



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 7PBJ / pdb_00007pbj
EMDB ID : EMD-13293
Title : Cryo-EM structure of the GroEL-GroES complex with ADP bound to both rings ("wide" conformation).
Authors : Pichkur, E.B.; Stanishneva-Konovalova, T.B.
Deposited on : 2021-08-02
Resolution : 3.40 Å(reported)
Based on initial model : 1SX4

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

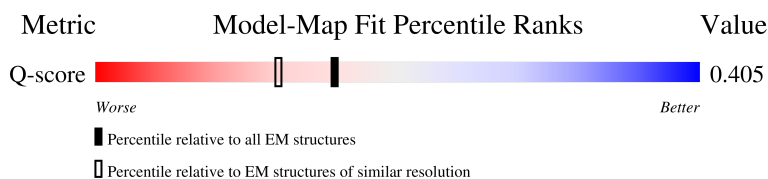
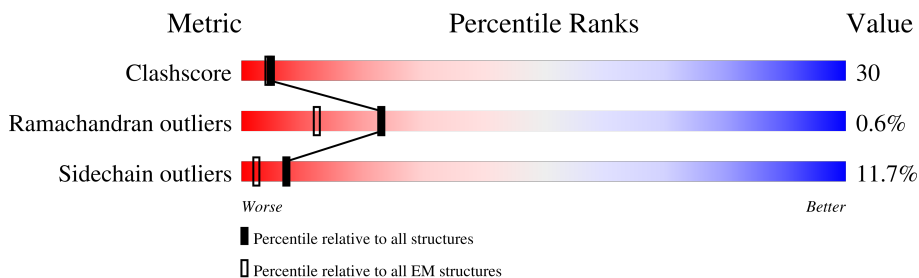
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Ad	524	
1	Ae	524	
1	Ak	524	
1	Al	524	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ar	524	
1	As	524	
1	Ay	524	
1	Az	524	
1	Bf	524	
1	Bg	524	
1	Bm	524	
1	Bn	524	
1	Bt	524	
1	Bu	524	
2	Af	97	
2	Am	97	
2	At	97	
2	Ba	97	
2	Bh	97	
2	Bo	97	
2	Bv	97	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 59486 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ad	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ae	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ak	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Al	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ar	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	As	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Ay	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Az	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bf	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bg	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bm	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bn	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bt	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		
1	Bu	524	Total	C	N	O	S	0	0
			3856	2397	665	774	20		

- Molecule 2 is a protein called 10 kDa chaperonin.

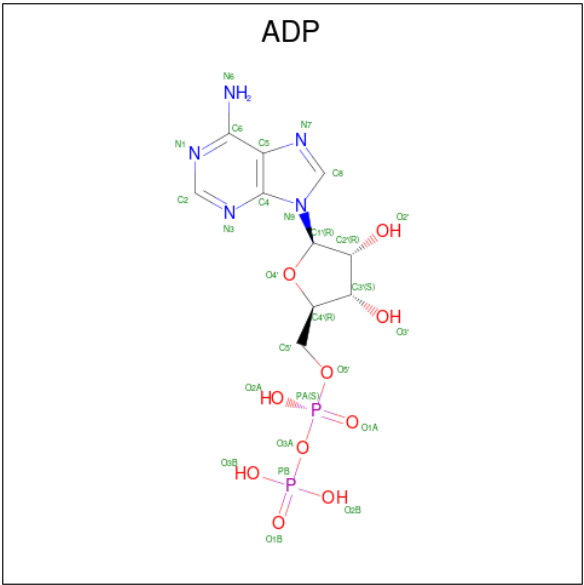
Mol	Chain	Residues	Atoms					AltConf	Trace
2	Af	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Am	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	At	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Ba	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Bh	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Bo	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Bv	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	Ad	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ae	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ak	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Al	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ar	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
3	As	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Ay	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Az	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bf	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bg	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bm	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bn	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bt	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Bu	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	Ad	1	Total	Mg	0
			1	1	
4	Ae	1	Total	Mg	0
			1	1	
4	Ak	1	Total	Mg	0
			1	1	
4	Al	1	Total	Mg	0
			1	1	
4	Ar	1	Total	Mg	0
			1	1	
4	As	1	Total	Mg	0
			1	1	
4	Ay	1	Total	Mg	0
			1	1	
4	Az	1	Total	Mg	0
			1	1	
4	Bf	1	Total	Mg	0
			1	1	
4	Bg	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	Bm	1	Total 1	Mg 1	0
4	Bn	1	Total 1	Mg 1	0
4	Bt	1	Total 1	Mg 1	0
4	Bu	1	Total 1	Mg 1	0

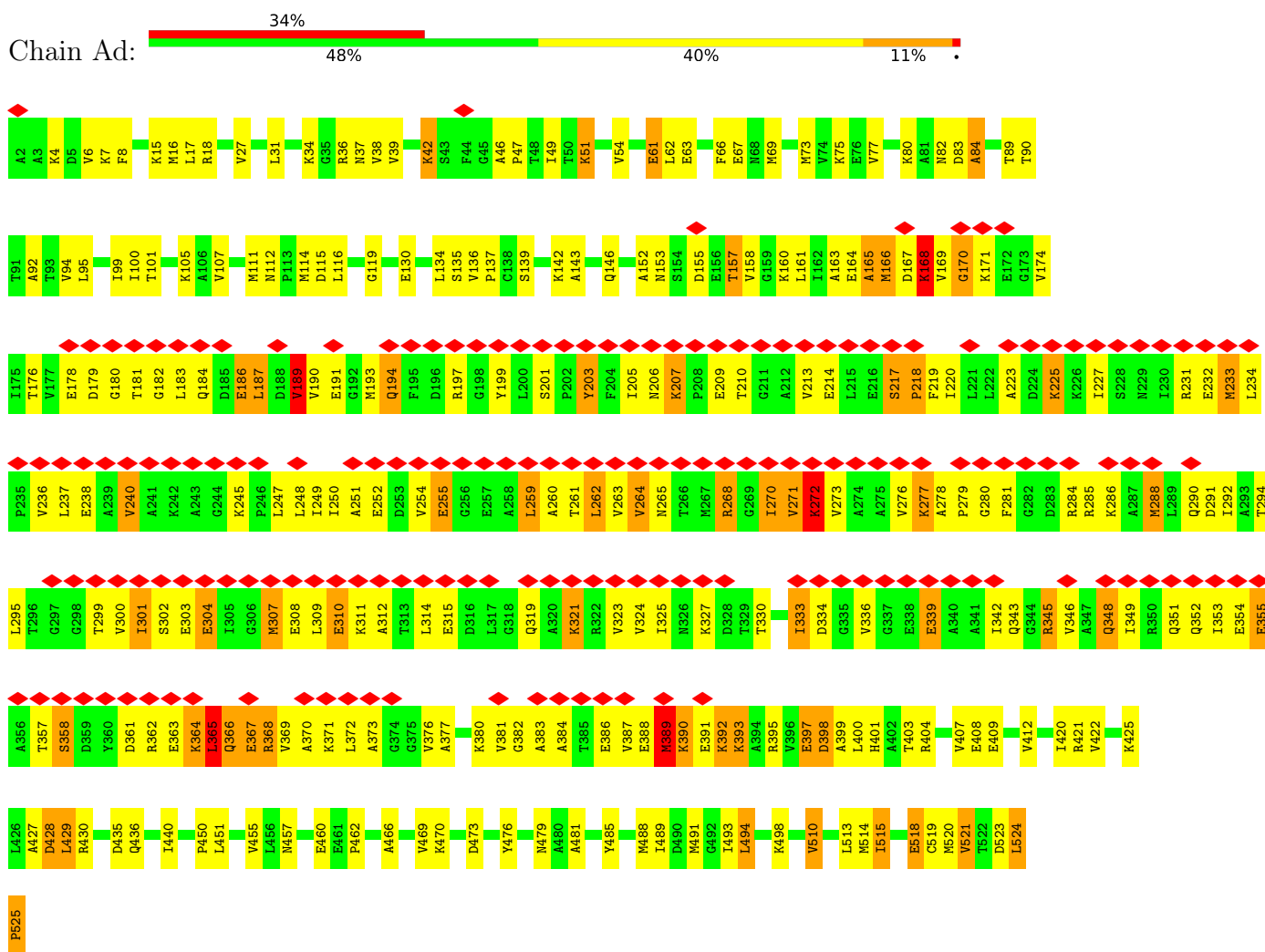
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	Ad	2	Total 2	O 2	0
5	Ak	2	Total 2	O 2	0
5	Ar	2	Total 2	O 2	0
5	Ay	2	Total 2	O 2	0
5	Bf	2	Total 2	O 2	0
5	Bm	2	Total 2	O 2	0
5	Bt	2	Total 2	O 2	0

3 Residue-property plots

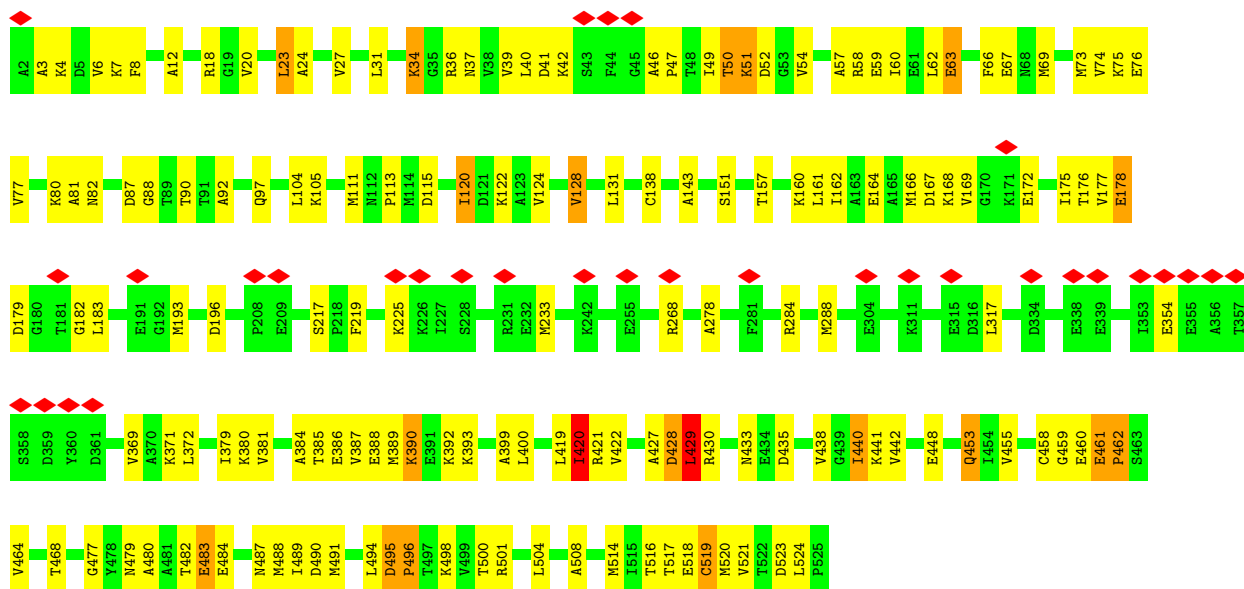
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 60 kDa chaperonin

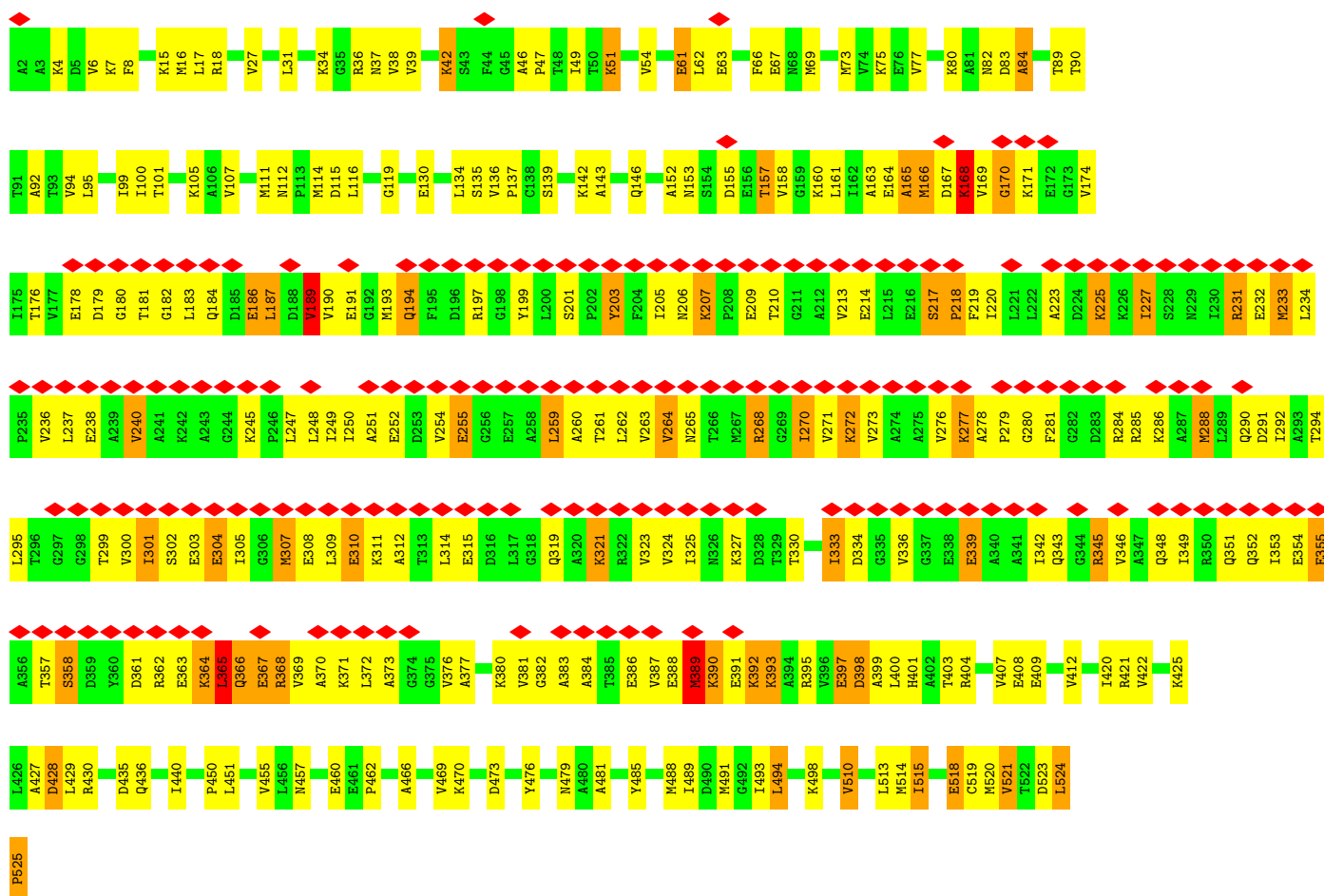


• Molecule 1: 60 kDa chaperonin

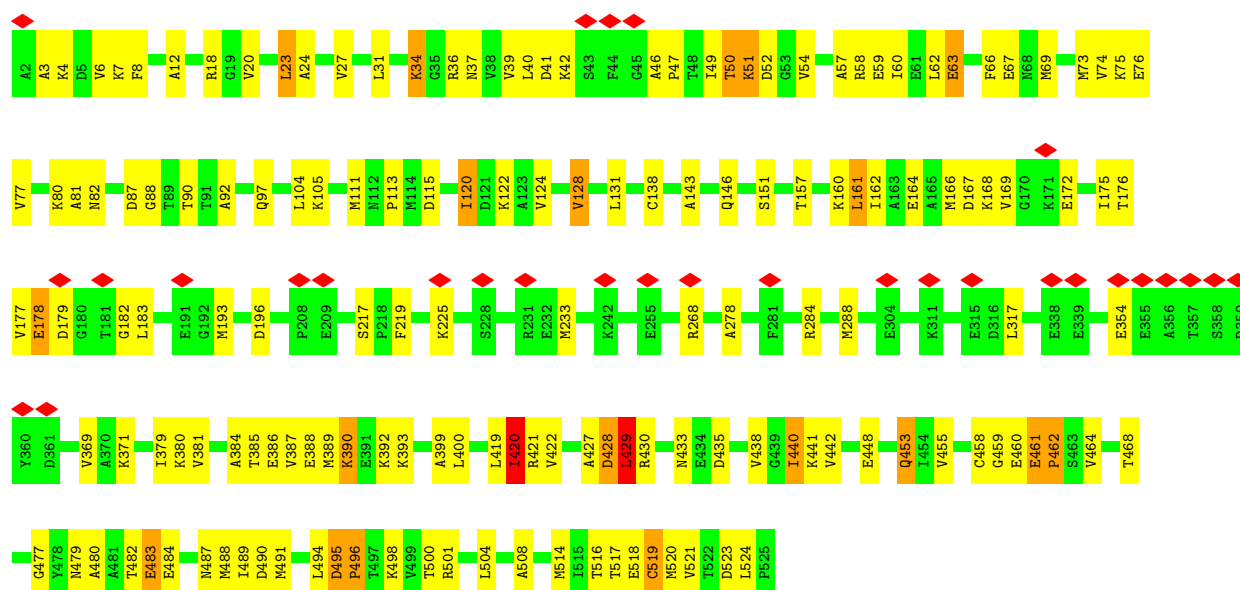
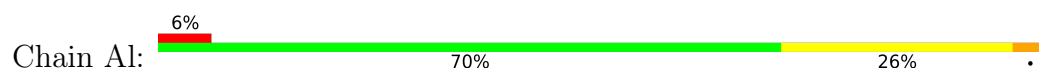




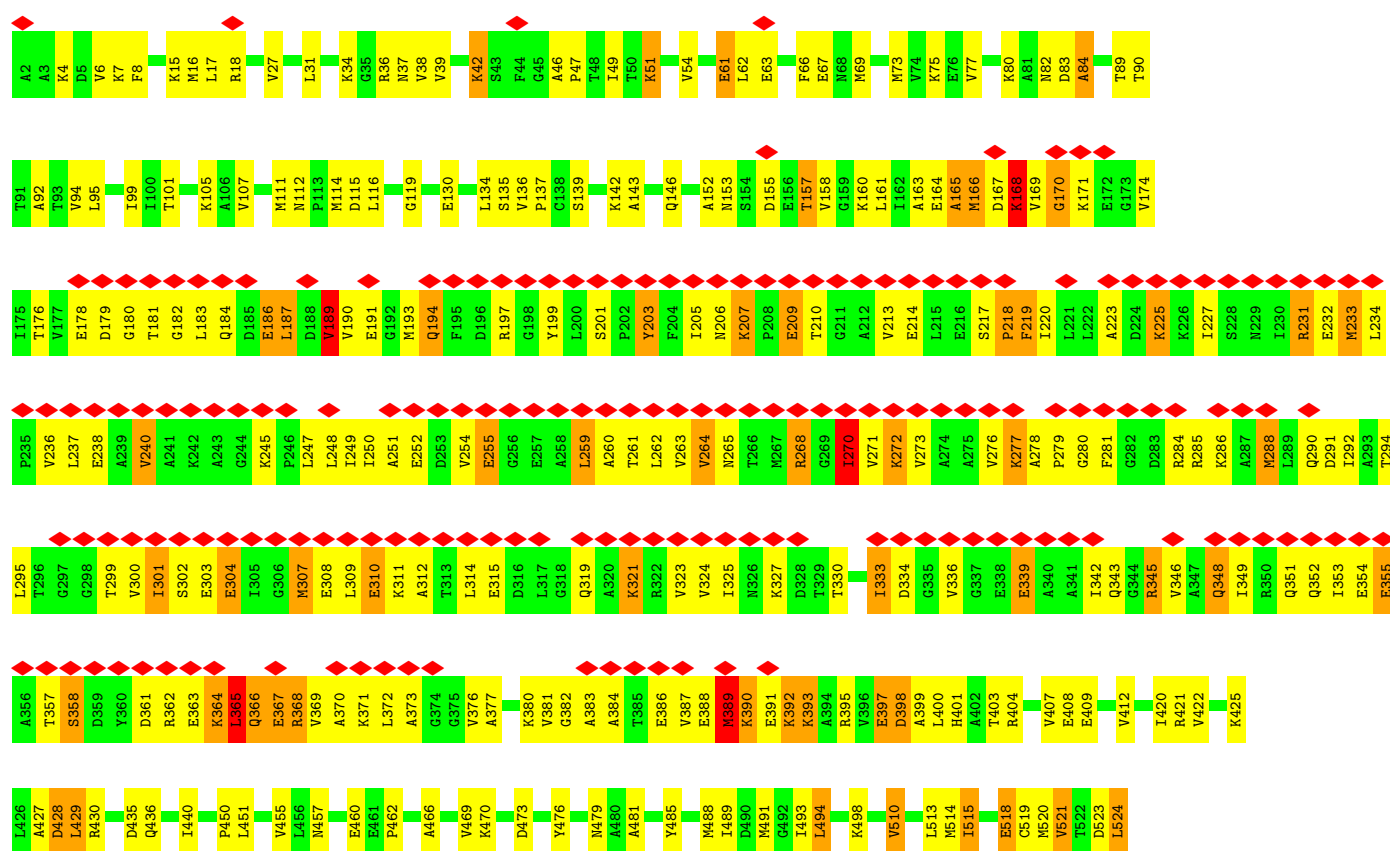
• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin

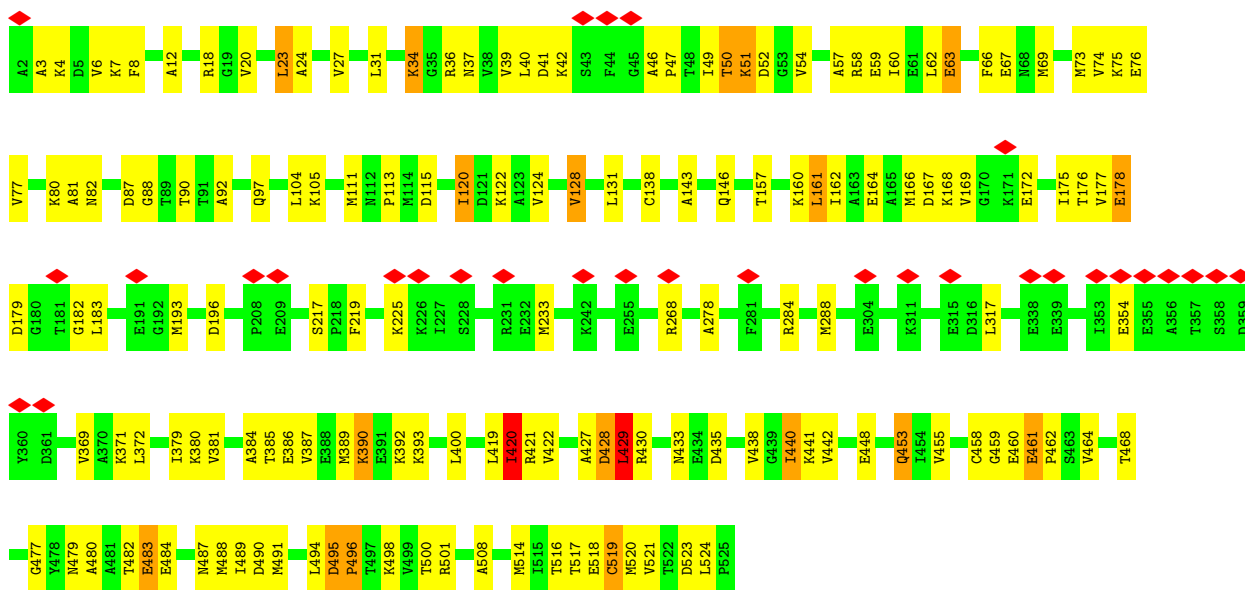
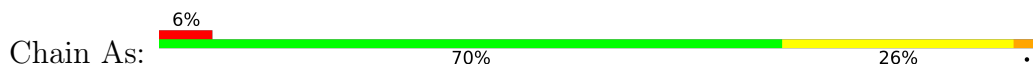


• Molecule 1: 60 kDa chaperonin

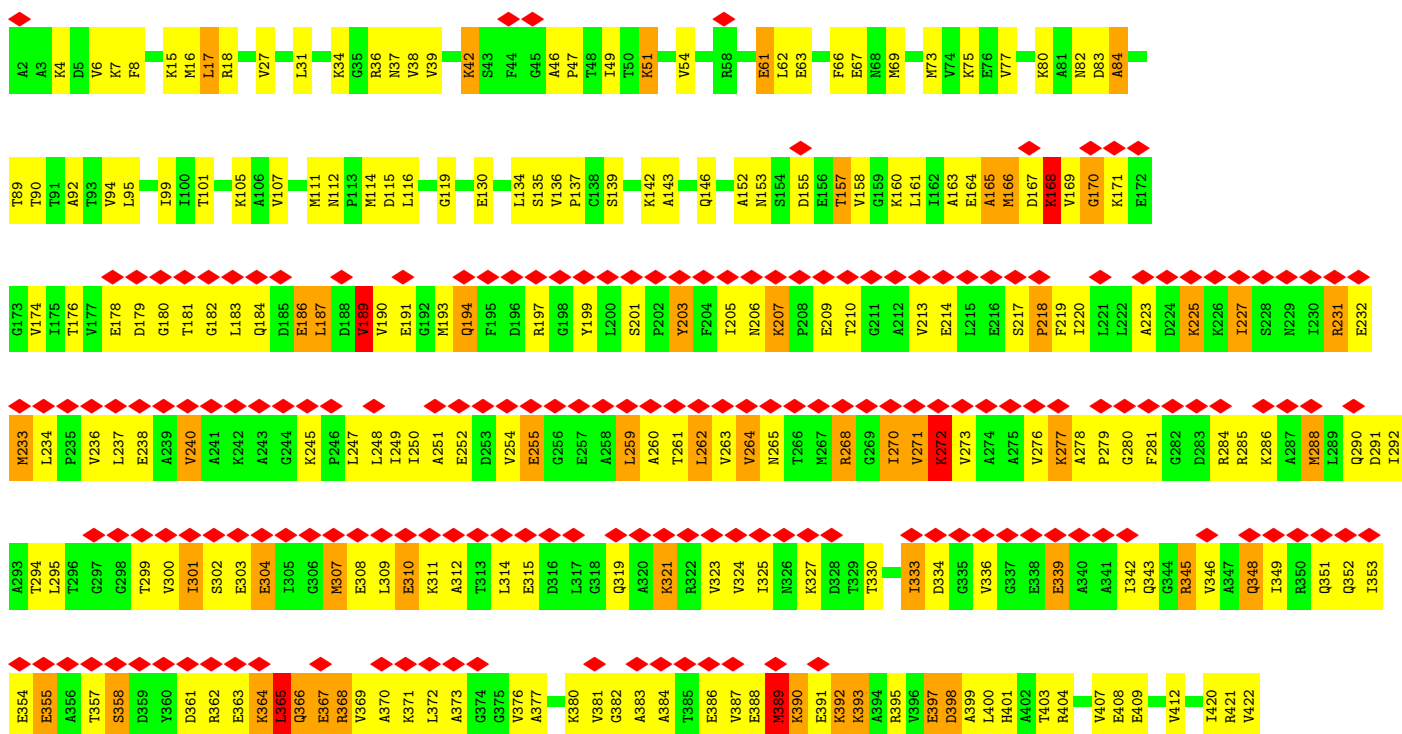


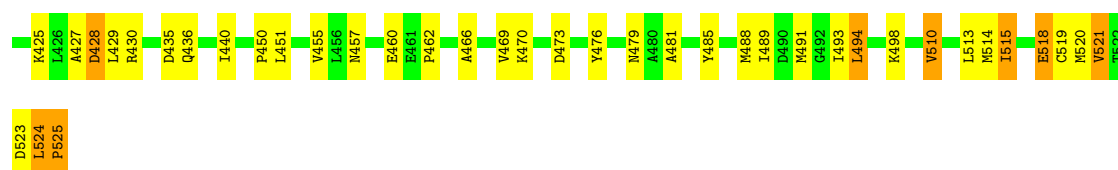
P525

- Molecule 1: 60 kDa chaperonin

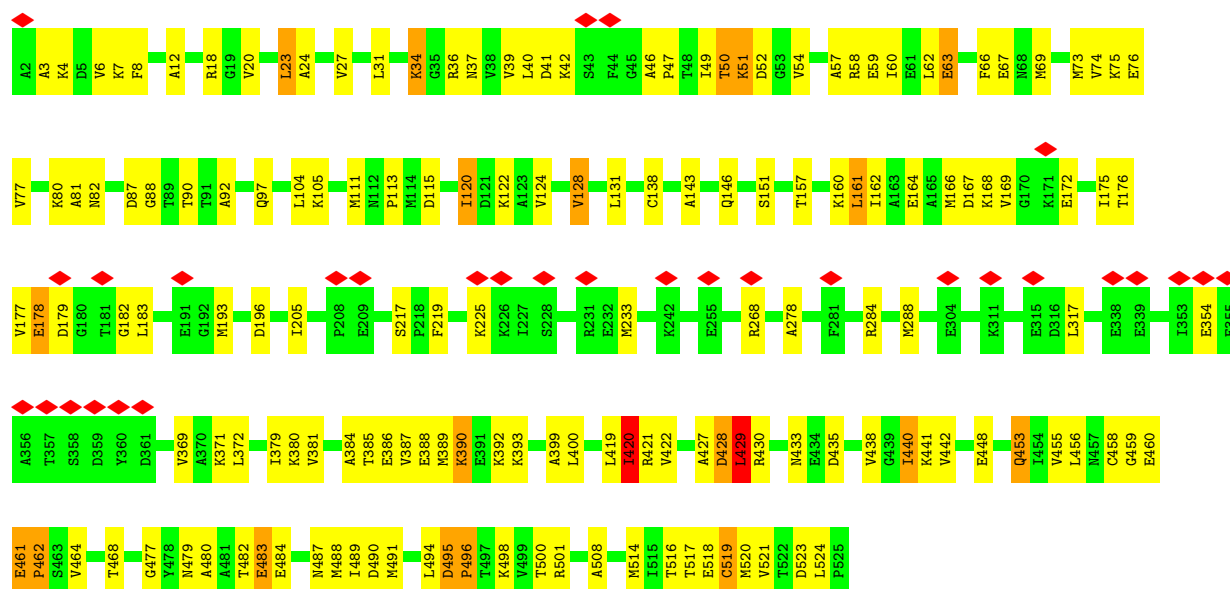


- Molecule 1: 60 kDa chaperonin

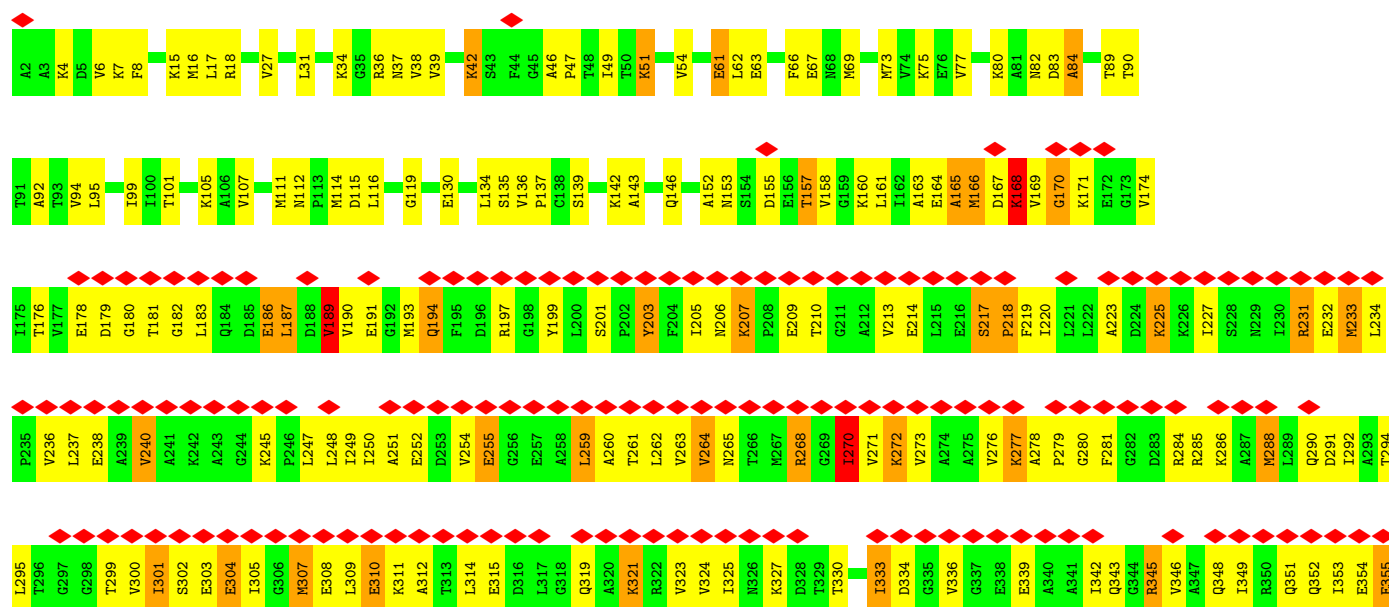


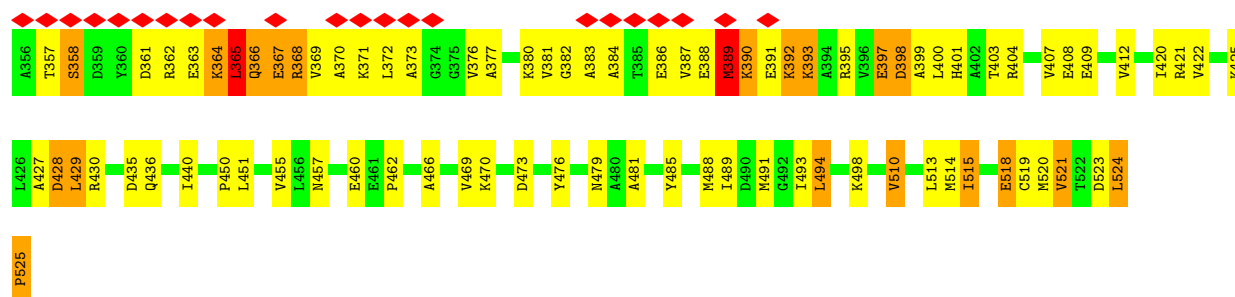


• Molecule 1: 60 kDa chaperonin

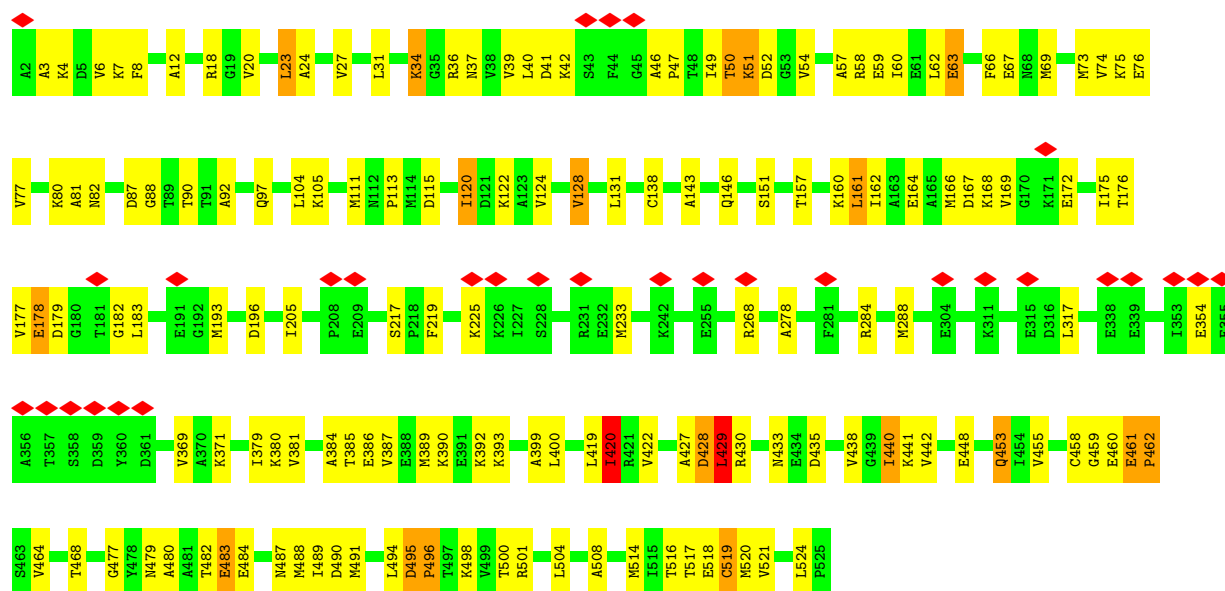
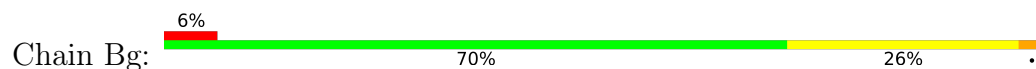


• Molecule 1: 60 kDa chaperonin

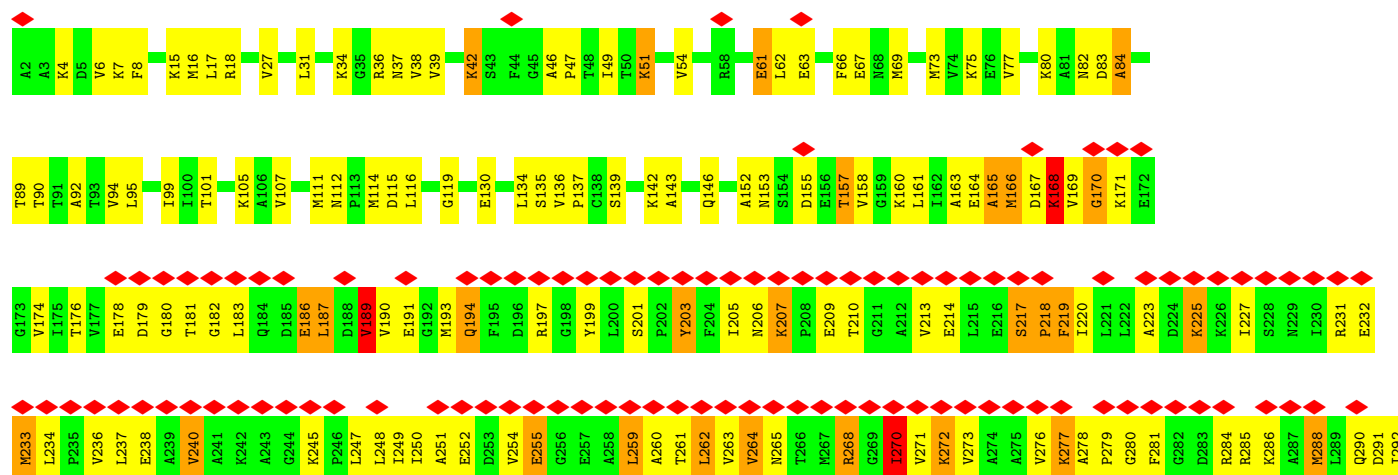


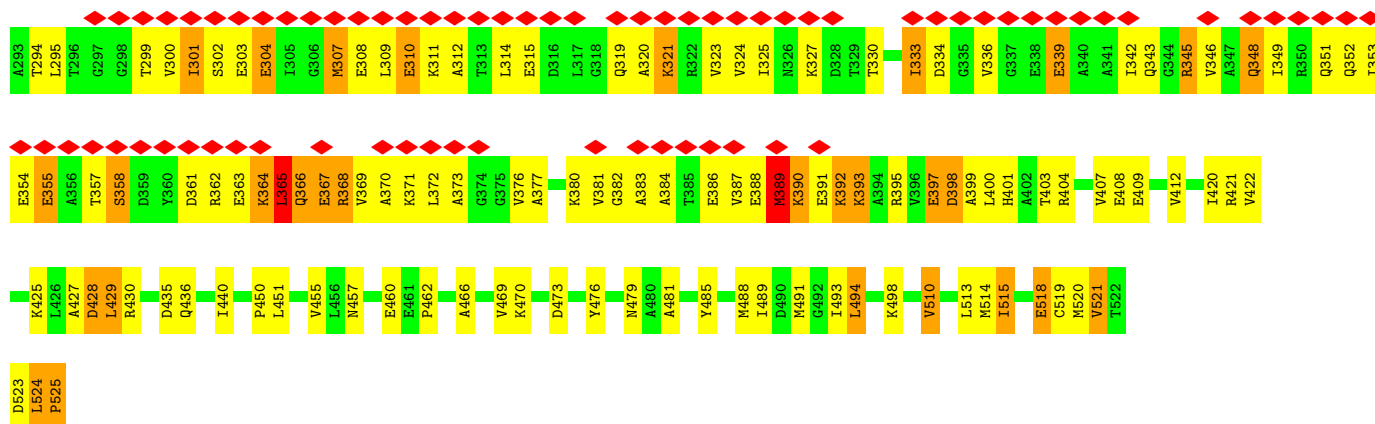


- Molecule 1: 60 kDa chaperonin

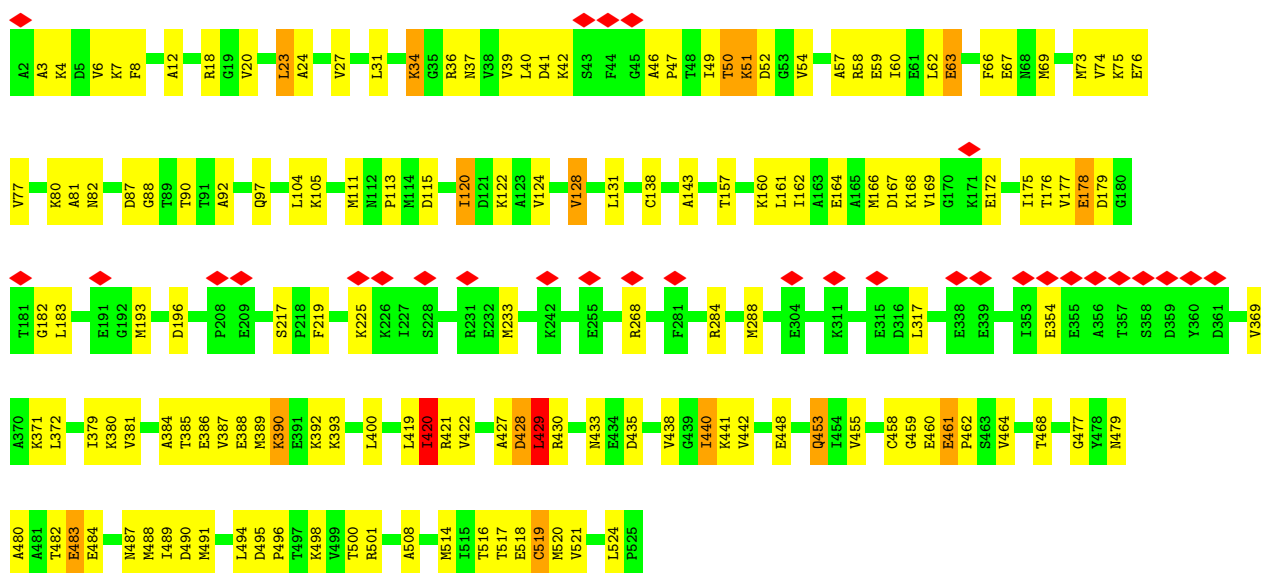
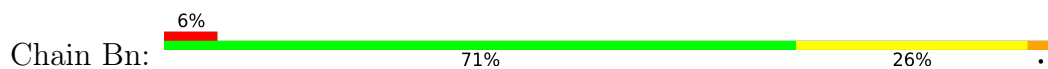


- Molecule 1: 60 kDa chaperonin

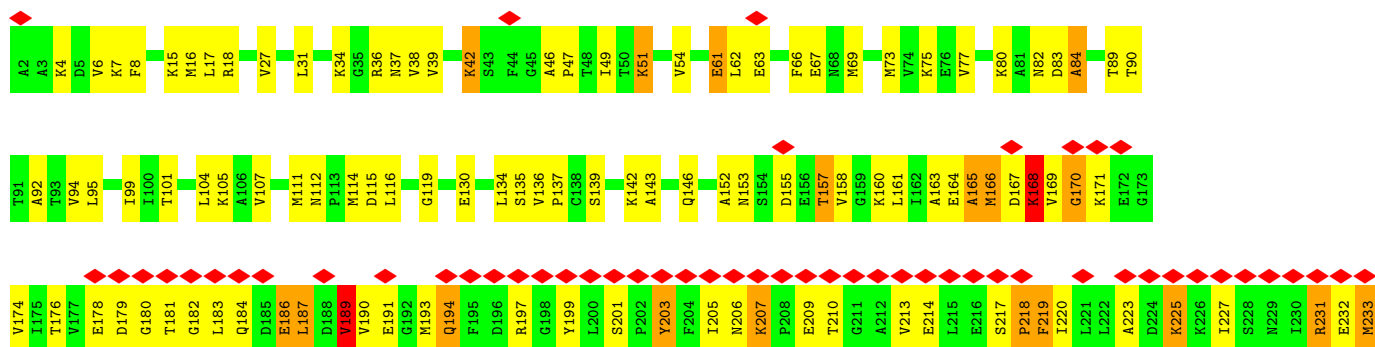


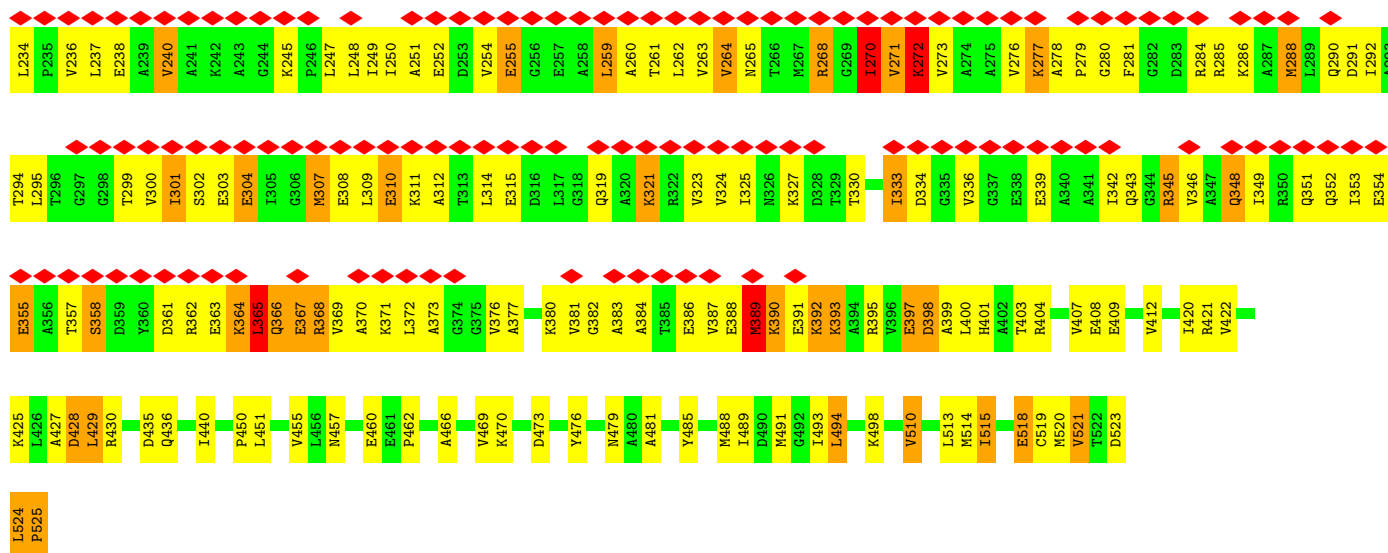


• Molecule 1: 60 kDa chaperonin

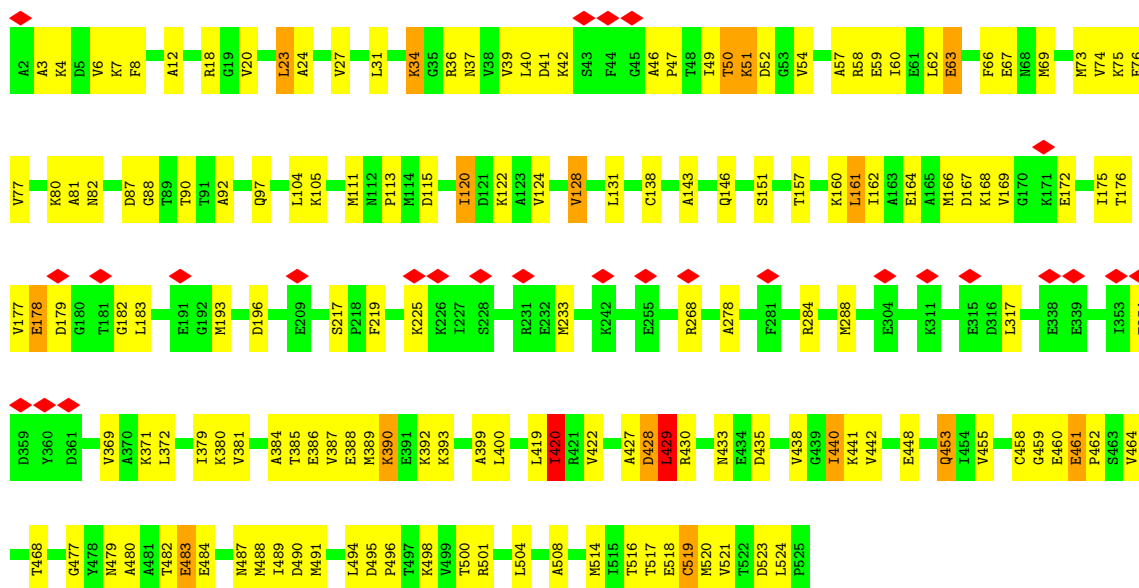


• Molecule 1: 60 kDa chaperonin

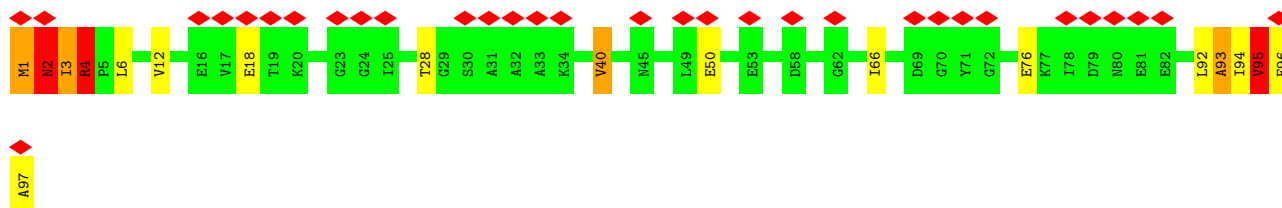
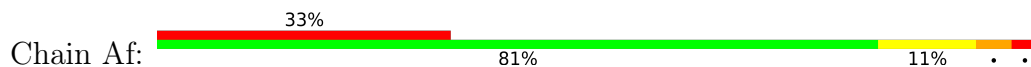




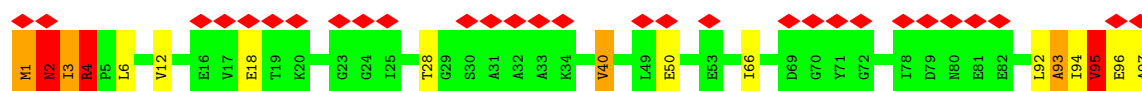
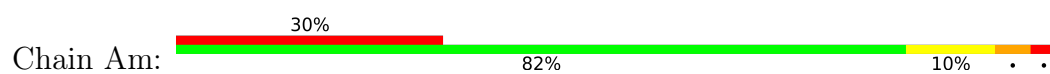
• Molecule 1: 60 kDa chaperonin



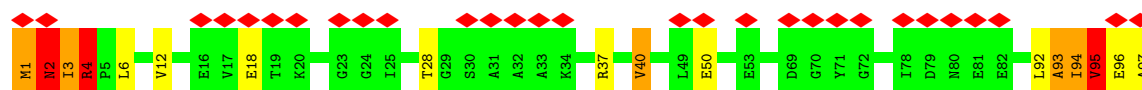
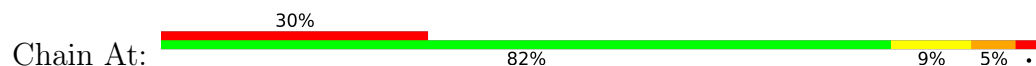
• Molecule 2: 10 kDa chaperonin



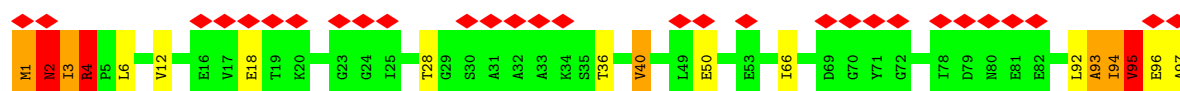
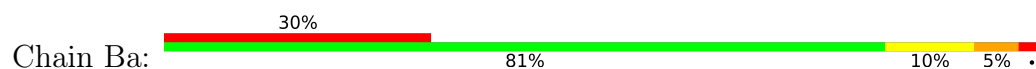
• Molecule 2: 10 kDa chaperonin



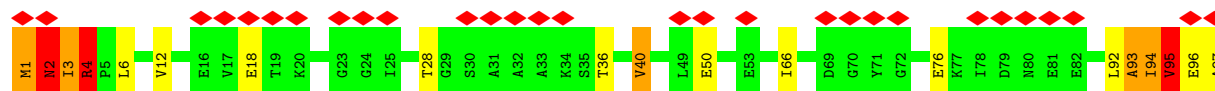
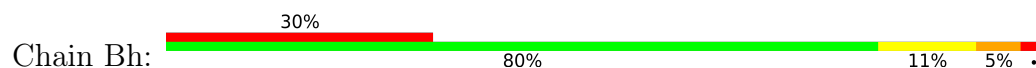
- Molecule 2: 10 kDa chaperonin



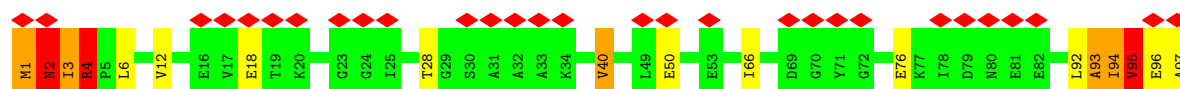
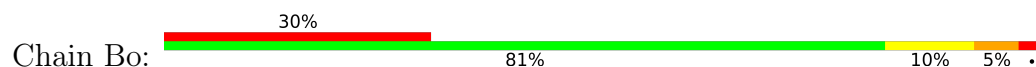
- Molecule 2: 10 kDa chaperonin



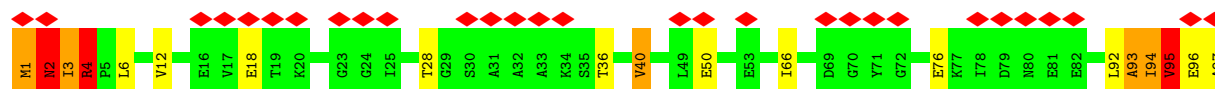
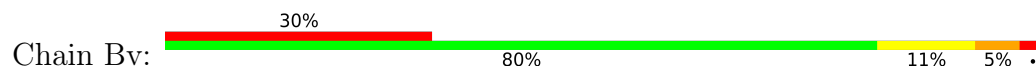
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	41000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	6.071	Depositor
Minimum map value	-1.209	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	425.088, 425.088, 425.088	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.107, 1.107, 1.107	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	Ad	1.27	5/3884 (0.1%)	1.58	54/5243 (1.0%)
1	Ae	0.95	2/3884 (0.1%)	1.48	26/5243 (0.5%)
1	Ak	1.27	5/3884 (0.1%)	1.58	54/5243 (1.0%)
1	Al	0.95	2/3884 (0.1%)	1.48	26/5243 (0.5%)
1	Ar	1.27	5/3884 (0.1%)	1.58	53/5243 (1.0%)
1	As	0.95	2/3884 (0.1%)	1.48	26/5243 (0.5%)
1	Ay	1.27	5/3884 (0.1%)	1.58	53/5243 (1.0%)
1	Az	0.95	2/3884 (0.1%)	1.48	26/5243 (0.5%)
1	Bf	1.27	5/3884 (0.1%)	1.58	54/5243 (1.0%)
1	Bg	0.95	2/3884 (0.1%)	1.48	26/5243 (0.5%)
1	Bm	1.26	5/3884 (0.1%)	1.58	54/5243 (1.0%)
1	Bn	0.95	2/3884 (0.1%)	1.48	25/5243 (0.5%)
1	Bt	1.27	5/3884 (0.1%)	1.58	53/5243 (1.0%)
1	Bu	0.95	2/3884 (0.1%)	1.48	26/5243 (0.5%)
2	Af	1.02	0/732	1.63	8/983 (0.8%)
2	Am	1.02	0/732	1.63	8/983 (0.8%)
2	At	1.02	0/732	1.63	8/983 (0.8%)
2	Ba	1.02	0/732	1.63	8/983 (0.8%)
2	Bh	1.02	0/732	1.63	8/983 (0.8%)
2	Bo	1.02	0/732	1.63	8/983 (0.8%)
2	Bv	1.02	0/732	1.63	8/983 (0.8%)
All	All	1.11	49/59500 (0.1%)	1.54	612/80283 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ad	0	1
1	Ae	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ak	0	1
1	Al	0	1
1	Ar	0	1
1	As	0	1
1	Ay	0	1
1	Az	0	1
1	Bf	0	1
1	Bg	0	1
1	Bm	0	1
1	Bn	0	1
1	Bt	0	1
1	Bu	0	1
2	Af	0	2
2	Am	0	2
2	At	0	2
2	Ba	0	2
2	Bh	0	2
2	Bo	0	2
2	Bv	0	2
All	All	0	28

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ay	525	PRO	C-O	49.21	2.21	1.23
1	Ad	525	PRO	C-O	49.20	2.21	1.23
1	Bt	525	PRO	C-O	49.20	2.21	1.23
1	Bm	525	PRO	C-O	49.20	2.21	1.23
1	Ak	525	PRO	C-O	49.19	2.21	1.23
1	Bf	525	PRO	C-O	49.19	2.21	1.23
1	Ar	525	PRO	C-O	49.17	2.21	1.23
1	Bf	189	VAL	C-N	10.85	1.49	1.33
1	Bm	189	VAL	C-N	10.80	1.49	1.33
1	Ad	189	VAL	C-N	10.79	1.49	1.33
1	Bt	189	VAL	C-N	10.78	1.49	1.33
1	Ak	189	VAL	C-N	10.78	1.49	1.33
1	Ay	189	VAL	C-N	10.77	1.49	1.33
1	Ar	189	VAL	C-N	10.77	1.49	1.33
1	Al	462	PRO	N-CD	-8.71	1.35	1.47
1	Bg	462	PRO	N-CD	-8.66	1.35	1.47
1	Az	462	PRO	N-CD	-8.65	1.35	1.47
1	Bn	462	PRO	N-CD	-8.65	1.35	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ae	462	PRO	N-CD	-8.64	1.35	1.47
1	Bu	462	PRO	N-CD	-8.64	1.35	1.47
1	As	462	PRO	N-CD	-8.63	1.35	1.47
1	Bn	496	PRO	N-CD	-8.09	1.36	1.47
1	Bg	496	PRO	N-CD	-8.08	1.36	1.47
1	Bu	496	PRO	N-CD	-8.06	1.36	1.47
1	Al	496	PRO	N-CD	-8.06	1.36	1.47
1	As	496	PRO	N-CD	-8.05	1.36	1.47
1	Ae	496	PRO	N-CD	-8.05	1.36	1.47
1	Az	496	PRO	N-CD	-8.04	1.36	1.47
1	Ar	137	PRO	N-CD	-6.65	1.38	1.47
1	Ad	137	PRO	N-CD	-6.60	1.38	1.47
1	Ak	137	PRO	N-CD	-6.59	1.38	1.47
1	Bf	137	PRO	N-CD	-6.59	1.38	1.47
1	Bt	137	PRO	N-CD	-6.58	1.38	1.47
1	Bm	137	PRO	N-CD	-6.56	1.38	1.47
1	Ay	137	PRO	N-CD	-6.56	1.38	1.47
1	Ak	366	GLN	CA-C	6.05	1.60	1.52
1	Bf	366	GLN	CA-C	6.05	1.60	1.52
1	Ay	366	GLN	CA-C	6.04	1.60	1.52
1	Ad	366	GLN	CA-C	6.02	1.60	1.52
1	Ar	366	GLN	CA-C	6.01	1.60	1.52
1	Bt	366	GLN	CA-C	5.97	1.60	1.52
1	Bm	366	GLN	CA-C	5.94	1.60	1.52
1	Bf	462	PRO	N-CD	5.30	1.55	1.47
1	Ak	462	PRO	N-CD	5.28	1.55	1.47
1	Bt	462	PRO	N-CD	5.28	1.55	1.47
1	Ad	462	PRO	N-CD	5.26	1.55	1.47
1	Ar	462	PRO	N-CD	5.25	1.55	1.47
1	Ay	462	PRO	N-CD	5.22	1.55	1.47
1	Bm	462	PRO	N-CD	5.22	1.55	1.47

