



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:06 AM UTC

PDB ID : 5A0Q / pdb_00005a0q
EMDB ID : EMD-2981
Title : Cryo-EM reveals the conformation of a substrate analogue in the human 20S proteasome core
Authors : daFonseca, P.C.A.; Morris, E.P.
Deposited on : 2015-04-22
Resolution : 3.50 Å(reported)
Based on initial model : 3UNE

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

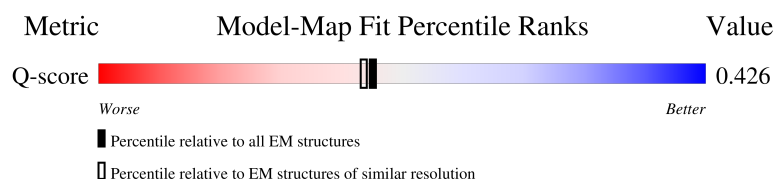
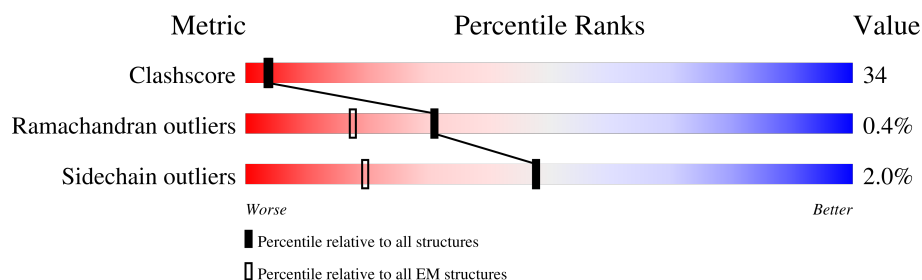
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



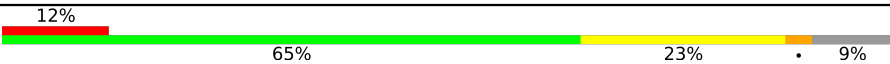
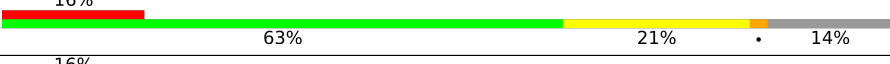
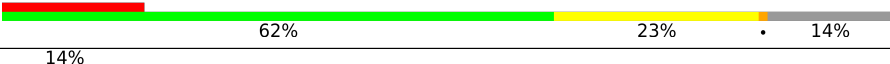
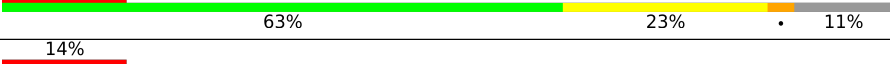
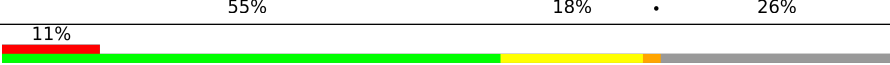
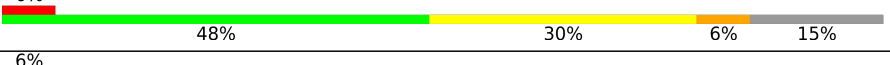
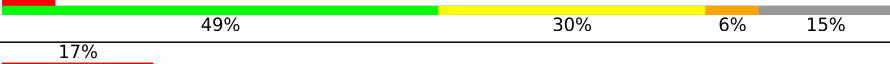
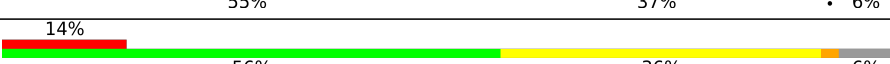
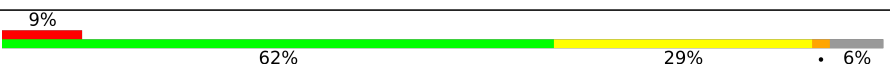
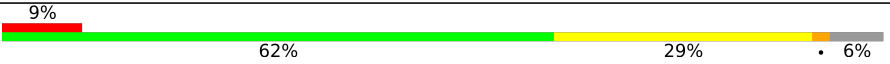
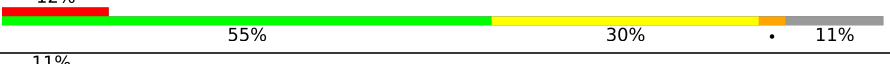
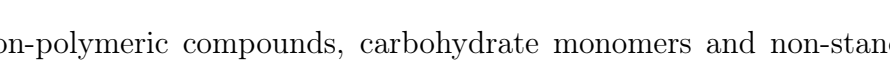
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	A	246	11% 63% 15% 21%
1	O	246	11% 63% 15% 21%
2	B	234	12% 59% 26% 6% 9%
2	P	234	12% 59% 26% 6% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	261	
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	204	
10	X	204	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	213	
13	a	213	
14	N	219	
14	b	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	KNM	H	300	-	-	X	-
15	KNM	I	300	-	-	X	-
15	KNM	L	300	-	-	X	-
15	KNM	V	300	-	-	X	-
15	KNM	W	300	-	-	X	-
15	KNM	Z	300	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 43448 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 PROTEASOME SUBUNIT ALPHA TYPE-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	195	Total	C	N	O	S	0	0
			1514	963	254	284	13		
1	O	195	Total	C	N	O	S	0	0
			1514	963	254	284	13		

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1671	1072	285	309	5		
2	P	214	Total	C	N	O	S	0	0
			1671	1072	285	309	5		

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1860	1175	321	354	10		
3	Q	237	Total	C	N	O	S	0	0
			1860	1175	321	354	10		

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	214	Total	C	N	O	S	0	0
			1674	1056	300	313	5		
4	R	214	Total	C	N	O	S	0	0
			1674	1056	300	313	5		

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1643	1036	272	325	10		
5	S	215	Total	C	N	O	S	0	0
			1643	1036	272	325	10		

- Molecule 6 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	195	Total	C	N	O	S	0	0
			1535	969	278	278	10		
6	T	195	Total	C	N	O	S	0	0
			1535	969	278	278	10		

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	209	Total	C	N	O	S	0	0
			1626	1032	279	304	11		
7	U	209	Total	C	N	O	S	0	0
			1626	1032	279	304	11		

- Molecule 8 is a protein called PROTEASOME SUBUNIT BETA TYPE-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	183	Total	C	N	O	S	0	0
			1372	858	236	266	12		
8	V	183	Total	C	N	O	S	0	0
			1372	858	236	266	12		

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	198	Total	C	N	O	S	0	0
			1490	939	251	288	12		
9	W	198	Total	C	N	O	S	0	0
			1490	939	251	288	12		

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1374	882	227	251	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	176	Total	C	N	O	S	0	0
			1374	882	227	251	14		

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	189	Total	C	N	O	S	0	0
			1512	970	259	275	8		
11	Y	189	Total	C	N	O	S	0	0
			1512	970	259	275	8		

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	192	Total	C	N	O	S	0	0
			1480	933	258	280	9		
12	Z	192	Total	C	N	O	S	0	0
			1480	933	258	280	9		

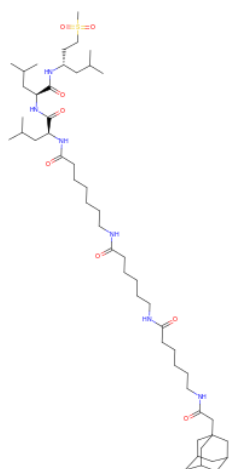
- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	190	Total	C	N	O	S	0	0
			1453	919	250	275	9		
13	a	190	Total	C	N	O	S	0	0
			1453	919	250	275	9		

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	184	Total	C	N	O	S	0	0
			1428	905	245	267	11		
14	b	184	Total	C	N	O	S	0	0
			1428	905	245	267	11		

- Molecule 15 is ADA-(AHX)3-(LEU)3-VINYLSULFONE (CCD ID: KNM) (formula: C₅₁H₉₂N₆O₈S).

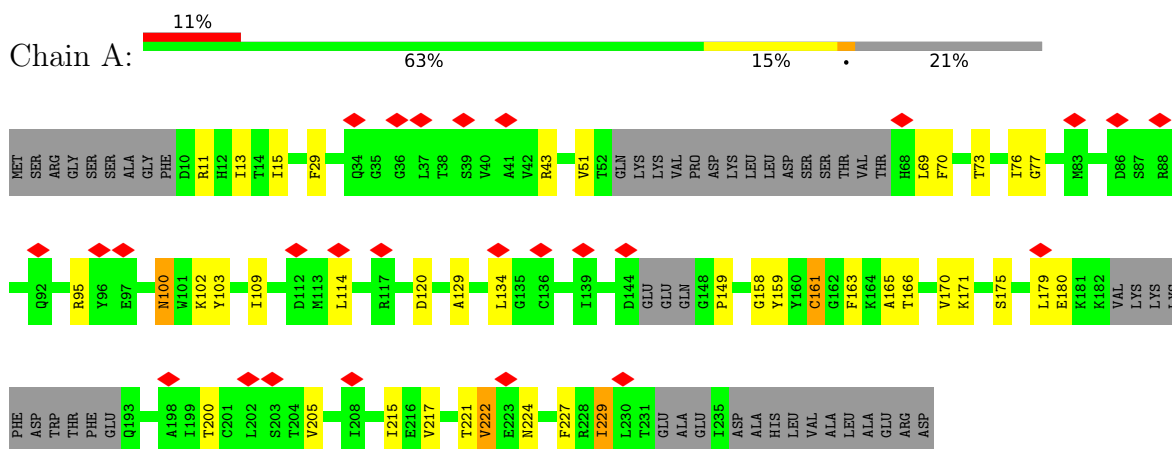


Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total 31	C 22	N 3	O 5	S 1	0
15	I	1	Total 30	C 22	N 3	O 4	S 1	0
15	L	1	Total 31	C 22	N 3	O 5	S 1	0
15	V	1	Total 31	C 22	N 3	O 5	S 1	0
15	W	1	Total 30	C 22	N 3	O 4	S 1	0
15	Z	1	Total 31	C 22	N 3	O 5	S 1	0

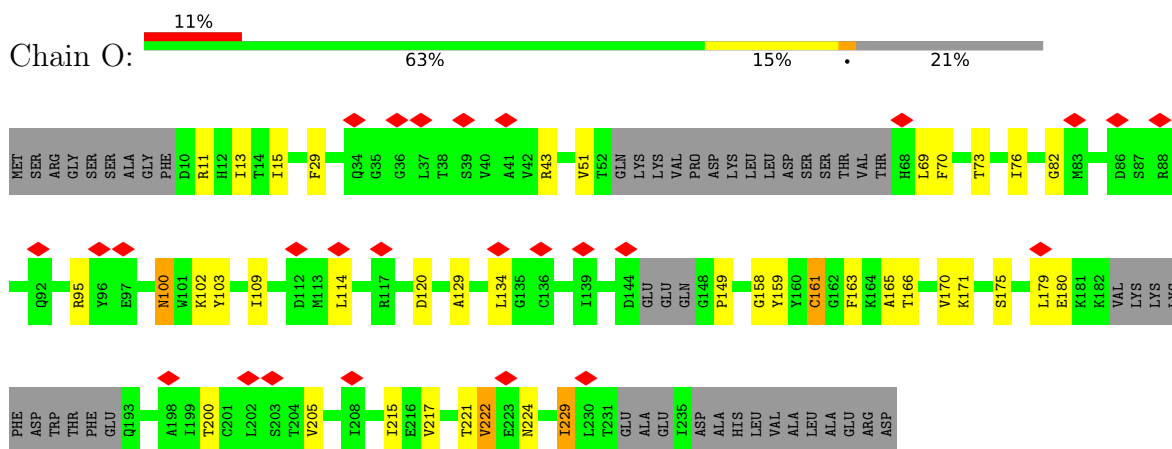
3 Residue-property plots

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.

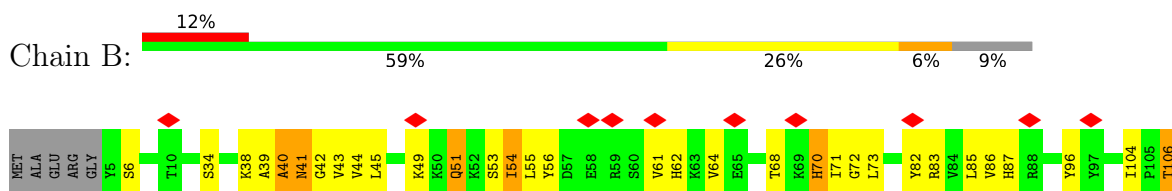
• Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-6

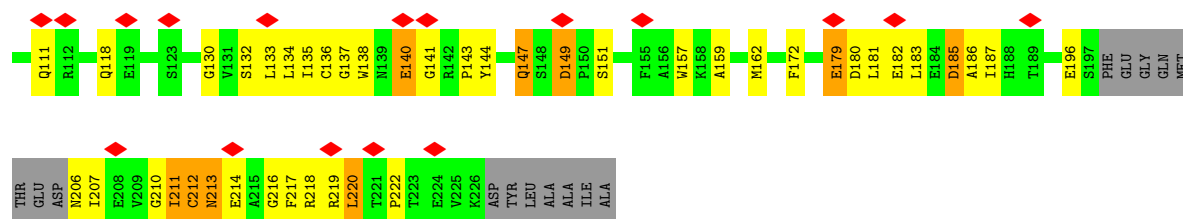


• Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-6

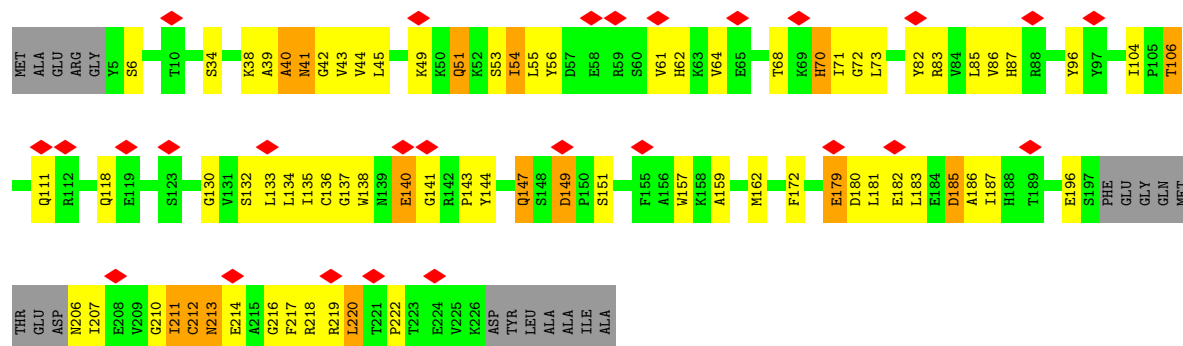


• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-2

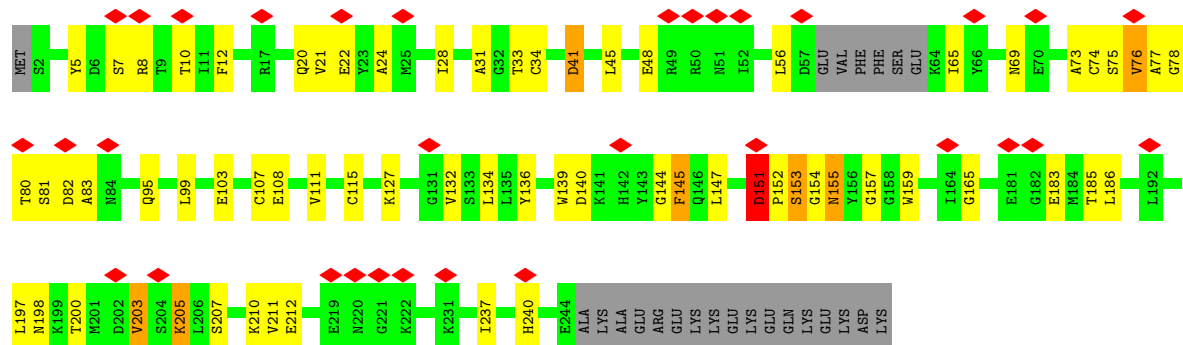




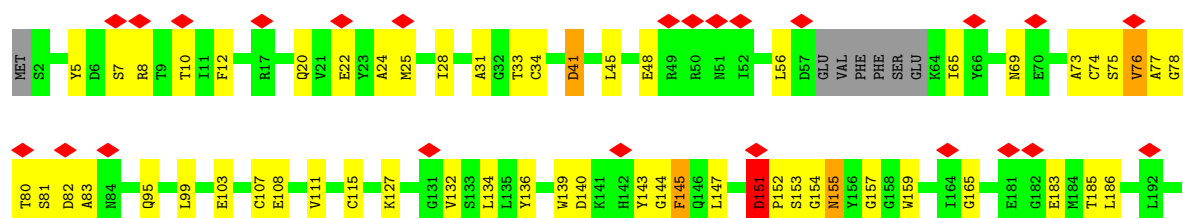
• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-2

