.0
2	BC	159	ILE	3.0
1	B0	332	LEU	3.0
2	AA	208	VAL	3.0
3	BV	281	LEU	3.0
1	B0	265	ALA	3.0
2	AB	97	VAL	2.9
1	AZ	158	ALA	2.9
2	AP	153	MET	2.9
3	BX	82	PHE	2.9
2	AA	185	LEU	2.9
2	BQ	27	TYR	2.9
2	AG	208	VAL	2.9
2	BR	2	THR	2.9
1	A0	328	GLU	2.9
2	AF	3	ILE	2.9
2	BA	77	LYS	2.9
2	BH	186	VAL	2.9
3	AU	227	ILE	2.9
2	BP	90	LEU	2.9
3	BV	197	PHE	2.9
3	BX	297	PHE	2.9
1	BZ	206	ILE	2.9
2	AL	251	THR	2.9
2	BQ	148	ILE	2.9
1	BZ	51	TYR	2.9
2	AI	197	ILE	2.9
2	AM	189	ARG	2.9
2	AM	218	GLN	2.9
2	BP	191	PHE	2.9
2	AJ	137	LYS	2.9
3	BU	202	ILE	2.9
1	AY	19	ASP	2.9
2	BE	146	ASP	2.9
3	BS	79	MET	2.9
2	BF	141	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BM	64	GLY	2.9
3	BW	76	TYR	2.9
2	AO	30	LEU	2.9
3	BV	31	PRO	2.9
2	AB	235	ILE	2.9
2	AR	148	ILE	2.9
1	AY	265	ALA	2.9
2	AI	198	GLN	2.9
3	AS	34	LEU	2.9
3	BU	288	GLU	2.9
3	BX	287	ALA	2.9
2	BM	173	GLY	2.9
2	BK	181	LYS	2.9
2	AH	259	GLY	2.9
2	BA	29	MET	2.9
2	BK	66	TYR	2.9
2	BL	27	TYR	2.9
2	BF	190	PHE	2.9
2	BG	184	ASP	2.9
1	AY	127	LYS	2.9
2	AR	256	ARG	2.9
2	BE	260	SER	2.9
2	BI	30	LEU	2.9
3	BT	76	TYR	2.9
3	BX	36	LEU	2.9
1	AY	161	ALA	2.9
2	BM	218	GLN	2.9
3	BS	51	MET	2.9
1	B0	225	LYS	2.9
2	AD	63	GLY	2.9
1	B0	204	LEU	2.9
2	BR	123	PHE	2.9
2	BF	194	VAL	2.9
2	BI	250	LYS	2.9
1	BY	318	ILE	2.9
2	BM	159	ILE	2.9
2	AQ	217	VAL	2.9
3	BV	118	TYR	2.9
2	BC	153	MET	2.9
3	BV	79	MET	2.9
1	A0	278	HIS	2.9
1	B0	63	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BO	148	ILE	2.9
3	AS	31	PRO	2.9
2	AG	255	THR	2.9
2	BD	258	ASN	2.9
1	A0	69	VAL	2.8
1	B0	247	PHE	2.8
2	AK	55	TYR	2.8
2	BD	26	LEU	2.8
3	BS	274	ILE	2.8
2	BD	259	GLY	2.8
3	AV	214	VAL	2.8
3	BV	195	GLU	2.8
1	A0	329	LEU	2.8
2	BP	225	ALA	2.8
1	BZ	120	ASP	2.8
3	BV	250	GLN	2.8
2	AA	76	LEU	2.8
2	AR	233	ILE	2.8
2	BB	31	THR	2.8
1	AY	133	ILE	2.8
2	BD	183	ASN	2.8
2	BN	55	TYR	2.8
2	BO	256	ARG	2.8
2	BE	61	ILE	2.8
2	AF	178	LEU	2.8
2	BF	233	ILE	2.8
2	BO	74	VAL	2.8
3	BT	34	LEU	2.8
2	BH	161	VAL	2.8
2	BD	84	ILE	2.8
2	BG	219	SER	2.8
2	AB	243	TRP	2.8
2	BK	33	MET	2.8
2	BF	145	LEU	2.8
3	AX	2	VAL	2.8
1	BZ	10	PHE	2.8
3	AU	247	GLU	2.8
1	A0	6	VAL	2.8
2	AG	145	LEU	2.8
2	AL	259	GLY	2.8
2	BM	76	LEU	2.8
2	BR	76	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AU	99	GLU	2.8
3	BT	238	ILE	2.8
2	BK	65	ARG	2.8
1	B0	304	PRO	2.8
2	AE	27	TYR	2.8
2	AE	190	PHE	2.8
2	AH	27	TYR	2.8
1	B0	179	ILE	2.8
2	BF	120	LYS	2.8
1	BZ	89	LEU	2.8
2	BL	257	GLY	2.8
3	BW	298	VAL	2.8
2	AR	189	ARG	2.8
2	BM	33	MET	2.8
1	AZ	125	ILE	2.8
2	AF	27	TYR	2.8
2	AI	221	VAL	2.8
2	AQ	38	ILE	2.8
2	BL	196	ASN	2.8