All (612) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bt	525	PRO	CA-C-O	13.22	160.67	121.00
1	Ar	525	PRO	CA-C-O	13.22	160.66	121.00
1	Ad	525	PRO	CA-C-O	13.21	160.63	121.00
1	Ak	525	PRO	CA-C-O	13.21	160.62	121.00
1	Bf	525	PRO	CA-C-O	13.20	160.61	121.00
1	Bm	525	PRO	CA-C-O	13.20	160.60	121.00
1	Ay	525	PRO	CA-C-O	13.19	160.58	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ak	367	GLU	N-CA-C	-12.79	96.15	112.90
1	Bm	367	GLU	N-CA-C	-12.78	96.16	112.90
1	Ar	367	GLU	N-CA-C	-12.77	96.17	112.90
1	Bf	367	GLU	N-CA-C	-12.77	96.18	112.90
1	Ad	367	GLU	N-CA-C	-12.76	96.19	112.90
1	Bt	367	GLU	N-CA-C	-12.75	96.19	112.90
1	Ay	367	GLU	N-CA-C	-12.73	96.22	112.90
1	Ak	429	LEU	N-CA-C	-12.45	91.28	109.96
1	Ak	399	ALA	N-CA-C	-12.45	97.71	111.28
1	Bt	399	ALA	N-CA-C	-12.45	97.71	111.28
1	Bt	429	LEU	N-CA-C	-12.44	91.29	109.96
1	Bf	429	LEU	N-CA-C	-12.44	91.30	109.96
1	Ad	399	ALA	N-CA-C	-12.44	97.72	111.28
1	Ay	429	LEU	N-CA-C	-12.44	91.31	109.96
1	Ay	399	ALA	N-CA-C	-12.43	97.73	111.28
1	Bm	399	ALA	N-CA-C	-12.43	97.73	111.28
1	Bf	399	ALA	N-CA-C	-12.43	97.73	111.28
1	Ar	399	ALA	N-CA-C	-12.42	97.74	111.28
1	Ad	429	LEU	N-CA-C	-12.42	91.33	109.96
1	Ar	429	LEU	N-CA-C	-12.42	91.34	109.96
1	Bm	429	LEU	N-CA-C	-12.39	91.37	109.96
1	Ar	166	MET	N-CA-C	-12.02	98.26	111.36
1	Ay	166	MET	N-CA-C	-12.01	98.27	111.36
1	Ad	166	MET	N-CA-C	-12.00	98.28	111.36
1	Bm	166	MET	N-CA-C	-12.00	98.28	111.36
1	Ak	166	MET	N-CA-C	-11.99	98.29	111.36
1	Bf	166	MET	N-CA-C	-11.98	98.30	111.36
1	Bt	166	MET	N-CA-C	-11.98	98.30	111.36
1	Ay	389	MET	N-CA-C	-11.88	98.36	111.07
1	Ak	389	MET	N-CA-C	-11.86	98.38	111.07
1	Bt	389	MET	N-CA-C	-11.86	98.39	111.07
1	Ad	389	MET	N-CA-C	-11.84	98.40	111.07
1	Bf	389	MET	N-CA-C	-11.84	98.41	111.07
1	Ar	389	MET	N-CA-C	-11.83	98.42	111.07
1	Bm	389	MET	N-CA-C	-11.81	98.43	111.07
1	Ak	365	LEU	N-CA-C	11.73	125.80	110.43
1	Bt	365	LEU	N-CA-C	11.73	125.80	110.43
1	Ar	365	LEU	N-CA-C	11.72	125.79	110.43
1	Ay	365	LEU	N-CA-C	11.71	125.78	110.43
1	Ad	365	LEU	N-CA-C	11.71	125.77	110.43
1	Bm	365	LEU	N-CA-C	11.70	125.76	110.43
1	Bm	368	ARG	N-CA-C	-11.70	98.22	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bf	365	LEU	N-CA-C	11.69	125.74	110.43
1	Bf	368	ARG	N-CA-C	-11.67	98.25	110.97
1	Bt	368	ARG	N-CA-C	-11.67	98.25	110.97
1	Ad	368	ARG	N-CA-C	-11.66	98.25	110.97
1	Ay	368	ARG	N-CA-C	-11.66	98.26	110.97
1	Ak	368	ARG	N-CA-C	-11.64	98.28	110.97
1	Ar	368	ARG	N-CA-C	-11.63	98.29	110.97
1	Bg	34	LYS	N-CA-C	-9.85	100.81	112.92
1	Al	34	LYS	N-CA-C	-9.84	100.81	112.92
1	Ae	34	LYS	N-CA-C	-9.84	100.81	112.92
1	As	34	LYS	N-CA-C	-9.83	100.82	112.92
1	Bn	34	LYS	N-CA-C	-9.83	100.82	112.92
1	Az	34	LYS	N-CA-C	-9.83	100.83	112.92
1	Bu	34	LYS	N-CA-C	-9.82	100.84	112.92
1	Az	496	PRO	N-CA-CB	-9.45	95.13	103.35
1	Bu	496	PRO	N-CA-CB	-9.42	95.15	103.35
1	As	496	PRO	N-CA-CB	-9.42	95.16	103.35
1	Bg	496	PRO	N-CA-CB	-9.42	95.15	103.35
1	Ae	496	PRO	N-CA-CB	-9.40	95.17	103.35
1	Al	496	PRO	N-CA-CB	-9.40	95.17	103.35
1	Bn	496	PRO	N-CA-CB	-9.38	95.19	103.35
1	Ak	368	ARG	N-CA-CB	9.03	123.09	109.91
1	Ay	368	ARG	N-CA-CB	9.02	123.08	109.91
1	Bt	368	ARG	N-CA-CB	9.02	123.08	109.91
1	Ad	368	ARG	N-CA-CB	9.02	123.07	109.91
1	Ar	368	ARG	N-CA-CB	9.01	123.06	109.91
1	Bm	368	ARG	N-CA-CB	9.01	123.06	109.91
1	Bf	368	ARG	N-CA-CB	8.99	123.04	109.91
1	As	166	MET	N-CA-C	-8.31	102.30	111.36
1	Bg	166	MET	N-CA-C	-8.30	102.31	111.36
1	Al	166	MET	N-CA-C	-8.28	102.33	111.36
1	Az	166	MET	N-CA-C	-8.28	102.33	111.36
1	Ae	166	MET	N-CA-C	-8.28	102.34	111.36
1	Bn	166	MET	N-CA-C	-8.27	102.34	111.36
1	Bu	166	MET	N-CA-C	-8.27	102.35	111.36
1	Ar	366	GLN	N-CA-C	8.15	128.17	110.80
1	Ak	366	GLN	N-CA-C	8.15	128.16	110.80
1	Bf	366	GLN	N-CA-C	8.15	128.16	110.80
1	Bm	366	GLN	N-CA-C	8.14	128.14	110.80
1	Ad	366	GLN	N-CA-C	8.14	128.14	110.80
1	Bt	366	GLN	N-CA-C	8.14	128.14	110.80
1	Ay	366	GLN	N-CA-C	8.14	128.13	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Az	483	GLU	CB-CA-C	8.02	123.51	111.80
1	Al	483	GLU	CB-CA-C	8.00	123.48	111.80
1	Bn	483	GLU	CB-CA-C	8.00	123.48	111.80
1	Ae	483	GLU	CB-CA-C	7.99	123.47	111.80
1	Bg	483	GLU	CB-CA-C	7.99	123.46	111.80
1	Bt	365	LEU	N-CA-CB	-7.98	98.85	110.26
1	As	483	GLU	CB-CA-C	7.97	123.44	111.80
1	Ay	365	LEU	N-CA-CB	-7.97	98.86	110.26
1	Bu	483	GLU	CB-CA-C	7.97	123.44	111.80
1	Bm	365	LEU	N-CA-CB	-7.97	98.86	110.26
1	Ar	365	LEU	N-CA-CB	-7.97	98.87	110.26
1	Ak	365	LEU	N-CA-CB	-7.96	98.88	110.26
1	Ad	365	LEU	N-CA-CB	-7.95	98.90	110.26
1	Bf	365	LEU	N-CA-CB	-7.94	98.90	110.26
1	Ay	364	LYS	N-CA-CB	7.81	121.69	109.82
1	Bt	513	LEU	N-CA-C	-7.81	102.85	111.36
1	Bf	364	LYS	N-CA-CB	7.80	121.68	109.82
1	Ay	364	LYS	N-CA-C	-7.80	101.50	111.02
1	Bm	364	LYS	N-CA-CB	7.80	121.68	109.82
1	Ak	364	LYS	N-CA-CB	7.79	121.67	109.82
1	Bm	364	LYS	N-CA-C	-7.79	101.51	111.02
1	Ad	364	LYS	N-CA-CB	7.79	121.66	109.82
1	Bf	513	LEU	N-CA-C	-7.79	102.87	111.36
1	Bm	513	LEU	N-CA-C	-7.79	102.87	111.36
1	Bt	364	LYS	N-CA-CB	7.79	121.66	109.82
1	Ad	513	LEU	N-CA-C	-7.78	102.88	111.36
1	Ay	513	LEU	N-CA-C	-7.78	102.88	111.36
1	Ar	513	LEU	N-CA-C	-7.78	102.88	111.36
1	Ar	364	LYS	N-CA-CB	7.77	121.63	109.82
1	Ar	364	LYS	N-CA-C	-7.76	101.55	111.02
1	Ak	513	LEU	N-CA-C	-7.76	102.90	111.36
1	Ad	364	LYS	N-CA-C	-7.76	101.55	111.02
1	Bf	364	LYS	N-CA-C	-7.76	101.55	111.02
1	Bt	364	LYS	N-CA-C	-7.75	101.56	111.02
1	Ak	364	LYS	N-CA-C	-7.75	101.57	111.02
1	Bf	170	GLY	N-CA-C	7.71	122.23	112.83
1	Ad	170	GLY	N-CA-C	7.67	122.19	112.83
1	Ak	170	GLY	N-CA-C	7.66	122.18	112.83
1	Bt	170	GLY	N-CA-C	7.66	122.18	112.83
1	Ar	170	GLY	N-CA-C	7.65	122.17	112.83
1	Bm	170	GLY	N-CA-C	7.65	122.16	112.83
1	Ay	170	GLY	N-CA-C	7.65	122.16	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bm	84	ALA	N-CA-C	-7.60	102.69	110.97
1	Bt	84	ALA	N-CA-C	-7.59	102.69	110.97
1	Ak	84	ALA	N-CA-C	-7.58	102.71	110.97
1	Ad	84	ALA	N-CA-C	-7.57	102.72	110.97
1	Ay	84	ALA	N-CA-C	-7.55	102.74	110.97
1	Ar	84	ALA	N-CA-C	-7.55	102.74	110.97
1	Bf	84	ALA	N-CA-C	-7.52	102.77	110.97
2	At	95	VAL	N-CA-C	7.51	124.96	109.34
2	Bh	95	VAL	N-CA-C	7.50	124.95	109.34
2	Ba	95	VAL	N-CA-C	7.50	124.94	109.34
2	Bo	95	VAL	N-CA-C	7.50	124.93	109.34
2	Af	95	VAL	N-CA-C	7.50	124.93	109.34
2	Am	95	VAL	N-CA-C	7.49	124.93	109.34
2	Bv	95	VAL	N-CA-C	7.49	124.92	109.34
1	Al	81	ALA	N-CA-C	-7.36	103.34	111.36
1	Bg	81	ALA	N-CA-C	-7.34	103.35	111.36
1	Bu	81	ALA	N-CA-C	-7.33	103.37	111.36
1	Ae	81	ALA	N-CA-C	-7.33	103.38	111.36
1	As	81	ALA	N-CA-C	-7.31	103.39	111.36
1	Az	81	ALA	N-CA-C	-7.31	103.40	111.36
1	Bn	81	ALA	N-CA-C	-7.29	103.41	111.36
1	Bt	389	MET	N-CA-CB	7.10	120.31	110.01
1	Bf	389	MET	N-CA-CB	7.07	120.26	110.01
1	Ay	168	LYS	N-CA-C	7.06	125.84	110.80
1	Bm	168	LYS	N-CA-C	7.06	125.84	110.80
1	Bm	389	MET	N-CA-CB	7.06	120.24	110.01
1	Ad	389	MET	N-CA-CB	7.05	120.24	110.01
1	Ay	389	MET	N-CA-CB	7.05	120.24	110.01
1	Ak	168	LYS	N-CA-C	7.05	125.82	110.80
1	Ad	168	LYS	N-CA-C	7.05	125.82	110.80
1	Ak	389	MET	N-CA-CB	7.05	120.23	110.01
1	Ar	389	MET	N-CA-CB	7.05	120.23	110.01
1	Bt	168	LYS	N-CA-C	7.05	125.81	110.80
1	Ar	168	LYS	N-CA-C	7.04	125.80	110.80
1	Bf	168	LYS	N-CA-C	7.04	125.79	110.80
2	Bo	2	ASN	CA-CB-CG	6.87	119.47	112.60
2	Bh	2	ASN	CA-CB-CG	6.87	119.47	112.60
2	Af	2	ASN	CA-CB-CG	6.86	119.46	112.60
1	Ar	427	ALA	N-CA-C	6.86	118.76	111.28
2	Am	2	ASN	CA-CB-CG	6.86	119.46	112.60
1	Bt	427	ALA	N-CA-C	6.86	118.76	111.28
2	Ba	2	ASN	CA-CB-CG	6.85	119.45	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ak	427	ALA	N-CA-C	6.85	118.74	111.28
2	At	2	ASN	CA-CB-CG	6.85	119.45	112.60
1	Bm	427	ALA	N-CA-C	6.84	118.74	111.28
1	Ad	427	ALA	N-CA-C	6.84	118.74	111.28
2	Bv	2	ASN	CA-CB-CG	6.83	119.43	112.60
1	Ay	427	ALA	N-CA-C	6.82	118.71	111.28
1	Bf	427	ALA	N-CA-C	6.82	118.71	111.28
1	Ar	390	LYS	N-CA-C	-6.80	103.94	111.36
1	Bt	390	LYS	N-CA-C	-6.80	103.94	111.36
1	Ay	390	LYS	N-CA-C	-6.79	103.96	111.36
1	Bm	390	LYS	N-CA-C	-6.79	103.96	111.36
1	Ad	390	LYS	N-CA-C	-6.78	103.97	111.36
1	Bf	390	LYS	N-CA-C	-6.77	103.98	111.36
1	Ak	390	LYS	N-CA-C	-6.74	104.01	111.36
1	Az	519	CYS	N-CA-CB	-6.70	99.17	111.37
1	Bg	519	CYS	N-CA-CB	-6.69	99.19	111.37
1	Al	519	CYS	N-CA-CB	-6.69	99.20	111.37
1	Ae	519	CYS	N-CA-CB	-6.68	99.20	111.37
1	As	519	CYS	N-CA-CB	-6.68	99.21	111.37
1	Bn	519	CYS	N-CA-CB	-6.68	99.21	111.37
1	Bu	519	CYS	N-CA-CB	-6.67	99.23	111.37
1	Az	168	LYS	N-CA-C	6.62	118.49	111.28
2	Am	4	ARG	CB-CA-C	-6.61	101.67	109.47
1	Bu	168	LYS	N-CA-C	6.61	118.48	111.28
1	Ae	168	LYS	N-CA-C	6.60	118.48	111.28
1	As	168	LYS	N-CA-C	6.60	118.47	111.28
1	Bn	168	LYS	N-CA-C	6.60	118.47	111.28
1	Al	168	LYS	N-CA-C	6.59	118.47	111.28
2	Bo	4	ARG	CB-CA-C	-6.59	101.69	109.47
2	Ba	4	ARG	CB-CA-C	-6.59	101.69	109.47
1	Bg	168	LYS	N-CA-C	6.59	118.46	111.28
2	At	4	ARG	CB-CA-C	-6.58	101.71	109.47
2	Af	4	ARG	CB-CA-C	-6.57	101.71	109.47
2	Bv	4	ARG	CB-CA-C	-6.57	101.71	109.47
1	Ak	393	LYS	N-CA-C	-6.55	104.14	111.28
2	Bh	4	ARG	CB-CA-C	-6.55	101.74	109.47
1	Bt	393	LYS	N-CA-C	-6.54	104.14	111.28
1	Bm	393	LYS	N-CA-C	-6.54	104.15	111.28
1	Ay	393	LYS	N-CA-C	-6.53	104.16	111.28
1	Bf	393	LYS	N-CA-C	-6.53	104.16	111.28
1	Ad	393	LYS	N-CA-C	-6.53	104.17	111.28
1	Ar	393	LYS	N-CA-C	-6.51	104.18	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bu	496	PRO	CA-N-CD	6.44	121.02	112.00
1	Az	496	PRO	CA-N-CD	6.43	121.01	112.00
1	Al	429	LEU	N-CA-C	-6.42	100.40	109.96
1	Bg	496	PRO	CA-N-CD	6.42	120.98	112.00
1	As	429	LEU	N-CA-C	-6.42	100.40	109.96
1	Ak	137	PRO	CA-C-N	-6.41	113.94	122.85
1	Ak	137	PRO	C-N-CA	-6.41	113.94	122.85
1	Bu	429	LEU	N-CA-C	-6.41	100.41	109.96
1	Bm	137	PRO	CA-C-N	-6.41	113.94	122.85
1	Bm	137	PRO	C-N-CA	-6.41	113.94	122.85
1	Ad	137	PRO	CA-C-N	-6.40	113.96	122.85
1	Ad	137	PRO	C-N-CA	-6.40	113.96	122.85
1	Ae	496	PRO	CA-N-CD	6.40	120.95	112.00
1	Ae	429	LEU	N-CA-C	-6.39	100.44	109.96
1	Bt	137	PRO	CA-C-N	-6.39	113.97	122.85
1	Bt	137	PRO	C-N-CA	-6.39	113.97	122.85
1	As	496	PRO	CA-N-CD	6.39	120.94	112.00
1	Ay	137	PRO	CA-C-N	-6.39	113.97	122.85
1	Ay	137	PRO	C-N-CA	-6.39	113.97	122.85
1	Bf	137	PRO	CA-C-N	-6.38	113.98	122.85
1	Bf	137	PRO	C-N-CA	-6.38	113.98	122.85
1	Ay	75	LYS	N-CA-C	-6.38	104.40	111.36
1	Al	496	PRO	CA-N-CD	6.38	120.93	112.00
1	Bn	429	LEU	N-CA-C	-6.38	100.45	109.96
1	Bn	496	PRO	CA-N-CD	6.38	120.93	112.00
1	Ar	137	PRO	CA-C-N	-6.37	113.99	122.85
1	Ar	137	PRO	C-N-CA	-6.37	113.99	122.85
1	Bg	429	LEU	N-CA-C	-6.36	100.48	109.96
1	Ar	75	LYS	N-CA-C	-6.36	104.42	111.36
1	Az	429	LEU	N-CA-C	-6.36	100.48	109.96
1	Ad	75	LYS	N-CA-C	-6.34	104.45	111.36
1	Bm	75	LYS	N-CA-C	-6.34	104.45	111.36
1	Ak	75	LYS	N-CA-C	-6.34	104.45	111.36
1	Bf	75	LYS	N-CA-C	-6.34	104.45	111.36
1	Bt	75	LYS	N-CA-C	-6.33	104.46	111.36
1	Ar	398	ASP	N-CA-C	6.32	120.82	113.18
1	Ay	398	ASP	N-CA-C	6.31	120.82	113.18
1	Bt	398	ASP	N-CA-C	6.31	120.81	113.18
1	Ad	398	ASP	N-CA-C	6.30	120.81	113.18
1	Ar	367	GLU	N-CA-CB	6.30	119.78	110.33
1	Bf	398	ASP	N-CA-C	6.30	120.81	113.18
1	Ay	403	THR	N-CA-C	-6.29	104.43	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ar	403	THR	N-CA-C	-6.28	104.43	111.28
1	Bm	398	ASP	N-CA-C	6.28	120.78	113.18
1	Ak	367	GLU	N-CA-CB	6.28	119.75	110.33
1	Ak	398	ASP	N-CA-C	6.28	120.78	113.18
1	Ad	367	GLU	N-CA-CB	6.28	119.75	110.33
1	Ad	403	THR	N-CA-C	-6.28	104.44	111.28
1	Bm	367	GLU	N-CA-CB	6.28	119.74	110.33
1	Bt	403	THR	N-CA-C	-6.27	104.45	111.28
1	Ak	403	THR	N-CA-C	-6.26	104.45	111.28
1	Ay	367	GLU	N-CA-CB	6.26	119.72	110.33
1	Bf	367	GLU	N-CA-CB	6.25	119.71	110.33
1	Bm	403	THR	N-CA-C	-6.25	104.47	111.28
1	Bt	367	GLU	N-CA-CB	6.25	119.70	110.33
1	Bf	403	THR	N-CA-C	-6.23	104.49	111.28
1	Bg	462	PRO	CA-N-CD	6.21	120.69	112.00
1	Al	161	LEU	N-CA-C	-6.19	104.44	111.07
1	Bt	392	LYS	N-CA-C	6.19	118.83	111.71
1	Bu	161	LEU	N-CA-C	-6.19	104.45	111.07
1	Al	462	PRO	CA-N-CD	6.19	120.66	112.00
1	Bg	161	LEU	N-CA-C	-6.18	104.45	111.07
1	Bn	50	THR	N-CA-C	6.18	119.47	109.40
1	Ae	161	LEU	N-CA-C	-6.17	104.46	111.07
1	Bn	161	LEU	N-CA-C	-6.17	104.46	111.07
1	Bn	462	PRO	CA-N-CD	6.17	120.64	112.00
1	Ae	462	PRO	CA-N-CD	6.17	120.64	112.00
1	Ak	392	LYS	N-CA-C	6.17	118.81	111.71
1	Ar	392	LYS	N-CA-C	6.17	118.80	111.71
1	Ay	392	LYS	N-CA-C	6.17	118.80	111.71
1	Az	50	THR	N-CA-C	6.17	119.45	109.40
1	Bu	50	THR	N-CA-C	6.16	119.45	109.40
1	As	462	PRO	CA-N-CD	6.16	120.63	112.00
1	As	161	LEU	N-CA-C	-6.16	104.48	111.07
1	Bt	165	ALA	N-CA-C	-6.15	104.48	111.07
1	Ae	50	THR	N-CA-C	6.15	119.43	109.40
1	Bg	50	THR	N-CA-C	6.15	119.43	109.40
2	Bo	94	ILE	CB-CA-C	-6.15	102.11	110.42
2	Bh	94	ILE	CB-CA-C	-6.15	102.12	110.42
1	Bf	392	LYS	N-CA-C	6.15	118.78	111.71
1	Bm	392	LYS	N-CA-C	6.15	118.78	111.71
1	Az	462	PRO	CA-N-CD	6.15	120.61	112.00
1	Ad	392	LYS	N-CA-C	6.14	118.78	111.71
1	Ad	165	ALA	N-CA-C	-6.14	104.50	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	At	94	ILE	CB-CA-C	-6.14	102.14	110.42
1	Bf	165	ALA	N-CA-C	-6.14	104.50	111.07
2	Af	94	ILE	CB-CA-C	-6.13	102.14	110.42
1	Ak	165	ALA	N-CA-C	-6.13	104.51	111.07
1	Ar	165	ALA	N-CA-C	-6.13	104.51	111.07
1	Bn	51	LYS	N-CA-C	-6.13	104.42	113.61
2	Am	94	ILE	CB-CA-C	-6.13	102.15	110.42
1	As	50	THR	N-CA-C	6.13	119.39	109.40
1	Az	161	LEU	N-CA-C	-6.13	104.51	111.07
1	Bu	51	LYS	N-CA-C	-6.13	104.42	113.61
1	Ay	165	ALA	N-CA-C	-6.13	104.52	111.07
1	Bm	165	ALA	N-CA-C	-6.12	104.52	111.07
1	Bu	462	PRO	CA-N-CD	6.12	120.58	112.00
2	Bv	94	ILE	CB-CA-C	-6.12	102.15	110.42
2	Ba	94	ILE	CB-CA-C	-6.12	102.16	110.42
1	Bg	51	LYS	N-CA-C	-6.11	104.44	113.61
1	As	51	LYS	N-CA-C	-6.11	104.44	113.61
1	Az	51	LYS	N-CA-C	-6.10	104.45	113.61
1	Ae	51	LYS	N-CA-C	-6.10	104.46	113.61
1	Al	51	LYS	N-CA-C	-6.09	104.48	113.61
1	Al	50	THR	N-CA-C	6.08	119.45	109.72
1	As	461	GLU	N-CA-C	-6.04	102.05	109.65
1	Ay	182	GLY	N-CA-C	-6.03	104.36	112.14
1	Bf	182	GLY	N-CA-C	-6.03	104.36	112.14
1	Bt	428	ASP	CB-CA-C	-6.03	101.42	111.13
1	Az	461	GLU	N-CA-C	-6.03	102.05	109.65
1	Bf	428	ASP	CB-CA-C	-6.03	101.42	111.13
1	Ak	428	ASP	CB-CA-C	-6.02	101.43	111.13
1	Ad	182	GLY	N-CA-C	-6.02	104.37	112.14
1	Ad	428	ASP	CB-CA-C	-6.02	101.44	111.13
1	Ak	61	GLU	N-CA-C	-6.02	99.54	108.99
1	Al	420	ILE	N-CA-C	-6.02	104.48	110.62
1	Ar	428	ASP	CB-CA-C	-6.02	101.44	111.13
1	Bt	182	GLY	N-CA-C	-6.02	104.38	112.14
1	Ay	61	GLU	N-CA-C	-6.02	99.54	108.99
1	Ar	182	GLY	N-CA-C	-6.01	104.38	112.14
1	Ae	461	GLU	N-CA-C	-6.01	102.08	109.65
1	Bm	182	GLY	N-CA-C	-6.01	104.39	112.14
1	Ak	182	GLY	N-CA-C	-6.01	104.39	112.14
1	Bm	428	ASP	CB-CA-C	-6.01	101.45	111.13
1	Bt	61	GLU	N-CA-C	-6.01	99.56	108.99
1	Ad	61	GLU	N-CA-C	-6.01	99.56	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bn	420	ILE	N-CA-C	-6.01	104.49	110.62
1	Al	461	GLU	N-CA-C	-6.00	102.09	109.65
1	Bu	420	ILE	N-CA-C	-6.00	104.50	110.62
1	Bf	61	GLU	N-CA-C	-6.00	99.57	108.99
1	Bn	461	GLU	N-CA-C	-6.00	102.09	109.65
1	Ay	428	ASP	CB-CA-C	-6.00	101.47	111.13
1	Bu	461	GLU	N-CA-C	-6.00	102.09	109.65
1	Ar	61	GLU	N-CA-C	-5.99	99.58	108.99
1	Bm	61	GLU	N-CA-C	-5.99	99.58	108.99
1	As	420	ILE	N-CA-C	-5.98	104.52	110.62
1	Bg	461	GLU	N-CA-C	-5.98	102.11	109.65
1	Ae	420	ILE	N-CA-C	-5.98	104.52	110.62
1	Bf	493	ILE	CB-CA-C	5.96	121.07	111.29
1	Ay	493	ILE	CB-CA-C	5.96	121.07	111.29
1	Ak	493	ILE	CB-CA-C	5.95	121.05	111.29
1	Az	420	ILE	N-CA-C	-5.95	104.55	110.62
1	Bg	420	ILE	N-CA-C	-5.95	104.55	110.62
1	Ar	493	ILE	CB-CA-C	5.95	121.04	111.29
1	Ad	493	ILE	CB-CA-C	5.94	121.03	111.29
1	Bm	493	ILE	CB-CA-C	5.94	121.03	111.29
1	Bt	493	ILE	CB-CA-C	5.92	121.01	111.29
1	Ak	408	GLU	N-CA-C	5.92	117.41	111.07
1	Bt	408	GLU	N-CA-C	5.92	117.41	111.07
1	Ad	408	GLU	N-CA-C	5.90	117.38	111.07
1	Ay	408	GLU	N-CA-C	5.90	117.38	111.07
1	Ar	365	LEU	CA-C-O	-5.90	115.38	121.87
1	Bm	408	GLU	N-CA-C	5.90	117.38	111.07
1	Bf	408	GLU	N-CA-C	5.89	117.37	111.07
1	Ar	408	GLU	N-CA-C	5.88	117.36	111.07
1	Bf	365	LEU	CA-C-O	-5.88	115.41	121.87
1	Ad	365	LEU	CA-C-O	-5.87	115.41	121.87
1	Ak	365	LEU	CA-C-O	-5.87	115.42	121.87
1	Bt	365	LEU	CA-C-O	-5.86	115.42	121.87
1	Bm	365	LEU	CA-C-O	-5.86	115.43	121.87
2	Am	3	ILE	CB-CA-C	5.84	120.04	110.69
2	Ba	3	ILE	CB-CA-C	5.84	120.04	110.69
2	Af	3	ILE	CB-CA-C	5.84	120.04	110.69
1	Ay	365	LEU	CA-C-O	-5.84	115.44	121.87
2	Bh	3	ILE	CB-CA-C	5.84	120.03	110.69
2	At	3	ILE	CB-CA-C	5.83	120.02	110.69
2	Bv	3	ILE	CB-CA-C	5.83	120.02	110.69
2	Bo	3	ILE	CB-CA-C	5.83	120.02	110.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Al	496	PRO	N-CA-C	5.82	120.46	111.21
2	Am	93	ALA	N-CA-C	5.81	117.37	108.42
2	Bo	93	ALA	N-CA-C	5.81	117.37	108.42
1	Bg	496	PRO	N-CA-C	5.81	120.44	111.21
1	Az	496	PRO	N-CA-C	5.80	120.44	111.21
1	Bu	496	PRO	N-CA-C	5.80	120.44	111.21
1	Ae	496	PRO	N-CA-C	5.80	120.43	111.21
1	As	496	PRO	N-CA-C	5.80	120.43	111.21
1	Bg	495	ASP	CB-CA-C	5.79	118.47	108.91
1	Bu	495	ASP	CB-CA-C	5.79	118.47	108.91
2	At	93	ALA	N-CA-C	5.79	117.33	108.42
2	Af	93	ALA	N-CA-C	5.79	117.33	108.42
1	Al	495	ASP	CB-CA-C	5.77	118.44	108.91
1	Bn	496	PRO	N-CA-C	5.77	120.39	111.21
1	Ae	495	ASP	CB-CA-C	5.77	118.43	108.91
1	Az	495	ASP	CB-CA-C	5.77	118.43	108.91
2	Bh	93	ALA	N-CA-C	5.77	117.31	108.42
2	Bv	93	ALA	N-CA-C	5.77	117.31	108.42
2	Am	94	ILE	O-C-N	-5.77	117.18	123.18
1	As	495	ASP	CB-CA-C	5.76	118.41	108.91
2	Ba	93	ALA	N-CA-C	5.76	117.29	108.42
2	Ba	94	ILE	O-C-N	-5.75	117.20	123.18
1	Bn	495	ASP	CB-CA-C	5.75	118.39	108.91
2	Af	94	ILE	O-C-N	-5.73	117.22	123.18
2	Bo	94	ILE	O-C-N	-5.73	117.22	123.18
2	At	94	ILE	O-C-N	-5.71	117.24	123.18
2	Bh	94	ILE	O-C-N	-5.71	117.25	123.18
1	Ak	399	ALA	N-CA-CB	5.70	118.50	110.12
1	Bt	399	ALA	N-CA-CB	5.70	118.49	110.12
2	Bv	94	ILE	O-C-N	-5.69	117.26	123.18
1	Ad	399	ALA	N-CA-CB	5.68	118.47	110.12
1	Ar	399	ALA	N-CA-CB	5.68	118.47	110.12
1	Ak	218	PRO	N-CA-C	5.67	120.09	111.19
1	Ay	399	ALA	N-CA-CB	5.67	118.45	110.12
1	Bt	218	PRO	N-CA-C	5.66	120.08	111.19
1	Ar	218	PRO	N-CA-C	5.66	120.08	111.19
1	Bf	399	ALA	N-CA-CB	5.66	118.44	110.12
1	Bm	399	ALA	N-CA-CB	5.66	118.44	110.12
1	Bm	218	PRO	N-CA-C	5.65	120.06	111.19
1	Ad	218	PRO	N-CA-C	5.65	120.06	111.19
1	Ay	218	PRO	N-CA-C	5.64	120.05	111.19
1	Bf	218	PRO	N-CA-C	5.64	120.05	111.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bt	139	SER	N-CA-C	-5.63	105.62	112.88
1	Ar	139	SER	N-CA-C	-5.62	105.62	112.88
1	Ay	139	SER	N-CA-C	-5.62	105.63	112.88
1	Ak	139	SER	N-CA-C	-5.61	105.64	112.88
1	Ad	139	SER	N-CA-C	-5.60	105.65	112.88
1	Ak	366	GLN	CB-CA-C	-5.60	99.27	110.42
1	Bf	366	GLN	CB-CA-C	-5.59	99.29	110.42
1	Bt	366	GLN	CB-CA-C	-5.59	99.30	110.42
1	Ad	366	GLN	CB-CA-C	-5.59	99.30	110.42
1	Ay	366	GLN	CB-CA-C	-5.58	99.31	110.42
1	Bf	139	SER	N-CA-C	-5.58	105.68	112.88
1	Bm	139	SER	N-CA-C	-5.57	105.69	112.88
1	Ar	366	GLN	CB-CA-C	-5.57	99.34	110.42
1	Az	442	VAL	N-CA-C	-5.57	105.08	110.42
1	Bm	366	GLN	CB-CA-C	-5.57	99.34	110.42
1	Bu	442	VAL	N-CA-C	-5.55	105.09	110.42
1	Bg	442	VAL	N-CA-C	-5.54	105.10	110.42
1	As	442	VAL	N-CA-C	-5.53	105.11	110.42
1	Ae	442	VAL	N-CA-C	-5.52	105.12	110.42
1	Bn	442	VAL	N-CA-C	-5.51	105.13	110.42
1	Bm	494	LEU	N-CA-C	5.47	117.88	109.07
1	Ar	494	LEU	N-CA-C	5.47	117.87	109.07
1	Al	442	VAL	N-CA-C	-5.47	105.17	110.42
1	Ay	494	LEU	N-CA-C	5.47	117.87	109.07
1	Ak	157	THR	N-CA-C	5.46	117.99	111.71
1	Ak	494	LEU	N-CA-C	5.46	117.86	109.07
1	Ad	494	LEU	N-CA-C	5.46	117.86	109.07
1	Bt	494	LEU	N-CA-C	5.45	117.85	109.07
1	Bf	92	ALA	N-CA-C	-5.45	105.24	111.07
1	Bf	494	LEU	N-CA-C	5.45	117.84	109.07
1	Bm	157	THR	N-CA-C	5.45	117.97	111.71
1	Bm	92	ALA	N-CA-C	-5.44	105.25	111.07
1	Bu	459	GLY	N-CA-C	-5.43	107.17	115.00
1	Ad	157	THR	N-CA-C	5.43	117.96	111.71
1	Ar	157	THR	N-CA-C	5.43	117.95	111.71
1	Ad	92	ALA	N-CA-C	-5.42	105.27	111.07
1	Ay	92	ALA	N-CA-C	-5.42	105.27	111.07
1	Ay	157	THR	N-CA-C	5.42	117.94	111.71
1	Ak	92	ALA	N-CA-C	-5.41	105.28	111.07
1	Al	459	GLY	N-CA-C	-5.41	107.20	115.00
1	Ae	459	GLY	N-CA-C	-5.41	107.21	115.00
1	Bf	157	THR	N-CA-C	5.41	117.93	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bt	143	ALA	N-CA-C	-5.41	105.46	111.36
1	As	459	GLY	N-CA-C	-5.41	107.21	115.00
1	Bg	459	GLY	N-CA-C	-5.40	107.22	115.00
1	Bt	157	THR	N-CA-C	5.40	117.92	111.71
1	Bf	143	ALA	N-CA-C	-5.40	105.47	111.36
1	Bt	92	ALA	N-CA-C	-5.40	105.29	111.07
1	Bm	143	ALA	N-CA-C	-5.40	105.48	111.36
1	Ad	143	ALA	N-CA-C	-5.40	105.48	111.36
1	Bn	459	GLY	N-CA-C	-5.39	107.23	115.00
1	Ar	92	ALA	N-CA-C	-5.39	105.30	111.07
1	Az	459	GLY	N-CA-C	-5.39	107.24	115.00
1	Ar	143	ALA	N-CA-C	-5.39	105.49	111.36
1	Ay	143	ALA	N-CA-C	-5.39	105.49	111.36
1	Ak	143	ALA	N-CA-C	-5.37	105.50	111.36
1	Az	182	GLY	N-CA-C	5.37	119.05	111.42
1	Bn	182	GLY	N-CA-C	5.37	119.04	111.42
1	Ae	182	GLY	N-CA-C	5.36	119.03	111.42
1	Al	182	GLY	N-CA-C	5.36	119.03	111.42
1	Bg	182	GLY	N-CA-C	5.35	119.02	111.42
1	Bu	182	GLY	N-CA-C	5.35	119.02	111.42
1	As	182	GLY	N-CA-C	5.33	118.99	111.42
1	Bn	427	ALA	N-CA-C	5.33	117.78	111.33
1	Al	427	ALA	N-CA-C	5.32	117.77	111.33
1	Az	427	ALA	N-CA-C	5.32	117.77	111.33
1	Az	217	SER	CB-CA-C	-5.32	106.37	111.00
1	Bf	271	VAL	CA-C-O	-5.32	115.42	120.95
1	Ae	427	ALA	N-CA-C	5.31	117.75	111.33
1	Bg	427	ALA	N-CA-C	5.31	117.75	111.33
1	Ar	271	VAL	CA-C-O	-5.30	115.43	120.95
1	As	427	ALA	N-CA-C	5.30	117.74	111.33
1	Bn	217	SER	CB-CA-C	-5.30	106.39	111.00
1	Bm	397	GLU	N-CA-C	5.29	117.48	111.02
1	Bu	42	LYS	N-CA-C	-5.29	101.07	109.59
1	Az	42	LYS	N-CA-C	-5.29	101.07	109.59
1	Bm	271	VAL	CA-C-O	-5.29	115.45	120.95
1	Ad	271	VAL	CA-C-O	-5.29	115.45	120.95
1	Al	42	LYS	N-CA-C	-5.29	101.08	109.59
1	Ak	397	GLU	N-CA-C	5.29	117.47	111.02
1	Bu	427	ALA	N-CA-C	5.29	117.73	111.33
1	Ay	271	VAL	CA-C-O	-5.28	115.45	120.95
1	Bn	42	LYS	N-CA-C	-5.28	101.08	109.59
1	Ae	42	LYS	N-CA-C	-5.28	101.09	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bt	397	GLU	N-CA-C	5.28	117.46	111.02
1	Ar	485	TYR	CB-CA-C	-5.28	100.59	109.72
1	Bt	271	VAL	CA-C-O	-5.28	115.46	120.95
1	Ay	485	TYR	CB-CA-C	-5.27	100.60	109.72
1	Ay	397	GLU	N-CA-C	5.27	117.45	111.02
1	Bf	397	GLU	N-CA-C	5.27	117.45	111.02
1	Bg	42	LYS	N-CA-C	-5.27	101.11	109.59
1	Bt	51	LYS	N-CA-C	-5.27	106.44	112.92
1	Ad	397	GLU	N-CA-C	5.26	117.44	111.02
1	Bt	485	TYR	CB-CA-C	-5.26	100.61	109.72
1	Ad	485	TYR	CB-CA-C	-5.26	100.62	109.72
1	Bm	51	LYS	N-CA-C	-5.26	106.45	112.92
1	Ak	485	TYR	CB-CA-C	-5.26	100.62	109.72
1	Bf	485	TYR	CB-CA-C	-5.26	100.62	109.72
1	Ay	51	LYS	N-CA-C	-5.25	106.46	112.92
1	Bm	485	TYR	CB-CA-C	-5.25	100.63	109.72
1	Ae	217	SER	CB-CA-C	-5.25	106.43	111.00
1	Ar	397	GLU	N-CA-C	5.25	117.43	111.02
1	As	42	LYS	N-CA-C	-5.25	101.13	109.59
1	Ak	271	VAL	CA-C-O	-5.25	115.49	120.95
1	Ay	515	ILE	N-CA-C	5.24	115.96	110.62
1	Bm	515	ILE	N-CA-C	5.24	115.96	110.62
1	Ad	51	LYS	N-CA-C	-5.24	106.48	112.92
1	Bf	51	LYS	N-CA-C	-5.23	106.48	112.92
1	Al	217	SER	CB-CA-C	-5.23	106.45	111.00
1	Ak	515	ILE	N-CA-C	5.23	115.95	110.62
1	Ar	515	ILE	N-CA-C	5.23	115.95	110.62
1	Bu	217	SER	CB-CA-C	-5.22	106.45	111.00
1	Bg	217	SER	CB-CA-C	-5.22	106.46	111.00
1	Ak	51	LYS	N-CA-C	-5.22	106.50	112.92
1	Ar	51	LYS	N-CA-C	-5.22	106.50	112.92
1	As	217	SER	CB-CA-C	-5.21	106.46	111.00
1	Ad	515	ILE	N-CA-C	5.20	115.93	110.62
1	Bt	515	ILE	N-CA-C	5.20	115.92	110.62
1	Ay	17	LEU	N-CA-C	-5.19	105.62	111.28
1	Ak	387	VAL	N-CA-C	5.19	115.81	110.36
1	Bt	387	VAL	N-CA-C	5.19	115.81	110.36
1	Bf	387	VAL	N-CA-C	5.18	115.80	110.36
1	Ad	387	VAL	N-CA-C	5.18	115.80	110.36
1	Bg	428	ASP	CB-CA-C	-5.18	99.61	110.17
2	Bo	40	VAL	N-CA-C	5.17	115.77	109.30
1	Ak	17	LEU	N-CA-C	-5.17	105.64	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Az	428	ASP	CB-CA-C	-5.17	99.62	110.17
1	Bt	84	ALA	N-CA-CB	5.17	117.46	109.91
1	Bu	428	ASP	CB-CA-C	-5.17	99.63	110.17
1	Ad	17	LEU	N-CA-C	-5.16	105.65	111.28
1	Ae	428	ASP	CB-CA-C	-5.16	99.64	110.17
1	As	428	ASP	CB-CA-C	-5.16	99.64	110.17
1	Bf	515	ILE	N-CA-C	5.16	115.89	110.62
1	Bt	17	LEU	N-CA-C	-5.16	105.65	111.28
1	Bn	428	ASP	CB-CA-C	-5.16	99.64	110.17
1	Ak	84	ALA	N-CA-CB	5.16	117.44	109.91
1	Bm	84	ALA	N-CA-CB	5.16	117.44	109.91
1	Ar	17	LEU	N-CA-C	-5.15	105.66	111.28
1	Ay	387	VAL	N-CA-C	5.15	115.77	110.36
2	Bv	40	VAL	N-CA-C	5.15	115.74	109.30
2	Af	40	VAL	N-CA-C	5.15	115.74	109.30
1	Al	428	ASP	CB-CA-C	-5.15	99.67	110.17
1	Ar	387	VAL	N-CA-C	5.15	115.77	110.36
1	Ad	84	ALA	N-CA-CB	5.15	117.42	109.91
1	Ar	84	ALA	N-CA-CB	5.14	117.42	109.91
1	Ay	84	ALA	N-CA-CB	5.14	117.42	109.91
1	Bm	387	VAL	N-CA-C	5.14	115.76	110.36
2	At	40	VAL	N-CA-C	5.14	115.72	109.30
1	Bf	84	ALA	N-CA-CB	5.14	117.41	109.91
2	Bh	40	VAL	N-CA-C	5.14	115.72	109.30
2	Am	40	VAL	N-CA-C	5.14	115.72	109.30
1	Bm	17	LEU	N-CA-C	-5.13	105.69	111.28
2	Ba	40	VAL	N-CA-C	5.13	115.71	109.30
1	Bf	17	LEU	N-CA-C	-5.12	105.70	111.28
1	Bf	158	VAL	N-CA-C	-5.10	105.42	110.62
1	Ar	158	VAL	N-CA-C	-5.09	105.43	110.62
1	Bm	42	LYS	N-CA-C	-5.08	102.97	110.48
1	Az	278	ALA	N-CA-C	5.07	116.08	109.64
1	Bt	158	VAL	N-CA-C	-5.07	105.45	110.62
1	Ak	42	LYS	N-CA-C	-5.07	102.98	110.48
1	Al	278	ALA	N-CA-C	5.07	116.08	109.64
1	Ad	42	LYS	N-CA-C	-5.07	102.98	110.48
1	Ad	158	VAL	N-CA-C	-5.06	105.46	110.62
1	Ar	42	LYS	N-CA-C	-5.06	103.00	110.48
1	Ay	158	VAL	N-CA-C	-5.06	105.46	110.62
1	Ak	158	VAL	N-CA-C	-5.05	105.47	110.62
1	Bt	42	LYS	N-CA-C	-5.05	103.01	110.48
1	Ay	42	LYS	N-CA-C	-5.05	103.01	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bm	158	VAL	N-CA-C	-5.04	105.47	110.62
1	Bf	42	LYS	N-CA-C	-5.04	103.02	110.48
1	Bg	278	ALA	N-CA-C	5.04	116.04	109.64
1	Ae	278	ALA	N-CA-C	5.04	116.04	109.64
1	Al	233	MET	N-CA-C	5.03	116.85	111.36
1	Bg	233	MET	N-CA-C	5.03	116.84	111.36
1	Bm	217	SER	CA-C-O	-5.03	117.00	120.47
1	Bu	233	MET	N-CA-C	5.03	116.84	111.36
1	Bu	278	ALA	N-CA-C	5.02	116.02	109.64
1	Ae	233	MET	N-CA-C	5.01	116.82	111.36
1	Bn	233	MET	N-CA-C	5.01	116.82	111.36
1	Bf	217	SER	CA-C-O	-5.01	117.01	120.47
1	As	233	MET	N-CA-C	5.01	116.82	111.36
1	Az	233	MET	N-CA-C	5.00	116.81	111.36
1	Ad	217	SER	CA-C-O	-5.00	117.02	120.47
1	Ak	217	SER	CA-C-O	-5.00	117.02	120.47
1	As	278	ALA	N-CA-C	5.00	115.99	109.64