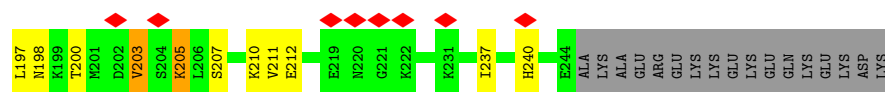


• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

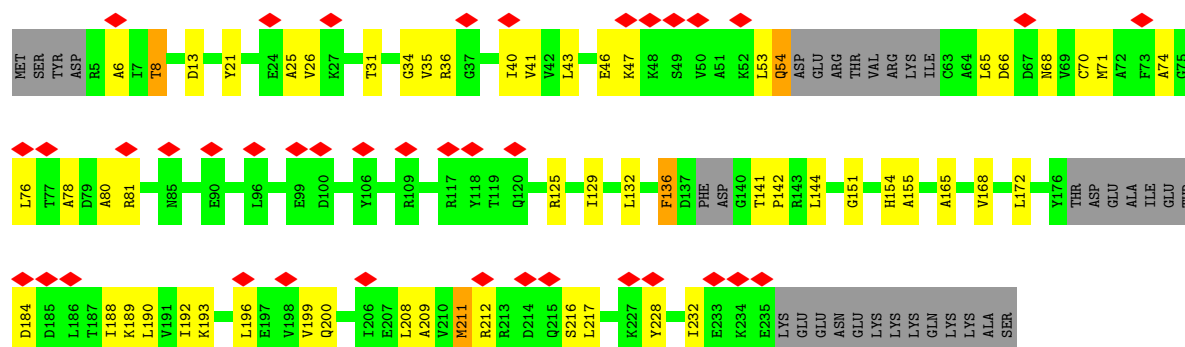


• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

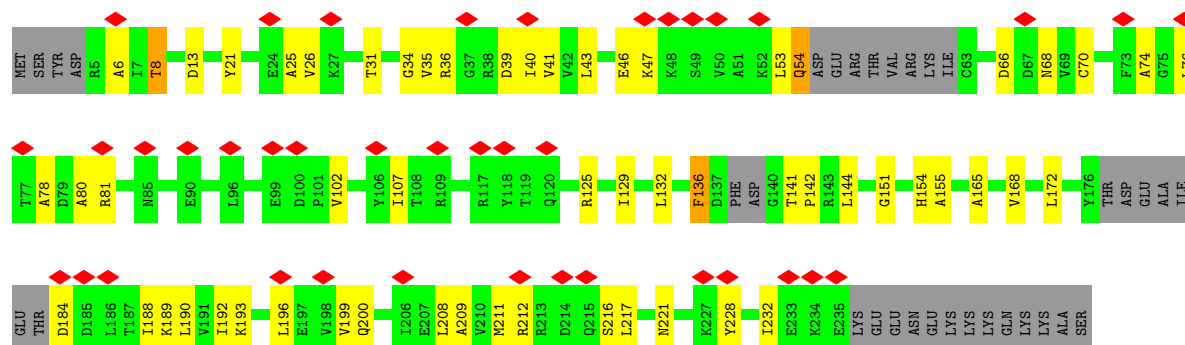




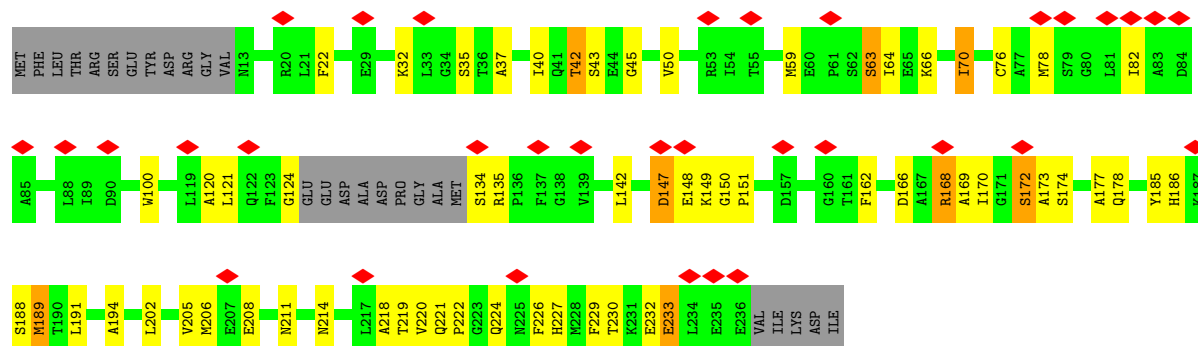
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-7



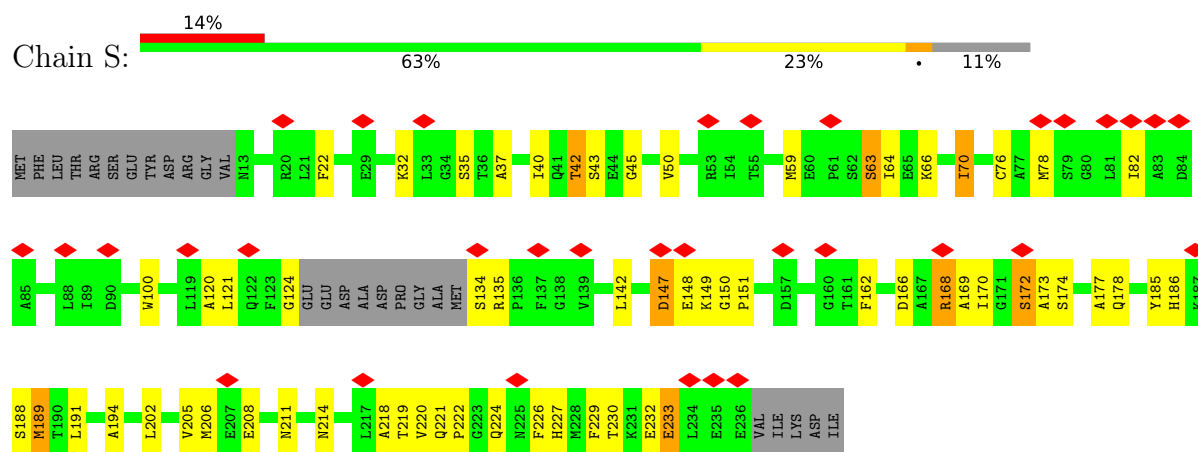
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-7



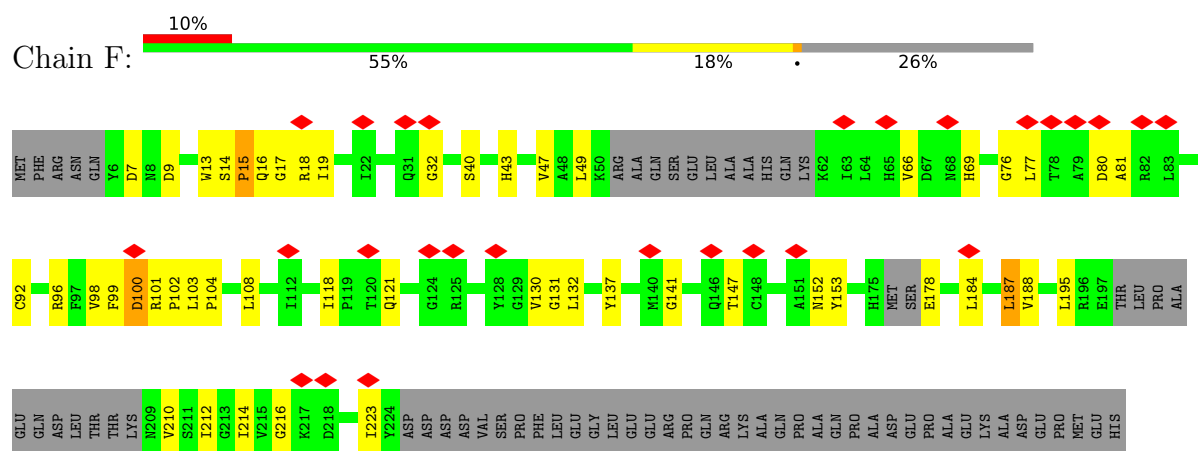
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-5



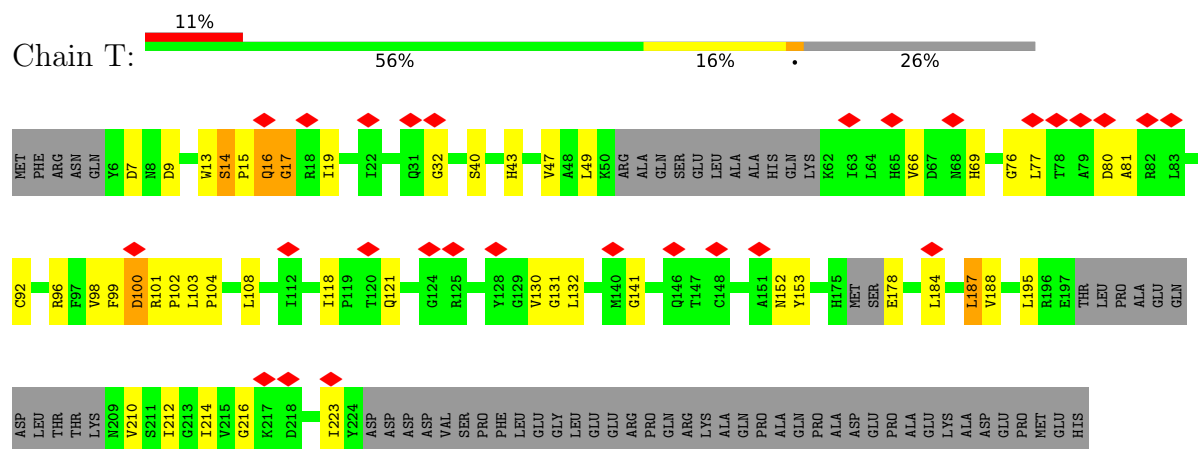
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-5



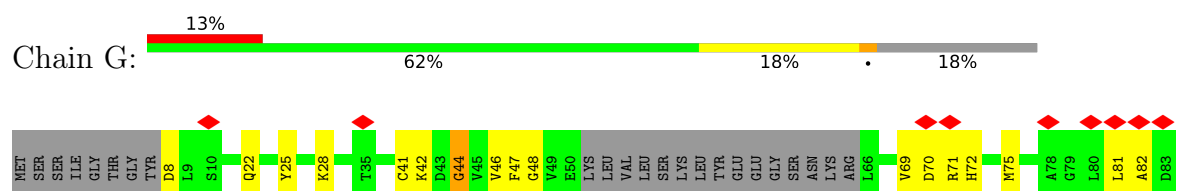
- Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-1

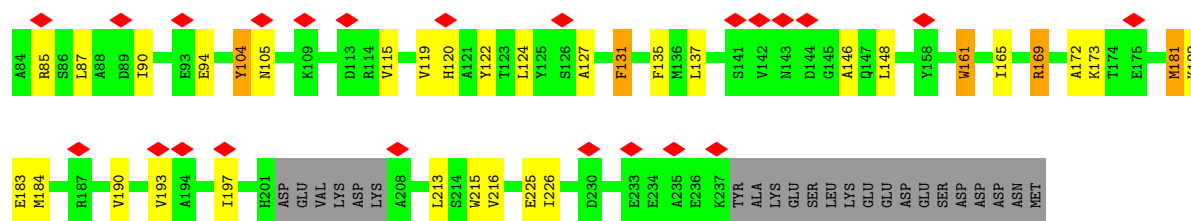


- Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-1

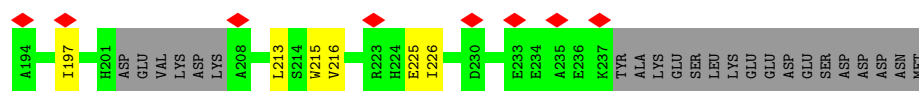
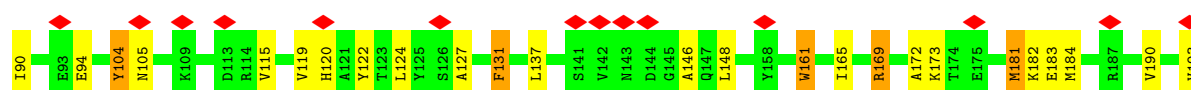
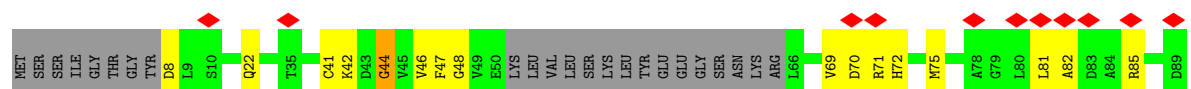


- Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-3

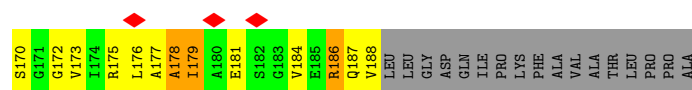
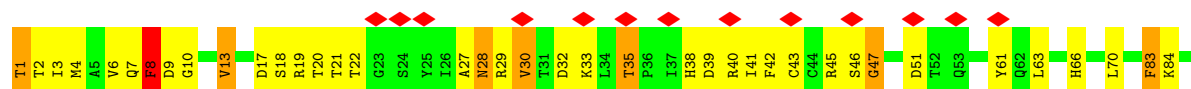




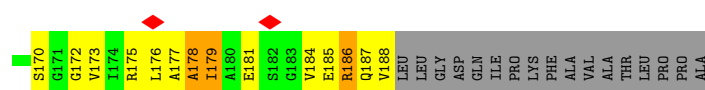
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-3



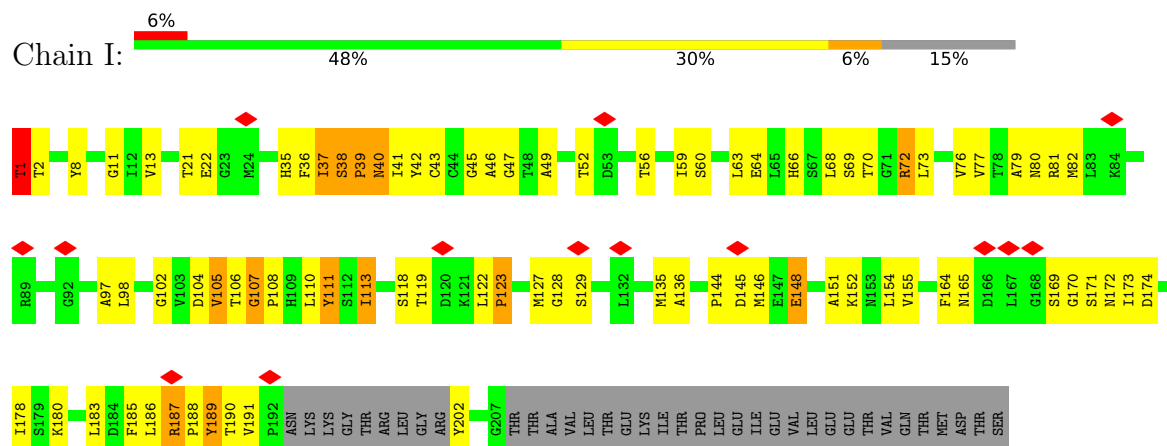
• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-6