3	BV	238	ILE	2.8
1	A0	150	TYR	2.8
2	AC	3	ILE	2.8
2	BC	199	LYS	2.8
2	BD	3	ILE	2.8
2	BD	126	VAL	2.8
3	BT	176	TYR	2.8
3	BV	29	TYR	2.8
3	AX	199	PHE	2.8
2	AP	119	LEU	2.8
2	AQ	209	ASP	2.8
1	AY	304	PRO	2.8
2	BM	251	THR	2.8
2	BC	246	ALA	2.8
2	AJ	88	ILE	2.8
2	BG	191	PHE	2.8
2	BL	249	ASP	2.8
3	AV	51	MET	2.8
3	AV	279	MET	2.8
1	A0	354	ARG	2.8
1	AZ	65	VAL	2.8
1	BZ	352	ALA	2.8
2	BG	18	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AG	29	MET	2.8
2	AO	26	LEU	2.8
1	BZ	210	SER	2.8
2	BD	190	PHE	2.8
3	AU	1	MET	2.8
3	BW	79	MET	2.8
2	AH	61	ILE	2.8
2	AF	255	THR	2.7
2	AQ	37	THR	2.7
2	BL	68	GLU	2.7
2	AF	258	ASN	2.7
2	BF	258	ASN	2.7
2	AR	28	MET	2.7
2	AD	257	GLY	2.7
2	AI	178	LEU	2.7
2	BL	3	ILE	2.7
2	AQ	232	HIS	2.7
1	AZ	320	THR	2.7
2	BK	258	ASN	2.7
3	BX	227	ILE	2.7
2	AM	262	PHE	2.7
2	AR	74	VAL	2.7
3	BU	55	SER	2.7
1	AZ	199	ASP	2.7
2	AI	114	ASN	2.7
3	BS	125	SER	2.7
1	A0	166	LYS	2.7
2	BD	30	LEU	2.7
2	BQ	33	MET	2.7
1	AY	359	PHE	2.7
2	AC	212	PHE	2.7
2	AK	99	LEU	2.7
1	BY	34	ILE	2.7
1	BY	119	LEU	2.7
2	AF	139	ILE	2.7
2	AQ	252	PRO	2.7
3	BU	5	TYR	2.7
2	AD	190	PHE	2.7
3	AV	197	PHE	2.7
3	AX	274	ILE	2.7
2	AF	261	TYR	2.7
2	AI	34	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AN	179	THR	2.7
3	AU	271	THR	2.7
1	AZ	347	TYR	2.7
2	AO	3	ILE	2.7
2	AN	222	GLY	2.7
2	AP	235	ILE	2.7
3	AS	214	VAL	2.7
2	BN	23	ASP	2.7
3	AV	239	LEU	2.7
2	AJ	260	SER	2.7
2	BF	121	VAL	2.7
1	B0	33	PRO	2.7
2	BC	211	PRO	2.7
1	B0	185	PHE	2.7
2	AL	185	LEU	2.7
2	BB	187	ILE	2.7
3	AV	294	LYS	2.7
1	A0	67	ASP	2.7
2	BH	249	ASP	2.7
1	BY	179	ILE	2.7
2	AP	118	VAL	2.7
2	BF	263	ILE	2.7
3	AS	297	PHE	2.7
3	AV	281	LEU	2.7
2	BM	256	ARG	2.7
2	BR	36	ARG	2.7
1	AZ	142	LYS	2.7
1	BY	225	LYS	2.7
2	AI	222	GLY	2.7
2	AN	64	GLY	2.7
2	AQ	246	ALA	2.7
2	BG	225	ALA	2.7
1	A0	314	SER	2.7
2	AF	144	THR	2.7
2	AL	110	VAL	2.7
2	AP	252	PRO	2.7
3	BW	178	TYR	2.7
3	BS	228	VAL	2.7
2	AB	62	ALA	2.7
2	AO	77	LYS	2.7
2	AN	190	PHE	2.6
3	BV	214	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BR	32	GLY	2.6
3	BS	117	GLY	2.6
3	BT	157	SER	2.6
2	BC	220	LEU	2.6
3	AX	297	PHE	2.6
3	BT	249	TYR	2.6
3	BX	249	TYR	2.6
1	BZ	145	LEU	2.6
2	AA	84	ILE	2.6
2	BC	30	LEU	2.6
3	AS	100	ILE	2.6
1	BY	121	VAL	2.6
2	AB	67	PHE	2.6
2	AN	101	ALA	2.6
2	BR	57	ASN	2.6
2	BF	187	ILE	2.6
3	AU	86	ILE	2.6
2	BR	145	LEU	2.6
3	AU	249	TYR	2.6
1	AZ	369	GLY	2.6
1	AZ	133	ILE	2.6
1	B0	134	ILE	2.6
2	BK	88	ILE	2.6
2	BG	259	GLY	2.6
3	AT	120	LYS	2.6
3	AV	288	GLU	2.6
2	AE	97	VAL	2.6
2	AP	175	GLN	2.6
2	AL	252	PRO	2.6
2	BA	17	PRO	2.6
3	BT	296	ASP	2.6
3	BV	140	GLU	2.6