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Ad	136	VAL	Mainchain
1	Ae	268	ARG	Sidechain
2	Af	1	MET	Peptide
2	Af	4	ARG	Sidechain
1	Ak	136	VAL	Mainchain
1	Al	268	ARG	Sidechain
2	Am	1	MET	Peptide
2	Am	4	ARG	Sidechain
1	Ar	136	VAL	Mainchain
1	As	268	ARG	Sidechain
2	At	1	MET	Peptide
2	At	4	ARG	Sidechain
1	Ay	136	VAL	Mainchain
1	Az	268	ARG	Sidechain
2	Ba	1	MET	Peptide
2	Ba	4	ARG	Sidechain
1	Bf	136	VAL	Mainchain
1	Bg	268	ARG	Sidechain
2	Bh	1	MET	Peptide
2	Bh	4	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	Bm	136	VAL	Mainchain
1	Bn	268	ARG	Sidechain
2	Bo	1	MET	Peptide
2	Bo	4	ARG	Sidechain
1	Bt	136	VAL	Mainchain
1	Bu	268	ARG	Sidechain
2	Bv	1	MET	Peptide
2	Bv	4	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ad	3856	0	3976	332	0
1	Ae	3856	0	3976	236	0
1	Ak	3856	0	3976	331	0
1	Al	3856	0	3976	234	0
1	Ar	3856	0	3976	329	0
1	As	3856	0	3976	232	0
1	Ay	3856	0	3976	330	0
1	Az	3856	0	3976	229	0
1	Bf	3856	0	3976	324	0
1	Bg	3856	0	3976	226	0
1	Bm	3856	0	3976	334	0
1	Bn	3856	0	3976	230	0
1	Bt	3856	0	3976	334	0
1	Bu	3856	0	3976	231	0
2	Af	728	0	762	22	0
2	Am	728	0	762	21	0
2	At	728	0	762	23	0
2	Ba	728	0	762	25	0
2	Bh	728	0	762	25	0
2	Bo	728	0	762	23	0
2	Bv	728	0	762	26	0
3	Ad	27	0	11	0	0
3	Ae	27	0	11	0	0
3	Ak	27	0	11	0	0
3	Al	27	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ar	27	0	11	0	0
3	As	27	0	11	0	0
3	Ay	27	0	11	0	0
3	Az	27	0	11	0	0
3	Bf	27	0	11	0	0
3	Bg	27	0	11	0	0
3	Bm	27	0	11	0	0
3	Bn	27	0	11	0	0
3	Bt	27	0	11	0	0
3	Bu	27	0	11	0	0
4	Ad	1	0	0	0	0
4	Ae	1	0	0	0	0
4	Ak	1	0	0	0	0
4	Al	1	0	0	0	0
4	Ar	1	0	0	0	0
4	As	1	0	0	0	0
4	Ay	1	0	0	0	0
4	Az	1	0	0	0	0
4	Bf	1	0	0	0	0
4	Bg	1	0	0	0	0
4	Bm	1	0	0	0	0
4	Bn	1	0	0	0	0
4	Bt	1	0	0	0	0
4	Bu	1	0	0	0	0
5	Ad	2	0	0	1	0
5	Ak	2	0	0	1	0
5	Ar	2	0	0	1	0
5	Ay	2	0	0	1	0
5	Bf	2	0	0	1	0
5	Bm	2	0	0	1	0
5	Bt	2	0	0	1	0
All	All	59486	0	61152	3596	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (3596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:134:LEU:HD11	1:Bf:425:LYS:NZ	1.41	1.35
1:Ay:134:LEU:HD11	1:Ay:425:LYS:NZ	1.42	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:134:LEU:HD11	1:Ar:425:LYS:NZ	1.41	1.33
1:Bt:134:LEU:HD11	1:Bt:425:LYS:NZ	1.42	1.32
1:Bm:134:LEU:HD11	1:Bm:425:LYS:NZ	1.42	1.32
1:Ad:134:LEU:HD11	1:Ad:425:LYS:NZ	1.41	1.31
1:Ak:134:LEU:HD11	1:Ak:425:LYS:NZ	1.42	1.30
1:Ar:363:GLU:HA	1:Ar:366:GLN:NE2	1.47	1.29
1:Ad:363:GLU:HA	1:Ad:366:GLN:NE2	1.47	1.29
1:Bm:363:GLU:HA	1:Bm:366:GLN:NE2	1.47	1.29
1:Ak:363:GLU:HA	1:Ak:366:GLN:NE2	1.47	1.28
1:Ay:363:GLU:HA	1:Ay:366:GLN:NE2	1.47	1.28
1:Bf:363:GLU:HA	1:Bf:366:GLN:NE2	1.47	1.27
1:Bt:363:GLU:HA	1:Bt:366:GLN:NE2	1.47	1.27
1:Ay:36:ARG:NE	1:Bt:114:MET:HE2	1.47	1.26
1:Bm:363:GLU:CA	1:Bm:366:GLN:HE22	1.49	1.26
1:Ad:36:ARG:NE	1:Ak:114:MET:HE2	1.51	1.25
1:Bf:36:ARG:NE	1:Bm:114:MET:HE2	1.48	1.25
1:Ar:114:MET:HE2	1:Bm:36:ARG:NE	1.49	1.25
1:Bt:363:GLU:CA	1:Bt:366:GLN:HE22	1.49	1.25
1:Ad:114:MET:HE2	1:Ar:36:ARG:NE	1.49	1.25
1:Ay:489:ILE:HD13	1:Ay:494:LEU:CD2	1.67	1.25
1:Ak:489:ILE:HD13	1:Ak:494:LEU:CD2	1.67	1.25
1:Al:24:ALA:HB1	1:Al:97:GLN:OE1	1.37	1.25
1:Ar:363:GLU:CA	1:Ar:366:GLN:HE22	1.49	1.25
1:Ak:36:ARG:NE	1:Ay:114:MET:HE2	1.49	1.25
1:Bf:114:MET:HE2	1:Bt:36:ARG:NE	1.48	1.25
1:Bf:489:ILE:HD13	1:Bf:494:LEU:CD2	1.67	1.25
1:Bm:489:ILE:HD13	1:Bm:494:LEU:CD2	1.67	1.24
1:Ad:363:GLU:CA	1:Ad:366:GLN:HE22	1.49	1.24
1:Ak:363:GLU:CA	1:Ak:366:GLN:HE22	1.49	1.24
1:Bu:24:ALA:HB1	1:Bu:97:GLN:OE1	1.37	1.24
1:Ad:489:ILE:HD13	1:Ad:494:LEU:CD2	1.67	1.24
1:Al:54:VAL:HG11	1:Al:82:ASN:ND2	1.53	1.24
1:Ay:363:GLU:CA	1:Ay:366:GLN:HE22	1.49	1.24
1:Bf:363:GLU:CA	1:Bf:366:GLN:HE22	1.49	1.24
1:Ae:54:VAL:HG11	1:Ae:82:ASN:ND2	1.53	1.23
1:Ar:489:ILE:HD13	1:Ar:494:LEU:CD2	1.67	1.23
1:Bn:54:VAL:HG11	1:Bn:82:ASN:ND2	1.53	1.23
1:Bu:54:VAL:HG11	1:Bu:82:ASN:ND2	1.53	1.22
1:Bt:489:ILE:HD13	1:Bt:494:LEU:CD2	1.67	1.22
1:Az:24:ALA:HB1	1:Az:97:GLN:OE1	1.37	1.21
1:As:24:ALA:HB1	1:As:97:GLN:OE1	1.37	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:54:VAL:HG11	1:Az:82:ASN:ND2	1.53	1.21
1:As:54:VAL:HG11	1:As:82:ASN:ND2	1.53	1.20
1:Bn:24:ALA:HB1	1:Bn:97:GLN:OE1	1.37	1.20
1:Ae:24:ALA:HB1	1:Ae:97:GLN:OE1	1.37	1.20
1:Bg:54:VAL:HG11	1:Bg:82:ASN:ND2	1.53	1.19
1:Bn:482:THR:OG1	1:Bn:484:GLU:HG2	1.42	1.19
1:As:482:THR:OG1	1:As:484:GLU:HG2	1.42	1.19
1:Ae:518:GLU:OE1	1:Al:37:ASN:N	1.76	1.18
1:Bg:482:THR:OG1	1:Bg:484:GLU:HG2	1.42	1.18
1:Bg:34:LYS:NZ	1:Bg:483:GLU:OE2	1.77	1.18
1:Bg:24:ALA:HB1	1:Bg:97:GLN:OE1	1.37	1.18
1:Az:482:THR:OG1	1:Az:484:GLU:HG2	1.42	1.18
1:Bn:34:LYS:NZ	1:Bn:483:GLU:OE2	1.77	1.18
1:As:37:ASN:N	1:Bn:518:GLU:OE1	1.77	1.17
1:Ae:482:THR:OG1	1:Ae:484:GLU:HG2	1.42	1.17
1:Al:518:GLU:OE1	1:Az:37:ASN:N	1.77	1.17
1:Az:34:LYS:NZ	1:Az:483:GLU:OE2	1.77	1.17
1:Az:518:GLU:OE1	1:Bu:37:ASN:N	1.77	1.17
1:Bg:37:ASN:N	1:Bu:518:GLU:OE1	1.77	1.17
1:Bg:518:GLU:OE1	1:Bn:37:ASN:N	1.78	1.16
1:Al:34:LYS:NZ	1:Al:483:GLU:OE2	1.77	1.16
1:As:34:LYS:NZ	1:As:483:GLU:OE2	1.77	1.16
1:Bu:482:THR:OG1	1:Bu:484:GLU:HG2	1.42	1.16
1:Bu:34:LYS:NZ	1:Bu:483:GLU:OE2	1.77	1.16
1:Ae:34:LYS:NZ	1:Ae:483:GLU:OE2	1.76	1.15
1:Ae:37:ASN:N	1:As:518:GLU:OE1	1.78	1.15
1:Al:482:THR:OG1	1:Al:484:GLU:HG2	1.42	1.14
1:Bt:368:ARG:O	1:Bt:372:LEU:HD23	1.48	1.14
1:Bm:368:ARG:O	1:Bm:372:LEU:HD23	1.48	1.13
1:Ad:368:ARG:O	1:Ad:372:LEU:HD23	1.48	1.13
1:Al:24:ALA:CB	1:Al:97:GLN:OE1	1.97	1.12
1:Az:24:ALA:CB	1:Az:97:GLN:OE1	1.97	1.12
1:Bu:24:ALA:CB	1:Bu:97:GLN:OE1	1.97	1.12
1:Ay:134:LEU:CD1	1:Ay:425:LYS:HZ2	1.62	1.12
1:Ay:368:ARG:O	1:Ay:372:LEU:HD23	1.48	1.12
1:Bm:134:LEU:CD1	1:Bm:425:LYS:HZ2	1.61	1.12
1:Bf:368:ARG:O	1:Bf:372:LEU:HD23	1.48	1.12
1:Ae:24:ALA:CB	1:Ae:97:GLN:OE1	1.97	1.11
1:Bg:24:ALA:CB	1:Bg:97:GLN:OE1	1.97	1.11
1:Ak:368:ARG:O	1:Ak:372:LEU:HD23	1.48	1.11
1:Bf:489:ILE:CD1	1:Bf:494:LEU:CD2	2.28	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:489:ILE:CD1	1:Ay:494:LEU:CD2	2.28	1.11
1:Ak:489:ILE:CD1	1:Ak:494:LEU:CD2	2.28	1.10
1:Bn:24:ALA:CB	1:Bn:97:GLN:OE1	1.97	1.10
1:Bt:489:ILE:CD1	1:Bt:494:LEU:CD2	2.28	1.10
1:Ad:489:ILE:CD1	1:Ad:494:LEU:CD2	2.28	1.10
1:Ar:489:ILE:CD1	1:Ar:494:LEU:CD2	2.28	1.10
1:As:24:ALA:CB	1:As:97:GLN:OE1	1.97	1.10
1:Ar:368:ARG:O	1:Ar:372:LEU:HD23	1.48	1.10
1:Bm:489:ILE:CD1	1:Bm:494:LEU:CD2	2.28	1.10
1:Ad:49:ILE:HD11	1:Ak:73:MET:CE	1.83	1.09
1:Al:3:ALA:C	1:Al:524:LEU:HD13	1.78	1.09
1:Az:3:ALA:C	1:Az:524:LEU:HD13	1.78	1.09
1:Ak:420:ILE:HD12	1:Ak:451:LEU:HD13	1.35	1.09
1:Bf:489:ILE:HD13	1:Bf:494:LEU:HD23	1.35	1.09
1:Ad:525:PRO:OXT	1:Ad:525:PRO:O	1.71	1.09
1:Ar:525:PRO:OXT	1:Ar:525:PRO:O	1.71	1.09
1:Ay:489:ILE:HD13	1:Ay:494:LEU:HD23	1.35	1.09
1:Ad:420:ILE:HD12	1:Ad:451:LEU:HD13	1.35	1.09
1:As:3:ALA:C	1:As:524:LEU:HD13	1.78	1.09
1:Bf:134:LEU:CD1	1:Bf:425:LYS:NZ	2.16	1.09
1:Bt:134:LEU:CD1	1:Bt:425:LYS:NZ	2.16	1.09
1:Ay:36:ARG:HE	1:Bt:114:MET:CE	1.65	1.08
1:Bm:134:LEU:CD1	1:Bm:425:LYS:NZ	2.16	1.08
1:Ak:284:ARG:NE	1:Ak:364:LYS:HG2	1.69	1.08
1:Ak:525:PRO:OXT	1:Ak:525:PRO:O	1.71	1.08
1:Bm:525:PRO:OXT	1:Bm:525:PRO:O	1.71	1.08
1:Ad:284:ARG:NE	1:Ad:364:LYS:HG2	1.69	1.08
1:Ay:420:ILE:HD12	1:Ay:451:LEU:HD13	1.35	1.08
1:Ae:3:ALA:C	1:Ae:524:LEU:HD13	1.78	1.08
1:Bg:3:ALA:C	1:Bg:524:LEU:HD13	1.78	1.08
1:Bt:284:ARG:NE	1:Bt:364:LYS:HG2	1.69	1.08
1:Ad:134:LEU:CD1	1:Ad:425:LYS:NZ	2.16	1.07
1:Bt:510:VAL:O	1:Bt:514:MET:HG2	1.54	1.07
1:Bu:3:ALA:C	1:Bu:524:LEU:HD13	1.78	1.07
1:Bm:284:ARG:NE	1:Bm:364:LYS:HG2	1.69	1.07
1:Ak:134:LEU:CD1	1:Ak:425:LYS:NZ	2.16	1.07
1:Ar:284:ARG:NE	1:Ar:364:LYS:HG2	1.69	1.07
1:Ar:420:ILE:HD12	1:Ar:451:LEU:HD13	1.35	1.07
1:Ar:489:ILE:HD13	1:Ar:494:LEU:HD23	1.35	1.07
1:Bf:114:MET:CE	1:Bt:36:ARG:HE	1.66	1.07
1:Bf:525:PRO:OXT	1:Bf:525:PRO:O	1.71	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bn:3:ALA:C	1:Bn:524:LEU:HD13	1.78	1.07
1:Ak:36:ARG:HE	1:Ay:114:MET:CE	1.67	1.06
1:Bf:510:VAL:O	1:Bf:514:MET:HG2	1.54	1.06
1:Al:7:LYS:HG3	1:Al:66:PHE:CZ	1.90	1.06
1:Ar:134:LEU:CD1	1:Ar:425:LYS:NZ	2.16	1.06
1:Ay:284:ARG:NE	1:Ay:364:LYS:HG2	1.69	1.06
1:Ay:525:PRO:OXT	1:Ay:525:PRO:O	1.71	1.06
1:Bf:36:ARG:HE	1:Bm:114:MET:CE	1.66	1.06
1:Bt:525:PRO:O	1:Bt:525:PRO:OXT	1.71	1.06
1:Ad:489:ILE:HD13	1:Ad:494:LEU:HD23	1.35	1.06
1:Ae:7:LYS:HG3	1:Ae:66:PHE:CZ	1.90	1.06
1:Ad:36:ARG:HE	1:Ak:114:MET:CE	1.68	1.06
1:As:7:LYS:HG3	1:As:66:PHE:CZ	1.90	1.06
1:Ay:510:VAL:O	1:Ay:514:MET:HG2	1.54	1.06
1:Bf:134:LEU:CD1	1:Bf:425:LYS:HZ2	1.66	1.06
1:Bg:7:LYS:HG3	1:Bg:66:PHE:CZ	1.90	1.05
1:Bm:510:VAL:O	1:Bm:514:MET:HG2	1.54	1.05
1:Bn:7:LYS:HG3	1:Bn:66:PHE:CZ	1.90	1.05
1:Az:7:LYS:HG3	1:Az:66:PHE:CZ	1.90	1.05
1:Bt:420:ILE:HD12	1:Bt:451:LEU:HD13	1.35	1.05
1:Ad:510:VAL:O	1:Ad:514:MET:HG2	1.53	1.05
1:Ar:6:VAL:HG22	1:Ar:521:VAL:HG13	1.37	1.05
1:Ar:73:MET:CE	1:Bm:49:ILE:HD11	1.87	1.05
1:Ar:114:MET:CE	1:Bm:36:ARG:HE	1.67	1.05
1:Bf:284:ARG:NE	1:Bf:364:LYS:HG2	1.69	1.05
1:Bu:7:LYS:HG3	1:Bu:66:PHE:CZ	1.90	1.05
1:Ak:489:ILE:HD13	1:Ak:494:LEU:HD23	1.35	1.05
1:Ad:114:MET:CE	1:Ar:36:ARG:HE	1.68	1.05
1:Ae:34:LYS:NZ	1:Ae:483:GLU:CD	2.15	1.05
1:Ak:510:VAL:O	1:Ak:514:MET:HG2	1.54	1.05
1:Ar:510:VAL:O	1:Ar:514:MET:HG2	1.54	1.05
1:Ay:134:LEU:CD1	1:Ay:425:LYS:NZ	2.16	1.05
1:Bf:73:MET:CE	1:Bt:49:ILE:HD11	1.86	1.05
1:Bm:6:VAL:HG22	1:Bm:521:VAL:HG13	1.37	1.05
1:As:34:LYS:NZ	1:As:483:GLU:CD	2.15	1.04
1:Ak:49:ILE:HD11	1:Ay:73:MET:CE	1.87	1.04
1:Bn:34:LYS:NZ	1:Bn:483:GLU:CD	2.15	1.04
1:Bf:49:ILE:HD11	1:Bm:73:MET:CE	1.87	1.04
1:Bt:489:ILE:HD13	1:Bt:494:LEU:HD23	1.35	1.04
1:Ay:134:LEU:HD11	1:Ay:425:LYS:HZ2	0.95	1.04
1:Bm:183:LEU:HG	1:Bm:384:ALA:HB2	1.39	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:420:ILE:HD12	1:Bm:451:LEU:HD13	1.35	1.04
1:Ae:54:VAL:HG21	1:Ae:82:ASN:HD22	1.22	1.04
1:Bf:183:LEU:HG	1:Bf:384:ALA:HB2	1.39	1.04
1:Ar:155:ASP:HB3	1:Ar:395:ARG:HH22	1.23	1.03
1:Az:34:LYS:NZ	1:Az:483:GLU:CD	2.15	1.03
1:Bg:34:LYS:NZ	1:Bg:483:GLU:CD	2.15	1.03
1:Bu:34:LYS:NZ	1:Bu:483:GLU:CD	2.15	1.03
1:Ad:49:ILE:CD1	1:Ak:73:MET:HE3	1.87	1.03
1:Al:34:LYS:NZ	1:Al:483:GLU:CD	2.15	1.03
1:As:54:VAL:HG21	1:As:82:ASN:HD22	1.22	1.03
1:Bf:420:ILE:HD12	1:Bf:451:LEU:HD13	1.35	1.03
1:Bm:489:ILE:HD13	1:Bm:494:LEU:HD23	1.35	1.03
1:Ad:73:MET:CE	1:Ar:49:ILE:HD11	1.88	1.03
1:Al:54:VAL:HG21	1:Al:82:ASN:HD22	1.22	1.03
1:Ay:49:ILE:HD11	1:Bt:73:MET:CE	1.89	1.02
1:Az:54:VAL:HG21	1:Az:82:ASN:HD22	1.22	1.02
1:Bf:6:VAL:HG22	1:Bf:521:VAL:HG13	1.37	1.02
1:Ak:183:LEU:HG	1:Ak:384:ALA:HB2	1.39	1.02
1:Bf:155:ASP:HB3	1:Bf:395:ARG:HH22	1.23	1.02
1:Bt:183:LEU:HG	1:Bt:384:ALA:HB2	1.39	1.02
1:Ae:524:LEU:CD1	1:Al:63:GLU:CD	2.29	1.02
1:Ad:6:VAL:HG22	1:Ad:521:VAL:HG13	1.37	1.02
1:Ak:36:ARG:HE	1:Ay:114:MET:HE2	0.85	1.02
1:Az:40:LEU:HB3	1:Az:59:GLU:OE1	1.60	1.02
1:Ad:114:MET:HE2	1:Ar:36:ARG:HE	0.86	1.02
1:Ak:155:ASP:HB3	1:Ak:395:ARG:HH22	1.23	1.02
1:Al:518:GLU:OE1	1:Az:36:ARG:C	1.98	1.01
1:Bg:488:MET:CE	1:Bg:491:MET:CE	2.38	1.01
1:Bg:518:GLU:OE1	1:Bn:36:ARG:C	1.98	1.01
1:Bn:40:LEU:HB3	1:Bn:59:GLU:OE1	1.60	1.01
1:Bu:488:MET:CE	1:Bu:491:MET:CE	2.38	1.01
1:Ae:488:MET:CE	1:Ae:491:MET:CE	2.38	1.01
1:Bg:54:VAL:HG21	1:Bg:82:ASN:HD22	1.22	1.01
1:Bn:54:VAL:HG21	1:Bn:82:ASN:HD22	1.22	1.01
1:Bt:6:VAL:HG22	1:Bt:521:VAL:HG13	1.37	1.01
1:As:36:ARG:C	1:Bn:518:GLU:OE1	1.98	1.01
1:Bm:155:ASP:HB3	1:Bm:395:ARG:HH22	1.23	1.01
1:Bt:155:ASP:HB3	1:Bt:395:ARG:HH22	1.23	1.01
1:Ad:134:LEU:CD1	1:Ad:425:LYS:HZ2	1.71	1.01
1:Ad:155:ASP:HB3	1:Ad:395:ARG:HH22	1.23	1.01
1:Al:488:MET:CE	1:Al:491:MET:CE	2.38	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bn:488:MET:CE	1:Bn:491:MET:CE	2.38	1.01
1:Ae:518:GLU:OE1	1:Al:37:ASN:O	1.79	1.00
1:Ak:6:VAL:HG22	1:Ak:521:VAL:HG13	1.37	1.00
1:Ay:183:LEU:HG	1:Ay:384:ALA:HB2	1.39	1.00
1:Al:40:LEU:HB3	1:Al:59:GLU:OE1	1.60	1.00
1:As:40:LEU:HB3	1:As:59:GLU:OE1	1.60	1.00
1:As:488:MET:CE	1:As:491:MET:CE	2.38	1.00
1:Bf:114:MET:HE2	1:Bt:36:ARG:HE	0.84	1.00
1:Az:488:MET:CE	1:Az:491:MET:CE	2.38	1.00
1:Al:524:LEU:CD1	1:Az:63:GLU:CD	2.31	1.00
1:Ad:73:MET:HE3	1:Ar:49:ILE:HD11	1.01	1.00
1:Ae:63:GLU:CD	1:As:524:LEU:CD1	2.27	1.00
1:Bg:36:ARG:C	1:Bu:518:GLU:OE1	1.97	1.00
1:Ad:36:ARG:HE	1:Ak:114:MET:HE2	0.84	1.00
1:Ad:183:LEU:HG	1:Ad:384:ALA:HB2	1.39	1.00
1:Ak:49:ILE:HD11	1:Ay:73:MET:HE3	1.00	1.00
1:Ar:183:LEU:HG	1:Ar:384:ALA:HB2	1.39	1.00
1:Bf:49:ILE:HD11	1:Bm:73:MET:HE3	1.00	1.00
1:Ar:134:LEU:CD1	1:Ar:425:LYS:HZ2	1.72	0.99
1:Bt:134:LEU:CD1	1:Bt:425:LYS:HZ2	1.72	0.99
1:Ay:6:VAL:HG22	1:Ay:521:VAL:HG13	1.37	0.99
1:Ae:40:LEU:HB3	1:Ae:59:GLU:OE1	1.60	0.99
1:Ay:49:ILE:HD11	1:Bt:73:MET:HE3	1.02	0.99
1:Bn:34:LYS:HZ1	1:Bn:483:GLU:CD	1.69	0.99
1:Bu:40:LEU:HB3	1:Bu:59:GLU:OE1	1.60	0.99
1:Ar:114:MET:HE2	1:Bm:36:ARG:HE	0.84	0.99
1:Ar:73:MET:HE3	1:Bm:49:ILE:HD11	0.99	0.99
1:Ay:155:ASP:HB3	1:Ay:395:ARG:HH22	1.23	0.99
1:Ak:49:ILE:CD1	1:Ay:73:MET:HE3	1.93	0.99
1:Bf:49:ILE:CD1	1:Bm:73:MET:HE3	1.92	0.99
1:Ak:142:LYS:HG3	1:Ak:146:GLN:NE2	1.78	0.99
1:Ar:73:MET:HE3	1:Bm:49:ILE:CD1	1.92	0.99
1:Ae:36:ARG:C	1:As:518:GLU:OE1	1.98	0.98
1:Bf:73:MET:HE3	1:Bt:49:ILE:CD1	1.91	0.98
1:Bg:40:LEU:HB3	1:Bg:59:GLU:OE1	1.60	0.98
1:Bg:36:ARG:NE	1:Bu:113:PRO:HG2	1.78	0.98
1:Bt:142:LYS:HG3	1:Bt:146:GLN:NE2	1.78	0.98
1:Ad:73:MET:HE3	1:Ar:49:ILE:CD1	1.94	0.98
1:Ae:34:LYS:HZ1	1:Ae:483:GLU:CD	1.70	0.98
1:Al:518:GLU:OE1	1:Az:37:ASN:O	1.82	0.98
1:As:36:ARG:NE	1:Bn:113:PRO:HG2	1.79	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:524:LEU:CD1	1:Bu:63:GLU:CD	2.31	0.98
1:Bf:36:ARG:HE	1:Bm:114:MET:HE2	0.84	0.98
1:Bu:34:LYS:HZ1	1:Bu:483:GLU:CD	1.71	0.98
1:Ae:46:ALA:CB	1:As:76:GLU:OE2	2.11	0.98
1:Bf:73:MET:HE3	1:Bt:49:ILE:HD11	0.99	0.98
1:Bf:142:LYS:HG3	1:Bf:146:GLN:NE2	1.78	0.98
1:Bm:142:LYS:HG3	1:Bm:146:GLN:NE2	1.78	0.98
1:Ad:157:THR:O	1:Ad:161:LEU:HD13	1.64	0.98
1:Ay:157:THR:O	1:Ay:161:LEU:HD13	1.64	0.98
1:Bg:63:GLU:CD	1:Bu:524:LEU:CD1	2.29	0.98
1:Ae:46:ALA:HB1	1:As:76:GLU:OE2	1.64	0.98
1:Az:34:LYS:HZ1	1:Az:483:GLU:CD	1.70	0.98
1:Al:172:GLU:OE2	1:Al:369:VAL:CG1	2.12	0.98
1:Bu:54:VAL:HG21	1:Bu:82:ASN:HD22	1.22	0.98
1:Ae:37:ASN:O	1:As:518:GLU:OE1	1.81	0.98
1:As:172:GLU:OE2	1:As:369:VAL:CG1	2.12	0.98
1:Bn:172:GLU:OE2	1:Bn:369:VAL:CG1	2.12	0.98
1:Ae:172:GLU:OE2	1:Ae:369:VAL:CG1	2.12	0.98
1:Az:172:GLU:OE2	1:Az:369:VAL:CG1	2.12	0.98
1:Bg:172:GLU:OE2	1:Bg:369:VAL:CG1	2.12	0.98
1:Bm:134:LEU:HD11	1:Bm:425:LYS:HZ2	0.94	0.98
1:Bf:169:VAL:HG12	1:Bf:377:ALA:HB2	1.46	0.97
1:Bu:172:GLU:OE2	1:Bu:369:VAL:CG1	2.12	0.97
1:Ae:36:ARG:NE	1:As:113:PRO:HG2	1.79	0.97
1:Ae:113:PRO:HG2	1:Al:36:ARG:NE	1.79	0.97
1:Ay:36:ARG:HE	1:Bt:114:MET:HE2	0.83	0.97
1:Ak:400:LEU:O	1:Ak:404:ARG:HG2	1.65	0.97
1:Az:518:GLU:OE1	1:Bu:36:ARG:C	1.97	0.97
1:Bm:400:LEU:O	1:Bm:404:ARG:HG2	1.65	0.97
1:Ar:142:LYS:HG3	1:Ar:146:GLN:NE2	1.78	0.97
1:Ay:169:VAL:HG12	1:Ay:377:ALA:HB2	1.47	0.97
1:Bg:37:ASN:O	1:Bu:518:GLU:OE1	1.82	0.97
1:Bg:113:PRO:HG2	1:Bn:36:ARG:NE	1.77	0.97
1:Al:113:PRO:HG2	1:Az:36:ARG:NE	1.80	0.97
1:Al:34:LYS:HZ1	1:Al:483:GLU:CD	1.70	0.97
1:Bm:169:VAL:HG12	1:Bm:377:ALA:HB2	1.47	0.97
1:Bt:157:THR:O	1:Bt:161:LEU:HD13	1.64	0.97
1:Ad:142:LYS:HG3	1:Ad:146:GLN:NE2	1.78	0.97
1:Ak:134:LEU:CD1	1:Ak:425:LYS:HZ2	1.72	0.97
1:As:37:ASN:O	1:Bn:518:GLU:OE1	1.81	0.97
1:Ar:157:THR:O	1:Ar:161:LEU:HD13	1.64	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:169:VAL:HG12	1:Ak:377:ALA:HB2	1.46	0.97
1:Ay:142:LYS:HG3	1:Ay:146:GLN:NE2	1.78	0.97
1:Bg:518:GLU:OE1	1:Bn:37:ASN:O	1.83	0.97
1:Bf:400:LEU:O	1:Bf:404:ARG:HG2	1.65	0.97
1:Bt:169:VAL:HG12	1:Bt:377:ALA:HB2	1.46	0.97
1:Ad:36:ARG:CG	1:Ak:518:GLU:OE2	2.13	0.96
1:Ar:134:LEU:HD11	1:Ar:425:LYS:HZ1	1.28	0.96
1:Ar:400:LEU:O	1:Ar:404:ARG:HG2	1.65	0.96
1:Ak:157:THR:O	1:Ak:161:LEU:HD13	1.64	0.96
1:As:63:GLU:CD	1:Bn:524:LEU:CD1	2.30	0.96
1:Ay:400:LEU:O	1:Ay:404:ARG:HG2	1.65	0.96
1:Bg:524:LEU:CD1	1:Bn:63:GLU:CD	2.29	0.96
1:Bm:157:THR:O	1:Bm:161:LEU:HD13	1.64	0.96
1:Ak:489:ILE:CD1	1:Ak:494:LEU:HD21	1.95	0.96
1:Az:113:PRO:HG2	1:Bu:36:ARG:NE	1.79	0.96
1:Ak:194:GLN:O	1:Ak:371:LYS:NZ	1.98	0.96
1:Ay:194:GLN:O	1:Ay:371:LYS:NZ	1.98	0.96
1:Bf:157:THR:O	1:Bf:161:LEU:HD13	1.64	0.96
1:Ad:400:LEU:O	1:Ad:404:ARG:HG2	1.65	0.96
1:Ay:388:GLU:HA	1:Ay:391:GLU:CB	1.95	0.96
1:Bt:194:GLN:O	1:Bt:371:LYS:NZ	1.98	0.96
1:Ay:49:ILE:CD1	1:Bt:73:MET:HE3	1.94	0.96
1:Ad:169:VAL:HG12	1:Ad:377:ALA:HB2	1.46	0.96
1:Ad:194:GLN:O	1:Ad:371:LYS:NZ	1.98	0.96
1:Ar:169:VAL:HG12	1:Ar:377:ALA:HB2	1.47	0.96
1:Ar:388:GLU:HA	1:Ar:391:GLU:CB	1.96	0.96
1:Bf:194:GLN:O	1:Bf:371:LYS:NZ	1.98	0.96
1:Ak:388:GLU:HA	1:Ak:391:GLU:CB	1.95	0.96
1:Az:518:GLU:OE1	1:Bu:37:ASN:O	1.84	0.96
1:Ad:489:ILE:CD1	1:Ad:494:LEU:HD21	1.95	0.96
1:Ar:194:GLN:O	1:Ar:371:LYS:NZ	1.98	0.96
1:Bg:76:GLU:OE2	1:Bn:46:ALA:CB	2.14	0.96
1:Ae:518:GLU:OE1	1:Al:36:ARG:C	1.98	0.95
1:Ae:76:GLU:OE2	1:Al:46:ALA:CB	2.14	0.95
1:Bm:194:GLN:O	1:Bm:371:LYS:NZ	1.98	0.95
1:Bt:400:LEU:O	1:Bt:404:ARG:HG2	1.65	0.95
1:Ar:489:ILE:CD1	1:Ar:494:LEU:HD21	1.95	0.95
1:Bf:489:ILE:CD1	1:Bf:494:LEU:HD21	1.95	0.95
1:Bg:46:ALA:CB	1:Bu:76:GLU:OE2	2.14	0.95
1:Bm:388:GLU:HA	1:Bm:391:GLU:CB	1.96	0.95
1:Ad:466:ALA:O	1:Ad:470:LYS:HG3	1.66	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:63:GLU:CD	1:As:524:LEU:HD13	1.91	0.95
1:Ay:489:ILE:CD1	1:Ay:494:LEU:HD21	1.95	0.95
1:Ar:466:ALA:O	1:Ar:470:LYS:HG3	1.66	0.95
1:Bt:388:GLU:HA	1:Bt:391:GLU:CB	1.96	0.95
1:Ad:134:LEU:HD11	1:Ad:425:LYS:HZ1	1.30	0.95
1:Ad:388:GLU:HA	1:Ad:391:GLU:CB	1.95	0.95
1:Ay:466:ALA:O	1:Ay:470:LYS:HG3	1.66	0.95
1:Ak:466:ALA:O	1:Ak:470:LYS:HG3	1.66	0.94
1:Al:76:GLU:OE2	1:Az:46:ALA:CB	2.16	0.94
1:Bf:388:GLU:HA	1:Bf:391:GLU:CB	1.95	0.94
1:Bm:489:ILE:CD1	1:Bm:494:LEU:HD21	1.95	0.94
1:Bm:466:ALA:O	1:Bm:470:LYS:HG3	1.66	0.94
1:As:46:ALA:HB1	1:Bn:76:GLU:OE2	1.67	0.94
1:Ae:76:GLU:OE2	1:Al:46:ALA:HB1	1.68	0.94
1:As:46:ALA:CB	1:Bn:76:GLU:OE2	2.15	0.94
1:Bf:466:ALA:O	1:Bf:470:LYS:HG3	1.66	0.94
1:Bt:489:ILE:CD1	1:Bt:494:LEU:HD21	1.95	0.94
1:Ak:134:LEU:HD11	1:Ak:425:LYS:HZ1	1.28	0.94
1:Bf:518:GLU:OE2	1:Bt:36:ARG:CG	2.16	0.94
1:Bt:466:ALA:O	1:Bt:470:LYS:HG3	1.66	0.94
1:Al:488:MET:HE2	1:Al:491:MET:CE	1.98	0.94
1:Bf:36:ARG:CG	1:Bm:518:GLU:OE2	2.16	0.94
1:Ar:518:GLU:OE2	1:Bm:36:ARG:CG	2.16	0.93
1:Ad:518:GLU:OE2	1:Ar:36:ARG:CG	2.16	0.93
1:Az:76:GLU:OE2	1:Bu:46:ALA:CB	2.16	0.93
1:Ae:488:MET:HE2	1:Ae:491:MET:CE	1.98	0.93
1:Bg:63:GLU:CD	1:Bu:524:LEU:HD13	1.93	0.93
1:Bg:76:GLU:OE2	1:Bn:46:ALA:HB1	1.66	0.93
1:Ae:111:MET:HE3	1:Ae:438:VAL:HG21	1.50	0.93
1:Bg:46:ALA:HB1	1:Bu:76:GLU:OE2	1.67	0.93
1:Al:76:GLU:OE2	1:Az:46:ALA:HB1	1.69	0.93
1:Bn:488:MET:HE1	1:Bn:491:MET:CE	1.99	0.93
1:Ad:284:ARG:CZ	1:Ad:364:LYS:HG2	1.99	0.93
1:Ar:284:ARG:CZ	1:Ar:364:LYS:HG2	1.99	0.93
1:As:111:MET:HE3	1:As:438:VAL:HG21	1.50	0.93
1:Az:488:MET:HE1	1:Az:491:MET:CE	1.99	0.93
1:Ad:36:ARG:HG3	1:Ak:518:GLU:OE2	1.69	0.92
1:Al:111:MET:HE3	1:Al:438:VAL:HG21	1.50	0.92
1:Bn:111:MET:HE3	1:Bn:438:VAL:HG21	1.50	0.92
1:Bt:168:LYS:HE2	1:Bt:187:LEU:HD21	1.51	0.92
1:Bm:284:ARG:CZ	1:Bm:364:LYS:HG2	1.99	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:488:MET:HE1	1:Ae:491:MET:HE1	1.50	0.92
1:Ak:284:ARG:CZ	1:Ak:364:LYS:HG2	1.99	0.92
1:Ak:36:ARG:CG	1:Ay:518:GLU:OE2	2.17	0.92
1:Ae:488:MET:HE1	1:Ae:491:MET:CE	1.99	0.92
1:As:488:MET:HE1	1:As:491:MET:CE	1.99	0.92
1:Ay:168:LYS:HE2	1:Ay:187:LEU:HD21	1.51	0.92
1:Bn:488:MET:CE	1:Bn:491:MET:HE3	2.00	0.92
1:Al:488:MET:HE1	1:Al:491:MET:CE	1.99	0.92
1:Ay:284:ARG:CZ	1:Ay:364:LYS:HG2	1.99	0.92
1:Bf:168:LYS:HE2	1:Bf:187:LEU:HD21	1.51	0.92
1:Bu:488:MET:CE	1:Bu:491:MET:HE3	2.00	0.92
1:Bu:488:MET:HE1	1:Bu:491:MET:CE	1.99	0.92
1:Al:488:MET:HE1	1:Al:491:MET:HE1	1.50	0.91
1:Bg:488:MET:CE	1:Bg:491:MET:HE3	2.00	0.91
1:As:488:MET:HE1	1:As:491:MET:HE1	1.50	0.91
1:Bg:34:LYS:HZ1	1:Bg:483:GLU:CD	1.74	0.91
1:Bg:488:MET:HE1	1:Bg:491:MET:CE	1.99	0.91
1:Bg:524:LEU:HD13	1:Bn:63:GLU:CD	1.92	0.91
1:Bt:284:ARG:CZ	1:Bt:364:LYS:HG2	1.99	0.91
1:Bf:284:ARG:CZ	1:Bf:364:LYS:HG2	1.99	0.91
1:Az:111:MET:HE3	1:Az:438:VAL:HG21	1.50	0.91
1:Az:524:LEU:HD13	1:Bu:63:GLU:CD	1.94	0.91
1:Ae:524:LEU:HD13	1:Al:63:GLU:CD	1.96	0.91
1:Ar:489:ILE:HD13	1:Ar:494:LEU:HD21	1.52	0.91
1:Az:76:GLU:OE2	1:Bu:46:ALA:HB1	1.68	0.91
1:Bm:168:LYS:HE2	1:Bm:187:LEU:HD21	1.51	0.91
1:Ar:183:LEU:HG	1:Ar:384:ALA:CB	2.01	0.91
1:Bg:111:MET:HE3	1:Bg:438:VAL:HG21	1.50	0.91
1:Bg:488:MET:HE2	1:Bg:491:MET:CE	1.98	0.91
1:Az:488:MET:HE2	1:Az:491:MET:CE	1.98	0.91
1:Bn:488:MET:HE2	1:Bn:491:MET:CE	1.98	0.91
1:Bu:111:MET:HE3	1:Bu:438:VAL:HG21	1.50	0.91
1:As:488:MET:CE	1:As:491:MET:HE3	2.00	0.91
1:Bg:7:LYS:HD2	1:Bg:66:PHE:CE2	2.06	0.91
1:Ad:183:LEU:HG	1:Ad:384:ALA:CB	2.01	0.91
1:Al:488:MET:CE	1:Al:491:MET:HE3	2.00	0.91
1:Bm:183:LEU:HG	1:Bm:384:ALA:CB	2.01	0.91
1:Bu:488:MET:HE1	1:Bu:491:MET:HE1	1.50	0.91
1:Bu:488:MET:HE2	1:Bu:491:MET:CE	1.98	0.91
1:Ae:7:LYS:HD2	1:Ae:66:PHE:CE2	2.06	0.90
1:As:488:MET:HE2	1:As:491:MET:CE	1.98	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:7:LYS:HD2	1:As:66:PHE:CE2	2.06	0.90
1:Bg:488:MET:HE2	1:Bg:491:MET:HE3	1.53	0.90
1:Bn:488:MET:HE2	1:Bn:491:MET:HE3	1.53	0.90
1:Bt:134:LEU:HD11	1:Bt:425:LYS:HZ1	1.28	0.90
1:Ay:36:ARG:CG	1:Bt:518:GLU:OE2	2.18	0.90
1:Az:488:MET:CE	1:Az:491:MET:HE3	2.00	0.90
1:Bg:488:MET:HE1	1:Bg:491:MET:HE1	1.50	0.90
1:Ak:168:LYS:HE2	1:Ak:187:LEU:HD21	1.51	0.90
1:Bm:489:ILE:HD13	1:Bm:494:LEU:HD21	1.52	0.90
1:Ak:183:LEU:HG	1:Ak:384:ALA:CB	2.01	0.90
1:Bf:518:GLU:OE2	1:Bt:36:ARG:HG3	1.72	0.90
1:Bt:489:ILE:HD13	1:Bt:494:LEU:HD21	1.52	0.90
1:Bu:54:VAL:CG2	1:Bu:82:ASN:HD22	1.85	0.90
1:Ae:488:MET:CE	1:Ae:491:MET:HE3	2.00	0.90
1:Az:488:MET:HE1	1:Az:491:MET:HE1	1.50	0.90
1:Ad:168:LYS:HE2	1:Ad:187:LEU:HD21	1.51	0.90
1:Az:7:LYS:HD2	1:Az:66:PHE:CE2	2.06	0.90
1:Az:54:VAL:CG2	1:Az:82:ASN:HD22	1.85	0.90
1:Bf:36:ARG:HG3	1:Bm:518:GLU:OE2	1.72	0.90
1:Bf:183:LEU:HG	1:Bf:384:ALA:CB	2.01	0.90
1:Bg:54:VAL:CG2	1:Bg:82:ASN:HD22	1.85	0.90
1:Al:7:LYS:HD2	1:Al:66:PHE:CE2	2.06	0.89
1:Ar:168:LYS:HE2	1:Ar:187:LEU:HD21	1.51	0.89
1:As:63:GLU:CD	1:Bn:524:LEU:HD13	1.94	0.89
1:Bn:488:MET:HE1	1:Bn:491:MET:HE1	1.50	0.89
1:Bu:7:LYS:HD2	1:Bu:66:PHE:CE2	2.06	0.89
1:Bn:7:LYS:HD2	1:Bn:66:PHE:CE2	2.06	0.89
1:Bu:488:MET:HE2	1:Bu:491:MET:HE3	1.53	0.89
1:Ad:49:ILE:HD11	1:Ak:73:MET:HE3	0.95	0.89
1:Bt:183:LEU:HG	1:Bt:384:ALA:CB	2.01	0.89
1:Ar:518:GLU:OE2	1:Bm:36:ARG:HG3	1.72	0.89
1:Ae:54:VAL:CG2	1:Ae:82:ASN:HD22	1.85	0.89
1:As:487:ASN:OD1	1:As:489:ILE:HG13	1.73	0.89
1:Az:487:ASN:OD1	1:Az:489:ILE:HG13	1.73	0.89
1:Al:487:ASN:OD1	1:Al:489:ILE:HG13	1.73	0.89
1:Bn:54:VAL:CG2	1:Bn:82:ASN:HD22	1.85	0.89
1:Ae:517:THR:HG23	1:Al:39:VAL:HG23	1.52	0.89
1:Al:54:VAL:CG2	1:Al:82:ASN:HD22	1.85	0.89
1:Al:178:GLU:OE2	1:Al:380:LYS:HE3	1.73	0.89
1:Ay:363:GLU:HA	1:Ay:366:GLN:HE22	0.72	0.89
1:Bf:363:GLU:HA	1:Bf:366:GLN:HE22	0.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:487:ASN:OD1	1:Bu:489:ILE:HG13	1.73	0.89
1:Ak:134:LEU:HD11	1:Ak:425:LYS:HZ2	1.08	0.89
1:As:34:LYS:HZ1	1:As:483:GLU:CD	1.75	0.89
1:Az:178:GLU:OE2	1:Az:380:LYS:HE3	1.73	0.89
1:As:54:VAL:CG2	1:As:82:ASN:HD22	1.85	0.88
1:Ay:183:LEU:HG	1:Ay:384:ALA:CB	2.01	0.88
1:Bg:178:GLU:OE2	1:Bg:380:LYS:HE3	1.73	0.88
1:As:488:MET:HE2	1:As:491:MET:HE3	1.53	0.88
1:Bn:178:GLU:OE2	1:Bn:380:LYS:HE3	1.73	0.88
1:Ae:178:GLU:OE2	1:Ae:380:LYS:HE3	1.73	0.88
1:Ar:363:GLU:HA	1:Ar:366:GLN:HE22	0.72	0.88
1:Bn:487:ASN:OD1	1:Bn:489:ILE:HG13	1.73	0.88
1:Bu:54:VAL:HG11	1:Bu:82:ASN:HD22	1.35	0.88
1:Bf:134:LEU:HD11	1:Bf:425:LYS:HZ1	1.35	0.88
1:Ae:488:MET:HE2	1:Ae:491:MET:HE3	1.53	0.88
1:Az:488:MET:HE2	1:Az:491:MET:HE3	1.54	0.88
1:Bu:178:GLU:OE2	1:Bu:380:LYS:HE3	1.73	0.88
1:Ak:36:ARG:HG3	1:Ay:518:GLU:OE2	1.74	0.88
1:Ak:363:GLU:HA	1:Ak:366:GLN:HE22	0.72	0.88
1:Bg:487:ASN:OD1	1:Bg:489:ILE:HG13	1.73	0.88
1:Al:524:LEU:HD13	1:Az:63:GLU:CD	1.95	0.88
1:Ad:518:GLU:OE2	1:Ar:36:ARG:HG3	1.73	0.87
1:Ay:36:ARG:HG3	1:Bt:518:GLU:OE2	1.74	0.87
1:Bt:134:LEU:HD11	1:Bt:425:LYS:HZ2	1.08	0.87
1:Ae:487:ASN:OD1	1:Ae:489:ILE:HG13	1.73	0.87
1:Ak:489:ILE:HD13	1:Ak:494:LEU:HD21	1.52	0.87
1:Al:488:MET:HE2	1:Al:491:MET:HE3	1.53	0.87
1:Al:54:VAL:HG11	1:Al:82:ASN:HD22	1.35	0.87
1:Ar:134:LEU:HD11	1:Ar:425:LYS:HZ2	1.08	0.87
1:As:39:VAL:HG23	1:Bn:517:THR:HG23	1.55	0.87
1:Bt:363:GLU:HA	1:Bt:366:GLN:HE22	0.72	0.87
1:Ae:39:VAL:HG23	1:As:517:THR:HG23	1.55	0.87
1:Ak:366:GLN:HA	1:Ak:369:VAL:HG23	1.57	0.87
1:As:178:GLU:OE2	1:As:380:LYS:HE3	1.73	0.87
1:Bf:193:MET:CE	1:Bf:371:LYS:HD2	2.05	0.87
1:Bm:366:GLN:HA	1:Bm:369:VAL:HG23	1.57	0.87
1:Bf:388:GLU:HA	1:Bf:391:GLU:HB3	1.56	0.87
1:Bt:388:GLU:HA	1:Bt:391:GLU:HB3	1.56	0.87
1:Ak:193:MET:CE	1:Ak:371:LYS:HD2	2.05	0.87
1:Ar:388:GLU:HA	1:Ar:391:GLU:HB3	1.56	0.87
1:Bf:366:GLN:HA	1:Bf:369:VAL:HG23	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:366:GLN:HA	1:Ad:369:VAL:HG23	1.57	0.87
1:Bn:54:VAL:HG11	1:Bn:82:ASN:HD22	1.35	0.87
1:Ae:54:VAL:HG11	1:Ae:82:ASN:HD22	1.35	0.87
1:Ar:366:GLN:HA	1:Ar:369:VAL:HG23	1.57	0.87
1:Bf:489:ILE:HD13	1:Bf:494:LEU:HD21	1.52	0.86
1:Ad:388:GLU:HA	1:Ad:391:GLU:HB3	1.56	0.86
1:Ay:366:GLN:HA	1:Ay:369:VAL:HG23	1.57	0.86
1:Al:517:THR:HG23	1:Az:39:VAL:HG23	1.55	0.86
1:Az:54:VAL:CG1	1:Az:82:ASN:ND2	2.39	0.86
1:Bm:164:GLU:CD	1:Bm:187:LEU:HD22	2.01	0.86
1:Ar:193:MET:CE	1:Ar:371:LYS:HD2	2.05	0.86
1:Ak:388:GLU:HA	1:Ak:391:GLU:HB3	1.56	0.86
1:Ay:388:GLU:HA	1:Ay:391:GLU:HB3	1.56	0.86
1:Bg:517:THR:HG23	1:Bn:39:VAL:HG23	1.57	0.86
1:Bt:193:MET:CE	1:Bt:371:LYS:HD2	2.05	0.86
1:Bf:352:GLN:HB3	1:Bf:365:LEU:HD23	1.58	0.86
1:Ak:473:ASP:O	1:Ak:473:ASP:OD1	1.94	0.86
1:Bm:193:MET:CE	1:Bm:371:LYS:HD2	2.05	0.86
1:Bt:164:GLU:CD	1:Bt:187:LEU:HD22	2.01	0.86
1:Ay:489:ILE:HD13	1:Ay:494:LEU:HD21	1.52	0.85
1:Bm:363:GLU:HA	1:Bm:366:GLN:HE22	0.72	0.85
1:Bu:3:ALA:O	1:Bu:524:LEU:HD13	1.76	0.85
1:Ad:164:GLU:CD	1:Ad:187:LEU:HD22	2.01	0.85
1:Ay:473:ASP:O	1:Ay:473:ASP:OD1	1.94	0.85
1:Bm:352:GLN:HB3	1:Bm:365:LEU:HD23	1.58	0.85
1:Ae:54:VAL:CG1	1:Ae:82:ASN:ND2	2.39	0.85
1:Bt:473:ASP:OD1	1:Bt:473:ASP:O	1.94	0.85
1:Bf:473:ASP:OD1	1:Bf:473:ASP:O	1.95	0.85
1:Bm:388:GLU:HA	1:Bm:391:GLU:HB3	1.56	0.85
1:Bn:54:VAL:CG1	1:Bn:82:ASN:ND2	2.38	0.85
1:Bt:365:LEU:N	1:Bt:365:LEU:CD1	2.40	0.85
1:Ad:193:MET:CE	1:Ad:371:LYS:HD2	2.05	0.85
1:Ad:473:ASP:OD1	1:Ad:473:ASP:O	1.94	0.85
1:Az:54:VAL:HG11	1:Az:82:ASN:HD22	1.35	0.85
1:Ad:353:ILE:HD11	1:Ad:366:GLN:HB3	1.59	0.85
1:Ar:420:ILE:CD1	1:Ar:451:LEU:HD13	2.07	0.85
1:Bf:420:ILE:CD1	1:Bf:451:LEU:HD13	2.07	0.85
1:Ad:15:LYS:HE2	1:Ad:18:ARG:NH1	1.92	0.85
1:Ad:489:ILE:HD13	1:Ad:494:LEU:HD21	1.52	0.85
1:Ay:193:MET:CE	1:Ay:371:LYS:HD2	2.05	0.85
1:Bt:420:ILE:CD1	1:Bt:451:LEU:HD13	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:179:ASP:OD1	1:As:393:LYS:HD2	1.77	0.85
1:Ay:365:LEU:N	1:Ay:365:LEU:CD1	2.40	0.85
1:Bn:179:ASP:OD1	1:Bn:393:LYS:HD2	1.77	0.85
1:Ak:352:GLN:HB3	1:Ak:365:LEU:HD23	1.58	0.85
1:Al:3:ALA:O	1:Al:524:LEU:HD13	1.76	0.85
1:As:54:VAL:HG11	1:As:82:ASN:HD22	1.35	0.85
1:Bm:420:ILE:CD1	1:Bm:451:LEU:HD13	2.07	0.85
1:Ak:420:ILE:CD1	1:Ak:451:LEU:HD13	2.07	0.84
1:Ar:15:LYS:HE2	1:Ar:18:ARG:NH1	1.92	0.84
1:Ar:164:GLU:CD	1:Ar:187:LEU:HD22	2.01	0.84
1:Bf:164:GLU:CD	1:Bf:187:LEU:HD22	2.01	0.84
1:Bg:3:ALA:O	1:Bg:524:LEU:HD13	1.76	0.84
1:Ad:284:ARG:CD	1:Ad:364:LYS:HG2	2.08	0.84
1:Ad:363:GLU:HA	1:Ad:366:GLN:HE22	0.72	0.84
1:Ak:365:LEU:N	1:Ak:365:LEU:CD1	2.40	0.84
1:Ak:366:GLN:HA	1:Ak:369:VAL:CG2	2.08	0.84
1:Az:179:ASP:OD1	1:Az:393:LYS:HD2	1.77	0.84
1:Bg:179:ASP:OD1	1:Bg:393:LYS:HD2	1.77	0.84
1:Bm:473:ASP:OD1	1:Bm:473:ASP:O	1.94	0.84
1:Ad:366:GLN:HA	1:Ad:369:VAL:CG2	2.08	0.84
1:Bg:39:VAL:HG23	1:Bu:517:THR:HG23	1.55	0.84
1:Bm:353:ILE:HD11	1:Bm:366:GLN:HB3	1.59	0.84
1:Ak:353:ILE:HD11	1:Ak:366:GLN:HB3	1.59	0.84
1:Ar:473:ASP:OD1	1:Ar:473:ASP:O	1.94	0.84
1:Ay:366:GLN:HA	1:Ay:369:VAL:CG2	2.07	0.84
1:Az:517:THR:HG23	1:Bu:39:VAL:HG23	1.57	0.84
1:Bt:15:LYS:HE2	1:Bt:18:ARG:NH1	1.92	0.84
1:Bt:284:ARG:CD	1:Bt:364:LYS:HG2	2.08	0.84
1:Bu:40:LEU:HD22	1:Bu:59:GLU:OE1	1.78	0.84
1:Ak:15:LYS:HE2	1:Ak:18:ARG:NH1	1.92	0.84
1:Ak:164:GLU:CD	1:Ak:187:LEU:HD22	2.01	0.84
1:Ak:284:ARG:CD	1:Ak:364:LYS:HG2	2.08	0.84
1:Ay:15:LYS:HE2	1:Ay:18:ARG:NH1	1.92	0.84
1:Az:178:GLU:OE2	1:Az:380:LYS:CE	2.26	0.84
1:Bg:54:VAL:CG1	1:Bg:82:ASN:ND2	2.39	0.84
1:Bm:284:ARG:CD	1:Bm:364:LYS:HG2	2.08	0.84
1:Ad:134:LEU:HD11	1:Ad:425:LYS:HZ2	1.07	0.84
1:Ar:352:GLN:HB3	1:Ar:365:LEU:HD23	1.58	0.84
1:Ay:164:GLU:CD	1:Ay:187:LEU:HD22	2.01	0.84
1:Ay:368:ARG:O	1:Ay:372:LEU:CD2	2.26	0.84
1:Ay:420:ILE:CD1	1:Ay:451:LEU:HD13	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:3:ALA:O	1:Az:524:LEU:HD13	1.76	0.84
1:Bm:134:LEU:HD11	1:Bm:425:LYS:HZ1	1.42	0.84
1:Ad:420:ILE:CD1	1:Ad:451:LEU:HD13	2.07	0.84
1:Ar:366:GLN:HA	1:Ar:369:VAL:CG2	2.08	0.84
1:Az:40:LEU:HD22	1:Az:59:GLU:OE1	1.78	0.84
1:Bn:40:LEU:HD22	1:Bn:59:GLU:OE1	1.78	0.84
1:Bn:178:GLU:OE2	1:Bn:380:LYS:CE	2.26	0.84
1:Bt:366:GLN:HA	1:Bt:369:VAL:HG23	1.57	0.84
1:Al:178:GLU:OE2	1:Al:380:LYS:CE	2.26	0.84
1:As:40:LEU:HD22	1:As:59:GLU:OE1	1.78	0.84
1:Bg:40:LEU:HD22	1:Bg:59:GLU:OE1	1.78	0.84
1:Bg:54:VAL:HG11	1:Bg:82:ASN:HD22	1.35	0.84
1:Bt:352:GLN:HB3	1:Bt:365:LEU:HD23	1.58	0.84
1:Bt:368:ARG:O	1:Bt:372:LEU:CD2	2.26	0.84
1:Ay:352:GLN:HB3	1:Ay:365:LEU:HD23	1.58	0.84
1:Ae:3:ALA:O	1:Ae:524:LEU:HD13	1.76	0.84
1:Bn:3:ALA:O	1:Bn:524:LEU:HD13	1.76	0.84
1:Bt:366:GLN:HA	1:Bt:369:VAL:CG2	2.07	0.84
1:Ae:179:ASP:OD1	1:Ae:393:LYS:HD2	1.77	0.83
1:Al:179:ASP:OD1	1:Al:393:LYS:HD2	1.77	0.83
1:As:3:ALA:O	1:As:524:LEU:HD13	1.76	0.83
1:As:178:GLU:OE2	1:As:380:LYS:CE	2.26	0.83
1:Ad:352:GLN:HB3	1:Ad:365:LEU:HD23	1.58	0.83
1:Ar:353:ILE:HD11	1:Ar:366:GLN:HB3	1.59	0.83
1:Al:3:ALA:C	1:Al:524:LEU:CD1	2.52	0.83
1:Bg:178:GLU:OE2	1:Bg:380:LYS:CE	2.26	0.83
1:Ak:368:ARG:O	1:Ak:372:LEU:CD2	2.26	0.83
1:Ar:284:ARG:CD	1:Ar:364:LYS:HG2	2.08	0.83
1:Ay:134:LEU:HD11	1:Ay:425:LYS:HZ1	1.41	0.83
1:Bf:15:LYS:HE2	1:Bf:18:ARG:NH1	1.92	0.83
1:Bf:366:GLN:HA	1:Bf:369:VAL:CG2	2.07	0.83
1:Bg:54:VAL:HG21	1:Bg:82:ASN:ND2	1.94	0.83
1:Bt:525:PRO:O	1:Bt:525:PRO:C	2.21	0.83
1:Bm:15:LYS:HE2	1:Bm:18:ARG:NH1	1.92	0.83
1:Ay:284:ARG:CD	1:Ay:364:LYS:HG2	2.08	0.83
1:Ay:525:PRO:O	1:Ay:525:PRO:C	2.22	0.83
1:Az:54:VAL:HG21	1:Az:82:ASN:ND2	1.94	0.83
1:Bf:114:MET:HE3	1:Bt:457:ASN:O	1.79	0.83
1:Bf:353:ILE:HD11	1:Bf:366:GLN:HB3	1.59	0.83
1:As:3:ALA:C	1:As:524:LEU:CD1	2.52	0.83
1:Bu:54:VAL:CG1	1:Bu:82:ASN:ND2	2.39	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:178:GLU:OE2	1:Ae:380:LYS:CE	2.26	0.83
1:Ay:353:ILE:HD11	1:Ay:366:GLN:HB3	1.59	0.83
1:Bf:457:ASN:O	1:Bm:114:MET:HE3	1.79	0.83
1:Al:40:LEU:HD22	1:Al:59:GLU:OE1	1.78	0.83
1:As:54:VAL:CG1	1:As:82:ASN:ND2	2.39	0.83
1:Bf:284:ARG:CD	1:Bf:364:LYS:HG2	2.07	0.83
1:Bf:368:ARG:O	1:Bf:372:LEU:CD2	2.26	0.83
1:Bm:366:GLN:HA	1:Bm:369:VAL:CG2	2.08	0.83
1:Ae:3:ALA:C	1:Ae:524:LEU:CD1	2.52	0.82
1:Ae:40:LEU:HD22	1:Ae:59:GLU:OE1	1.78	0.82
1:Bf:525:PRO:O	1:Bf:525:PRO:C	2.21	0.82
1:Bt:353:ILE:HD11	1:Bt:366:GLN:HB3	1.59	0.82
1:Bu:179:ASP:OD1	1:Bu:393:LYS:HD2	1.77	0.82
1:Bf:134:LEU:HD11	1:Bf:425:LYS:HZ2	1.01	0.82
1:Ad:457:ASN:O	1:Ak:114:MET:HE3	1.77	0.82
1:Al:54:VAL:CG1	1:Al:82:ASN:ND2	2.38	0.82
1:Bm:365:LEU:N	1:Bm:365:LEU:CD1	2.40	0.82
1:Bm:368:ARG:O	1:Bm:372:LEU:CD2	2.26	0.82
1:Bu:178:GLU:OE2	1:Bu:380:LYS:CE	2.26	0.82
1:Ad:365:LEU:N	1:Ad:365:LEU:CD1	2.40	0.82
1:Ar:525:PRO:O	1:Ar:525:PRO:C	2.21	0.82
1:Ay:457:ASN:O	1:Bt:114:MET:HE3	1.79	0.82
1:Az:3:ALA:C	1:Az:524:LEU:CD1	2.52	0.82
1:Bm:525:PRO:O	1:Bm:525:PRO:C	2.21	0.82
1:Bu:3:ALA:C	1:Bu:524:LEU:CD1	2.52	0.82
1:Ad:368:ARG:O	1:Ad:372:LEU:CD2	2.26	0.82
1:Ae:54:VAL:HG21	1:Ae:82:ASN:ND2	1.94	0.82
1:Bm:363:GLU:O	1:Bm:367:GLU:OE1	1.98	0.82
1:Ay:365:LEU:N	1:Ay:365:LEU:HD12	1.95	0.82
1:Bg:3:ALA:C	1:Bg:524:LEU:CD1	2.52	0.82
1:Ak:525:PRO:O	1:Ak:525:PRO:C	2.21	0.82
1:Bf:365:LEU:N	1:Bf:365:LEU:CD1	2.40	0.82
1:Bn:3:ALA:C	1:Bn:524:LEU:CD1	2.52	0.82
1:Bt:363:GLU:O	1:Bt:367:GLU:OE1	1.98	0.82
1:Ad:365:LEU:N	1:Ad:365:LEU:HD12	1.95	0.82
1:Ar:368:ARG:O	1:Ar:372:LEU:CD2	2.26	0.82
1:Bf:363:GLU:O	1:Bf:367:GLU:OE1	1.98	0.82
1:Ak:134:LEU:CD1	1:Ak:425:LYS:HZ1	1.89	0.81
1:Ar:365:LEU:N	1:Ar:365:LEU:CD1	2.40	0.81
1:As:54:VAL:HG21	1:As:82:ASN:ND2	1.94	0.81
1:Bm:365:LEU:N	1:Bm:365:LEU:HD12	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:365:LEU:N	1:Bt:365:LEU:HD12	1.95	0.81
1:Bu:54:VAL:HG21	1:Bu:82:ASN:ND2	1.94	0.81
1:Ad:363:GLU:O	1:Ad:367:GLU:OE1	1.98	0.81
1:Ad:525:PRO:O	1:Ad:525:PRO:C	2.21	0.81
1:Ar:363:GLU:O	1:Ar:367:GLU:OE1	1.98	0.81
1:Bn:54:VAL:HG21	1:Bn:82:ASN:ND2	1.94	0.81
1:Al:54:VAL:HG21	1:Al:82:ASN:ND2	1.94	0.81
1:Bu:54:VAL:CG1	1:Bu:82:ASN:HD22	1.94	0.81
1:Bn:54:VAL:CG1	1:Bn:82:ASN:HD22	1.94	0.81
1:Bm:388:GLU:HA	1:Bm:391:GLU:HB2	1.62	0.81
1:Bf:388:GLU:HA	1:Bf:391:GLU:HB2	1.62	0.81
1:Ay:363:GLU:O	1:Ay:367:GLU:OE1	1.98	0.81
1:Bg:54:VAL:CG1	1:Bg:82:ASN:HD22	1.94	0.81
1:Ae:54:VAL:CG1	1:Ae:82:ASN:HD22	1.94	0.81
1:Ar:114:MET:HE3	1:Bm:457:ASN:O	1.80	0.81
1:Ak:363:GLU:O	1:Ak:367:GLU:OE1	1.98	0.80
1:Ak:388:GLU:HA	1:Ak:391:GLU:HB2	1.62	0.80
1:Bn:172:GLU:OE2	1:Bn:369:VAL:HG12	1.82	0.80
1:Az:54:VAL:CG1	1:Az:82:ASN:HD22	1.94	0.80
1:Ar:365:LEU:N	1:Ar:365:LEU:HD12	1.95	0.80
1:As:482:THR:OG1	1:As:484:GLU:CG	2.29	0.80
1:Bf:365:LEU:N	1:Bf:365:LEU:HD12	1.95	0.80
1:Ak:365:LEU:N	1:Ak:365:LEU:HD12	1.95	0.80
1:As:54:VAL:CG1	1:As:82:ASN:HD22	1.94	0.80
1:As:172:GLU:OE2	1:As:369:VAL:HG12	1.82	0.80
1:Bg:172:GLU:OE2	1:Bg:369:VAL:HG12	1.82	0.80
1:Ar:388:GLU:HA	1:Ar:391:GLU:HB2	1.62	0.80
1:Al:54:VAL:CG1	1:Al:82:ASN:HD22	1.94	0.80
1:Al:477:GLY:C	1:Al:488:MET:HE3	2.07	0.80
1:Ae:172:GLU:OE2	1:Ae:369:VAL:HG12	1.82	0.80
1:Bg:477:GLY:C	1:Bg:488:MET:HE3	2.07	0.80
1:Ae:381:VAL:HG12	1:Ae:389:MET:SD	2.22	0.79
1:Ak:457:ASN:O	1:Ay:114:MET:HE3	1.81	0.79
1:Bt:388:GLU:HA	1:Bt:391:GLU:HB2	1.62	0.79
1:Ae:477:GLY:C	1:Ae:488:MET:HE3	2.07	0.79
1:Ad:114:MET:HE3	1:Ar:457:ASN:O	1.81	0.79
1:As:477:GLY:C	1:As:488:MET:HE3	2.07	0.79
1:Bg:381:VAL:HG12	1:Bg:389:MET:SD	2.22	0.79
1:As:381:VAL:HG12	1:As:389:MET:SD	2.22	0.79
1:Az:477:GLY:C	1:Az:488:MET:HE3	2.07	0.79
1:Bn:381:VAL:HG12	1:Bn:389:MET:SD	2.22	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:477:GLY:C	1:Bu:488:MET:HE3	2.07	0.79
1:Ad:388:GLU:HA	1:Ad:391:GLU:HB2	1.62	0.79
1:Az:381:VAL:HG12	1:Az:389:MET:SD	2.22	0.79
1:Bu:172:GLU:OE2	1:Bu:369:VAL:HG12	1.82	0.79
1:Bu:482:THR:OG1	1:Bu:484:GLU:CG	2.29	0.79
1:Al:482:THR:OG1	1:Al:484:GLU:CG	2.29	0.79
1:Bf:169:VAL:CG1	1:Bf:377:ALA:HB2	2.13	0.78
1:Bu:381:VAL:HG12	1:Bu:389:MET:SD	2.22	0.78
1:Al:172:GLU:OE2	1:Al:369:VAL:HG12	1.82	0.78
1:Al:381:VAL:HG12	1:Al:389:MET:SD	2.22	0.78
1:Bf:284:ARG:HD2	1:Bf:364:LYS:CG	2.14	0.78
1:Ay:169:VAL:CG1	1:Ay:377:ALA:HB2	2.14	0.78
1:Ay:388:GLU:HA	1:Ay:391:GLU:HB2	1.62	0.78
1:Bn:482:THR:OG1	1:Bn:484:GLU:CG	2.29	0.78
1:Bm:169:VAL:CG1	1:Bm:377:ALA:HB2	2.14	0.78
1:Bn:477:GLY:C	1:Bn:488:MET:HE3	2.07	0.78
1:Bm:284:ARG:HD2	1:Bm:364:LYS:CG	2.14	0.77
1:Bt:284:ARG:HD2	1:Bt:364:LYS:CG	2.14	0.77
1:Bt:421:ARG:HH12	1:Bt:469:VAL:HG12	1.49	0.77
1:Az:172:GLU:OE2	1:Az:369:VAL:HG12	1.82	0.77
1:Bn:50:THR:HG23	1:Bn:52:ASP:OD1	1.84	0.77
1:Ad:169:VAL:CG1	1:Ad:377:ALA:HB2	2.13	0.77
1:Bt:169:VAL:CG1	1:Bt:377:ALA:HB2	2.13	0.77
1:Bu:50:THR:HG23	1:Bu:52:ASP:OD1	1.84	0.77
1:Ar:169:VAL:CG1	1:Ar:377:ALA:HB2	2.13	0.77
1:As:34:LYS:HZ1	1:As:483:GLU:CG	1.96	0.77
1:Az:50:THR:HG23	1:Az:52:ASP:OD1	1.84	0.77
1:Bg:50:THR:HG23	1:Bg:52:ASP:OD1	1.84	0.77
1:Ad:489:ILE:HD12	1:Ad:494:LEU:CD2	2.15	0.77
2:Af:3:ILE:HA	2:At:95:VAL:HA	1.65	0.77
1:Ak:169:VAL:CG1	1:Ak:377:ALA:HB2	2.13	0.77
1:Az:482:THR:OG1	1:Az:484:GLU:CG	2.29	0.77
1:Ad:421:ARG:HH12	1:Ad:469:VAL:HG12	1.49	0.77
1:Ae:50:THR:HG23	1:Ae:52:ASP:OD1	1.84	0.77
1:Bf:421:ARG:HH12	1:Bf:469:VAL:HG12	1.48	0.77
1:Ad:284:ARG:HD2	1:Ad:364:LYS:CG	2.14	0.77
1:Ar:421:ARG:HH12	1:Ar:469:VAL:HG12	1.48	0.77
1:Ad:36:ARG:CD	1:Ak:518:GLU:OE2	2.33	0.76
1:Ak:421:ARG:HH12	1:Ak:469:VAL:HG12	1.48	0.76
1:As:50:THR:HG23	1:As:52:ASP:OD1	1.85	0.76
1:Ay:168:LYS:HZ1	1:Ay:187:LEU:HG	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:284:ARG:HD2	1:Ay:364:LYS:CG	2.14	0.76
1:Ak:284:ARG:HD2	1:Ak:364:LYS:CG	2.14	0.76
1:Ar:134:LEU:CD1	1:Ar:425:LYS:HZ1	1.89	0.76
1:Ar:152:ALA:O	1:Ar:395:ARG:NH2	2.19	0.76
1:Ar:284:ARG:HD2	1:Ar:364:LYS:CG	2.14	0.76
1:Al:50:THR:HG23	1:Al:52:ASP:OD1	1.84	0.76
1:Bf:455:VAL:HG13	1:Bf:460:GLU:HG2	1.68	0.76
1:Ay:152:ALA:O	1:Ay:395:ARG:NH2	2.19	0.76
1:Ad:168:LYS:CE	1:Ad:187:LEU:HD21	2.16	0.76
1:Ar:168:LYS:CE	1:Ar:187:LEU:HD21	2.16	0.76
1:Ak:152:ALA:O	1:Ak:395:ARG:NH2	2.19	0.76
1:Ak:168:LYS:CE	1:Ak:187:LEU:HD21	2.16	0.76
1:Al:7:LYS:CG	1:Al:66:PHE:CZ	2.69	0.76
1:Bt:455:VAL:HG13	1:Bt:460:GLU:HG2	1.68	0.76
1:Ar:489:ILE:HD12	1:Ar:494:LEU:CD2	2.15	0.76
1:Bg:34:LYS:HZ1	1:Bg:483:GLU:CG	1.98	0.76
1:Bf:489:ILE:HD12	1:Bf:494:LEU:CD2	2.15	0.76
1:Bm:421:ARG:HH12	1:Bm:469:VAL:HG12	1.49	0.76
1:Bt:183:LEU:CG	1:Bt:384:ALA:HB2	2.16	0.76
1:Ak:489:ILE:HD12	1:Ak:494:LEU:CD2	2.15	0.75
1:Bm:152:ALA:O	1:Bm:395:ARG:NH2	2.19	0.75
1:Bm:168:LYS:CE	1:Bm:187:LEU:HD21	2.16	0.75
1:Bm:455:VAL:HG13	1:Bm:460:GLU:HG2	1.68	0.75
1:Ad:134:LEU:CD1	1:Ad:425:LYS:HZ1	1.90	0.75
1:Ar:455:VAL:HG13	1:Ar:460:GLU:HG2	1.68	0.75
1:Ay:383:ALA:CB	1:Ay:388:GLU:HG3	2.17	0.75
2:Bh:95:VAL:HA	2:Bo:3:ILE:HA	1.68	0.75
1:Bm:489:ILE:HD12	1:Bm:494:LEU:CD2	2.15	0.75
1:Bm:168:LYS:HZ1	1:Bm:187:LEU:HG	1.50	0.75
1:Bt:119:GLY:O	1:Bt:440:ILE:HD13	1.87	0.75
1:Ad:152:ALA:O	1:Ad:395:ARG:NH2	2.19	0.75
1:Ay:421:ARG:HH12	1:Ay:469:VAL:HG12	1.48	0.75
1:Bt:152:ALA:O	1:Bt:395:ARG:NH2	2.19	0.75
1:Ad:361:ASP:O	1:Ad:365:LEU:HD13	1.87	0.75
1:Ar:142:LYS:HG3	1:Ar:146:GLN:HE21	1.51	0.75
1:Bf:361:ASP:O	1:Bf:365:LEU:HD13	1.87	0.75
1:Ad:119:GLY:O	1:Ad:440:ILE:HD13	1.87	0.75
1:Ad:455:VAL:HG13	1:Ad:460:GLU:HG2	1.68	0.75
1:Ak:142:LYS:HG3	1:Ak:146:GLN:HE21	1.52	0.75
1:Ay:455:VAL:HG13	1:Ay:460:GLU:HG2	1.68	0.75
1:Bt:161:LEU:O	1:Bt:164:GLU:HG2	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:168:LYS:CE	1:Bf:187:LEU:HD21	2.16	0.75
1:Bf:183:LEU:CG	1:Bf:384:ALA:HB2	2.16	0.75
1:Bn:7:LYS:CG	1:Bn:66:PHE:CZ	2.69	0.75
1:Bt:383:ALA:CB	1:Bt:388:GLU:HG3	2.17	0.75
1:Bu:7:LYS:CG	1:Bu:66:PHE:CZ	2.69	0.75
1:Ak:455:VAL:HG13	1:Ak:460:GLU:HG2	1.68	0.75
1:Ay:168:LYS:CE	1:Ay:187:LEU:HD21	2.16	0.75
1:Bf:119:GLY:O	1:Bf:440:ILE:HD13	1.87	0.75
1:Ae:482:THR:OG1	1:Ae:484:GLU:CG	2.29	0.74
1:Ak:119:GLY:O	1:Ak:440:ILE:HD13	1.87	0.74
1:Ak:361:ASP:O	1:Ak:365:LEU:HD13	1.87	0.74
1:Ak:383:ALA:CB	1:Ak:388:GLU:HG3	2.17	0.74
1:Ar:361:ASP:O	1:Ar:365:LEU:HD13	1.87	0.74
1:Ar:119:GLY:O	1:Ar:440:ILE:HD13	1.87	0.74
1:As:7:LYS:CG	1:As:66:PHE:CZ	2.69	0.74
1:Bm:361:ASP:O	1:Bm:365:LEU:HD13	1.87	0.74
1:Bt:489:ILE:HD12	1:Bt:494:LEU:CD2	2.15	0.74
1:Ad:142:LYS:HG3	1:Ad:146:GLN:HE21	1.51	0.74
1:Ay:489:ILE:HD12	1:Ay:494:LEU:CD2	2.15	0.74
1:Bg:482:THR:OG1	1:Bg:484:GLU:CG	2.29	0.74
1:Ad:161:LEU:O	1:Ad:164:GLU:HG2	1.87	0.74
1:Ae:428:ASP:O	1:Ae:430:ARG:HG2	1.88	0.74
1:Ay:161:LEU:O	1:Ay:164:GLU:HG2	1.87	0.74
1:Bf:152:ALA:O	1:Bf:395:ARG:NH2	2.19	0.74
1:Bf:168:LYS:HZ1	1:Bf:187:LEU:HG	1.50	0.74
1:Bg:7:LYS:CG	1:Bg:66:PHE:CZ	2.69	0.74
1:Bm:142:LYS:HG3	1:Bm:146:GLN:HE21	1.52	0.74
1:Bm:383:ALA:CB	1:Bm:388:GLU:HG3	2.17	0.74
1:Bt:168:LYS:CE	1:Bt:187:LEU:HD21	2.16	0.74
1:Ad:383:ALA:CB	1:Ad:388:GLU:HG3	2.17	0.74
1:Ar:161:LEU:O	1:Ar:164:GLU:HG2	1.87	0.74
1:Bn:428:ASP:O	1:Bn:430:ARG:HG2	1.88	0.74
1:Bt:142:LYS:HG3	1:Bt:146:GLN:HE21	1.52	0.74
1:Bt:361:ASP:O	1:Bt:365:LEU:HD13	1.87	0.74
1:Ad:388:GLU:CA	1:Ad:391:GLU:HB3	2.18	0.74
1:Ar:168:LYS:HZ1	1:Ar:187:LEU:HG	1.51	0.74
1:Bf:142:LYS:HG3	1:Bf:146:GLN:HE21	1.52	0.74
2:Bh:3:ILE:HA	2:Bv:95:VAL:HA	1.69	0.74
1:Ae:47:PRO:HG2	1:As:73:MET:HG3	1.68	0.74
1:Ae:73:MET:HG3	1:Al:47:PRO:HG2	1.69	0.74
1:Ar:518:GLU:OE2	1:Bm:36:ARG:CD	2.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ba:95:VAL:HA	2:Bv:3:ILE:HA	1.68	0.74
1:Ak:36:ARG:CD	1:Ay:518:GLU:OE2	2.36	0.74
1:Al:428:ASP:O	1:Al:430:ARG:HG2	1.87	0.74
1:As:178:GLU:OE2	1:As:380:LYS:CD	2.36	0.74
1:As:428:ASP:O	1:As:430:ARG:HG2	1.88	0.74
1:Ay:119:GLY:O	1:Ay:440:ILE:HD13	1.87	0.74
1:Az:428:ASP:O	1:Az:430:ARG:HG2	1.88	0.74
1:Bf:153:ASN:OD1	5:Bf:702:HOH:O	2.06	0.74
1:Bf:161:LEU:O	1:Bf:164:GLU:HG2	1.87	0.74
1:Bf:518:GLU:OE2	1:Bt:36:ARG:CD	2.36	0.74
1:Bt:153:ASN:OD1	5:Bt:702:HOH:O	2.06	0.74
1:Ak:161:LEU:O	1:Ak:164:GLU:HG2	1.87	0.74
1:Al:178:GLU:OE2	1:Al:380:LYS:CD	2.36	0.74
1:Ar:155:ASP:CB	1:Ar:395:ARG:HH22	2.00	0.74
1:Bg:47:PRO:HG2	1:Bu:73:MET:HG3	1.69	0.74
1:Bg:178:GLU:OE2	1:Bg:380:LYS:CD	2.36	0.74
1:Bm:119:GLY:O	1:Bm:440:ILE:HD13	1.87	0.74
1:Ak:388:GLU:CA	1:Ak:391:GLU:HB3	2.18	0.73
1:Ar:436:GLN:O	1:Ar:440:ILE:HG12	1.88	0.73
1:Az:178:GLU:OE2	1:Az:380:LYS:CD	2.36	0.73
1:Bf:155:ASP:CB	1:Bf:395:ARG:HH22	2.00	0.73
1:Bm:183:LEU:CG	1:Bm:384:ALA:HB2	2.16	0.73
1:Bm:436:GLN:O	1:Bm:440:ILE:HG12	1.88	0.73
1:Ad:183:LEU:CG	1:Ad:384:ALA:HB2	2.16	0.73
1:Ad:436:GLN:O	1:Ad:440:ILE:HG12	1.89	0.73
1:Ad:518:GLU:OE2	1:Ar:36:ARG:CD	2.36	0.73
1:Bf:36:ARG:CD	1:Bm:518:GLU:OE2	2.36	0.73
1:Bf:383:ALA:CB	1:Bf:388:GLU:HG3	2.17	0.73
1:Bu:428:ASP:O	1:Bu:430:ARG:HG2	1.88	0.73
1:Bm:153:ASN:OD1	5:Bm:702:HOH:O	2.06	0.73
1:Bu:178:GLU:OE2	1:Bu:380:LYS:CD	2.36	0.73
1:Al:18:ARG:HD2	1:Al:67:GLU:OE2	1.89	0.73
1:Ar:383:ALA:CB	1:Ar:388:GLU:HG3	2.17	0.73
1:Ar:388:GLU:CA	1:Ar:391:GLU:HB3	2.18	0.73
1:Ay:361:ASP:O	1:Ay:365:LEU:HD13	1.87	0.73
1:Ak:16:MET:HE2	1:Ak:514:MET:HE1	1.71	0.73
1:Ar:284:ARG:HG2	1:Ar:368:ARG:NH1	2.04	0.73
1:Ad:16:MET:HE2	1:Ad:514:MET:HE1	1.71	0.73
1:Ae:178:GLU:OE2	1:Ae:380:LYS:CD	2.36	0.73
1:Ar:168:LYS:NZ	1:Ar:187:LEU:HG	2.04	0.73
1:Ay:284:ARG:HG2	1:Ay:368:ARG:NH1	2.04	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:436:GLN:O	1:Bf:440:ILE:HG12	1.89	0.73
1:Bn:18:ARG:HD2	1:Bn:67:GLU:OE2	1.89	0.73
1:Bn:482:THR:HG1	1:Bn:484:GLU:HG2	1.54	0.73
1:Bt:16:MET:HE2	1:Bt:514:MET:HE1	1.71	0.73
1:Bu:18:ARG:HD2	1:Bu:67:GLU:OE2	1.89	0.73
1:Ad:168:LYS:NZ	1:Ad:187:LEU:HG	2.04	0.73
1:Ae:7:LYS:CG	1:Ae:66:PHE:CZ	2.69	0.73
1:Ay:153:ASN:OD1	5:Ay:702:HOH:O	2.06	0.73
1:Az:18:ARG:HD2	1:Az:67:GLU:OE2	1.89	0.73
1:Ak:436:GLN:O	1:Ak:440:ILE:HG12	1.88	0.73
1:Bt:155:ASP:CB	1:Bt:395:ARG:HH22	2.00	0.73
1:Bt:284:ARG:HG2	1:Bt:368:ARG:NH1	2.04	0.73
1:Bt:388:GLU:CA	1:Bt:391:GLU:HB3	2.18	0.73
1:Ad:69:MET:HE3	1:Ad:520:MET:HE2	1.71	0.73
1:Ad:284:ARG:HG2	1:Ad:368:ARG:NH1	2.04	0.73
1:Ar:352:GLN:OE1	1:Ar:368:ARG:NH2	2.22	0.73
1:Bf:519:CYS:HB3	1:Bt:38:VAL:HG13	1.71	0.73
1:Bg:37:ASN:N	1:Bu:518:GLU:CD	2.31	0.73
1:Bm:161:LEU:O	1:Bm:164:GLU:HG2	1.87	0.73
1:Ad:193:MET:SD	1:Ad:371:LYS:HD2	2.29	0.73
1:Ak:155:ASP:CB	1:Ak:395:ARG:HH22	2.00	0.73
1:Ay:16:MET:HE2	1:Ay:514:MET:HE1	1.71	0.73
1:Bn:178:GLU:OE2	1:Bn:380:LYS:CD	2.36	0.73
1:Bt:352:GLN:OE1	1:Bt:368:ARG:NH2	2.22	0.73
1:Ad:352:GLN:OE1	1:Ad:368:ARG:NH2	2.22	0.72
1:Ar:153:ASN:OD1	5:Ar:702:HOH:O	2.06	0.72
1:Ar:193:MET:SD	1:Ar:371:LYS:HD2	2.29	0.72
1:Bn:34:LYS:NZ	1:Bn:483:GLU:CG	2.52	0.72
1:Bt:134:LEU:CD1	1:Bt:425:LYS:HZ1	1.89	0.72
1:Ak:168:LYS:NZ	1:Ak:187:LEU:HG	2.04	0.72
1:Ak:352:GLN:OE1	1:Ak:368:ARG:NH2	2.22	0.72
1:Ar:69:MET:HE3	1:Ar:520:MET:HE2	1.71	0.72
1:Bg:34:LYS:NZ	1:Bg:483:GLU:CG	2.52	0.72
1:Ae:18:ARG:HD2	1:Ae:67:GLU:OE2	1.89	0.72
1:Bf:16:MET:HE2	1:Bf:514:MET:HE1	1.70	0.72
1:Bm:155:ASP:CB	1:Bm:395:ARG:HH22	2.00	0.72
1:Bm:168:LYS:NZ	1:Bm:187:LEU:HG	2.04	0.72
1:Bt:436:GLN:O	1:Bt:440:ILE:HG12	1.89	0.72
1:Ar:16:MET:HE2	1:Ar:514:MET:HE1	1.71	0.72
1:Ar:176:THR:HG22	1:Ar:178:GLU:OE2	1.90	0.72
1:Ay:436:GLN:O	1:Ay:440:ILE:HG12	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:352:GLN:OE1	1:Bf:368:ARG:NH2	2.22	0.72
1:Bm:388:GLU:CA	1:Bm:391:GLU:HB3	2.18	0.72
1:Ak:284:ARG:HG2	1:Ak:368:ARG:NH1	2.04	0.72
1:Ay:388:GLU:CA	1:Ay:391:GLU:HB3	2.18	0.72
1:Bg:18:ARG:HD2	1:Bg:67:GLU:OE2	1.89	0.72
1:Bt:176:THR:HG22	1:Bt:178:GLU:OE2	1.90	0.72
1:Ad:519:CYS:HB3	1:Ar:38:VAL:HG13	1.71	0.72
1:Ae:40:LEU:CB	1:Ae:59:GLU:OE1	2.38	0.72
1:Ay:142:LYS:HG3	1:Ay:146:GLN:HE21	1.52	0.72
1:Az:7:LYS:CG	1:Az:66:PHE:CZ	2.69	0.72
1:Bm:193:MET:SD	1:Bm:371:LYS:HD2	2.29	0.72
1:Bm:284:ARG:HG2	1:Bm:368:ARG:NH1	2.04	0.72
1:Ak:176:THR:HG22	1:Ak:178:GLU:OE2	1.90	0.72
1:Ak:183:LEU:CG	1:Ak:384:ALA:HB2	2.16	0.72
1:Bg:428:ASP:O	1:Bg:430:ARG:HG2	1.88	0.72
1:Ae:428:ASP:OD1	1:Ae:429:LEU:N	2.23	0.72
1:As:428:ASP:OD1	1:As:429:LEU:N	2.23	0.72
1:Ay:193:MET:SD	1:Ay:371:LYS:HD2	2.29	0.72
1:Bf:388:GLU:CA	1:Bf:391:GLU:HB3	2.18	0.72
1:Ak:153:ASN:OD1	5:Ak:702:HOH:O	2.06	0.72
1:Ak:193:MET:SD	1:Ak:371:LYS:HD2	2.29	0.72
1:Bf:284:ARG:HG2	1:Bf:368:ARG:NH1	2.04	0.72
1:Bm:176:THR:HG22	1:Bm:178:GLU:OE2	1.90	0.72
1:Bu:34:LYS:NZ	1:Bu:483:GLU:CG	2.52	0.72
1:Ae:34:LYS:NZ	1:Ae:483:GLU:CG	2.52	0.72
1:Al:34:LYS:NZ	1:Al:483:GLU:CG	2.52	0.72
2:At:3:ILE:HA	2:Bo:95:VAL:HA	1.71	0.72
1:Ay:36:ARG:CD	1:Bt:518:GLU:OE2	2.38	0.72
1:Bt:168:LYS:NZ	1:Bt:187:LEU:HG	2.04	0.72
1:Ak:69:MET:HE3	1:Ak:520:MET:HE2	1.71	0.71
1:Al:40:LEU:CB	1:Al:59:GLU:OE1	2.38	0.71
1:Ay:176:THR:HG22	1:Ay:178:GLU:OE2	1.90	0.71
1:Ay:352:GLN:OE1	1:Ay:368:ARG:NH2	2.22	0.71
1:Bf:168:LYS:NZ	1:Bf:187:LEU:HG	2.04	0.71
1:Bf:193:MET:SD	1:Bf:371:LYS:HD2	2.29	0.71
1:Bg:113:PRO:CG	1:Bn:36:ARG:NE	2.52	0.71
1:Bg:428:ASP:OD1	1:Bg:429:LEU:N	2.23	0.71
1:Bm:352:GLN:OE1	1:Bm:368:ARG:NH2	2.22	0.71
1:Ad:38:VAL:HG13	1:Ak:519:CYS:HB3	1.71	0.71
1:Ad:153:ASN:OD1	5:Ad:702:HOH:O	2.06	0.71
1:Ay:168:LYS:NZ	1:Ay:187:LEU:HG	2.04	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:73:MET:HG3	1:Bu:47:PRO:HG2	1.72	0.71
1:Ad:36:ARG:HD2	1:Ak:518:GLU:OE2	1.90	0.71
1:Ar:183:LEU:CG	1:Ar:384:ALA:HB2	2.16	0.71
1:As:18:ARG:HD2	1:As:67:GLU:OE2	1.89	0.71
1:Bt:193:MET:SD	1:Bt:371:LYS:HD2	2.29	0.71
1:Bu:428:ASP:OD1	1:Bu:429:LEU:N	2.23	0.71
1:As:37:ASN:N	1:Bn:518:GLU:CD	2.31	0.71
1:As:47:PRO:HG2	1:Bn:73:MET:HG3	1.70	0.71
1:Bm:16:MET:HE2	1:Bm:514:MET:HE1	1.71	0.71
1:Bn:428:ASP:OD1	1:Bn:429:LEU:N	2.23	0.71
1:Ar:157:THR:O	1:Ar:161:LEU:CD1	2.39	0.71
1:Ay:155:ASP:CB	1:Ay:395:ARG:HH22	2.00	0.71
1:Bg:73:MET:HG3	1:Bn:47:PRO:HG2	1.70	0.71
1:Bn:124:VAL:HG21	1:Bn:508:ALA:CB	2.21	0.71
1:Ad:157:THR:O	1:Ad:161:LEU:CD1	2.39	0.71
1:Ad:176:THR:HG22	1:Ad:178:GLU:OE2	1.90	0.71
1:Ae:113:PRO:CG	1:Al:36:ARG:NE	2.52	0.71
1:Al:428:ASP:OD1	1:Al:429:LEU:N	2.23	0.71
1:Ar:180:GLY:O	1:Ar:382:GLY:HA2	1.91	0.71
1:Ar:519:CYS:HB3	1:Bm:38:VAL:HG13	1.71	0.71
1:As:124:VAL:HG21	1:As:508:ALA:CB	2.21	0.71
1:Ay:38:VAL:HG13	1:Bt:519:CYS:HB3	1.72	0.71
1:Az:428:ASP:OD1	1:Az:429:LEU:N	2.23	0.71
1:Az:489:ILE:HG22	1:Az:494:LEU:HD21	1.72	0.71
1:Bf:38:VAL:HG13	1:Bm:519:CYS:HB3	1.72	0.71
1:Bf:176:THR:HG22	1:Bf:178:GLU:OE2	1.90	0.71
1:Ak:38:VAL:HG13	1:Ay:519:CYS:HB3	1.71	0.71
1:Az:34:LYS:NZ	1:Az:483:GLU:CG	2.52	0.71
1:Ad:82:ASN:HB2	1:Ad:89:THR:OG1	1.91	0.71
1:Bg:124:VAL:HG21	1:Bg:508:ALA:CB	2.21	0.71
1:Ad:111:MET:SD	1:Ad:435:ASP:OD1	2.49	0.71
1:Ak:111:MET:SD	1:Ak:435:ASP:OD1	2.49	0.71
1:Ak:489:ILE:HD12	1:Ak:494:LEU:HD21	1.73	0.71
1:Ay:180:GLY:O	1:Ay:382:GLY:HA2	1.91	0.71
1:Az:124:VAL:HG21	1:Az:508:ALA:CB	2.21	0.71
1:Bf:69:MET:HE3	1:Bf:520:MET:HE2	1.71	0.71
1:Bm:69:MET:HE3	1:Bm:520:MET:HE2	1.71	0.71
1:Bt:69:MET:HE3	1:Bt:520:MET:HE2	1.71	0.71
1:Ak:82:ASN:HB2	1:Ak:89:THR:OG1	1.91	0.71
1:Bf:180:GLY:O	1:Bf:382:GLY:HA2	1.91	0.71
1:Ad:489:ILE:HD12	1:Ad:494:LEU:HD21	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:124:VAL:HG21	1:Ae:508:ALA:CB	2.21	0.70
1:Al:73:MET:HG3	1:Az:47:PRO:HG2	1.71	0.70
1:Al:489:ILE:HG22	1:Al:494:LEU:HD21	1.73	0.70
1:As:34:LYS:HZ1	1:As:483:GLU:HG3	1.54	0.70
1:Bg:40:LEU:CB	1:Bg:59:GLU:OE1	2.38	0.70
1:Ak:180:GLY:O	1:Ak:382:GLY:HA2	1.91	0.70
1:Ar:111:MET:SD	1:Ar:435:ASP:OD1	2.49	0.70
1:Az:40:LEU:CB	1:Az:59:GLU:OE1	2.38	0.70
1:Bg:36:ARG:NE	1:Bu:113:PRO:CG	2.53	0.70
1:Ad:155:ASP:CB	1:Ad:395:ARG:HH22	2.00	0.70
1:As:36:ARG:NE	1:Bn:113:PRO:CG	2.53	0.70
1:Ay:111:MET:SD	1:Ay:435:ASP:OD1	2.49	0.70
1:Ay:489:ILE:HD12	1:Ay:494:LEU:HD21	1.73	0.70
1:Bf:157:THR:O	1:Bf:161:LEU:CD1	2.39	0.70
1:Bm:157:THR:O	1:Bm:161:LEU:CD1	2.39	0.70
1:Bt:82:ASN:HB2	1:Bt:89:THR:OG1	1.91	0.70
1:Bt:180:GLY:O	1:Bt:382:GLY:HA2	1.91	0.70
1:Bu:124:VAL:HG21	1:Bu:508:ALA:CB	2.21	0.70
1:Bu:489:ILE:HG22	1:Bu:494:LEU:HD21	1.73	0.70
1:Ae:36:ARG:NE	1:As:113:PRO:CG	2.53	0.70
1:Ak:157:THR:O	1:Ak:161:LEU:CD1	2.39	0.70
2:Am:95:VAL:HA	2:Ba:3:ILE:HA	1.71	0.70
1:Ar:82:ASN:HB2	1:Ar:89:THR:OG1	1.91	0.70
1:Ar:489:ILE:HD12	1:Ar:494:LEU:HD21	1.73	0.70
1:Ak:36:ARG:HD2	1:Ay:518:GLU:OE2	1.90	0.70
1:Ay:82:ASN:HB2	1:Ay:89:THR:OG1	1.91	0.70
1:Ay:183:LEU:CG	1:Ay:384:ALA:HB2	2.16	0.70
1:Bg:384:ALA:O	1:Bu:80:LYS:HE2	1.92	0.70
1:Bm:82:ASN:HB2	1:Bm:89:THR:OG1	1.91	0.70
1:Ad:180:GLY:O	1:Ad:382:GLY:HA2	1.91	0.70
1:Ak:349:ILE:HG23	1:Ak:368:ARG:HD2	1.74	0.70
1:Ay:69:MET:HE3	1:Ay:520:MET:HE2	1.71	0.70
1:Az:80:LYS:HE2	1:Bu:384:ALA:O	1.91	0.70
1:Bu:40:LEU:CB	1:Bu:59:GLU:OE1	2.38	0.70
1:Ad:518:GLU:OE2	1:Ar:36:ARG:HD2	1.90	0.70
1:As:34:LYS:NZ	1:As:483:GLU:CG	2.52	0.70
1:Bn:40:LEU:CB	1:Bn:59:GLU:OE1	2.38	0.70
1:Ay:349:ILE:HG23	1:Ay:368:ARG:HD2	1.74	0.70
1:Bf:111:MET:SD	1:Bf:435:ASP:OD1	2.49	0.70
1:Bf:349:ILE:HG23	1:Bf:368:ARG:HD2	1.74	0.70
1:Al:113:PRO:CG	1:Az:36:ARG:NE	2.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bn:489:ILE:HG22	1:Bn:494:LEU:HD21	1.73	0.70
1:Bt:157:THR:O	1:Bt:161:LEU:CD1	2.39	0.70
1:Bt:489:ILE:HD12	1:Bt:494:LEU:HD21	1.73	0.70
1:Ad:349:ILE:HG23	1:Ad:368:ARG:HD2	1.74	0.69
1:Ar:518:GLU:OE2	1:Bm:36:ARG:HD2	1.90	0.69
1:As:482:THR:HG1	1:As:484:GLU:HG2	1.57	0.69
1:Bm:489:ILE:HD12	1:Bm:494:LEU:HD21	1.73	0.69
2:Af:95:VAL:HB	2:Am:1:MET:HB3	1.74	0.69
1:Al:124:VAL:HG21	1:Al:508:ALA:CB	2.21	0.69
1:Bg:80:LYS:HE2	1:Bn:384:ALA:O	1.91	0.69
1:Bm:111:MET:SD	1:Bm:435:ASP:OD1	2.49	0.69
1:Bt:349:ILE:HG23	1:Bt:368:ARG:HD2	1.74	0.69
1:As:489:ILE:HG22	1:As:494:LEU:HD21	1.73	0.69
1:Az:162:ILE:HG12	1:Az:400:LEU:CD2	2.23	0.69
1:Bm:349:ILE:HG23	1:Bm:368:ARG:HD2	1.74	0.69
1:Bt:161:LEU:HA	1:Bt:164:GLU:OE2	1.93	0.69
1:Ad:161:LEU:HA	1:Ad:164:GLU:OE2	1.93	0.69
1:Ae:69:MET:SD	1:Al:41:ASP:OD1	2.51	0.69
1:Ae:489:ILE:HG22	1:Ae:494:LEU:HD21	1.73	0.69
1:Al:162:ILE:HG12	1:Al:400:LEU:CD2	2.23	0.69
1:Ay:36:ARG:HD2	1:Bt:518:GLU:OE2	1.93	0.69
1:Ay:157:THR:O	1:Ay:161:LEU:CD1	2.39	0.69
1:Bf:82:ASN:HB2	1:Bf:89:THR:OG1	1.91	0.69
1:Bm:180:GLY:O	1:Bm:382:GLY:HA2	1.91	0.69
1:Ar:349:ILE:HG23	1:Ar:368:ARG:HD2	1.74	0.69
1:Ay:161:LEU:HA	1:Ay:164:GLU:OE2	1.93	0.69
1:Ak:161:LEU:HA	1:Ak:164:GLU:OE2	1.93	0.69
1:Bn:162:ILE:HG12	1:Bn:400:LEU:CD2	2.23	0.69
1:Bu:162:ILE:HG12	1:Bu:400:LEU:CD2	2.23	0.69
1:Ae:162:ILE:HG12	1:Ae:400:LEU:CD2	2.23	0.69
1:Ar:161:LEU:HA	1:Ar:164:GLU:OE2	1.93	0.69
1:As:162:ILE:HG12	1:As:400:LEU:CD2	2.23	0.69
1:Bf:489:ILE:HD12	1:Bf:494:LEU:HD21	1.73	0.69
1:Bg:162:ILE:HG12	1:Bg:400:LEU:CD2	2.23	0.69
1:Bg:489:ILE:HG22	1:Bg:494:LEU:HD21	1.73	0.69
1:Bm:176:THR:HG21	1:Bm:333:ILE:HD11	1.75	0.69
1:Bt:176:THR:HG21	1:Bt:333:ILE:HD11	1.75	0.69
1:Ae:63:GLU:CD	1:As:524:LEU:HD11	2.18	0.69
1:Ar:166:MET:HA	1:Ar:170:GLY:HA3	1.75	0.69
1:Bf:36:ARG:HD2	1:Bm:518:GLU:OE2	1.91	0.69
1:Bf:161:LEU:HA	1:Bf:164:GLU:OE2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:111:MET:SD	1:Bt:435:ASP:OD1	2.49	0.69
1:Az:113:PRO:CG	1:Bu:36:ARG:NE	2.54	0.69
1:Ad:365:LEU:CD1	1:Ad:365:LEU:H	2.07	0.68
1:Bg:518:GLU:CD	1:Bn:37:ASN:N	2.33	0.68
1:As:384:ALA:O	1:Bn:80:LYS:HE2	1.93	0.68
1:Ay:176:THR:HG21	1:Ay:333:ILE:HD11	1.75	0.68
1:Ae:41:ASP:OD1	1:As:69:MET:SD	2.51	0.68
1:Ak:366:GLN:HA	1:Ak:369:VAL:HB	1.75	0.68
1:Ar:365:LEU:CD1	1:Ar:365:LEU:H	2.07	0.68
1:Bm:366:GLN:HA	1:Bm:369:VAL:HB	1.75	0.68
1:Ae:69:MET:HE3	1:Al:41:ASP:CG	2.19	0.68
1:Bm:366:GLN:HA	1:Bm:369:VAL:CB	2.24	0.68
1:Bt:366:GLN:HA	1:Bt:369:VAL:CB	2.23	0.68
1:Bf:366:GLN:HA	1:Bf:369:VAL:CB	2.24	0.68
1:Bf:366:GLN:HA	1:Bf:369:VAL:HB	1.75	0.68
1:As:40:LEU:CB	1:As:59:GLU:OE1	2.38	0.68
1:Bf:518:GLU:OE2	1:Bt:36:ARG:HD2	1.91	0.68
1:Bg:49:ILE:HD11	1:Bu:73:MET:SD	2.33	0.68
1:Ad:166:MET:HA	1:Ad:170:GLY:HA3	1.75	0.68
1:Ae:73:MET:SD	1:Al:49:ILE:HD11	2.34	0.68
1:Ae:524:LEU:HD11	1:Al:63:GLU:CD	2.17	0.68
1:Al:80:LYS:HE2	1:Az:384:ALA:O	1.93	0.68
1:Bm:166:MET:HA	1:Bm:170:GLY:HA3	1.75	0.68
1:Bf:181:THR:HA	1:Bf:389:MET:SD	2.34	0.68
1:Ar:176:THR:HG21	1:Ar:333:ILE:HD11	1.75	0.68
1:Ay:366:GLN:HA	1:Ay:369:VAL:HB	1.75	0.68
1:Bf:176:THR:HG21	1:Bf:333:ILE:HD11	1.75	0.68
1:Ad:164:GLU:HG3	1:Ad:187:LEU:HD22	1.76	0.68
1:Ad:366:GLN:HA	1:Ad:369:VAL:HB	1.75	0.68
1:Ak:365:LEU:CD1	1:Ak:365:LEU:H	2.07	0.68
1:Ar:16:MET:HE2	1:Ar:514:MET:CE	2.24	0.68
1:As:7:LYS:CD	1:As:66:PHE:CE2	2.78	0.68
1:Bg:41:ASP:OD1	1:Bu:69:MET:SD	2.52	0.68
1:Az:73:MET:SD	1:Bu:49:ILE:HD11	2.34	0.67
1:Bt:168:LYS:HZ1	1:Bt:187:LEU:HG	1.59	0.67
1:Bt:181:THR:HA	1:Bt:389:MET:SD	2.34	0.67
1:Ad:366:GLN:HA	1:Ad:369:VAL:CB	2.24	0.67
1:Ad:181:THR:HA	1:Ad:389:MET:SD	2.34	0.67
1:Ar:164:GLU:HG3	1:Ar:187:LEU:HD22	1.76	0.67
1:Ar:366:GLN:HA	1:Ar:369:VAL:CB	2.24	0.67
1:Ay:181:THR:HA	1:Ay:389:MET:SD	2.34	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:7:LYS:CD	1:Bg:66:PHE:CE2	2.77	0.67
1:Bg:34:LYS:HZ1	1:Bg:483:GLU:HG3	1.56	0.67
1:Bm:365:LEU:CD1	1:Bm:365:LEU:H	2.07	0.67
1:Ad:16:MET:HE2	1:Ad:514:MET:CE	2.24	0.67
1:Ae:80:LYS:HE2	1:Al:384:ALA:O	1.94	0.67
1:Ak:164:GLU:HG3	1:Ak:187:LEU:HD22	1.76	0.67
1:Ar:181:THR:HA	1:Ar:389:MET:SD	2.34	0.67
1:As:49:ILE:HD11	1:Bn:73:MET:SD	2.34	0.67
1:Ay:366:GLN:HA	1:Ay:369:VAL:CB	2.23	0.67
1:Bg:482:THR:HG1	1:Bg:484:GLU:HG2	1.57	0.67
1:Bt:366:GLN:HA	1:Bt:369:VAL:HB	1.75	0.67
1:Ad:291:ASP:HA	1:Ad:345:ARG:HE	1.60	0.67
1:Ad:353:ILE:CD1	1:Ad:366:GLN:HB3	2.24	0.67
1:Ae:49:ILE:HD11	1:As:73:MET:SD	2.34	0.67
1:Bf:69:MET:O	1:Bf:73:MET:HG3	1.94	0.67
1:Bm:161:LEU:HA	1:Bm:164:GLU:OE2	1.93	0.67
1:Ae:518:GLU:OE1	1:Al:37:ASN:C	2.36	0.67
1:Ak:181:THR:HA	1:Ak:389:MET:SD	2.34	0.67
1:Ay:16:MET:HE2	1:Ay:514:MET:CE	2.24	0.67
1:Bg:73:MET:SD	1:Bn:49:ILE:HD11	2.34	0.67
1:Bm:16:MET:HE2	1:Bm:514:MET:CE	2.24	0.67
1:Bt:353:ILE:CD1	1:Bt:366:GLN:HB3	2.24	0.67
1:Ak:353:ILE:CD1	1:Ak:366:GLN:HB3	2.24	0.67
1:Ar:353:ILE:HG12	1:Ar:366:GLN:OE1	1.95	0.67
1:Bt:16:MET:HE2	1:Bt:514:MET:CE	2.24	0.67
1:Ae:384:ALA:O	1:As:80:LYS:HE2	1.95	0.67
1:Ak:391:GLU:OE2	1:Ak:395:ARG:HD2	1.95	0.67
1:Bg:63:GLU:CD	1:Bu:524:LEU:HD11	2.19	0.67
1:Bt:291:ASP:HA	1:Bt:345:ARG:HE	1.60	0.67
1:Ad:421:ARG:NH2	1:Ad:476:TYR:O	2.28	0.67
1:Ar:353:ILE:CD1	1:Ar:366:GLN:HB3	2.24	0.67
1:As:41:ASP:OD1	1:Bn:69:MET:SD	2.52	0.67
1:Bf:291:ASP:HA	1:Bf:345:ARG:HE	1.60	0.67
1:Bg:41:ASP:CG	1:Bu:69:MET:HE3	2.20	0.67
1:Bg:69:MET:SD	1:Bn:41:ASP:OD1	2.53	0.67
1:Bg:386:GLU:OE2	1:Bu:76:GLU:HG2	1.95	0.67
1:Ad:391:GLU:OE2	1:Ad:395:ARG:HD2	1.95	0.67
1:Ae:7:LYS:CD	1:Ae:66:PHE:CE2	2.77	0.67
1:Ak:166:MET:HA	1:Ak:170:GLY:HA3	1.75	0.67
1:Ak:353:ILE:HG12	1:Ak:366:GLN:OE1	1.95	0.67
1:Ay:421:ARG:NH2	1:Ay:476:TYR:O	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:181:THR:HA	1:Bm:389:MET:SD	2.34	0.67
1:Bt:166:MET:HA	1:Bt:170:GLY:HA3	1.75	0.67
1:Ak:16:MET:HE2	1:Ak:514:MET:CE	2.24	0.66
1:Ak:176:THR:HG21	1:Ak:333:ILE:HD11	1.75	0.66
1:Bf:16:MET:HE2	1:Bf:514:MET:CE	2.24	0.66
1:Bf:421:ARG:NH2	1:Bf:476:TYR:O	2.28	0.66
1:Bm:291:ASP:HA	1:Bm:345:ARG:HE	1.60	0.66
1:Bm:363:GLU:CA	1:Bm:366:GLN:NE2	2.28	0.66
1:Bt:164:GLU:HG3	1:Bt:187:LEU:HD22	1.76	0.66
1:Ad:164:GLU:CG	1:Ad:187:LEU:HD22	2.25	0.66
1:Ad:176:THR:HG21	1:Ad:333:ILE:HD11	1.75	0.66
1:Ak:366:GLN:HA	1:Ak:369:VAL:CB	2.24	0.66
1:As:386:GLU:OE2	1:Bn:76:GLU:HG2	1.96	0.66
1:Bf:166:MET:HA	1:Bf:170:GLY:HA3	1.75	0.66
1:Bf:353:ILE:CD1	1:Bf:366:GLN:HB3	2.25	0.66
1:Bm:421:ARG:NH2	1:Bm:476:TYR:O	2.28	0.66
1:Bn:7:LYS:CD	1:Bn:66:PHE:CE2	2.78	0.66
1:Ar:69:MET:O	1:Ar:73:MET:HG3	1.95	0.66
1:Ar:363:GLU:CA	1:Ar:366:GLN:NE2	2.28	0.66
1:Bf:164:GLU:HG3	1:Bf:187:LEU:HD22	1.76	0.66
1:Bm:353:ILE:CD1	1:Bm:366:GLN:HB3	2.24	0.66
1:Bt:421:ARG:NH2	1:Bt:476:TYR:O	2.28	0.66
1:Bu:7:LYS:CD	1:Bu:66:PHE:CE2	2.78	0.66
1:Ad:69:MET:O	1:Ad:73:MET:HG3	1.95	0.66
1:Ak:291:ASP:HA	1:Ak:345:ARG:HE	1.60	0.66
1:Al:69:MET:SD	1:Az:41:ASP:OD1	2.53	0.66
1:Ar:366:GLN:HA	1:Ar:369:VAL:HB	1.75	0.66
1:Ar:391:GLU:OE2	1:Ar:395:ARG:HD2	1.95	0.66
1:As:111:MET:CE	1:As:438:VAL:HG21	2.25	0.66
1:Bf:365:LEU:CD1	1:Bf:365:LEU:H	2.07	0.66
1:Bm:164:GLU:CG	1:Bm:187:LEU:HD22	2.25	0.66
1:Bn:138:CYS:SG	1:Bn:143:ALA:CB	2.84	0.66
1:Ad:161:LEU:HD12	1:Ad:161:LEU:N	2.11	0.66
1:Al:73:MET:SD	1:Az:49:ILE:HD11	2.35	0.66
1:Ay:166:MET:HA	1:Ay:170:GLY:HA3	1.75	0.66
1:Bf:193:MET:SD	1:Bf:372:LEU:HD22	2.35	0.66
1:Bm:164:GLU:HG3	1:Bm:187:LEU:HD22	1.76	0.66
1:Ad:284:ARG:CD	1:Ad:364:LYS:CG	2.74	0.66
1:Ak:363:GLU:CA	1:Ak:366:GLN:NE2	2.28	0.66
1:Ak:421:ARG:NH2	1:Ak:476:TYR:O	2.28	0.66
1:Ar:164:GLU:CG	1:Ar:187:LEU:HD22	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:365:LEU:CD1	1:Ay:365:LEU:H	2.07	0.66
1:Bg:138:CYS:SG	1:Bg:143:ALA:CB	2.84	0.66
1:Bt:193:MET:SD	1:Bt:372:LEU:HD22	2.36	0.66
1:Ae:518:GLU:CD	1:Al:37:ASN:N	2.28	0.66
1:Ar:421:ARG:NH2	1:Ar:476:TYR:O	2.28	0.66
1:Ay:164:GLU:CG	1:Ay:187:LEU:HD22	2.25	0.66
1:Ay:353:ILE:CD1	1:Ay:366:GLN:HB3	2.24	0.66
1:Ae:76:GLU:HG2	1:Al:386:GLU:OE2	1.95	0.66
1:Ae:138:CYS:SG	1:Ae:143:ALA:CB	2.84	0.66
1:Ak:321:LYS:HB2	1:Ak:334:ASP:HB3	1.78	0.66
1:Al:138:CYS:SG	1:Al:143:ALA:CB	2.84	0.66
1:As:138:CYS:SG	1:As:143:ALA:CB	2.84	0.66
1:Ay:69:MET:O	1:Ay:73:MET:HG3	1.95	0.66
1:Az:138:CYS:SG	1:Az:143:ALA:CB	2.84	0.66
1:Bt:353:ILE:HG12	1:Bt:366:GLN:OE1	1.95	0.66
1:Bt:365:LEU:CD1	1:Bt:365:LEU:H	2.07	0.66
1:Bu:138:CYS:SG	1:Bu:143:ALA:CB	2.84	0.66
1:Ak:161:LEU:HD12	1:Ak:161:LEU:N	2.11	0.66
1:Ar:161:LEU:HD12	1:Ar:161:LEU:N	2.11	0.66
1:Ay:164:GLU:HG3	1:Ay:187:LEU:HD22	1.76	0.66
1:Ay:291:ASP:HA	1:Ay:345:ARG:HE	1.60	0.66
1:Az:518:GLU:HG3	1:Bu:36:ARG:CD	2.25	0.66
1:Bm:69:MET:O	1:Bm:73:MET:HG3	1.95	0.66
1:Bm:321:LYS:HB2	1:Bm:334:ASP:HB3	1.78	0.66
1:Bt:164:GLU:CG	1:Bt:187:LEU:HD22	2.25	0.66
1:Ak:69:MET:O	1:Ak:73:MET:HG3	1.95	0.66
1:Al:76:GLU:HG2	1:Az:386:GLU:OE2	1.96	0.66
1:Ar:291:ASP:HA	1:Ar:345:ARG:HE	1.60	0.66
1:As:41:ASP:CG	1:Bn:69:MET:HE3	2.21	0.66
1:Ay:193:MET:SD	1:Ay:372:LEU:HD22	2.35	0.66
1:Ay:391:GLU:OE2	1:Ay:395:ARG:HD2	1.95	0.66
1:Bf:353:ILE:HG12	1:Bf:366:GLN:OE1	1.95	0.66
1:Bg:76:GLU:HG2	1:Bn:386:GLU:OE2	1.96	0.66
1:Ad:321:LYS:HB2	1:Ad:334:ASP:HB3	1.78	0.65
1:Ak:193:MET:SD	1:Ak:372:LEU:HD22	2.35	0.65
1:Al:7:LYS:CD	1:Al:66:PHE:CE2	2.77	0.65
1:Bt:69:MET:O	1:Bt:73:MET:HG3	1.95	0.65
1:Ad:36:ARG:HH11	1:Ak:518:GLU:CD	2.03	0.65
1:Ae:47:PRO:HG2	1:As:73:MET:CG	2.26	0.65
1:Ak:284:ARG:CD	1:Ak:364:LYS:CG	2.74	0.65
1:Al:518:GLU:OE1	1:Az:37:ASN:C	2.39	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:321:LYS:HB2	1:Ar:334:ASP:HB3	1.78	0.65
1:Az:7:LYS:CD	1:Az:66:PHE:CE2	2.77	0.65
1:Bf:164:GLU:CG	1:Bf:187:LEU:HD22	2.25	0.65
1:Bf:321:LYS:HB2	1:Bf:334:ASP:HB3	1.78	0.65
1:Bm:193:MET:SD	1:Bm:372:LEU:HD22	2.35	0.65
1:Bm:353:ILE:HG12	1:Bm:366:GLN:OE1	1.95	0.65
1:Ad:353:ILE:HG12	1:Ad:366:GLN:OE1	1.95	0.65
1:Ae:386:GLU:OE2	1:As:76:GLU:HG2	1.96	0.65
1:Ak:111:MET:HB2	1:Ak:116:LEU:HD11	1.79	0.65
1:Ak:164:GLU:CG	1:Ak:187:LEU:HD22	2.25	0.65
1:Al:69:MET:HE3	1:Az:41:ASP:CG	2.21	0.65
1:As:37:ASN:C	1:Bn:518:GLU:OE1	2.39	0.65
1:Ay:111:MET:HB2	1:Ay:116:LEU:HD11	1.79	0.65
1:Ay:321:LYS:HB2	1:Ay:334:ASP:HB3	1.78	0.65
1:Az:24:ALA:HB3	1:Az:97:GLN:OE1	1.96	0.65
1:Bm:391:GLU:OE2	1:Bm:395:ARG:HD2	1.95	0.65
1:Bu:24:ALA:HB3	1:Bu:97:GLN:OE1	1.96	0.65
1:Ad:193:MET:SD	1:Ad:372:LEU:HD22	2.35	0.65
1:Ar:193:MET:SD	1:Ar:372:LEU:HD22	2.35	0.65
1:Az:69:MET:HE3	1:Bu:41:ASP:CG	2.22	0.65
1:Ae:41:ASP:CG	1:As:69:MET:HE3	2.21	0.65
1:Ay:353:ILE:HG12	1:Ay:366:GLN:OE1	1.95	0.65
1:Bg:111:MET:CE	1:Bg:438:VAL:HG21	2.25	0.65
1:Ae:37:ASN:C	1:As:518:GLU:OE1	2.39	0.65
1:Ae:111:MET:CE	1:Ae:438:VAL:HG21	2.25	0.65
1:Ae:518:GLU:OE1	1:Al:37:ASN:CA	2.45	0.65
1:Al:518:GLU:HG3	1:Az:36:ARG:CD	2.27	0.65
1:Bf:391:GLU:OE2	1:Bf:395:ARG:HD2	1.95	0.65
1:Bg:524:LEU:HD11	1:Bn:63:GLU:CD	2.19	0.65
1:Bt:391:GLU:OE2	1:Bt:395:ARG:HD2	1.95	0.65
2:Af:96:GLU:O	2:Am:2:ASN:N	2.29	0.65
1:Bf:161:LEU:N	1:Bf:161:LEU:HD12	2.11	0.65
1:Bg:69:MET:HE3	1:Bn:41:ASP:CG	2.21	0.65
1:Ay:168:LYS:HZ1	1:Ay:187:LEU:CG	2.10	0.65
1:Az:69:MET:SD	1:Bu:41:ASP:OD1	2.54	0.65
1:Az:111:MET:CE	1:Az:438:VAL:HG21	2.25	0.65
1:Bt:284:ARG:CD	1:Bt:364:LYS:CG	2.74	0.65
1:Ad:111:MET:HB2	1:Ad:116:LEU:HD11	1.79	0.65
1:Bm:391:GLU:OE1	1:Bm:392:LYS:HG3	1.97	0.65
1:Bt:321:LYS:HB2	1:Bt:334:ASP:HB3	1.78	0.65
1:Ad:391:GLU:OE1	1:Ad:392:LYS:HG3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:34:LYS:HZ1	1:Bu:483:GLU:CG	2.08	0.64
1:Ae:34:LYS:NZ	1:Ae:483:GLU:HG3	2.13	0.64
1:Ay:391:GLU:OE1	1:Ay:392:LYS:HG3	1.97	0.64
1:Bf:363:GLU:CA	1:Bf:366:GLN:NE2	2.28	0.64
1:Bt:111:MET:HB2	1:Bt:116:LEU:HD11	1.79	0.64
1:Bt:164:GLU:HA	1:Bt:167:ASP:HB2	1.79	0.64
1:Bt:391:GLU:OE1	1:Bt:392:LYS:HG3	1.97	0.64
1:As:34:LYS:NZ	1:As:483:GLU:HG3	2.13	0.64
1:Az:76:GLU:HG2	1:Bu:386:GLU:OE2	1.96	0.64
1:Bn:34:LYS:NZ	1:Bn:483:GLU:HG3	2.13	0.64
1:Ak:168:LYS:HZ1	1:Ak:187:LEU:HG	1.61	0.64
1:Ay:161:LEU:HD12	1:Ay:161:LEU:N	2.11	0.64
1:Bg:36:ARG:CD	1:Bu:518:GLU:HG3	2.27	0.64
1:Bg:162:ILE:HG12	1:Bg:400:LEU:HD21	1.80	0.64
1:Bg:518:GLU:HG3	1:Bn:36:ARG:CD	2.28	0.64
1:Bm:164:GLU:HA	1:Bm:167:ASP:HB2	1.79	0.64
1:Ae:73:MET:CG	1:Al:47:PRO:HG2	2.28	0.64
1:Ae:482:THR:HG1	1:Ae:484:GLU:HG2	1.62	0.64
1:Al:524:LEU:HD11	1:Az:63:GLU:CD	2.20	0.64
1:Az:524:LEU:HD11	1:Bu:63:GLU:CD	2.21	0.64
1:Bf:164:GLU:HA	1:Bf:167:ASP:HB2	1.79	0.64
1:Bu:162:ILE:HG12	1:Bu:400:LEU:HD21	1.80	0.64
1:Ak:391:GLU:OE1	1:Ak:392:LYS:HG3	1.97	0.64
1:Al:162:ILE:HG12	1:Al:400:LEU:HD21	1.80	0.64
1:As:23:LEU:HD21	1:As:57:ALA:HA	1.80	0.64
1:Ay:164:GLU:HA	1:Ay:167:ASP:HB2	1.80	0.64
1:Bf:391:GLU:OE1	1:Bf:392:LYS:HG3	1.97	0.64
1:Bg:37:ASN:C	1:Bu:518:GLU:OE1	2.40	0.64
1:Ae:69:MET:CE	1:Al:41:ASP:CG	2.70	0.64
1:As:36:ARG:CD	1:Bn:518:GLU:HG3	2.28	0.64
1:Az:23:LEU:HD21	1:Az:57:ALA:HA	1.80	0.64
1:Bf:142:LYS:HG3	1:Bf:146:GLN:HE22	1.62	0.64
1:Bg:41:ASP:CG	1:Bu:69:MET:CE	2.70	0.64
1:Bg:87:ASP:OD1	1:Bg:88:GLY:N	2.29	0.64
1:Bm:161:LEU:HD12	1:Bm:161:LEU:N	2.11	0.64
1:Bn:23:LEU:HD21	1:Bn:57:ALA:HA	1.80	0.64
1:Bn:162:ILE:HG12	1:Bn:400:LEU:HD21	1.80	0.64
1:Ae:23:LEU:HD21	1:Ae:57:ALA:HA	1.80	0.64
1:Al:23:LEU:HD21	1:Al:57:ALA:HA	1.80	0.64
1:Ar:391:GLU:OE1	1:Ar:392:LYS:HG3	1.97	0.64
1:Ar:518:GLU:CD	1:Bm:36:ARG:HH11	2.05	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:162:ILE:HG12	1:Az:400:LEU:HD21	1.80	0.64
1:Bm:111:MET:HB2	1:Bm:116:LEU:HD11	1.79	0.64
1:Bt:161:LEU:N	1:Bt:161:LEU:HD12	2.11	0.64
1:Bu:34:LYS:NZ	1:Bu:483:GLU:HG3	2.13	0.64
1:Ae:36:ARG:CD	1:As:518:GLU:HG3	2.28	0.64
1:Ak:42:LYS:HE2	1:Ak:46:ALA:O	1.98	0.64
1:Bf:42:LYS:HE2	1:Bf:46:ALA:O	1.98	0.64
1:Bu:87:ASP:OD1	1:Bu:88:GLY:N	2.29	0.64
1:Ad:42:LYS:HE2	1:Ad:46:ALA:O	1.98	0.63
1:Ad:518:GLU:CD	1:Ar:36:ARG:HH11	2.06	0.63
1:Ae:3:ALA:O	1:Ae:524:LEU:CD1	2.46	0.63
1:Ae:162:ILE:HG12	1:Ae:400:LEU:HD21	1.80	0.63
1:Al:3:ALA:O	1:Al:524:LEU:CD1	2.46	0.63
1:Ar:42:LYS:HE2	1:Ar:46:ALA:O	1.98	0.63
1:Ar:142:LYS:HG3	1:Ar:146:GLN:HE22	1.62	0.63
1:Ay:42:LYS:HE2	1:Ay:46:ALA:O	1.98	0.63
1:Bm:284:ARG:CD	1:Bm:364:LYS:CG	2.74	0.63
1:Bt:42:LYS:HE2	1:Bt:46:ALA:O	1.98	0.63
1:Bt:363:GLU:CA	1:Bt:366:GLN:NE2	2.28	0.63
1:Bu:23:LEU:HD21	1:Bu:57:ALA:HA	1.80	0.63
1:As:162:ILE:HG12	1:As:400:LEU:HD21	1.80	0.63
1:Ay:349:ILE:CG2	1:Ay:368:ARG:HD2	2.29	0.63
1:Bf:36:ARG:HH11	1:Bm:518:GLU:CD	2.05	0.63
1:Bg:34:LYS:NZ	1:Bg:483:GLU:HG3	2.13	0.63
1:Bt:349:ILE:CG2	1:Bt:368:ARG:HD2	2.29	0.63
1:Az:518:GLU:OE1	1:Bu:37:ASN:C	2.42	0.63
1:Bf:168:LYS:HZ1	1:Bf:187:LEU:CG	2.12	0.63
1:Bg:518:GLU:OE1	1:Bn:37:ASN:C	2.40	0.63
1:Ar:164:GLU:HA	1:Ar:167:ASP:HB2	1.79	0.63
1:Az:477:GLY:CA	1:Az:488:MET:HE3	2.29	0.63
1:Ak:163:ALA:O	1:Ak:167:ASP:CG	2.42	0.63
1:Ak:193:MET:HE3	1:Ak:371:LYS:HD2	1.81	0.63
1:Bf:111:MET:HB2	1:Bf:116:LEU:HD11	1.79	0.63
1:Bf:518:GLU:CD	1:Bt:36:ARG:HH11	2.06	0.63
1:Bn:34:LYS:HZ2	1:Bn:483:GLU:CG	2.11	0.63
1:Ad:193:MET:HE3	1:Ad:371:LYS:HD2	1.81	0.63
1:Ae:24:ALA:CB	1:Ae:97:GLN:CD	2.72	0.63
1:Ae:41:ASP:CG	1:As:69:MET:CE	2.71	0.63
1:Ak:36:ARG:HH11	1:Ay:518:GLU:CD	2.06	0.63
1:Al:34:LYS:NZ	1:Al:483:GLU:HG3	2.13	0.63
1:As:477:GLY:CA	1:As:488:MET:HE3	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:3:ALA:O	1:Az:524:LEU:CD1	2.46	0.63
1:Bf:163:ALA:O	1:Bf:167:ASP:CG	2.42	0.63
1:Ad:163:ALA:O	1:Ad:167:ASP:CG	2.42	0.63
1:Ae:63:GLU:OE1	1:As:524:LEU:HD13	1.99	0.63
1:Ak:164:GLU:HA	1:Ak:167:ASP:HB2	1.80	0.63
1:Ak:398:ASP:HA	1:Ak:401:HIS:ND1	2.14	0.63
1:Al:69:MET:CE	1:Az:41:ASP:CG	2.72	0.63
1:Al:111:MET:CE	1:Al:438:VAL:HG21	2.25	0.63
1:Ar:383:ALA:HB1	1:Ar:388:GLU:HG3	1.81	0.63
1:As:63:GLU:CD	1:Bn:524:LEU:HD11	2.19	0.63
1:Bg:23:LEU:HD21	1:Bg:57:ALA:HA	1.80	0.63
1:Bm:163:ALA:O	1:Bm:167:ASP:CG	2.42	0.63
1:Bn:164:GLU:O	1:Bn:167:ASP:HB2	1.99	0.63
1:Ad:349:ILE:CG2	1:Ad:368:ARG:HD2	2.29	0.63
1:Ae:164:GLU:O	1:Ae:167:ASP:HB2	1.99	0.63
1:Ar:349:ILE:CG2	1:Ar:368:ARG:HD2	2.29	0.63
1:As:164:GLU:O	1:As:167:ASP:HB2	1.99	0.63
1:Ay:163:ALA:O	1:Ay:167:ASP:CG	2.42	0.63
1:Az:69:MET:CE	1:Bu:41:ASP:CG	2.72	0.63
1:Bf:15:LYS:HE2	1:Bf:18:ARG:HH12	1.64	0.63
1:Bf:134:LEU:CD1	1:Bf:425:LYS:HZ1	1.95	0.63
1:Bg:69:MET:CE	1:Bn:41:ASP:CG	2.72	0.63
1:Bm:42:LYS:HE2	1:Bm:46:ALA:O	1.98	0.63
1:Bu:111:MET:CE	1:Bu:438:VAL:HG21	2.25	0.63
1:Ad:398:ASP:HA	1:Ad:401:HIS:ND1	2.14	0.63
1:Ae:477:GLY:CA	1:Ae:488:MET:HE3	2.29	0.63
2:Af:66:ILE:HG13	2:Am:3:ILE:HD12	1.79	0.63
1:Ar:15:LYS:HE2	1:Ar:18:ARG:HH12	1.64	0.63
1:Ar:111:MET:HB2	1:Ar:116:LEU:HD11	1.79	0.63
1:As:3:ALA:O	1:As:524:LEU:CD1	2.46	0.63
1:Ay:398:ASP:HA	1:Ay:401:HIS:ND1	2.14	0.63
1:Bn:87:ASP:OD1	1:Bn:88:GLY:N	2.29	0.63
1:Bt:163:ALA:O	1:Bt:167:ASP:CG	2.42	0.63
1:Ad:164:GLU:HA	1:Ad:167:ASP:HB2	1.79	0.62
1:Ad:383:ALA:HB1	1:Ad:388:GLU:HG3	1.81	0.62
2:Af:95:VAL:HA	2:Am:3:ILE:HA	1.80	0.62
1:As:24:ALA:CB	1:As:97:GLN:CD	2.72	0.62
1:As:41:ASP:CG	1:Bn:69:MET:CE	2.71	0.62
1:Ay:193:MET:HE3	1:Ay:371:LYS:HD2	1.81	0.62
1:Bm:383:ALA:HB1	1:Bm:388:GLU:HG3	1.81	0.62
1:Bm:398:ASP:HA	1:Bm:401:HIS:ND1	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:15:LYS:HE2	1:Bt:18:ARG:HH12	1.64	0.62
1:Bt:349:ILE:HD13	1:Bt:368:ARG:HG2	1.81	0.62
1:Al:518:GLU:CD	1:Az:37:ASN:N	2.31	0.62
1:Ar:193:MET:HE3	1:Ar:371:LYS:HD2	1.81	0.62
1:Bf:36:ARG:NE	1:Bm:114:MET:CE	2.40	0.62
1:Bf:398:ASP:HA	1:Bf:401:HIS:ND1	2.14	0.62
1:Bg:47:PRO:HG2	1:Bu:73:MET:CG	2.28	0.62
1:As:47:PRO:HG2	1:Bn:73:MET:CG	2.29	0.62
1:Az:34:LYS:NZ	1:Az:483:GLU:HG3	2.13	0.62
1:Bg:164:GLU:O	1:Bg:167:ASP:HB2	1.99	0.62
1:Bn:477:GLY:CA	1:Bn:488:MET:HE3	2.29	0.62
1:Bu:54:VAL:CB	1:Bu:82:ASN:HD22	2.12	0.62
1:Ae:288:MET:HE1	1:Ae:371:LYS:NZ	2.15	0.62
1:Ak:349:ILE:CG2	1:Ak:368:ARG:HD2	2.29	0.62
1:Az:131:LEU:HD11	1:Az:500:THR:HG22	1.82	0.62
1:Ae:34:LYS:HZ1	1:Ae:483:GLU:CG	2.09	0.62
1:As:87:ASP:OD1	1:As:88:GLY:N	2.29	0.62
1:Ay:349:ILE:HD13	1:Ay:368:ARG:HG2	1.81	0.62
1:Bf:383:ALA:HB1	1:Bf:388:GLU:HG3	1.81	0.62
1:Bm:349:ILE:CG2	1:Bm:368:ARG:HD2	2.29	0.62
1:Ae:498:LYS:HG3	1:Ae:501:ARG:HH21	1.65	0.62
1:Bg:288:MET:HE1	1:Bg:371:LYS:NZ	2.15	0.62
1:Bm:168:LYS:HZ1	1:Bm:187:LEU:CG	2.12	0.62
1:Bt:193:MET:HE3	1:Bt:371:LYS:HD2	1.81	0.62
1:Bu:3:ALA:O	1:Bu:524:LEU:CD1	2.46	0.62
1:Bu:288:MET:HE1	1:Bu:371:LYS:NZ	2.15	0.62
1:Bu:477:GLY:CA	1:Bu:488:MET:HE3	2.29	0.62
1:Al:54:VAL:CB	1:Al:82:ASN:HD22	2.12	0.62
1:Al:518:GLU:OE1	1:Az:37:ASN:CA	2.48	0.62
1:Ar:168:LYS:HZ1	1:Ar:187:LEU:CG	2.13	0.62
1:Bn:24:ALA:CB	1:Bn:97:GLN:CD	2.72	0.62
1:Bu:131:LEU:HD11	1:Bu:500:THR:HG22	1.82	0.62
1:Al:34:LYS:HZ1	1:Al:483:GLU:CG	2.12	0.62
1:Al:131:LEU:HD11	1:Al:500:THR:HG22	1.82	0.62
1:Ay:36:ARG:HH11	1:Bt:518:GLU:CD	2.07	0.62
1:Ay:164:GLU:O	1:Ay:167:ASP:HB2	2.00	0.62
1:Az:288:MET:HE1	1:Az:371:LYS:NZ	2.15	0.62
1:Bf:164:GLU:O	1:Bf:167:ASP:HB2	2.00	0.62
1:Bn:3:ALA:O	1:Bn:524:LEU:CD1	2.46	0.62
1:Ad:164:GLU:O	1:Ad:167:ASP:HB2	2.00	0.62
1:Ak:284:ARG:HD2	1:Ak:364:LYS:HG2	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:383:ALA:HB1	1:Ak:388:GLU:HG3	1.81	0.62
1:Al:477:GLY:CA	1:Al:488:MET:HE3	2.29	0.62
1:Ar:398:ASP:HA	1:Ar:401:HIS:ND1	2.14	0.62
1:As:54:VAL:CB	1:As:82:ASN:HD22	2.12	0.62
1:Ay:183:LEU:HG	1:Ay:384:ALA:CA	2.30	0.62
1:Az:54:VAL:CB	1:Az:82:ASN:HD22	2.12	0.62
1:Bn:54:VAL:CB	1:Bn:82:ASN:HD22	2.12	0.62
1:Bt:398:ASP:HA	1:Bt:401:HIS:ND1	2.14	0.62
1:Al:164:GLU:O	1:Al:167:ASP:HB2	1.99	0.62
1:Ar:163:ALA:O	1:Ar:167:ASP:CG	2.42	0.62
1:Az:87:ASP:OD1	1:Az:88:GLY:N	2.29	0.62
1:Bf:349:ILE:CG2	1:Bf:368:ARG:HD2	2.29	0.62
1:Bg:54:VAL:CB	1:Bg:82:ASN:HD22	2.12	0.62
1:Bg:477:GLY:CA	1:Bg:488:MET:HE3	2.29	0.62
1:Bn:34:LYS:HZ2	1:Bn:483:GLU:HG3	1.65	0.62
1:Ad:349:ILE:HD13	1:Ad:368:ARG:HG2	1.81	0.61
1:Ad:383:ALA:HB1	1:Ad:388:GLU:CD	2.25	0.61
1:Ae:37:ASN:CA	1:As:518:GLU:OE1	2.48	0.61
1:Ae:54:VAL:CB	1:Ae:82:ASN:HD22	2.12	0.61
1:Ay:134:LEU:CD1	1:Ay:425:LYS:HZ1	2.00	0.61
1:Bf:349:ILE:HD13	1:Bf:368:ARG:HG2	1.81	0.61
1:Bg:3:ALA:O	1:Bg:524:LEU:CD1	2.46	0.61
1:Bg:73:MET:CG	1:Bn:47:PRO:HG2	2.29	0.61
1:Bm:349:ILE:HD13	1:Bm:368:ARG:HG2	1.81	0.61
1:Bt:383:ALA:HB1	1:Bt:388:GLU:HG3	1.81	0.61
1:Ae:131:LEU:HD11	1:Ae:500:THR:HG22	1.82	0.61
1:Bm:193:MET:HE3	1:Bm:371:LYS:HD2	1.81	0.61
1:Bn:288:MET:HE1	1:Bn:371:LYS:NZ	2.15	0.61
1:Bu:138:CYS:SG	1:Bu:143:ALA:HB1	2.40	0.61
1:Al:73:MET:CG	1:Az:47:PRO:HG2	2.30	0.61
1:Ar:284:ARG:HD2	1:Ar:364:LYS:HG2	1.79	0.61
1:Ar:383:ALA:HB1	1:Ar:388:GLU:CD	2.25	0.61
1:As:288:MET:HE1	1:As:371:LYS:NZ	2.15	0.61
1:As:480:ALA:O	1:As:483:GLU:HG3	2.01	0.61
2:At:1:MET:HB3	2:Bo:95:VAL:HB	1.82	0.61
1:Bg:37:ASN:CA	1:Bu:518:GLU:OE1	2.48	0.61
1:Bn:111:MET:CE	1:Bn:438:VAL:HG21	2.25	0.61
1:Bt:164:GLU:O	1:Bt:167:ASP:HB2	2.00	0.61
1:Bu:24:ALA:CB	1:Bu:97:GLN:CD	2.72	0.61
2:Af:6:LEU:HD23	2:At:92:LEU:C	2.25	0.61
1:Ay:428:ASP:O	1:Ay:430:ARG:HG2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:193:MET:HE3	1:Bf:371:LYS:HD2	1.81	0.61
1:Bg:498:LYS:HG3	1:Bg:501:ARG:HH21	1.65	0.61
1:Bm:428:ASP:O	1:Bm:430:ARG:HG2	2.01	0.61
1:Ak:183:LEU:HG	1:Ak:384:ALA:CA	2.30	0.61
1:Ak:349:ILE:HD13	1:Ak:368:ARG:HG2	1.81	0.61
1:Al:288:MET:HE1	1:Al:371:LYS:NZ	2.15	0.61
1:Al:480:ALA:O	1:Al:483:GLU:HG3	2.01	0.61
1:Bg:138:CYS:SG	1:Bg:143:ALA:HB1	2.40	0.61
1:Bt:428:ASP:O	1:Bt:430:ARG:HG2	2.01	0.61
1:Ae:385:THR:OG1	1:Ae:387:VAL:HG12	2.01	0.61
1:Ae:524:LEU:HD13	1:Al:63:GLU:OE1	2.01	0.61
1:Ar:80:LYS:O	1:Ar:83:ASP:OD1	2.19	0.61
1:As:37:ASN:CA	1:Bn:518:GLU:OE1	2.48	0.61
1:Ay:363:GLU:CA	1:Ay:366:GLN:NE2	2.28	0.61
1:Ay:383:ALA:HB1	1:Ay:388:GLU:HG3	1.81	0.61
1:Az:518:GLU:HG3	1:Bu:36:ARG:HD2	1.83	0.61
1:Bg:24:ALA:CB	1:Bg:97:GLN:CD	2.72	0.61
1:Bn:480:ALA:O	1:Bn:483:GLU:HG3	2.01	0.61
1:Bu:164:GLU:O	1:Bu:167:ASP:HB2	1.99	0.61
1:Ad:80:LYS:O	1:Ad:83:ASP:OD1	2.19	0.61
1:Ak:383:ALA:HB1	1:Ak:388:GLU:CD	2.25	0.61
1:Al:385:THR:OG1	1:Al:387:VAL:HG12	2.01	0.61
1:Al:498:LYS:HG3	1:Al:501:ARG:HH21	1.65	0.61
1:Ar:6:VAL:CG2	1:Ar:521:VAL:HG13	2.24	0.61
1:Ar:349:ILE:HD13	1:Ar:368:ARG:HG2	1.81	0.61
1:As:385:THR:OG1	1:As:387:VAL:HG12	2.01	0.61
1:Ay:349:ILE:HB	1:Ay:369:VAL:HG22	1.83	0.61
1:Bf:383:ALA:HB1	1:Bf:388:GLU:CD	2.25	0.61
1:Bm:6:VAL:CG2	1:Bm:521:VAL:HG13	2.24	0.61
1:Ad:142:LYS:HG3	1:Ad:146:GLN:HE22	1.62	0.61
1:Ad:183:LEU:HG	1:Ad:384:ALA:CA	2.30	0.61
1:Ad:288:MET:HE1	1:Ad:364:LYS:HE3	1.83	0.61
1:Ae:138:CYS:SG	1:Ae:143:ALA:HB1	2.40	0.61
1:Ae:518:GLU:HG3	1:Al:36:ARG:CD	2.31	0.61
1:Az:480:ALA:O	1:Az:483:GLU:HG3	2.01	0.61
1:Bf:183:LEU:HG	1:Bf:384:ALA:CA	2.30	0.61
1:Ae:87:ASP:OD1	1:Ae:88:GLY:N	2.29	0.61
1:Ak:15:LYS:HE2	1:Ak:18:ARG:HH12	1.63	0.61
2:Am:95:VAL:HB	2:Ba:1:MET:HB3	1.82	0.61
1:As:131:LEU:HD11	1:As:500:THR:HG22	1.82	0.61
1:Ay:383:ALA:HB1	1:Ay:388:GLU:CD	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:498:LYS:HG3	1:Az:501:ARG:HH21	1.65	0.61
1:Bg:385:THR:OG1	1:Bg:387:VAL:HG12	2.01	0.61
1:Ak:349:ILE:HB	1:Ak:369:VAL:HG22	1.83	0.61
1:Al:138:CYS:SG	1:Al:143:ALA:HB1	2.40	0.61
1:Ar:164:GLU:O	1:Ar:167:ASP:HB2	2.00	0.61
1:Az:138:CYS:SG	1:Az:143:ALA:HB1	2.40	0.61
1:Bf:428:ASP:O	1:Bf:430:ARG:HG2	2.01	0.61
1:Bm:80:LYS:O	1:Bm:83:ASP:OD1	2.19	0.61
1:Bm:164:GLU:O	1:Bm:167:ASP:HB2	2.00	0.61
1:Bn:488:MET:CE	1:Bn:491:MET:HE1	2.19	0.61
1:Bt:183:LEU:HG	1:Bt:384:ALA:CA	2.30	0.61
1:Bt:383:ALA:HB1	1:Bt:388:GLU:CD	2.25	0.61
1:Ar:428:ASP:O	1:Ar:430:ARG:HG2	2.01	0.60
1:As:138:CYS:SG	1:As:143:ALA:HB1	2.40	0.60
1:Az:164:GLU:O	1:Az:167:ASP:HB2	1.99	0.60
1:Bg:131:LEU:HD11	1:Bg:500:THR:HG22	1.82	0.60
1:Bg:480:ALA:O	1:Bg:483:GLU:HG3	2.01	0.60
1:Bm:142:LYS:HG3	1:Bm:146:GLN:HE22	1.62	0.60
1:Bt:349:ILE:HB	1:Bt:369:VAL:HG22	1.83	0.60
1:Bu:498:LYS:HG3	1:Bu:501:ARG:HH21	1.65	0.60
1:Ad:168:LYS:HZ1	1:Ad:187:LEU:HG	1.66	0.60
1:Ae:113:PRO:HG2	1:Al:36:ARG:CD	2.30	0.60
1:Ak:80:LYS:O	1:Ak:83:ASP:OD1	2.19	0.60
1:Ak:428:ASP:O	1:Ak:430:ARG:HG2	2.01	0.60
1:Ar:183:LEU:HG	1:Ar:384:ALA:CA	2.30	0.60
1:Ar:284:ARG:CD	1:Ar:364:LYS:CG	2.74	0.60
1:Az:482:THR:HG1	1:Az:484:GLU:HG2	1.60	0.60
1:Bf:288:MET:HE1	1:Bf:364:LYS:HE3	1.83	0.60
1:Bm:183:LEU:HG	1:Bm:384:ALA:CA	2.30	0.60
1:Ak:164:GLU:O	1:Ak:167:ASP:HB2	2.00	0.60
1:Ak:186:GLU:HG3	1:Ak:380:LYS:HB2	1.84	0.60
1:Ar:288:MET:HE1	1:Ar:364:LYS:HE3	1.83	0.60
1:As:498:LYS:HG3	1:As:501:ARG:HH21	1.65	0.60
1:Ay:206:ASN:HB2	1:Ay:213:VAL:HG13	1.83	0.60
1:Ay:366:GLN:O	1:Ay:370:ALA:N	2.34	0.60
1:Az:24:ALA:CB	1:Az:97:GLN:CD	2.72	0.60
1:Bg:63:GLU:OE1	1:Bu:524:LEU:HD13	1.99	0.60
1:Bm:288:MET:HE1	1:Bm:364:LYS:HE3	1.82	0.60
1:Bn:138:CYS:SG	1:Bn:143:ALA:HB1	2.40	0.60
1:Bt:428:ASP:C	1:Bt:428:ASP:OD1	2.45	0.60
1:Ad:186:GLU:HG3	1:Ad:380:LYS:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:206:ASN:HB2	1:Ak:213:VAL:HG13	1.83	0.60
1:Az:385:THR:OG1	1:Az:387:VAL:HG12	2.01	0.60
1:Bf:428:ASP:C	1:Bf:428:ASP:OD1	2.45	0.60
1:Bg:113:PRO:HG2	1:Bn:36:ARG:CD	2.31	0.60
1:Bm:383:ALA:HB1	1:Bm:388:GLU:CD	2.25	0.60
1:Bn:131:LEU:HD11	1:Bn:500:THR:HG22	1.82	0.60
1:Bn:385:THR:OG1	1:Bn:387:VAL:HG12	2.01	0.60
1:Bn:498:LYS:HG3	1:Bn:501:ARG:HH21	1.65	0.60
1:Ak:288:MET:HE1	1:Ak:364:LYS:HE3	1.83	0.60
1:Bm:366:GLN:O	1:Bm:370:ALA:N	2.34	0.60
1:Bu:385:THR:OG1	1:Bu:387:VAL:HG12	2.01	0.60
1:Bu:482:THR:HG1	1:Bu:484:GLU:HG2	1.59	0.60
1:Ad:428:ASP:C	1:Ad:428:ASP:OD1	2.45	0.60
1:Ak:366:GLN:O	1:Ak:370:ALA:N	2.34	0.60
1:Ay:7:LYS:HG3	1:Ay:66:PHE:CZ	2.37	0.60
1:Ad:7:LYS:HG3	1:Ad:66:PHE:CZ	2.37	0.60
1:Ad:206:ASN:HB2	1:Ad:213:VAL:HG13	1.83	0.60
1:Ad:349:ILE:HB	1:Ad:369:VAL:HG22	1.83	0.60
1:Ak:7:LYS:HG3	1:Ak:66:PHE:CZ	2.37	0.60
1:Ay:186:GLU:HG3	1:Ay:380:LYS:HB2	1.84	0.60
1:Bf:284:ARG:CD	1:Bf:364:LYS:CG	2.74	0.60
1:Bg:524:LEU:HD13	1:Bn:63:GLU:OE1	2.00	0.60
1:Bt:205:ILE:HA	1:Bt:213:VAL:HG22	1.84	0.60
1:Ae:7:LYS:CD	1:Ae:66:PHE:CZ	2.85	0.60
1:Ar:352:GLN:HA	1:Ar:355:GLU:HB3	1.83	0.60
1:As:7:LYS:CD	1:As:66:PHE:CZ	2.85	0.60
1:As:24:ALA:HB3	1:As:97:GLN:OE1	1.96	0.60
1:As:63:GLU:OE1	1:Bn:524:LEU:HD13	2.01	0.60
1:Ay:15:LYS:HE2	1:Ay:18:ARG:HH12	1.63	0.60
1:Az:73:MET:CG	1:Bu:47:PRO:HG2	2.31	0.60
1:Bf:349:ILE:HB	1:Bf:369:VAL:HG22	1.83	0.60
1:Bm:7:LYS:HG3	1:Bm:66:PHE:CZ	2.37	0.60
1:Bt:288:MET:HE1	1:Bt:364:LYS:HE3	1.83	0.60
1:Ad:363:GLU:CA	1:Ad:366:GLN:NE2	2.28	0.60
1:Ad:428:ASP:O	1:Ad:430:ARG:HG2	2.01	0.60
1:Ar:186:GLU:HG3	1:Ar:380:LYS:HB2	1.84	0.60
1:Ar:284:ARG:HD2	1:Ar:364:LYS:HB3	1.84	0.60
1:Ay:205:ILE:HA	1:Ay:213:VAL:HG22	1.84	0.60
1:Bg:36:ARG:CD	1:Bu:113:PRO:HG2	2.32	0.60
1:Bg:518:GLU:OE1	1:Bn:37:ASN:CA	2.49	0.60
1:Bn:7:LYS:CD	1:Bn:66:PHE:CZ	2.85	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:80:LYS:O	1:Bt:83:ASP:OD1	2.19	0.60
1:Bu:480:ALA:O	1:Bu:483:GLU:HG3	2.01	0.60
1:Al:178:GLU:OE2	1:Al:380:LYS:HD3	2.02	0.60
1:Ar:206:ASN:HB2	1:Ar:213:VAL:HG13	1.83	0.60
1:Ay:428:ASP:C	1:Ay:428:ASP:OD1	2.45	0.60
1:Bf:164:GLU:CD	1:Bf:187:LEU:CD2	2.75	0.60
1:Bm:15:LYS:HE2	1:Bm:18:ARG:HH12	1.64	0.60
1:Bt:206:ASN:HB2	1:Bt:213:VAL:HG13	1.83	0.60
1:As:178:GLU:OE2	1:As:380:LYS:HD3	2.02	0.59
1:Az:178:GLU:OE2	1:Az:380:LYS:HD3	2.02	0.59
1:Az:518:GLU:OE1	1:Bu:37:ASN:CA	2.49	0.59
2:Ba:95:VAL:HB	2:Bv:1:MET:HB3	1.83	0.59
1:Bm:164:GLU:CD	1:Bm:187:LEU:CD2	2.75	0.59
1:Bt:168:LYS:NZ	1:Bt:187:LEU:CG	2.65	0.59
1:Ad:15:LYS:HE2	1:Ad:18:ARG:HH12	1.64	0.59
1:Ae:480:ALA:O	1:Ae:483:GLU:HG3	2.01	0.59
1:Ak:428:ASP:C	1:Ak:428:ASP:OD1	2.45	0.59
1:Al:24:ALA:CB	1:Al:97:GLN:CD	2.72	0.59
1:Ar:7:LYS:HG3	1:Ar:66:PHE:CZ	2.37	0.59
1:Ay:80:LYS:O	1:Ay:83:ASP:OD1	2.19	0.59
1:Ay:288:MET:HE1	1:Ay:364:LYS:HE3	1.83	0.59
1:Bm:168:LYS:HD2	1:Bm:189:VAL:CG2	2.32	0.59
1:Bt:368:ARG:C	1:Bt:372:LEU:HD23	2.26	0.59
1:Ad:284:ARG:HD2	1:Ad:364:LYS:HB3	1.84	0.59
1:Ad:352:GLN:HA	1:Ad:355:GLU:HB3	1.83	0.59
1:Al:87:ASP:OD1	1:Al:88:GLY:N	2.30	0.59
1:Al:524:LEU:HD13	1:Az:63:GLU:OE1	2.02	0.59
1:Ay:168:LYS:NZ	1:Ay:187:LEU:CG	2.65	0.59
1:Az:34:LYS:HZ1	1:Az:483:GLU:CG	2.13	0.59
1:Bf:168:LYS:NZ	1:Bf:187:LEU:CG	2.66	0.59
1:Bm:206:ASN:HB2	1:Bm:213:VAL:HG13	1.83	0.59
1:Bm:284:ARG:HD2	1:Bm:364:LYS:HB3	1.84	0.59
1:Ae:36:ARG:CD	1:As:113:PRO:HG2	2.32	0.59
1:Ak:349:ILE:HD11	1:Ak:372:LEU:HG	1.84	0.59
1:Bg:381:VAL:HG11	1:Bg:393:LYS:HG3	1.85	0.59
2:Bh:95:VAL:HB	2:Bo:1:MET:HB3	1.84	0.59
1:Bm:352:GLN:HA	1:Bm:355:GLU:HB3	1.83	0.59
1:Bt:186:GLU:HG3	1:Bt:380:LYS:HB2	1.84	0.59
1:Bu:178:GLU:OE2	1:Bu:380:LYS:HD3	2.02	0.59
1:Ad:6:VAL:CG2	1:Ad:521:VAL:HG13	2.24	0.59
1:Ad:349:ILE:HD11	1:Ad:372:LEU:HG	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:178:GLU:OE2	1:Ae:380:LYS:HD3	2.02	0.59
1:Al:482:THR:HG1	1:Al:484:GLU:HG2	1.63	0.59
1:As:122:LYS:HE2	1:As:430:ARG:O	2.03	0.59
1:Bf:6:VAL:CG2	1:Bf:521:VAL:HG13	2.24	0.59
1:Bf:168:LYS:HD2	1:Bf:189:VAL:CG2	2.33	0.59
1:Bm:349:ILE:HB	1:Bm:369:VAL:HG22	1.83	0.59
1:Bt:7:LYS:HG3	1:Bt:66:PHE:CZ	2.37	0.59
1:Bt:366:GLN:O	1:Bt:370:ALA:N	2.34	0.59
1:Ak:168:LYS:HD2	1:Ak:189:VAL:CG2	2.33	0.59
1:Al:122:LYS:HE2	1:Al:430:ARG:O	2.03	0.59
1:Bf:206:ASN:HB2	1:Bf:213:VAL:HG13	1.83	0.59
1:Bg:7:LYS:CD	1:Bg:66:PHE:CZ	2.85	0.59
1:Bg:20:VAL:CG2	1:Bg:514:MET:HE1	2.33	0.59
1:Bg:36:ARG:HD2	1:Bu:518:GLU:HG3	1.85	0.59
1:Bm:168:LYS:NZ	1:Bm:187:LEU:CG	2.65	0.59
1:Bu:381:VAL:HG11	1:Bu:393:LYS:HG3	1.85	0.59
1:Ae:138:CYS:SG	1:Ae:143:ALA:HB3	2.43	0.59
1:Al:7:LYS:CD	1:Al:66:PHE:CZ	2.85	0.59
1:Ay:352:GLN:HA	1:Ay:355:GLU:HB3	1.83	0.59
1:Az:7:LYS:CD	1:Az:66:PHE:CZ	2.85	0.59
1:Az:122:LYS:HE2	1:Az:430:ARG:O	2.03	0.59
1:Az:381:VAL:HG11	1:Az:393:LYS:HG3	1.85	0.59
1:Bf:7:LYS:HG3	1:Bf:66:PHE:CZ	2.37	0.59
1:Bf:80:LYS:O	1:Bf:83:ASP:OD1	2.19	0.59
1:Bf:205:ILE:HA	1:Bf:213:VAL:HG22	1.84	0.59
1:Bt:168:LYS:HD2	1:Bt:189:VAL:CG2	2.33	0.59
1:Bu:20:VAL:CG2	1:Bu:514:MET:HE1	2.33	0.59
1:Ak:142:LYS:HG3	1:Ak:146:GLN:HE22	1.62	0.59
1:Ak:352:GLN:HA	1:Ak:355:GLU:HB3	1.83	0.59
1:Al:381:VAL:HG11	1:Al:393:LYS:HG3	1.85	0.59
1:Ar:349:ILE:HB	1:Ar:369:VAL:HG22	1.83	0.59
1:Ar:349:ILE:HD11	1:Ar:372:LEU:HG	1.84	0.59
1:As:138:CYS:SG	1:As:143:ALA:HB3	2.43	0.59
1:Ay:142:LYS:HG3	1:Ay:146:GLN:HE22	1.62	0.59
1:Bf:161:LEU:CD1	1:Bf:161:LEU:N	2.66	0.59
1:Bg:178:GLU:OE2	1:Bg:380:LYS:HD3	2.02	0.59
1:Bt:161:LEU:CD1	1:Bt:161:LEU:N	2.66	0.59
1:Ad:366:GLN:O	1:Ad:370:ALA:N	2.34	0.59
1:Ae:24:ALA:HB3	1:Ae:97:GLN:OE1	1.96	0.59
1:Ak:164:GLU:CD	1:Ak:187:LEU:CD2	2.75	0.59
1:Ak:168:LYS:NZ	1:Ak:187:LEU:CG	2.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:138:CYS:SG	1:Al:143:ALA:HB3	2.43	0.59
1:Ar:168:LYS:HD2	1:Ar:189:VAL:CG2	2.33	0.59
1:As:36:ARG:CD	1:Bn:113:PRO:HG2	2.32	0.59
1:As:40:LEU:CD2	1:As:59:GLU:OE1	2.50	0.59
1:Az:20:VAL:CG2	1:Az:514:MET:HE1	2.33	0.59
1:Bf:352:GLN:HA	1:Bf:355:GLU:HB3	1.83	0.59
1:Bg:518:GLU:HG3	1:Bn:36:ARG:HD2	1.84	0.59
1:Bm:383:ALA:HB3	1:Bm:388:GLU:HG3	1.85	0.59
1:Bm:428:ASP:OD1	1:Bm:428:ASP:C	2.45	0.59
1:Bn:381:VAL:HG11	1:Bn:393:LYS:HG3	1.85	0.59
2:At:2:ASN:N	2:Bo:96:GLU:O	2.35	0.59
1:Bf:366:GLN:O	1:Bf:370:ALA:N	2.34	0.59
1:Ae:20:VAL:CG2	1:Ae:514:MET:HE1	2.33	0.58
1:Ak:383:ALA:HB3	1:Ak:388:GLU:HG3	1.85	0.58
1:Al:20:VAL:CG2	1:Al:514:MET:HE1	2.33	0.58
1:Bf:186:GLU:HG3	1:Bf:380:LYS:HB2	1.84	0.58
1:Bm:161:LEU:CD1	1:Bm:161:LEU:N	2.66	0.58
1:Bm:186:GLU:HG3	1:Bm:380:LYS:HB2	1.84	0.58
1:Bn:124:VAL:HG21	1:Bn:508:ALA:HB2	1.85	0.58
1:Bt:352:GLN:HA	1:Bt:355:GLU:HB3	1.83	0.58
1:Bu:122:LYS:HE2	1:Bu:430:ARG:O	2.03	0.58
1:Ae:69:MET:CE	1:Al:41:ASP:OD1	2.51	0.58
1:Bn:138:CYS:SG	1:Bn:143:ALA:HB3	2.43	0.58
1:Ad:161:LEU:CD1	1:Ad:161:LEU:N	2.66	0.58
1:Ae:381:VAL:HG11	1:Ae:393:LYS:HG3	1.85	0.58
1:Ak:205:ILE:HA	1:Ak:213:VAL:HG22	1.84	0.58
1:Ar:383:ALA:HB3	1:Ar:388:GLU:HG3	1.85	0.58
1:As:124:VAL:HG21	1:As:508:ALA:HB2	1.85	0.58
1:Ay:349:ILE:HD11	1:Ay:372:LEU:HG	1.84	0.58
1:Az:138:CYS:SG	1:Az:143:ALA:HB3	2.43	0.58
2:Ba:96:GLU:O	2:Bv:2:ASN:N	2.36	0.58
1:Bf:349:ILE:HD11	1:Bf:372:LEU:HG	1.84	0.58
1:Bg:288:MET:HE1	1:Bg:371:LYS:HZ3	1.69	0.58
2:Bh:1:MET:HB3	2:Bv:95:VAL:HB	1.84	0.58
2:Bh:2:ASN:N	2:Bv:96:GLU:O	2.37	0.58
1:Bn:24:ALA:HB3	1:Bn:97:GLN:OE1	1.96	0.58
1:Bn:122:LYS:HE2	1:Bn:430:ARG:O	2.03	0.58
1:Bt:164:GLU:CD	1:Bt:187:LEU:CD2	2.75	0.58
1:Bu:7:LYS:CD	1:Bu:66:PHE:CZ	2.85	0.58
1:Bf:409:GLU:OE1	1:Bf:498:LYS:HB2	2.03	0.58
1:Bg:177:VAL:HG23	1:Bg:400:LEU:CD1	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bn:20:VAL:CG2	1:Bn:514:MET:HE1	2.33	0.58
1:Bt:37:ASN:HD21	1:Bt:51:LYS:HZ1	1.50	0.58
1:Ad:168:LYS:HD2	1:Ad:189:VAL:CG2	2.33	0.58
1:Ak:409:GLU:OE1	1:Ak:498:LYS:HB2	2.03	0.58
1:Ar:168:LYS:NZ	1:Ar:187:LEU:CG	2.65	0.58
1:As:381:VAL:HG11	1:As:393:LYS:HG3	1.85	0.58
1:Az:524:LEU:HD13	1:Bu:63:GLU:OE1	2.01	0.58
1:Bn:40:LEU:CD2	1:Bn:59:GLU:OE1	2.50	0.58
1:Bn:177:VAL:HG23	1:Bn:400:LEU:CD1	2.34	0.58
1:Bt:142:LYS:HG3	1:Bt:146:GLN:HE22	1.62	0.58
1:Ad:168:LYS:NZ	1:Ad:187:LEU:CG	2.65	0.58
1:Ar:428:ASP:C	1:Ar:428:ASP:OD1	2.45	0.58
1:Bg:41:ASP:OD1	1:Bu:69:MET:CE	2.52	0.58
1:Bm:368:ARG:C	1:Bm:372:LEU:HD23	2.26	0.58
1:Bm:409:GLU:OE1	1:Bm:498:LYS:HB2	2.03	0.58
1:Bt:349:ILE:HD11	1:Bt:372:LEU:HG	1.84	0.58
1:Ae:47:PRO:CG	1:As:73:MET:HG3	2.33	0.58
1:Ak:161:LEU:CD1	1:Ak:161:LEU:N	2.66	0.58
1:Ak:284:ARG:HD2	1:Ak:364:LYS:HB3	1.84	0.58
1:Al:455:VAL:HG13	1:Al:460:GLU:HB2	1.86	0.58
1:Ar:164:GLU:CD	1:Ar:187:LEU:CD2	2.75	0.58
1:Ar:409:GLU:OE1	1:Ar:498:LYS:HB2	2.03	0.58
1:As:20:VAL:CG2	1:As:514:MET:HE1	2.33	0.58
1:Ay:161:LEU:CD1	1:Ay:161:LEU:N	2.66	0.58
1:Bf:284:ARG:HD2	1:Bf:364:LYS:HB3	1.84	0.58
1:Bg:122:LYS:HE2	1:Bg:430:ARG:O	2.03	0.58
1:Bg:124:VAL:HG21	1:Bg:508:ALA:HB2	1.85	0.58
1:Ad:368:ARG:C	1:Ad:372:LEU:HD23	2.26	0.58
1:Ae:76:GLU:OE2	1:Al:46:ALA:HB2	2.02	0.58
1:Ak:174:VAL:HG12	1:Ak:376:VAL:HG13	1.86	0.58
1:Ak:368:ARG:C	1:Ak:372:LEU:HD23	2.26	0.58
1:As:177:VAL:HG23	1:As:400:LEU:CD1	2.34	0.58
1:Ay:174:VAL:HG12	1:Ay:376:VAL:HG13	1.86	0.58
1:Az:455:VAL:HG13	1:Az:460:GLU:HB2	1.86	0.58
1:Bf:37:ASN:HD21	1:Bf:51:LYS:HZ1	1.52	0.58
1:Bf:155:ASP:HB3	1:Bf:395:ARG:NH2	2.08	0.58
1:Bm:349:ILE:HD11	1:Bm:372:LEU:HG	1.84	0.58
1:Bt:409:GLU:OE1	1:Bt:498:LYS:HB2	2.03	0.58
1:Bu:177:VAL:HG23	1:Bu:400:LEU:CD1	2.34	0.58
1:Ad:194:GLN:H	1:Ad:371:LYS:HD3	1.69	0.58
1:Ae:455:VAL:HG13	1:Ae:460:GLU:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Af:6:LEU:CD2	2:At:92:LEU:C	2.77	0.58
1:Al:518:GLU:HG3	1:Az:36:ARG:HD2	1.85	0.58
1:Ay:168:LYS:HD2	1:Ay:189:VAL:CG2	2.32	0.58
1:Bn:178:GLU:OE2	1:Bn:380:LYS:HD3	2.02	0.58
1:Ad:174:VAL:HG12	1:Ad:376:VAL:HG13	1.86	0.58
1:Ad:205:ILE:HA	1:Ad:213:VAL:HG22	1.84	0.58
1:Al:69:MET:CE	1:Az:41:ASP:OD1	2.52	0.58
1:Ar:161:LEU:CD1	1:Ar:161:LEU:N	2.66	0.58
1:Ar:194:GLN:H	1:Ar:371:LYS:HD3	1.69	0.58
1:Ay:155:ASP:HB3	1:Ay:395:ARG:NH2	2.08	0.58
1:Ay:164:GLU:HG3	1:Ay:165:ALA:N	2.19	0.58
1:Az:177:VAL:HG23	1:Az:400:LEU:CD1	2.34	0.58
1:Bg:40:LEU:CD2	1:Bg:59:GLU:OE1	2.50	0.58
1:Bm:205:ILE:HA	1:Bm:213:VAL:HG22	1.84	0.58
1:Ad:383:ALA:HB3	1:Ad:388:GLU:HG3	1.85	0.57
1:Ad:409:GLU:OE1	1:Ad:498:LYS:HB2	2.03	0.57
1:Ae:46:ALA:HB2	1:As:76:GLU:OE2	2.01	0.57
1:Ar:205:ILE:HA	1:Ar:213:VAL:HG22	1.84	0.57
1:Ad:155:ASP:HB3	1:Ad:395:ARG:NH2	2.08	0.57
1:Ae:122:LYS:HE2	1:Ae:430:ARG:O	2.03	0.57
1:Ae:124:VAL:HG21	1:Ae:508:ALA:HB2	1.85	0.57
1:Ak:365:LEU:HD13	1:Ak:365:LEU:H	1.69	0.57
1:Az:113:PRO:HG2	1:Bu:36:ARG:CD	2.34	0.57
1:Bt:383:ALA:HB3	1:Bt:388:GLU:HG3	1.85	0.57
1:Al:177:VAL:HG23	1:Al:400:LEU:CD1	2.34	0.57
1:Ay:409:GLU:OE1	1:Ay:498:LYS:HB2	2.03	0.57
1:Bm:164:GLU:HG3	1:Bm:165:ALA:N	2.19	0.57