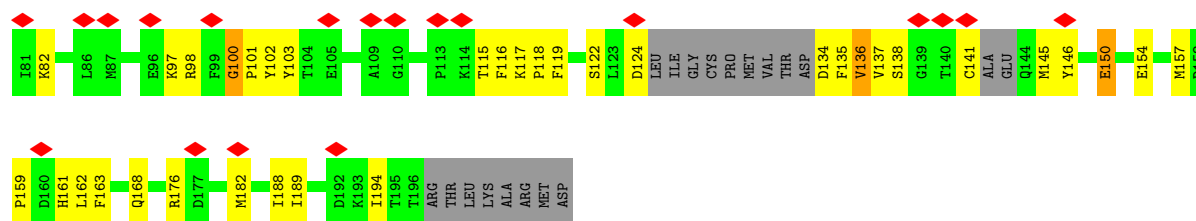


• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-6

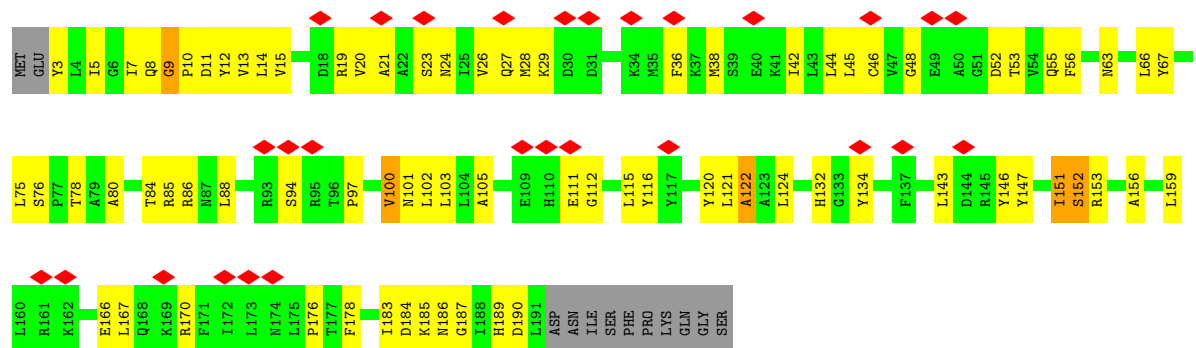


- Molecule 9: PROTEASOME SUBUNIT BETA TYPE-7

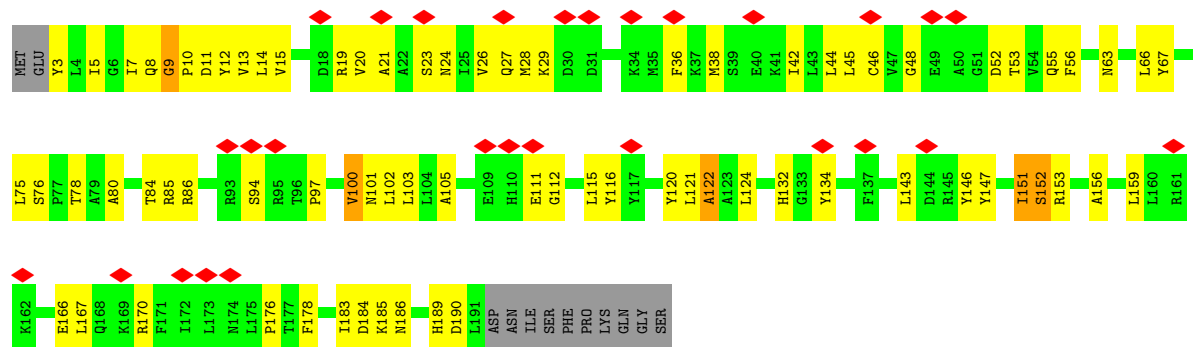




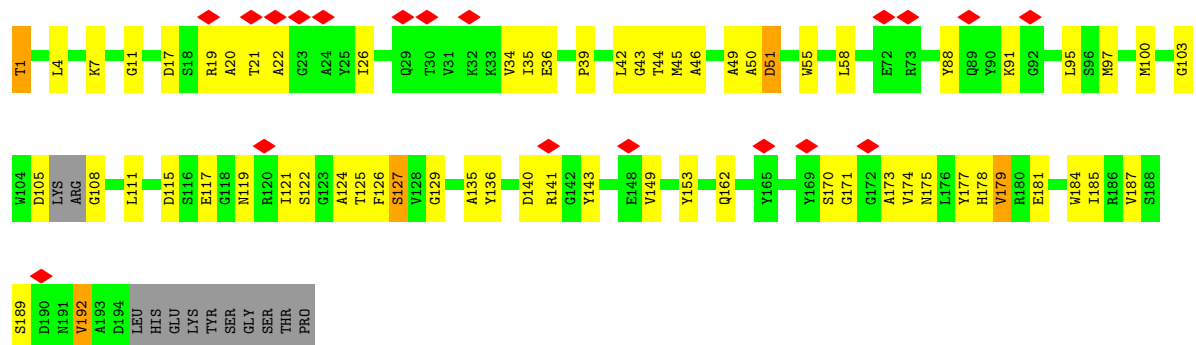
• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-2



• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-2

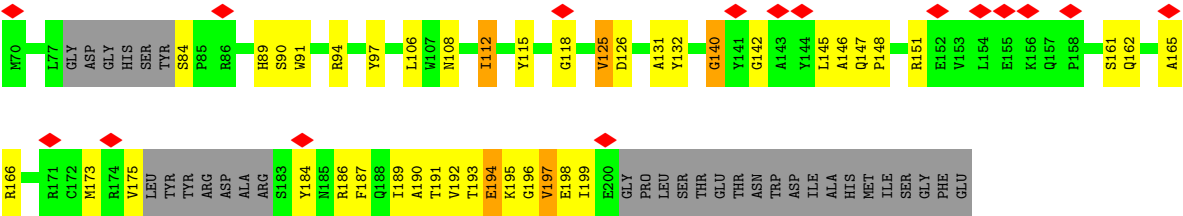


• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-5

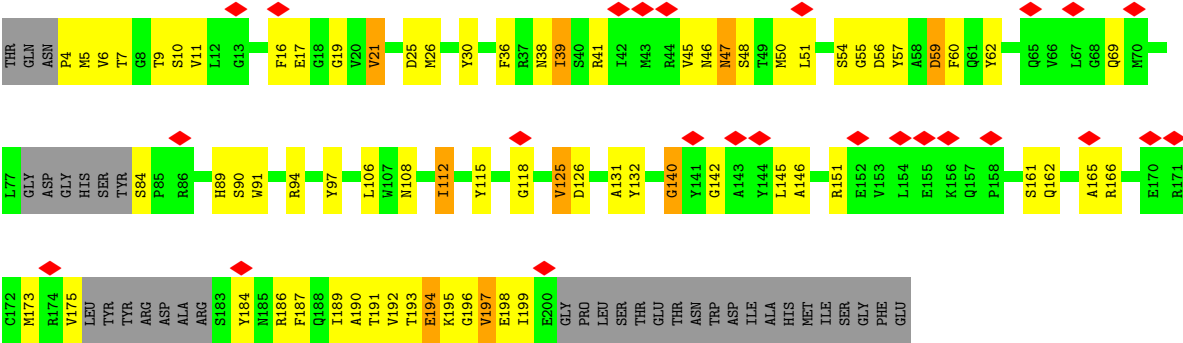


Chain Z: 9% 62% 29% 6%





• Molecule 14: PROTEASOME SUBUNIT BETA TYPE-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	76500	Depositor
Resolution determination method	Not provided	
CTF correction method	FULL RECORDED IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.8	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134461	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	16.752	Depositor
Minimum map value	-13.472	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.2	Depositor
Map size ($\text{\AA}$)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.33	2/1537 (0.1%)	1.48	12/2073 (0.6%)
1	O	1.33	3/1537 (0.2%)	1.48	12/2073 (0.6%)
2	B	1.25	0/1707	1.47	10/2312 (0.4%)
2	P	1.25	0/1707	1.47	10/2312 (0.4%)
3	C	1.31	3/1887 (0.2%)	1.54	16/2542 (0.6%)
3	Q	1.31	3/1887 (0.2%)	1.54	16/2542 (0.6%)
4	D	1.39	4/1695 (0.2%)	1.50	10/2283 (0.4%)
4	R	1.39	3/1695 (0.2%)	1.50	12/2283 (0.5%)
5	E	1.19	2/1668 (0.1%)	1.52	15/2252 (0.7%)
5	S	1.19	2/1668 (0.1%)	1.52	15/2252 (0.7%)
6	F	1.38	2/1562 (0.1%)	1.56	12/2105 (0.6%)
6	T	1.39	4/1562 (0.3%)	1.63	14/2105 (0.7%)
7	G	1.36	2/1656 (0.1%)	1.61	15/2232 (0.7%)
7	U	1.36	2/1656 (0.1%)	1.61	15/2232 (0.7%)
8	H	1.60	4/1394 (0.3%)	1.57	13/1884 (0.7%)
8	V	1.60	4/1394 (0.3%)	1.56	14/1884 (0.7%)
9	I	1.39	5/1515 (0.3%)	1.64	29/2050 (1.4%)
9	W	1.39	5/1515 (0.3%)	1.64	29/2050 (1.4%)
10	J	1.33	2/1398 (0.1%)	1.51	22/1884 (1.2%)
10	X	1.33	2/1398 (0.1%)	1.51	22/1884 (1.2%)
11	K	1.24	0/1543	1.48	24/2088 (1.1%)
11	Y	1.25	0/1543	1.48	24/2088 (1.1%)
12	L	1.49	4/1508 (0.3%)	1.54	19/2038 (0.9%)
12	Z	1.49	4/1508 (0.3%)	1.54	19/2038 (0.9%)
13	M	1.32	2/1477 (0.1%)	1.48	17/1990 (0.9%)
13	a	1.32	2/1477 (0.1%)	1.48	17/1990 (0.9%)
14	N	1.30	2/1451 (0.1%)	1.44	16/1957 (0.8%)
14	b	1.30	2/1451 (0.1%)	1.45	16/1957 (0.8%)
All	All	1.35	70/43996 (0.2%)	1.53	465/59380 (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	A	0	1
1	O	0	1
5	E	0	1
5	S	0	1
7	G	0	1
7	U	0	1
9	I	0	2
9	W	0	2
10	J	0	1
10	X	0	1
11	K	0	1
11	Y	0	1
13	M	0	2
13	a	0	2
All	All	0	18

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	THR	C-N	34.70	1.78	1.33
8	V	1	THR	C-N	34.70	1.78	1.33
12	L	1	THR	C-N	11.26	1.49	1.33
12	Z	1	THR	C-N	11.26	1.49	1.33
9	I	123	PRO	N-CD	-7.56	1.37	1.47
9	W	123	PRO	N-CD	-7.56	1.37	1.47
12	L	162	GLN	CD-OE1	7.26	1.37	1.23
12	Z	162	GLN	CD-OE1	7.26	1.37	1.23
4	D	54	GLN	CD-OE1	7.00	1.36	1.23
6	T	131	GLY	CA-C	-6.98	1.47	1.52
4	R	54	GLN	CD-OE1	6.98	1.36	1.23
10	J	168	GLN	CD-OE1	6.97	1.36	1.23
10	X	168	GLN	CD-OE1	6.97	1.36	1.23
3	C	20	GLN	CD-OE1	6.95	1.36	1.23
14	b	69	GLN	CD-OE1	6.95	1.36	1.23
3	Q	20	GLN	CD-OE1	6.93	1.36	1.23
14	N	69	GLN	CD-OE1	6.92	1.36	1.23
6	F	131	GLY	CA-C	-6.88	1.47	1.52
3	C	95	GLN	CD-OE1	6.82	1.36	1.23
3	Q	95	GLN	CD-OE1	6.82	1.36	1.23
8	H	90	TYR	CA-C	-6.69	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	90	TYR	CA-C	-6.69	1.45	1.52
10	X	100	GLY	C-N	6.34	1.40	1.33
10	J	100	GLY	C-N	6.28	1.40	1.33
12	L	7	LYS	CA-C	-5.80	1.45	1.52
12	Z	7	LYS	CA-C	-5.80	1.45	1.52
4	D	154	HIS	CA-C	-5.70	1.45	1.52
4	R	154	HIS	CA-C	-5.70	1.45	1.52
8	H	41	ILE	CA-C	-5.68	1.45	1.52
6	T	14	SER	CA-C	-5.68	1.46	1.53
8	V	41	ILE	CA-C	-5.68	1.45	1.52
4	D	193	LYS	CA-C	-5.64	1.45	1.52
4	R	193	LYS	CA-C	-5.64	1.45	1.52
5	E	22	PHE	CA-C	-5.64	1.47	1.53
5	S	22	PHE	CA-C	-5.64	1.47	1.53
9	I	110	LEU	CA-C	-5.50	1.47	1.53
9	W	110	LEU	CA-C	-5.50	1.47	1.53
12	L	51	ASP	CA-C	-5.42	1.46	1.52
12	Z	51	ASP	CA-C	-5.42	1.46	1.52
14	N	51	LEU	CA-C	-5.39	1.46	1.52
14	b	51	LEU	CA-C	-5.35	1.46	1.52
9	I	174	ASP	CA-C	-5.29	1.46	1.52
9	W	174	ASP	CA-C	-5.29	1.46	1.52
1	A	70	PHE	CA-C	-5.29	1.46	1.52
1	O	70	PHE	CA-C	-5.29	1.46	1.52
6	F	223	ILE	CA-C	-5.24	1.47	1.52
13	a	35	ILE	CA-C	-5.24	1.46	1.52
6	T	223	ILE	CA-C	-5.24	1.47	1.52
9	I	38	SER	C-N	5.23	1.41	1.34
9	W	38	SER	C-N	5.23	1.41	1.34
13	M	35	ILE	CA-C	-5.19	1.46	1.52
5	E	162	PHE	CA-C	-5.19	1.46	1.52
5	S	162	PHE	CA-C	-5.19	1.46	1.52
3	Q	152	PRO	N-CD	5.19	1.55	1.47
3	C	152	PRO	N-CD	5.18	1.55	1.47
9	I	39	PRO	N-CD	5.17	1.54	1.47
9	W	39	PRO	N-CD	5.17	1.54	1.47
1	A	161	CYS	CA-C	-5.16	1.46	1.52
1	O	161	CYS	CA-C	-5.16	1.46	1.52
13	M	22	ILE	CA-C	-5.15	1.47	1.53
8	H	139	VAL	CA-C	-5.12	1.46	1.52
6	T	14	SER	C-N	5.12	1.40	1.34
8	V	139	VAL	CA-C	-5.12	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	22	ILE	CA-C	-5.12	1.47	1.53
7	U	44	GLY	CA-C	-5.12	1.47	1.52
7	G	44	GLY	CA-C	-5.11	1.47	1.52
7	G	148	LEU	CA-C	-5.05	1.47	1.53
4	D	211	MET	CA-C	-5.04	1.46	1.52
7	U	148	LEU	CA-C	-5.03	1.47	1.53
1	O	82	GLY	CA-C	-5.02	1.46	1.52