2	AQ	258	ASN	2.6
2	BL	46	PRO	2.6
3	BU	61	ILE	2.6
3	BV	240	ILE	2.6
2	BA	67	PHE	2.6
3	AV	213	GLY	2.6
3	AT	239	LEU	2.6
3	AS	29	TYR	2.6
2	AA	122	CYS	2.6
2	AQ	251	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AB	252	PRO	2.6
2	AO	67	PHE	2.6
2	AQ	2	THR	2.6
3	AU	202	ILE	2.6
2	BF	30	LEU	2.6
1	AY	339	ASP	2.6
1	B0	133	ILE	2.6
1	B0	294	PHE	2.6
2	AJ	125	ILE	2.6
2	AQ	208	VAL	2.6
2	BC	235	ILE	2.6
2	BF	252	PRO	2.6
2	BG	53	VAL	2.6
2	AD	29	MET	2.6
1	B0	312	GLU	2.6
2	BC	212	PHE	2.6
2	BF	131	THR	2.6
3	AS	205	PRO	2.6
3	AW	282	ILE	2.6
3	AW	298	VAL	2.6
1	A0	178	ARG	2.6
2	AH	31	THR	2.6
1	BY	208	PHE	2.6
2	BA	190	PHE	2.6
2	AJ	153	MET	2.6
3	BT	1	MET	2.6
2	AF	88	ILE	2.6
2	BO	31	THR	2.6
1	B0	10	PHE	2.6
2	AM	185	LEU	2.6
3	BW	34	LEU	2.6
2	BD	124	ASP	2.6
1	A0	167	ALA	2.6
1	A0	300	HIS	2.6
1	BZ	265	ALA	2.6
2	BJ	59	SER	2.6
2	AH	39	ARG	2.6
3	BV	258	LEU	2.6
2	AP	62	ALA	2.6
3	AV	247	GLU	2.6
2	AB	30	LEU	2.6
2	AB	164	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BQ	30	LEU	2.6
3	AT	286	LYS	2.6
3	AU	214	VAL	2.6
2	BK	68	GLU	2.6
3	AU	107	LEU	2.6
3	BS	29	TYR	2.6
2	AH	36	ARG	2.5
2	BN	67	PHE	2.5
1	AY	348	SER	2.5
2	BB	62	ALA	2.5
2	AL	99	LEU	2.5
3	BU	116	GLU	2.5
2	AL	233	ILE	2.5
2	AP	61	ILE	2.5
3	AS	250	GLN	2.5
1	A0	204	LEU	2.5
1	B0	2	LEU	2.5
2	AD	39	ARG	2.5
3	AT	227	ILE	2.5
2	AM	178	LEU	2.5
2	BG	122	CYS	2.5
2	BN	184	ASP	2.5
2	AG	257	GLY	2.5
3	AV	143	THR	2.5
2	BN	62	ALA	2.5
2	BA	60	ILE	2.5
2	BB	241	ILE	2.5
2	BD	133	VAL	2.5
3	BV	1	MET	2.5
1	AZ	303	PRO	2.5
1	B0	260	PRO	2.5
2	AL	257	GLY	2.5
2	BF	231	PHE	2.5
2	BI	258	ASN	2.5
2	BG	168	VAL	2.5
3	AS	279	MET	2.5
3	AU	79	MET	2.5
2	BQ	115	GLY	2.5
2	AC	41	LYS	2.5
2	AF	159	ILE	2.5
2	BH	153	MET	2.5
2	BL	97	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BM	81	VAL	2.5
1	B0	188	THR	2.5
2	BP	58	THR	2.5
2	AG	177	GLN	2.5
1	AZ	2	LEU	2.5
2	BJ	211	PRO	2.5
3	BV	48	ILE	2.5
2	AI	67	PHE	2.5
3	AT	116	GLU	2.5
3	BS	126	GLU	2.5
2	BE	176	LEU	2.5
3	AT	100	ILE	2.5
2	BQ	189	ARG	2.5
3	BX	214	VAL	2.5
2	BD	66	TYR	2.5
3	AT	200	MET	2.5
3	AX	34	LEU	2.5
2	AC	260	SER	2.5
2	AH	30	LEU	2.5
2	BF	119	LEU	2.5
2	AR	32	GLY	2.5
2	BE	33	MET	2.5
2	BH	97	VAL	2.5
2	BM	171	GLY	2.5
2	AH	216	ALA	2.5
2	AI	62	ALA	2.5
2	AB	255	THR	2.5
2	AF	217	VAL	2.5
3	AS	213	GLY	2.5
3	AS	260	LEU	2.5
2	BL	48	ASN	2.5
2	BC	184	ASP	2.5
1	AZ	29	LYS	2.5
3	BW	170	TYR	2.5
2	AI	232	HIS	2.5
1	B0	32	LEU	2.5
2	AD	159	ILE	2.5
2	AK	63	GLY	2.5
2	AR	211	PRO	2.5
2	AK	262	PHE	2.5
2	AP	123	PHE	2.5
2	AP	170	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BH	190	PHE	2.5