1:Bm:174:VAL:HG12	1:Bm:376:VAL:HG13	1.86	0.57
1:Bt:161:LEU:CD1	1:Bt:161:LEU:H	2.18	0.57
1:Bt:164:GLU:HG3	1:Bt:165:ALA:N	2.19	0.57
1:Bu:455:VAL:HG13	1:Bu:460:GLU:HB2	1.86	0.57
1:Ar:114:MET:CE	1:Bm:36:ARG:NE	2.41	0.57
1:As:455:VAL:HG13	1:As:460:GLU:HB2	1.86	0.57
1:Ay:365:LEU:HD13	1:Ay:365:LEU:H	1.69	0.57
1:Bm:194:GLN:H	1:Bm:371:LYS:HD3	1.69	0.57
1:Bt:284:ARG:HD2	1:Bt:364:LYS:HB3	1.84	0.57
1:Bt:489:ILE:CD1	1:Bt:494:LEU:HD22	2.33	0.57
1:Bu:40:LEU:CD2	1:Bu:59:GLU:OE1	2.50	0.57
1:Bu:138:CYS:SG	1:Bu:143:ALA:HB3	2.43	0.57
1:Ae:177:VAL:HG23	1:Ae:400:LEU:CD1	2.34	0.57
1:Ak:194:GLN:H	1:Ak:371:LYS:HD3	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:284:ARG:HD2	1:Ay:364:LYS:HB3	1.84	0.57
1:Az:40:LEU:CD2	1:Az:59:GLU:OE1	2.50	0.57
1:Bg:46:ALA:HB2	1:Bu:76:GLU:OE2	2.04	0.57
1:Bg:138:CYS:SG	1:Bg:143:ALA:HB3	2.43	0.57
1:Bt:174:VAL:HG12	1:Bt:376:VAL:HG13	1.86	0.57
1:Ad:365:LEU:HD13	1:Ad:365:LEU:H	1.69	0.57
1:Ae:7:LYS:HD2	1:Ae:66:PHE:CD2	2.40	0.57
1:Ar:161:LEU:CD1	1:Ar:161:LEU:H	2.18	0.57
1:Ar:164:GLU:HG3	1:Ar:165:ALA:N	2.19	0.57
1:Ar:366:GLN:O	1:Ar:370:ALA:N	2.34	0.57
1:Ar:368:ARG:C	1:Ar:372:LEU:HD23	2.26	0.57
1:Bf:164:GLU:HG3	1:Bf:165:ALA:N	2.19	0.57
1:Bf:365:LEU:HD13	1:Bf:365:LEU:H	1.69	0.57
1:Bn:288:MET:HE1	1:Bn:371:LYS:HZ3	1.67	0.57
1:Ad:130:GLU:O	1:Ad:134:LEU:HD13	2.05	0.57
1:Ae:73:MET:HG3	1:Al:47:PRO:CG	2.35	0.57
1:Ak:164:GLU:HG3	1:Ak:165:ALA:N	2.19	0.57
1:Al:115:ASP:HB3	1:Al:435:ASP:HB2	1.85	0.57
1:Ar:130:GLU:O	1:Ar:134:LEU:HD13	2.05	0.57
1:Ay:37:ASN:HD21	1:Ay:51:LYS:HZ1	1.53	0.57
1:Ay:194:GLN:H	1:Ay:371:LYS:HD3	1.69	0.57
1:Ay:383:ALA:HB3	1:Ay:388:GLU:HG3	1.85	0.57
1:Az:7:LYS:HD2	1:Az:66:PHE:CD2	2.40	0.57
1:Az:115:ASP:HB3	1:Az:435:ASP:HB2	1.85	0.57
1:Bf:161:LEU:CD1	1:Bf:161:LEU:H	2.18	0.57
1:Bm:223:ALA:HB3	1:Bm:251:ALA:HA	1.87	0.57
1:Bt:223:ALA:HB3	1:Bt:251:ALA:HA	1.87	0.57
1:Ae:115:ASP:HB3	1:Ae:435:ASP:HB2	1.85	0.57
1:Ak:161:LEU:CD1	1:Ak:161:LEU:H	2.18	0.57
1:Bm:161:LEU:CD1	1:Bm:161:LEU:H	2.18	0.57
1:Bt:130:GLU:O	1:Bt:134:LEU:HD13	2.05	0.57
1:Ae:40:LEU:CD2	1:Ae:59:GLU:OE1	2.50	0.57
1:As:41:ASP:OD1	1:Bn:69:MET:CE	2.52	0.57
1:As:115:ASP:HB3	1:As:435:ASP:HB2	1.85	0.57
1:Bm:237:LEU:HD22	1:Bm:273:VAL:HG21	1.87	0.57
1:Bm:395:ARG:O	1:Bm:398:ASP:OD1	2.23	0.57
1:Bt:6:VAL:CG2	1:Bt:521:VAL:HG13	2.24	0.57
1:Bt:155:ASP:HB3	1:Bt:395:ARG:NH2	2.08	0.57
1:Bt:194:GLN:H	1:Bt:371:LYS:HD3	1.69	0.57
1:Bt:365:LEU:HD13	1:Bt:365:LEU:H	1.69	0.57
1:Ak:155:ASP:HB3	1:Ak:395:ARG:NH2	2.08	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:223:ALA:HB3	1:Ar:251:ALA:HA	1.87	0.56
1:As:36:ARG:HD2	1:Bn:518:GLU:HG3	1.86	0.56
1:Ay:36:ARG:NE	1:Bt:114:MET:CE	2.38	0.56
1:Ay:489:ILE:CD1	1:Ay:494:LEU:HD22	2.33	0.56
1:Bf:174:VAL:HG12	1:Bf:376:VAL:HG13	1.86	0.56
1:Bf:237:LEU:HD22	1:Bf:273:VAL:HG21	1.87	0.56
1:Bf:395:ARG:O	1:Bf:398:ASP:OD1	2.23	0.56
1:Bm:130:GLU:O	1:Bm:134:LEU:HD13	2.05	0.56
1:Ae:36:ARG:HD2	1:As:518:GLU:HG3	1.86	0.56
1:Ak:6:VAL:CG2	1:Ak:521:VAL:HG13	2.24	0.56
1:Al:113:PRO:HG2	1:Az:36:ARG:CD	2.33	0.56
1:Ay:161:LEU:CD1	1:Ay:161:LEU:H	2.18	0.56
1:Ay:223:ALA:HB3	1:Ay:251:ALA:HA	1.87	0.56
1:Bf:130:GLU:O	1:Bf:134:LEU:HD13	2.05	0.56
1:Bf:368:ARG:C	1:Bf:372:LEU:HD23	2.26	0.56
1:Bn:115:ASP:HB3	1:Bn:435:ASP:HB2	1.85	0.56
1:Ad:164:GLU:CD	1:Ad:187:LEU:CD2	2.75	0.56
1:Al:76:GLU:OE2	1:Az:46:ALA:HB2	2.04	0.56
1:Az:69:MET:CE	1:Bu:41:ASP:OD1	2.53	0.56
1:Bg:455:VAL:HG13	1:Bg:460:GLU:HB2	1.86	0.56
1:Bu:115:ASP:HB3	1:Bu:435:ASP:HB2	1.85	0.56
1:Bu:124:VAL:HG21	1:Bu:508:ALA:HB2	1.85	0.56
1:Al:40:LEU:CD2	1:Al:59:GLU:OE1	2.50	0.56
1:Bn:455:VAL:HG13	1:Bn:460:GLU:HB2	1.86	0.56
1:Ae:41:ASP:OD1	1:As:69:MET:CE	2.53	0.56
1:Ak:237:LEU:HD22	1:Ak:273:VAL:HG21	1.87	0.56
1:Ak:395:ARG:O	1:Ak:398:ASP:OD1	2.23	0.56
1:Ar:365:LEU:HD13	1:Ar:365:LEU:H	1.69	0.56
1:Az:34:LYS:HZ2	1:Az:483:GLU:CG	2.19	0.56
1:Bg:24:ALA:HB3	1:Bg:97:GLN:OE1	1.96	0.56
1:Ad:36:ARG:CB	1:Ak:518:GLU:OE2	2.54	0.56
1:Al:24:ALA:HB3	1:Al:97:GLN:OE1	1.96	0.56
1:Ar:395:ARG:O	1:Ar:398:ASP:OD1	2.23	0.56
1:Ay:395:ARG:O	1:Ay:398:ASP:OD1	2.23	0.56
1:Bf:194:GLN:H	1:Bf:371:LYS:HD3	1.69	0.56
1:Bf:383:ALA:HB3	1:Bf:388:GLU:HG3	1.85	0.56
1:Bg:69:MET:CE	1:Bn:41:ASP:OD1	2.53	0.56
1:Al:7:LYS:HD2	1:Al:66:PHE:CD2	2.40	0.56
1:Al:124:VAL:HG21	1:Al:508:ALA:HB2	1.85	0.56
1:Ay:130:GLU:O	1:Ay:134:LEU:HD13	2.05	0.56
1:Ay:368:ARG:C	1:Ay:372:LEU:HD23	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:73:MET:HG3	1:Bn:47:PRO:CG	2.35	0.56
1:Bg:115:ASP:HB3	1:Bg:435:ASP:HB2	1.85	0.56
1:Bu:3:ALA:CB	1:Bu:524:LEU:HD13	2.36	0.56
1:Ad:164:GLU:HG3	1:Ad:165:ALA:N	2.19	0.56
1:Ae:157:THR:HA	1:Ae:160:LYS:HE3	1.88	0.56
1:Ar:174:VAL:HG12	1:Ar:376:VAL:HG13	1.86	0.56
1:As:157:THR:HA	1:As:160:LYS:HE3	1.88	0.56
1:Az:3:ALA:CB	1:Az:524:LEU:HD13	2.36	0.56
1:Bm:134:LEU:CD1	1:Bm:425:LYS:HZ1	2.01	0.56
1:Bm:365:LEU:HD13	1:Bm:365:LEU:H	1.69	0.56
1:Ar:237:LEU:HD22	1:Ar:273:VAL:HG21	1.87	0.56
1:Ad:223:ALA:HB3	1:Ad:251:ALA:HA	1.87	0.56
1:Ad:237:LEU:HD22	1:Ad:273:VAL:HG21	1.87	0.56
1:Ad:395:ARG:O	1:Ad:398:ASP:OD1	2.23	0.56
1:Ak:130:GLU:O	1:Ak:134:LEU:HD13	2.05	0.56
1:Bg:3:ALA:CB	1:Bg:524:LEU:HD13	2.36	0.56
2:Bh:96:GLU:O	2:Bo:2:ASN:N	2.36	0.56
1:Ak:223:ALA:HB3	1:Ak:251:ALA:HA	1.87	0.55
1:Ay:237:LEU:HD22	1:Ay:273:VAL:HG21	1.87	0.55
1:Ay:284:ARG:HD2	1:Ay:364:LYS:CB	2.36	0.55
1:Bf:223:ALA:HB3	1:Bf:251:ALA:HA	1.87	0.55
1:Bg:7:LYS:HD2	1:Bg:66:PHE:CD2	2.40	0.55
1:Bt:395:ARG:O	1:Bt:398:ASP:OD1	2.23	0.55
1:Al:157:THR:HA	1:Al:160:LYS:HE3	1.88	0.55
1:Az:76:GLU:OE2	1:Bu:46:ALA:HB2	2.06	0.55
1:Bg:76:GLU:OE2	1:Bn:46:ALA:HB2	2.04	0.55
1:Bm:155:ASP:HB3	1:Bm:395:ARG:NH2	2.08	0.55
1:Ad:161:LEU:CD1	1:Ad:161:LEU:H	2.18	0.55
1:Ad:489:ILE:CD1	1:Ad:494:LEU:HD22	2.33	0.55
1:Al:3:ALA:CB	1:Al:524:LEU:HD13	2.36	0.55
1:Ay:164:GLU:CD	1:Ay:187:LEU:CD2	2.75	0.55
1:Bf:346:VAL:HB	1:Bf:369:VAL:HG13	1.88	0.55
1:Ar:155:ASP:HB3	1:Ar:395:ARG:NH2	2.08	0.55
1:Bn:7:LYS:HD2	1:Bn:66:PHE:CD2	2.40	0.55
1:Bt:361:ASP:O	1:Bt:364:LYS:HB3	2.07	0.55
1:Ad:168:LYS:HZ3	1:Ad:187:LEU:CD2	2.19	0.55
1:Ae:3:ALA:CB	1:Ae:524:LEU:HD13	2.36	0.55
1:As:47:PRO:CG	1:Bn:73:MET:HG3	2.36	0.55
1:As:288:MET:HE1	1:As:371:LYS:HZ3	1.71	0.55
1:Bm:37:ASN:HD21	1:Bm:51:LYS:HZ1	1.53	0.55
1:Bt:346:VAL:HB	1:Bt:369:VAL:HG13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:349:ILE:CD1	1:Ak:372:LEU:HG	2.37	0.55
1:Ar:112:ASN:HB3	1:Ar:115:ASP:HB2	1.89	0.55
1:As:7:LYS:HD2	1:As:66:PHE:CD2	2.40	0.55
1:Bm:361:ASP:O	1:Bm:364:LYS:HB3	2.07	0.55
1:Ad:36:ARG:NH1	1:Ak:518:GLU:OE2	2.36	0.55
1:Ad:346:VAL:HB	1:Ad:369:VAL:HG13	1.88	0.55
1:Ad:361:ASP:O	1:Ad:364:LYS:HB3	2.07	0.55
1:Ak:284:ARG:HD2	1:Ak:364:LYS:CB	2.36	0.55
1:Ak:361:ASP:O	1:Ak:364:LYS:HB3	2.07	0.55
1:Az:124:VAL:HG21	1:Az:508:ALA:HB2	1.85	0.55
1:Az:479:ASN:HB2	1:Az:491:MET:SD	2.47	0.55
1:Bm:255:GLU:HB3	1:Bm:259:LEU:HB2	1.89	0.55
1:Bt:237:LEU:HD22	1:Bt:273:VAL:HG21	1.87	0.55
1:Ak:199:TYR:HA	1:Ak:276:VAL:HG12	1.89	0.55
1:Ak:489:ILE:CD1	1:Ak:494:LEU:HD22	2.33	0.55
2:Am:96:GLU:O	2:Ba:2:ASN:N	2.35	0.55
1:Ar:346:VAL:HB	1:Ar:369:VAL:HG13	1.88	0.55
2:At:3:ILE:HD12	2:Bo:66:ILE:HG13	1.88	0.55
1:Bn:3:ALA:CB	1:Bn:524:LEU:HD13	2.36	0.55
1:Bn:157:THR:HA	1:Bn:160:LYS:HE3	1.88	0.55
1:Bn:479:ASN:HB2	1:Bn:491:MET:SD	2.47	0.55
1:Bt:284:ARG:HD2	1:Bt:364:LYS:CB	2.36	0.55
1:Bu:7:LYS:HD2	1:Bu:66:PHE:CD2	2.40	0.55
1:Al:34:LYS:HZ2	1:Al:483:GLU:CG	2.20	0.55
1:As:479:ASN:HB2	1:As:491:MET:SD	2.47	0.55
1:Bg:169:VAL:HG21	1:Bg:175:ILE:HD11	1.89	0.55
1:Ad:112:ASN:HB3	1:Ad:115:ASP:HB2	1.89	0.55
1:Ad:114:MET:CE	1:Ar:36:ARG:NE	2.41	0.55
1:Ay:6:VAL:CG2	1:Ay:521:VAL:HG13	2.24	0.55
1:Bf:255:GLU:HB3	1:Bf:259:LEU:HB2	1.89	0.55
1:Bf:284:ARG:HD2	1:Bf:364:LYS:CB	2.36	0.55
1:Bf:361:ASP:O	1:Bf:364:LYS:HB3	2.07	0.55
1:Bm:112:ASN:HB3	1:Bm:115:ASP:HB2	1.89	0.55
1:Bm:346:VAL:HB	1:Bm:369:VAL:HG13	1.88	0.55
1:Bn:162:ILE:HG12	1:Bn:400:LEU:HD23	1.89	0.55
1:Bu:169:VAL:HG21	1:Bu:175:ILE:HD11	1.89	0.55
1:Ae:37:ASN:N	1:As:518:GLU:CD	2.31	0.54
1:Ae:517:THR:CG2	1:Al:39:VAL:HG23	2.32	0.54
1:As:12:ALA:HB1	1:As:520:MET:HG3	1.90	0.54
1:Ay:346:VAL:HB	1:Ay:369:VAL:HG13	1.88	0.54
1:Bu:288:MET:HE1	1:Bu:371:LYS:HZ2	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:37:ASN:HD21	1:Ad:51:LYS:HZ1	1.54	0.54
1:Ar:284:ARG:HD2	1:Ar:364:LYS:CB	2.37	0.54
1:As:162:ILE:HG12	1:As:400:LEU:HD23	1.89	0.54
1:Ay:366:GLN:O	1:Ay:369:VAL:HB	2.08	0.54
1:Bf:518:GLU:OE2	1:Bt:36:ARG:CB	2.55	0.54
1:Bu:157:THR:HA	1:Bu:160:LYS:HE3	1.88	0.54
1:Ad:199:TYR:HA	1:Ad:276:VAL:HG12	1.89	0.54
1:Ad:349:ILE:CD1	1:Ad:372:LEU:HG	2.37	0.54
1:Ak:27:VAL:HG12	1:Ak:90:THR:HG23	1.90	0.54
1:Ak:36:ARG:NE	1:Ay:114:MET:CE	2.40	0.54
1:Ak:288:MET:HE1	1:Ak:364:LYS:CE	2.38	0.54
1:Al:479:ASN:HB2	1:Al:491:MET:SD	2.47	0.54
2:Am:66:ILE:HG13	2:Ba:3:ILE:HD12	1.88	0.54
1:Ar:288:MET:HE1	1:Ar:364:LYS:CE	2.38	0.54
1:Ar:361:ASP:O	1:Ar:364:LYS:HB3	2.07	0.54
1:Ay:112:ASN:HB3	1:Ay:115:ASP:HB2	1.89	0.54
1:Az:157:THR:HA	1:Az:160:LYS:HE3	1.88	0.54
1:Bf:27:VAL:HG12	1:Bf:90:THR:HG23	1.90	0.54
1:Bf:288:MET:HE1	1:Bf:364:LYS:CE	2.38	0.54
1:Bg:162:ILE:HG12	1:Bg:400:LEU:HD23	1.89	0.54
1:As:3:ALA:CB	1:As:524:LEU:HD13	2.36	0.54
1:Az:169:VAL:HG21	1:Az:175:ILE:HD11	1.89	0.54
1:Bg:479:ASN:HB2	1:Bg:491:MET:SD	2.47	0.54
1:Ad:27:VAL:HG12	1:Ad:90:THR:HG23	1.90	0.54
1:Ar:349:ILE:CD1	1:Ar:372:LEU:HG	2.37	0.54
1:Ay:361:ASP:O	1:Ay:364:LYS:HB3	2.07	0.54
1:Bt:27:VAL:HG12	1:Bt:90:THR:HG23	1.90	0.54
1:Bt:366:GLN:O	1:Bt:369:VAL:HB	2.08	0.54
1:Ae:381:VAL:HG13	1:Ae:392:LYS:HG3	1.90	0.54
1:Ak:366:GLN:O	1:Ak:369:VAL:HB	2.08	0.54
1:As:381:VAL:HG13	1:As:392:LYS:HG3	1.90	0.54
1:Bg:39:VAL:HG23	1:Bu:517:THR:CG2	2.35	0.54
1:Bg:157:THR:HA	1:Bg:160:LYS:HE3	1.88	0.54
1:Bg:381:VAL:HG13	1:Bg:392:LYS:HG3	1.90	0.54
1:Bm:27:VAL:HG12	1:Bm:90:THR:HG23	1.90	0.54
1:Bm:284:ARG:HD2	1:Bm:364:LYS:CB	2.36	0.54
1:Bn:169:VAL:HG21	1:Bn:175:ILE:HD11	1.89	0.54
1:Bu:12:ALA:HB1	1:Bu:520:MET:HG3	1.89	0.54
1:Bu:479:ASN:HB2	1:Bu:491:MET:SD	2.47	0.54
1:Ad:255:GLU:HB3	1:Ad:259:LEU:HB2	1.89	0.54
1:Ad:284:ARG:HD2	1:Ad:364:LYS:CB	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:518:GLU:OE2	1:Ar:36:ARG:CB	2.55	0.54
1:Ae:12:ALA:HB1	1:Ae:520:MET:HG3	1.90	0.54
1:Ae:489:ILE:CD1	1:Ae:490:ASP:OD1	2.56	0.54
1:Al:73:MET:HG3	1:Az:47:PRO:CG	2.37	0.54
1:Al:517:THR:CG2	1:Az:39:VAL:HG23	2.35	0.54
1:Ay:199:TYR:HA	1:Ay:276:VAL:HG12	1.90	0.54
1:Az:518:GLU:CD	1:Bu:37:ASN:N	2.32	0.54
1:Bf:112:ASN:HB3	1:Bf:115:ASP:HB2	1.89	0.54
1:Bg:12:ALA:HB1	1:Bg:520:MET:HG3	1.90	0.54
1:Bt:112:ASN:HB3	1:Bt:115:ASP:HB2	1.89	0.54
1:Ae:479:ASN:HB2	1:Ae:491:MET:SD	2.47	0.54
1:Ak:255:GLU:HB3	1:Ak:259:LEU:HB2	1.89	0.54
1:Ar:518:GLU:OE2	1:Bm:36:ARG:CB	2.56	0.54
1:Az:461:GLU:O	1:Az:461:GLU:HG2	2.08	0.54
1:Bg:47:PRO:CG	1:Bu:73:MET:HG3	2.35	0.54
1:Bu:489:ILE:CD1	1:Bu:490:ASP:OD1	2.56	0.54
1:Ae:162:ILE:HG12	1:Ae:400:LEU:HD23	1.89	0.54
1:Ak:346:VAL:HB	1:Ak:369:VAL:HG13	1.88	0.54
1:Ar:27:VAL:HG12	1:Ar:90:THR:HG23	1.90	0.54
1:Ar:255:GLU:HB3	1:Ar:259:LEU:HB2	1.89	0.54
1:As:458:CYS:SG	1:As:480:ALA:HB1	2.48	0.54
1:Ay:27:VAL:HG12	1:Ay:90:THR:HG23	1.90	0.54
1:Bf:349:ILE:CD1	1:Bf:372:LEU:HG	2.37	0.54
1:Bn:381:VAL:HG13	1:Bn:392:LYS:HG3	1.90	0.54
1:Bn:489:ILE:CD1	1:Bn:490:ASP:OD1	2.56	0.54
1:Ad:366:GLN:O	1:Ad:369:VAL:HB	2.08	0.54
1:Al:169:VAL:HG21	1:Al:175:ILE:HD11	1.89	0.54
1:Az:120:ILE:O	1:Az:124:VAL:HG23	2.08	0.54
1:Bf:366:GLN:O	1:Bf:369:VAL:HB	2.08	0.54
1:Bm:288:MET:HE1	1:Bm:364:LYS:CE	2.38	0.54
1:Bm:349:ILE:CD1	1:Bm:372:LEU:HG	2.37	0.54
1:Bt:349:ILE:CD1	1:Bt:372:LEU:HG	2.37	0.54
1:Bt:366:GLN:CA	1:Bt:369:VAL:HB	2.38	0.54
1:Ae:518:GLU:HG3	1:Al:36:ARG:HD2	1.89	0.53
1:Ak:112:ASN:HB3	1:Ak:115:ASP:HB2	1.89	0.53
1:Al:381:VAL:HG13	1:Al:392:LYS:HG3	1.90	0.53
1:Al:458:CYS:SG	1:Al:480:ALA:HB1	2.48	0.53
1:Al:461:GLU:O	1:Al:461:GLU:HG2	2.08	0.53
1:Ay:281:PHE:HA	1:Ay:285:ARG:HD2	1.90	0.53
1:Ay:288:MET:HE1	1:Ay:364:LYS:CE	2.38	0.53
1:Az:73:MET:HG3	1:Bu:47:PRO:CG	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:458:CYS:SG	1:Az:480:ALA:HB1	2.48	0.53
1:Bf:281:PHE:HA	1:Bf:285:ARG:HD2	1.90	0.53
1:Bm:281:PHE:HA	1:Bm:285:ARG:HD2	1.90	0.53
1:Bn:120:ILE:O	1:Bn:124:VAL:HG23	2.08	0.53
1:Bu:381:VAL:HG13	1:Bu:392:LYS:HG3	1.90	0.53
1:Ae:120:ILE:O	1:Ae:124:VAL:HG23	2.08	0.53
1:Al:120:ILE:O	1:Al:124:VAL:HG23	2.08	0.53
1:Al:461:GLU:OE2	1:Al:464:VAL:HB	2.09	0.53
1:Ar:281:PHE:HA	1:Ar:285:ARG:HD2	1.90	0.53
1:As:169:VAL:HG21	1:As:175:ILE:HD11	1.89	0.53
1:Ay:349:ILE:CD1	1:Ay:372:LEU:HG	2.37	0.53
1:Bt:135:SER:HA	1:Bt:412:VAL:HG12	1.90	0.53
1:Bt:255:GLU:HB3	1:Bt:259:LEU:HB2	1.89	0.53
1:Bt:409:GLU:OE2	1:Bt:498:LYS:HD3	2.09	0.53
1:Ad:135:SER:HA	1:Ad:412:VAL:HG12	1.90	0.53
1:Ae:169:VAL:HG21	1:Ae:175:ILE:HD11	1.89	0.53
1:Ak:281:PHE:HA	1:Ak:285:ARG:HD2	1.90	0.53
1:Al:162:ILE:HG12	1:Al:400:LEU:HD23	1.89	0.53
1:Ar:366:GLN:O	1:Ar:369:VAL:HB	2.08	0.53
1:Ay:255:GLU:HB3	1:Ay:259:LEU:HB2	1.89	0.53
1:Ay:409:GLU:OE2	1:Ay:498:LYS:HD3	2.09	0.53
1:Ay:523:ASP:OD1	1:Ay:524:LEU:N	2.42	0.53
1:Az:489:ILE:CD1	1:Az:490:ASP:OD1	2.56	0.53
1:Bg:113:PRO:HD3	1:Bn:36:ARG:HH11	1.74	0.53
1:Bg:458:CYS:SG	1:Bg:480:ALA:HB1	2.48	0.53
1:Bn:12:ALA:HB1	1:Bn:520:MET:HG3	1.90	0.53
1:Bt:281:PHE:HA	1:Bt:285:ARG:HD2	1.90	0.53
1:Bt:288:MET:HE1	1:Bt:364:LYS:CE	2.38	0.53
1:Bu:162:ILE:HG12	1:Bu:400:LEU:HD23	1.89	0.53
1:Ae:461:GLU:HG2	1:Ae:461:GLU:O	2.08	0.53
1:Ar:135:SER:HA	1:Ar:412:VAL:HG12	1.90	0.53
1:As:120:ILE:O	1:As:124:VAL:HG23	2.08	0.53
1:As:461:GLU:OE2	1:As:464:VAL:HB	2.09	0.53
1:Az:162:ILE:HG12	1:Az:400:LEU:HD23	1.89	0.53
1:Az:381:VAL:HG13	1:Az:392:LYS:HG3	1.90	0.53
2:Ba:66:ILE:HG13	2:Bv:3:ILE:HD12	1.90	0.53
1:Bf:366:GLN:CA	1:Bf:369:VAL:HB	2.38	0.53
1:Bf:523:ASP:OD1	1:Bf:524:LEU:N	2.42	0.53
1:Bg:489:ILE:CD1	1:Bg:490:ASP:OD1	2.56	0.53
1:Bm:366:GLN:O	1:Bm:369:VAL:HB	2.08	0.53
1:Bn:458:CYS:SG	1:Bn:480:ALA:HB1	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:24:ALA:HB3	1:Bu:97:GLN:CD	2.34	0.53
1:Bu:120:ILE:O	1:Bu:124:VAL:HG23	2.09	0.53
1:Bu:461:GLU:O	1:Bu:461:GLU:HG2	2.08	0.53
1:Ae:77:VAL:HG22	1:Ae:92:ALA:HB1	1.91	0.53
1:Al:489:ILE:CD1	1:Al:490:ASP:OD1	2.56	0.53
1:Ar:199:TYR:HA	1:Ar:276:VAL:HG12	1.90	0.53
1:Ay:366:GLN:CA	1:Ay:369:VAL:HB	2.38	0.53
1:Az:461:GLU:HG3	1:Az:464:VAL:HG23	1.91	0.53
1:Bf:114:MET:CE	1:Bt:36:ARG:NE	2.40	0.53
1:Bg:24:ALA:HB3	1:Bg:97:GLN:CD	2.34	0.53
2:Bh:3:ILE:HD12	2:Bv:66:ILE:HG13	1.90	0.53
1:Bt:365:LEU:HD11	1:Bt:368:ARG:NH1	2.24	0.53
1:Bu:461:GLU:OE2	1:Bu:464:VAL:HB	2.09	0.53
1:Ad:134:LEU:HD11	1:Ad:425:LYS:CE	2.36	0.53
1:Ad:168:LYS:HZ3	1:Ad:187:LEU:HG	1.72	0.53
1:Ad:281:PHE:HA	1:Ad:285:ARG:HD2	1.90	0.53
1:Ad:288:MET:HE1	1:Ad:364:LYS:CE	2.38	0.53
1:Ar:518:GLU:OE2	1:Bm:36:ARG:NH1	2.37	0.53
1:As:77:VAL:HG22	1:As:92:ALA:HB1	1.91	0.53
1:Ay:365:LEU:HD11	1:Ay:368:ARG:NH1	2.24	0.53
1:Az:12:ALA:HB1	1:Az:520:MET:HG3	1.90	0.53
1:Bf:135:SER:HA	1:Bf:412:VAL:HG12	1.90	0.53
1:Bf:409:GLU:OE2	1:Bf:498:LYS:HD3	2.09	0.53
1:Bm:366:GLN:CA	1:Bm:369:VAL:HB	2.38	0.53
1:Ad:47:PRO:HG3	1:Ak:69:MET:HG2	1.91	0.53
1:Ad:61:GLU:C	1:Ad:62:LEU:HD12	2.34	0.53
1:Ae:24:ALA:HB3	1:Ae:97:GLN:CD	2.34	0.53
1:Ae:386:GLU:HG2	1:Ae:387:VAL:N	2.24	0.53
1:Ak:409:GLU:OE2	1:Ak:498:LYS:HD3	2.09	0.53
1:Al:12:ALA:HB1	1:Al:520:MET:HG3	1.90	0.53
1:Al:461:GLU:HG3	1:Al:464:VAL:HG23	1.91	0.53
1:Ay:36:ARG:CD	1:Bt:114:MET:HE2	2.37	0.53
1:Ay:61:GLU:C	1:Ay:62:LEU:HD12	2.34	0.53
1:Ay:135:SER:HA	1:Ay:412:VAL:HG12	1.90	0.53
1:Bf:36:ARG:CB	1:Bm:518:GLU:OE2	2.57	0.53
1:Bf:365:LEU:HD11	1:Bf:368:ARG:NH1	2.24	0.53
1:Ad:365:LEU:HD11	1:Ad:368:ARG:NH1	2.24	0.53
1:Ad:409:GLU:OE2	1:Ad:498:LYS:HD3	2.09	0.53
1:Ad:523:ASP:OD1	1:Ad:524:LEU:N	2.42	0.53
1:Ae:458:CYS:SG	1:Ae:480:ALA:HB1	2.48	0.53
1:Ak:135:SER:HA	1:Ak:412:VAL:HG12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:77:VAL:HG22	1:Al:92:ALA:HB1	1.91	0.53
1:Ar:134:LEU:HD11	1:Ar:425:LYS:CE	2.36	0.53
1:As:489:ILE:CD1	1:As:490:ASP:OD1	2.56	0.53
1:Bm:61:GLU:C	1:Bm:62:LEU:HD12	2.34	0.53
1:Ae:428:ASP:OD1	1:Ae:428:ASP:C	2.52	0.53
1:Ar:366:GLN:CA	1:Ar:369:VAL:HB	2.38	0.53
1:Ar:409:GLU:OE2	1:Ar:498:LYS:HD3	2.09	0.53
1:Az:24:ALA:HB3	1:Az:97:GLN:CD	2.34	0.53
1:Bg:120:ILE:O	1:Bg:124:VAL:HG23	2.09	0.53
2:Bh:66:ILE:HG13	2:Bo:3:ILE:HD12	1.91	0.53
1:Bm:523:ASP:OD1	1:Bm:524:LEU:N	2.42	0.53
1:Bn:24:ALA:HB3	1:Bn:97:GLN:CD	2.34	0.53
1:Bu:461:GLU:HG3	1:Bu:464:VAL:HG23	1.91	0.53
1:Ae:517:THR:HG23	1:Al:39:VAL:CG2	2.35	0.53
1:Ak:366:GLN:CA	1:Ak:369:VAL:HB	2.38	0.53
1:Ak:523:ASP:OD1	1:Ak:524:LEU:N	2.42	0.53
1:As:24:ALA:HB3	1:As:97:GLN:CD	2.34	0.53
1:Ay:36:ARG:CB	1:Bt:518:GLU:OE2	2.57	0.53
1:Bf:199:TYR:HA	1:Bf:276:VAL:HG12	1.89	0.53
1:Bm:409:GLU:OE2	1:Bm:498:LYS:HD3	2.09	0.53
1:Bn:34:LYS:HZ1	1:Bn:483:GLU:CG	2.20	0.53
1:Bn:77:VAL:HG22	1:Bn:92:ALA:HB1	1.91	0.53
1:Bt:199:TYR:HA	1:Bt:276:VAL:HG12	1.89	0.53
1:Ad:366:GLN:CA	1:Ad:369:VAL:HB	2.38	0.52
1:Ak:61:GLU:C	1:Ak:62:LEU:HD12	2.34	0.52
1:As:386:GLU:HG2	1:As:387:VAL:N	2.24	0.52
1:Az:288:MET:HE1	1:Az:371:LYS:HZ3	1.74	0.52
1:Bu:458:CYS:SG	1:Bu:480:ALA:HB1	2.48	0.52
1:Ae:461:GLU:HG3	1:Ae:464:VAL:HG23	1.91	0.52
1:Al:24:ALA:HB3	1:Al:97:GLN:CD	2.34	0.52
1:Al:386:GLU:HG2	1:Al:387:VAL:N	2.24	0.52
1:Bm:199:TYR:HA	1:Bm:276:VAL:HG12	1.89	0.52
1:Ak:36:ARG:CB	1:Ay:518:GLU:OE2	2.56	0.52
1:Ar:365:LEU:HD11	1:Ar:368:ARG:NH1	2.24	0.52
1:As:39:VAL:HG23	1:Bn:517:THR:CG2	2.35	0.52
1:As:461:GLU:HG2	1:As:461:GLU:O	2.08	0.52
1:Az:517:THR:CG2	1:Bu:39:VAL:HG23	2.37	0.52
1:Bm:135:SER:HA	1:Bm:412:VAL:HG12	1.90	0.52
1:Bt:61:GLU:C	1:Bt:62:LEU:HD12	2.34	0.52
1:Bt:523:ASP:OD1	1:Bt:524:LEU:N	2.42	0.52
1:Ad:174:VAL:CG1	1:Ad:376:VAL:HG13	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:365:LEU:HD11	1:Ak:368:ARG:NH1	2.24	0.52
1:Ay:174:VAL:CG1	1:Ay:376:VAL:HG13	2.39	0.52
1:Bm:174:VAL:CG1	1:Bm:376:VAL:HG13	2.39	0.52
1:Bm:383:ALA:HB1	1:Bm:388:GLU:CG	2.40	0.52
1:Ad:383:ALA:HB1	1:Ad:388:GLU:CG	2.40	0.52
1:Ar:174:VAL:CG1	1:Ar:376:VAL:HG13	2.39	0.52
1:As:46:ALA:HB2	1:Bn:76:GLU:OE2	2.03	0.52
1:Az:461:GLU:OE2	1:Az:464:VAL:HB	2.09	0.52
1:Bf:174:VAL:CG1	1:Bf:376:VAL:HG13	2.39	0.52
2:Bh:6:LEU:HD23	2:Bv:92:LEU:C	2.35	0.52
1:Bm:134:LEU:HD11	1:Bm:425:LYS:CE	2.36	0.52
1:Bm:365:LEU:HD11	1:Bm:368:ARG:NH1	2.24	0.52
1:Ae:461:GLU:OE2	1:Ae:464:VAL:HB	2.09	0.52
1:Ak:36:ARG:NH1	1:Ay:518:GLU:OE2	2.37	0.52
1:Bg:461:GLU:OE2	1:Bg:464:VAL:HB	2.09	0.52
1:Bt:174:VAL:CG1	1:Bt:376:VAL:HG13	2.39	0.52
1:Ar:383:ALA:HB1	1:Ar:388:GLU:CG	2.40	0.52
1:Ar:523:ASP:OD1	1:Ar:524:LEU:N	2.42	0.52
1:Bn:461:GLU:OE2	1:Bn:464:VAL:HB	2.09	0.52
1:Ak:134:LEU:HD11	1:Ak:425:LYS:CE	2.36	0.52
1:Ar:61:GLU:C	1:Ar:62:LEU:HD12	2.34	0.52
1:Az:77:VAL:HG22	1:Az:92:ALA:HB1	1.91	0.52
1:Az:428:ASP:OD1	1:Az:428:ASP:C	2.52	0.52
1:Bf:61:GLU:C	1:Bf:62:LEU:HD12	2.34	0.52
1:Bf:134:LEU:HD11	1:Bf:425:LYS:CE	2.36	0.52
1:Bu:428:ASP:OD1	1:Bu:428:ASP:C	2.52	0.52
1:Ak:479:ASN:HB2	1:Ak:491:MET:CE	2.40	0.52
1:As:461:GLU:HG3	1:As:464:VAL:HG23	1.91	0.52
1:Ay:284:ARG:HG2	1:Ay:368:ARG:HH12	1.75	0.52
1:Ay:479:ASN:HB2	1:Ay:491:MET:CE	2.40	0.52
1:Bn:386:GLU:HG2	1:Bn:387:VAL:N	2.24	0.52
1:Bn:461:GLU:O	1:Bn:461:GLU:HG2	2.08	0.52
1:Ad:479:ASN:HB2	1:Ad:491:MET:CE	2.40	0.52
1:Ak:174:VAL:CG1	1:Ak:376:VAL:HG13	2.39	0.52
1:As:489:ILE:HD12	1:As:490:ASP:OD1	2.10	0.52
1:Bf:36:ARG:NH1	1:Bm:518:GLU:OE2	2.36	0.52
1:Bg:6:VAL:HG13	1:Bg:519:CYS:SG	2.50	0.52
1:Bg:77:VAL:HG22	1:Bg:92:ALA:HB1	1.91	0.52
1:Bn:461:GLU:HG3	1:Bn:464:VAL:HG23	1.91	0.52
1:Al:489:ILE:HD12	1:Al:490:ASP:OD1	2.10	0.51
1:Bf:489:ILE:CD1	1:Bf:494:LEU:HD22	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:428:ASP:OD1	1:Bg:428:ASP:C	2.52	0.51
1:Bg:461:GLU:O	1:Bg:461:GLU:HG2	2.08	0.51
1:Bg:461:GLU:HG3	1:Bg:464:VAL:HG23	1.91	0.51
1:Bt:134:LEU:HD11	1:Bt:425:LYS:CE	2.36	0.51
1:Ae:113:PRO:HD3	1:Al:36:ARG:HH11	1.75	0.51
1:Ak:18:ARG:HB2	1:Ak:67:GLU:HG2	1.93	0.51
1:Ay:284:ARG:CD	1:Ay:364:LYS:CG	2.74	0.51
1:Bf:18:ARG:HB2	1:Bf:67:GLU:HG2	1.93	0.51
1:Bt:203:TYR:HB2	1:Bt:264:VAL:HG11	1.92	0.51
1:Bt:325:ILE:HG12	1:Bt:330:THR:HG23	1.92	0.51
1:Bu:34:LYS:HZ2	1:Bu:483:GLU:CG	2.24	0.51
1:Bu:489:ILE:HD12	1:Bu:490:ASP:OD1	2.10	0.51
1:Ad:265:ASN:HA	1:Ad:268:ARG:HE	1.76	0.51
1:Ae:489:ILE:HD12	1:Ae:490:ASP:OD1	2.10	0.51
1:Ay:18:ARG:HB2	1:Ay:67:GLU:HG2	1.93	0.51
1:Ay:203:TYR:HB2	1:Ay:264:VAL:HG11	1.92	0.51
1:Ay:325:ILE:HG12	1:Ay:330:THR:HG23	1.92	0.51
1:Az:386:GLU:HG2	1:Az:387:VAL:N	2.24	0.51
1:Bf:383:ALA:HB1	1:Bf:388:GLU:CG	2.40	0.51
1:Bf:479:ASN:HB2	1:Bf:491:MET:CE	2.40	0.51
1:Bg:386:GLU:HG2	1:Bg:387:VAL:N	2.24	0.51
2:Bh:6:LEU:CD2	2:Bv:92:LEU:C	2.83	0.51
1:Bm:479:ASN:HB2	1:Bm:491:MET:CE	2.40	0.51
1:Ad:203:TYR:HB2	1:Ad:264:VAL:HG11	1.92	0.51
1:Al:113:PRO:HD3	1:Az:36:ARG:HH11	1.76	0.51
2:Am:92:LEU:C	2:Ba:6:LEU:CD2	2.84	0.51
1:Ar:479:ASN:HB2	1:Ar:491:MET:CE	2.40	0.51
2:At:6:LEU:CD2	2:Bo:92:LEU:C	2.83	0.51
1:Bg:489:ILE:HD12	1:Bg:490:ASP:OD1	2.10	0.51
2:Bh:92:LEU:C	2:Bo:6:LEU:HD23	2.36	0.51
1:Bm:18:ARG:HB2	1:Bm:67:GLU:HG2	1.93	0.51
1:Bn:6:VAL:HG13	1:Bn:519:CYS:SG	2.50	0.51
1:Bn:489:ILE:HD12	1:Bn:490:ASP:OD1	2.10	0.51
1:Ad:18:ARG:HB2	1:Ad:67:GLU:HG2	1.93	0.51
1:Ad:284:ARG:HG2	1:Ad:368:ARG:HH12	1.75	0.51
1:Ae:36:ARG:HH11	1:As:113:PRO:HD3	1.76	0.51
2:Af:2:ASN:N	2:At:96:GLU:O	2.42	0.51
1:Ar:265:ASN:HA	1:Ar:268:ARG:HE	1.76	0.51
1:Ay:197:ARG:HD2	1:Ay:277:LYS:HB2	1.93	0.51
1:Ay:383:ALA:HB1	1:Ay:388:GLU:CG	2.40	0.51
1:Bf:325:ILE:HG12	1:Bf:330:THR:HG23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:181:THR:HG22	1:Bm:389:MET:HE1	1.93	0.51
1:Bn:128:VAL:HG22	1:Bn:501:ARG:HG3	1.92	0.51
1:Bn:428:ASP:OD1	1:Bn:428:ASP:C	2.52	0.51
1:Bt:479:ASN:HB2	1:Bt:491:MET:CE	2.40	0.51
1:Bu:386:GLU:HG2	1:Bu:387:VAL:N	2.24	0.51
1:Ak:284:ARG:HG2	1:Ak:368:ARG:HH12	1.75	0.51
1:Ar:18:ARG:HB2	1:Ar:67:GLU:HG2	1.93	0.51
1:Az:113:PRO:HD3	1:Bu:36:ARG:HH11	1.75	0.51
1:Az:489:ILE:HD12	1:Az:490:ASP:OD1	2.10	0.51
1:Bg:128:VAL:HG22	1:Bg:501:ARG:HG3	1.92	0.51
1:Bt:18:ARG:HB2	1:Bt:67:GLU:HG2	1.93	0.51
1:Ak:181:THR:HG22	1:Ak:389:MET:HE1	1.93	0.51
1:Ak:325:ILE:HG12	1:Ak:330:THR:HG23	1.92	0.51
1:Ak:383:ALA:HB1	1:Ak:388:GLU:CG	2.40	0.51
1:Ar:69:MET:HG2	1:Bm:47:PRO:HG3	1.93	0.51
1:As:36:ARG:HH11	1:Bn:113:PRO:HD3	1.75	0.51
1:Bf:181:THR:HG22	1:Bf:389:MET:HE1	1.93	0.51
1:Bf:265:ASN:HA	1:Bf:268:ARG:HE	1.76	0.51
1:Bm:15:LYS:CE	1:Bm:18:ARG:NH1	2.72	0.51
1:Bm:203:TYR:HB2	1:Bm:264:VAL:HG11	1.92	0.51
1:Bt:197:ARG:HD2	1:Bt:277:LYS:HB2	1.92	0.51
1:Ae:6:VAL:HG13	1:Ae:519:CYS:SG	2.51	0.51
1:As:128:VAL:HG22	1:As:501:ARG:HG3	1.92	0.51
1:Bm:265:ASN:HA	1:Bm:268:ARG:HE	1.76	0.51
1:Bt:265:ASN:HA	1:Bt:268:ARG:HE	1.76	0.51
1:Bu:6:VAL:HG13	1:Bu:519:CYS:SG	2.50	0.51
1:Ak:197:ARG:HD2	1:Ak:277:LYS:HB2	1.92	0.51
1:Al:6:VAL:HG13	1:Al:519:CYS:SG	2.51	0.51
1:Bu:77:VAL:HG22	1:Bu:92:ALA:HB1	1.90	0.51
1:Ad:181:THR:HG22	1:Ad:389:MET:HE1	1.93	0.51
1:Ar:203:TYR:HB2	1:Ar:264:VAL:HG11	1.92	0.51
1:As:6:VAL:HG13	1:As:519:CYS:SG	2.50	0.51
2:At:6:LEU:HD23	2:Bo:92:LEU:C	2.36	0.51
1:Bm:363:GLU:C	1:Bm:366:GLN:HE22	2.17	0.51
1:Bu:128:VAL:HG22	1:Bu:501:ARG:HG3	1.92	0.51
1:Ae:183:LEU:CD2	1:Ae:384:ALA:HA	2.41	0.50
1:Ak:168:LYS:HZ3	1:Ak:187:LEU:CD2	2.24	0.50
1:Al:183:LEU:CD2	1:Al:384:ALA:HA	2.41	0.50
1:Al:428:ASP:OD1	1:Al:428:ASP:C	2.52	0.50
1:Ar:197:ARG:HD2	1:Ar:277:LYS:HB2	1.92	0.50
1:Bf:203:TYR:HB2	1:Bf:264:VAL:HG11	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:518:GLU:OE2	1:Bt:36:ARG:NH1	2.37	0.50
1:Ad:36:ARG:NE	1:Ak:114:MET:CE	2.43	0.50
1:Ak:265:ASN:HA	1:Ak:268:ARG:HE	1.76	0.50
1:Bm:197:ARG:HD2	1:Bm:277:LYS:HB2	1.92	0.50
1:Bm:489:ILE:CD1	1:Bm:494:LEU:HD22	2.33	0.50
1:Bt:168:LYS:HZ1	1:Bt:187:LEU:CG	2.22	0.50
1:Ae:288:MET:HE1	1:Ae:371:LYS:HZ3	1.75	0.50
1:As:183:LEU:CD2	1:As:384:ALA:HA	2.41	0.50
1:Ay:181:THR:HG22	1:Ay:389:MET:HE1	1.93	0.50
1:Ay:353:ILE:HG23	1:Ay:362:ARG:O	2.12	0.50
1:Bg:36:ARG:HH11	1:Bu:113:PRO:HD3	1.75	0.50
1:Bm:353:ILE:HG23	1:Bm:362:ARG:O	2.12	0.50
1:Bn:183:LEU:CD2	1:Bn:384:ALA:HA	2.41	0.50
1:Bt:181:THR:HG22	1:Bt:389:MET:HE1	1.93	0.50
1:Bt:383:ALA:HB1	1:Bt:388:GLU:CG	2.40	0.50
1:Ak:203:TYR:HB2	1:Ak:264:VAL:HG11	1.92	0.50
1:Al:128:VAL:HG22	1:Al:501:ARG:HG3	1.92	0.50
1:Ar:83:ASP:OD1	1:Ar:84:ALA:N	2.45	0.50
1:Az:6:VAL:HG13	1:Az:519:CYS:SG	2.51	0.50
1:Az:183:LEU:CD2	1:Az:384:ALA:HA	2.42	0.50
1:Bf:69:MET:HG2	1:Bt:47:PRO:HG3	1.94	0.50
1:Bm:325:ILE:HG12	1:Bm:330:THR:HG23	1.92	0.50
1:Ae:128:VAL:HG22	1:Ae:501:ARG:HG3	1.92	0.50
1:Ak:42:LYS:CE	1:Ak:46:ALA:O	2.60	0.50
1:Al:122:LYS:HE3	1:Al:429:LEU:HD11	1.94	0.50
1:Ay:183:LEU:CD2	1:Ay:384:ALA:HB2	2.42	0.50
1:Ay:420:ILE:CG2	1:Ay:470:LYS:HG2	2.42	0.50
1:Bg:113:PRO:CG	1:Bn:36:ARG:CZ	2.89	0.50
1:Bm:409:GLU:CD	1:Bm:498:LYS:HD3	2.37	0.50
1:Bt:420:ILE:CG2	1:Bt:470:LYS:HG2	2.42	0.50
1:Ad:42:LYS:CE	1:Ad:46:ALA:O	2.60	0.50
1:Ad:325:ILE:HG12	1:Ad:330:THR:HG23	1.92	0.50
1:Ad:409:GLU:CD	1:Ad:498:LYS:HD3	2.37	0.50
1:Ak:47:PRO:HG3	1:Ay:69:MET:HG2	1.93	0.50
1:Ak:353:ILE:HG23	1:Ak:362:ARG:O	2.12	0.50
2:Am:92:LEU:C	2:Ba:6:LEU:HD23	2.36	0.50
1:Ar:409:GLU:CD	1:Ar:498:LYS:HD3	2.37	0.50
1:Ar:420:ILE:CG2	1:Ar:470:LYS:HG2	2.42	0.50
1:As:428:ASP:OD1	1:As:428:ASP:C	2.52	0.50
2:Ba:92:LEU:C	2:Bv:6:LEU:HD23	2.37	0.50
1:Bg:183:LEU:CD2	1:Bg:384:ALA:HA	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:42:LYS:CE	1:Bm:46:ALA:O	2.60	0.50
1:Bm:420:ILE:CG2	1:Bm:470:LYS:HG2	2.42	0.50
1:Bt:164:GLU:CG	1:Bt:165:ALA:N	2.75	0.50
1:Bu:183:LEU:CD2	1:Bu:384:ALA:HA	2.41	0.50
1:Ad:83:ASP:OD1	1:Ad:84:ALA:N	2.45	0.50
1:Ak:183:LEU:CD2	1:Ak:384:ALA:HB2	2.42	0.50
1:Ar:164:GLU:CG	1:Ar:165:ALA:N	2.75	0.50
1:Ar:325:ILE:HG12	1:Ar:330:THR:HG23	1.92	0.50
1:Ay:42:LYS:CE	1:Ay:46:ALA:O	2.60	0.50
1:Ay:265:ASN:HA	1:Ay:268:ARG:HE	1.76	0.50
1:Bf:42:LYS:CE	1:Bf:46:ALA:O	2.60	0.50
1:Bf:420:ILE:CG2	1:Bf:470:LYS:HG2	2.42	0.50
2:Bh:92:LEU:C	2:Bo:6:LEU:CD2	2.84	0.50
1:Bm:83:ASP:OD1	1:Bm:84:ALA:N	2.45	0.50
1:Bm:164:GLU:CG	1:Bm:165:ALA:N	2.75	0.50
1:Bt:284:ARG:HG2	1:Bt:368:ARG:HH12	1.75	0.50
1:Ae:34:LYS:HZ2	1:Ae:483:GLU:CG	2.23	0.50
1:Ae:122:LYS:HE3	1:Ae:429:LEU:HD11	1.94	0.50
1:Ar:42:LYS:CE	1:Ar:46:ALA:O	2.60	0.50
1:Bf:197:ARG:HD2	1:Bf:277:LYS:HB2	1.92	0.50
1:Bf:479:ASN:CB	1:Bf:491:MET:HE1	2.42	0.50
1:Bt:363:GLU:C	1:Bt:366:GLN:HE22	2.17	0.50
1:Ak:409:GLU:CD	1:Ak:498:LYS:HD3	2.37	0.50
1:Ar:15:LYS:CE	1:Ar:18:ARG:NH1	2.72	0.50
1:Ar:181:THR:HG22	1:Ar:389:MET:HE1	1.93	0.50
1:Ar:353:ILE:HG23	1:Ar:362:ARG:O	2.12	0.50
1:Bf:409:GLU:CD	1:Bf:498:LYS:HD3	2.37	0.50
1:Bm:168:LYS:HD2	1:Bm:189:VAL:HG21	1.94	0.50
1:Bm:183:LEU:CD2	1:Bm:384:ALA:HB2	2.42	0.50
1:Bt:479:ASN:CB	1:Bt:491:MET:HE1	2.42	0.50
1:Ad:197:ARG:HD2	1:Ad:277:LYS:HB2	1.92	0.49
1:Ae:381:VAL:HG13	1:Ae:392:LYS:CG	2.42	0.49
1:Ak:31:LEU:HD22	1:Ak:94:VAL:HG21	1.93	0.49
1:Al:7:LYS:HG3	1:Al:66:PHE:CE1	2.45	0.49
1:As:122:LYS:HE3	1:As:429:LEU:HD11	1.94	0.49
1:Ay:83:ASP:OD1	1:Ay:84:ALA:N	2.45	0.49
1:Ay:164:GLU:CG	1:Ay:165:ALA:N	2.75	0.49
1:Az:128:VAL:HG22	1:Az:501:ARG:HG3	1.92	0.49
2:Ba:92:LEU:C	2:Bv:6:LEU:CD2	2.85	0.49
1:Bf:168:LYS:HD2	1:Bf:189:VAL:HG21	1.94	0.49
1:Bt:42:LYS:CE	1:Bt:46:ALA:O	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:353:ILE:HG23	1:Ad:362:ARG:O	2.12	0.49
1:Ad:420:ILE:CG2	1:Ad:470:LYS:HG2	2.42	0.49
1:Ay:409:GLU:CD	1:Ay:498:LYS:HD3	2.37	0.49
1:Az:122:LYS:HE3	1:Az:429:LEU:HD11	1.94	0.49
1:Bf:353:ILE:HG23	1:Bf:362:ARG:O	2.12	0.49
1:Bm:479:ASN:CB	1:Bm:491:MET:HE1	2.42	0.49
1:Bt:31:LEU:HD22	1:Bt:94:VAL:HG21	1.93	0.49
1:Bt:168:LYS:HZ3	1:Bt:187:LEU:CD2	2.25	0.49
1:Bt:183:LEU:CD2	1:Bt:384:ALA:HB2	2.42	0.49
1:Bt:301:ILE:HG21	1:Bt:312:ALA:HB2	1.94	0.49
1:Ad:69:MET:HG2	1:Ar:47:PRO:HG3	1.95	0.49
2:Af:92:LEU:C	2:Am:6:LEU:CD2	2.86	0.49
1:Ak:164:GLU:CA	1:Ak:167:ASP:HB2	2.43	0.49
1:Ak:168:LYS:HZ1	1:Ak:187:LEU:CG	2.24	0.49
1:Ak:225:LYS:HG3	1:Ak:304:GLU:HB2	1.94	0.49
1:Ay:479:ASN:CB	1:Ay:491:MET:HE1	2.42	0.49
1:Bf:47:PRO:HG3	1:Bm:69:MET:HG2	1.95	0.49
1:Bm:39:VAL:HG22	1:Bm:49:ILE:HG12	1.95	0.49
1:Bm:284:ARG:HG2	1:Bm:368:ARG:HH12	1.75	0.49
1:Bt:353:ILE:HG23	1:Bt:362:ARG:O	2.12	0.49
1:Bt:409:GLU:CD	1:Bt:498:LYS:HD3	2.37	0.49
1:Ad:31:LEU:HD22	1:Ad:94:VAL:HG21	1.93	0.49
1:Ad:301:ILE:HG21	1:Ad:312:ALA:HB2	1.94	0.49
1:Ak:83:ASP:OD1	1:Ak:84:ALA:N	2.45	0.49
1:Ak:363:GLU:C	1:Ak:366:GLN:HE22	2.17	0.49
1:Ak:420:ILE:CG2	1:Ak:470:LYS:HG2	2.42	0.49
1:Al:288:MET:HE1	1:Al:371:LYS:HZ3	1.75	0.49
1:Ar:284:ARG:HG2	1:Ar:368:ARG:HH12	1.75	0.49
1:Ay:31:LEU:HD22	1:Ay:94:VAL:HG21	1.93	0.49
1:Az:169:VAL:HG21	1:Az:175:ILE:CD1	2.42	0.49
1:Bg:169:VAL:HG21	1:Bg:175:ILE:CD1	2.42	0.49
1:Bn:381:VAL:HG13	1:Bn:392:LYS:CG	2.42	0.49
1:Bu:461:GLU:OE2	1:Bu:464:VAL:HG21	2.13	0.49
1:Ay:164:GLU:CA	1:Ay:167:ASP:HB2	2.43	0.49
1:Bf:31:LEU:HD22	1:Bf:94:VAL:HG21	1.93	0.49
1:Bf:83:ASP:OD1	1:Bf:84:ALA:N	2.45	0.49
1:Bf:164:GLU:CG	1:Bf:165:ALA:N	2.75	0.49
1:Bg:381:VAL:HG13	1:Bg:392:LYS:CG	2.42	0.49
1:Bu:381:VAL:HG13	1:Bu:392:LYS:CG	2.42	0.49
1:Ak:248:LEU:HD22	1:Ak:323:VAL:HG11	1.95	0.49
1:Ar:39:VAL:HG22	1:Ar:49:ILE:HG12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:36:ARG:NH1	1:Bt:518:GLU:OE2	2.37	0.49
1:Bf:39:VAL:HG22	1:Bf:49:ILE:HG12	1.95	0.49
1:Bf:301:ILE:HG21	1:Bf:312:ALA:HB2	1.94	0.49
1:Ad:39:VAL:HG22	1:Ad:49:ILE:HG12	1.95	0.49
1:Ad:225:LYS:HG3	1:Ad:304:GLU:HB2	1.94	0.49
1:Ad:248:LEU:HD22	1:Ad:323:VAL:HG11	1.95	0.49
1:Ak:37:ASN:HD21	1:Ak:51:LYS:HZ1	1.59	0.49
1:Ar:183:LEU:CD2	1:Ar:384:ALA:HB2	2.42	0.49
1:Ay:301:ILE:HG21	1:Ay:312:ALA:HB2	1.94	0.49
1:Az:113:PRO:CG	1:Bu:36:ARG:CZ	2.91	0.49
1:Az:461:GLU:OE2	1:Az:464:VAL:HG21	2.13	0.49
1:Bg:36:ARG:CZ	1:Bu:113:PRO:CG	2.91	0.49
1:Bn:122:LYS:HE3	1:Bn:429:LEU:HD11	1.94	0.49
1:Bt:83:ASP:OD1	1:Bt:84:ALA:N	2.45	0.49
1:Bt:164:GLU:CA	1:Bt:167:ASP:HB2	2.42	0.49
1:Bu:7:LYS:HG3	1:Bu:66:PHE:CE1	2.45	0.49
1:Ad:183:LEU:CD2	1:Ad:384:ALA:HB2	2.42	0.49
1:Ak:479:ASN:CB	1:Ak:491:MET:HE1	2.42	0.49
1:Ar:301:ILE:HG21	1:Ar:312:ALA:HB2	1.94	0.49
1:Ar:479:ASN:CB	1:Ar:491:MET:HE1	2.42	0.49
1:As:381:VAL:HG13	1:As:392:LYS:CG	2.42	0.49
1:Ay:225:LYS:HG3	1:Ay:304:GLU:HB2	1.94	0.49
1:Az:34:LYS:HZ2	1:Az:483:GLU:HG3	1.76	0.49
1:Bf:164:GLU:CA	1:Bf:167:ASP:HB2	2.42	0.49
1:Bf:284:ARG:HG2	1:Bf:368:ARG:HH12	1.75	0.49
1:Bg:461:GLU:OE2	1:Bg:464:VAL:HG21	2.13	0.49
1:Ad:164:GLU:CG	1:Ad:165:ALA:N	2.75	0.49
1:Ae:36:ARG:CZ	1:As:113:PRO:CG	2.91	0.49
1:Al:461:GLU:OE2	1:Al:464:VAL:HG21	2.13	0.49
1:Ar:37:ASN:HD21	1:Ar:51:LYS:HZ1	1.59	0.49
1:Ar:168:LYS:HD2	1:Ar:189:VAL:HG21	1.94	0.49
1:Bt:168:LYS:HD2	1:Bt:189:VAL:HG21	1.94	0.49
1:Ae:461:GLU:OE2	1:Ae:464:VAL:HG21	2.13	0.49
1:Al:169:VAL:HG21	1:Al:175:ILE:CD1	2.42	0.49
2:Am:12:VAL:HG12	2:Am:40:VAL:HA	1.95	0.49
1:Ay:134:LEU:HD11	1:Ay:425:LYS:CE	2.36	0.49
1:Bf:225:LYS:HG3	1:Bf:304:GLU:HB2	1.94	0.49
1:Bn:169:VAL:HG21	1:Bn:175:ILE:CD1	2.42	0.49
1:Bu:169:VAL:HG21	1:Bu:175:ILE:CD1	2.43	0.49
1:Bu:461:GLU:OE2	1:Bu:464:VAL:CB	2.61	0.49
1:Ae:461:GLU:OE2	1:Ae:464:VAL:CB	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:248:LEU:HD22	1:Ar:323:VAL:HG11	1.95	0.48
1:As:7:LYS:HG3	1:As:66:PHE:CE1	2.45	0.48
1:Az:488:MET:CE	1:Az:491:MET:HE1	2.19	0.48
1:Bg:461:GLU:OE2	1:Bg:464:VAL:CB	2.61	0.48
1:Bm:225:LYS:HG3	1:Bm:304:GLU:HB2	1.94	0.48
1:Ad:363:GLU:C	1:Ad:366:GLN:HE22	2.17	0.48
1:Ad:479:ASN:CB	1:Ad:491:MET:HE1	2.42	0.48
1:Ae:113:PRO:CG	1:Al:36:ARG:CZ	2.91	0.48
1:Ak:39:VAL:HG22	1:Ak:49:ILE:HG12	1.95	0.48
1:Ak:301:ILE:HG21	1:Ak:312:ALA:HB2	1.94	0.48
1:Ar:31:LEU:HD22	1:Ar:94:VAL:HG21	1.93	0.48
1:Ar:168:LYS:NZ	1:Ar:187:LEU:CD2	2.77	0.48
1:Ay:6:VAL:HG12	1:Ay:8:PHE:CE1	2.49	0.48
2:Ba:12:VAL:HG12	2:Ba:40:VAL:HA	1.95	0.48
1:Bg:122:LYS:HE3	1:Bg:429:LEU:HD11	1.94	0.48
1:Bm:6:VAL:HG12	1:Bm:8:PHE:CE1	2.49	0.48
1:Ad:345:ARG:O	1:Ad:349:ILE:HG13	2.14	0.48
2:Af:97:ALA:OXT	2:Am:1:MET:N	2.46	0.48
1:Ak:168:LYS:HZ3	1:Ak:187:LEU:HG	1.77	0.48
1:Ar:69:MET:CE	1:Ar:520:MET:HE2	2.42	0.48
1:Ar:176:THR:CG2	1:Ar:178:GLU:OE2	2.61	0.48
1:Ar:381:VAL:HG21	1:Ar:393:LYS:HA	1.95	0.48
1:Ay:248:LEU:HD22	1:Ay:323:VAL:HG11	1.95	0.48
1:Az:381:VAL:HG13	1:Az:392:LYS:CG	2.42	0.48
1:Bf:6:VAL:HG12	1:Bf:8:PHE:CE1	2.49	0.48
1:Bf:183:LEU:CD2	1:Bf:384:ALA:HB2	2.42	0.48
1:Bt:39:VAL:HG22	1:Bt:49:ILE:HG12	1.95	0.48
1:Ak:280:GLY:HA2	1:Ak:284:ARG:HH21	1.79	0.48
1:Al:381:VAL:HG13	1:Al:392:LYS:CG	2.42	0.48
1:As:36:ARG:CZ	1:Bn:113:PRO:CG	2.91	0.48
1:Bf:280:GLY:HA2	1:Bf:284:ARG:HH21	1.79	0.48
1:Bu:122:LYS:HE3	1:Bu:429:LEU:HD11	1.94	0.48
1:As:169:VAL:HG21	1:As:175:ILE:CD1	2.42	0.48
1:As:461:GLU:OE2	1:As:464:VAL:HG21	2.12	0.48
1:Ay:47:PRO:HG3	1:Bt:69:MET:HG2	1.95	0.48
1:Bm:31:LEU:HD22	1:Bm:94:VAL:HG21	1.93	0.48
1:Bm:301:ILE:HG21	1:Bm:312:ALA:HB2	1.94	0.48
1:Bm:345:ARG:O	1:Bm:349:ILE:HG13	2.14	0.48
1:Bm:381:VAL:HG21	1:Bm:393:LYS:HA	1.95	0.48
1:Bn:461:GLU:OE2	1:Bn:464:VAL:HG21	2.13	0.48
1:Bt:345:ARG:O	1:Bt:349:ILE:HG13	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:177:VAL:CG2	1:Bu:400:LEU:CD1	2.92	0.48
1:Ad:168:LYS:NZ	1:Ad:187:LEU:HD21	2.29	0.48
1:Ad:381:VAL:HG21	1:Ad:393:LYS:HA	1.95	0.48
1:Ae:169:VAL:HG21	1:Ae:175:ILE:CD1	2.42	0.48
1:Ae:177:VAL:CG2	1:Ae:400:LEU:CD1	2.92	0.48
1:Ak:164:GLU:CG	1:Ak:165:ALA:N	2.75	0.48
1:Ak:207:LYS:H	1:Ak:207:LYS:HG3	1.42	0.48
1:Al:4:LYS:N	1:Al:524:LEU:CD1	2.77	0.48
1:Al:461:GLU:OE2	1:Al:464:VAL:CB	2.61	0.48
1:As:54:VAL:HG11	1:As:82:ASN:HD21	1.68	0.48
1:As:461:GLU:OE2	1:As:464:VAL:CB	2.61	0.48
1:Ay:107:VAL:HG21	1:Ay:515:ILE:HG23	1.96	0.48
1:Ay:168:LYS:NZ	1:Ay:187:LEU:CD2	2.77	0.48
1:Bg:4:LYS:N	1:Bg:524:LEU:CD1	2.77	0.48
2:Bh:76:GLU:OE1	2:Bv:36:THR:OG1	2.30	0.48
1:Bn:4:LYS:N	1:Bn:524:LEU:CD1	2.77	0.48
1:Bt:6:VAL:HG12	1:Bt:8:PHE:CE1	2.49	0.48
1:Bt:225:LYS:HG3	1:Bt:304:GLU:HB2	1.94	0.48
1:Ad:280:GLY:HA2	1:Ad:284:ARG:HH21	1.79	0.48
1:Ak:6:VAL:HG12	1:Ak:8:PHE:CE1	2.49	0.48
1:Ar:6:VAL:HG12	1:Ar:8:PHE:CE1	2.49	0.48
1:Bf:248:LEU:HD22	1:Bf:323:VAL:HG11	1.95	0.48
1:Bm:280:GLY:HA2	1:Bm:284:ARG:HH21	1.79	0.48
1:Bt:107:VAL:HG21	1:Bt:515:ILE:HG23	1.96	0.48
1:Ad:168:LYS:NZ	1:Ad:187:LEU:CD2	2.77	0.48
2:Af:4:ARG:HB3	2:At:94:ILE:O	2.14	0.48
1:Ak:168:LYS:NZ	1:Ak:187:LEU:CD2	2.77	0.48
1:Al:177:VAL:CG2	1:Al:400:LEU:CD1	2.92	0.48
1:Ar:345:ARG:O	1:Ar:349:ILE:HG13	2.14	0.48
1:Ar:524:LEU:HD23	1:Ar:525:PRO:HD2	1.96	0.48
1:Ay:39:VAL:HG22	1:Ay:49:ILE:HG12	1.95	0.48
1:Ay:168:LYS:HD2	1:Ay:189:VAL:HG21	1.94	0.48
1:Bf:409:GLU:OE1	1:Bf:498:LYS:CB	2.62	0.48
1:Bf:524:LEU:HD23	1:Bf:525:PRO:HD2	1.96	0.48
1:Bm:409:GLU:OE1	1:Bm:498:LYS:CB	2.62	0.48
1:Bn:461:GLU:OE2	1:Bn:464:VAL:CB	2.61	0.48
1:Bt:168:LYS:NZ	1:Bt:187:LEU:CD2	2.77	0.48
1:Bt:524:LEU:HD23	1:Bt:525:PRO:HD2	1.96	0.48
1:Ae:419:LEU:HA	1:Ae:422:VAL:HG22	1.96	0.48
1:Ak:107:VAL:HG21	1:Ak:515:ILE:HG23	1.96	0.48
1:Ak:321:LYS:HD3	1:Ak:321:LYS:HA	1.50	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:225:LYS:HG3	1:Ar:304:GLU:HB2	1.94	0.48
1:Ay:321:LYS:HD3	1:Ay:321:LYS:HA	1.50	0.48
1:Bg:177:VAL:CG2	1:Bg:400:LEU:CD1	2.92	0.48
1:Bm:524:LEU:HD23	1:Bm:525:PRO:HD2	1.96	0.48
1:Ad:168:LYS:HD2	1:Ad:189:VAL:HG21	1.94	0.48
1:Ad:524:LEU:HD23	1:Ad:525:PRO:HD2	1.96	0.48
1:As:177:VAL:CG2	1:As:400:LEU:CD1	2.92	0.48
1:Ay:168:LYS:NZ	1:Ay:187:LEU:HD21	2.29	0.48
1:Bf:168:LYS:NZ	1:Bf:187:LEU:CD2	2.77	0.48
1:Bt:409:GLU:OE1	1:Bt:498:LYS:CB	2.62	0.48
2:Bv:12:VAL:HG12	2:Bv:40:VAL:HA	1.95	0.48
1:Al:419:LEU:HA	1:Al:422:VAL:HG22	1.96	0.47
1:Ar:280:GLY:HA2	1:Ar:284:ARG:HH21	1.79	0.47
1:Ar:321:LYS:HD3	1:Ar:321:LYS:HA	1.50	0.47
2:At:12:VAL:HG12	2:At:40:VAL:HA	1.95	0.47
1:Ay:280:GLY:HA2	1:Ay:284:ARG:HH21	1.79	0.47
1:Az:419:LEU:HA	1:Az:422:VAL:HG22	1.96	0.47
1:Bf:345:ARG:O	1:Bf:349:ILE:HG13	2.14	0.47
1:Bg:517:THR:CG2	1:Bn:39:VAL:HG23	2.36	0.47
1:Bu:419:LEU:HA	1:Bu:422:VAL:HG22	1.96	0.47
1:Ae:36:ARG:CZ	1:As:113:PRO:HG2	2.44	0.47
1:Ae:39:VAL:CG2	1:As:517:THR:HG23	2.38	0.47
2:Af:12:VAL:HG12	2:Af:40:VAL:HA	1.95	0.47
1:Ak:168:LYS:HD2	1:Ak:189:VAL:HG21	1.94	0.47
1:Ar:168:LYS:NZ	1:Ar:187:LEU:HD21	2.29	0.47
1:Bf:107:VAL:HG21	1:Bf:515:ILE:HG23	1.96	0.47
1:Bt:168:LYS:NZ	1:Bt:187:LEU:HD21	2.29	0.47
1:Bt:248:LEU:HD22	1:Bt:323:VAL:HG11	1.95	0.47
1:Ad:6:VAL:HG12	1:Ad:8:PHE:CE1	2.49	0.47
1:Ad:69:MET:CE	1:Ad:520:MET:HE2	2.42	0.47
2:Af:3:ILE:HG23	2:At:95:VAL:N	2.29	0.47
1:Ak:69:MET:CE	1:Ak:520:MET:HE2	2.42	0.47
1:Ak:524:LEU:HD23	1:Ak:525:PRO:HD2	1.96	0.47
1:Ay:207:LYS:H	1:Ay:207:LYS:HG3	1.42	0.47
1:Ay:381:VAL:HG21	1:Ay:393:LYS:HA	1.95	0.47
1:Ay:409:GLU:OE1	1:Ay:498:LYS:CB	2.62	0.47
1:Ay:524:LEU:HD23	1:Ay:525:PRO:HD2	1.96	0.47
1:Az:461:GLU:OE2	1:Az:464:VAL:CB	2.61	0.47
1:Bf:381:VAL:HG21	1:Bf:393:LYS:HA	1.96	0.47
1:Bm:168:LYS:NZ	1:Bm:187:LEU:CD2	2.77	0.47
1:Bn:177:VAL:CG2	1:Bn:400:LEU:CD1	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:107:VAL:HG21	1:Ad:515:ILE:HG23	1.96	0.47
1:Ad:457:ASN:O	1:Ak:114:MET:CE	2.59	0.47
1:Ae:488:MET:CE	1:Ae:491:MET:HE1	2.19	0.47
1:Ak:168:LYS:NZ	1:Ak:187:LEU:HD21	2.29	0.47
1:Ak:345:ARG:O	1:Ak:349:ILE:HG13	2.14	0.47
1:As:4:LYS:N	1:As:524:LEU:CD1	2.77	0.47
1:Bf:168:LYS:NZ	1:Bf:187:LEU:HD21	2.29	0.47
1:Bf:391:GLU:OE1	1:Bf:392:LYS:CG	2.62	0.47
2:Bo:12:VAL:HG12	2:Bo:40:VAL:HA	1.95	0.47
1:Bu:4:LYS:N	1:Bu:524:LEU:CD1	2.77	0.47
1:Ad:15:LYS:CE	1:Ad:18:ARG:NH1	2.72	0.47
1:Ae:34:LYS:HZ1	1:Ae:483:GLU:HG3	1.74	0.47
1:As:419:LEU:HA	1:As:422:VAL:HG22	1.96	0.47
1:Az:177:VAL:CG2	1:Az:400:LEU:CD1	2.92	0.47
1:Bg:419:LEU:HA	1:Bg:422:VAL:HG22	1.96	0.47
1:Bm:95:LEU:HD23	1:Bm:450:PRO:HD3	1.97	0.47
1:Bm:168:LYS:NZ	1:Bm:187:LEU:HD21	2.29	0.47
1:Bm:248:LEU:HD22	1:Bm:323:VAL:HG11	1.95	0.47
1:Bt:381:VAL:HG21	1:Bt:393:LYS:HA	1.95	0.47
1:Ad:518:GLU:OE2	1:Ar:36:ARG:NH1	2.37	0.47
1:Ae:4:LYS:N	1:Ae:524:LEU:CD1	2.77	0.47
1:Ak:381:VAL:HG21	1:Ak:393:LYS:HA	1.95	0.47
1:Ar:107:VAL:HG21	1:Ar:515:ILE:HG23	1.95	0.47
1:Ar:409:GLU:OE1	1:Ar:498:LYS:CB	2.62	0.47
1:As:36:ARG:CZ	1:Bn:113:PRO:HG2	2.44	0.47
1:Ay:348:GLN:HE21	1:Ay:348:GLN:HB3	1.54	0.47
1:Bf:95:LEU:HD23	1:Bf:450:PRO:HD3	1.97	0.47
2:Bh:12:VAL:HG12	2:Bh:40:VAL:HA	1.95	0.47
1:Bm:164:GLU:CA	1:Bm:167:ASP:HB2	2.42	0.47
1:Bm:366:GLN:C	1:Bm:369:VAL:HB	2.40	0.47
1:Bn:58:ARG:HA	1:Bn:75:LYS:HD3	1.97	0.47
1:Ad:114:MET:HE2	1:Ar:36:ARG:CD	2.37	0.47
1:Ae:60:ILE:HG12	1:As:521:VAL:HG11	1.97	0.47
1:Ak:349:ILE:HA	1:Ak:352:GLN:HB2	1.97	0.47
1:Ak:421:ARG:HH12	1:Ak:469:VAL:CG1	2.24	0.47
1:Al:488:MET:CE	1:Al:491:MET:HE1	2.19	0.47
1:Ar:95:LEU:HD23	1:Ar:450:PRO:HD3	1.97	0.47
1:Ar:363:GLU:C	1:Ar:366:GLN:HE22	2.17	0.47
1:Ay:176:THR:CG2	1:Ay:178:GLU:OE2	2.61	0.47
1:Ay:349:ILE:HA	1:Ay:352:GLN:HB2	1.97	0.47
1:Ay:391:GLU:OE1	1:Ay:392:LYS:CG	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:366:GLN:C	1:Bf:369:VAL:HB	2.40	0.47
1:Bf:366:GLN:HG2	1:Bf:367:GLU:N	2.30	0.47
1:Bg:60:ILE:HG12	1:Bu:521:VAL:HG11	1.97	0.47
1:Bm:107:VAL:HG21	1:Bm:515:ILE:HG23	1.96	0.47
1:Bt:280:GLY:HA2	1:Bt:284:ARG:HH21	1.79	0.47
1:Bu:58:ARG:HA	1:Bu:75:LYS:HD3	1.97	0.47
1:Ad:288:MET:CE	1:Ad:364:LYS:HE3	2.45	0.47
1:Al:113:PRO:CG	1:Az:36:ARG:CZ	2.92	0.47
1:Al:131:LEU:HD23	1:Al:131:LEU:HA	1.76	0.47
1:Ar:489:ILE:CD1	1:Ar:494:LEU:HD22	2.33	0.47
1:Ay:345:ARG:O	1:Ay:349:ILE:HG13	2.14	0.47
1:Az:4:LYS:N	1:Az:524:LEU:CD1	2.77	0.47
1:Bg:58:ARG:HA	1:Bg:75:LYS:HD3	1.97	0.47
1:Bm:176:THR:CG2	1:Bm:178:GLU:OE2	2.61	0.47
1:Bm:288:MET:CE	1:Bm:364:LYS:HE3	2.45	0.47
1:Ad:349:ILE:HA	1:Ad:352:GLN:HB2	1.97	0.47
1:Ad:409:GLU:OE1	1:Ad:498:LYS:CB	2.62	0.47
1:Ar:164:GLU:CA	1:Ar:167:ASP:HB2	2.42	0.47
1:Ar:366:GLN:C	1:Ar:369:VAL:HB	2.40	0.47
1:Bn:23:LEU:HD23	1:Bn:60:ILE:HB	1.97	0.47
1:Bn:419:LEU:HA	1:Bn:422:VAL:HG22	1.96	0.47
1:Bt:176:THR:CG2	1:Bt:178:GLU:OE2	2.61	0.47
1:Bt:366:GLN:C	1:Bt:369:VAL:HB	2.40	0.47
1:Bt:404:ARG:O	1:Bt:407:VAL:HG22	2.15	0.47
1:Bt:422:VAL:HA	1:Bt:425:LYS:HD2	1.97	0.47
1:Ae:39:VAL:HG23	1:As:517:THR:CG2	2.35	0.47
1:Ak:277:LYS:H	1:Ak:277:LYS:HG3	1.53	0.47
1:Ar:349:ILE:HA	1:Ar:352:GLN:HB2	1.97	0.47
1:As:58:ARG:HA	1:As:75:LYS:HD3	1.97	0.47
1:Az:58:ARG:HA	1:Az:75:LYS:HD3	1.97	0.47
1:Bf:176:THR:CG2	1:Bf:178:GLU:OE2	2.61	0.47
1:Bg:20:VAL:HG21	1:Bg:514:MET:HE1	1.97	0.47
1:Bm:421:ARG:NH1	1:Bm:469:VAL:O	2.48	0.47
1:Bu:430:ARG:NH1	1:Bu:441:LYS:NZ	2.63	0.47
1:Ak:307:MET:HE3	1:Ak:307:MET:HB3	1.64	0.46
1:Ak:366:GLN:CA	1:Ak:369:VAL:H	2.29	0.46
1:Ar:352:GLN:CB	1:Ar:365:LEU:HD23	2.39	0.46
1:Ar:404:ARG:O	1:Ar:407:VAL:HG22	2.16	0.46
1:As:430:ARG:NH1	1:As:441:LYS:NZ	2.63	0.46
1:Az:113:PRO:HG2	1:Bu:36:ARG:CZ	2.43	0.46
1:Bf:69:MET:CE	1:Bf:520:MET:HE2	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:430:ARG:NH1	1:Bg:441:LYS:NZ	2.63	0.46
1:Bm:366:GLN:CA	1:Bm:369:VAL:H	2.29	0.46
1:Ae:430:ARG:NH1	1:Ae:441:LYS:NZ	2.63	0.46
1:Ak:366:GLN:C	1:Ak:369:VAL:HB	2.40	0.46
1:Bm:366:GLN:HG2	1:Bm:367:GLU:N	2.30	0.46
1:Bn:20:VAL:HG21	1:Bn:514:MET:HE1	1.97	0.46
1:Bt:95:LEU:HD23	1:Bt:450:PRO:HD3	1.97	0.46
1:Bt:345:ARG:HD3	1:Bt:345:ARG:HA	1.68	0.46
1:Ad:366:GLN:C	1:Ad:369:VAL:HB	2.40	0.46
1:Ad:404:ARG:O	1:Ad:407:VAL:HG22	2.16	0.46
1:Ak:409:GLU:OE1	1:Ak:498:LYS:CB	2.62	0.46
1:Al:20:VAL:HG21	1:Al:514:MET:HE1	1.97	0.46
1:Ar:366:GLN:HG2	1:Ar:367:GLU:N	2.30	0.46
1:As:23:LEU:HD23	1:As:60:ILE:HB	1.97	0.46
1:Ay:184:GLN:H	1:Ay:184:GLN:HG3	1.43	0.46
1:Ay:366:GLN:CA	1:Ay:369:VAL:H	2.29	0.46
1:Bf:422:VAL:HA	1:Bf:425:LYS:HD2	1.97	0.46
1:Bg:23:LEU:HD23	1:Bg:60:ILE:HB	1.97	0.46
1:Bm:352:GLN:HB3	1:Bm:365:LEU:CD2	2.40	0.46
1:Bt:349:ILE:HA	1:Bt:352:GLN:HB2	1.97	0.46
1:Bt:366:GLN:HG2	1:Bt:367:GLU:N	2.30	0.46
1:Ad:164:GLU:CA	1:Ad:167:ASP:HB2	2.42	0.46
1:Ad:421:ARG:NH1	1:Ad:469:VAL:O	2.48	0.46
1:Ak:184:GLN:H	1:Ak:184:GLN:HG3	1.43	0.46
1:Ar:207:LYS:H	1:Ar:207:LYS:HG3	1.42	0.46
1:Ay:422:VAL:HA	1:Ay:425:LYS:HD2	1.97	0.46
1:Bf:366:GLN:CA	1:Bf:369:VAL:H	2.29	0.46
1:Bg:521:VAL:HG11	1:Bn:60:ILE:HG12	1.98	0.46
1:Bm:349:ILE:HA	1:Bm:352:GLN:HB2	1.97	0.46
1:Bt:421:ARG:NH1	1:Bt:469:VAL:O	2.48	0.46
1:Ad:518:GLU:OE2	1:Ar:36:ARG:HB3	2.15	0.46
1:Ak:404:ARG:O	1:Ak:407:VAL:HG22	2.15	0.46
1:Ak:422:VAL:HA	1:Ak:425:LYS:HD2	1.97	0.46
1:Al:122:LYS:HD3	1:Al:440:ILE:HD11	1.98	0.46
1:Al:172:GLU:OE2	1:Al:369:VAL:HG13	2.12	0.46
1:Ar:421:ARG:NH1	1:Ar:469:VAL:O	2.48	0.46
1:Az:430:ARG:NH1	1:Az:441:LYS:NZ	2.63	0.46
2:Ba:95:VAL:HG12	2:Bv:2:ASN:O	2.15	0.46
1:Bm:404:ARG:O	1:Bm:407:VAL:HG22	2.16	0.46
1:Ad:366:GLN:CA	1:Ad:369:VAL:H	2.29	0.46
1:Ad:421:ARG:HH12	1:Ad:469:VAL:CG1	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Af:76:GLU:OE1	2:At:37:ARG:NH1	2.49	0.46
2:Af:95:VAL:HA	2:Am:2:ASN:O	2.15	0.46
1:Ak:36:ARG:HB3	1:Ay:518:GLU:OE2	2.16	0.46
1:Al:477:GLY:C	1:Al:488:MET:CE	2.85	0.46
1:Al:517:THR:HG23	1:Az:39:VAL:CG2	2.37	0.46
1:Ar:366:GLN:CA	1:Ar:369:VAL:H	2.29	0.46
1:Ar:473:ASP:OD1	1:Ar:473:ASP:C	2.58	0.46
1:Bf:352:GLN:HB3	1:Bf:365:LEU:CD2	2.40	0.46
1:Ad:95:LEU:HD23	1:Ad:450:PRO:HD3	1.97	0.46
1:Ak:95:LEU:HD23	1:Ak:450:PRO:HD3	1.97	0.46
1:Al:430:ARG:NH1	1:Al:441:LYS:NZ	2.63	0.46
1:As:20:VAL:HG21	1:As:514:MET:HE1	1.97	0.46
1:As:172:GLU:OE2	1:As:369:VAL:HG13	2.12	0.46
1:Bf:421:ARG:NH1	1:Bf:469:VAL:O	2.48	0.46
1:Bg:420:ILE:HD11	1:Bg:448:GLU:HA	1.98	0.46
1:Bm:391:GLU:OE1	1:Bm:392:LYS:CG	2.62	0.46
1:Bn:6:VAL:CG1	1:Bn:8:PHE:CZ	2.99	0.46
1:Bt:186:GLU:CG	1:Bt:380:LYS:HB2	2.46	0.46
1:Bu:23:LEU:HD23	1:Bu:60:ILE:HB	1.97	0.46
1:Bu:122:LYS:HD3	1:Bu:440:ILE:HD11	1.98	0.46
1:Ad:36:ARG:HB3	1:Ak:518:GLU:OE2	2.15	0.46
1:Ak:301:ILE:HD13	1:Ak:307:MET:HB2	1.97	0.46
1:Ak:366:GLN:HG2	1:Ak:367:GLU:N	2.30	0.46
1:Al:58:ARG:HA	1:Al:75:LYS:HD3	1.97	0.46
1:Al:420:ILE:HD11	1:Al:448:GLU:HA	1.98	0.46
1:Bg:36:ARG:CZ	1:Bu:113:PRO:HG2	2.44	0.46
1:Bg:516:THR:O	1:Bn:36:ARG:HB3	2.16	0.46
1:Bu:131:LEU:HD23	1:Bu:131:LEU:HA	1.76	0.46
1:Ad:301:ILE:HD13	1:Ad:307:MET:HB2	1.97	0.46
1:Ad:363:GLU:C	1:Ad:366:GLN:NE2	2.74	0.46
1:Ae:23:LEU:HD23	1:Ae:60:ILE:HB	1.97	0.46
1:Ae:58:ARG:HA	1:Ae:75:LYS:HD3	1.97	0.46
2:Af:93:ALA:HA	2:Am:4:ARG:O	2.16	0.46
1:Ak:479:ASN:HB3	1:Ak:491:MET:HE1	1.98	0.46
1:Ar:391:GLU:OE1	1:Ar:392:LYS:CG	2.62	0.46
1:Ay:288:MET:CE	1:Ay:364:LYS:HE3	2.45	0.46
1:Ay:366:GLN:C	1:Ay:369:VAL:HB	2.40	0.46
1:Ay:421:ARG:NH1	1:Ay:469:VAL:O	2.48	0.46
1:Az:7:LYS:HG3	1:Az:66:PHE:CE1	2.45	0.46
1:Az:20:VAL:HG21	1:Az:514:MET:HE1	1.97	0.46
1:Az:420:ILE:HD11	1:Az:448:GLU:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:521:VAL:HG11	1:Bu:60:ILE:HG12	1.98	0.46
1:Bf:186:GLU:CG	1:Bf:380:LYS:HB2	2.46	0.46
1:Bf:349:ILE:HA	1:Bf:352:GLN:HB2	1.97	0.46
1:Bf:420:ILE:HD11	1:Bf:451:LEU:CB	2.46	0.46
1:Bm:301:ILE:HD13	1:Bm:307:MET:HB2	1.97	0.46
1:Bn:420:ILE:HD11	1:Bn:448:GLU:HA	1.98	0.46
1:Bt:421:ARG:HH12	1:Bt:469:VAL:CG1	2.24	0.46
1:Bu:54:VAL:HG11	1:Bu:82:ASN:HD21	1.68	0.46
1:Bu:420:ILE:HD11	1:Bu:448:GLU:HA	1.98	0.46
1:Ad:184:GLN:H	1:Ad:184:GLN:HG3	1.43	0.46
1:Ae:420:ILE:HD11	1:Ae:448:GLU:HA	1.98	0.46
1:Ak:421:ARG:NH1	1:Ak:469:VAL:O	2.48	0.46
1:Ar:518:GLU:OE2	1:Bm:36:ARG:HB3	2.16	0.46
1:Ay:366:GLN:HG2	1:Ay:367:GLU:N	2.30	0.46
1:Bf:301:ILE:HD13	1:Bf:307:MET:HB2	1.98	0.46
1:Bf:363:GLU:C	1:Bf:366:GLN:HE22	2.17	0.46
1:Bf:479:ASN:HB3	1:Bf:491:MET:HE1	1.98	0.46
1:Bn:131:LEU:HD23	1:Bn:131:LEU:HA	1.76	0.46
1:Bn:430:ARG:NH1	1:Bn:441:LYS:NZ	2.63	0.46
1:Bu:6:VAL:CG1	1:Bu:8:PHE:CZ	2.99	0.46
1:Ad:47:PRO:CG	1:Ak:69:MET:HG2	2.46	0.45
1:Ad:391:GLU:OE1	1:Ad:392:LYS:CG	2.62	0.45
1:Ar:288:MET:CE	1:Ar:364:LYS:HE3	2.45	0.45
1:Ay:95:LEU:HD23	1:Ay:450:PRO:HD3	1.97	0.45
1:Ay:420:ILE:HD11	1:Ay:451:LEU:CB	2.47	0.45
1:Az:169:VAL:CG2	1:Az:175:ILE:HD11	2.46	0.45
1:Bf:163:ALA:O	1:Bf:167:ASP:N	2.46	0.45
1:Bf:404:ARG:O	1:Bf:407:VAL:HG22	2.16	0.45
1:Bf:518:GLU:OE2	1:Bt:36:ARG:HB3	2.16	0.45
1:Bg:6:VAL:CG1	1:Bg:8:PHE:CZ	2.99	0.45
1:Bg:113:PRO:HG2	1:Bn:36:ARG:CZ	2.42	0.45
1:Bg:169:VAL:CG2	1:Bg:175:ILE:HD11	2.46	0.45
1:Bn:390:LYS:HE2	1:Bn:390:LYS:HB2	1.77	0.45
1:Bt:288:MET:CE	1:Bt:364:LYS:HE3	2.45	0.45
1:Bt:301:ILE:HD13	1:Bt:307:MET:HB2	1.97	0.45
1:Bu:20:VAL:HG21	1:Bu:514:MET:HE1	1.97	0.45
1:Ad:479:ASN:HB3	1:Ad:491:MET:HE1	1.98	0.45
1:Ae:34:LYS:HZ2	1:Ae:483:GLU:HG3	1.81	0.45
1:Ak:284:ARG:CD	1:Ak:364:LYS:HB3	2.47	0.45
1:Ak:363:GLU:C	1:Ak:366:GLN:NE2	2.74	0.45
1:Al:6:VAL:CG1	1:Al:8:PHE:CZ	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:7:LYS:HD2	1:Ar:66:PHE:CE2	2.52	0.45
1:Ay:95:LEU:CD2	1:Ay:450:PRO:HD3	2.46	0.45
1:Ay:301:ILE:HD13	1:Ay:307:MET:HB2	1.97	0.45
1:Ay:404:ARG:O	1:Ay:407:VAL:HG22	2.16	0.45
1:Az:23:LEU:HD23	1:Az:60:ILE:HB	1.97	0.45
2:Ba:36:THR:OG1	2:Bv:76:GLU:OE1	2.29	0.45
1:Bf:95:LEU:CD2	1:Bf:450:PRO:HD3	2.47	0.45
2:Bh:95:VAL:HG12	2:Bo:2:ASN:O	2.16	0.45
1:Bm:95:LEU:CD2	1:Bm:450:PRO:HD3	2.47	0.45
1:Bm:479:ASN:HB3	1:Bm:491:MET:HE1	1.98	0.45
1:Bn:62:LEU:HD12	1:Bn:62:LEU:HA	1.78	0.45
1:Bt:184:GLN:H	1:Bt:184:GLN:HG3	1.43	0.45
1:Bt:284:ARG:CD	1:Bt:364:LYS:HB3	2.47	0.45
1:Ad:422:VAL:HA	1:Ad:425:LYS:HD2	1.97	0.45
1:Ad:524:LEU:CD1	1:Ar:63:GLU:HB2	2.47	0.45
1:Ar:95:LEU:CD2	1:Ar:450:PRO:HD3	2.47	0.45
1:Ar:301:ILE:HD13	1:Ar:307:MET:HB2	1.97	0.45
1:As:177:VAL:CG2	1:As:400:LEU:HD11	2.47	0.45
1:As:420:ILE:HD11	1:As:448:GLU:HA	1.98	0.45
1:Bg:36:ARG:HB3	1:Bu:516:THR:O	2.16	0.45
1:Bm:422:VAL:HA	1:Bm:425:LYS:HD2	1.97	0.45
1:Bt:366:GLN:CA	1:Bt:369:VAL:H	2.29	0.45
1:Bt:479:ASN:HB3	1:Bt:491:MET:HE1	1.98	0.45
1:Bu:34:LYS:HZ1	1:Bu:483:GLU:HG3	1.72	0.45
1:Ad:61:GLU:HG2	1:Ak:4:LYS:HG2	1.98	0.45
1:Ad:95:LEU:CD2	1:Ad:450:PRO:HD3	2.47	0.45
1:Ae:177:VAL:CG2	1:Ae:400:LEU:HD11	2.47	0.45
1:Ar:363:GLU:C	1:Ar:366:GLN:NE2	2.74	0.45
1:As:172:GLU:OE2	1:As:369:VAL:HG11	2.12	0.45
1:Ay:479:ASN:HB3	1:Ay:491:MET:HE1	1.98	0.45
1:Az:177:VAL:CG2	1:Az:400:LEU:HD11	2.47	0.45
1:Bg:122:LYS:HD3	1:Bg:440:ILE:HD11	1.98	0.45
1:Bm:363:GLU:C	1:Bm:366:GLN:NE2	2.74	0.45
1:Bu:177:VAL:CG2	1:Bu:400:LEU:HD11	2.47	0.45
1:Ad:7:LYS:HD2	1:Ad:66:PHE:CE2	2.52	0.45
1:Ae:169:VAL:CG2	1:Ae:175:ILE:HD11	2.46	0.45
1:Ak:176:THR:CG2	1:Ak:178:GLU:OE2	2.61	0.45
1:Al:495:ASP:HA	1:Al:496:PRO:HD3	1.75	0.45
1:Ar:420:ILE:HD11	1:Ar:451:LEU:CB	2.46	0.45
1:Ar:422:VAL:HA	1:Ar:425:LYS:HD2	1.97	0.45
1:Ar:479:ASN:HB3	1:Ar:491:MET:HE1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:488:MET:CE	1:As:491:MET:HE1	2.19	0.45
1:Ay:112:ASN:ND2	1:Ay:114:MET:HB2	2.32	0.45
1:Ay:363:GLU:C	1:Ay:366:GLN:HE22	2.17	0.45
1:Bf:524:LEU:CD1	1:Bt:63:GLU:HB2	2.47	0.45
1:Bg:54:VAL:HG11	1:Bg:82:ASN:HD21	1.68	0.45
1:Ad:155:ASP:CB	1:Ad:395:ARG:NH2	2.76	0.45
1:Ad:420:ILE:HD11	1:Ad:451:LEU:HB3	1.99	0.45
2:Af:92:LEU:C	2:Am:6:LEU:HD23	2.42	0.45
1:Ak:7:LYS:HD2	1:Ak:66:PHE:CE2	2.52	0.45
1:Ar:420:ILE:HD11	1:Ar:451:LEU:HB3	1.99	0.45
1:Ay:227:ILE:HD12	1:Ay:227:ILE:HA	1.62	0.45
1:Ay:262:LEU:HD12	1:Ay:262:LEU:HA	1.75	0.45
1:Bf:4:LYS:HG2	1:Bt:61:GLU:HG2	1.98	0.45
1:Bn:7:LYS:HG3	1:Bn:66:PHE:CE1	2.45	0.45
1:Ad:161:LEU:O	1:Ad:164:GLU:CG	2.63	0.45
1:Ad:366:GLN:HG2	1:Ad:367:GLU:N	2.30	0.45
1:Ak:112:ASN:ND2	1:Ak:114:MET:HB2	2.32	0.45
1:Ak:288:MET:CE	1:Ak:364:LYS:HE3	2.45	0.45
1:Al:23:LEU:HD23	1:Al:60:ILE:HB	1.97	0.45
1:Al:113:PRO:HG2	1:Az:36:ARG:CZ	2.45	0.45
1:Ar:114:MET:HE2	1:Bm:36:ARG:CD	2.38	0.45
1:Ar:352:GLN:HB3	1:Ar:365:LEU:CD2	2.40	0.45
1:Ay:421:ARG:HH12	1:Ay:469:VAL:CG1	2.24	0.45
1:Az:6:VAL:CG1	1:Az:8:PHE:CZ	2.99	0.45
1:Az:122:LYS:HD3	1:Az:440:ILE:HD11	1.98	0.45
1:Bf:284:ARG:HG2	1:Bf:368:ARG:HH11	1.80	0.45
1:Bg:495:ASP:HA	1:Bg:496:PRO:HD3	1.75	0.45
1:Bm:186:GLU:CG	1:Bm:380:LYS:HB2	2.46	0.45
1:Bt:7:LYS:HD2	1:Bt:66:PHE:CE2	2.52	0.45
1:Bt:366:GLN:HA	1:Bt:369:VAL:H	1.82	0.45
1:Bu:62:LEU:HD23	1:Bu:67:GLU:HB3	1.99	0.45
1:Ad:348:GLN:HE21	1:Ad:348:GLN:HB3	1.54	0.45
1:Ad:352:GLN:HB3	1:Ad:365:LEU:CD2	2.39	0.45
1:Ae:6:VAL:CG1	1:Ae:8:PHE:CZ	2.99	0.45
1:Ae:6:VAL:HG22	1:Ae:521:VAL:HG13	1.99	0.45
1:Ae:122:LYS:HD3	1:Ae:440:ILE:HD11	1.98	0.45
1:Ak:420:ILE:HD11	1:Ak:451:LEU:HB3	1.99	0.45
1:Ar:310:GLU:HG3	1:Ar:311:LYS:HG2	1.98	0.45
1:As:60:ILE:HG12	1:Bn:521:VAL:HG11	1.99	0.45
1:Bf:107:VAL:CG2	1:Bf:515:ILE:HG23	2.47	0.45
1:Bg:177:VAL:CG2	1:Bg:400:LEU:HD11	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bh:2:ASN:O	2:Bv:95:VAL:HG12	2.16	0.45
1:Bm:310:GLU:HG3	1:Bm:311:LYS:HG2	1.98	0.45
1:Bu:169:VAL:CG2	1:Bu:175:ILE:HD11	2.46	0.45
1:Ad:420:ILE:HD11	1:Ad:451:LEU:CB	2.46	0.45
1:Ad:429:LEU:HD12	1:Ad:429:LEU:HA	1.90	0.45
1:Ae:7:LYS:HG3	1:Ae:66:PHE:CE1	2.45	0.45
1:Ae:477:GLY:C	1:Ae:488:MET:CE	2.85	0.45
1:Al:177:VAL:CG2	1:Al:400:LEU:HD11	2.46	0.45
1:Ay:63:GLU:HB2	1:Bt:524:LEU:CD1	2.47	0.45
1:Ay:363:GLU:C	1:Ay:366:GLN:NE2	2.74	0.45
1:Az:516:THR:O	1:Bu:36:ARG:HB3	2.17	0.45
1:Bf:310:GLU:HG3	1:Bf:311:LYS:HG2	1.98	0.45
1:Bm:69:MET:CE	1:Bm:520:MET:HE2	2.42	0.45
1:Bt:37:ASN:ND2	1:Bt:51:LYS:HZ1	2.15	0.45
1:Bt:112:ASN:ND2	1:Bt:114:MET:HB2	2.32	0.45
2:Af:6:LEU:CD2	2:At:92:LEU:O	2.65	0.45
1:Ak:391:GLU:OE1	1:Ak:392:LYS:CG	2.62	0.45
1:Ar:510:VAL:O	1:Ar:514:MET:CG	2.45	0.45
1:As:39:VAL:CG2	1:Bn:517:THR:HG23	2.37	0.45
1:Ay:231:ARG:H	1:Ay:231:ARG:HG2	1.48	0.45
1:Bg:62:LEU:HD23	1:Bg:67:GLU:HB3	1.99	0.45
1:Bm:107:VAL:CG2	1:Bm:515:ILE:HG23	2.47	0.45
1:Bm:262:LEU:HD12	1:Bm:262:LEU:HA	1.75	0.45
1:Bm:284:ARG:CD	1:Bm:364:LYS:HB3	2.47	0.45
1:Bn:477:GLY:C	1:Bn:488:MET:CE	2.85	0.45
1:Bt:391:GLU:OE1	1:Bt:392:LYS:CG	2.62	0.45
1:Bu:477:GLY:C	1:Bu:488:MET:CE	2.85	0.45
1:Ae:36:ARG:HB3	1:As:516:THR:O	2.17	0.44
1:Ae:504:LEU:HD23	1:Ae:504:LEU:HA	1.83	0.44
1:Ak:107:VAL:CG2	1:Ak:515:ILE:HG23	2.47	0.44
1:Al:6:VAL:HG22	1:Al:521:VAL:HG13	1.99	0.44
1:Ar:284:ARG:CD	1:Ar:364:LYS:HB3	2.47	0.44
1:As:6:VAL:CG1	1:As:8:PHE:CZ	2.99	0.44
1:Az:177:VAL:HG23	1:Az:400:LEU:HD12	1.99	0.44
1:Az:390:LYS:HE2	1:Az:390:LYS:HB2	1.77	0.44
1:Bf:429:LEU:HD12	1:Bf:429:LEU:HA	1.90	0.44
1:Bt:95:LEU:CD2	1:Bt:450:PRO:HD3	2.47	0.44
1:Ad:112:ASN:ND2	1:Ad:114:MET:HB2	2.32	0.44
1:Ad:262:LEU:HD12	1:Ad:262:LEU:HA	1.75	0.44
1:Ad:352:GLN:CB	1:Ad:365:LEU:HD23	2.39	0.44
1:Ae:20:VAL:HG21	1:Ae:514:MET:HE1	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:27:VAL:HG12	1:Ae:90:THR:HG23	2.00	0.44
1:Ak:15:LYS:CE	1:Ak:18:ARG:NH1	2.72	0.44
1:Ar:366:GLN:HA	1:Ar:369:VAL:H	1.82	0.44
1:As:122:LYS:HD3	1:As:440:ILE:HD11	1.98	0.44
1:As:169:VAL:CG2	1:As:175:ILE:HD11	2.46	0.44
1:Bf:288:MET:CE	1:Bf:364:LYS:HE3	2.45	0.44
1:Bm:7:LYS:HD2	1:Bm:66:PHE:CE2	2.52	0.44
1:Bm:421:ARG:HH12	1:Bm:469:VAL:CG1	2.24	0.44
1:Bn:122:LYS:HD3	1:Bn:440:ILE:HD11	1.98	0.44
1:Bn:177:VAL:CG2	1:Bn:400:LEU:HD11	2.47	0.44
1:Bt:69:MET:CE	1:Bt:520:MET:HE2	2.42	0.44
1:Bt:420:ILE:HD11	1:Bt:451:LEU:CB	2.46	0.44
1:Ad:107:VAL:CG2	1:Ad:515:ILE:HG23	2.47	0.44
1:Ad:168:LYS:HZ3	1:Ad:187:LEU:CG	2.29	0.44
1:Ad:207:LYS:H	1:Ad:207:LYS:HG3	1.42	0.44
1:Ae:131:LEU:CD1	1:Ae:500:THR:HG22	2.47	0.44
1:Ak:279:PRO:O	1:Ak:285:ARG:HA	2.18	0.44
1:Ak:420:ILE:HD11	1:Ak:451:LEU:CB	2.46	0.44
1:Ar:107:VAL:CG2	1:Ar:515:ILE:HG23	2.47	0.44
1:Ar:279:PRO:O	1:Ar:285:ARG:HA	2.18	0.44
1:As:27:VAL:HG12	1:As:90:THR:HG23	2.00	0.44
1:Ay:36:ARG:HB3	1:Bt:518:GLU:OE2	2.17	0.44
1:Ay:284:ARG:CD	1:Ay:364:LYS:HB3	2.47	0.44
1:Az:6:VAL:HG22	1:Az:521:VAL:HG13	1.99	0.44
1:Bf:277:LYS:H	1:Bf:277:LYS:HG3	1.53	0.44
1:Bm:348:GLN:HE21	1:Bm:348:GLN:HB3	1.54	0.44
1:Bn:62:LEU:HD23	1:Bn:67:GLU:HB3	1.99	0.44
1:Bt:107:VAL:CG2	1:Bt:515:ILE:HG23	2.47	0.44
1:Bt:284:ARG:HG2	1:Bt:368:ARG:HH11	1.81	0.44
1:Bt:352:GLN:HB3	1:Bt:365:LEU:CD2	2.39	0.44
1:Ad:367:GLU:HA	1:Ad:370:ALA:HB3	2.00	0.44
1:Ae:288:MET:HE1	1:Ae:371:LYS:HZ2	1.83	0.44
1:Al:169:VAL:CG2	1:Al:175:ILE:HD11	2.46	0.44
1:Ar:163:ALA:O	1:Ar:167:ASP:N	2.46	0.44
1:Ar:186:GLU:CG	1:Ar:380:LYS:HB2	2.46	0.44
1:Ay:307:MET:H	1:Ay:307:MET:HG2	1.44	0.44
1:Ay:310:GLU:HG3	1:Ay:311:LYS:HG2	1.98	0.44
1:Az:62:LEU:HD12	1:Az:62:LEU:HA	1.78	0.44
1:Az:161:LEU:HD12	1:Az:161:LEU:HA	1.87	0.44
1:Bf:7:LYS:HD2	1:Bf:66:PHE:CE2	2.52	0.44
1:Bf:112:ASN:ND2	1:Bf:114:MET:HB2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:284:ARG:CD	1:Bf:364:LYS:HB3	2.47	0.44
1:Bf:321:LYS:HD3	1:Bf:321:LYS:HA	1.50	0.44
1:Bg:6:VAL:HG22	1:Bg:521:VAL:HG13	1.99	0.44
1:Bm:307:MET:H	1:Bm:307:MET:HG2	1.45	0.44
1:Bm:420:ILE:HD11	1:Bm:451:LEU:CB	2.46	0.44
1:Bm:420:ILE:HD11	1:Bm:451:LEU:HB3	1.99	0.44
1:Bn:169:VAL:CG2	1:Bn:175:ILE:HD11	2.46	0.44
1:Bt:310:GLU:HG3	1:Bt:311:LYS:HG2	1.98	0.44
1:Ad:310:GLU:HG3	1:Ad:311:LYS:HG2	1.98	0.44
1:Ae:390:LYS:HE2	1:Ae:390:LYS:HB2	1.77	0.44
1:Ak:367:GLU:HA	1:Ak:370:ALA:HB3	2.00	0.44
1:Al:288:MET:HE1	1:Al:371:LYS:HZ2	1.83	0.44
1:Ay:367:GLU:HA	1:Ay:370:ALA:HB3	2.00	0.44
1:Az:62:LEU:HD23	1:Az:67:GLU:HB3	1.99	0.44
1:Bu:131:LEU:CD1	1:Bu:500:THR:HG22	2.47	0.44
1:Ad:321:LYS:HA	1:Ad:321:LYS:HD3	1.50	0.44
1:Ad:339:GLU:H	1:Ad:339:GLU:HG2	1.54	0.44
2:Af:1:MET:HB3	2:At:95:VAL:HB	2.00	0.44
1:Ak:95:LEU:CD2	1:Ak:450:PRO:HD3	2.47	0.44
1:Ar:112:ASN:ND2	1:Ar:114:MET:HB2	2.32	0.44
1:As:6:VAL:HG22	1:As:521:VAL:HG13	1.99	0.44
1:Ay:107:VAL:CG2	1:Ay:515:ILE:HG23	2.47	0.44
1:Ay:166:MET:HA	1:Ay:170:GLY:CA	2.47	0.44
1:Bf:279:PRO:O	1:Bf:285:ARG:HA	2.18	0.44
1:Bf:366:GLN:HA	1:Bf:369:VAL:H	1.82	0.44
1:Bg:131:LEU:CD1	1:Bg:500:THR:HG22	2.47	0.44
1:Bm:270:ILE:H	1:Bm:270:ILE:HG12	1.58	0.44
1:Bm:284:ARG:HG2	1:Bm:368:ARG:HH11	1.81	0.44
1:Bm:429:LEU:HD12	1:Bm:429:LEU:HA	1.90	0.44
1:Bt:363:GLU:C	1:Bt:366:GLN:NE2	2.74	0.44
1:Ad:63:GLU:HB2	1:Ak:524:LEU:CD1	2.48	0.44
1:Ak:166:MET:HA	1:Ak:170:GLY:CA	2.47	0.44
1:Ak:310:GLU:HG3	1:Ak:311:LYS:HG2	1.98	0.44
1:Ak:358:SER:O	1:Ak:362:ARG:HG3	2.18	0.44
1:Al:27:VAL:HG12	1:Al:90:THR:HG23	2.00	0.44
2:Am:95:VAL:HG12	2:Ba:2:ASN:O	2.18	0.44
1:Az:39:VAL:HG13	1:Az:49:ILE:HG13	2.00	0.44
1:Bf:36:ARG:CD	1:Bm:114:MET:HE2	2.39	0.44
1:Bf:352:GLN:CB	1:Bf:365:LEU:HD23	2.39	0.44
1:Bm:219:PHE:HD1	1:Bm:219:PHE:HA	1.70	0.44
1:Bm:277:LYS:H	1:Bm:277:LYS:HG3	1.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bn:27:VAL:HG12	1:Bn:90:THR:HG23	2.00	0.44
1:Bu:39:VAL:HG13	1:Bu:49:ILE:HG13	2.00	0.44
1:Bu:430:ARG:NH1	1:Bu:441:LYS:HZ3	2.16	0.44
1:Ad:366:GLN:HA	1:Ad:369:VAL:H	1.82	0.44
1:Ad:489:ILE:HD12	1:Ad:494:LEU:HD22	1.97	0.44
1:Ae:177:VAL:HG23	1:Ae:400:LEU:HD12	1.99	0.44
1:Ae:516:THR:O	1:Al:36:ARG:HB3	2.18	0.44
1:Ak:366:GLN:HA	1:Ak:369:VAL:H	1.82	0.44
1:Al:131:LEU:CD1	1:Al:500:THR:HG22	2.48	0.44
1:Ar:339:GLU:H	1:Ar:339:GLU:HG2	1.54	0.44
1:As:390:LYS:HE2	1:As:390:LYS:HB2	1.76	0.44
1:Ay:240:VAL:HG21	1:Ay:247:LEU:HB2	2.00	0.44
1:Ay:279:PRO:O	1:Ay:285:ARG:HA	2.18	0.44
1:Az:176:THR:HG22	1:Az:177:VAL:N	2.33	0.44
1:Bf:233:MET:HE1	1:Bf:263:VAL:HG22	2.00	0.44
1:Bf:421:ARG:HH12	1:Bf:469:VAL:CG1	2.24	0.44
1:Bg:63:GLU:H	1:Bg:63:GLU:HG2	1.66	0.44
2:Bh:94:ILE:O	2:Bo:4:ARG:HB3	2.18	0.44
1:Bm:112:ASN:ND2	1:Bm:114:MET:HB2	2.32	0.44
1:Bt:207:LYS:H	1:Bt:207:LYS:HG3	1.42	0.44
1:Bt:358:SER:O	1:Bt:362:ARG:HG3	2.18	0.44
1:Bu:161:LEU:HD12	1:Bu:161:LEU:HA	1.86	0.44
1:Ad:163:ALA:O	1:Ad:167:ASP:N	2.46	0.44
1:Ad:166:MET:HA	1:Ad:170:GLY:CA	2.47	0.44
1:Ad:284:ARG:CD	1:Ad:364:LYS:HB3	2.47	0.44
1:Ad:473:ASP:OD1	1:Ad:473:ASP:C	2.58	0.44
1:Ae:517:THR:CG2	1:Al:39:VAL:CG2	2.96	0.44
1:Ar:288:MET:SD	1:Ar:368:ARG:NH1	2.91	0.44
1:As:36:ARG:HB3	1:Bn:516:THR:O	2.17	0.44
1:As:62:LEU:HD23	1:As:67:GLU:HB3	1.99	0.44
1:As:494:LEU:HD23	1:As:494:LEU:HA	1.86	0.44
1:Ay:420:ILE:HD11	1:Ay:451:LEU:HB3	1.99	0.44
1:Az:131:LEU:CD1	1:Az:500:THR:HG22	2.48	0.44
1:Bf:15:LYS:CE	1:Bf:18:ARG:NH1	2.72	0.44
1:Bf:63:GLU:HB2	1:Bm:524:LEU:CD1	2.47	0.44
1:Bg:39:VAL:HG13	1:Bg:49:ILE:HG13	2.00	0.44
2:Bh:4:ARG:HB3	2:Bv:94:ILE:O	2.18	0.44
1:Bt:168:LYS:HZ3	1:Bt:187:LEU:HG	1.78	0.44
1:Bt:183:LEU:HG	1:Bt:384:ALA:HA	1.99	0.44
1:Bt:279:PRO:O	1:Bt:285:ARG:HA	2.18	0.44
1:Bt:352:GLN:CB	1:Bt:365:LEU:HD23	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:279:PRO:O	1:Ad:285:ARG:HA	2.18	0.43
1:Ad:288:MET:SD	1:Ad:368:ARG:NH1	2.91	0.43
1:Ak:186:GLU:CG	1:Ak:380:LYS:HB2	2.46	0.43
1:Ak:240:VAL:HG21	1:Ak:247:LEU:HB2	2.00	0.43
1:Ar:161:LEU:O	1:Ar:164:GLU:CG	2.63	0.43
1:Ar:233:MET:HE1	1:Ar:263:VAL:HG22	2.00	0.43
1:Ar:367:GLU:HA	1:Ar:370:ALA:HB3	2.00	0.43
1:Ar:429:LEU:HD12	1:Ar:429:LEU:HA	1.91	0.43
2:At:1:MET:N	2:Bo:97:ALA:OXT	2.50	0.43
2:At:2:ASN:O	2:Bo:95:VAL:HG12	2.18	0.43
1:Bf:270:ILE:H	1:Bf:270:ILE:HG12	1.58	0.43
1:Bn:461:GLU:OE2	1:Bn:464:VAL:CG2	2.66	0.43
1:Bt:321:LYS:HD3	1:Bt:321:LYS:HA	1.50	0.43
1:Bt:409:GLU:OE1	1:Bt:498:LYS:CA	2.66	0.43
1:Bu:177:VAL:HG23	1:Bu:400:LEU:HD12	1.99	0.43
1:Ad:233:MET:HE1	1:Ad:263:VAL:HG22	2.00	0.43
1:Ad:240:VAL:HG21	1:Ad:247:LEU:HB2	2.00	0.43
1:Ad:279:PRO:HG2	1:Ad:288:MET:HB3	2.00	0.43
1:Ad:409:GLU:OE1	1:Ad:498:LYS:CA	2.66	0.43
1:Ae:113:PRO:CD	1:Al:36:ARG:HE	2.31	0.43
1:Al:516:THR:O	1:Az:36:ARG:HB3	2.18	0.43
1:Ar:101:THR:O	1:Ar:105:LYS:HG3	2.18	0.43
1:Ar:201:SER:HB3	1:Ar:260:ALA:HB1	2.01	0.43
1:Ar:358:SER:O	1:Ar:362:ARG:HG3	2.18	0.43
1:Ay:207:LYS:HD2	1:Ay:214:GLU:HB3	2.00	0.43
1:Bf:36:ARG:HB3	1:Bm:518:GLU:OE2	2.17	0.43
1:Bf:346:VAL:HG11	1:Bf:373:ALA:HB2	2.00	0.43
1:Bf:420:ILE:HD11	1:Bf:451:LEU:HB3	1.99	0.43
1:Bm:288:MET:SD	1:Bm:368:ARG:NH1	2.91	0.43
1:Bm:366:GLN:HA	1:Bm:369:VAL:H	1.82	0.43
1:Bm:409:GLU:OE1	1:Bm:498:LYS:CA	2.66	0.43
1:Bt:207:LYS:HD2	1:Bt:214:GLU:HB3	2.00	0.43
1:Bt:219:PHE:HD1	1:Bt:219:PHE:HA	1.70	0.43
1:Bt:420:ILE:HD11	1:Bt:451:LEU:HB3	1.99	0.43
1:Ad:201:SER:HB3	1:Ad:260:ALA:HB1	2.01	0.43
1:Al:430:ARG:NH1	1:Al:441:LYS:HZ3	2.16	0.43
1:Al:521:VAL:HG11	1:Az:60:ILE:HG12	2.00	0.43
1:Ar:270:ILE:H	1:Ar:270:ILE:HG12	1.58	0.43
1:Ar:346:VAL:HG11	1:Ar:373:ALA:HB2	2.00	0.43
1:Ay:7:LYS:HD2	1:Ay:66:PHE:CE2	2.52	0.43
1:Bf:161:LEU:O	1:Bf:164:GLU:CG	2.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:27:VAL:HG12	1:Bg:90:THR:HG23	2.00	0.43
1:Bm:358:SER:O	1:Bm:362:ARG:HG3	2.18	0.43
1:Bn:39:VAL:HG13	1:Bn:49:ILE:HG13	2.00	0.43
1:Bn:494:LEU:HD23	1:Bn:494:LEU:HA	1.86	0.43
1:Bt:37:ASN:ND2	1:Bt:51:LYS:NZ	2.66	0.43
1:Bt:119:GLY:C	1:Bt:440:ILE:HD13	2.44	0.43
1:Bt:201:SER:HB3	1:Bt:260:ALA:HB1	2.00	0.43
1:Bt:346:VAL:HG11	1:Bt:373:ALA:HB2	2.00	0.43
1:Bu:172:GLU:OE2	1:Bu:369:VAL:HG11	2.12	0.43
1:Ad:277:LYS:H	1:Ad:277:LYS:HG3	1.53	0.43
1:Ae:62:LEU:HD23	1:Ae:67:GLU:HB3	1.99	0.43
1:Ak:101:THR:O	1:Ak:105:LYS:HG3	2.19	0.43
1:Ak:163:ALA:O	1:Ak:167:ASP:N	2.46	0.43
1:Ak:346:VAL:HG11	1:Ak:373:ALA:HB2	2.00	0.43
1:Al:39:VAL:HG13	1:Al:49:ILE:HG13	2.00	0.43
1:Al:62:LEU:HD23	1:Al:67:GLU:HB3	1.99	0.43
1:Ar:37:ASN:ND2	1:Ar:51:LYS:NZ	2.66	0.43
1:Ay:61:GLU:HG2	1:Bt:4:LYS:HG2	2.00	0.43
1:Ay:155:ASP:CB	1:Ay:395:ARG:NH2	2.76	0.43
1:Ay:201:SER:HB3	1:Ay:260:ALA:HB1	2.01	0.43
1:Ay:409:GLU:OE1	1:Ay:498:LYS:CA	2.66	0.43
1:Bf:61:GLU:HG2	1:Bm:4:LYS:HG2	1.99	0.43
1:Bf:101:THR:O	1:Bf:105:LYS:HG3	2.19	0.43
1:Bg:177:VAL:HG23	1:Bg:400:LEU:HD12	1.99	0.43
2:Bh:97:ALA:OXT	2:Bo:1:MET:N	2.52	0.43
1:Bm:349:ILE:HG21	1:Bm:368:ARG:HB3	2.00	0.43
1:Bn:6:VAL:HG22	1:Bn:521:VAL:HG13	1.99	0.43
1:Bn:177:VAL:HG23	1:Bn:400:LEU:HD12	1.99	0.43
1:Bt:231:ARG:H	1:Bt:231:ARG:HG2	1.48	0.43
1:Bt:233:MET:HE1	1:Bt:263:VAL:HG22	2.00	0.43
1:Bt:240:VAL:HG21	1:Bt:247:LEU:HB2	2.00	0.43
1:Bu:176:THR:HG22	1:Bu:177:VAL:N	2.33	0.43
1:Ad:4:LYS:HG2	1:Ar:61:GLU:HG2	1.99	0.43
1:Ad:346:VAL:HG11	1:Ad:373:ALA:HB2	2.00	0.43
1:Ae:521:VAL:HG11	1:Al:60:ILE:HG12	2.00	0.43
1:Ak:279:PRO:HG2	1:Ak:288:MET:HB3	2.01	0.43
1:Ak:288:MET:SD	1:Ak:368:ARG:NH1	2.91	0.43
1:Ar:207:LYS:HD2	1:Ar:214:GLU:HB3	2.00	0.43
1:Ar:240:VAL:HG21	1:Ar:247:LEU:HB2	2.00	0.43
1:Ar:524:LEU:CD1	1:Bm:63:GLU:HB2	2.48	0.43
1:Ay:346:VAL:HG11	1:Ay:373:ALA:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:461:GLU:OE2	1:Az:464:VAL:CG2	2.67	0.43
1:Bf:37:ASN:ND2	1:Bf:51:LYS:NZ	2.66	0.43
1:Bf:278:ALA:HB3	1:Bf:285:ARG:HE	1.84	0.43
1:Bm:201:SER:HB3	1:Bm:260:ALA:HB1	2.01	0.43
1:Bm:279:PRO:O	1:Bm:285:ARG:HA	2.18	0.43
1:Bm:279:PRO:HG2	1:Bm:288:MET:HB3	2.01	0.43
1:Bu:390:LYS:HE2	1:Bu:390:LYS:HB2	1.77	0.43
1:Bu:489:ILE:HG22	1:Bu:494:LEU:CD2	2.47	0.43
1:Ad:101:THR:O	1:Ad:105:LYS:HG3	2.19	0.43
1:Ad:358:SER:O	1:Ad:362:ARG:HG3	2.18	0.43
2:Af:1:MET:N	2:At:97:ALA:OXT	2.50	0.43
1:Ak:201:SER:HB3	1:Ak:260:ALA:HB1	2.01	0.43
1:Ak:305:ILE:HD13	1:Ak:305:ILE:HA	1.89	0.43
1:Ak:409:GLU:OE1	1:Ak:498:LYS:CA	2.66	0.43
1:Al:34:LYS:HZ2	1:Al:483:GLU:HG3	1.77	0.43
1:Al:461:GLU:OE2	1:Al:464:VAL:CG2	2.66	0.43
1:Ar:155:ASP:CB	1:Ar:395:ARG:NH2	2.76	0.43
1:Ar:279:PRO:HG2	1:Ar:288:MET:HB3	2.01	0.43
1:As:461:GLU:OE2	1:As:464:VAL:CG2	2.66	0.43
1:Ay:37:ASN:ND2	1:Ay:51:LYS:NZ	2.66	0.43
1:Ay:183:LEU:HG	1:Ay:384:ALA:HA	2.00	0.43
1:Ay:186:GLU:CG	1:Ay:380:LYS:HB2	2.46	0.43
1:Bf:409:GLU:OE1	1:Bf:498:LYS:CA	2.66	0.43
1:Bg:461:GLU:OE2	1:Bg:464:VAL:CG2	2.67	0.43
1:Bg:504:LEU:HD23	1:Bg:504:LEU:HA	1.83	0.43
2:Bh:95:VAL:N	2:Bo:3:ILE:HG23	2.34	0.43
1:Bm:161:LEU:O	1:Bm:164:GLU:CG	2.63	0.43
1:Bm:346:VAL:HG11	1:Bm:373:ALA:HB2	2.00	0.43
1:Bm:352:GLN:CB	1:Bm:365:LEU:HD23	2.39	0.43
1:Bn:430:ARG:NH1	1:Bn:441:LYS:HZ3	2.16	0.43
1:Bt:429:LEU:HD12	1:Bt:429:LEU:HA	1.90	0.43
1:Bu:6:VAL:HG22	1:Bu:521:VAL:HG13	1.99	0.43
1:Ad:37:ASN:ND2	1:Ad:51:LYS:NZ	2.66	0.43
1:Ad:207:LYS:HD2	1:Ad:214:GLU:HB3	2.00	0.43
1:Ae:495:ASP:HA	1:Ae:496:PRO:HD3	1.75	0.43
1:Ak:349:ILE:HG21	1:Ak:368:ARG:HB3	2.00	0.43
1:Al:455:VAL:CG1	1:Al:460:GLU:HB2	2.49	0.43
1:As:176:THR:HG22	1:As:177:VAL:N	2.33	0.43
1:Ay:349:ILE:HG21	1:Ay:368:ARG:HB3	2.00	0.43
1:Bf:201:SER:HB3	1:Bf:260:ALA:HB1	2.01	0.43
1:Bf:207:LYS:HD2	1:Bf:214:GLU:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bf:367:GLU:HA	1:Bf:370:ALA:HB3	1.99	0.43
1:Bg:477:GLY:C	1:Bg:488:MET:CE	2.85	0.43
1:Bm:183:LEU:HG	1:Bm:384:ALA:HA	1.99	0.43
1:Bm:240:VAL:HG21	1:Bm:247:LEU:HB2	2.00	0.43
1:Bt:367:GLU:HA	1:Bt:370:ALA:HB3	2.00	0.43
1:Bu:461:GLU:OE2	1:Bu:464:VAL:CG2	2.66	0.43
1:Ae:455:VAL:CG1	1:Ae:460:GLU:HB2	2.49	0.43
1:Ak:63:GLU:HB2	1:Ay:524:LEU:CD1	2.49	0.43
1:Ak:489:ILE:HD12	1:Ak:494:LEU:HD22	1.97	0.43
1:Al:176:THR:HG22	1:Al:177:VAL:N	2.33	0.43
1:Al:177:VAL:HG23	1:Al:400:LEU:HD12	1.99	0.43
1:Ar:4:LYS:HG2	1:Bm:61:GLU:HG2	2.00	0.43
1:Ar:278:ALA:HB3	1:Ar:285:ARG:HE	1.84	0.43
1:Ar:409:GLU:OE1	1:Ar:498:LYS:CA	2.66	0.43
1:Ar:489:ILE:HD12	1:Ar:494:LEU:HD22	1.97	0.43
1:Ay:278:ALA:HB3	1:Ay:285:ARG:HE	1.84	0.43
1:Ay:366:GLN:HA	1:Ay:369:VAL:H	1.82	0.43
1:Az:421:ARG:HD3	1:Az:421:ARG:HA	1.85	0.43
2:Ba:97:ALA:OXT	2:Bv:1:MET:N	2.52	0.43
1:Bf:240:VAL:HG21	1:Bf:247:LEU:HB2	2.00	0.43
1:Bf:363:GLU:C	1:Bf:366:GLN:NE2	2.74	0.43
1:Bm:16:MET:HG3	1:Bm:520:MET:SD	2.59	0.43
1:Bm:367:GLU:HA	1:Bm:370:ALA:HB3	2.00	0.43
1:Bn:372:LEU:HD23	1:Bn:372:LEU:HA	1.92	0.43
1:Bt:294:THR:HB	1:Bt:345:ARG:HG2	2.01	0.43
1:Ad:186:GLU:CG	1:Ad:380:LYS:HB2	2.46	0.43
1:Ak:16:MET:HG3	1:Ak:520:MET:SD	2.59	0.43
1:Ak:119:GLY:C	1:Ak:440:ILE:HD13	2.44	0.43
1:Ak:207:LYS:HD2	1:Ak:214:GLU:HB3	2.00	0.43
1:Al:421:ARG:HA	1:Al:421:ARG:HD3	1.85	0.43
1:Ar:166:MET:HA	1:Ar:170:GLY:CA	2.47	0.43
1:As:39:VAL:HG13	1:As:49:ILE:HG13	2.00	0.43
1:As:131:LEU:HD23	1:As:131:LEU:HA	1.76	0.43
1:As:177:VAL:HG23	1:As:400:LEU:HD12	1.99	0.43
1:As:455:VAL:CG1	1:As:460:GLU:HB2	2.49	0.43
1:Ay:284:ARG:HG2	1:Ay:368:ARG:HH11	1.80	0.43
1:Az:455:VAL:CG1	1:Az:460:GLU:HB2	2.49	0.43
1:Bf:358:SER:O	1:Bf:362:ARG:HG3	2.18	0.43
1:Bf:473:ASP:OD1	1:Bf:473:ASP:C	2.58	0.43
1:Bg:477:GLY:O	1:Bg:488:MET:HE3	2.19	0.43
1:Bm:37:ASN:ND2	1:Bm:51:LYS:NZ	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:155:ASP:CB	1:Bt:395:ARG:NH2	2.76	0.43
1:Bt:288:MET:SD	1:Bt:368:ARG:NH1	2.91	0.43
1:Bu:477:GLY:O	1:Bu:488:MET:HE3	2.19	0.43
1:Ad:176:THR:CG2	1:Ad:178:GLU:OE2	2.61	0.43
1:Ae:172:GLU:OE2	1:Ae:369:VAL:HG13	2.12	0.43
1:Ae:461:GLU:HA	1:Ae:462:PRO:HD3	1.80	0.43
1:Ak:352:GLN:CB	1:Ak:365:LEU:HD23	2.39	0.43
1:Ay:49:ILE:CD1	1:Bt:73:MET:CE	2.76	0.43
1:Ay:358:SER:O	1:Ay:362:ARG:HG3	2.18	0.43
1:Az:27:VAL:HG12	1:Az:90:THR:HG23	1.99	0.43
1:Az:288:MET:HE1	1:Az:371:LYS:HZ2	1.84	0.43
1:Bm:321:LYS:HA	1:Bm:321:LYS:HD3	1.50	0.43
1:Bu:31:LEU:HD23	1:Bu:453:GLN:HB3	2.01	0.43
1:Ad:49:ILE:CD1	1:Ak:73:MET:CE	2.70	0.42
1:Ae:7:LYS:HG3	1:Ae:66:PHE:HZ	1.72	0.42
1:Ak:278:ALA:HB3	1:Ak:285:ARG:HE	1.84	0.42
1:Ar:16:MET:HG3	1:Ar:520:MET:SD	2.59	0.42
1:Ar:69:MET:HG2	1:Bm:47:PRO:CG	2.48	0.42
1:As:421:ARG:HD3	1:As:421:ARG:HA	1.85	0.42
1:Ay:15:LYS:CE	1:Ay:18:ARG:NH1	2.72	0.42
1:Ay:16:MET:HG3	1:Ay:520:MET:SD	2.59	0.42
1:Ay:69:MET:CE	1:Ay:520:MET:HE2	2.42	0.42
1:Ay:294:THR:HB	1:Ay:345:ARG:HG2	2.01	0.42
1:Ay:352:GLN:CB	1:Ay:365:LEU:HD23	2.39	0.42
1:Bf:279:PRO:HG2	1:Bf:288:MET:HB3	2.01	0.42
1:Bf:294:THR:HB	1:Bf:345:ARG:HG2	2.01	0.42
1:Bg:176:THR:HG22	1:Bg:177:VAL:N	2.33	0.42
1:Bu:455:VAL:CG1	1:Bu:460:GLU:HB2	2.49	0.42
1:Bu:494:LEU:HD23	1:Bu:494:LEU:HA	1.86	0.42
1:Ae:461:GLU:OE2	1:Ae:464:VAL:CG2	2.66	0.42
1:Ak:36:ARG:CD	1:Ay:114:MET:HE2	2.38	0.42
1:Ak:47:PRO:CG	1:Ay:69:MET:HG2	2.49	0.42
1:Ak:397:GLU:O	1:Ak:400:LEU:HB3	2.19	0.42
1:Ak:455:VAL:HG13	1:Ak:460:GLU:CG	2.45	0.42
1:Ay:277:LYS:H	1:Ay:277:LYS:HG3	1.53	0.42
1:Ay:288:MET:SD	1:Ay:368:ARG:NH1	2.91	0.42
1:Bf:69:MET:HG2	1:Bt:47:PRO:CG	2.49	0.42
1:Bf:114:MET:HE2	1:Bt:36:ARG:CD	2.38	0.42
2:Bh:36:THR:OG1	2:Bo:76:GLU:OE1	2.30	0.42
1:Bn:176:THR:HG22	1:Bn:177:VAL:N	2.33	0.42
1:Bt:15:LYS:CE	1:Bt:18:ARG:NH1	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:397:GLU:O	1:Bt:400:LEU:HB3	2.19	0.42
1:Bu:27:VAL:HG12	1:Bu:90:THR:HG23	2.00	0.42
1:Ak:231:ARG:H	1:Ak:231:ARG:HG2	1.48	0.42
1:Al:390:LYS:HE2	1:Al:390:LYS:HB2	1.77	0.42
1:Al:461:GLU:HA	1:Al:462:PRO:HD3	1.80	0.42
1:Ar:183:LEU:HG	1:Ar:384:ALA:HA	1.99	0.42
1:Ar:284:ARG:HG2	1:Ar:368:ARG:HH11	1.81	0.42
1:Ar:294:THR:HB	1:Ar:345:ARG:HG2	2.01	0.42
1:Ay:119:GLY:C	1:Ay:440:ILE:HD13	2.44	0.42
1:Ay:233:MET:HE1	1:Ay:263:VAL:HG22	2.00	0.42
1:Bf:183:LEU:HG	1:Bf:384:ALA:HA	1.99	0.42
1:Bf:288:MET:SD	1:Bf:368:ARG:NH1	2.91	0.42
1:Bg:455:VAL:CG1	1:Bg:460:GLU:HB2	2.49	0.42
1:Bg:461:GLU:HA	1:Bg:462:PRO:HD3	1.80	0.42
2:Bh:4:ARG:O	2:Bv:93:ALA:HA	2.20	0.42
1:Bm:207:LYS:HD2	1:Bm:214:GLU:HB3	2.00	0.42
1:Bn:455:VAL:CG1	1:Bn:460:GLU:HB2	2.49	0.42
1:Bt:16:MET:HG3	1:Bt:520:MET:SD	2.59	0.42
1:Ad:278:ALA:HB3	1:Ad:285:ARG:HE	1.84	0.42
1:Ae:176:THR:HG22	1:Ae:177:VAL:N	2.33	0.42
1:Ar:349:ILE:HG21	1:Ar:368:ARG:HB3	2.00	0.42
1:As:372:LEU:HD23	1:As:372:LEU:HA	1.92	0.42
1:As:477:GLY:C	1:As:488:MET:CE	2.85	0.42
1:Ay:279:PRO:HG2	1:Ay:288:MET:HB3	2.00	0.42
1:Ay:397:GLU:O	1:Ay:400:LEU:HB3	2.19	0.42
1:Bf:47:PRO:CG	1:Bm:69:MET:HG2	2.50	0.42
1:Bt:101:THR:O	1:Bt:105:LYS:HG3	2.19	0.42
1:Bt:270:ILE:HB	1:Bt:271:VAL:H	1.67	0.42
1:Bt:349:ILE:HG21	1:Bt:368:ARG:HB3	2.00	0.42
1:Bt:510:VAL:O	1:Bt:514:MET:CG	2.45	0.42
1:Ae:39:VAL:HG13	1:Ae:49:ILE:HG13	2.00	0.42
1:Ae:183:LEU:HD21	1:Ae:384:ALA:HA	2.02	0.42
1:Ak:77:VAL:HG21	1:Ak:510:VAL:HB	2.01	0.42
1:Ak:233:MET:HE1	1:Ak:263:VAL:HG22	2.00	0.42
1:Ak:352:GLN:HB3	1:Ak:365:LEU:CD2	2.39	0.42
1:Al:161:LEU:HD12	1:Al:161:LEU:HA	1.87	0.42
1:Ay:352:GLN:HB3	1:Ay:365:LEU:CD2	2.40	0.42
1:Az:372:LEU:HD23	1:Az:372:LEU:HA	1.91	0.42
2:Ba:93:ALA:HA	2:Bv:4:ARG:O	2.19	0.42
2:Ba:94:ILE:O	2:Bv:4:ARG:HB3	2.18	0.42
2:Ba:95:VAL:N	2:Bv:3:ILE:HG23	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:31:LEU:HD23	1:Bg:453:GLN:HB3	2.01	0.42
1:Bm:233:MET:HE1	1:Bm:263:VAL:HG22	2.00	0.42
1:Bm:397:GLU:O	1:Bm:400:LEU:HB3	2.19	0.42
1:Bt:278:ALA:HB3	1:Bt:285:ARG:HE	1.84	0.42
1:Ad:16:MET:HG3	1:Ad:520:MET:SD	2.59	0.42
1:Ad:294:THR:HB	1:Ad:345:ARG:HG2	2.01	0.42
1:Ad:349:ILE:HG21	1:Ad:368:ARG:HB3	2.00	0.42
2:Af:6:LEU:HD23	2:At:92:LEU:O	2.20	0.42
1:Ak:37:ASN:ND2	1:Ak:51:LYS:NZ	2.66	0.42
1:Ak:61:GLU:HG2	1:Ay:4:LYS:HG2	2.01	0.42
1:Ak:183:LEU:HG	1:Ak:384:ALA:HA	1.99	0.42
1:Ak:186:GLU:O	1:Ak:380:LYS:N	2.52	0.42
1:Ak:339:GLU:H	1:Ak:339:GLU:HG2	1.54	0.42
1:As:146:GLN:HE21	1:As:146:GLN:HB2	1.62	0.42
1:Ay:186:GLU:O	1:Ay:380:LYS:N	2.52	0.42
1:Bg:113:PRO:CD	1:Bn:36:ARG:HE	2.33	0.42
1:Ad:218:PRO:HG3	1:Ad:323:VAL:HB	2.02	0.42
1:Ae:494:LEU:HD23	1:Ae:494:LEU:HA	1.86	0.42
1:Ak:218:PRO:HG3	1:Ak:323:VAL:HB	2.02	0.42
1:Al:183:LEU:HD21	1:Al:384:ALA:HA	2.02	0.42
1:Ar:218:PRO:HG3	1:Ar:323:VAL:HB	2.02	0.42
1:As:124:VAL:HG21	1:As:508:ALA:HB1	2.01	0.42
1:As:161:LEU:HD12	1:As:161:LEU:HA	1.86	0.42
1:Ay:489:ILE:HG23	1:Ay:494:LEU:HD21	2.02	0.42
1:Bf:166:MET:HA	1:Bf:170:GLY:CA	2.47	0.42
1:Bf:349:ILE:HG21	1:Bf:368:ARG:HB3	2.00	0.42
1:Bm:101:THR:O	1:Bm:105:LYS:HG3	2.19	0.42
1:Bm:119:GLY:C	1:Bm:440:ILE:HD13	2.44	0.42
1:Bt:489:ILE:HG23	1:Bt:494:LEU:HD21	2.02	0.42
1:Ak:233:MET:HB2	1:Ak:233:MET:HE2	1.67	0.42
1:As:183:LEU:HD21	1:As:384:ALA:HA	2.02	0.42
1:Ay:194:GLN:H	1:Ay:371:LYS:CD	2.33	0.42
1:Ay:339:GLU:H	1:Ay:339:GLU:HG2	1.54	0.42
1:Az:31:LEU:HD23	1:Az:453:GLN:HB3	2.01	0.42
1:Bf:119:GLY:C	1:Bf:440:ILE:HD13	2.44	0.42
1:Bg:381:VAL:O	1:Bg:389:MET:SD	2.78	0.42
1:Bt:163:ALA:O	1:Bt:167:ASP:N	2.46	0.42
1:Bu:372:LEU:HD23	1:Bu:372:LEU:HA	1.92	0.42
1:Ad:77:VAL:HG21	1:Ad:510:VAL:HB	2.01	0.42
1:Ak:155:ASP:CB	1:Ak:395:ARG:NH2	2.76	0.42
1:Ak:294:THR:HB	1:Ak:345:ARG:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:231:ARG:H	1:Ar:231:ARG:HG2	1.48	0.42
1:Ar:479:ASN:CB	1:Ar:491:MET:CE	2.98	0.42
1:Ay:16:MET:CG	1:Ay:520:MET:SD	3.08	0.42
1:Ay:77:VAL:HG21	1:Ay:510:VAL:HB	2.01	0.42
1:Ay:218:PRO:HG3	1:Ay:323:VAL:HB	2.02	0.42
1:Bm:155:ASP:CB	1:Bm:395:ARG:NH2	2.76	0.42
1:Bt:279:PRO:HG2	1:Bt:288:MET:HB3	2.01	0.42
1:Bt:479:ASN:CB	1:Bt:491:MET:CE	2.98	0.42
1:Ad:284:ARG:HG2	1:Ad:368:ARG:HH11	1.81	0.42
1:As:31:LEU:HD23	1:As:453:GLN:HB3	2.01	0.42
2:At:4:ARG:O	2:Bo:93:ALA:HA	2.20	0.42
1:Ay:101:THR:O	1:Ay:105:LYS:HG3	2.19	0.42
1:Az:524:LEU:HD21	1:Bu:63:GLU:HG3	0.99	0.42
1:Bf:16:MET:HG3	1:Bf:520:MET:SD	2.59	0.42
1:Bf:77:VAL:HG21	1:Bf:510:VAL:HB	2.01	0.42
1:Bf:345:ARG:HD3	1:Bf:345:ARG:HA	1.68	0.42
1:Bm:16:MET:CG	1:Bm:520:MET:SD	3.08	0.42
1:Bm:77:VAL:HG21	1:Bm:510:VAL:HB	2.01	0.42
1:Bm:207:LYS:H	1:Bm:207:LYS:HG3	1.42	0.42
1:Bm:278:ALA:HB3	1:Bm:285:ARG:HE	1.84	0.42
1:Bm:294:THR:HB	1:Bm:345:ARG:HG2	2.01	0.42
1:Bu:62:LEU:HD12	1:Bu:62:LEU:HA	1.78	0.42
1:Ad:36:ARG:CD	1:Ak:114:MET:HE2	2.40	0.41
1:Ad:397:GLU:O	1:Ad:400:LEU:HB3	2.19	0.41
1:Ae:381:VAL:O	1:Ae:389:MET:SD	2.78	0.41
1:Ae:421:ARG:HD3	1:Ae:421:ARG:HA	1.85	0.41
1:Ak:489:ILE:HG23	1:Ak:494:LEU:HD21	2.02	0.41
2:Am:93:ALA:HA	2:Ba:4:ARG:O	2.19	0.41
1:Ar:16:MET:CG	1:Ar:520:MET:SD	3.08	0.41
1:Az:477:GLY:C	1:Az:488:MET:CE	2.85	0.41
1:Bf:16:MET:CG	1:Bf:520:MET:SD	3.08	0.41
1:Bf:397:GLU:O	1:Bf:400:LEU:HB3	2.19	0.41
1:Bf:489:ILE:HG23	1:Bf:494:LEU:HD21	2.02	0.41
1:Bg:161:LEU:HD12	1:Bg:161:LEU:HA	1.86	0.41
1:Bm:164:GLU:C	1:Bm:167:ASP:HB2	2.45	0.41
1:Bt:284:ARG:CG	1:Bt:368:ARG:NH1	2.81	0.41
1:Bu:381:VAL:O	1:Bu:389:MET:SD	2.78	0.41
1:Ad:479:ASN:CB	1:Ad:491:MET:CE	2.98	0.41
1:Ad:510:VAL:O	1:Ad:514:MET:CG	2.45	0.41
1:Ak:194:GLN:H	1:Ak:371:LYS:CD	2.33	0.41
1:Ak:284:ARG:HG2	1:Ak:368:ARG:HH11	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:381:VAL:O	1:Al:389:MET:SD	2.78	0.41
1:Ar:119:GLY:C	1:Ar:440:ILE:HD13	2.44	0.41
1:Ar:209:GLU:H	1:Ar:209:GLU:HG2	1.60	0.41
1:Ar:386:GLU:HG3	1:Ar:390:LYS:NZ	2.35	0.41
1:Bm:218:PRO:HG3	1:Bm:323:VAL:HB	2.02	0.41
1:Bm:386:GLU:HG3	1:Bm:390:LYS:NZ	2.35	0.41
1:Bn:31:LEU:HD23	1:Bn:453:GLN:HB3	2.01	0.41
1:Ar:77:VAL:HG21	1:Ar:510:VAL:HB	2.01	0.41
1:Ar:164:GLU:C	1:Ar:167:ASP:HB2	2.45	0.41
1:Ar:184:GLN:H	1:Ar:184:GLN:HG3	1.43	0.41
1:Ay:307:MET:HE3	1:Ay:307:MET:HB3	1.64	0.41
1:Az:183:LEU:HD21	1:Az:384:ALA:HA	2.02	0.41
1:Bf:164:GLU:C	1:Bf:167:ASP:HB2	2.45	0.41
1:Bf:479:ASN:HB2	1:Bf:491:MET:HE1	2.03	0.41
1:Bm:194:GLN:H	1:Bm:371:LYS:CD	2.33	0.41
1:Bm:479:ASN:CB	1:Bm:491:MET:CE	2.98	0.41
1:Bn:421:ARG:HD3	1:Bn:421:ARG:HA	1.85	0.41
1:Bt:16:MET:CG	1:Bt:520:MET:SD	3.08	0.41
1:Ad:194:GLN:H	1:Ad:371:LYS:CD	2.33	0.41
1:Ad:307:MET:H	1:Ad:307:MET:HG2	1.44	0.41
1:Ad:489:ILE:HG23	1:Ad:494:LEU:HD21	2.02	0.41
1:Ak:16:MET:CG	1:Ak:520:MET:SD	3.08	0.41
1:Ak:479:ASN:CB	1:Ak:491:MET:CE	2.98	0.41
1:Ar:34:LYS:HE3	1:Ar:481:ALA:HA	2.01	0.41
1:Ar:194:GLN:H	1:Ar:371:LYS:CD	2.33	0.41
1:As:36:ARG:HE	1:Bn:113:PRO:CD	2.33	0.41
1:As:495:ASP:HA	1:As:496:PRO:HD3	1.75	0.41
1:Az:63:GLU:H	1:Az:63:GLU:HG2	1.66	0.41
1:Az:461:GLU:HA	1:Az:462:PRO:HD3	1.80	0.41
1:Bf:284:ARG:CD	1:Bf:364:LYS:CB	2.99	0.41
1:Bg:494:LEU:HD23	1:Bg:494:LEU:HA	1.86	0.41
1:Bg:517:THR:HG23	1:Bn:39:VAL:CG2	2.39	0.41
1:Bm:233:MET:HB2	1:Bm:233:MET:HE2	1.67	0.41
1:Bn:183:LEU:HD21	1:Bn:384:ALA:HA	2.02	0.41
1:Bt:34:LYS:HE3	1:Bt:481:ALA:HA	2.01	0.41
1:Bt:218:PRO:HG3	1:Bt:323:VAL:HB	2.02	0.41
1:Bt:479:ASN:HB2	1:Bt:491:MET:HE1	2.03	0.41
1:Bu:151:SER:HB3	1:Bu:399:ALA:HA	2.02	0.41
1:Ad:34:LYS:HE3	1:Ad:481:ALA:HA	2.01	0.41
1:Ad:479:ASN:HB2	1:Ad:491:MET:HE1	2.03	0.41
1:Ae:36:ARG:HE	1:As:113:PRO:CD	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:124:VAL:HG21	1:Ae:508:ALA:HB1	2.01	0.41
1:Al:6:VAL:HG12	1:Al:8:PHE:CZ	2.56	0.41
1:Ar:134:LEU:HD12	1:Ar:425:LYS:NZ	2.26	0.41
1:Ay:34:LYS:HE3	1:Ay:481:ALA:HA	2.01	0.41
1:Ay:455:VAL:HG13	1:Ay:460:GLU:CG	2.45	0.41
1:Ay:479:ASN:HB2	1:Ay:491:MET:HE1	2.03	0.41
1:Az:381:VAL:O	1:Az:389:MET:SD	2.78	0.41
2:Bh:3:ILE:HG23	2:Bv:95:VAL:N	2.35	0.41
1:Bm:339:GLU:H	1:Bm:339:GLU:HG2	1.54	0.41
2:Af:4:ARG:O	2:At:93:ALA:HB1	2.21	0.41
1:Al:151:SER:HB3	1:Al:399:ALA:HA	2.02	0.41
1:Ar:397:GLU:O	1:Ar:400:LEU:HB3	2.19	0.41
1:Az:151:SER:HB3	1:Az:399:ALA:HA	2.02	0.41
1:Az:489:ILE:HG22	1:Az:494:LEU:CD2	2.47	0.41
1:Bf:386:GLU:HG3	1:Bf:390:LYS:NZ	2.35	0.41
1:Bg:146:GLN:HE21	1:Bg:146:GLN:HB2	1.61	0.41
2:Bh:93:ALA:HA	2:Bo:4:ARG:O	2.21	0.41
1:Bm:37:ASN:ND2	1:Bm:51:LYS:HZ1	2.18	0.41
1:Bm:479:ASN:HB2	1:Bm:491:MET:HE1	2.03	0.41
1:Bn:172:GLU:OE2	1:Bn:369:VAL:HG11	2.12	0.41
1:Bt:77:VAL:HG21	1:Bt:510:VAL:HB	2.01	0.41
1:Bu:219:PHE:HB3	1:Bu:317:LEU:HD23	2.02	0.41
1:Ae:31:LEU:HD23	1:Ae:453:GLN:HB3	2.01	0.41
1:Ae:219:PHE:HB3	1:Ae:317:LEU:HD23	2.02	0.41
1:Ak:479:ASN:HB2	1:Ak:491:MET:HE1	2.03	0.41
1:Al:31:LEU:HD23	1:Al:453:GLN:HB3	2.01	0.41
2:Am:97:ALA:OXT	2:Ba:1:MET:N	2.51	0.41
1:Ar:219:PHE:HD1	1:Ar:219:PHE:HA	1.70	0.41
1:Ar:479:ASN:HB2	1:Ar:491:MET:HE1	2.03	0.41
1:Ar:489:ILE:HG23	1:Ar:494:LEU:HD21	2.02	0.41
1:As:62:LEU:HD12	1:As:62:LEU:HA	1.78	0.41
1:As:219:PHE:HB3	1:As:317:LEU:HD23	2.02	0.41
1:Ay:489:ILE:HD12	1:Ay:494:LEU:HD22	1.98	0.41
1:Bf:34:LYS:HE3	1:Bf:481:ALA:HA	2.01	0.41
1:Bf:155:ASP:CB	1:Bf:395:ARG:NH2	2.76	0.41
1:Bf:218:PRO:HG3	1:Bf:323:VAL:HB	2.02	0.41
1:Bm:284:ARG:CD	1:Bm:364:LYS:CB	2.99	0.41
1:Bm:473:ASP:OD1	1:Bm:473:ASP:C	2.58	0.41
1:Bm:489:ILE:HG23	1:Bm:494:LEU:HD21	2.02	0.41
1:Ad:16:MET:CG	1:Ad:520:MET:SD	3.08	0.41
1:Ad:69:MET:HG2	1:Ar:47:PRO:CG	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:119:GLY:C	1:Ad:440:ILE:HD13	2.44	0.41
1:Ad:164:GLU:C	1:Ad:167:ASP:HB2	2.45	0.41
1:Ad:168:LYS:HZ1	1:Ad:187:LEU:CG	2.29	0.41
1:Ak:386:GLU:HG3	1:Ak:390:LYS:NZ	2.35	0.41
1:Al:504:LEU:HD23	1:Al:504:LEU:HA	1.83	0.41
1:Ar:307:MET:HB3	1:Ar:307:MET:HE3	1.64	0.41
1:As:381:VAL:O	1:As:389:MET:SD	2.78	0.41
1:Ay:479:ASN:CB	1:Ay:491:MET:CE	2.98	0.41
1:Az:172:GLU:OE2	1:Az:369:VAL:HG11	2.12	0.41
1:Bg:151:SER:HB3	1:Bg:399:ALA:HA	2.02	0.41
1:Bg:219:PHE:HB3	1:Bg:317:LEU:HD23	2.02	0.41
1:Bn:6:VAL:HG12	1:Bn:8:PHE:CZ	2.56	0.41
1:Bn:39:VAL:HG22	1:Bn:49:ILE:HG13	2.03	0.41
1:Bt:284:ARG:CD	1:Bt:364:LYS:CB	2.99	0.41
1:Ad:186:GLU:O	1:Ad:380:LYS:N	2.52	0.41
1:Ad:386:GLU:HG3	1:Ad:390:LYS:NZ	2.35	0.41
1:Ae:40:LEU:CG	1:Ae:59:GLU:OE1	2.69	0.41
1:Ae:54:VAL:HG11	1:Ae:82:ASN:HD21	1.68	0.41
1:Ae:151:SER:HB3	1:Ae:399:ALA:HA	2.02	0.41
1:As:40:LEU:CG	1:As:59:GLU:OE1	2.69	0.41
1:Ay:233:MET:H	1:Ay:233:MET:HG3	1.71	0.41
1:Ay:457:ASN:O	1:Bt:114:MET:CE	2.61	0.41
1:Az:146:GLN:HE21	1:Az:146:GLN:HB2	1.62	0.41
1:Az:219:PHE:HB3	1:Az:317:LEU:HD23	2.02	0.41
1:Bf:207:LYS:H	1:Bf:207:LYS:HG3	1.42	0.41
1:Bg:6:VAL:HG12	1:Bg:8:PHE:CZ	2.56	0.41
1:Bg:7:LYS:HG3	1:Bg:66:PHE:CE1	2.45	0.41
1:Bg:36:ARG:HE	1:Bu:113:PRO:CD	2.33	0.41
1:Bg:39:VAL:HG22	1:Bg:49:ILE:HG13	2.03	0.41
1:Bg:113:PRO:HG2	1:Bn:36:ARG:HE	1.77	0.41
1:Bn:40:LEU:CG	1:Bn:59:GLU:OE1	2.69	0.41
1:Bn:381:VAL:O	1:Bn:389:MET:SD	2.78	0.41
1:Bt:164:GLU:C	1:Bt:167:ASP:HB2	2.45	0.41
1:Bt:186:GLU:O	1:Bt:380:LYS:N	2.52	0.41
1:Bt:194:GLN:H	1:Bt:371:LYS:CD	2.33	0.41
1:Bu:75:LYS:HE2	1:Bu:75:LYS:HB2	1.89	0.41
1:Bu:146:GLN:HE21	1:Bu:146:GLN:HB2	1.62	0.41
1:Ae:4:LYS:HD3	1:Ae:523:ASP:HA	2.03	0.41
1:Ae:6:VAL:HG12	1:Ae:8:PHE:CZ	2.56	0.41
1:Ae:372:LEU:HD23	1:Ae:372:LEU:HA	1.92	0.41
1:Ak:34:LYS:HE3	1:Ak:481:ALA:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:4:LYS:HD3	1:Al:523:ASP:HA	2.03	0.41
1:Al:18:ARG:HD2	1:Al:67:GLU:CD	2.46	0.41
1:Al:387:VAL:HG13	1:Al:388:GLU:N	2.36	0.41
2:Am:95:VAL:HA	2:Ba:2:ASN:O	2.21	0.41
1:As:6:VAL:HG12	1:As:8:PHE:CZ	2.56	0.41
1:Ay:47:PRO:CG	1:Bt:69:MET:HG2	2.51	0.41
1:Az:517:THR:HG23	1:Bu:39:VAL:CG2	2.40	0.41
2:Ba:95:VAL:HA	2:Bv:2:ASN:O	2.21	0.41
1:Bf:233:MET:HE2	1:Bf:233:MET:HB2	1.67	0.41
1:Bf:305:ILE:HD13	1:Bf:305:ILE:HA	1.89	0.41
1:Bg:39:VAL:CG2	1:Bu:517:THR:HG23	2.38	0.41
1:Bg:524:LEU:HD21	1:Bn:63:GLU:HG3	0.98	0.41
1:Bm:166:MET:HA	1:Bm:170:GLY:CA	2.47	0.41
1:Bn:489:ILE:HD11	1:Bn:490:ASP:OD1	2.21	0.41
1:Bt:104:LEU:HD23	1:Bt:104:LEU:HA	1.83	0.41
1:Bt:233:MET:HE2	1:Bt:233:MET:HB2	1.67	0.41
1:Bu:18:ARG:HD2	1:Bu:67:GLU:CD	2.46	0.41
1:Bu:387:VAL:HG13	1:Bu:388:GLU:N	2.36	0.41
1:Ad:100:ILE:HD11	1:Ad:510:VAL:HG13	2.03	0.40
1:Ae:6:VAL:HG21	1:Al:60:ILE:HD13	2.03	0.40
1:Al:62:LEU:HD12	1:Al:62:LEU:HA	1.78	0.40
1:Ay:386:GLU:HG3	1:Ay:390:LYS:NZ	2.35	0.40
1:Az:4:LYS:HD3	1:Az:523:ASP:HA	2.03	0.40
1:Az:6:VAL:HG12	1:Az:8:PHE:CZ	2.56	0.40
1:Az:20:VAL:HG22	1:Az:514:MET:HE1	2.04	0.40
1:Az:387:VAL:HG13	1:Az:388:GLU:N	2.37	0.40
1:Bf:479:ASN:CB	1:Bf:491:MET:CE	2.98	0.40
1:Bg:62:LEU:HD12	1:Bg:62:LEU:HA	1.78	0.40
1:Bg:183:LEU:HD21	1:Bg:384:ALA:HA	2.02	0.40
1:Bg:489:ILE:HD11	1:Bg:490:ASP:OD1	2.21	0.40
1:Bm:163:ALA:O	1:Bm:167:ASP:N	2.46	0.40
1:Bn:18:ARG:HD2	1:Bn:67:GLU:CD	2.46	0.40
1:Bn:131:LEU:CD1	1:Bn:500:THR:HG22	2.48	0.40
1:Bt:271:VAL:O	1:Bt:272:LYS:HB3	2.21	0.40
1:Bt:386:GLU:HG3	1:Bt:390:LYS:NZ	2.35	0.40
1:Bt:455:VAL:HG13	1:Bt:460:GLU:CG	2.45	0.40
1:Bt:489:ILE:HD12	1:Bt:494:LEU:HD22	1.97	0.40
1:Bu:183:LEU:HD21	1:Bu:384:ALA:HA	2.02	0.40
1:Bu:489:ILE:HD11	1:Bu:490:ASP:OD1	2.21	0.40
1:Ad:183:LEU:HG	1:Ad:384:ALA:HA	2.00	0.40
1:Ae:477:GLY:O	1:Ae:488:MET:HE3	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:489:ILE:HD11	1:Ae:490:ASP:OD1	2.21	0.40
1:Al:40:LEU:CG	1:Al:59:GLU:OE1	2.69	0.40
1:Al:428:ASP:O	1:Al:429:LEU:C	2.65	0.40
1:Al:458:CYS:HB3	1:Al:483:GLU:OE2	2.21	0.40
1:Ar:111:MET:CB	1:Ar:116:LEU:HD11	2.50	0.40
1:Ar:114:MET:CE	1:Bm:457:ASN:O	2.62	0.40
1:Ar:421:ARG:HH12	1:Ar:469:VAL:CG1	2.24	0.40
1:As:18:ARG:HD2	1:As:67:GLU:CD	2.46	0.40
1:Ay:17:LEU:HD12	1:Ay:17:LEU:HA	1.86	0.40
1:Ay:163:ALA:O	1:Ay:167:ASP:N	2.46	0.40
1:Ay:284:ARG:CD	1:Ay:364:LYS:CB	2.99	0.40
2:Bh:1:MET:N	2:Bv:97:ALA:OXT	2.52	0.40
1:Bm:34:LYS:HE3	1:Bm:481:ALA:HA	2.01	0.40
1:Bu:20:VAL:HG22	1:Bu:514:MET:HE1	2.04	0.40
1:Ae:20:VAL:HG22	1:Ae:514:MET:HE1	2.04	0.40
1:Ae:387:VAL:HG13	1:Ae:388:GLU:N	2.36	0.40
1:Ae:458:CYS:HB3	1:Ae:483:GLU:OE2	2.21	0.40
1:Ak:284:ARG:CD	1:Ak:364:LYS:CB	2.99	0.40
1:Al:146:GLN:HE21	1:Al:146:GLN:HB2	1.62	0.40
1:Al:489:ILE:HD11	1:Al:490:ASP:OD1	2.21	0.40
1:As:4:LYS:HD3	1:As:523:ASP:HA	2.03	0.40
2:At:4:ARG:HB3	2:Bo:94:ILE:O	2.21	0.40
1:Ay:164:GLU:C	1:Ay:167:ASP:HB2	2.46	0.40
1:Ay:271:VAL:O	1:Ay:272:LYS:HB3	2.22	0.40
1:Az:456:LEU:HB2	1:Az:462:PRO:HG3	2.04	0.40
1:Bf:49:ILE:CD1	1:Bm:73:MET:CE	2.75	0.40
1:Bf:510:VAL:O	1:Bf:514:MET:CG	2.45	0.40
1:Bm:142:LYS:CG	1:Bm:146:GLN:NE2	2.68	0.40
1:Bm:233:MET:H	1:Bm:233:MET:HG3	1.71	0.40
1:Bm:248:LEU:HD13	1:Bm:325:ILE:HD11	2.03	0.40
1:Bn:428:ASP:O	1:Bn:429:LEU:C	2.65	0.40
1:Bn:458:CYS:HB3	1:Bn:483:GLU:OE2	2.21	0.40
1:Bu:504:LEU:HD23	1:Bu:504:LEU:HA	1.83	0.40
1:Ad:248:LEU:HD13	1:Ad:325:ILE:HD11	2.03	0.40
1:Ae:524:LEU:HD21	1:Al:63:GLU:HG3	1.02	0.40
1:Ak:100:ILE:HD11	1:Ak:510:VAL:HG13	2.04	0.40
1:Ak:164:GLU:C	1:Ak:167:ASP:HB2	2.46	0.40
1:Ak:227:ILE:HD12	1:Ak:227:ILE:HA	1.62	0.40
1:Al:20:VAL:HG22	1:Al:514:MET:HE1	2.04	0.40
1:Al:219:PHE:HB3	1:Al:317:LEU:HD23	2.02	0.40
2:Am:95:VAL:N	2:Ba:3:ILE:HG23	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:348:GLN:HE21	1:Ar:348:GLN:HB3	1.54	0.40
1:As:20:VAL:HG22	1:As:514:MET:HE1	2.03	0.40
1:As:39:VAL:HG22	1:As:49:ILE:HG13	2.03	0.40
1:As:477:GLY:O	1:As:488:MET:HE3	2.19	0.40
1:As:489:ILE:HD11	1:As:490:ASP:OD1	2.21	0.40
1:Bf:307:MET:HB3	1:Bf:307:MET:HE3	1.64	0.40
1:Bm:524:LEU:HA	1:Bm:525:PRO:HD2	1.92	0.40
1:Bn:54:VAL:HG11	1:Bn:82:ASN:HD21	1.68	0.40
1:Bt:112:ASN:HD21	1:Bt:114:MET:HB2	1.87	0.40
1:Bt:348:GLN:HE21	1:Bt:348:GLN:HB3	1.54	0.40
1:Bu:428:ASP:O	1:Bu:429:LEU:C	2.65	0.40
1:Ad:271:VAL:O	1:Ad:272:LYS:HB3	2.21	0.40
1:Ae:50:THR:CG2	1:Ae:52:ASP:OD1	2.65	0.40
1:Ak:473:ASP:OD1	1:Ak:473:ASP:C	2.58	0.40
1:As:7:LYS:CD	1:As:66:PHE:CD2	3.05	0.40
1:As:428:ASP:O	1:As:429:LEU:C	2.65	0.40
1:Az:131:LEU:HD23	1:Az:131:LEU:HA	1.76	0.40
1:Az:495:ASP:HA	1:Az:496:PRO:HD3	1.75	0.40
1:Bf:231:ARG:H	1:Bf:231:ARG:HG2	1.48	0.40
1:Bg:40:LEU:CG	1:Bg:59:GLU:OE1	2.69	0.40
1:Bm:112:ASN:HD21	1:Bm:114:MET:HB2	1.87	0.40
1:Bm:218:PRO:HG2	1:Bm:320:ALA:HB3	2.03	0.40
1:Bm:489:ILE:HD12	1:Bm:494:LEU:HD22	1.97	0.40
1:Bn:219:PHE:HB3	1:Bn:317:LEU:HD23	2.02	0.40
1:Bn:387:VAL:HG13	1:Bn:388:GLU:N	2.36	0.40
1:Bt:307:MET:HB3	1:Bt:307:MET:HE3	1.64	0.40
1:Bu:4:LYS:HD3	1:Bu:523:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	Ad	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	Ae	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	43	71
1	Ak	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	Al	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	43	71
1	Ar	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	As	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	43	71
1	Ay	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	Az	522/524 (100%)	516 (99%)	4 (1%)	2 (0%)	30	59
1	Bf	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	Bg	522/524 (100%)	516 (99%)	4 (1%)	2 (0%)	30	59
1	Bm	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	Bn	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	43	71
1	Bt	522/524 (100%)	508 (97%)	11 (2%)	3 (1%)	21	50
1	Bu	522/524 (100%)	515 (99%)	6 (1%)	1 (0%)	43	71
2	Af	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
2	Am	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
2	At	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
2	Ba	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
2	Bh	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
2	Bo	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
2	Bv	95/97 (98%)	80 (84%)	12 (13%)	3 (3%)	3	17
All	All	7973/8015 (100%)	7723 (97%)	199 (2%)	51 (1%)	23	50