All (465) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	17	GLY	N-CA-C	16.20	151.57	113.18
5	E	172	SER	N-CA-C	13.64	125.87	111.14
5	S	172	SER	N-CA-C	13.58	125.81	111.14
3	Q	153	SER	N-CA-C	-12.77	89.26	108.79
3	C	153	SER	N-CA-C	-12.75	89.28	108.79
12	L	1	THR	CA-C-N	11.54	137.10	120.95
12	L	1	THR	C-N-CA	11.54	137.10	120.95
12	Z	1	THR	CA-C-N	11.54	137.10	120.95
12	Z	1	THR	C-N-CA	11.54	137.10	120.95
8	V	179	ILE	N-CA-C	-10.91	92.21	108.46
8	H	179	ILE	N-CA-C	-10.89	92.23	108.46
9	W	189	TYR	N-CA-C	10.69	127.43	112.04
9	I	189	TYR	N-CA-C	10.68	127.42	112.04
6	T	16	GLN	N-CA-C	-10.59	100.03	113.16
9	I	119	THR	N-CA-C	-10.32	91.32	108.76
9	W	119	THR	N-CA-C	-10.32	91.32	108.76
8	H	47	GLY	N-CA-C	-9.83	89.87	113.18
8	V	47	GLY	N-CA-C	-9.83	89.87	113.18
8	H	8	PHE	N-CA-C	9.26	130.51	110.80
9	I	69	SER	N-CA-C	9.24	121.12	111.14
9	W	69	SER	N-CA-C	9.24	121.12	111.14
10	X	8	GLY	N-CA-C	-9.20	99.50	111.37
10	J	8	GLY	N-CA-C	-9.19	99.51	111.37
5	E	64	ILE	N-CA-C	-8.73	97.50	109.55
5	S	64	ILE	N-CA-C	-8.73	97.50	109.55
3	C	151	ASP	CA-C-N	-8.70	112.87	121.65
3	C	151	ASP	C-N-CA	-8.70	112.87	121.65
3	Q	151	ASP	CA-C-N	-8.70	112.87	121.65
3	Q	151	ASP	C-N-CA	-8.70	112.87	121.65
9	I	148	GLU	N-CA-C	8.46	120.28	111.14
9	W	148	GLU	N-CA-C	8.46	120.27	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	103	GLU	N-CA-C	-8.43	100.63	108.22
3	Q	103	GLU	N-CA-C	-8.43	100.63	108.22
7	G	169	ARG	N-CA-C	8.27	121.49	111.40
7	U	169	ARG	N-CA-C	8.27	121.49	111.40
9	I	155	VAL	N-CA-C	-8.24	104.72	112.96
9	W	155	VAL	N-CA-C	-8.24	104.72	112.96
6	F	18	ARG	N-CA-C	8.24	120.95	110.33
13	M	186	ASP	N-CA-C	-8.11	96.54	109.59
13	a	186	ASP	N-CA-C	-8.11	96.54	109.59
13	M	35	ILE	N-CA-CB	8.05	119.75	110.49
13	a	35	ILE	N-CA-CB	8.01	119.70	110.49
12	Z	126	PHE	CA-CB-CG	-7.60	106.20	113.80
12	L	126	PHE	CA-CB-CG	-7.57	106.23	113.80
9	W	77	VAL	CA-C-N	7.50	130.19	120.44
9	W	77	VAL	C-N-CA	7.50	130.19	120.44
9	I	77	VAL	CA-C-N	7.48	130.16	120.44
9	I	77	VAL	C-N-CA	7.48	130.16	120.44
12	L	1	THR	O-C-N	-7.42	111.12	123.00
12	Z	1	THR	O-C-N	-7.42	111.12	123.00
14	N	47	ASN	N-CA-C	-7.38	102.75	112.34
14	b	47	ASN	N-CA-C	-7.38	102.75	112.34
3	Q	155	ASN	N-CA-C	-7.33	97.00	108.14
3	C	155	ASN	N-CA-C	-7.32	97.02	108.14
14	N	140	GLY	N-CA-C	7.31	119.92	111.36
14	b	140	GLY	N-CA-C	7.31	119.92	111.36
7	U	161	TRP	N-CA-C	-7.28	104.92	113.88
7	G	161	TRP	N-CA-C	-7.26	104.95	113.88
11	K	178	PHE	CA-CB-CG	-7.24	106.56	113.80
10	X	58	ASP	CA-CB-CG	-7.23	105.37	112.60
7	G	70	ASP	N-CA-C	-7.22	98.06	108.60
7	U	70	ASP	N-CA-C	-7.22	98.06	108.60
11	Y	178	PHE	CA-CB-CG	-7.20	106.60	113.80
10	J	58	ASP	CA-CB-CG	-7.20	105.40	112.60
9	I	119	THR	N-CA-CB	7.18	123.22	110.80
9	W	119	THR	N-CA-CB	7.18	123.22	110.80
10	X	54	GLY	N-CA-C	-7.15	96.22	113.18
11	K	183	ILE	N-CA-C	-7.15	97.73	108.17
10	J	54	GLY	N-CA-C	-7.15	96.24	113.18
11	Y	183	ILE	N-CA-C	-7.13	97.76	108.17
11	K	111	GLU	N-CA-C	-7.12	105.12	114.31
11	Y	111	GLU	N-CA-C	-7.11	105.14	114.31
6	T	17	GLY	CA-C-N	7.06	133.63	122.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	17	GLY	C-N-CA	7.06	133.63	122.62
8	V	97	GLY	N-CA-C	-7.05	96.47	113.18
8	H	97	GLY	N-CA-C	-7.04	96.51	113.18
13	a	28	ARG	N-CA-C	6.96	120.32	110.23
13	M	28	ARG	N-CA-C	6.95	120.30	110.23
10	J	98	ARG	N-CA-C	-6.94	104.48	114.12
10	X	98	ARG	N-CA-C	-6.92	104.50	114.12
8	V	7	GLN	CB-CA-C	-6.81	96.81	110.30
11	Y	66	LEU	CA-C-N	6.73	129.19	120.44
11	Y	66	LEU	C-N-CA	6.73	129.19	120.44
11	K	66	LEU	CA-C-N	6.68	129.13	120.44
11	K	66	LEU	C-N-CA	6.68	129.13	120.44
2	B	185	ASP	CA-CB-CG	-6.65	105.95	112.60
2	P	185	ASP	CA-CB-CG	-6.65	105.95	112.60
11	K	152	SER	N-CA-CB	6.63	121.83	111.56
11	Y	152	SER	N-CA-CB	6.63	121.83	111.56
9	I	165	ASN	CA-CB-CG	-6.57	106.03	112.60
13	a	124	PHE	CA-CB-CG	-6.57	107.23	113.80
9	I	2	THR	N-CA-C	-6.57	97.82	108.52
13	M	124	PHE	CA-CB-CG	-6.56	107.24	113.80
9	W	2	THR	N-CA-C	-6.56	97.83	108.52
9	W	165	ASN	CA-CB-CG	-6.55	106.05	112.60
8	H	91	ARG	N-CA-C	-6.54	105.61	113.97
1	A	73	THR	N-CA-C	-6.53	99.15	109.07
1	O	73	THR	N-CA-C	-6.53	99.15	109.07
8	V	91	ARG	N-CA-C	-6.51	105.63	113.97
7	G	71	ARG	CA-C-N	6.51	129.54	120.29
7	G	71	ARG	C-N-CA	6.51	129.54	120.29
7	U	71	ARG	CA-C-N	6.51	129.54	120.29
7	U	71	ARG	C-N-CA	6.51	129.54	120.29
12	L	192	VAL	N-CA-C	-6.49	105.82	113.42
9	I	66	HIS	CA-CB-CG	6.49	120.29	113.80
12	Z	192	VAL	N-CA-C	-6.49	105.83	113.42
9	W	66	HIS	CA-CB-CG	6.48	120.28	113.80
10	X	117	LYS	CA-C-N	6.46	126.41	119.76
10	X	117	LYS	C-N-CA	6.46	126.41	119.76
10	J	117	LYS	CA-C-N	6.43	126.38	119.76
10	J	117	LYS	C-N-CA	6.43	126.38	119.76
1	A	166	THR	N-CA-C	6.40	118.82	110.43
1	O	166	THR	N-CA-C	6.40	118.82	110.43
8	H	179	ILE	N-CA-CB	6.40	121.93	111.44
8	V	179	ILE	N-CA-CB	6.38	121.91	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	69	ASN	CA-CB-CG	-6.37	106.23	112.60
3	Q	69	ASN	CA-CB-CG	-6.33	106.27	112.60
9	W	1	THR	CA-C-N	-6.31	114.21	123.05
9	W	1	THR	C-N-CA	-6.31	114.21	123.05
9	I	1	THR	CA-C-N	-6.31	114.22	123.05
9	I	1	THR	C-N-CA	-6.31	114.22	123.05
13	M	40	SER	N-CA-C	-6.29	98.04	108.23
13	a	40	SER	N-CA-C	-6.29	98.04	108.23
1	A	129	ALA	CA-C-N	6.27	128.68	120.28
1	A	129	ALA	C-N-CA	6.27	128.68	120.28
1	O	129	ALA	CA-C-N	6.27	128.68	120.28
1	O	129	ALA	C-N-CA	6.27	128.68	120.28
2	B	41	ASN	N-CA-C	-6.27	105.28	113.12
8	H	178	ALA	N-CA-C	-6.27	98.06	108.34
9	I	180	LYS	CA-C-N	6.27	128.68	120.28
9	I	180	LYS	C-N-CA	6.27	128.68	120.28
8	V	178	ALA	N-CA-C	-6.27	98.06	108.34
9	W	180	LYS	CA-C-N	6.27	128.68	120.28
9	W	180	LYS	C-N-CA	6.27	128.68	120.28
11	Y	38	MET	CG-SD-CE	-6.26	87.13	100.90
6	T	9	ASP	CA-C-N	6.26	129.03	120.46
6	T	9	ASP	C-N-CA	6.26	129.03	120.46
1	A	171	LYS	N-CA-C	-6.25	105.51	112.57
1	O	171	LYS	N-CA-C	-6.25	105.51	112.57
2	P	41	ASN	N-CA-C	-6.25	105.31	113.12
11	K	38	MET	CG-SD-CE	-6.25	87.16	100.90
6	F	9	ASP	CA-C-N	6.23	129.00	120.46
6	F	9	ASP	C-N-CA	6.23	129.00	120.46
6	F	131	GLY	N-CA-C	-6.21	100.13	111.25
6	T	131	GLY	N-CA-C	-6.21	100.13	111.25
10	X	100	GLY	CA-C-N	-6.18	113.15	120.13
10	X	100	GLY	C-N-CA	-6.18	113.15	120.13
10	J	100	GLY	CA-C-N	-6.17	113.16	120.13
10	J	100	GLY	C-N-CA	-6.17	113.16	120.13
5	E	173	ALA	CA-C-N	6.17	129.16	120.28
5	E	173	ALA	C-N-CA	6.17	129.16	120.28
14	N	17	GLU	N-CA-C	-6.13	100.32	109.15
14	b	17	GLU	N-CA-C	-6.13	100.32	109.15
5	S	173	ALA	CA-C-N	6.12	129.09	120.28
5	S	173	ALA	C-N-CA	6.12	129.09	120.28
14	N	197	VAL	N-CA-C	6.11	122.04	109.34
14	b	197	VAL	N-CA-C	6.09	122.00	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	8	ASP	CA-CB-CG	6.07	118.67	112.60
7	G	8	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	100	ASN	CA-CB-CG	6.05	118.65	112.60
3	C	205	LYS	N-CA-C	-6.05	100.22	109.41
3	Q	205	LYS	N-CA-C	-6.05	100.22	109.41
1	O	100	ASN	CA-CB-CG	6.04	118.64	112.60
4	D	53	LEU	N-CA-C	-6.04	104.29	112.26
4	R	53	LEU	N-CA-C	-6.01	104.33	112.26
8	H	13	VAL	N-CA-C	-5.99	99.49	108.12
8	V	13	VAL	N-CA-C	-5.99	99.49	108.12
1	A	170	VAL	CB-CA-C	-5.98	104.21	112.04
1	O	170	VAL	CB-CA-C	-5.98	104.21	112.04
7	G	82	ALA	CA-C-N	5.96	129.37	120.31
7	G	82	ALA	C-N-CA	5.96	129.37	120.31
7	U	82	ALA	CA-C-N	5.96	129.37	120.31
7	U	82	ALA	C-N-CA	5.96	129.37	120.31
6	F	15	PRO	N-CA-C	-5.95	105.26	113.53
6	F	99	PHE	CA-CB-CG	-5.95	107.85	113.80
6	T	99	PHE	CA-CB-CG	-5.95	107.85	113.80
13	a	48	ASP	N-CA-C	-5.95	104.87	111.71
12	L	175	ASN	CB-CA-C	-5.94	103.59	112.09
12	Z	175	ASN	CB-CA-C	-5.94	103.59	112.09
7	G	127	ALA	N-CA-C	5.94	117.42	111.07
7	U	127	ALA	N-CA-C	5.94	117.42	111.07
12	L	135	ALA	CA-C-N	5.93	128.22	120.28
12	L	135	ALA	C-N-CA	5.93	128.22	120.28
13	M	48	ASP	N-CA-C	-5.93	104.89	111.71
12	Z	135	ALA	CA-C-N	5.93	128.22	120.28
12	Z	135	ALA	C-N-CA	5.93	128.22	120.28
1	A	70	PHE	CA-CB-CG	-5.91	107.89	113.80
1	O	70	PHE	CA-CB-CG	-5.91	107.89	113.80
4	R	189	LYS	N-CA-CB	5.90	118.79	110.12
3	C	185	THR	N-CA-C	-5.90	102.59	110.55
2	B	111	GLN	CB-CA-C	-5.88	101.61	110.90
4	D	189	LYS	N-CA-CB	5.88	118.76	110.12
3	Q	185	THR	N-CA-C	-5.88	102.62	110.55
2	P	111	GLN	CB-CA-C	-5.86	101.64	110.90
5	E	42	THR	N-CA-C	-5.83	100.79	110.17
4	R	151	GLY	N-CA-C	-5.81	106.48	116.01
5	S	42	THR	N-CA-C	-5.80	100.82	110.17
6	T	187	LEU	CB-CA-C	-5.80	101.77	110.88
6	F	187	LEU	CB-CA-C	-5.80	101.77	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	47	VAL	N-CA-C	-5.79	99.72	108.17
6	T	47	VAL	N-CA-C	-5.79	99.72	108.17
4	D	151	GLY	N-CA-C	-5.79	106.52	116.01
14	N	194	GLU	N-CA-C	-5.78	104.35	111.75
14	b	194	GLU	N-CA-C	-5.78	104.35	111.75
11	K	152	SER	N-CA-C	-5.78	99.95	108.79
11	Y	152	SER	N-CA-C	-5.78	99.95	108.79
13	M	146	GLN	CA-C-O	-5.76	113.09	118.73
13	a	146	GLN	CA-C-O	-5.76	113.09	118.73
10	X	136	VAL	N-CA-C	-5.70	99.29	107.78
5	E	124	GLY	N-CA-C	-5.68	96.83	113.30
5	S	124	GLY	N-CA-C	-5.68	96.83	113.30
1	A	158	GLY	N-CA-C	-5.68	106.70	116.01
1	O	158	GLY	N-CA-C	-5.68	106.70	116.01
9	I	38	SER	CA-C-N	-5.67	112.75	119.05
9	I	38	SER	C-N-CA	-5.67	112.75	119.05
9	W	38	SER	CA-C-N	-5.67	112.75	119.05
9	W	38	SER	C-N-CA	-5.67	112.75	119.05
10	J	136	VAL	N-CA-C	-5.67	99.34	107.78
13	M	138	GLY	N-CA-C	-5.67	103.38	111.42
13	a	138	GLY	N-CA-C	-5.65	103.39	111.42
14	N	126	ASP	CA-CB-CG	5.64	118.24	112.60
13	M	167	SER	N-CA-C	-5.64	101.70	110.10
13	a	167	SER	N-CA-C	-5.63	101.71	110.10
14	b	126	ASP	CA-CB-CG	5.61	118.21	112.60
8	H	35	THR	N-CA-C	5.61	117.63	109.84
8	V	35	THR	N-CA-C	5.61	117.63	109.84
13	a	121	VAL	N-CA-C	-5.60	100.16	108.45
13	M	121	VAL	N-CA-C	-5.59	100.18	108.45
11	K	13	VAL	N-CA-C	-5.58	100.09	108.12
11	Y	13	VAL	N-CA-C	-5.58	100.09	108.12
11	K	7	ILE	N-CA-C	-5.54	101.04	108.35
11	Y	7	ILE	N-CA-C	-5.54	101.04	108.35
8	H	124	SER	N-CA-C	-5.53	106.89	113.97