3	BT	298	VAL	2.5
2	BC	263	ILE	2.5
2	AD	67	PHE	2.5
2	AO	167	THR	2.5
2	AR	124	ASP	2.5
1	AZ	214	ASN	2.5
2	BD	188	VAL	2.5
3	AW	287	ALA	2.5
1	BY	2	LEU	2.5
1	BZ	332	LEU	2.5
2	AN	3	ILE	2.5
2	AQ	88	ILE	2.5
2	AQ	176	LEU	2.5
3	BS	248	THR	2.5
3	BW	144	PHE	2.5
1	AZ	36	LYS	2.5
1	B0	335	ASN	2.5
1	BY	356	LYS	2.5
1	BZ	87	LYS	2.5
1	AY	286	ASP	2.4
1	BY	122	PRO	2.4
2	BJ	159	ILE	2.5
3	AV	114	LYS	2.4
2	AI	60	ILE	2.4
2	BG	64	GLY	2.4
2	AA	241	ILE	2.4
2	BL	88	ILE	2.4
1	B0	108	LEU	2.4
1	AZ	51	TYR	2.4
2	BC	256	ARG	2.4
3	AT	96	TYR	2.4
1	B0	293	LEU	2.4
2	AL	174	LEU	2.4
2	AN	207	TRP	2.4
1	B0	115	MET	2.4
2	AH	264	LYS	2.4
2	AP	38	ILE	2.4
3	AU	240	ILE	2.4
2	AD	174	LEU	2.4
2	AG	122	CYS	2.4
2	AO	176	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BM	27	TYR	2.4
3	AT	289	PHE	2.4
2	BG	4	LYS	2.4
1	B0	207	ASN	2.4
1	B0	52	LEU	2.4
2	AG	222	GLY	2.4
2	BJ	83	TYR	2.4
3	AU	237	TYR	2.4
3	BS	281	LEU	2.4
1	A0	264	ILE	2.4
1	BY	216	LYS	2.4
2	AM	122	CYS	2.4
3	BT	154	ALA	2.4
2	AD	40	ARG	2.4
2	AG	86	ALA	2.4
1	B0	264	ILE	2.4
2	AP	169	GLU	2.4
3	AS	62	GLU	2.4
3	BS	287	ALA	2.4
2	AJ	47	LEU	2.4
2	AL	217	VAL	2.4
2	AN	162	PRO	2.4
1	A0	233	GLU	2.4
2	AK	79	ASP	2.4
2	BF	170	ALA	2.4
2	BL	62	ALA	2.4
2	BQ	209	ASP	2.4
2	AJ	176	LEU	2.4
2	BE	30	LEU	2.4
2	BN	220	LEU	2.4
2	BO	161	VAL	2.4
3	AS	67	THR	2.4
2	AR	84	ILE	2.4
1	AZ	228	VAL	2.4
2	AH	7	THR	2.4
1	BZ	146	MET	2.4
2	AL	225	ALA	2.4
2	BM	262	PHE	2.4
1	AZ	356	LYS	2.4
3	AX	139	TYR	2.4
2	AD	123	PHE	2.4
3	BV	134	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AO	159	ILE	2.4
3	AU	133	ILE	2.4
1	AY	370	ASP	2.4
1	AY	163	ILE	2.4
2	AD	181	LYS	2.4
3	AU	5	TYR	2.4
2	AE	30	LEU	2.4
2	BC	264	LYS	2.4
2	BK	6	PHE	2.4
3	AV	291	ILE	2.4
3	AU	204	TYR	2.4
3	BV	269	TYR	2.4
1	AY	336	ASP	2.4
2	AF	214	PRO	2.4
2	BG	23	ASP	2.4
1	BZ	141	ASN	2.4
2	AM	67	PHE	2.4
3	BT	289	PHE	2.4
1	A0	136	TYR	2.4
2	AN	261	TYR	2.4
3	BS	76	TYR	2.4
1	AY	368	SER	2.4
1	B0	305	GLU	2.4
1	A0	207	ASN	2.4
2	AB	215	ALA	2.4
2	BN	162	PRO	2.4
2	AI	233	ILE	2.4
2	BI	88	ILE	2.4
2	BN	3	ILE	2.4
1	AY	300	HIS	2.4
2	BI	97	VAL	2.4
1	BZ	260	PRO	2.4
2	AA	176	LEU	2.4
3	BX	34	LEU	2.4
3	BX	204	TYR	2.4
2	AF	67	PHE	2.4
3	AT	73	GLU	2.4
2	BI	60	ILE	2.4
2	BC	55	TYR	2.4
2	AI	235	ILE	2.4
2	AL	61	ILE	2.4
3	BU	114	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	BV	114	LYS	2.4
2	AG	193	SER	2.4
3	AT	249	TYR	2.4
2	BR	203	MET	2.4
2	BF	218	GLN	2.4
2	BD	165	THR	2.3
2	BG	255	THR	2.3
2	BK	167	THR	2.3
1	A0	277	TYR	2.3
1	A0	330	LEU	2.3
1	B0	46	LEU	2.3
2	BF	61	ILE	2.3