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Af	95	VAL
2	Am	95	VAL
2	At	95	VAL
2	Ba	95	VAL
2	Bh	95	VAL
2	Bo	95	VAL
2	Bv	95	VAL
1	Ad	270	ILE
1	Ak	270	ILE
1	Ar	270	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ay	270	ILE
1	Bf	270	ILE
1	Bm	270	ILE
1	Bt	270	ILE
1	Ad	272	LYS
1	Ak	272	LYS
1	Ar	272	LYS
1	Ay	272	LYS
1	Bf	272	LYS
1	Bm	272	LYS
1	Bt	272	LYS
1	Ae	225	LYS
1	Al	225	LYS
1	As	225	LYS
1	Az	225	LYS
1	Bg	225	LYS
1	Bn	225	LYS
1	Bu	225	LYS
2	Af	18	GLU
2	Af	50	GLU
2	Am	18	GLU
2	Am	50	GLU
2	At	18	GLU
2	At	50	GLU
2	Ba	18	GLU
2	Ba	50	GLU
2	Bh	18	GLU
2	Bh	50	GLU
2	Bo	18	GLU
2	Bo	50	GLU
2	Bv	18	GLU
2	Bv	50	GLU
1	Ad	168	LYS
1	Ak	168	LYS
1	Ar	168	LYS
1	Ay	168	LYS
1	Bf	168	LYS
1	Bm	168	LYS
1	Bt	168	LYS
1	Az	205	ILE
1	Bg	205	ILE