8	V	124	SER	N-CA-C	-5.53	106.89	113.97
14	N	184	TYR	N-CA-C	-5.53	99.73	108.14
14	b	184	TYR	N-CA-C	-5.53	99.73	108.14
1	O	29	PHE	N-CA-CB	5.51	118.22	110.12
1	A	29	PHE	N-CA-CB	5.51	118.22	110.12
10	J	80	GLN	CA-C-N	5.49	127.86	120.50
10	J	80	GLN	C-N-CA	5.49	127.86	120.50
10	X	80	GLN	CA-C-N	5.49	127.86	120.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	80	GLN	C-N-CA	5.49	127.86	120.50
9	I	105	VAL	N-CA-C	-5.48	103.60	111.17
9	W	105	VAL	N-CA-C	-5.48	103.60	111.17
7	G	225	GLU	CA-C-N	5.46	128.73	120.75
7	G	225	GLU	C-N-CA	5.46	128.73	120.75
6	T	100	ASP	N-CA-C	5.46	119.16	111.52
10	X	194	ILE	CA-C-N	5.46	128.62	120.87
10	X	194	ILE	C-N-CA	5.46	128.62	120.87
3	C	212	GLU	N-CA-C	-5.45	99.44	108.75
10	J	194	ILE	CA-C-N	5.45	128.60	120.87
10	J	194	ILE	C-N-CA	5.45	128.60	120.87
7	U	225	GLU	CA-C-N	5.45	128.70	120.75
7	U	225	GLU	C-N-CA	5.45	128.70	120.75
3	Q	212	GLU	N-CA-C	-5.44	99.44	108.75
9	I	2	THR	N-CA-CB	5.43	119.08	110.55
14	N	84	SER	CA-C-N	5.43	125.25	119.28
14	N	84	SER	C-N-CA	5.43	125.25	119.28
9	W	2	THR	N-CA-CB	5.43	119.07	110.55
6	F	100	ASP	N-CA-C	5.42	119.11	111.52
3	C	22	GLU	CB-CA-C	-5.42	101.79	110.79
3	Q	22	GLU	CB-CA-C	-5.42	101.79	110.79
10	J	115	THR	N-CA-C	-5.42	106.68	113.72
10	X	115	THR	N-CA-C	-5.42	106.68	113.72
14	N	125	VAL	CA-C-N	5.41	129.44	120.94
14	N	125	VAL	C-N-CA	5.41	129.44	120.94
9	I	107	GLY	CA-C-N	5.41	125.33	119.76
9	I	107	GLY	C-N-CA	5.41	125.33	119.76
12	L	173	ALA	CA-C-N	5.41	127.75	120.50
12	L	173	ALA	C-N-CA	5.41	127.75	120.50
12	Z	173	ALA	CA-C-N	5.41	127.75	120.50
12	Z	173	ALA	C-N-CA	5.41	127.75	120.50
14	b	84	SER	CA-C-N	5.41	125.23	119.28
14	b	84	SER	C-N-CA	5.41	125.23	119.28
10	J	159	PRO	CA-C-N	5.40	127.51	120.28
10	J	159	PRO	C-N-CA	5.40	127.51	120.28
10	X	159	PRO	CA-C-N	5.40	127.51	120.28
10	X	159	PRO	C-N-CA	5.40	127.51	120.28
14	b	125	VAL	CA-C-N	5.40	129.41	120.94
14	b	125	VAL	C-N-CA	5.40	129.41	120.94
9	I	113	ILE	CA-C-N	5.40	128.88	120.68
9	I	113	ILE	C-N-CA	5.40	128.88	120.68
9	W	113	ILE	CA-C-N	5.40	128.88	120.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	113	ILE	C-N-CA	5.40	128.88	120.68
9	W	107	GLY	CA-C-N	5.38	125.31	119.76
9	W	107	GLY	C-N-CA	5.38	125.31	119.76
13	a	101	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	200	THR	N-CA-CB	5.38	118.61	110.28
8	H	117	GLY	N-CA-C	-5.37	106.21	113.24
13	M	101	PHE	CA-CB-CG	-5.37	108.43	113.80
1	O	200	THR	N-CA-CB	5.37	118.60	110.28
8	V	117	GLY	N-CA-C	-5.37	106.21	113.24
2	B	149	ASP	CA-C-N	5.37	126.55	119.84
2	B	149	ASP	C-N-CA	5.37	126.55	119.84
2	P	149	ASP	CA-C-N	5.37	126.55	119.84
2	P	149	ASP	C-N-CA	5.37	126.55	119.84
11	K	28	MET	N-CA-C	-5.36	106.67	114.12
13	a	38	ARG	N-CA-C	-5.36	106.42	113.17
4	R	141	THR	CA-C-N	5.35	125.29	119.78
4	R	141	THR	C-N-CA	5.35	125.29	119.78
14	N	106	LEU	N-CA-C	-5.34	101.45	109.95
14	b	106	LEU	N-CA-C	-5.34	101.45	109.95
14	N	59	ASP	CA-CB-CG	-5.34	107.26	112.60
14	b	39	ILE	N-CA-CB	5.34	116.54	110.72
14	b	59	ASP	CA-CB-CG	-5.34	107.26	112.60
4	D	141	THR	CA-C-N	5.34	125.28	119.78
4	D	141	THR	C-N-CA	5.34	125.28	119.78
6	T	118	ILE	N-CA-CB	5.33	114.61	110.45
13	M	42	LYS	N-CA-C	-5.33	106.91	113.41
11	Y	28	MET	N-CA-C	-5.33	106.72	114.12
12	L	35	ILE	CA-C-N	5.32	128.43	120.87
12	L	35	ILE	C-N-CA	5.32	128.43	120.87
14	N	39	ILE	N-CA-CB	5.32	116.52	110.72
11	K	9	GLY	N-CA-C	5.32	123.19	112.34
13	M	38	ARG	N-CA-C	-5.32	106.47	113.17
11	Y	9	GLY	N-CA-C	5.32	123.19	112.34
5	E	230	THR	CA-C-N	5.32	127.93	120.28
5	E	230	THR	C-N-CA	5.32	127.93	120.28
11	Y	63	ASN	CA-CB-CG	-5.32	107.28	112.60
5	E	59	MET	CG-SD-CE	-5.31	89.23	100.90
5	S	59	MET	CG-SD-CE	-5.31	89.23	100.90
13	a	42	LYS	N-CA-C	-5.31	106.94	113.41
12	Z	35	ILE	CA-C-N	5.30	128.39	120.87
12	Z	35	ILE	C-N-CA	5.30	128.39	120.87
6	F	118	ILE	N-CA-CB	5.29	114.57	110.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	63	ASN	CA-CB-CG	-5.29	107.31	112.60
7	G	172	ALA	CA-C-N	5.28	127.88	120.28
7	G	172	ALA	C-N-CA	5.28	127.88	120.28
7	U	172	ALA	CA-C-N	5.28	127.88	120.28
7	U	172	ALA	C-N-CA	5.28	127.88	120.28
11	K	134	TYR	N-CA-C	-5.28	106.86	113.72
5	S	230	THR	CA-C-N	5.27	127.87	120.28
5	S	230	THR	C-N-CA	5.27	127.87	120.28
7	U	104	TYR	N-CA-C	5.26	117.51	110.35
7	G	104	TYR	N-CA-C	5.26	117.50	110.35
11	Y	134	TYR	N-CA-C	-5.25	106.90	113.72
5	E	168	ARG	N-CA-C	-5.24	100.15	109.06
5	S	168	ARG	N-CA-C	-5.24	100.15	109.06
11	K	76	SER	CA-C-N	5.24	124.86	119.05
11	K	76	SER	C-N-CA	5.24	124.86	119.05
11	Y	76	SER	CA-C-N	5.24	124.86	119.05
11	Y	76	SER	C-N-CA	5.24	124.86	119.05
5	E	142	LEU	CB-CA-C	-5.23	103.82	111.77
14	N	51	LEU	N-CA-CB	5.23	119.93	110.83
5	S	142	LEU	CB-CA-C	-5.23	103.82	111.77
14	b	51	LEU	N-CA-CB	5.23	119.93	110.83
3	Q	165	GLY	CA-C-N	5.23	128.19	120.82
3	Q	165	GLY	C-N-CA	5.23	128.19	120.82
10	X	82	LYS	CA-C-N	5.23	125.03	119.28
10	X	82	LYS	C-N-CA	5.23	125.03	119.28
3	C	78	GLY	N-CA-C	5.22	119.00	112.73
10	J	82	LYS	CA-C-N	5.22	125.03	119.28
10	J	82	LYS	C-N-CA	5.22	125.03	119.28
3	C	165	GLY	CA-C-N	5.22	128.18	120.82
3	C	165	GLY	C-N-CA	5.22	128.18	120.82
6	F	141	GLY	CA-C-N	5.22	125.21	119.89
6	F	141	GLY	C-N-CA	5.22	125.21	119.89
6	T	141	GLY	CA-C-N	5.22	125.21	119.89
6	T	141	GLY	C-N-CA	5.22	125.21	119.89
10	X	59	VAL	N-CA-C	-5.22	105.63	110.53
3	Q	78	GLY	N-CA-C	5.21	118.98	112.73
5	E	232	GLU	CA-C-N	5.20	128.22	120.31
5	E	232	GLU	C-N-CA	5.20	128.22	120.31
5	S	232	GLU	CA-C-N	5.20	128.22	120.31
5	S	232	GLU	C-N-CA	5.20	128.22	120.31
11	K	27	GLN	N-CA-CB	5.19	118.18	110.29
11	Y	27	GLN	N-CA-CB	5.19	118.18	110.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	80	ASN	CA-CB-CG	-5.19	107.41	112.60
10	J	59	VAL	N-CA-C	-5.18	105.66	110.53
8	H	30	VAL	N-CA-C	-5.18	108.08	113.10
9	I	72	ARG	CA-C-N	5.18	127.69	120.65
9	I	72	ARG	C-N-CA	5.18	127.69	120.65
8	V	30	VAL	N-CA-C	-5.18	108.08	113.10
9	W	72	ARG	CA-C-N	5.18	127.69	120.65
9	W	72	ARG	C-N-CA	5.18	127.69	120.65
8	V	83	PHE	CA-CB-CG	-5.17	108.63	113.80
8	H	83	PHE	CA-CB-CG	-5.17	108.63	113.80
4	D	76	LEU	N-CA-C	-5.17	100.10	108.52
4	R	76	LEU	N-CA-C	-5.17	100.10	108.52
10	X	71	ASN	CA-CB-CG	-5.17	107.43	112.60
11	K	112	GLY	CA-C-N	5.16	125.08	119.76
11	K	112	GLY	C-N-CA	5.16	125.08	119.76
13	M	74	MET	CB-CA-C	-5.16	102.22	110.79
13	a	74	MET	CB-CA-C	-5.16	102.23	110.79
13	a	80	ASN	CA-CB-CG	-5.15	107.45	112.60
10	X	42	PHE	CA-CB-CG	-5.15	108.65	113.80
10	J	71	ASN	CA-CB-CG	-5.14	107.46	112.60
8	V	9	ASP	N-CA-C	5.14	116.12	108.31
11	Y	112	GLY	CA-C-N	5.13	125.05	119.76
11	Y	112	GLY	C-N-CA	5.13	125.05	119.76
11	Y	94	SER	CA-C-N	5.12	127.14	120.28
11	Y	94	SER	C-N-CA	5.12	127.14	120.28
2	B	130	GLY	CA-C-N	5.12	128.16	120.69
2	B	130	GLY	C-N-CA	5.12	128.16	120.69
2	P	130	GLY	CA-C-N	5.12	128.16	120.69
2	P	130	GLY	C-N-CA	5.12	128.16	120.69
9	I	40	ASN	N-CA-C	5.12	116.94	111.36
9	W	40	ASN	N-CA-C	5.12	116.94	111.36
9	I	135	MET	N-CA-CB	5.11	118.20	110.28
13	M	102	PHE	CA-C-O	-5.11	114.23	119.49
14	N	55	GLY	N-CA-C	-5.11	103.32	110.88
9	W	135	MET	N-CA-CB	5.11	118.20	110.28
14	b	55	GLY	N-CA-C	-5.11	103.32	110.88
7	G	131	PHE	CA-CB-CG	-5.11	108.69	113.80
12	L	127	SER	N-CA-C	-5.10	100.02	108.75
10	J	42	PHE	CA-CB-CG	-5.10	108.70	113.80
13	M	9	GLY	N-CA-C	-5.10	103.77	110.29
11	K	94	SER	CA-C-N	5.09	127.11	120.28
11	K	94	SER	C-N-CA	5.09	127.11	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	9	GLY	N-CA-C	-5.09	103.77	110.29
3	C	145	PHE	CA-CB-CG	-5.09	108.71	113.80
7	U	131	PHE	CA-CB-CG	-5.09	108.71	113.80
12	Z	177	TYR	N-CA-C	-5.09	100.74	109.24
12	Z	127	SER	N-CA-C	-5.09	100.05	108.75
12	L	177	TYR	N-CA-C	-5.09	100.75	109.24
2	P	179	GLU	CB-CA-C	-5.09	110.31	117.23
3	Q	145	PHE	CA-CB-CG	-5.08	108.72	113.80
11	K	11	ASP	CA-CB-CG	5.08	117.68	112.60
2	B	147	GLN	CA-C-O	-5.07	114.85	120.33
13	a	102	PHE	CA-C-O	-5.07	114.26	119.49
2	B	179	GLU	CB-CA-C	-5.07	110.33	117.23
9	I	174	ASP	N-CA-C	-5.06	101.90	109.95
9	W	174	ASP	N-CA-C	-5.06	101.90	109.95
4	D	136	PHE	CA-CB-CG	-5.06	108.74	113.80
4	R	136	PHE	CA-CB-CG	-5.06	108.74	113.80
4	D	132	LEU	N-CA-CB	5.06	117.40	110.57
4	R	132	LEU	N-CA-CB	5.06	117.40	110.57
12	L	129	GLY	CA-C-N	5.05	127.05	120.28
12	L	129	GLY	C-N-CA	5.05	127.05	120.28
4	R	189	LYS	CB-CA-C	-5.05	102.41	110.79
12	L	189	SER	N-CA-C	-5.04	105.50	113.02
11	Y	11	ASP	CA-CB-CG	5.04	117.64	112.60
12	Z	189	SER	N-CA-C	-5.04	105.50	113.02
3	C	108	GLU	CA-C-N	5.04	127.45	120.29
3	C	108	GLU	C-N-CA	5.04	127.45	120.29
5	E	233	GLU	CA-C-N	5.04	127.97	120.31
5	E	233	GLU	C-N-CA	5.04	127.97	120.31
3	Q	108	GLU	CA-C-N	5.04	127.45	120.29
3	Q	108	GLU	C-N-CA	5.04	127.45	120.29
5	S	233	GLU	CA-C-N	5.04	127.97	120.31
5	S	233	GLU	C-N-CA	5.04	127.97	120.31
11	K	80	ALA	CA-C-N	5.04	127.30	120.44
11	K	80	ALA	C-N-CA	5.04	127.30	120.44
4	D	74	ALA	N-CA-C	-5.04	101.71	109.52
4	R	74	ALA	N-CA-C	-5.04	101.71	109.52
11	Y	80	ALA	CA-C-N	5.04	127.29	120.44
11	Y	80	ALA	C-N-CA	5.04	127.29	120.44
10	X	150	GLU	N-CA-C	5.03	117.50	111.71
12	Z	129	GLY	CA-C-N	5.03	127.02	120.28
12	Z	129	GLY	C-N-CA	5.03	127.02	120.28
1	A	11	ARG	N-CA-C	-5.03	106.46	112.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	11	ARG	N-CA-C	-5.03	106.46	112.59
4	D	189	LYS	CB-CA-C	-5.03	102.45	110.79
2	B	220	LEU	N-CA-C	-5.02	102.77	110.30
2	P	220	LEU	N-CA-C	-5.02	102.77	110.30
12	L	181	GLU	CA-C-N	5.02	126.97	120.44
12	L	181	GLU	C-N-CA	5.02	126.97	120.44
12	Z	181	GLU	CA-C-N	5.02	126.97	120.44
12	Z	181	GLU	C-N-CA	5.02	126.97	120.44
10	J	150	GLU	N-CA-C	5.02	117.48	111.71
4	R	221	ASN	CA-C-N	5.01	124.80	119.28
4	R	221	ASN	C-N-CA	5.01	124.80	119.28
9	I	187	ARG	CA-C-O	-5.01	113.29	120.16
9	W	187	ARG	CA-C-O	-5.01	113.29	120.16
2	P	147	GLN	CA-C-O	-5.01	114.92	120.33