3	AX	116	GLU	2.3
3	BV	76	TYR	2.3
1	B0	359	PHE	2.3
3	AS	79	MET	2.3
3	AV	199	PHE	2.3
3	AW	28	PHE	2.3
3	BW	51	MET	2.3
2	AL	226	GLY	2.3
2	BQ	258	ASN	2.3
2	BR	82	ASN	2.3
3	BS	120	LYS	2.3
1	AZ	318	ILE	2.3
1	B0	330	LEU	2.3
2	AC	139	ILE	2.3
2	AJ	225	ALA	2.3
3	BU	289	PHE	2.3
1	AY	225	LYS	2.3
2	AH	217	VAL	2.3
2	BM	186	VAL	2.3
1	AZ	316	SER	2.3
2	AM	222	GLY	2.3
3	AS	68	PHE	2.3
1	AZ	264	ILE	2.3
2	BP	159	ILE	2.3
3	BX	262	PRO	2.3
1	BZ	75	GLU	2.3
3	AT	170	TYR	2.3
3	AU	152	VAL	2.3
2	BM	99	LEU	2.3
2	BQ	64	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AV	290	LYS	2.3
1	BZ	235	ILE	2.3
2	AB	246	ALA	2.3
2	AC	235	ILE	2.3
3	BV	100	ILE	2.3
3	BW	86	ILE	2.3
1	AZ	8	ASP	2.3
2	AJ	43	TRP	2.3
2	AA	136	THR	2.3
3	AU	178	TYR	2.3
1	A0	147	SER	2.3
1	AY	113	TRP	2.3
2	AE	208	VAL	2.3
2	AP	174	LEU	2.3
2	BF	235	ILE	2.3
2	BH	174	LEU	2.3
2	BI	185	LEU	2.3
3	AX	26	VAL	2.3
2	AQ	262	PHE	2.3
3	AT	28	PHE	2.3
3	BS	229	PHE	2.3
2	BD	180	LYS	2.3
2	AE	176	LEU	2.3
2	BI	67	PHE	2.3
3	BV	68	PHE	2.3
1	BY	134	ILE	2.3
2	AJ	155	VAL	2.3
2	AN	164	GLN	2.3
2	AN	186	VAL	2.3
2	BR	71	ASN	2.3
3	BV	292	LYS	2.3
1	BZ	140	PRO	2.3
2	AE	153	MET	2.3
3	AV	54	ARG	2.3
3	BT	155	GLY	2.3
2	BH	137	LYS	2.3
2	AL	178	LEU	2.3
2	AM	191	PHE	2.3
2	BJ	61	ILE	2.3
3	AT	136	TRP	2.3
2	AA	216	ALA	2.3
3	BT	147	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AN	24	GLY	2.3
2	AQ	165	THR	2.3
2	BB	179	THR	2.3
2	BN	181	LYS	2.3
2	AO	78	GLY	2.3
2	BQ	235	ILE	2.3
3	AS	227	ILE	2.3
2	AE	155	VAL	2.3
1	BZ	68	ILE	2.3
2	AE	159	ILE	2.3
3	AV	169	LYS	2.3
2	BJ	99	LEU	2.3
3	BS	159	ILE	2.3
1	BZ	77	VAL	2.3
3	BT	116	GLU	2.3
1	A0	8	ASP	2.3
2	AR	137	LYS	2.3
2	BJ	181	LYS	2.3
1	AZ	132	ALA	2.3
3	AX	291	ILE	2.3
1	A0	201	ARG	2.3
1	AY	178	ARG	2.3
1	AZ	128	THR	2.3
2	BQ	229	THR	2.3
2	AG	123	PHE	2.3
2	AL	28	MET	2.3
3	AU	96	TYR	2.3
1	B0	215	ARG	2.3
2	AN	26	LEU	2.3
2	BL	26	LEU	2.3
2	BR	38	ILE	2.3
2	BG	97	VAL	2.3
3	AT	190	TRP	2.3
3	AT	204	TYR	2.3
2	BJ	233	ILE	2.3
3	BX	86	ILE	2.3
2	BK	50	ALA	2.3
3	BS	214	VAL	2.3
2	BH	23	ASP	2.3
3	BT	179	TYR	2.3
2	AD	256	ARG	2.3
2	AG	210	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AJ	97	VAL	2.3
2	BL	99	LEU	2.3
3	AW	214	VAL	2.3
3	BW	142	LEU	2.3
1	AY	259	PRO	2.3
1	BZ	234	THR	2.3
3	BV	279	MET	2.2
3	BW	26	VAL	2.2
2	AB	112	ILE	2.2
2	BG	55	TYR	2.2
3	AU	34	LEU	2.2
2	BG	74	VAL	2.2
2	BG	208	VAL	2.2
2	BQ	159	ILE	2.2
2	AG	218	GLN	2.2
2	AL	218	GLN	2.2
2	AR	39	ARG	2.2
2	BL	254	ALA	2.2
2	BR	243	TRP	2.2
3	BV	136	TRP	2.2
2	BP	76	LEU	2.2
3	BW	90	LYS	2.2
2	BE	188	VAL	2.2
2	AB	72	GLU	2.2