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 PDB entries followed by that with respect to all EM entries.

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	Ad	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	Ae	404/404 (100%)	383 (95%)	21 (5%)	21	48
1	Ak	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	Al	404/404 (100%)	383 (95%)	21 (5%)	21	48
1	Ar	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	As	404/404 (100%)	383 (95%)	21 (5%)	21	48
1	Ay	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	Az	404/404 (100%)	383 (95%)	21 (5%)	21	48
1	Bf	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	Bg	404/404 (100%)	383 (95%)	21 (5%)	21	48
1	Bm	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	Bn	404/404 (100%)	383 (95%)	21 (5%)	21	48
1	Bt	404/404 (100%)	323 (80%)	81 (20%)	1	4
1	Bu	404/404 (100%)	383 (95%)	21 (5%)	21	48
2	Af	80/80 (100%)	78 (98%)	2 (2%)	42	62
2	Am	80/80 (100%)	78 (98%)	2 (2%)	42	62
2	At	80/80 (100%)	78 (98%)	2 (2%)	42	62
2	Ba	80/80 (100%)	78 (98%)	2 (2%)	42	62
2	Bh	80/80 (100%)	78 (98%)	2 (2%)	42	62
2	Bo	80/80 (100%)	78 (98%)	2 (2%)	42	62
2	Bv	80/80 (100%)	78 (98%)	2 (2%)	42	62
All	All	6216/6216 (100%)	5488 (88%)	728 (12%)	7	20