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ARG	Sidechain
5	E	147	ASP	Peptide
7	G	181	MET	Peptide
9	I	1	THR	Mainchain
9	I	111	TYR	Sidechain
10	J	16	LYS	Peptide
11	K	153	ARG	Sidechain
13	M	18	GLU	Peptide
13	M	188	TYR	Sidechain
1	O	95	ARG	Sidechain
5	S	147	ASP	Peptide
7	U	181	MET	Peptide
9	W	1	THR	Mainchain
9	W	111	TYR	Sidechain
10	X	16	LYS	Peptide
11	Y	153	ARG	Sidechain
13	a	18	GLU	Peptide
13	a	188	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1514	0	1527	73	0
1	O	1514	0	1527	74	0
2	B	1671	0	1681	157	0
2	P	1671	0	1681	158	0
3	C	1860	0	1886	86	0
3	Q	1860	0	1886	88	0
4	D	1674	0	1712	67	0
4	R	1674	0	1712	68	0
5	E	1643	0	1636	97	0
5	S	1643	0	1636	97	0
6	F	1535	0	1540	75	0
6	T	1535	0	1540	74	0
7	G	1626	0	1602	98	0
7	U	1626	0	1602	93	0
8	H	1372	0	1338	139	0
8	V	1372	0	1338	146	0
9	I	1490	0	1490	172	0
9	W	1490	0	1490	167	0
10	J	1374	0	1383	90	0
10	X	1374	0	1383	92	0
11	K	1512	0	1520	123	0
11	Y	1512	0	1520	118	0
12	L	1480	0	1441	109	0
12	Z	1480	0	1441	106	0
13	M	1453	0	1455	164	0
13	a	1453	0	1455	160	0
14	N	1428	0	1432	191	0
14	b	1428	0	1432	186	0
15	H	31	0	39	35	0
15	I	30	0	39	46	0
15	L	31	0	39	31	0
15	V	31	0	39	33	0
15	W	30	0	39	45	0
15	Z	31	0	39	30	0
All	All	43448	0	43520	2938	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 34.