2	BR	78	GLY	2.2
3	AV	227	ILE	2.2
3	AW	61	ILE	2.2
3	BT	274	ILE	2.2
3	AV	235	GLN	2.2
1	AZ	34	ILE	2.2
2	AD	187	ILE	2.2
1	B0	59	LEU	2.2
2	AB	76	LEU	2.2
2	BH	181	LYS	2.2
1	BZ	147	SER	2.2
2	AP	192	GLY	2.2
2	BI	235	ILE	2.2
2	AD	264	LYS	2.2
1	B0	39	CYS	2.2
2	BP	206	THR	2.2
2	AB	53	VAL	2.2
3	BT	187	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	BT	287	ALA	2.2
2	AJ	23	ASP	2.2
1	B0	128	THR	2.2
2	BC	27	TYR	2.2
3	BU	76	TYR	2.2
3	BV	158	LYS	2.2
1	BZ	335	ASN	2.2
1	B0	79	ILE	2.2
2	AD	88	ILE	2.2
2	AI	159	ILE	2.2
2	AO	66	TYR	2.2
2	BI	187	ILE	2.2
3	BU	199	PHE	2.2
1	BY	211	ARG	2.2
2	AD	145	LEU	2.2
2	AG	260	SER	2.2
2	BN	204	SER	2.2
2	BQ	31	THR	2.2
3	AV	29	TYR	2.2
1	BZ	329	LEU	2.2
2	AI	241	ILE	2.2
2	AM	66	TYR	2.2
3	AU	197	PHE	2.2
3	AV	262	PRO	2.2
1	B0	291	LYS	2.2
2	AA	50	ALA	2.2
2	AA	181	LYS	2.2
2	AC	43	TRP	2.2
2	AM	64	GLY	2.2
2	BF	86	ALA	2.2
2	BR	69	LEU	2.2
1	B0	313	ILE	2.2
2	AC	60	ILE	2.2
2	BD	88	ILE	2.2
3	AV	205	PRO	2.2
3	AW	86	ILE	2.2
2	BG	83	TYR	2.2
2	AD	64	GLY	2.2
2	BQ	245	GLY	2.2
3	AT	201	GLY	2.2
1	AZ	208	PHE	2.2
1	BY	142	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BZ	230	MET	2.2
2	AF	97	VAL	2.2
2	BB	77	LYS	2.2
2	BJ	220	LEU	2.2
2	BN	6	PHE	2.2
2	BP	145	LEU	2.2
3	BV	25	LYS	2.2
1	A0	193	HIS	2.2
1	BZ	150	TYR	2.2
3	AS	262	PRO	2.2
2	AA	86	ALA	2.2
2	AN	76	LEU	2.2
2	AN	212	PHE	2.2
2	AO	225	ALA	2.2
2	BA	101	ALA	2.2
2	AK	26	LEU	2.2
3	AT	158	LYS	2.2
3	AX	114	LYS	2.2
1	AZ	229	THR	2.2
3	AU	288	GLU	2.2
3	AV	264	MET	2.2
3	BT	79	MET	2.2
2	AE	200	GLY	2.2
2	AJ	42	ASP	2.2
3	BV	96	TYR	2.2
2	AK	176	LEU	2.2
2	AQ	185	LEU	2.2
2	BG	88	ILE	2.2
3	BS	53	THR	2.2
2	AB	117	GLY	2.2
3	AS	51	MET	2.2
2	AA	133	VAL	2.2
2	BN	73	THR	2.2
2	AN	209	ASP	2.2
2	BJ	67	PHE	2.2
3	BV	190	TRP	2.2
2	AA	51	LEU	2.2
2	AO	109	GLY	2.2
2	BC	183	ASN	2.2
2	BH	208	VAL	2.2
2	BL	258	ASN	2.2
3	BU	34	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	BU	238	ILE	2.2
2	BI	62	ALA	2.2
3	BS	264	MET	2.2
2	AB	221	VAL	2.2
2	BF	26	LEU	2.2
2	AH	187	ILE	2.2
2	BN	77	LYS	2.2
3	AS	139	TYR	2.2
2	BD	256	ARG	2.2
3	AU	61	ILE	2.2
1	B0	206	ILE	2.2
2	AG	32	GLY	2.2
2	BF	251	THR	2.2
2	BG	261	TYR	2.2
3	AS	96	TYR	2.2
3	AX	281	LEU	2.2
3	BX	90	LYS	2.2
1	AY	269	GLY	2.1
2	BA	99	LEU	2.1
1	B0	111	TYR	2.1
2	AM	219	SER	2.1
1	A0	260	PRO	2.1
2	AE	26	LEU	2.1
2	AE	99	LEU	2.1
2	AG	33	MET	2.1
3	AT	281	LEU	2.1
3	BT	279	MET	2.1
2	BF	208	VAL	2.1
1	A0	25	GLY	2.1
2	AN	215	ALA	2.1
3	AU	212	ALA	2.1
1	AZ	203	LEU	2.1
2	BK	60	ILE	2.1
2	BR	99	LEU	2.1
2	AM	190	PHE	2.1
2	AO	235	ILE	2.1
2	BB	235	ILE	2.1