All (728) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ad	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ad	99	ILE
1	Ad	160	LYS
1	Ad	171	LYS
1	Ad	179	ASP
1	Ad	186	GLU
1	Ad	187	LEU
1	Ad	189	VAL
1	Ad	190	VAL
1	Ad	191	GLU
1	Ad	194	GLN
1	Ad	203	TYR
1	Ad	207	LYS
1	Ad	209	GLU
1	Ad	210	THR
1	Ad	217	SER
1	Ad	219	PHE
1	Ad	220	ILE
1	Ad	225	LYS
1	Ad	227	ILE
1	Ad	231	ARG
1	Ad	232	GLU
1	Ad	233	MET
1	Ad	234	LEU
1	Ad	236	VAL
1	Ad	238	GLU
1	Ad	240	VAL
1	Ad	245	LYS
1	Ad	249	ILE
1	Ad	250	ILE
1	Ad	252	GLU
1	Ad	254	VAL
1	Ad	255	GLU
1	Ad	259	LEU
1	Ad	261	THR
1	Ad	262	LEU
1	Ad	264	VAL
1	Ad	268	ARG
1	Ad	270	ILE
1	Ad	272	LYS
1	Ad	277	LYS
1	Ad	286	LYS
1	Ad	288	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ad	290	GLN
1	Ad	292	ILE
1	Ad	295	LEU
1	Ad	299	THR
1	Ad	300	VAL
1	Ad	301	ILE
1	Ad	302	SER
1	Ad	303	GLU
1	Ad	304	GLU
1	Ad	307	MET
1	Ad	308	GLU
1	Ad	309	LEU
1	Ad	310	GLU
1	Ad	314	LEU
1	Ad	315	GLU
1	Ad	319	GLN
1	Ad	321	LYS
1	Ad	324	VAL
1	Ad	327	LYS
1	Ad	333	ILE
1	Ad	336	VAL
1	Ad	339	GLU
1	Ad	342	ILE
1	Ad	343	GLN
1	Ad	345	ARG
1	Ad	348	GLN
1	Ad	351	GLN
1	Ad	354	GLU
1	Ad	355	GLU
1	Ad	357	THR
1	Ad	358	SER
1	Ad	365	LEU
1	Ad	389	MET
1	Ad	488	MET
1	Ad	510	VAL
1	Ad	518	GLU
1	Ad	521	VAL
1	Ad	524	LEU
1	Ae	23	LEU
1	Ae	51	LYS
1	Ae	63	GLU
1	Ae	74	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ae	104	LEU
1	Ae	105	LYS
1	Ae	120	ILE
1	Ae	128	VAL
1	Ae	178	GLU
1	Ae	193	MET
1	Ae	196	ASP
1	Ae	284	ARG
1	Ae	354	GLU
1	Ae	379	ILE
1	Ae	390	LYS
1	Ae	420	ILE
1	Ae	429	LEU
1	Ae	433	ASN
1	Ae	440	ILE
1	Ae	453	GLN
1	Ae	468	THR
2	Af	2	ASN
2	Af	28	THR
1	Ak	54	VAL
1	Ak	99	ILE
1	Ak	160	LYS
1	Ak	171	LYS
1	Ak	179	ASP
1	Ak	186	GLU
1	Ak	187	LEU
1	Ak	189	VAL
1	Ak	190	VAL
1	Ak	191	GLU
1	Ak	194	GLN
1	Ak	203	TYR
1	Ak	207	LYS
1	Ak	209	GLU
1	Ak	210	THR
1	Ak	217	SER
1	Ak	219	PHE
1	Ak	220	ILE
1	Ak	225	LYS
1	Ak	227	ILE
1	Ak	231	ARG
1	Ak	232	GLU
1	Ak	233	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ak	234	LEU
1	Ak	236	VAL
1	Ak	238	GLU
1	Ak	240	VAL
1	Ak	245	LYS
1	Ak	249	ILE
1	Ak	250	ILE
1	Ak	252	GLU
1	Ak	254	VAL
1	Ak	255	GLU
1	Ak	259	LEU
1	Ak	261	THR
1	Ak	262	LEU
1	Ak	264	VAL
1	Ak	268	ARG
1	Ak	270	ILE
1	Ak	272	LYS
1	Ak	277	LYS
1	Ak	286	LYS
1	Ak	288	MET
1	Ak	290	GLN
1	Ak	292	ILE
1	Ak	295	LEU
1	Ak	299	THR
1	Ak	300	VAL
1	Ak	301	ILE
1	Ak	302	SER
1	Ak	303	GLU
1	Ak	304	GLU
1	Ak	307	MET
1	Ak	308	GLU
1	Ak	309	LEU
1	Ak	310	GLU
1	Ak	314	LEU
1	Ak	315	GLU
1	Ak	319	GLN
1	Ak	321	LYS
1	Ak	324	VAL
1	Ak	327	LYS
1	Ak	333	ILE
1	Ak	336	VAL
1	Ak	339	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ak	342	ILE
1	Ak	343	GLN
1	Ak	345	ARG
1	Ak	348	GLN
1	Ak	351	GLN
1	Ak	354	GLU
1	Ak	355	GLU
1	Ak	357	THR
1	Ak	358	SER
1	Ak	365	LEU
1	Ak	389	MET
1	Ak	488	MET
1	Ak	510	VAL
1	Ak	518	GLU
1	Ak	521	VAL
1	Ak	524	LEU
1	Al	23	LEU
1	Al	51	LYS
1	Al	63	GLU
1	Al	74	VAL
1	Al	104	LEU
1	Al	105	LYS
1	Al	120	ILE
1	Al	128	VAL
1	Al	178	GLU
1	Al	193	MET
1	Al	196	ASP
1	Al	284	ARG
1	Al	354	GLU
1	Al	379	ILE
1	Al	390	LYS
1	Al	420	ILE
1	Al	429	LEU
1	Al	433	ASN
1	Al	440	ILE
1	Al	453	GLN
1	Al	468	THR
2	Am	2	ASN
2	Am	28	THR
1	Ar	54	VAL
1	Ar	99	ILE
1	Ar	160	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ar	171	LYS
1	Ar	179	ASP
1	Ar	186	GLU
1	Ar	187	LEU
1	Ar	189	VAL
1	Ar	190	VAL
1	Ar	191	GLU
1	Ar	194	GLN
1	Ar	203	TYR
1	Ar	207	LYS
1	Ar	209	GLU
1	Ar	210	THR
1	Ar	217	SER
1	Ar	219	PHE
1	Ar	220	ILE
1	Ar	225	LYS
1	Ar	227	ILE
1	Ar	231	ARG
1	Ar	232	GLU
1	Ar	233	MET
1	Ar	234	LEU
1	Ar	236	VAL
1	Ar	238	GLU
1	Ar	240	VAL
1	Ar	245	LYS
1	Ar	249	ILE
1	Ar	250	ILE
1	Ar	252	GLU
1	Ar	254	VAL
1	Ar	255	GLU
1	Ar	259	LEU
1	Ar	261	THR
1	Ar	262	LEU
1	Ar	264	VAL
1	Ar	268	ARG
1	Ar	270	ILE
1	Ar	272	LYS
1	Ar	277	LYS
1	Ar	286	LYS
1	Ar	288	MET
1	Ar	290	GLN
1	Ar	292	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ar	295	LEU
1	Ar	299	THR
1	Ar	300	VAL
1	Ar	301	ILE
1	Ar	302	SER
1	Ar	303	GLU
1	Ar	304	GLU
1	Ar	307	MET
1	Ar	308	GLU
1	Ar	309	LEU
1	Ar	310	GLU
1	Ar	314	LEU
1	Ar	315	GLU
1	Ar	319	GLN
1	Ar	321	LYS
1	Ar	324	VAL
1	Ar	327	LYS
1	Ar	333	ILE
1	Ar	336	VAL
1	Ar	339	GLU
1	Ar	342	ILE
1	Ar	343	GLN
1	Ar	345	ARG
1	Ar	348	GLN
1	Ar	351	GLN
1	Ar	354	GLU
1	Ar	355	GLU
1	Ar	357	THR
1	Ar	358	SER
1	Ar	365	LEU
1	Ar	389	MET
1	Ar	488	MET
1	Ar	510	VAL
1	Ar	518	GLU
1	Ar	521	VAL
1	Ar	524	LEU
1	As	23	LEU
1	As	51	LYS
1	As	63	GLU
1	As	74	VAL
1	As	104	LEU
1	As	105	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	As	120	ILE
1	As	128	VAL
1	As	178	GLU
1	As	193	MET
1	As	196	ASP
1	As	284	ARG
1	As	354	GLU
1	As	379	ILE
1	As	390	LYS
1	As	420	ILE
1	As	429	LEU
1	As	433	ASN
1	As	440	ILE
1	As	453	GLN
1	As	468	THR
2	At	2	ASN
2	At	28	THR
1	Ay	54	VAL
1	Ay	99	ILE
1	Ay	160	LYS
1	Ay	171	LYS
1	Ay	179	ASP
1	Ay	186	GLU
1	Ay	187	LEU
1	Ay	189	VAL
1	Ay	190	VAL
1	Ay	191	GLU
1	Ay	194	GLN
1	Ay	203	TYR
1	Ay	207	LYS
1	Ay	209	GLU
1	Ay	210	THR
1	Ay	217	SER
1	Ay	219	PHE
1	Ay	220	ILE
1	Ay	225	LYS
1	Ay	227	ILE
1	Ay	231	ARG
1	Ay	232	GLU
1	Ay	233	MET
1	Ay	234	LEU
1	Ay	236	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ay	238	GLU
1	Ay	240	VAL
1	Ay	245	LYS
1	Ay	249	ILE
1	Ay	250	ILE
1	Ay	252	GLU
1	Ay	254	VAL
1	Ay	255	GLU
1	Ay	259	LEU
1	Ay	261	THR
1	Ay	262	LEU
1	Ay	264	VAL
1	Ay	268	ARG
1	Ay	270	ILE
1	Ay	272	LYS
1	Ay	277	LYS
1	Ay	286	LYS
1	Ay	288	MET
1	Ay	290	GLN
1	Ay	292	ILE
1	Ay	295	LEU
1	Ay	299	THR
1	Ay	300	VAL
1	Ay	301	ILE
1	Ay	302	SER
1	Ay	303	GLU
1	Ay	304	GLU
1	Ay	307	MET
1	Ay	308	GLU
1	Ay	309	LEU
1	Ay	310	GLU
1	Ay	314	LEU
1	Ay	315	GLU
1	Ay	319	GLN
1	Ay	321	LYS
1	Ay	324	VAL
1	Ay	327	LYS
1	Ay	333	ILE
1	Ay	336	VAL
1	Ay	339	GLU
1	Ay	342	ILE
1	Ay	343	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ay	345	ARG
1	Ay	348	GLN
1	Ay	351	GLN
1	Ay	354	GLU
1	Ay	355	GLU
1	Ay	357	THR
1	Ay	358	SER
1	Ay	365	LEU
1	Ay	389	MET
1	Ay	488	MET
1	Ay	510	VAL
1	Ay	518	GLU
1	Ay	521	VAL
1	Ay	524	LEU
1	Az	23	LEU
1	Az	51	LYS
1	Az	63	GLU
1	Az	74	VAL
1	Az	104	LEU
1	Az	105	LYS
1	Az	120	ILE
1	Az	128	VAL
1	Az	178	GLU
1	Az	193	MET
1	Az	196	ASP
1	Az	284	ARG
1	Az	354	GLU
1	Az	379	ILE
1	Az	390	LYS
1	Az	420	ILE
1	Az	429	LEU
1	Az	433	ASN
1	Az	440	ILE
1	Az	453	GLN
1	Az	468	THR
2	Ba	2	ASN
2	Ba	28	THR
1	Bf	54	VAL
1	Bf	99	ILE
1	Bf	160	LYS
1	Bf	171	LYS
1	Bf	179	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bf	186	GLU
1	Bf	187	LEU
1	Bf	189	VAL
1	Bf	190	VAL
1	Bf	191	GLU
1	Bf	194	GLN
1	Bf	203	TYR
1	Bf	207	LYS
1	Bf	209	GLU
1	Bf	210	THR
1	Bf	217	SER
1	Bf	219	PHE
1	Bf	220	ILE
1	Bf	225	LYS
1	Bf	227	ILE
1	Bf	231	ARG
1	Bf	232	GLU
1	Bf	233	MET
1	Bf	234	LEU
1	Bf	236	VAL
1	Bf	238	GLU
1	Bf	240	VAL
1	Bf	245	LYS
1	Bf	249	ILE
1	Bf	250	ILE
1	Bf	252	GLU
1	Bf	254	VAL
1	Bf	255	GLU
1	Bf	259	LEU
1	Bf	261	THR
1	Bf	262	LEU
1	Bf	264	VAL
1	Bf	268	ARG
1	Bf	270	ILE
1	Bf	272	LYS
1	Bf	277	LYS
1	Bf	286	LYS
1	Bf	288	MET
1	Bf	290	GLN
1	Bf	292	ILE
1	Bf	295	LEU
1	Bf	299	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bf	300	VAL
1	Bf	301	ILE
1	Bf	302	SER
1	Bf	303	GLU
1	Bf	304	GLU
1	Bf	307	MET
1	Bf	308	GLU
1	Bf	309	LEU
1	Bf	310	GLU
1	Bf	314	LEU
1	Bf	315	GLU
1	Bf	319	GLN
1	Bf	321	LYS
1	Bf	324	VAL
1	Bf	327	LYS
1	Bf	333	ILE
1	Bf	336	VAL
1	Bf	339	GLU
1	Bf	342	ILE
1	Bf	343	GLN
1	Bf	345	ARG
1	Bf	348	GLN
1	Bf	351	GLN
1	Bf	354	GLU
1	Bf	355	GLU
1	Bf	357	THR
1	Bf	358	SER
1	Bf	365	LEU
1	Bf	389	MET
1	Bf	488	MET
1	Bf	510	VAL
1	Bf	518	GLU
1	Bf	521	VAL
1	Bf	524	LEU
1	Bg	23	LEU
1	Bg	51	LYS
1	Bg	63	GLU
1	Bg	74	VAL
1	Bg	104	LEU
1	Bg	105	LYS
1	Bg	120	ILE
1	Bg	128	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bg	178	GLU
1	Bg	193	MET
1	Bg	196	ASP
1	Bg	284	ARG
1	Bg	354	GLU
1	Bg	379	ILE
1	Bg	390	LYS
1	Bg	420	ILE
1	Bg	429	LEU
1	Bg	433	ASN
1	Bg	440	ILE
1	Bg	453	GLN
1	Bg	468	THR
2	Bh	2	ASN
2	Bh	28	THR
1	Bm	54	VAL
1	Bm	99	ILE
1	Bm	160	LYS
1	Bm	171	LYS
1	Bm	179	ASP
1	Bm	186	GLU
1	Bm	187	LEU
1	Bm	189	VAL
1	Bm	190	VAL
1	Bm	191	GLU
1	Bm	194	GLN
1	Bm	203	TYR
1	Bm	207	LYS
1	Bm	209	GLU
1	Bm	210	THR
1	Bm	217	SER
1	Bm	219	PHE
1	Bm	220	ILE
1	Bm	225	LYS
1	Bm	227	ILE
1	Bm	231	ARG
1	Bm	232	GLU
1	Bm	233	MET
1	Bm	234	LEU
1	Bm	236	VAL
1	Bm	238	GLU
1	Bm	240	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bm	245	LYS
1	Bm	249	ILE
1	Bm	250	ILE
1	Bm	252	GLU
1	Bm	254	VAL
1	Bm	255	GLU
1	Bm	259	LEU
1	Bm	261	THR
1	Bm	262	LEU
1	Bm	264	VAL
1	Bm	268	ARG
1	Bm	270	ILE
1	Bm	272	LYS
1	Bm	277	LYS
1	Bm	286	LYS
1	Bm	288	MET
1	Bm	290	GLN
1	Bm	292	ILE
1	Bm	295	LEU
1	Bm	299	THR
1	Bm	300	VAL
1	Bm	301	ILE
1	Bm	302	SER
1	Bm	303	GLU
1	Bm	304	GLU
1	Bm	307	MET
1	Bm	308	GLU
1	Bm	309	LEU
1	Bm	310	GLU
1	Bm	314	LEU
1	Bm	315	GLU
1	Bm	319	GLN
1	Bm	321	LYS
1	Bm	324	VAL
1	Bm	327	LYS
1	Bm	333	ILE
1	Bm	336	VAL
1	Bm	339	GLU
1	Bm	342	ILE
1	Bm	343	GLN
1	Bm	345	ARG
1	Bm	348	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bm	351	GLN
1	Bm	354	GLU
1	Bm	355	GLU
1	Bm	357	THR
1	Bm	358	SER
1	Bm	365	LEU
1	Bm	389	MET
1	Bm	488	MET
1	Bm	510	VAL
1	Bm	518	GLU
1	Bm	521	VAL
1	Bm	524	LEU
1	Bn	23	LEU
1	Bn	51	LYS
1	Bn	63	GLU
1	Bn	74	VAL
1	Bn	104	LEU
1	Bn	105	LYS
1	Bn	120	ILE
1	Bn	128	VAL
1	Bn	178	GLU
1	Bn	193	MET
1	Bn	196	ASP
1	Bn	284	ARG
1	Bn	354	GLU
1	Bn	379	ILE
1	Bn	390	LYS
1	Bn	420	ILE
1	Bn	429	LEU
1	Bn	433	ASN
1	Bn	440	ILE
1	Bn	453	GLN
1	Bn	468	THR
2	Bo	2	ASN
2	Bo	28	THR
1	Bt	54	VAL
1	Bt	99	ILE
1	Bt	160	LYS
1	Bt	171	LYS
1	Bt	179	ASP
1	Bt	186	GLU
1	Bt	187	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bt	189	VAL
1	Bt	190	VAL
1	Bt	191	GLU
1	Bt	194	GLN
1	Bt	203	TYR
1	Bt	207	LYS
1	Bt	209	GLU
1	Bt	210	THR
1	Bt	217	SER
1	Bt	219	PHE
1	Bt	220	ILE
1	Bt	225	LYS
1	Bt	227	ILE
1	Bt	231	ARG
1	Bt	232	GLU
1	Bt	233	MET
1	Bt	234	LEU
1	Bt	236	VAL
1	Bt	238	GLU
1	Bt	240	VAL
1	Bt	245	LYS
1	Bt	249	ILE
1	Bt	250	ILE
1	Bt	252	GLU
1	Bt	254	VAL
1	Bt	255	GLU
1	Bt	259	LEU
1	Bt	261	THR
1	Bt	262	LEU
1	Bt	264	VAL
1	Bt	268	ARG
1	Bt	270	ILE
1	Bt	272	LYS
1	Bt	277	LYS
1	Bt	286	LYS
1	Bt	288	MET
1	Bt	290	GLN
1	Bt	292	ILE
1	Bt	295	LEU
1	Bt	299	THR
1	Bt	300	VAL
1	Bt	301	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bt	302	SER
1	Bt	303	GLU
1	Bt	304	GLU
1	Bt	307	MET
1	Bt	308	GLU
1	Bt	309	LEU
1	Bt	310	GLU
1	Bt	314	LEU
1	Bt	315	GLU
1	Bt	319	GLN
1	Bt	321	LYS
1	Bt	324	VAL
1	Bt	327	LYS
1	Bt	333	ILE
1	Bt	336	VAL
1	Bt	339	GLU
1	Bt	342	ILE
1	Bt	343	GLN
1	Bt	345	ARG
1	Bt	348	GLN
1	Bt	351	GLN
1	Bt	354	GLU
1	Bt	355	GLU
1	Bt	357	THR
1	Bt	358	SER
1	Bt	365	LEU
1	Bt	389	MET
1	Bt	488	MET
1	Bt	510	VAL
1	Bt	518	GLU
1	Bt	521	VAL
1	Bt	524	LEU
1	Bu	23	LEU
1	Bu	51	LYS
1	Bu	63	GLU
1	Bu	74	VAL
1	Bu	104	LEU
1	Bu	105	LYS
1	Bu	120	ILE
1	Bu	128	VAL
1	Bu	178	GLU
1	Bu	193	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bu	196	ASP
1	Bu	284	ARG
1	Bu	354	GLU
1	Bu	379	ILE
1	Bu	390	LYS
1	Bu	420	ILE
1	Bu	429	LEU
1	Bu	433	ASN
1	Bu	440	ILE
1	Bu	453	GLN
1	Bu	468	THR
2	Bv	2	ASN
2	Bv	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ad	37	ASN
1	Ad	72	GLN
1	Ad	112	ASN
1	Ad	146	GLN
1	Ad	348	GLN
1	Ad	366	GLN
1	Ad	453	GLN
1	Ad	475	ASN
1	Ad	487	ASN
1	Ae	21	ASN
1	Ae	72	GLN
1	Ae	82	ASN
1	Ae	146	GLN
1	Ae	153	ASN
1	Ak	37	ASN
1	Ak	112	ASN
1	Ak	146	GLN
1	Ak	348	GLN
1	Ak	366	GLN
1	Ak	453	GLN
1	Ak	475	ASN
1	Ak	487	ASN
1	Al	21	ASN
1	Al	72	GLN
1	Al	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Al	146	GLN
1	Al	153	ASN
1	Ar	37	ASN
1	Ar	112	ASN
1	Ar	146	GLN
1	Ar	348	GLN
1	Ar	366	GLN
1	Ar	453	GLN
1	Ar	475	ASN
1	Ar	487	ASN
1	As	21	ASN
1	As	72	GLN
1	As	82	ASN
1	As	146	GLN
1	As	153	ASN
1	Ay	37	ASN
1	Ay	112	ASN
1	Ay	146	GLN
1	Ay	348	GLN
1	Ay	366	GLN
1	Ay	453	GLN
1	Ay	475	ASN
1	Ay	487	ASN
1	Az	21	ASN
1	Az	72	GLN
1	Az	82	ASN
1	Az	146	GLN
1	Az	153	ASN
1	Bf	37	ASN
1	Bf	112	ASN
1	Bf	146	GLN
1	Bf	348	GLN
1	Bf	366	GLN
1	Bf	453	GLN
1	Bf	475	ASN
1	Bf	487	ASN
1	Bg	21	ASN
1	Bg	72	GLN
1	Bg	82	ASN
1	Bg	146	GLN
1	Bg	153	ASN
1	Bm	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bm	72	GLN
1	Bm	112	ASN
1	Bm	146	GLN
1	Bm	366	GLN
1	Bm	453	GLN
1	Bm	475	ASN
1	Bm	487	ASN
1	Bn	21	ASN
1	Bn	72	GLN
1	Bn	82	ASN
1	Bn	146	GLN
1	Bn	153	ASN
1	Bt	37	ASN
1	Bt	112	ASN
1	Bt	146	GLN
1	Bt	348	GLN
1	Bt	366	GLN
1	Bt	453	GLN
1	Bt	475	ASN
1	Bt	487	ASN
1	Bu	21	ASN
1	Bu	72	GLN
1	Bu	82	ASN
1	Bu	146	GLN
1	Bu	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	Ar	601	4	28,29,29	2.80	10 (35%)	43,45,45	1.85	8 (18%)
3	ADP	Bu	601	4	28,29,29	2.79	10 (35%)	43,45,45	1.80	10 (23%)
3	ADP	Az	601	4	28,29,29	2.79	10 (35%)	43,45,45	1.80	9 (20%)
3	ADP	Ak	601	4	28,29,29	2.80	10 (35%)	43,45,45	1.84	8 (18%)
3	ADP	Ay	601	4	28,29,29	2.79	10 (35%)	43,45,45	1.84	8 (18%)
3	ADP	Bm	601	4	28,29,29	2.79	10 (35%)	43,45,45	1.84	8 (18%)
3	ADP	Al	601	4	28,29,29	2.79	10 (35%)	43,45,45	1.80	9 (20%)
3	ADP	Ad	601	4	28,29,29	2.80	10 (35%)	43,45,45	1.84	8 (18%)
3	ADP	Bn	601	4	28,29,29	2.78	10 (35%)	43,45,45	1.80	9 (20%)
3	ADP	Bg	601	4	28,29,29	2.78	10 (35%)	43,45,45	1.79	9 (20%)
3	ADP	Bt	601	4	28,29,29	2.80	10 (35%)	43,45,45	1.84	8 (18%)
3	ADP	Ae	601	4	28,29,29	2.78	10 (35%)	43,45,45	1.80	9 (20%)
3	ADP	As	601	4	28,29,29	2.78	10 (35%)	43,45,45	1.80	10 (23%)
3	ADP	Bf	601	4	28,29,29	2.80	10 (35%)	43,45,45	1.84	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	Ar	601	4	-	3/16/32/32	0/3/3/3
3	ADP	Bu	601	4	-	6/16/32/32	0/3/3/3
3	ADP	Az	601	4	-	6/16/32/32	0/3/3/3
3	ADP	Ak	601	4	-	3/16/32/32	0/3/3/3
3	ADP	Ay	601	4	-	3/16/32/32	0/3/3/3
3	ADP	Bm	601	4	-	3/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	Al	601	4	-	6/16/32/32	0/3/3/3
3	ADP	Ad	601	4	-	3/16/32/32	0/3/3/3
3	ADP	Bn	601	4	-	6/16/32/32	0/3/3/3
3	ADP	Bg	601	4	-	6/16/32/32	0/3/3/3
3	ADP	Bt	601	4	-	3/16/32/32	0/3/3/3
3	ADP	Ae	601	4	-	6/16/32/32	0/3/3/3
3	ADP	As	601	4	-	6/16/32/32	0/3/3/3
3	ADP	Bf	601	4	-	3/16/32/32	0/3/3/3

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Bf	601	ADP	O4'-C1'	7.84	1.60	1.42
3	Ay	601	ADP	O4'-C1'	7.83	1.60	1.42
3	Ad	601	ADP	O4'-C1'	7.82	1.60	1.42
3	Ar	601	ADP	O4'-C1'	7.82	1.60	1.42
3	Ak	601	ADP	O4'-C1'	7.80	1.60	1.42
3	Bt	601	ADP	O4'-C1'	7.79	1.60	1.42
3	Bm	601	ADP	O4'-C1'	7.79	1.60	1.42
3	As	601	ADP	O4'-C1'	7.76	1.59	1.42
3	Bu	601	ADP	O4'-C1'	7.76	1.59	1.42
3	Az	601	ADP	O4'-C1'	7.76	1.59	1.42
3	Al	601	ADP	O4'-C1'	7.75	1.59	1.42
3	Ae	601	ADP	O4'-C1'	7.74	1.59	1.42
3	Bg	601	ADP	O4'-C1'	7.74	1.59	1.42
3	Bn	601	ADP	O4'-C1'	7.74	1.59	1.42
3	Ak	601	ADP	C2'-C1'	-6.19	1.34	1.53
3	Ay	601	ADP	C2'-C1'	-6.19	1.34	1.53
3	Bf	601	ADP	C2'-C1'	-6.19	1.34	1.53
3	Ar	601	ADP	C2'-C1'	-6.19	1.34	1.53
3	Bt	601	ADP	C2'-C1'	-6.19	1.34	1.53
3	Ad	601	ADP	C2'-C1'	-6.18	1.34	1.53
3	Bm	601	ADP	C2'-C1'	-6.14	1.34	1.53
3	As	601	ADP	C2'-C1'	-6.09	1.34	1.53
3	Az	601	ADP	C2'-C1'	-6.08	1.34	1.53
3	Ae	601	ADP	C2'-C1'	-6.07	1.34	1.53
3	Bg	601	ADP	C2'-C1'	-6.07	1.34	1.53
3	Bn	601	ADP	C2'-C1'	-6.07	1.34	1.53
3	Al	601	ADP	C2'-C1'	-6.06	1.34	1.53
3	Bu	601	ADP	C2'-C1'	-6.06	1.34	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Al	601	ADP	O4'-C4'	-5.70	1.32	1.45
3	Ae	601	ADP	O4'-C4'	-5.68	1.32	1.45
3	Bg	601	ADP	O4'-C4'	-5.68	1.32	1.45
3	Bn	601	ADP	O4'-C4'	-5.68	1.32	1.45
3	Bu	601	ADP	O4'-C4'	-5.68	1.32	1.45
3	Az	601	ADP	O4'-C4'	-5.67	1.32	1.45
3	As	601	ADP	O4'-C4'	-5.66	1.32	1.45
3	Ar	601	ADP	O4'-C4'	-5.58	1.32	1.45
3	Ay	601	ADP	O4'-C4'	-5.58	1.32	1.45
3	Ad	601	ADP	O4'-C4'	-5.57	1.32	1.45
3	Bt	601	ADP	O4'-C4'	-5.57	1.32	1.45
3	Ak	601	ADP	O4'-C4'	-5.55	1.32	1.45
3	Bf	601	ADP	O4'-C4'	-5.55	1.32	1.45
3	Bm	601	ADP	O4'-C4'	-5.54	1.32	1.45
3	Ar	601	ADP	C6-N6	5.34	1.47	1.34
3	Bm	601	ADP	C6-N6	5.33	1.47	1.34
3	Ad	601	ADP	C6-N6	5.31	1.47	1.34
3	Ak	601	ADP	C6-N6	5.30	1.47	1.34
3	Bt	601	ADP	C6-N6	5.29	1.47	1.34
3	Bf	601	ADP	C6-N6	5.29	1.47	1.34
3	Ay	601	ADP	C6-N6	5.28	1.47	1.34
3	Al	601	ADP	C6-N6	5.25	1.47	1.34
3	Bn	601	ADP	C6-N6	5.24	1.47	1.34
3	Ae	601	ADP	C6-N6	5.24	1.47	1.34
3	Bg	601	ADP	C6-N6	5.23	1.47	1.34
3	Bu	601	ADP	C6-N6	5.23	1.47	1.34
3	As	601	ADP	C6-N6	5.23	1.47	1.34
3	Az	601	ADP	C6-N6	5.22	1.47	1.34
3	Ak	601	ADP	PA-O3A	3.61	1.63	1.59
3	Bt	601	ADP	PA-O3A	3.59	1.63	1.59
3	Bm	601	ADP	PA-O3A	3.57	1.63	1.59
3	Ad	601	ADP	PA-O3A	3.56	1.63	1.59
3	Bf	601	ADP	PA-O3A	3.51	1.63	1.59
3	Ar	601	ADP	PA-O3A	3.51	1.63	1.59
3	Ay	601	ADP	PA-O3A	3.48	1.63	1.59
3	Bf	601	ADP	O3'-C3'	-3.18	1.35	1.43
3	Ak	601	ADP	O3'-C3'	-3.18	1.35	1.43
3	Bt	601	ADP	O3'-C3'	-3.18	1.35	1.43
3	Bm	601	ADP	O3'-C3'	-3.16	1.35	1.43
3	Ad	601	ADP	O3'-C3'	-3.16	1.35	1.43
3	Ar	601	ADP	O3'-C3'	-3.15	1.35	1.43
3	Ay	601	ADP	O3'-C3'	-3.15	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Az	601	ADP	O3'-C3'	-3.14	1.35	1.43
3	As	601	ADP	O3'-C3'	-3.13	1.35	1.43
3	Bn	601	ADP	O3'-C3'	-3.12	1.35	1.43
3	Ae	601	ADP	O3'-C3'	-3.11	1.35	1.43
3	Al	601	ADP	O3'-C3'	-3.11	1.35	1.43
3	Bu	601	ADP	O3'-C3'	-3.09	1.35	1.43
3	Bg	601	ADP	O3'-C3'	-3.08	1.35	1.43
3	Bu	601	ADP	C8-N9	-3.02	1.32	1.37
3	Ae	601	ADP	C8-N9	-2.98	1.32	1.37
3	Al	601	ADP	C8-N9	-2.98	1.32	1.37
3	Bn	601	ADP	C8-N9	-2.97	1.32	1.37
3	As	601	ADP	C8-N9	-2.96	1.32	1.37
3	Bg	601	ADP	C8-N9	-2.96	1.32	1.37
3	Az	601	ADP	C8-N9	-2.96	1.32	1.37
3	Bu	601	ADP	PA-O3A	2.90	1.62	1.59
3	Al	601	ADP	PA-O3A	2.89	1.62	1.59
3	Bm	601	ADP	C8-N9	-2.89	1.32	1.37
3	Ae	601	ADP	PA-O3A	2.89	1.62	1.59
3	Bt	601	ADP	C8-N9	-2.88	1.32	1.37
3	As	601	ADP	PA-O3A	2.88	1.62	1.59
3	Az	601	ADP	PA-O3A	2.88	1.62	1.59
3	Bg	601	ADP	PA-O3A	2.86	1.62	1.59
3	Bn	601	ADP	PA-O3A	2.86	1.62	1.59
3	Ad	601	ADP	C8-N9	-2.85	1.32	1.37
3	Bf	601	ADP	C8-N9	-2.85	1.32	1.37
3	Ar	601	ADP	C8-N9	-2.84	1.32	1.37
3	Ay	601	ADP	C8-N9	-2.84	1.32	1.37
3	Ak	601	ADP	C8-N9	-2.82	1.32	1.37
3	Bn	601	ADP	O2'-C2'	2.39	1.48	1.43
3	Az	601	ADP	C5-N7	-2.38	1.34	1.39
3	Al	601	ADP	O2'-C2'	2.38	1.48	1.43
3	Bu	601	ADP	O2'-C2'	2.37	1.48	1.43
3	Bu	601	ADP	C5-N7	-2.37	1.34	1.39
3	As	601	ADP	O2'-C2'	2.37	1.48	1.43
3	Ae	601	ADP	O2'-C2'	2.37	1.48	1.43
3	Az	601	ADP	O2'-C2'	2.36	1.48	1.43
3	Bg	601	ADP	O2'-C2'	2.36	1.48	1.43
3	Al	601	ADP	C5-N7	-2.36	1.34	1.39
3	Ae	601	ADP	C5-N7	-2.36	1.34	1.39
3	Bn	601	ADP	C5-N7	-2.36	1.34	1.39
3	As	601	ADP	C5-N7	-2.32	1.34	1.39
3	Bg	601	ADP	C5-N7	-2.32	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Ay	601	ADP	PA-O5'	2.30	1.68	1.59
3	Bm	601	ADP	PA-O5'	2.28	1.68	1.59
3	Bf	601	ADP	C5-N7	-2.28	1.34	1.39
3	Bt	601	ADP	PA-O5'	2.28	1.68	1.59
3	Ak	601	ADP	C5-N7	-2.28	1.34	1.39
3	Bf	601	ADP	PA-O5'	2.28	1.68	1.59
3	Ad	601	ADP	PA-O5'	2.28	1.68	1.59
3	Bt	601	ADP	C5-N7	-2.27	1.34	1.39
3	Ay	601	ADP	C5-N7	-2.27	1.34	1.39
3	Ar	601	ADP	PA-O5'	2.27	1.68	1.59
3	Bf	601	ADP	O2'-C2'	2.27	1.48	1.43
3	Ak	601	ADP	PA-O5'	2.27	1.68	1.59
3	Ar	601	ADP	C5-N7	-2.26	1.34	1.39
3	Ad	601	ADP	C5-N7	-2.25	1.35	1.39
3	Ak	601	ADP	O2'-C2'	2.24	1.48	1.43
3	Ad	601	ADP	O2'-C2'	2.24	1.48	1.43
3	Ar	601	ADP	O2'-C2'	2.24	1.48	1.43
3	Ay	601	ADP	O2'-C2'	2.23	1.48	1.43
3	Bm	601	ADP	O2'-C2'	2.23	1.48	1.43
3	Bt	601	ADP	O2'-C2'	2.21	1.48	1.43
3	Bm	601	ADP	C5-N7	-2.21	1.35	1.39
3	As	601	ADP	PA-O5'	2.17	1.67	1.59
3	Bn	601	ADP	PA-O5'	2.16	1.67	1.59
3	Ae	601	ADP	PA-O5'	2.16	1.67	1.59
3	Az	601	ADP	PA-O5'	2.16	1.67	1.59
3	Bu	601	ADP	PA-O5'	2.16	1.67	1.59
3	Al	601	ADP	PA-O5'	2.15	1.67	1.59
3	Bg	601	ADP	PA-O5'	2.14	1.67	1.59

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Bm	601	ADP	C5-C4-N3	-5.14	119.64	126.72
3	Ar	601	ADP	C5-C4-N3	-5.13	119.65	126.72
3	Ad	601	ADP	C5-C4-N3	-5.13	119.66	126.72
3	Ay	601	ADP	C5-C4-N3	-5.11	119.68	126.72
3	Ak	601	ADP	C5-C4-N3	-5.11	119.68	126.72
3	Bt	601	ADP	C5-C4-N3	-5.11	119.68	126.72
3	Bf	601	ADP	C5-C4-N3	-5.07	119.74	126.72
3	Bu	601	ADP	C5-C4-N3	-4.68	120.27	126.72
3	As	601	ADP	C5-C4-N3	-4.67	120.28	126.72
3	Bg	601	ADP	C5-C4-N3	-4.66	120.30	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Ae	601	ADP	C5-C4-N3	-4.66	120.30	126.72
3	Bn	601	ADP	C5-C4-N3	-4.66	120.31	126.72
3	Al	601	ADP	C5-C4-N3	-4.65	120.31	126.72
3	Az	601	ADP	C5-C4-N3	-4.65	120.32	126.72
3	Al	601	ADP	N3-C2-N1	-4.52	121.74	128.58
3	As	601	ADP	N3-C2-N1	-4.52	121.75	128.58
3	Bn	601	ADP	N3-C2-N1	-4.50	121.77	128.58
3	Bu	601	ADP	N3-C2-N1	-4.49	121.78	128.58
3	Ae	601	ADP	N3-C2-N1	-4.48	121.80	128.58
3	Bm	601	ADP	N3-C2-N1	-4.48	121.81	128.58
3	Az	601	ADP	N3-C2-N1	-4.47	121.81	128.58
3	Bg	601	ADP	N3-C2-N1	-4.47	121.81	128.58
3	Ar	601	ADP	N3-C2-N1	-4.47	121.82	128.58
3	Bf	601	ADP	N3-C2-N1	-4.46	121.82	128.58
3	Ad	601	ADP	N3-C2-N1	-4.45	121.85	128.58
3	Ak	601	ADP	N3-C2-N1	-4.44	121.85	128.58
3	Ay	601	ADP	N3-C2-N1	-4.43	121.87	128.58
3	Bt	601	ADP	N3-C2-N1	-4.43	121.88	128.58
3	Bt	601	ADP	N3-C4-N9	4.16	134.24	127.17
3	Ad	601	ADP	N3-C4-N9	4.14	134.21	127.17
3	Ay	601	ADP	N3-C4-N9	4.14	134.21	127.17
3	Ar	601	ADP	N3-C4-N9	4.14	134.20	127.17
3	Bm	601	ADP	N3-C4-N9	4.13	134.19	127.17
3	Ak	601	ADP	N3-C4-N9	4.13	134.19	127.17
3	Bf	601	ADP	N3-C4-N9	4.10	134.15	127.17
3	Az	601	ADP	N9-C8-N7	-3.64	108.78	113.94
3	Bu	601	ADP	N3-C4-N9	3.62	133.33	127.17
3	Bf	601	ADP	N9-C8-N7	-3.62	108.80	113.94
3	Ar	601	ADP	N9-C8-N7	-3.60	108.83	113.94
3	Ae	601	ADP	N3-C4-N9	3.60	133.28	127.17
3	Ak	601	ADP	N9-C8-N7	-3.60	108.83	113.94
3	Az	601	ADP	N3-C4-N9	3.59	133.28	127.17
3	Ad	601	ADP	N9-C8-N7	-3.59	108.85	113.94
3	As	601	ADP	N3-C4-N9	3.59	133.27	127.17
3	Ae	601	ADP	N9-C8-N7	-3.58	108.85	113.94
3	Bn	601	ADP	N9-C8-N7	-3.58	108.85	113.94
3	Bt	601	ADP	N9-C8-N7	-3.58	108.85	113.94
3	Ay	601	ADP	N9-C8-N7	-3.58	108.85	113.94
3	Bg	601	ADP	N3-C4-N9	3.58	133.26	127.17
3	Bn	601	ADP	N3-C4-N9	3.58	133.26	127.17
3	Al	601	ADP	N3-C4-N9	3.58	133.25	127.17
3	Al	601	ADP	N9-C8-N7	-3.57	108.87	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Bu	601	ADP	N9-C8-N7	-3.57	108.87	113.94
3	As	601	ADP	N9-C8-N7	-3.57	108.87	113.94
3	Bg	601	ADP	N9-C8-N7	-3.55	108.89	113.94
3	Bm	601	ADP	N9-C8-N7	-3.55	108.90	113.94
3	Bt	601	ADP	C4-N9-C8	3.51	109.43	105.74
3	Bf	601	ADP	C4-N9-C8	3.51	109.42	105.74
3	Ad	601	ADP	C4-N9-C8	3.50	109.41	105.74
3	Ak	601	ADP	C4-N9-C8	3.49	109.41	105.74
3	Ar	601	ADP	C4-N9-C8	3.49	109.40	105.74
3	Ay	601	ADP	C4-N9-C8	3.48	109.39	105.74
3	Az	601	ADP	C4-N9-C8	3.48	109.39	105.74
3	Bm	601	ADP	C4-N9-C8	3.46	109.37	105.74
3	Bu	601	ADP	C4-N9-C8	3.44	109.35	105.74
3	Ae	601	ADP	C4-N9-C8	3.43	109.34	105.74
3	Ar	601	ADP	C2-N3-C4	3.42	120.18	111.83
3	Bm	601	ADP	C2-N3-C4	3.42	120.17	111.83
3	Bn	601	ADP	C4-N9-C8	3.41	109.32	105.74
3	Ad	601	ADP	C2-N3-C4	3.41	120.16	111.83
3	As	601	ADP	C4-N9-C8	3.41	109.32	105.74
3	Bg	601	ADP	C4-N9-C8	3.41	109.32	105.74
3	Ay	601	ADP	C2-N3-C4	3.41	120.15	111.83
3	Bt	601	ADP	C2-N3-C4	3.40	120.14	111.83
3	Ak	601	ADP	C2-N3-C4	3.40	120.14	111.83
3	Al	601	ADP	C4-N9-C8	3.39	109.30	105.74
3	Bf	601	ADP	C2-N3-C4	3.39	120.11	111.83
3	Bu	601	ADP	C2-N3-C4	3.23	119.71	111.83
3	As	601	ADP	C2-N3-C4	3.22	119.70	111.83
3	Bn	601	ADP	C2-N3-C4	3.22	119.69	111.83
3	Al	601	ADP	C2-N3-C4	3.22	119.69	111.83
3	Ae	601	ADP	C2-N3-C4	3.21	119.67	111.83
3	Az	601	ADP	C2-N3-C4	3.20	119.65	111.83
3	Bg	601	ADP	C2-N3-C4	3.19	119.63	111.83
3	Az	601	ADP	C5-N7-C8	3.04	108.23	103.45
3	Ar	601	ADP	C5-N7-C8	3.02	108.20	103.45
3	Al	601	ADP	C5-N7-C8	3.02	108.20	103.45
3	Bf	601	ADP	C5-N7-C8	3.02	108.19	103.45
3	Bn	601	ADP	C5-N7-C8	3.02	108.19	103.45
3	Ae	601	ADP	C5-N7-C8	3.01	108.18	103.45
3	Ay	601	ADP	C5-N7-C8	3.01	108.18	103.45
3	Bt	601	ADP	C5-N7-C8	3.01	108.17	103.45
3	Ad	601	ADP	C5-N7-C8	3.00	108.17	103.45
3	Bu	601	ADP	C5-N7-C8	3.00	108.16	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	As	601	ADP	C5-N7-C8	2.99	108.15	103.45
3	Ak	601	ADP	C5-N7-C8	2.99	108.15	103.45
3	Bg	601	ADP	C5-N7-C8	2.98	108.13	103.45
3	Bm	601	ADP	C5-N7-C8	2.98	108.13	103.45
3	Az	601	ADP	C4-C5-N7	-2.96	107.20	110.58
3	Al	601	ADP	C4-C5-N7	-2.96	107.20	110.58
3	Bn	601	ADP	C4-C5-N7	-2.96	107.20	110.58
3	As	601	ADP	C4-C5-N7	-2.95	107.21	110.58
3	Ae	601	ADP	C4-C5-N7	-2.95	107.21	110.58
3	Bu	601	ADP	C4-C5-N7	-2.94	107.22	110.58
3	Bg	601	ADP	C4-C5-N7	-2.94	107.22	110.58
3	Ar	601	ADP	C4-C5-N7	-2.76	107.42	110.58
3	Bm	601	ADP	C4-C5-N7	-2.75	107.43	110.58
3	Ad	601	ADP	C4-C5-N7	-2.75	107.44	110.58
3	Ay	601	ADP	C4-C5-N7	-2.73	107.46	110.58
3	Bf	601	ADP	C4-C5-N7	-2.73	107.46	110.58
3	Bt	601	ADP	C4-C5-N7	-2.73	107.46	110.58
3	Ak	601	ADP	C4-C5-N7	-2.71	107.48	110.58
3	Al	601	ADP	C5'-C4'-C3'	-2.07	107.75	115.21
3	Bg	601	ADP	C5'-C4'-C3'	-2.07	107.76	115.21
3	Bn	601	ADP	C5'-C4'-C3'	-2.07	107.76	115.21
3	Bu	601	ADP	C5'-C4'-C3'	-2.07	107.76	115.21
3	Ae	601	ADP	C5'-C4'-C3'	-2.07	107.78	115.21
3	Az	601	ADP	C5'-C4'-C3'	-2.06	107.80	115.21
3	As	601	ADP	C5'-C4'-C3'	-2.06	107.80	115.21
3	Bu	601	ADP	C2-N1-C6	2.01	122.03	118.73
3	As	601	ADP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Ae	601	ADP	C5'-O5'-PA-O1A
3	Ae	601	ADP	C5'-O5'-PA-O2A
3	Ae	601	ADP	C5'-O5'-PA-O3A
3	Al	601	ADP	C5'-O5'-PA-O1A
3	Al	601	ADP	C5'-O5'-PA-O2A
3	Al	601	ADP	C5'-O5'-PA-O3A
3	As	601	ADP	C5'-O5'-PA-O1A
3	As	601	ADP	C5'-O5'-PA-O2A
3	As	601	ADP	C5'-O5'-PA-O3A
3	Az	601	ADP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	Az	601	ADP	C5'-O5'-PA-O2A
3	Az	601	ADP	C5'-O5'-PA-O3A
3	Bg	601	ADP	C5'-O5'-PA-O1A
3	Bg	601	ADP	C5'-O5'-PA-O2A
3	Bg	601	ADP	C5'-O5'-PA-O3A
3	Bn	601	ADP	C5'-O5'-PA-O1A
3	Bn	601	ADP	C5'-O5'-PA-O2A
3	Bn	601	ADP	C5'-O5'-PA-O3A
3	Bu	601	ADP	C5'-O5'-PA-O1A
3	Bu	601	ADP	C5'-O5'-PA-O2A
3	Bu	601	ADP	C5'-O5'-PA-O3A
3	Ae	601	ADP	C3'-C4'-C5'-O5'
3	Al	601	ADP	C3'-C4'-C5'-O5'
3	As	601	ADP	C3'-C4'-C5'-O5'
3	Az	601	ADP	C3'-C4'-C5'-O5'
3	Bg	601	ADP	C3'-C4'-C5'-O5'
3	Bn	601	ADP	C3'-C4'-C5'-O5'
3	Bu	601	ADP	C3'-C4'-C5'-O5'
3	Ae	601	ADP	O4'-C4'-C5'-O5'
3	Al	601	ADP	O4'-C4'-C5'-O5'
3	As	601	ADP	O4'-C4'-C5'-O5'
3	Az	601	ADP	O4'-C4'-C5'-O5'
3	Bg	601	ADP	O4'-C4'-C5'-O5'
3	Bn	601	ADP	O4'-C4'-C5'-O5'
3	Bu	601	ADP	O4'-C4'-C5'-O5'
3	Ad	601	ADP	C3'-C4'-C5'-O5'
3	Ak	601	ADP	C3'-C4'-C5'-O5'
3	Ar	601	ADP	C3'-C4'-C5'-O5'
3	Ay	601	ADP	C3'-C4'-C5'-O5'
3	Bf	601	ADP	C3'-C4'-C5'-O5'
3	Bm	601	ADP	C3'-C4'-C5'-O5'
3	Bt	601	ADP	C3'-C4'-C5'-O5'
3	Ae	601	ADP	PB-O3A-PA-O5'
3	Al	601	ADP	PB-O3A-PA-O5'
3	As	601	ADP	PB-O3A-PA-O5'
3	Az	601	ADP	PB-O3A-PA-O5'
3	Bg	601	ADP	PB-O3A-PA-O5'
3	Bn	601	ADP	PB-O3A-PA-O5'
3	Bu	601	ADP	PB-O3A-PA-O5'
3	Ad	601	ADP	PB-O3A-PA-O2A
3	Ak	601	ADP	PB-O3A-PA-O2A
3	Ar	601	ADP	PB-O3A-PA-O2A

Continued on next page...

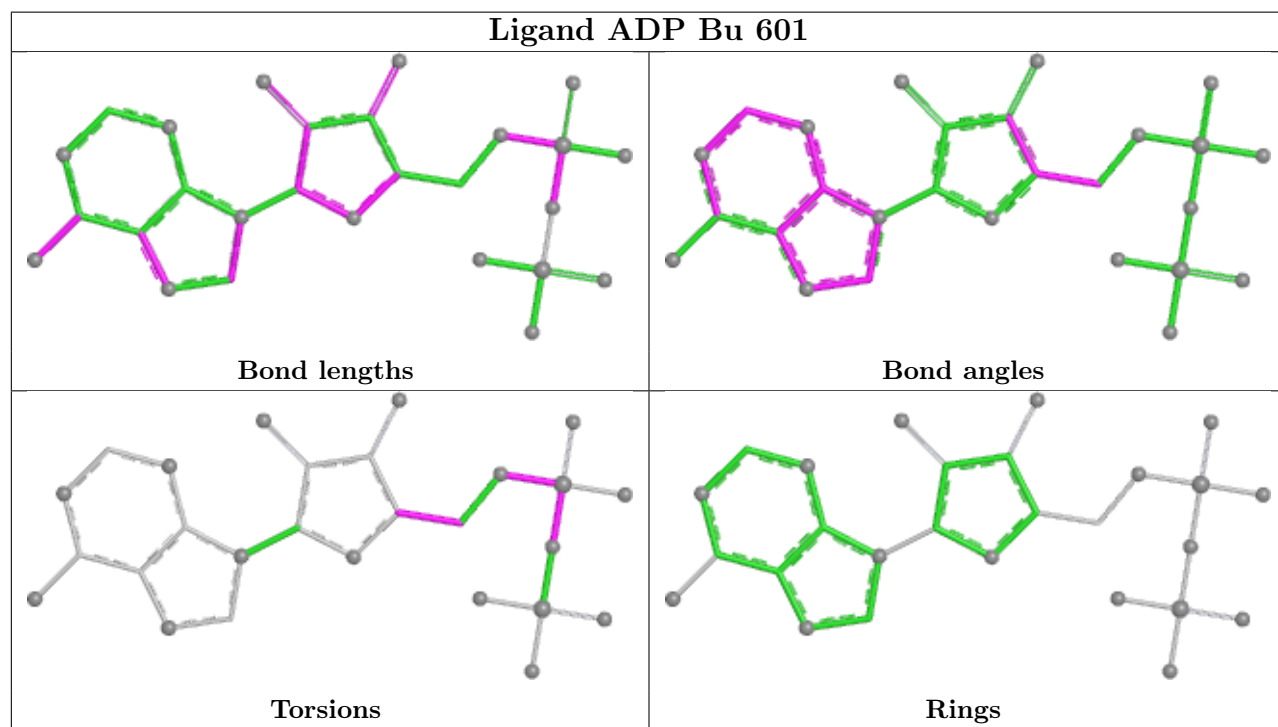
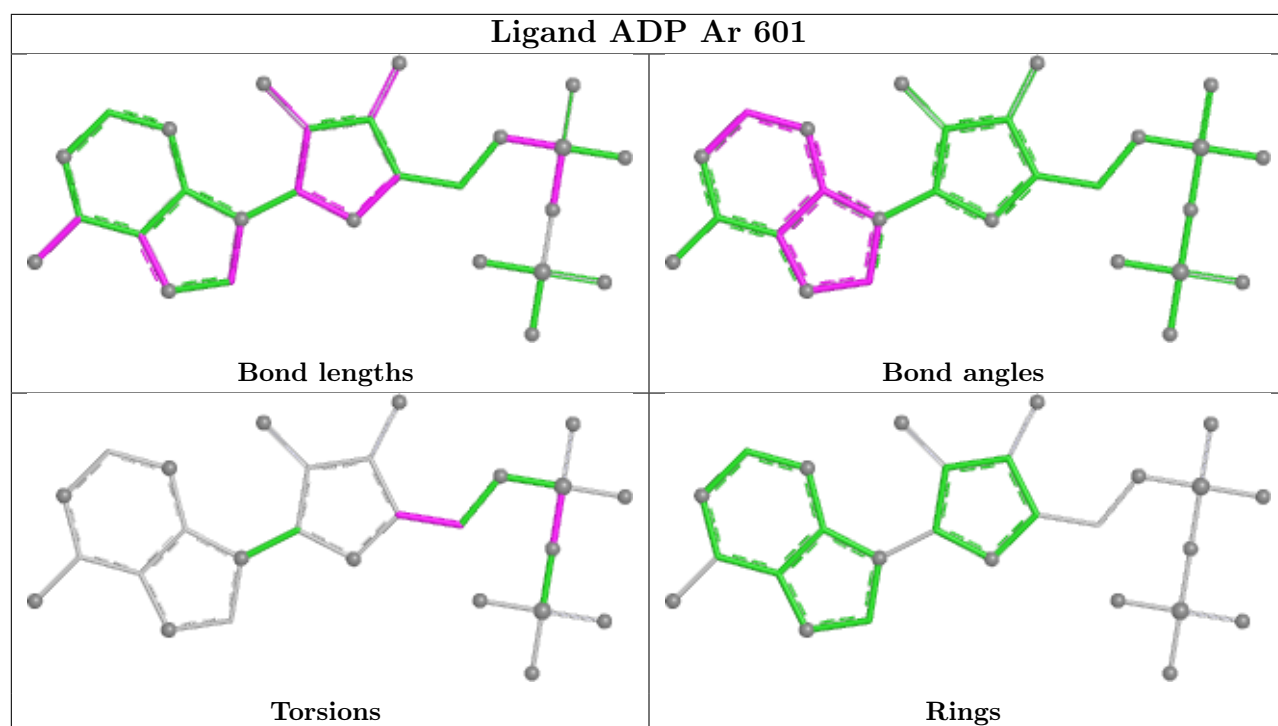
Continued from previous page...