All (2938) 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)
13:M:152:GLN:HG3	9:W:202:TYR:CD2	1.31	1.63
1:A:109:ILE:CG2	1:A:114:LEU:HD21	1.26	1.62
9:I:202:TYR:CD2	13:a:152:GLN:HG3	1.31	1.61
14:b:26:MET:CE	14:b:186:ARG:HH12	1.10	1.61
14:N:26:MET:CE	14:N:186:ARG:HH12	1.10	1.60
8:V:119:MET:HE3	14:b:57:TYR:CD2	1.34	1.60
8:H:119:MET:HE3	14:N:57:TYR:CD2	1.34	1.58
1:O:109:ILE:CG2	1:O:114:LEU:HD21	1.26	1.57
14:N:16:PHE:CE1	14:N:166:ARG:N	1.74	1.56
14:b:16:PHE:CE1	14:b:166:ARG:N	1.74	1.51
8:V:119:MET:CE	14:b:57:TYR:CD2	1.91	1.51
8:H:119:MET:CE	14:N:57:TYR:CD2	1.91	1.50
1:O:109:ILE:HG21	1:O:114:LEU:CD2	1.40	1.50
1:A:109:ILE:HG21	1:A:114:LEU:CD2	1.40	1.49
1:O:109:ILE:HD13	1:O:114:LEU:CD2	1.46	1.46
1:A:103:TYR:CA	9:I:81:ARG:NH2	1.78	1.45
13:M:99:ARG:HD3	13:M:104:TYR:CZ	1.51	1.44
13:a:99:ARG:HD3	13:a:104:TYR:CZ	1.51	1.44
14:N:16:PHE:CZ	14:N:166:ARG:N	1.83	1.43
1:O:103:TYR:CA	9:W:81:ARG:NH2	1.78	1.43
1:O:109:ILE:CD1	1:O:114:LEU:HD23	1.47	1.43
14:b:16:PHE:CZ	14:b:166:ARG:N	1.83	1.43
1:A:109:ILE:HD13	1:A:114:LEU:CD2	1.46	1.42
8:H:1:THR:C	8:H:2:THR:N	1.78	1.41
14:b:26:MET:CE	14:b:186:ARG:NH1	1.82	1.41
1:A:109:ILE:CD1	1:A:114:LEU:HD23	1.47	1.41
8:H:119:MET:HE1	14:N:57:TYR:CB	1.52	1.39
13:a:18:GLU:N	13:a:166:LEU:HD13	1.36	1.38
8:V:1:THR:C	8:V:2:THR:N	1.78	1.38
10:J:157:MET:HG2	10:J:161:HIS:CD2	1.58	1.38
13:M:18:GLU:N	13:M:166:LEU:HD13	1.36	1.37
11:K:23:SER:C	11:K:24:ASN:OD1	1.67	1.37
14:N:26:MET:CE	14:N:186:ARG:NH1	1.81	1.37
8:V:119:MET:HE1	14:b:57:TYR:CB	1.52	1.36
10:X:157:MET:HG2	10:X:161:HIS:CD2	1.58	1.36
12:L:50:ALA:HB1	13:M:97:TYR:OH	1.21	1.36
11:Y:23:SER:C	11:Y:24:ASN:OD1	1.67	1.36
13:M:152:GLN:CG	9:W:202:TYR:CD2	2.05	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:16:PHE:CE2	14:N:21:VAL:HB	1.61	1.36
1:O:103:TYR:HA	9:W:81:ARG:NH2	1.05	1.36
14:b:16:PHE:CE2	14:b:21:VAL:HB	1.61	1.36
8:H:20:THR:HG22	15:H:300:KNM:C20	1.56	1.35
10:X:157:MET:CG	10:X:161:HIS:HD2	1.37	1.35
1:A:103:TYR:HA	9:I:81:ARG:NH2	1.05	1.35
8:H:119:MET:CE	14:N:57:TYR:HB3	1.57	1.35
4:R:192:ILE:HG13	4:R:228:TYR:CD1	1.61	1.35
7:U:75:MET:HB2	7:U:137:LEU:CD2	1.56	1.35
8:V:20:THR:HG22	15:V:300:KNM:C20	1.56	1.35
9:I:202:TYR:CD2	13:a:152:GLN:CG	2.05	1.35
13:M:152:GLN:CG	9:W:202:TYR:HD2	1.39	1.34
4:D:192:ILE:HG13	4:D:228:TYR:CD1	1.61	1.34
10:J:157:MET:CG	10:J:161:HIS:HD2	1.37	1.34
8:V:119:MET:CE	14:b:57:TYR:HB3	1.57	1.33
5:E:42:THR:CG2	5:E:194:ALA:CB	2.06	1.33
7:G:75:MET:HB2	7:G:137:LEU:CD2	1.56	1.33
5:S:42:THR:CG2	5:S:194:ALA:CB	2.06	1.33
7:G:190:VAL:HG11	7:G:215:TRP:CZ2	1.65	1.31
5:S:229:PHE:CZ	5:S:233:GLU:HG2	1.63	1.31
12:L:140:ASP:OD2	11:Y:170:ARG:HD3	1.26	1.31
5:E:229:PHE:CZ	5:E:233:GLU:HG2	1.63	1.31
7:G:190:VAL:CG1	7:G:215:TRP:HZ2	1.44	1.30
7:U:190:VAL:HG11	7:U:215:TRP:CZ2	1.65	1.30
11:K:23:SER:O	11:K:24:ASN:CG	1.72	1.30
9:W:36:PHE:CE1	9:W:38:SER:C	2.10	1.30
7:U:190:VAL:CG1	7:U:215:TRP:HZ2	1.44	1.29
14:N:4:PRO:CB	14:N:56:ASP:OD2	1.80	1.29
12:Z:50:ALA:HB1	13:a:97:TYR:OH	1.21	1.29
9:I:36:PHE:CE1	9:I:38:SER:C	2.10	1.28
11:Y:23:SER:O	11:Y:24:ASN:CG	1.72	1.28
13:a:99:ARG:HD3	13:a:104:TYR:CE2	1.68	1.28
4:D:184:ASP:O	4:D:188:ILE:HD12	1.29	1.27
9:I:202:TYR:HD2	13:a:152:GLN:CG	1.39	1.27
4:R:184:ASP:O	4:R:188:ILE:HD12	1.29	1.27
6:T:184:LEU:HD11	6:T:214:ILE:CD1	1.65	1.27
11:K:170:ARG:HD3	12:Z:140:ASP:OD2	1.26	1.26
14:N:16:PHE:CZ	14:N:165:ALA:C	2.12	1.26
13:M:99:ARG:HD3	13:M:104:TYR:CE2	1.68	1.26
14:b:4:PRO:CB	14:b:56:ASP:OD2	1.80	1.26
2:B:138:TRP:NE1	2:B:143:PRO:HD3	1.49	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:16:PHE:CZ	14:b:165:ALA:C	2.12	1.26
13:M:17:GLY:HA3	13:M:166:LEU:CD2	1.66	1.26
2:P:138:TRP:NE1	2:P:143:PRO:HD3	1.49	1.25
5:E:229:PHE:CE2	5:E:233:GLU:CG	2.19	1.24
5:S:229:PHE:CE2	5:S:233:GLU:CG	2.19	1.24
12:L:50:ALA:CB	13:M:97:TYR:OH	1.84	1.24
12:Z:50:ALA:CB	13:a:97:TYR:OH	1.84	1.24
6:F:184:LEU:HD11	6:F:214:ILE:CD1	1.65	1.24
6:T:184:LEU:CD1	6:T:214:ILE:HD12	1.68	1.24
14:N:26:MET:HE2	14:N:186:ARG:NH1	1.48	1.23
4:R:184:ASP:O	4:R:188:ILE:CD1	1.86	1.23
6:F:184:LEU:CD1	6:F:214:ILE:HD12	1.68	1.22
7:G:190:VAL:HB	7:G:215:TRP:NE1	1.53	1.22
8:H:47:GLY:O	15:H:300:KNM:H24	1.37	1.22
13:a:17:GLY:HA3	13:a:166:LEU:CD2	1.66	1.22
9:I:36:PHE:HE1	9:I:39:PRO:N	1.37	1.22
4:D:184:ASP:O	4:D:188:ILE:CD1	1.86	1.22
10:X:137:VAL:HG23	10:X:146:TYR:CZ	1.74	1.22
14:N:16:PHE:HE2	14:N:21:VAL:CB	1.53	1.21
1:O:76:ILE:CD1	1:O:114:LEU:HD11	1.71	1.21
10:J:137:VAL:HG23	10:J:146:TYR:CE2	1.75	1.21
5:S:229:PHE:CE2	5:S:233:GLU:HG2	1.75	1.21
12:Z:55:TRP:HZ2	12:Z:95:LEU:CD1	1.53	1.21
14:b:16:PHE:HE2	14:b:21:VAL:CB	1.53	1.21
10:J:64:GLN:NE2	11:K:85:ARG:HH22	1.38	1.21
8:V:47:GLY:O	15:V:300:KNM:H24	1.37	1.21
10:X:64:GLN:NE2	11:Y:85:ARG:HH22	1.38	1.21
10:X:137:VAL:HG23	10:X:146:TYR:CE2	1.75	1.20
13:a:48:ASP:O	13:a:203:ILE:HG13	1.41	1.20
1:A:76:ILE:CD1	1:A:114:LEU:HD11	1.71	1.20
7:U:190:VAL:HB	7:U:215:TRP:NE1	1.53	1.20
9:W:36:PHE:HE1	9:W:39:PRO:N	1.37	1.20
13:M:48:ASP:O	13:M:203:ILE:HG13	1.41	1.20
10:X:64:GLN:NE2	11:Y:85:ARG:NH2	1.88	1.20
5:E:229:PHE:CE2	5:E:233:GLU:HG2	1.75	1.19
7:G:75:MET:CB	7:G:137:LEU:CD2	2.20	1.19
12:L:55:TRP:HZ2	12:L:95:LEU:CD1	1.53	1.19
10:J:137:VAL:HG23	10:J:146:TYR:CZ	1.74	1.19
10:J:64:GLN:NE2	11:K:85:ARG:NH2	1.88	1.19
5:S:166:ASP:CB	5:S:185:TYR:OH	1.91	1.18
9:W:47:GLY:H	15:W:300:KNM:C16	1.56	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:202:TYR:CE2	13:a:174:LEU:HD13	1.78	1.18
13:M:174:LEU:HD13	9:W:202:TYR:CE2	1.78	1.18
14:b:6:VAL:HG22	14:b:30:TYR:HB2	1.24	1.18
5:E:166:ASP:HB3	5:E:185:TYR:OH	1.02	1.18
7:U:75:MET:CB	7:U:137:LEU:CD2	2.20	1.18
5:S:166:ASP:HB3	5:S:185:TYR:OH	1.02	1.17
5:E:166:ASP:CB	5:E:185:TYR:OH	1.91	1.17
11:K:170:ARG:NH2	12:Z:136:TYR:CD1	2.13	1.17
4:R:40:ILE:HG21	4:R:211:MET:O	1.45	1.17
8:V:88:TYR:OH	14:b:62:TYR:CB	1.93	1.16
9:W:36:PHE:HE1	9:W:38:SER:C	1.49	1.16
8:H:119:MET:CE	14:N:57:TYR:CG	2.28	1.16
12:L:136:TYR:CD1	11:Y:170:ARG:NH2	2.13	1.16
2:B:41:ASN:HB2	2:B:183:LEU:HB2	1.28	1.16
3:C:207:SER:H	3:C:210:LYS:HD2	1.00	1.16
9:I:47:GLY:H	15:I:300:KNM:C16	1.56	1.16
14:N:50:MET:HE2	14:N:192:VAL:CG2	1.76	1.16
8:V:119:MET:CE	14:b:57:TYR:CG	2.28	1.16
8:H:88:TYR:OH	14:N:62:TYR:CB	1.93	1.15
9:W:1:THR:HG21	15:W:300:KNM:H42	1.28	1.15
12:L:26:ILE:HD12	10:X:176:ARG:O	1.44	1.15
4:R:40:ILE:CG2	4:R:211:MET:O	1.95	1.15
10:X:157:MET:SD	10:X:161:HIS:CD2	2.40	1.15
8:H:88:TYR:CZ	14:N:62:TYR:HB2	1.82	1.15
5:S:224:GLN:NE2	5:S:227:HIS:ND1	1.94	1.14
4:D:40:ILE:CG2	4:D:211:MET:O	1.95	1.14
5:E:166:ASP:HB3	5:E:185:TYR:CZ	1.82	1.14
9:I:36:PHE:HE1	9:I:38:SER:C	1.49	1.14
10:J:157:MET:SD	10:J:161:HIS:CD2	2.40	1.14
14:N:26:MET:HB2	14:N:186:ARG:NH2	1.63	1.14
14:N:50:MET:CE	14:N:192:VAL:HG23	1.77	1.14
14:b:50:MET:HE2	14:b:192:VAL:CG2	1.76	1.14
5:S:166:ASP:HB3	5:S:185:TYR:CZ	1.81	1.14
14:b:50:MET:CE	14:b:192:VAL:HG23	1.77	1.14
7:U:161:TRP:O	7:U:181:MET:HE1	1.48	1.13
12:Z:55:TRP:HZ2	12:Z:95:LEU:HD13	0.98	1.13
10:J:176:ARG:O	12:Z:26:ILE:HD12	1.43	1.13
5:E:224:GLN:NE2	5:E:227:HIS:ND1	1.94	1.13
8:V:88:TYR:CZ	14:b:62:TYR:HB2	1.82	1.13
1:A:76:ILE:HD13	1:A:114:LEU:CD1	1.78	1.12
4:D:40:ILE:HG21	4:D:211:MET:O	1.45	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:76:ILE:HD13	1:O:114:LEU:CD1	1.78	1.13
2:P:62:HIS:CE1	2:P:219:ARG:NH1	2.18	1.12
2:B:62:HIS:CE1	2:B:219:ARG:NH1	2.18	1.12
14:b:26:MET:HB2	14:b:186:ARG:NH2	1.63	1.12
7:G:161:TRP:O	7:G:181:MET:HE1	1.48	1.11
13:M:17:GLY:HA3	13:M:166:LEU:HD22	1.19	1.11
12:Z:50:ALA:C	13:a:97:TYR:OH	1.94	1.11
13:a:16:ALA:HB1	13:a:119:GLY:HA3	1.22	1.11
5:E:42:THR:HG21	5:E:194:ALA:CB	1.81	1.11
12:L:50:ALA:C	13:M:97:TYR:OH	1.94	1.11
14:b:26:MET:HE2	14:b:186:ARG:NH1	1.48	1.11
5:E:42:THR:CG2	5:E:194:ALA:HB2	1.79	1.11
12:L:55:TRP:HZ2	12:L:95:LEU:HD13	0.98	1.10
5:S:229:PHE:HE2	5:S:233:GLU:CB	1.65	1.10
2:P:73:LEU:HD22	2:P:133:LEU:HD13	1.10	1.10
7:U:190:VAL:HG21	7:U:215:TRP:CZ2	1.86	1.10
14:b:16:PHE:CE1	14:b:165:ALA:C	2.28	1.10
8:H:119:MET:CE	14:N:57:TYR:HD2	1.43	1.10
11:K:170:ARG:NH2	12:Z:136:TYR:CE1	2.20	1.10
12:L:55:TRP:CZ2	12:L:95:LEU:HD13	1.86	1.10
7:G:190:VAL:HG21	7:G:215:TRP:CZ2	1.86	1.10
7:U:190:VAL:CG1	7:U:215:TRP:CZ2	2.31	1.10
9:W:70:THR:HG23	9:W:72:ARG:H	1.16	1.10
12:Z:55:TRP:CZ2	12:Z:95:LEU:HD13	1.86	1.10
6:F:184:LEU:HD21	6:F:214:ILE:HG21	1.34	1.09
7:G:75:MET:HB2	7:G:137:LEU:HD21	1.26	1.09
8:H:20:THR:HG22	15:H:300:KNM:H36	1.12	1.09
9:I:1:THR:HG23	9:I:129:SER:H	1.05	1.09
12:L:136:TYR:CE1	11:Y:170:ARG:NH2	2.20	1.09
14:N:6:VAL:HG22	14:N:30:TYR:HB2	1.24	1.09
2:P:41:ASN:HB2	2:P:183:LEU:HB2	1.28	1.09
3:Q:207:SER:H	3:Q:210:LYS:HD2	1.00	1.09
5:S:42:THR:CG2	5:S:194:ALA:HB2	1.79	1.09
7:U:190:VAL:CB	7:U:215:TRP:CZ2	2.36	1.09
13:a:100:ARG:NH1	13:a:127:VAL:HB	1.68	1.09
1:A:103:TYR:C	9:I:81:ARG:NH2	2.11	1.09
5:E:229:PHE:HE2	5:E:233:GLU:CB	1.65	1.09
14:N:91:TRP:CE3	14:N:94:ARG:HB2	1.88	1.09
8:V:119:MET:CE	14:b:57:TYR:HD2	1.43	1.09
4:D:211:MET:HB2	4:D:217:LEU:HD13	1.35	1.09
4:R:40:ILE:HG23	4:R:136:PHE:HZ	1.14	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:184:LEU:HD21	6:T:214:ILE:HG21	1.34	1.09
9:W:1:THR:HG23	9:W:129:SER:H	1.05	1.08
9:I:70:THR:HG23	9:I:72:ARG:H	1.16	1.08
13:M:99:ARG:CD	13:M:104:TYR:CZ	2.35	1.08
4:R:211:MET:HB2	4:R:217:LEU:HD13	1.35	1.08
14:b:91:TRP:CE3	14:b:94:ARG:HB2	1.88	1.08
2:B:181:LEU:HD21	2:B:185:ASP:O	1.52	1.08
7:G:190:VAL:CB	7:G:215:TRP:CZ2	2.36	1.08
7:U:75:MET:HB2	7:U:137:LEU:HD21	1.26	1.08
13:M:16:ALA:HB1	13:M:119:GLY:HA3	1.22	1.08
2:P:181:LEU:HD21	2:P:185:ASP:O	1.52	1.08
9:I:1:THR:HG21	15:I:300:KNM:H42	1.28	1.08
9:W:1:THR:CG2	9:W:129:SER:H	1.65	1.08
13:M:100:ARG:NH1	13:M:127:VAL:HB	1.68	1.07
6:T:100:ASP:OD1	14:b:90:SER:OG	1.72	1.07
13:a:99:ARG:CD	13:a:104:TYR:CZ	2.35	1.07
5:S:42:THR:HG22	5:S:194:ALA:HB2	1.36	1.07
5:E:42:THR:HG22	5:E:194:ALA:HB2	1.36	1.07
1:O:103:TYR:C	9:W:81:ARG:NH2	2.11	1.07
13:a:17:GLY:HA3	13:a:166:LEU:HD22	1.19	1.07
2:B:73:LEU:HD22	2:B:133:LEU:HD13	1.10	1.07
9:I:1:THR:CG2	9:I:129:SER:H	1.65	1.07
12:L:50:ALA:C	13:M:97:TYR:HH	1.63	1.07
14:N:48:SER:HA	14:N:197:VAL:HG23	1.36	1.07
7:U:190:VAL:HG11	7:U:215:TRP:HZ2	0.90	1.07
14:N:91:TRP:CZ3	14:N:94:ARG:CB	2.38	1.06
13:M:146:GLN:HB3	10:X:176:ARG:HH22	1.16	1.06
5:S:42:THR:HG21	5:S:194:ALA:CB	1.81	1.06
14:b:4:PRO:HB3	14:b:56:ASP:OD2	1.51	1.06
14:N:4:PRO:HB3	14:N:56:ASP:OD2	1.51	1.06
8:H:32:ASP:OD2	8:H:186:ARG:NH2	1.89	1.06
5:S:229:PHE:HE2	5:S:233:GLU:CG	1.61	1.06
6:F:100:ASP:OD1	14:N:90:SER:OG	1.72	1.05
7:G:190:VAL:HB	7:G:215:TRP:CE2	1.91	1.05
5:S:42:THR:HG21	5:S:194:ALA:HB3	1.36	1.05
13:a:15:ILE:HG22	13:a:135:PHE:HB3	1.33	1.05
5:E:224:GLN:HE22	5:E:227:HIS:CE1	1.75	1.05
11:K:55:GLN:HG3	12:L:88:TYR:CD2	1.89	1.05
7:U:190:VAL:HB	7:U:215:TRP:CE2	1.91	1.05
8:V:32:ASP:OD2	8:V:186:ARG:NH2	1.89	1.05
11:Y:55:GLN:HG3	12:Z:88:TYR:CD2	1.89	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:8:GLN:OE1	11:K:115:LEU:HD23	1.57	1.05
12:L:19:ARG:HB2	12:L:171:GLY:O	1.55	1.05
14:N:16:PHE:CE1	14:N:165:ALA:C	2.28	1.05
14:b:48:SER:HA	14:b:197:VAL:HG23	1.36	1.05
7:G:190:VAL:HB	7:G:215:TRP:HE1	1.11	1.05
13:M:15:ILE:HG22	13:M:135:PHE:HB3	1.34	1.05
14:b:91:TRP:CZ3	14:b:94:ARG:CB	2.39	1.05
5:E:229:PHE:HE2	5:E:233:GLU:CG	1.61	1.05
9:I:202:TYR:OH	13:a:174:LEU:HB2	1.57	1.05
14:N:59:ASP:C	14:N:108:ASN:HD21	1.65	1.04
8:H:88:TYR:OH	14:N:62:TYR:HB2	1.51	1.04
1:A:109:ILE:CG2	1:A:114:LEU:CD2	2.14	1.04
10:J:157:MET:CG	10:J:161:HIS:CD2	2.23	1.04
2:P:140:GLU:HG2	2:P:141:GLY:H	1.22	1.04
14:b:16:PHE:CZ	14:b:166:ARG:CA	2.41	1.04
14:b:59:ASP:C	14:b:108:ASN:HD21	1.65	1.04
7:G:72:HIS:CG	7:G:105:ASN:HD21	1.75	1.04
8:V:20:THR:HG22	15:V:300:KNM:H36	1.12	1.04
11:Y:85:ARG:NH2	11:Y:86:ARG:HH22	1.55	1.04
14:b:91:TRP:CZ3	14:b:94:ARG:HB2	1.93	1.04
10:J:176:ARG:HH22	13:a:146:GLN:HB3	1.16	1.03
2:B:140:GLU:HG2	2:B:141:GLY:H	1.22	1.03
3:C:76:VAL:HG11	3:C:83:ALA:HB1	1.38	1.03
11:K:85:ARG:NH2	11:K:86:ARG:HH22	1.55	1.03
14:N:6:VAL:HG22	14:N:30:TYR:CB	1.88	1.03
14:N:16:PHE:CZ	14:N:166:ARG:CA	2.41	1.03
5:S:224:GLN:HE22	5:S:227:HIS:CE1	1.75	1.03
8:V:7:GLN:O	8:V:8:PHE:HD1	1.40	1.03
12:Z:19:ARG:HB2	12:Z:171:GLY:O	1.55	1.03
3:C:205:LYS:HB3	3:C:240:HIS:HD2	1.24	1.03
4:D:40:ILE:HG23	4:D:136:PHE:HZ	1.14	1.03
6:F:103:LEU:HD23	6:F:104:PRO:O	1.58	1.03
7:U:72:HIS:CG	7:U:105:ASN:HD21	1.75	1.03
11:Y:8:GLN:OE1	11:Y:115:LEU:HD23	1.57	1.03
3:C:24:ALA:O	3:C:28:ILE:CD1	2.07	1.03
3:Q:24:ALA:O	3:Q:28:ILE:CD1	2.07	1.03
6:T:103:LEU:HD23	6:T:104:PRO:O	1.58	1.03
8:V:1:THR:CB	15:V:300:KNM:O5	2.07	1.03
8:V:88:TYR:OH	14:b:62:TYR:HB2	1.51	1.03
11:Y:55:GLN:HG3	12:Z:88:TYR:CE2	1.94	1.03
5:E:218:ALA:HB1	5:E:226:PHE:CE1	1.95	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:229:PHE:CE2	5:E:233:GLU:HB3	1.94	1.02
7:G:75:MET:HA	7:G:137:LEU:HD23	1.41	1.02
8:H:119:MET:CE	14:N:57:TYR:CB	2.22	1.02
14:N:91:TRP:CZ3	14:N:94:ARG:HB2	1.93	1.02
3:Q:205:LYS:HB3	3:Q:240:HIS:HD2	1.24	1.02
5:S:229:PHE:HE2	5:S:233:GLU:HB3	1.22	1.02
11:K:55:GLN:HG3	12:L:88:TYR:CE2	1.94	1.02
8:V:20:THR:CG2	15:V:300:KNM:H36	1.89	1.02
13:M:174:LEU:HB2	9:W:202:TYR:OH	1.57	1.02