3	BS	239	LEU	2.1
1	AZ	184	GLN	2.1
2	AB	175	GLN	2.1
3	BU	286	LYS	2.1
3	BX	279	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AI	86	ALA	2.1
2	BQ	207	TRP	2.1
1	AZ	235	ILE	2.1
2	AD	69	LEU	2.1
2	AI	167	THR	2.1
2	AP	18	VAL	2.1
2	AR	38	ILE	2.1
2	BJ	125	ILE	2.1
2	BR	122	CYS	2.1
3	AS	99	GLU	2.1
3	AW	83	VAL	2.1
3	BT	91	PHE	2.1
1	AY	51	TYR	2.1
2	AO	33	MET	2.1
1	AY	130	ASN	2.1
2	AF	235	ILE	2.1
2	AN	126	VAL	2.1
2	BG	169	GLU	2.1
2	BP	37	THR	2.1
2	BR	56	THR	2.1
3	BS	50	VAL	2.1
1	BY	158	ALA	2.1
2	AH	40	ARG	2.1
2	BG	256	ARG	2.1
2	AF	153	MET	2.1
3	AW	178	TYR	2.1
3	AU	94	LEU	2.1
1	AY	195	PRO	2.1
1	B0	157	PHE	2.1
2	AI	74	VAL	2.1
2	AK	23	ASP	2.1
2	AO	97	VAL	2.1
2	BA	50	ALA	2.1
3	BT	82	PHE	2.1
1	A0	173	HIS	2.1
2	BR	23	ASP	2.1
3	AX	12	ASP	2.1
3	BT	85	ASP	2.1
2	AD	148	ILE	2.1
2	AG	139	ILE	2.1
2	AL	38	ILE	2.1
2	AO	190	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BB	43	TRP	2.1
2	BG	211	PRO	2.1
3	BW	287	ALA	2.1
1	BZ	330	LEU	2.1
2	AF	35	TYR	2.1
2	AM	257	GLY	2.1
2	AP	66	TYR	2.1
2	AQ	148	ILE	2.1
2	BA	88	ILE	2.1
2	BE	3	ILE	2.1
2	BE	63	GLY	2.1
3	BT	48	ILE	2.1
1	B0	73	PHE	2.1
3	BT	2	VAL	2.1
3	BV	297	PHE	2.1
3	BW	82	PHE	2.1
2	AP	260	SER	2.1
2	AG	252	PRO	2.1
2	AQ	214	PRO	2.1
2	BB	218	GLN	2.1
2	AF	194	VAL	2.1
2	AG	165	THR	2.1
2	AI	61	ILE	2.1
2	AO	187	ILE	2.1
2	BD	263	ILE	2.1
3	BU	94	LEU	2.1
1	A0	208	PHE	2.1
1	BY	157	PHE	2.1
2	AK	3	ILE	2.1
2	AK	66	TYR	2.1
2	AK	208	VAL	2.1
3	AW	109	LEU	2.1
3	BU	249	TYR	2.1
2	BG	62	ALA	2.1
2	BI	154	THR	2.1
2	BM	143	SER	2.1
3	AW	273	ILE	2.1
2	BL	174	LEU	2.1
3	AV	158	LYS	2.1
3	AX	141	ASN	2.1
2	BK	232	HIS	2.1
3	BX	213	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AN	214	PRO	2.1
2	AO	186	VAL	2.1
2	BD	38	ILE	2.1
3	AV	274	ILE	2.1
3	AW	2	VAL	2.1
2	AB	48	ASN	2.1
2	BA	258	ASN	2.1
3	BV	143	THR	2.1
2	AF	33	MET	2.1
2	AF	86	ALA	2.1
2	AP	23	ASP	2.1
2	BR	124	ASP	2.1
2	AP	110	VAL	2.1
2	BG	217	VAL	2.1
3	BV	293	ARG	2.1
3	BW	164	ALA	2.1
1	A0	23	PRO	2.1
1	AY	23	PRO	2.1
3	AV	141	ASN	2.1
3	AW	59	PRO	2.1
3	AV	203	LEU	2.1
2	BK	23	ASP	2.1
2	BN	161	VAL	2.1
1	A0	79	ILE	2.1
2	AF	61	ILE	2.1
1	AZ	219	THR	2.1
2	AM	167	THR	2.1
2	AO	29	MET	2.1
2	AH	257	GLY	2.1
2	BA	133	VAL	2.1
3	BV	63	PHE	2.1
2	AP	22	ASN	2.1
2	BL	215	ALA	2.1
2	BH	248	ILE	2.1
2	BL	159	ILE	2.1
3	AX	273	ILE	2.1
2	BG	190	PHE	2.1
3	BW	280	GLU	2.1
1	AY	66	GLY	2.1
2	BN	222	GLY	2.1
2	AJ	139	ILE	2.1
2	BQ	187	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AS	118	TYR	2.1
2	BP	214	PRO	2.1
1	AY	89	LEU	2.1
3	BS	30	GLN	2.1
2	AM	187	ILE	2.1
2	AP	6	PHE	2.1