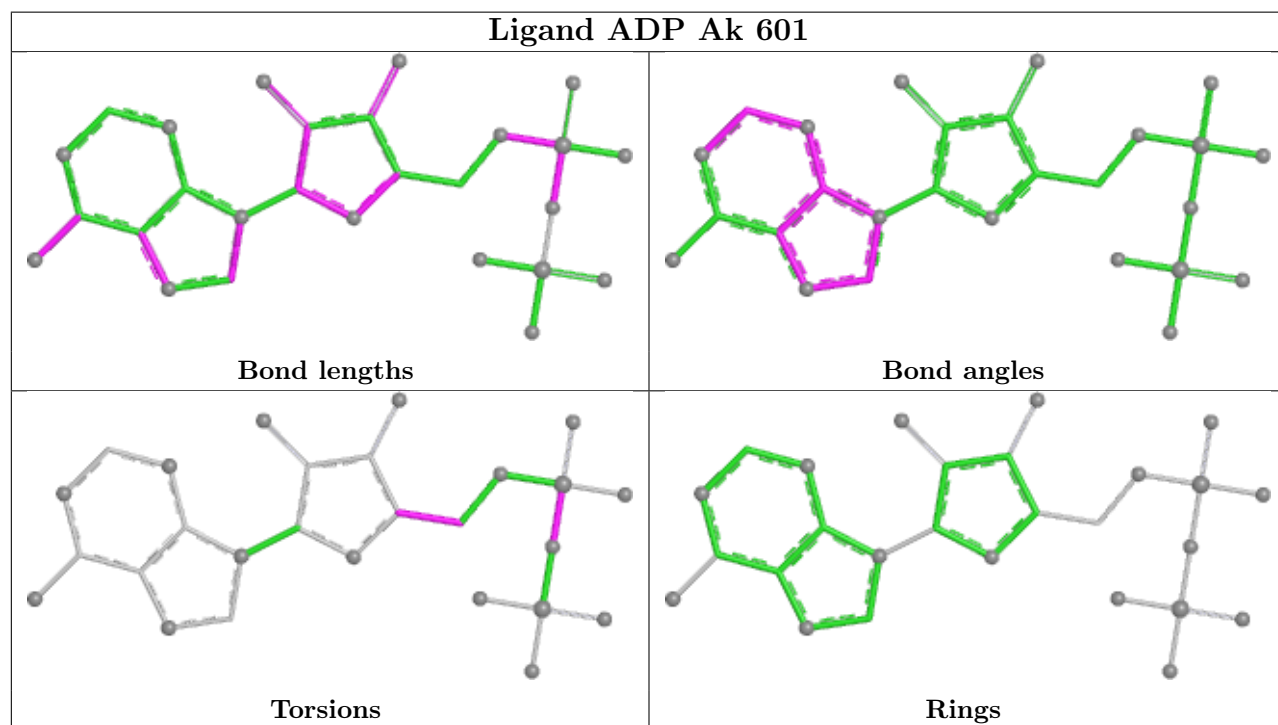
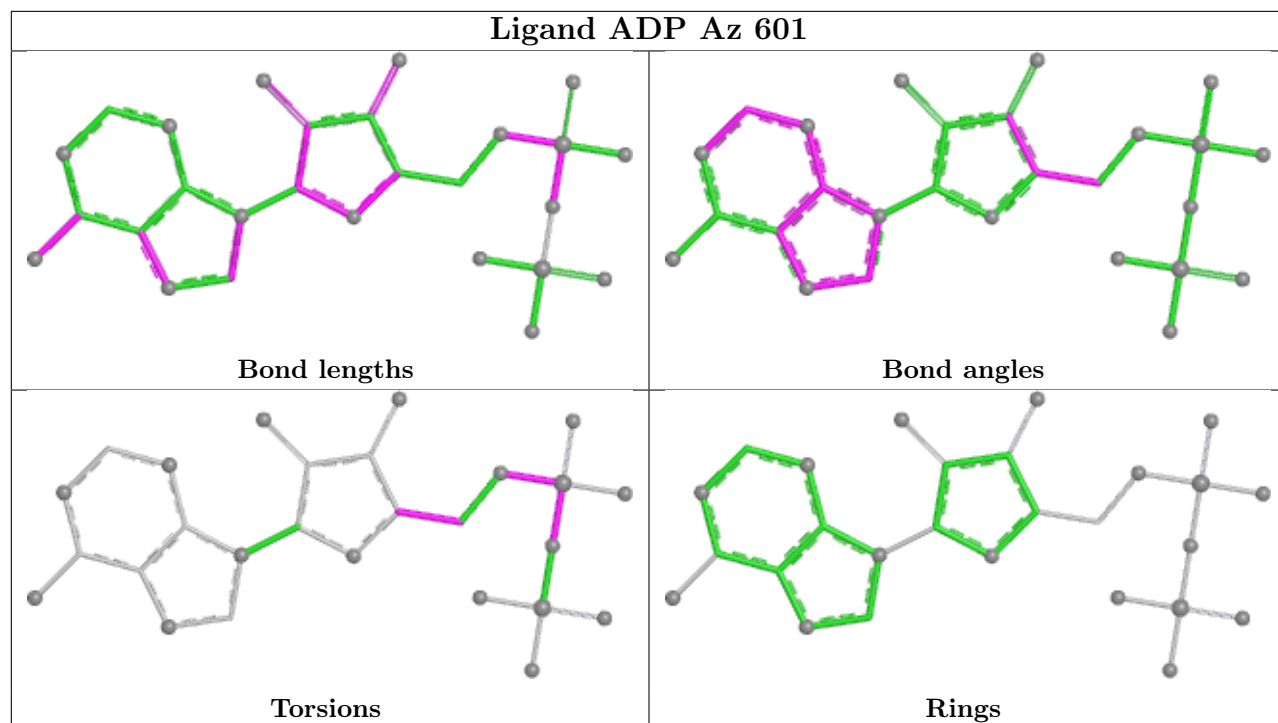
Mol	Chain	Res	Type	Atoms
3	Ay	601	ADP	PB-O3A-PA-O2A
3	Bf	601	ADP	PB-O3A-PA-O2A
3	Bm	601	ADP	PB-O3A-PA-O2A
3	Bt	601	ADP	PB-O3A-PA-O2A
3	Bm	601	ADP	O4'-C4'-C5'-O5'
3	Ad	601	ADP	O4'-C4'-C5'-O5'
3	Ak	601	ADP	O4'-C4'-C5'-O5'
3	Ar	601	ADP	O4'-C4'-C5'-O5'
3	Ay	601	ADP	O4'-C4'-C5'-O5'
3	Bf	601	ADP	O4'-C4'-C5'-O5'
3	Bt	601	ADP	O4'-C4'-C5'-O5'

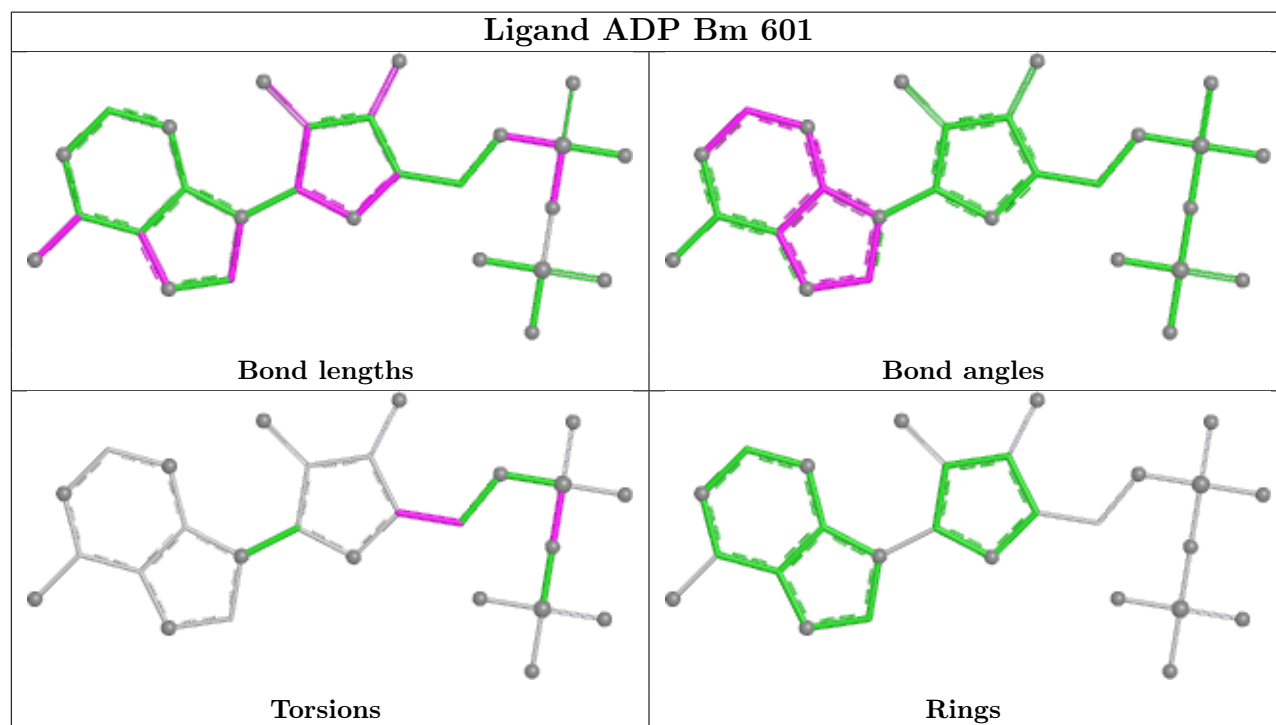
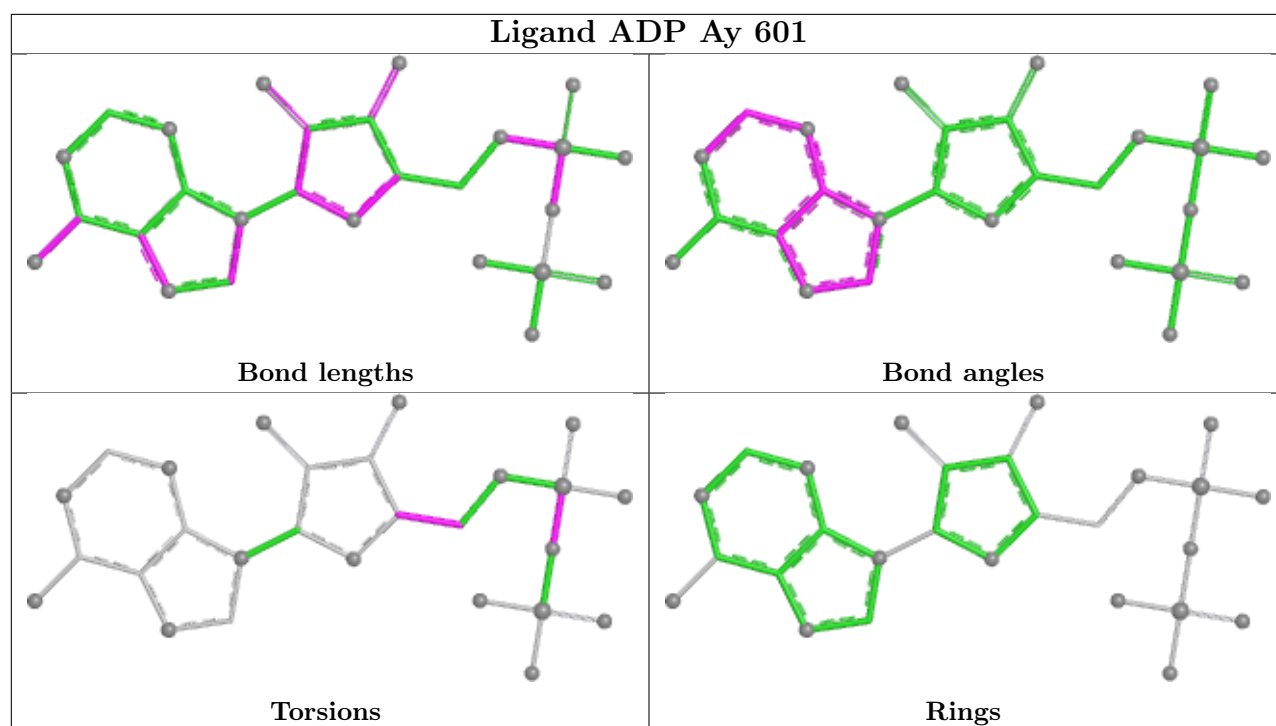
There are no ring outliers.

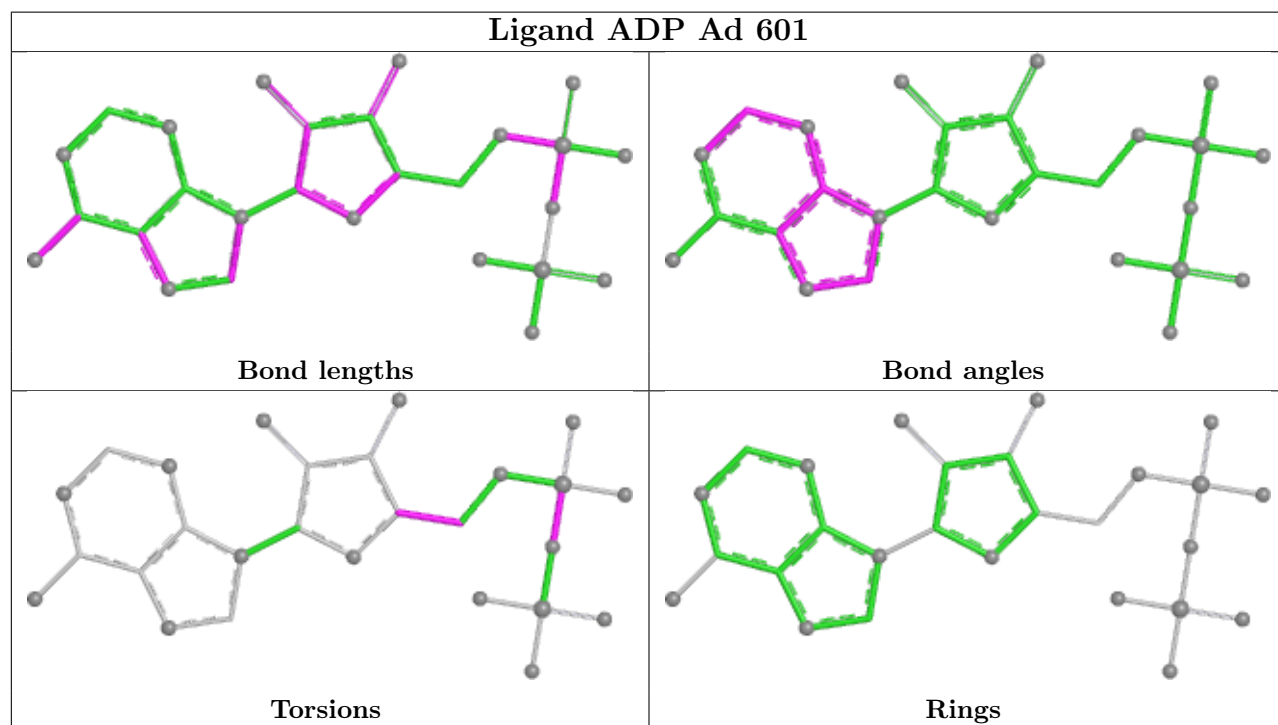
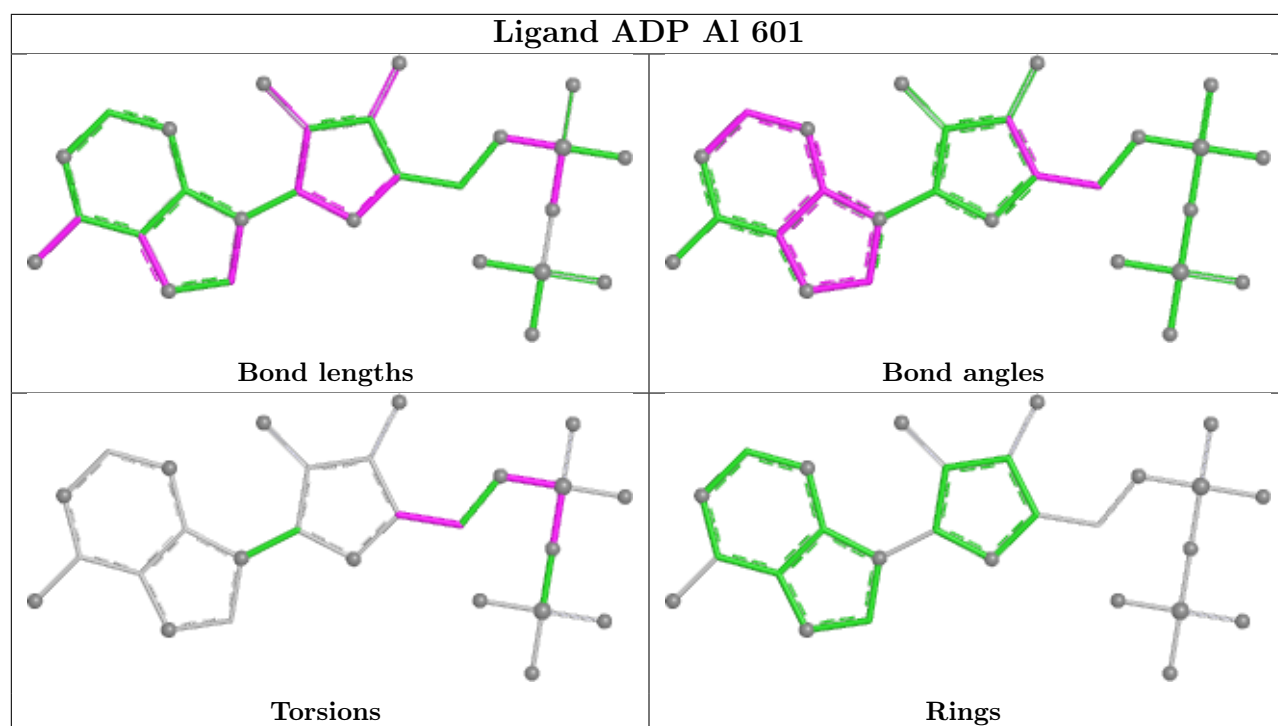
No monomer is involved in short contacts.

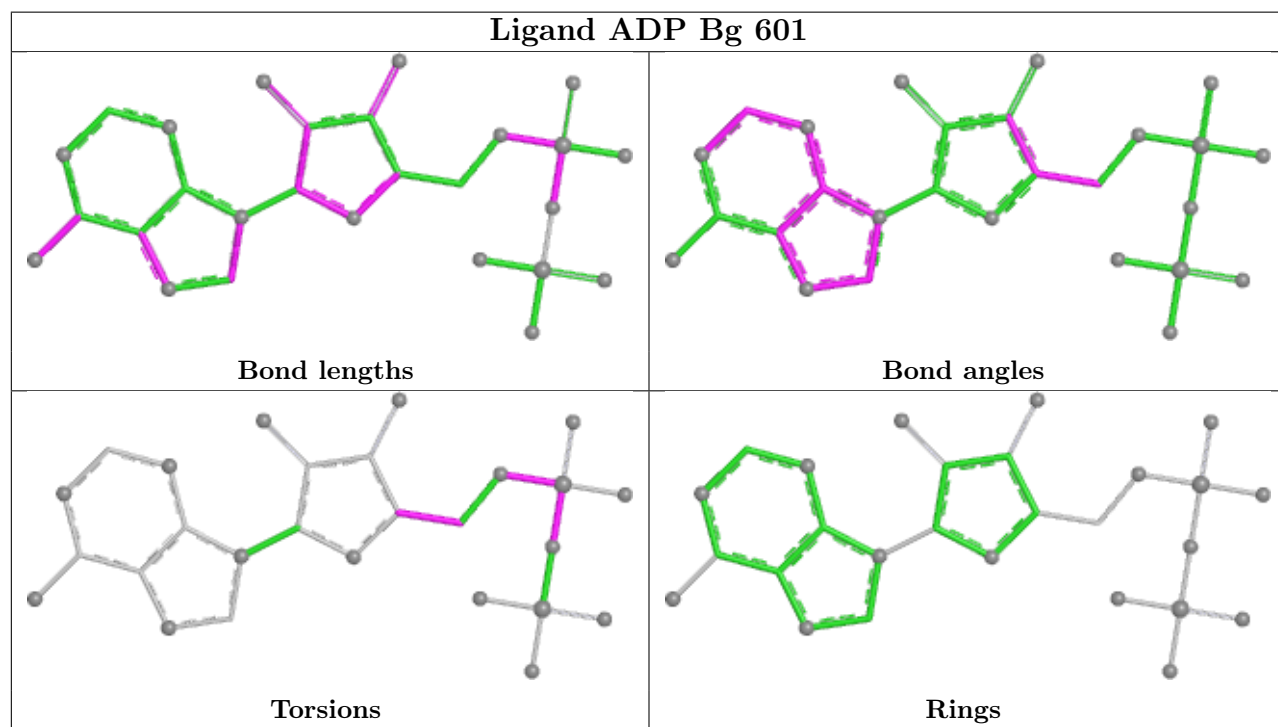
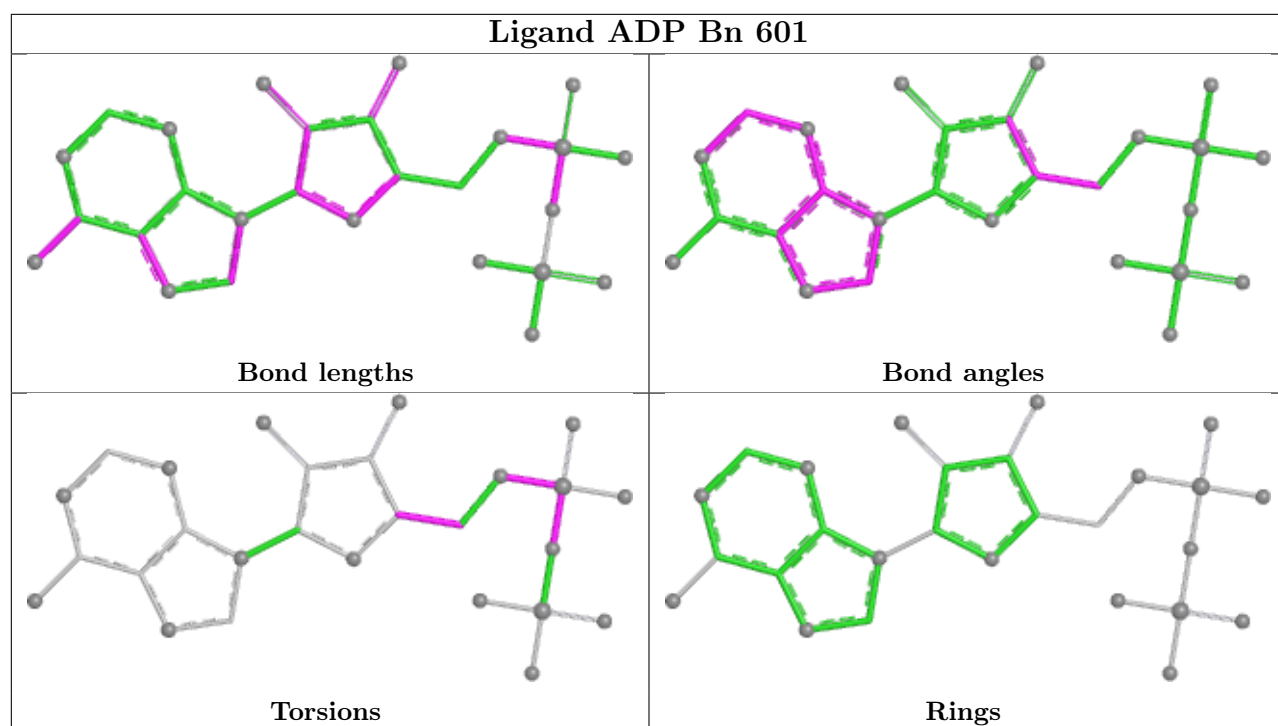
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

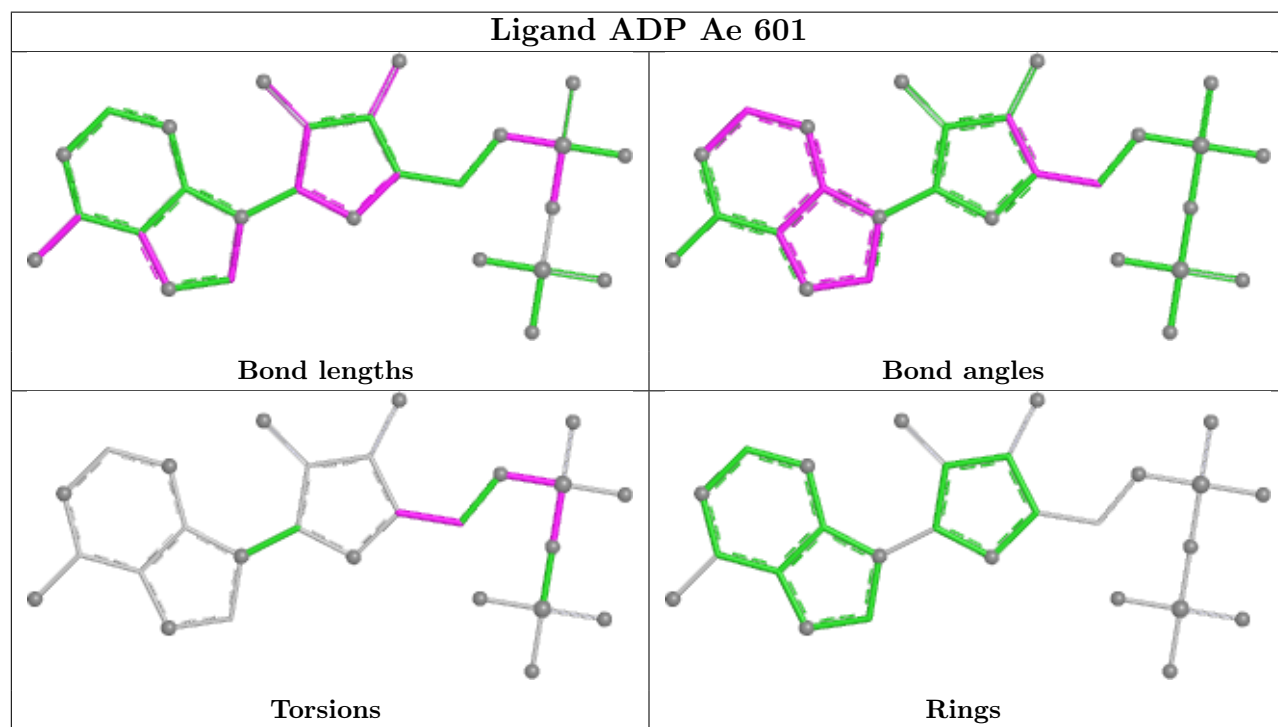
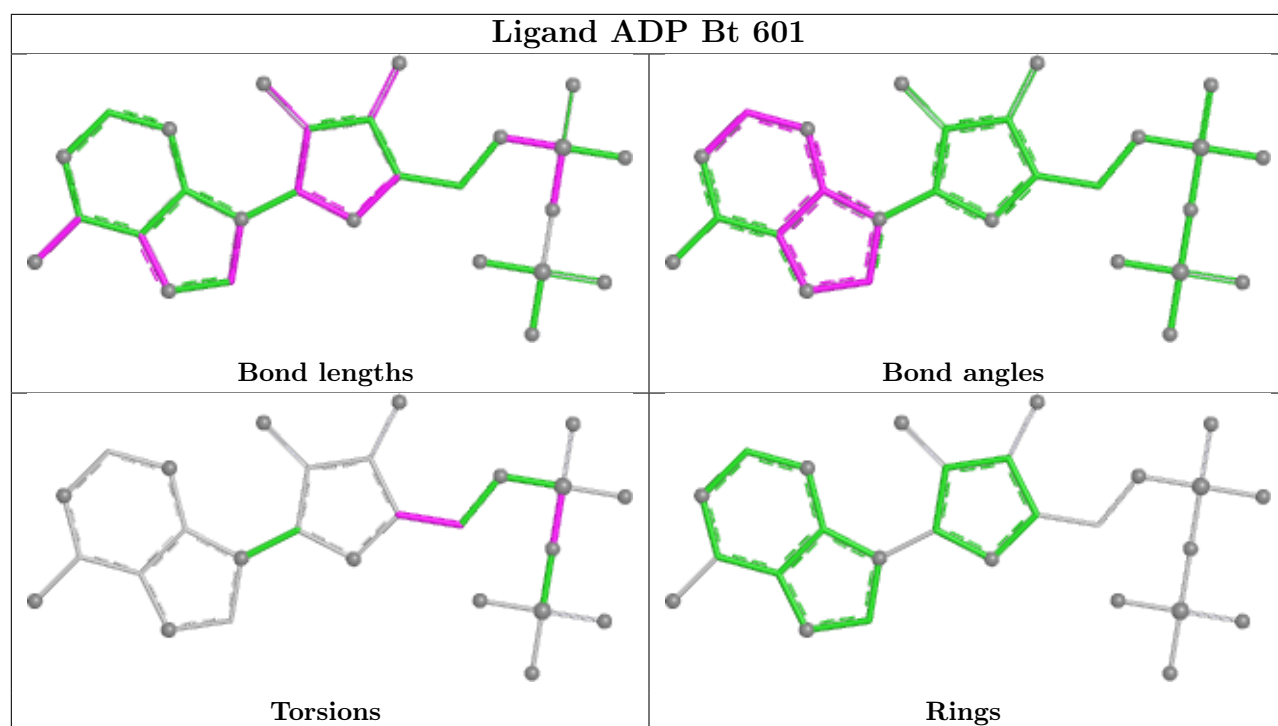


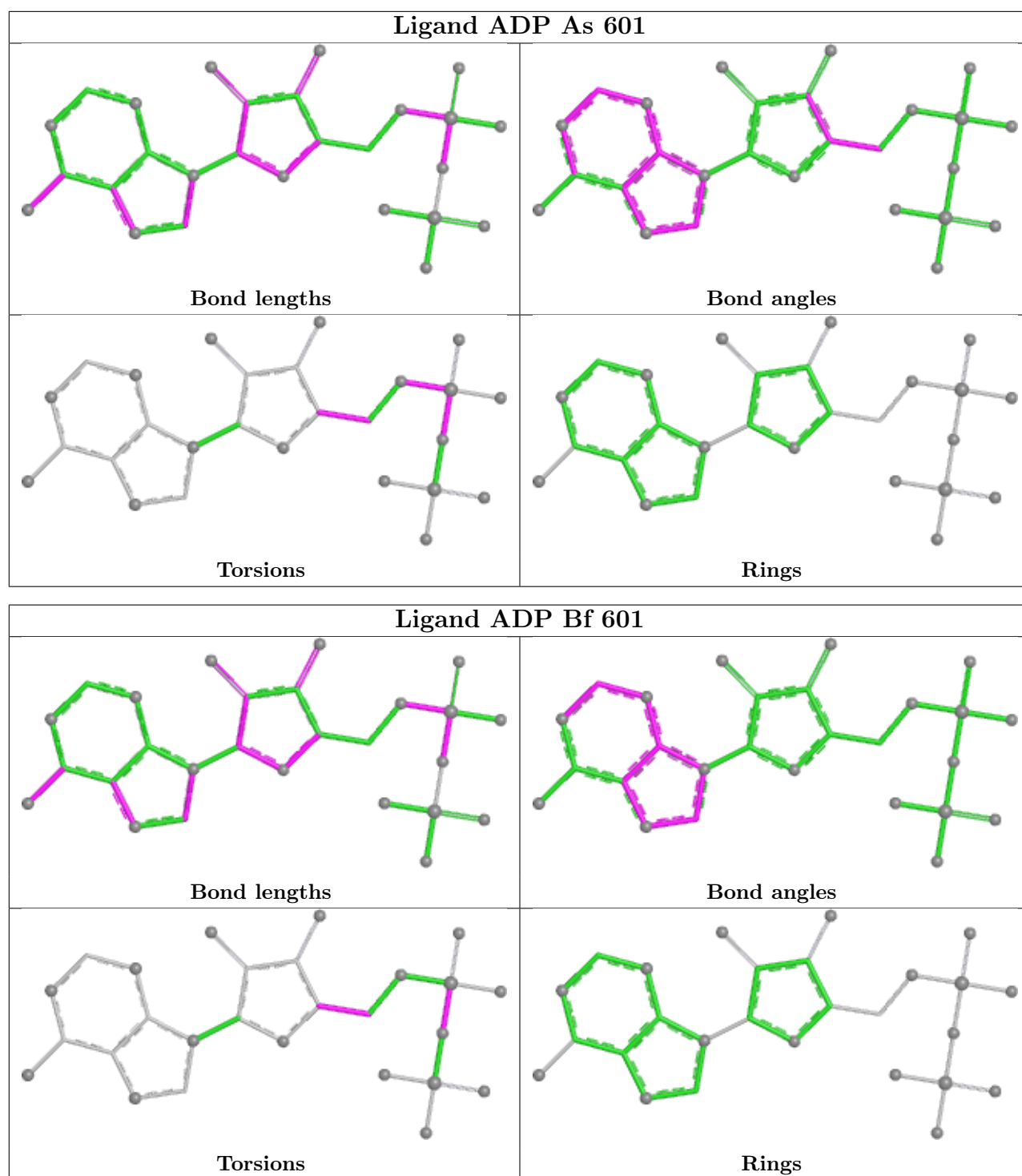












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13293. These allow visual inspection of the internal detail of the map and identification of artifacts.

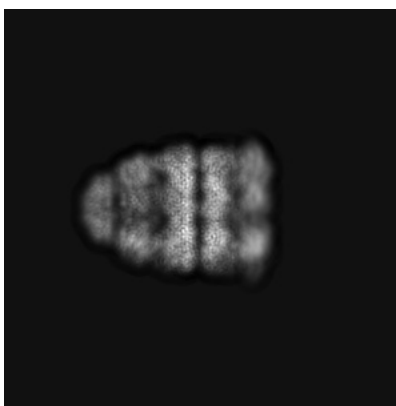
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

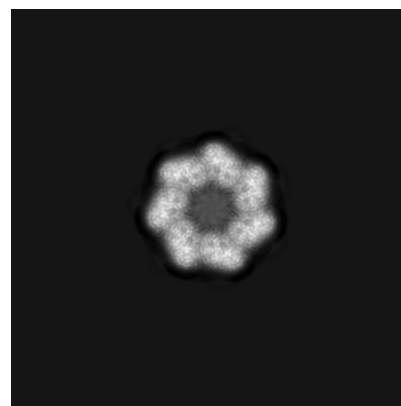
6.1.1 Primary map



X



Y

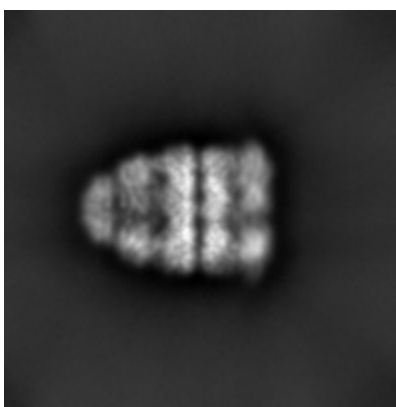


Z

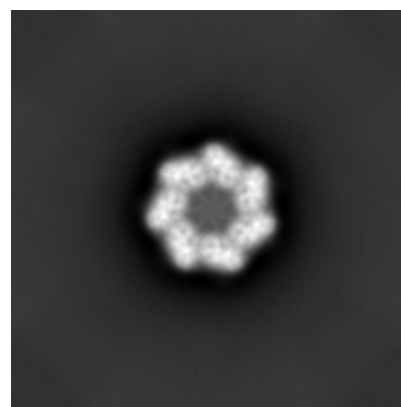
6.1.2 Raw map



X



Y

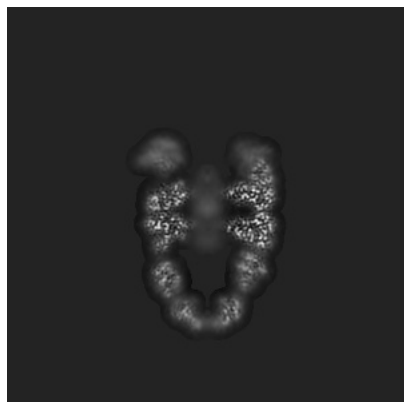


Z

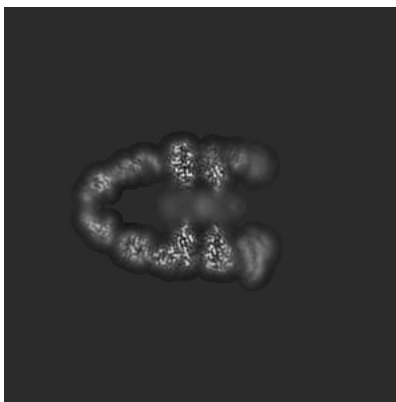
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

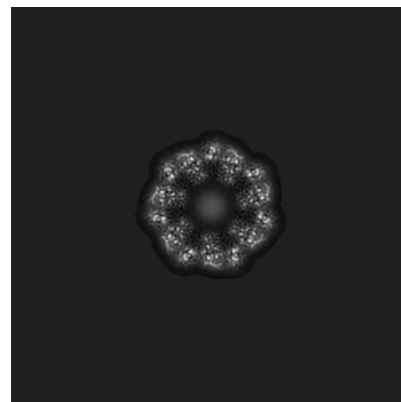
6.2.1 Primary map



X Index: 192

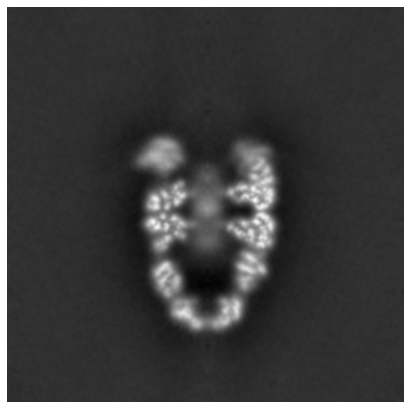


Y Index: 192

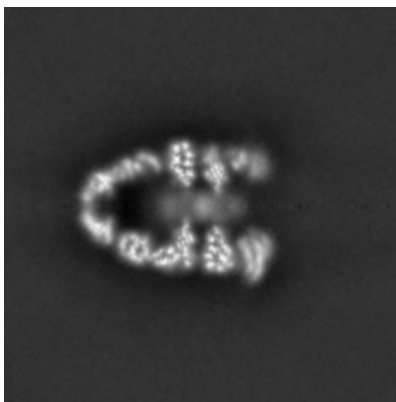


Z Index: 192

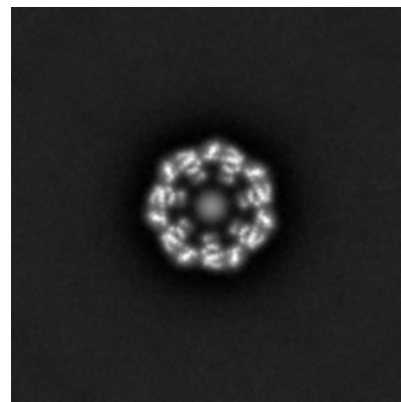
6.2.2 Raw map



X Index: 192



Y Index: 192

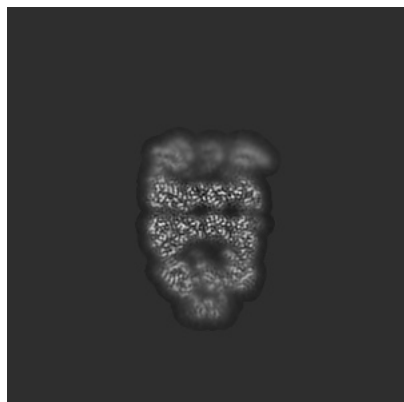


Z Index: 192

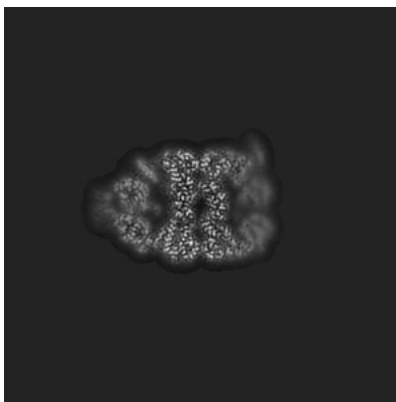
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

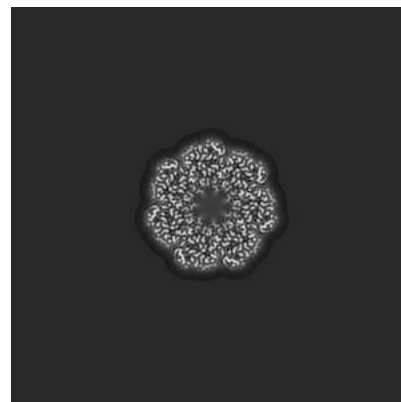
6.3.1 Primary map



X Index: 162

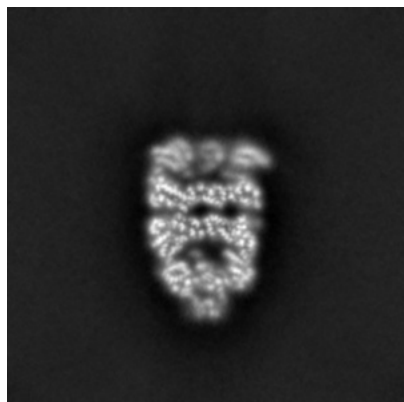


Y Index: 225

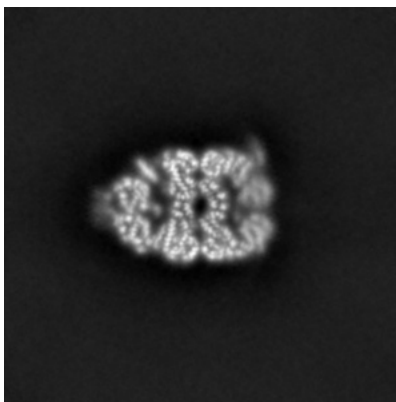


Z Index: 175

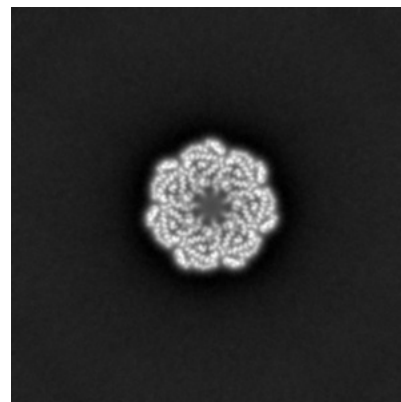
6.3.2 Raw map



X Index: 161



Y Index: 226

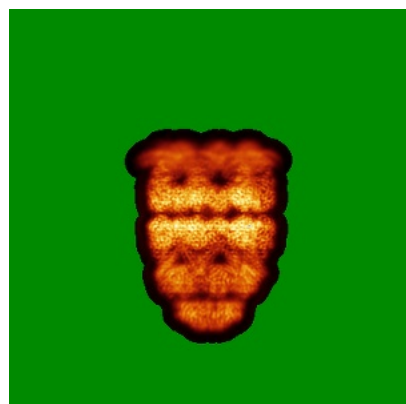


Z Index: 175

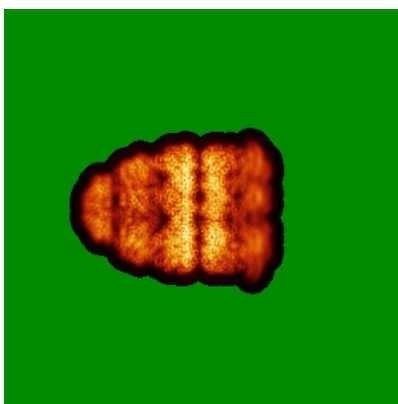
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

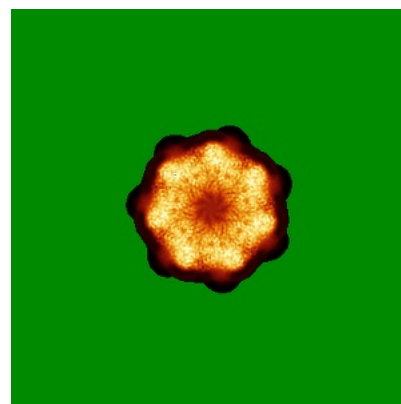
6.4.1 Primary map



X

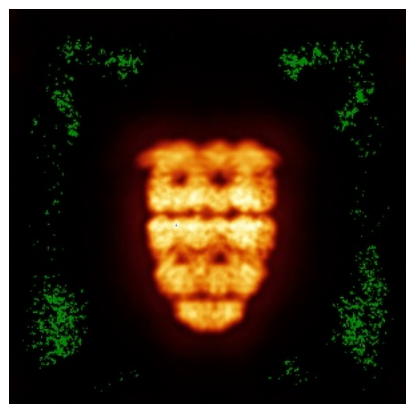


Y

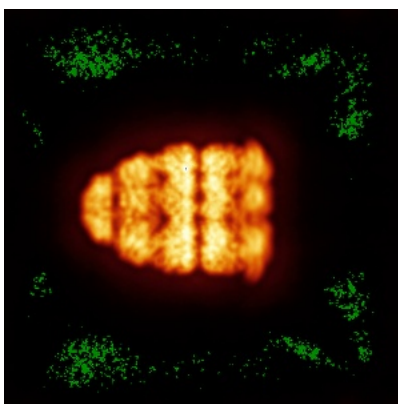


Z

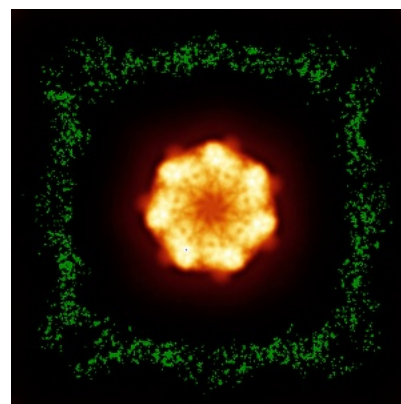
6.4.2 Raw map



X



Y

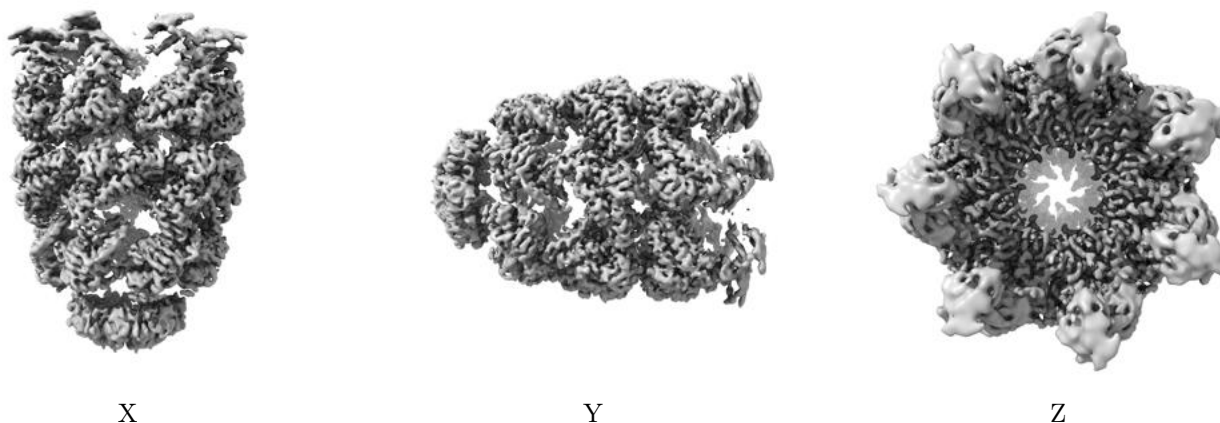


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

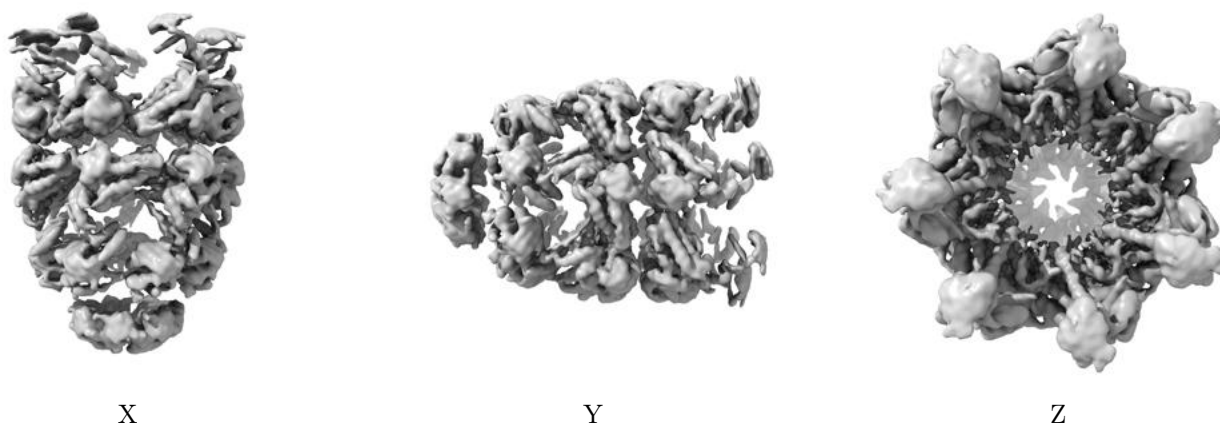
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

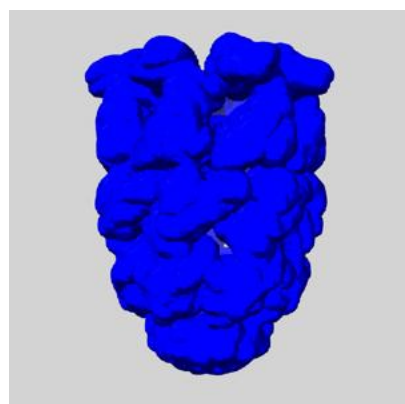
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

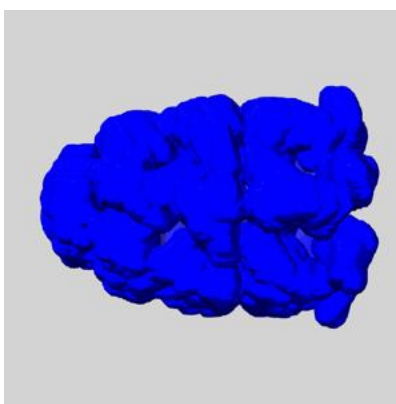
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

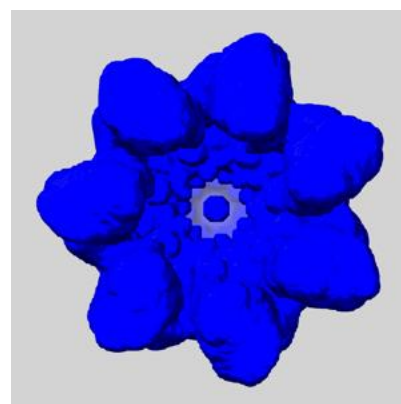
6.6.1 emd_13293_msk_1.map [i](#)



X



Y

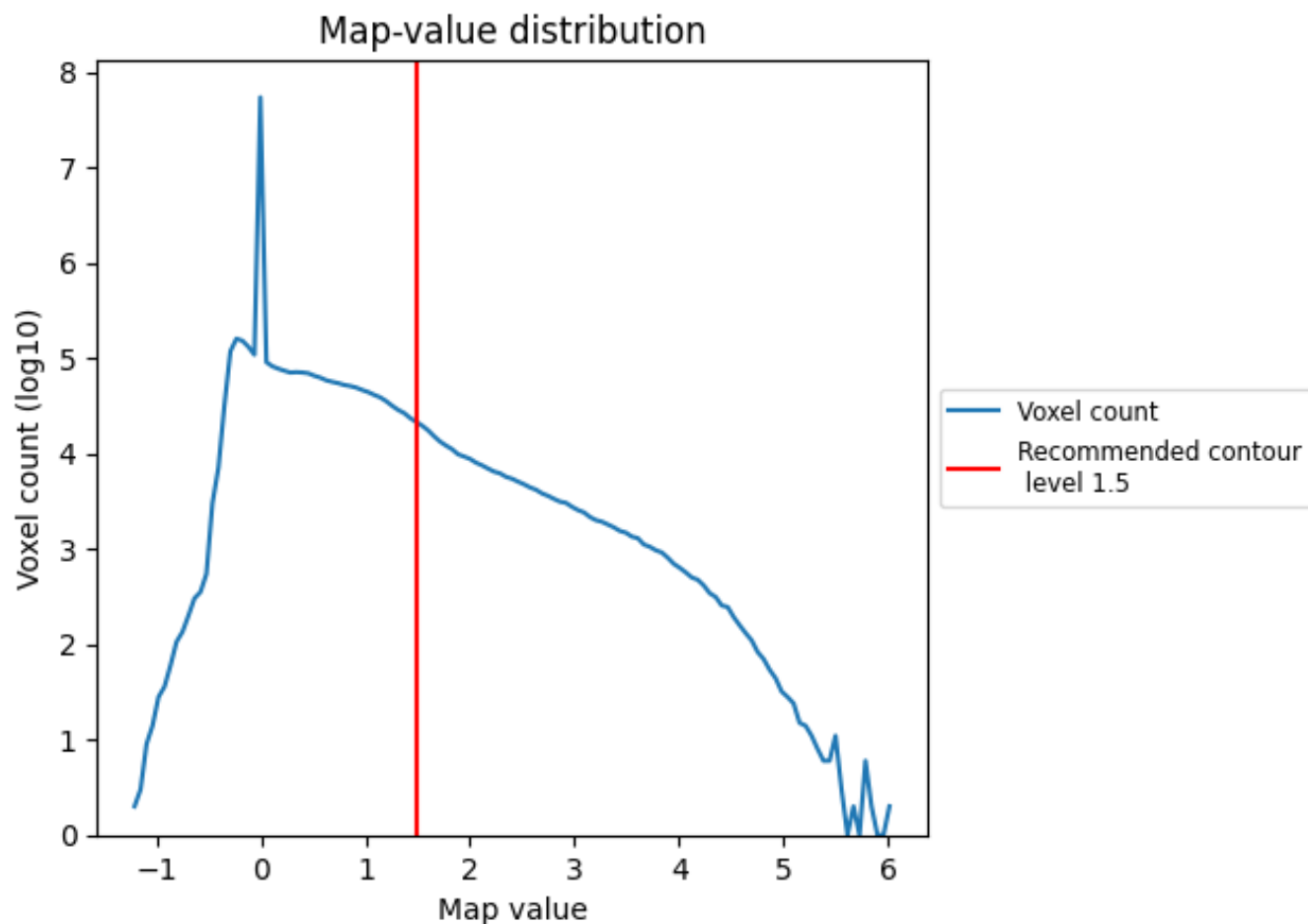


Z

7 Map analysis [i](#)

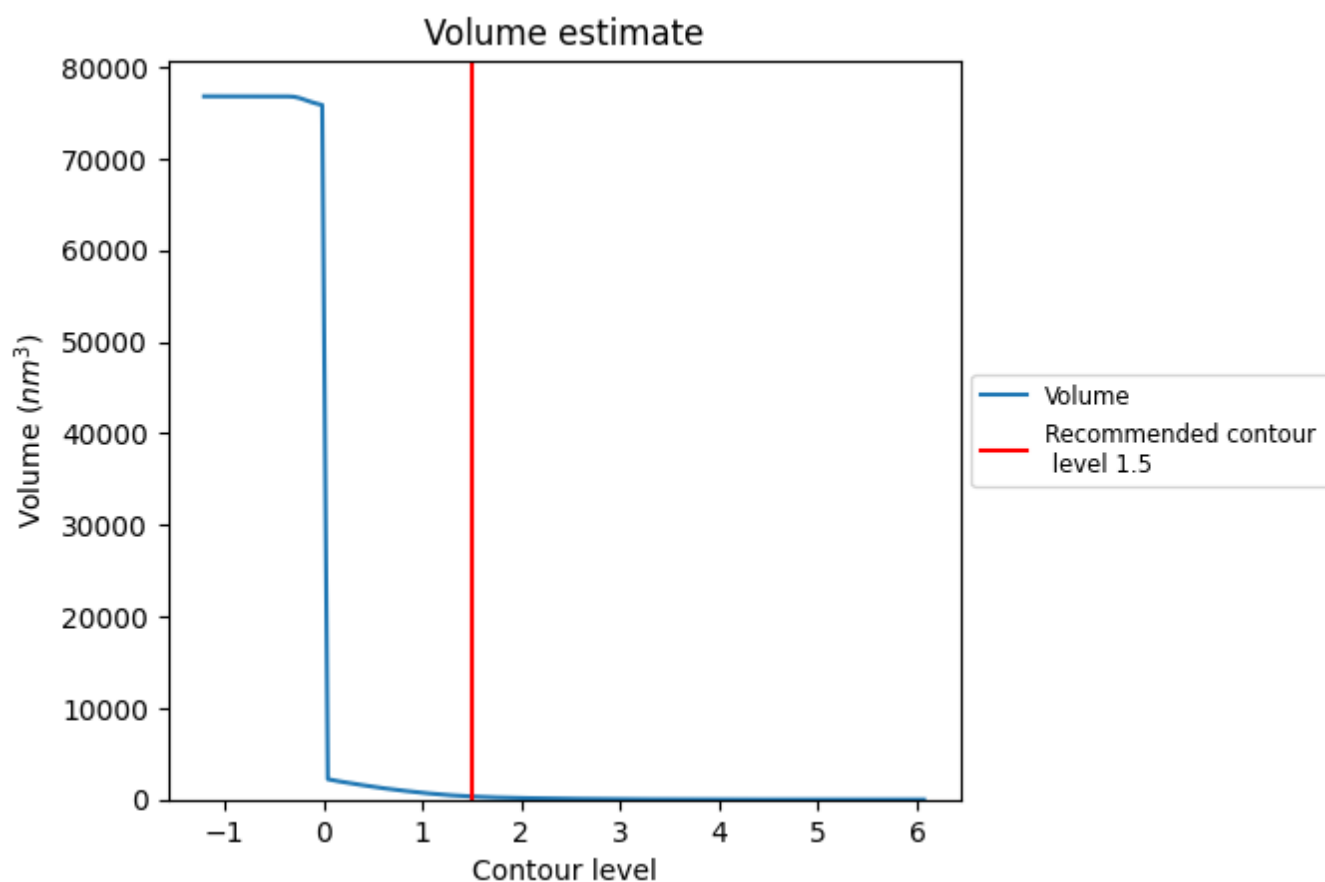
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

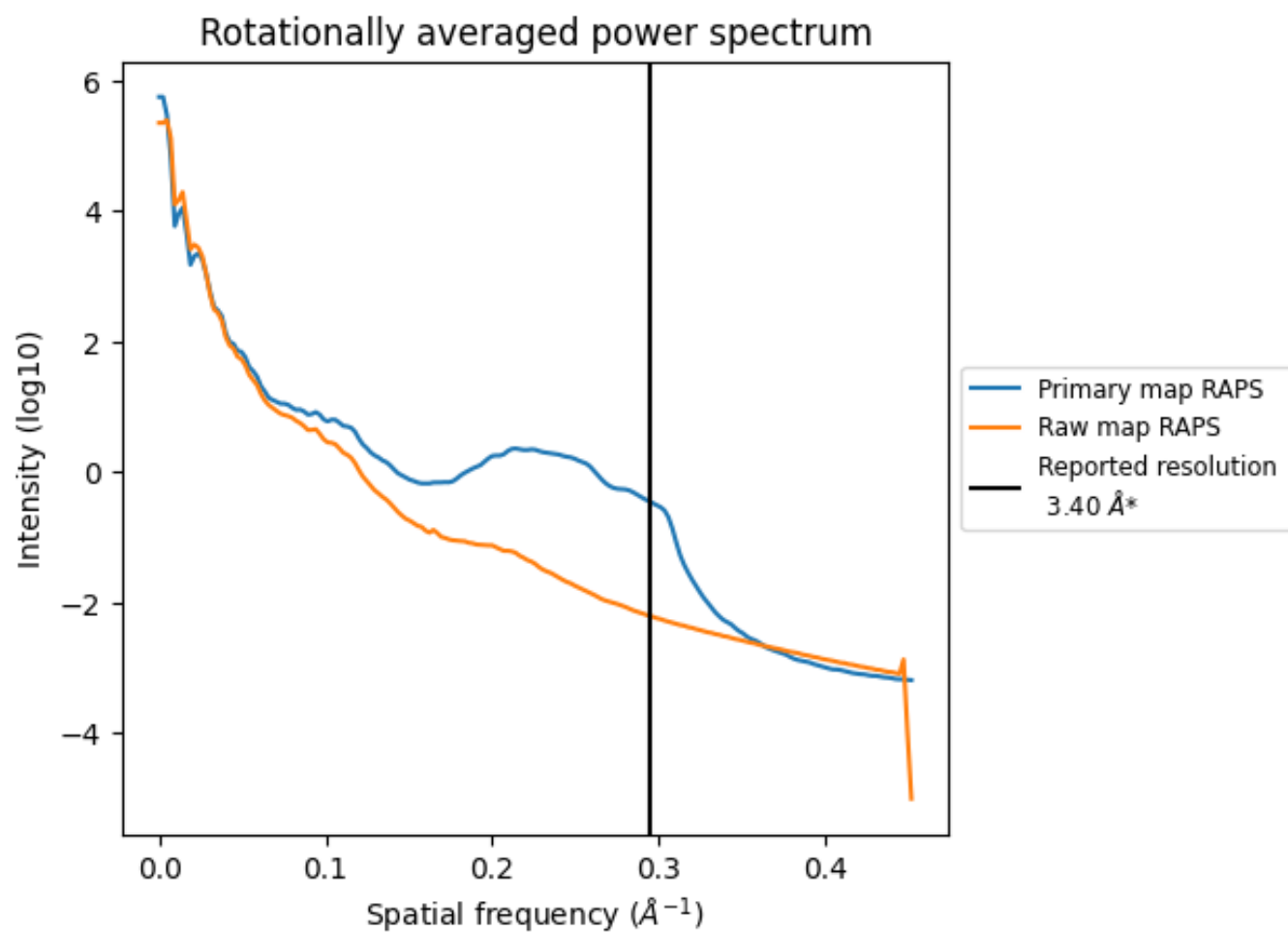
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 336 nm³; this corresponds to an approximate mass of 303 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

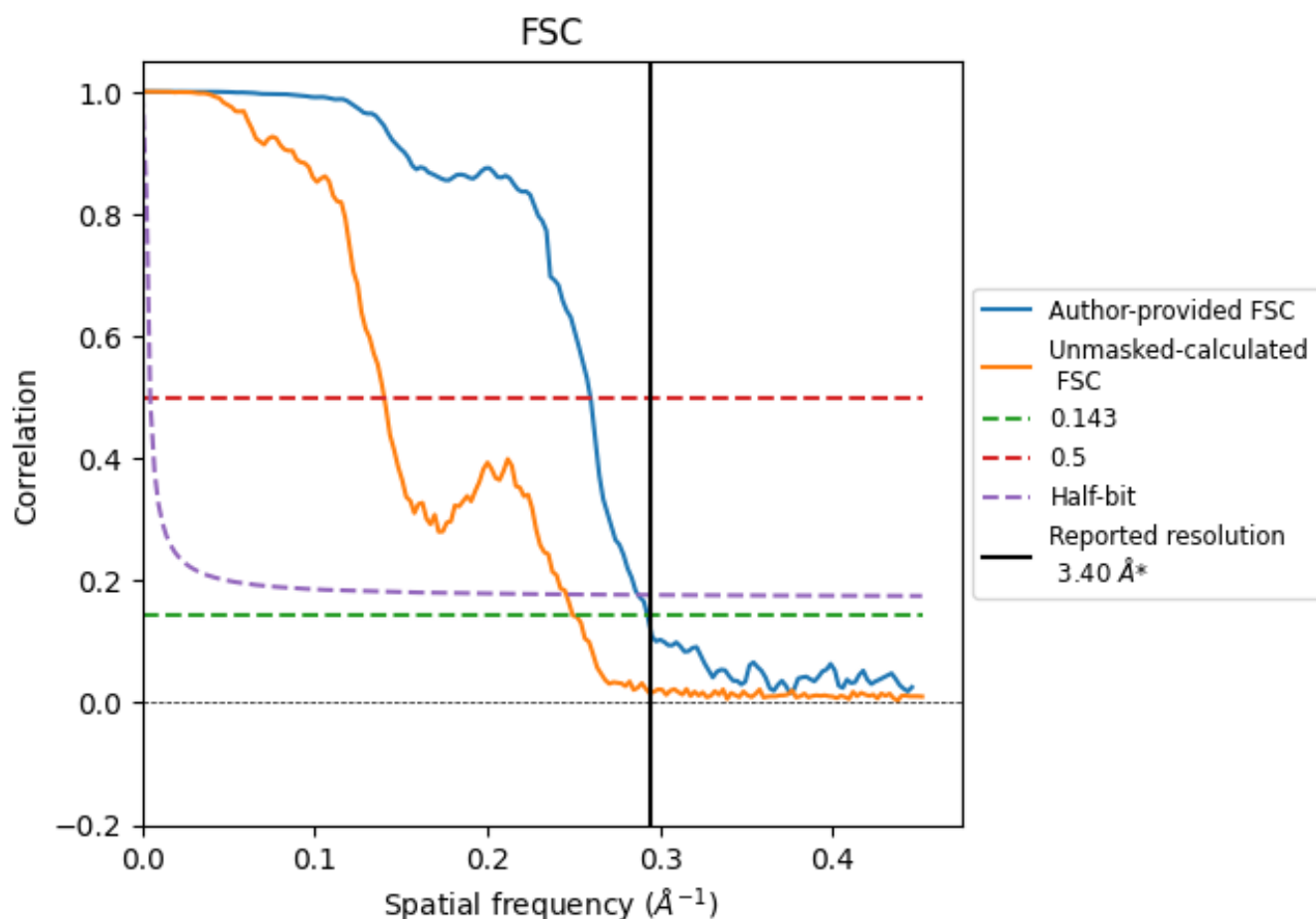


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

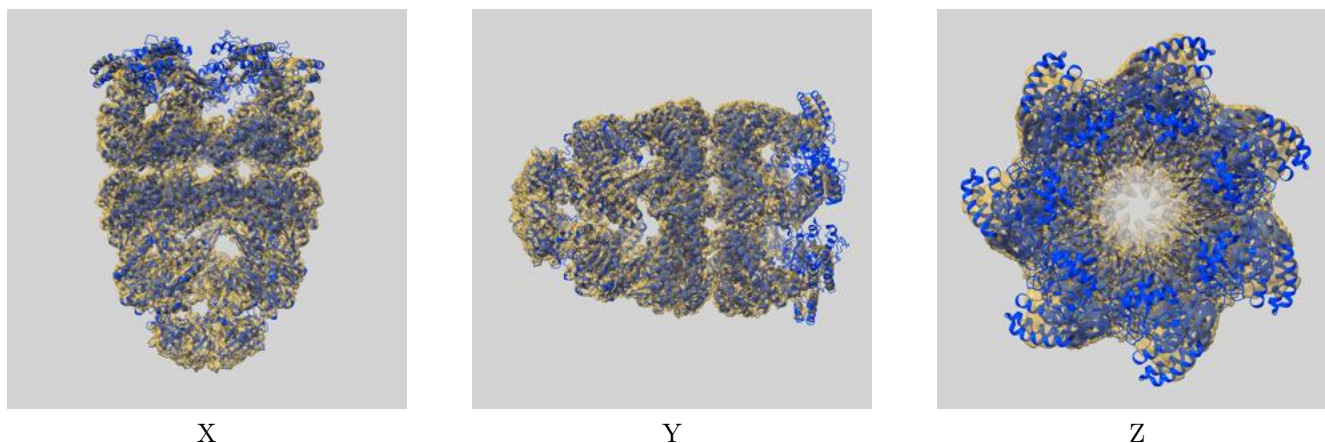
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.85	3.48
Unmasked-calculated*	4.01	7.14	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

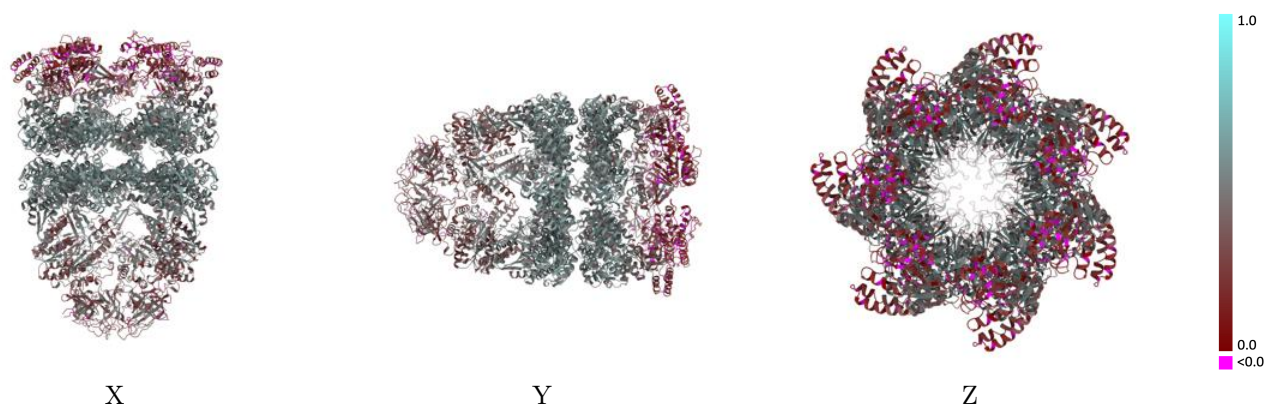
This section contains information regarding the fit between EMDB map EMD-13293 and PDB model 7PBJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



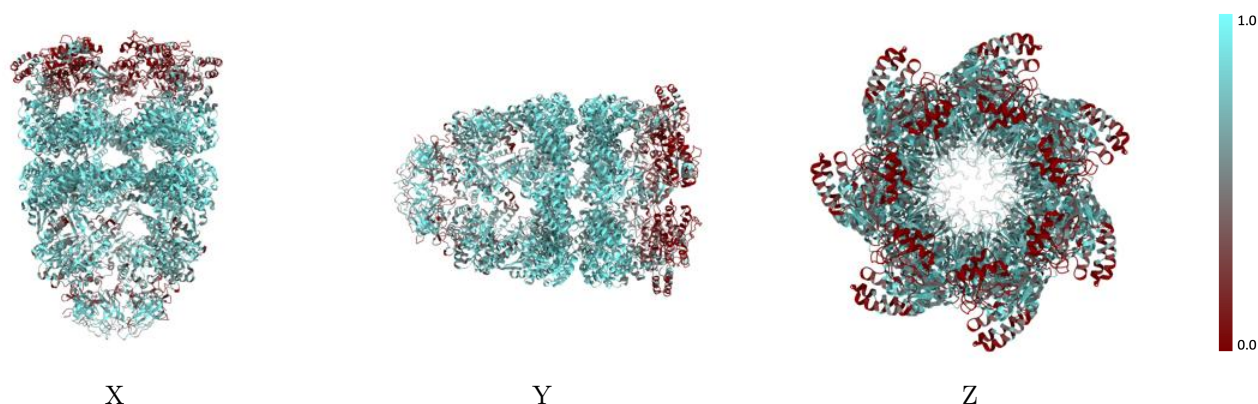
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



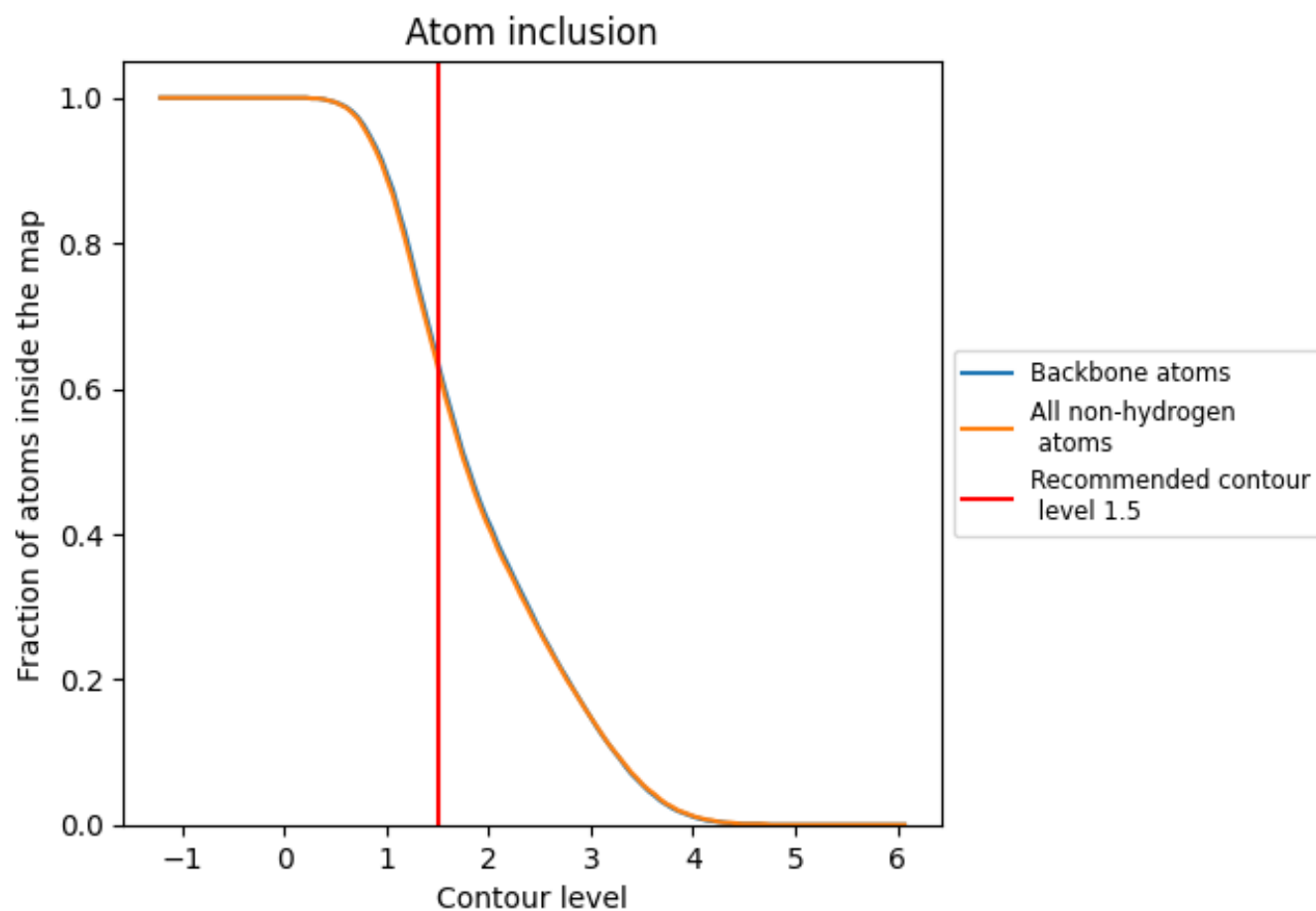
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6320	 0.4050
Ad	 0.5420	 0.3630
Ae	 0.7500	 0.4650
Af	 0.5440	 0.3120
Ak	 0.5390	 0.3620
Al	 0.7520	 0.4650
Am	 0.5540	 0.3100
Ar	 0.5410	 0.3630
As	 0.7520	 0.4640
At	 0.5520	 0.3100
Ay	 0.5400	 0.3610
Az	 0.7540	 0.4640
Ba	 0.5480	 0.3130
Bf	 0.5410	 0.3620
Bg	 0.7540	 0.4660
Bh	 0.5580	 0.3130
Bm	 0.5420	 0.3630
Bn	 0.7570	 0.4640
Bo	 0.5520	 0.3130
Bt	 0.5420	 0.3630
Bu	 0.7520	 0.4660
Bv	 0.5520	 0.3130