1	B0	145	LEU	2.1
2	AA	132	GLY	2.1
2	AL	229	THR	2.1
2	BD	17	PRO	2.1
3	BT	271	THR	2.1
2	BN	182	ASN	2.0
2	BF	188	VAL	2.0
3	BS	282	ILE	2.0
3	BU	139	TYR	2.0
2	BA	51	LEU	2.0
1	BZ	157	PHE	2.0
2	AA	125	ILE	2.0
2	AI	110	VAL	2.0
2	BE	233	ILE	2.0
2	BG	233	ILE	2.0
2	BQ	29	MET	2.0
3	AV	68	PHE	2.0
2	BM	222	GLY	2.0
1	AY	305	GLU	2.0
1	AZ	329	LEU	2.0
1	BZ	78	PRO	2.0
2	AQ	26	LEU	2.0
2	BE	7	THR	2.0
2	BP	55	TYR	2.0
2	BR	247	ASN	2.0
3	AV	260	LEU	2.0
2	BQ	123	PHE	2.0
3	AS	63	PHE	2.0
3	AT	213	GLY	2.0
1	AZ	337	LEU	2.0
2	AD	136	THR	2.0
2	AO	145	LEU	2.0
2	BF	211	PRO	2.0
2	BR	127	THR	2.0
3	AS	289	PHE	2.0
3	AU	168	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AJ	86	ALA	2.0
2	AK	259	GLY	2.0
2	BB	264	LYS	2.0
2	BD	18	VAL	2.0
2	BE	74	VAL	2.0
3	AX	158	LYS	2.0
1	AY	125	ILE	2.0
2	BB	148	ILE	2.0
3	AU	7	ILE	2.0
2	AR	228	ASP	2.0
2	BB	208	VAL	2.0
3	BS	298	VAL	2.0
1	A0	4	ALA	2.0
2	BE	190	PHE	2.0
2	BO	7	THR	2.0
2	BP	209	ASP	2.0
2	AN	210	ARG	2.0
2	AR	260	SER	2.0
3	BU	281	LEU	2.0
2	AN	84	ILE	2.0
2	AQ	190	PHE	2.0
2	BA	86	ALA	2.0
2	BN	170	ALA	2.0
3	AV	196	ILE	2.0
2	AN	161	VAL	2.0
2	AQ	34	ASP	2.0
2	BO	155	VAL	2.0
1	AZ	332	LEU	2.0
2	AM	166	LEU	2.0
2	BG	90	LEU	2.0
2	BJ	26	LEU	2.0
3	BV	203	LEU	2.0
2	AE	199	LYS	2.0
2	AK	18	VAL	2.0
2	AK	38	ILE	2.0
2	AQ	123	PHE	2.0
1	BY	287	VAL	2.0
2	AH	204	SER	2.0
2	AM	97	VAL	2.0
2	AR	159	ILE	2.0
2	BE	235	ILE	2.0
2	BL	264	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	AI	258	ASN	2.0
2	BD	35	TYR	2.0
2	BI	33	MET	2.0
2	AP	139	ILE	2.0
2	BA	208	VAL	2.0
2	BP	97	VAL	2.0
2	BR	148	ILE	2.0
3	AX	227	ILE	2.0
2	AK	30	LEU	2.0
2	BC	214	PRO	2.0
2	BI	123	PHE	2.0
3	AS	258	LEU	2.0
3	BS	28	PHE	2.0
1	A0	351	ILE	2.0
1	AY	183	VAL	2.0
2	AA	187	ILE	2.0
2	AR	3	ILE	2.0
2	BM	61	ILE	2.0
2	BO	181	LYS	2.0
3	BU	214	VAL	2.0
3	AS	190	TRP	2.0
2	AQ	212	PHE	2.0
3	AW	60	GLN	2.0
3	BU	91	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	AU	301	1/1	0.33	0.85	275,275,275,275	0
4	CA	AS	301	1/1	0.33	0.42	281,281,281,281	0
4	CA	BS	301	1/1	0.32	0.30	267,267,267,267	0
4	CA	AV	301	1/1	0.37	0.24	276,276,276,276	0
4	CA	AW	301	1/1	0.28	-0.43	266,266,266,266	0
4	CA	BU	301	1/1	0.31	-0.44	269,269,269,269	0
4	CA	AX	301	1/1	0.30	-0.51	275,275,275,275	0
4	CA	BT	301	1/1	0.32	-0.62	279,279,279,279	0
4	CA	BX	301	1/1	0.30	-0.76	287,287,287,287	0
4	CA	AT	301	1/1	0.24	-0.81	275,275,275,275	0
4	CA	BW	301	1/1	0.25	-0.90	268,268,268,268	0
4	CA	BV	301	1/1	0.28	-1.04	272,272,272,272	0

6.5 Other polymers ⓘ

There are no such residues in this entry.