12:Z:39:PRO:O	12:Z:184:TRP:CD1	2.13	1.02
12:Z:50:ALA:HB1	13:a:97:TYR:CZ	1.95	1.02
14:b:6:VAL:HG22	14:b:30:TYR:CB	1.88	1.02
7:G:94:GLU:OE1	7:G:115:VAL:CG2	2.08	1.02
12:L:39:PRO:O	12:L:184:TRP:CD1	2.13	1.02
8:H:1:THR:CB	15:H:300:KNM:O5	2.07	1.01
8:H:20:THR:CG2	15:H:300:KNM:H36	1.89	1.01
1:O:165:ALA:HB3	2:P:55:LEU:CD2	1.91	1.01
5:S:229:PHE:CE2	5:S:233:GLU:HB3	1.94	1.01
8:V:119:MET:HE1	14:b:57:TYR:HB3	1.01	1.01
12:Z:45:MET:SD	15:Z:300:KNM:C20	2.49	1.01
5:E:42:THR:HG21	5:E:194:ALA:HB3	1.36	1.01
9:I:1:THR:HG21	15:I:300:KNM:C22	1.90	1.01
7:U:75:MET:HA	7:U:137:LEU:HD23	1.41	1.01
12:L:50:ALA:HB1	13:M:97:TYR:CZ	1.95	1.01
7:U:75:MET:CB	7:U:137:LEU:HD23	1.89	1.01
7:U:94:GLU:OE1	7:U:115:VAL:CG2	2.08	1.01
9:W:1:THR:HG21	15:W:300:KNM:C22	1.90	1.01
2:B:62:HIS:CE1	2:B:219:ARG:HH12	1.78	1.00
12:L:45:MET:SD	15:L:300:KNM:C20	2.49	1.00
2:P:62:HIS:CE1	2:P:219:ARG:HH12	1.78	1.00
3:C:205:LYS:HB3	3:C:240:HIS:CD2	1.96	1.00
5:E:229:PHE:CZ	5:E:233:GLU:CG	2.39	1.00
7:G:190:VAL:HG11	7:G:215:TRP:HZ2	0.90	1.00
3:Q:76:VAL:HG11	3:Q:83:ALA:HB1	1.38	1.00
14:b:46:ASN:O	14:b:48:SER:N	1.93	1.00
13:M:18:GLU:H	13:M:166:LEU:HD13	0.89	1.00
5:S:218:ALA:HB1	5:S:226:PHE:CE1	1.95	1.00
8:V:119:MET:HE1	14:b:57:TYR:CG	1.93	1.00
7:G:190:VAL:CB	7:G:215:TRP:HZ2	1.74	1.00
14:N:46:ASN:O	14:N:48:SER:N	1.93	1.00
1:O:165:ALA:O	1:O:179:LEU:HD13	1.62	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:75:MET:CB	7:G:137:LEU:HD23	1.89	0.99
3:Q:205:LYS:HB3	3:Q:240:HIS:CD2	1.96	0.99
1:A:165:ALA:HB3	2:B:55:LEU:CD2	1.91	0.99
7:U:161:TRP:O	7:U:181:MET:CE	2.10	0.99
8:V:4:MET:HB3	8:V:160:LEU:HD21	1.42	0.99
7:G:161:TRP:O	7:G:181:MET:CE	2.10	0.99
2:P:157:TRP:CE3	2:P:159:ALA:O	2.15	0.99
8:H:17:ASP:OD2	8:H:170:SER:HB2	1.63	0.99
11:K:56:PHE:HZ	11:K:84:THR:HG1	1.11	0.99
2:P:73:LEU:HD22	2:P:133:LEU:CD1	1.93	0.99
14:N:26:MET:HE1	14:N:186:ARG:HH12	1.25	0.99
1:O:76:ILE:CD1	1:O:114:LEU:CD1	2.38	0.99
2:B:157:TRP:CE3	2:B:159:ALA:O	2.15	0.98
14:N:26:MET:SD	14:N:186:ARG:NH1	2.36	0.98
11:Y:85:ARG:NH2	11:Y:86:ARG:NH2	2.11	0.98
1:A:103:TYR:C	9:I:81:ARG:HH21	1.71	0.98
13:M:20:PHE:HD2	13:M:168:LEU:HD12	1.27	0.98
12:Z:50:ALA:CA	13:a:97:TYR:OH	2.11	0.98
14:b:26:MET:SD	14:b:186:ARG:NH1	2.36	0.98
2:B:73:LEU:HD22	2:B:133:LEU:CD1	1.93	0.98
11:K:85:ARG:NH2	11:K:86:ARG:NH2	2.11	0.98
12:Z:55:TRP:CZ2	12:Z:95:LEU:CD1	2.43	0.98
7:G:75:MET:CA	7:G:137:LEU:HD23	1.94	0.98
7:G:190:VAL:CG2	7:G:215:TRP:CZ2	2.46	0.98
7:U:190:VAL:CG2	7:U:215:TRP:CZ2	2.46	0.98
1:A:165:ALA:O	1:A:179:LEU:HD13	1.62	0.98
8:V:119:MET:CE	14:b:57:TYR:CB	2.22	0.98
2:B:68:THR:HG22	2:B:71:ILE:HB	1.46	0.98
9:I:36:PHE:CE1	9:I:39:PRO:N	2.29	0.98
12:Z:50:ALA:C	13:a:97:TYR:HH	1.67	0.98
7:G:72:HIS:HB2	7:G:105:ASN:HD21	1.29	0.97
7:G:94:GLU:OE1	7:G:115:VAL:HG22	1.63	0.97
8:H:4:MET:HB3	8:H:160:LEU:HD21	1.42	0.97
2:P:73:LEU:CD2	2:P:133:LEU:HD13	1.93	0.97
7:U:190:VAL:HB	7:U:215:TRP:HE1	1.11	0.97
14:b:26:MET:HE1	14:b:186:ARG:HH12	1.26	0.97
5:E:229:PHE:HE2	5:E:233:GLU:HB3	1.22	0.97
2:P:181:LEU:HD23	2:P:186:ALA:HA	1.46	0.97
8:V:7:GLN:NE2	8:V:109:GLY:O	1.97	0.97
8:H:119:MET:HE1	14:N:57:TYR:HB3	1.01	0.97
12:L:55:TRP:CZ2	12:L:95:LEU:CD1	2.43	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:174:LEU:HD22	9:W:202:TYR:OH	1.65	0.97
8:V:17:ASP:OD2	8:V:170:SER:HB2	1.63	0.97
9:I:47:GLY:H	15:I:300:KNM:H29	1.26	0.97
7:G:190:VAL:CG1	7:G:215:TRP:CZ2	2.31	0.97
14:N:16:PHE:HZ	14:N:166:ARG:N	1.54	0.97
8:V:119:MET:HE3	14:b:57:TYR:CG	1.97	0.97
7:U:72:HIS:HB2	7:U:105:ASN:HD21	1.29	0.97
7:U:94:GLU:OE1	7:U:115:VAL:HG22	1.63	0.97
2:B:181:LEU:HD23	2:B:186:ALA:HA	1.46	0.97
7:U:75:MET:CA	7:U:137:LEU:HD23	1.94	0.97
7:U:72:HIS:CB	7:U:105:ASN:HD21	1.78	0.97
12:Z:45:MET:CG	15:Z:300:KNM:H38	1.95	0.97
7:G:72:HIS:CB	7:G:105:ASN:HD21	1.78	0.96
8:H:119:MET:HE1	14:N:57:TYR:CG	1.93	0.96
12:L:50:ALA:CA	13:M:97:TYR:OH	2.11	0.96
10:X:157:MET:CG	10:X:161:HIS:CD2	2.24	0.96
9:I:202:TYR:OH	13:a:174:LEU:HD22	1.65	0.96
2:B:73:LEU:CD2	2:B:133:LEU:HD13	1.93	0.96
14:b:145:LEU:HD21	14:b:175:VAL:HG12	1.46	0.96
12:L:45:MET:CG	15:L:300:KNM:H38	1.95	0.96
13:M:15:ILE:CG2	13:M:135:PHE:HB3	1.95	0.96
8:V:119:MET:HE2	14:b:57:TYR:CD2	1.99	0.96
9:W:36:PHE:CE1	9:W:39:PRO:N	2.29	0.96
5:S:229:PHE:CZ	5:S:233:GLU:CG	2.39	0.96
13:a:20:PHE:HD2	13:a:168:LEU:HD12	1.27	0.96
14:N:16:PHE:CE1	14:N:165:ALA:HB3	2.01	0.96
1:O:103:TYR:CA	9:W:81:ARG:HH21	1.59	0.96
1:O:103:TYR:C	9:W:81:ARG:HH21	1.71	0.96
9:W:47:GLY:H	15:W:300:KNM:H29	1.26	0.96
2:B:38:LYS:HA	2:B:43:VAL:HG22	1.48	0.96
13:a:15:ILE:CG2	13:a:135:PHE:HB3	1.95	0.96
13:a:99:ARG:CD	13:a:104:TYR:CE2	2.48	0.96
15:L:300:KNM:H21	15:L:300:KNM:C8	1.96	0.96
2:B:181:LEU:HD11	2:B:185:ASP:HB3	1.48	0.95
9:I:172:ASN:OD1	9:I:191:VAL:HA	1.66	0.95
2:P:38:LYS:HA	2:P:43:VAL:HG22	1.48	0.95
9:W:172:ASN:OD1	9:W:191:VAL:HA	1.66	0.95
12:L:140:ASP:OD2	11:Y:170:ARG:CD	2.15	0.95
8:V:1:THR:N	15:V:300:KNM:O5	1.99	0.95
13:M:99:ARG:CD	13:M:104:TYR:CE2	2.48	0.95
3:C:76:VAL:HG11	3:C:83:ALA:CB	1.97	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:181:LEU:HD11	2:P:185:ASP:HB3	1.48	0.95
2:B:51:GLN:CG	2:B:54:ILE:HA	1.97	0.95
3:Q:76:VAL:HG11	3:Q:83:ALA:CB	1.97	0.95
9:W:146:MET:HE1	9:W:154:LEU:HD23	1.47	0.95
13:M:15:ILE:HD11	13:M:175:VAL:CG2	1.96	0.95
14:N:145:LEU:HD21	14:N:175:VAL:HG12	1.46	0.95
3:Q:198:ASN:OD1	3:Q:240:HIS:CE1	2.20	0.95
14:b:16:PHE:CE1	14:b:165:ALA:HB3	2.01	0.95
7:U:190:VAL:CB	7:U:215:TRP:HE1	1.79	0.95
3:C:24:ALA:O	3:C:28:ILE:HD12	1.64	0.95
8:H:119:MET:HE2	14:N:57:TYR:CD2	1.99	0.95
11:K:170:ARG:CD	12:Z:140:ASP:OD2	2.15	0.94
2:P:51:GLN:CG	2:P:54:ILE:HA	1.97	0.94
13:a:15:ILE:HD11	13:a:175:VAL:CG2	1.96	0.94
8:H:1:THR:N	15:H:300:KNM:O5	1.99	0.94
9:I:146:MET:HE1	9:I:154:LEU:HD23	1.47	0.94
1:A:76:ILE:CD1	1:A:114:LEU:CD1	2.38	0.94
2:B:137:GLY:O	2:B:144:TYR:N	2.00	0.94
11:Y:52:ASP:OD1	12:Z:88:TYR:OH	1.85	0.94
15:Z:300:KNM:C8	15:Z:300:KNM:H21	1.96	0.94
7:G:190:VAL:CB	7:G:215:TRP:HE1	1.79	0.94
8:H:88:TYR:CE2	14:N:62:TYR:HB2	2.01	0.94
10:J:176:ARG:NH2	13:a:146:GLN:HB3	1.83	0.94
7:U:190:VAL:CB	7:U:215:TRP:HZ2	1.74	0.94
2:P:157:TRP:HE3	2:P:159:ALA:O	1.49	0.94
4:R:192:ILE:CG1	4:R:228:TYR:CD1	2.50	0.94
8:V:88:TYR:CE2	14:b:62:TYR:HB2	2.01	0.94
2:P:68:THR:HG22	2:P:71:ILE:HB	1.46	0.94
2:P:133:LEU:CD1	2:P:135:ILE:HG12	1.98	0.94
3:C:198:ASN:OD1	3:C:240:HIS:CE1	2.20	0.94
14:N:59:ASP:CB	14:N:108:ASN:ND2	2.31	0.94
9:W:1:THR:N	9:W:169:SER:OG	2.01	0.94
14:b:59:ASP:CB	14:b:108:ASN:ND2	2.31	0.94
1:A:76:ILE:HD13	1:A:114:LEU:HD12	1.50	0.94
4:D:192:ILE:CG1	4:D:228:TYR:CD1	2.50	0.94
13:M:152:GLN:HB3	9:W:202:TYR:CE2	2.03	0.94
1:A:103:TYR:CA	9:I:81:ARG:HH21	1.59	0.93
1:A:161:CYS:SG	1:A:163:PHE:HE1	1.91	0.93
13:a:18:GLU:H	13:a:166:LEU:HD13	0.89	0.93
2:B:133:LEU:CD1	2:B:135:ILE:HG12	1.98	0.93
14:N:16:PHE:HZ	14:N:165:ALA:C	1.72	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:7:GLN:O	8:V:8:PHE:CD1	2.21	0.93
10:J:16:LYS:O	10:J:18:CYS:N	2.01	0.93
11:K:52:ASP:OD1	12:L:88:TYR:OH	1.85	0.93
1:O:161:CYS:SG	1:O:163:PHE:HE1	1.91	0.93
13:M:146:GLN:HB3	10:X:176:ARG:NH2	1.83	0.93
14:b:10:SER:OG	14:b:25:ASP:OD1	1.87	0.93
9:I:1:THR:N	9:I:169:SER:OG	2.01	0.93
12:L:17:ASP:OD2	12:L:170:SER:HB3	1.69	0.93
10:X:16:LYS:O	10:X:18:CYS:N	2.01	0.93
12:Z:17:ASP:OD2	12:Z:170:SER:HB3	1.69	0.93
14:b:16:PHE:HE2	14:b:21:VAL:HB	0.76	0.93
8:H:4:MET:CB	8:H:160:LEU:HD21	1.99	0.93
14:N:16:PHE:CE1	14:N:165:ALA:CA	2.52	0.93
1:O:109:ILE:CG2	1:O:114:LEU:CD2	2.14	0.93
3:Q:24:ALA:O	3:Q:28:ILE:HD12	1.64	0.93
9:I:202:TYR:CE2	13:a:152:GLN:HB3	2.03	0.93
2:P:137:GLY:O	2:P:144:TYR:N	2.00	0.93
13:M:152:GLN:CB	9:W:202:TYR:CE2	2.51	0.92
5:S:70:ILE:HD11	5:S:76:CYS:CB	1.99	0.92
12:L:45:MET:HG2	15:L:300:KNM:H38	1.50	0.92
2:B:157:TRP:HE3	2:B:159:ALA:O	1.48	0.92
9:I:104:ASP:O	9:I:107:GLY:N	2.03	0.92
4:D:40:ILE:HG23	4:D:136:PHE:CZ	2.04	0.92
9:I:202:TYR:CE2	13:a:152:GLN:CB	2.51	0.92
14:N:10:SER:OG	14:N:25:ASP:OD1	1.87	0.92
14:b:26:MET:HE2	14:b:186:ARG:HH12	0.76	0.92
8:V:4:MET:CB	8:V:160:LEU:HD21	1.99	0.91
14:b:16:PHE:CE1	14:b:165:ALA:CA	2.52	0.91
13:a:106:VAL:HG12	13:a:108:ASN:OD1	1.70	0.91
7:G:75:MET:CB	7:G:137:LEU:HD21	1.92	0.91
15:I:300:KNM:H12	10:J:124:ASP:OD1	1.71	0.91
11:K:44:LEU:HD23	11:K:102:LEU:CD1	2.01	0.91
14:N:91:TRP:CE3	14:N:94:ARG:CB	2.53	0.91
6:T:43:HIS:CG	6:T:184:LEU:HD22	2.06	0.91
4:D:36:ARG:HG3	4:D:142:PRO:HB2	1.53	0.91
5:E:70:ILE:HD11	5:E:76:CYS:CB	1.99	0.91
8:H:119:MET:HE3	14:N:57:TYR:CG	1.97	0.91
14:N:16:PHE:HE2	14:N:21:VAL:HB	0.76	0.91
1:A:76:ILE:HD12	1:A:114:LEU:HD11	1.52	0.91
7:G:190:VAL:CB	7:G:215:TRP:NE1	2.33	0.91
4:R:40:ILE:HG23	4:R:136:PHE:CZ	2.04	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:122:SER:HB3	10:X:136:VAL:HG11	1.52	0.91
2:B:138:TRP:NE1	2:B:143:PRO:CD	2.33	0.91
14:b:91:TRP:CE3	14:b:94:ARG:CB	2.53	0.91
14:N:26:MET:HE2	14:N:186:ARG:HH12	0.76	0.91
13:a:18:GLU:H	13:a:166:LEU:CD1	1.82	0.91
14:b:48:SER:CA	14:b:197:VAL:HG23	2.01	0.91
9:I:47:GLY:H	15:I:300:KNM:H28	1.35	0.91
13:M:106:VAL:HG12	13:M:108:ASN:OD1	1.70	0.91
11:Y:44:LEU:HD23	11:Y:102:LEU:CD1	2.01	0.91
11:Y:56:PHE:HZ	11:Y:84:THR:HG1	1.14	0.91
13:a:36:HIS:HB3	14:b:132:TYR:OH	1.70	0.91
8:H:45:ARG:HE	15:H:300:KNM:C19	1.84	0.91
14:N:193:THR:O	14:N:196:GLY:N	2.04	0.91
1:O:76:ILE:HD12	1:O:114:LEU:HD11	1.52	0.90
15:W:300:KNM:H12	10:X:124:ASP:OD1	1.71	0.90
14:b:193:THR:O	14:b:196:GLY:N	2.04	0.90
13:M:36:HIS:HB3	14:N:132:TYR:OH	1.70	0.90
14:N:48:SER:CA	14:N:197:VAL:HG23	2.01	0.90
14:b:4:PRO:HB2	14:b:56:ASP:OD2	1.71	0.90
3:C:207:SER:N	3:C:210:LYS:HD2	1.86	0.90
14:b:6:VAL:HG22	14:b:30:TYR:CG	2.07	0.90
2:P:138:TRP:NE1	2:P:143:PRO:CD	2.33	0.90
10:J:137:VAL:CG2	10:J:146:TYR:CZ	2.54	0.90
9:W:104:ASP:O	9:W:107:GLY:N	2.03	0.90
6:F:43:HIS:CG	6:F:184:LEU:HD22	2.05	0.90
10:J:122:SER:HB3	10:J:136:VAL:HG11	1.52	0.90
14:N:21:VAL:CG2	14:N:191:THR:HG22	2.02	0.90
7:U:75:MET:CB	7:U:137:LEU:HD21	1.92	0.90
14:N:6:VAL:HG22	14:N:30:TYR:CG	2.07	0.90
10:X:137:VAL:CG2	10:X:146:TYR:CZ	2.54	0.90
8:V:115:PRO:HD2	8:V:119:MET:O	1.71	0.89
13:a:20:PHE:CD2	13:a:168:LEU:HD12	2.07	0.89
1:O:76:ILE:HD13	1:O:114:LEU:HD12	1.50	0.89
13:a:18:GLU:N	13:a:166:LEU:CD1	2.31	0.89
5:E:229:PHE:CE2	5:E:233:GLU:CB	2.47	0.89
4:R:36:ARG:HG3	4:R:142:PRO:HB2	1.53	0.89
13:M:20:PHE:CD2	13:M:168:LEU:HD12	2.07	0.89
10:J:137:VAL:CG2	10:J:146:TYR:CE1	2.55	0.89
8:V:1:THR:OG1	15:V:300:KNM:O5	1.88	0.89
9:W:47:GLY:N	15:W:300:KNM:H28	1.88	0.89
10:X:137:VAL:CG2	10:X:146:TYR:CE1	2.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:21:VAL:CG2	14:b:191:THR:HG22	2.02	0.89
13:M:18:GLU:N	13:M:166:LEU:CD1	2.31	0.89
8:H:115:PRO:HD2	8:H:119:MET:O	1.71	0.89
14:N:9:THR:HG22	14:N:10:SER:H	1.38	0.89
9:W:47:GLY:N	15:W:300:KNM:C16	2.35	0.89
3:C:76:VAL:HG13	3:C:134:LEU:HD21	1.55	0.89
14:N:4:PRO:HB2	14:N:56:ASP:OD2	1.71	0.89
7:U:190:VAL:CB	7:U:215:TRP:NE1	2.33	0.89
8:V:45:ARG:HE	15:V:300:KNM:C19	1.84	0.89
9:W:47:GLY:H	15:W:300:KNM:H28	1.35	0.89
9:I:47:GLY:N	15:I:300:KNM:C16	2.35	0.88
9:I:1:THR:HG23	9:I:129:SER:N	1.87	0.88
14:N:6:VAL:CG2	14:N:30:TYR:HB2	2.03	0.88
5:S:35:SER:HB2	5:S:66:LYS:NZ	1.88	0.88
4:R:192:ILE:HG13	4:R:228:TYR:HD1	1.04	0.88
3:Q:207:SER:N	3:Q:210:LYS:HD2	1.86	0.88
9:W:1:THR:HG23	9:W:129:SER:N	1.87	0.88
5:E:35:SER:HB2	5:E:66:LYS:NZ	1.88	0.88
7:G:72:HIS:CG	7:G:105:ASN:ND2	2.42	0.88
14:N:25:ASP:O	14:N:41:ARG:NH1	2.07	0.88
5:S:229:PHE:CE2	5:S:233:GLU:CB	2.47	0.88
3:Q:76:VAL:HG13	3:Q:134:LEU:HD21	1.55	0.88
12:Z:45:MET:HG2	15:Z:300:KNM:H38	1.51	0.88
13:M:18:GLU:H	13:M:166:LEU:CD1	1.82	0.88
15:W:300:KNM:H12	10:X:124:ASP:CG	1.99	0.88
14:b:16:PHE:HZ	14:b:166:ARG:N	1.54	0.88
11:K:151:ILE:HG13	11:K:152:SER:H	1.40	0.87
9:I:59:ILE:HG22	9:I:63:LEU:HD13	1.57	0.87
15:I:300:KNM:H12	10:J:124:ASP:CG	1.99	0.87
11:K:78:THR:HG22	11:K:116:TYR:OH	1.74	0.87
13:M:49:LYS:HB3	13:M:113:LEU:H	1.40	0.87
4:D:192:ILE:HG13	4:D:228:TYR:HD1	1.04	0.87
9:I:47:GLY:N	15:I:300:KNM:H28	1.88	0.87
13:M:17:GLY:CA	13:M:166:LEU:HD22	2.04	0.87
14:b:16:PHE:HE1	14:b:166:ARG:N	1.34	0.87
3:C:157:GLY:O	3:C:159:TRP:HD1	1.56	0.87
6:F:13:TRP:CD1	7:G:22:GLN:HE21	1.93	0.87
7:U:190:VAL:CB	7:U:215:TRP:CE2	2.56	0.87
13:a:17:GLY:CA	13:a:166:LEU:HD22	2.04	0.87
10:J:134:ASP:OD1	10:J:135:PHE:N	2.07	0.87
14:N:9:THR:O	14:N:10:SER:OG	1.93	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:46:CYS:HB2	11:Y:102:LEU:HD12	1.55	0.87
11:K:85:ARG:HH22	11:K:86:ARG:HH22	1.18	0.87
12:L:45:MET:SD	15:L:300:KNM:H36	2.14	0.87
6:T:13:TRP:CD1	7:U:22:GLN:HE21	1.93	0.87
7:U:72:HIS:CG	7:U:105:ASN:ND2	2.42	0.87
14:b:6:VAL:CG2	14:b:30:TYR:HB2	2.03	0.87
14:N:16:PHE:CD1	14:N:165:ALA:HB3	2.10	0.86
5:S:166:ASP:HB3	5:S:185:TYR:HH	1.31	0.86
9:W:59:ILE:HG22	9:W:63:LEU:HD13	1.56	0.86
6:F:13:TRP:CD1	7:G:22:GLN:NE2	2.43	0.86
11:K:46:CYS:HB2	11:K:102:LEU:HD12	1.55	0.86
11:Y:151:ILE:HG13	11:Y:152:SER:H	1.40	0.86
14:b:9:THR:O	14:b:10:SER:OG	1.93	0.86
1:A:103:TYR:O	9:I:81:ARG:NH2	2.08	0.86
2:B:172:PHE:CE2	2:B:196:GLU:CD	2.54	0.86
1:O:103:TYR:O	9:W:81:ARG:NH2	2.08	0.86
9:W:1:THR:HG22	9:W:129:SER:HB2	1.57	0.86
13:a:49:LYS:HB3	13:a:113:LEU:H	1.40	0.86
12:Z:50:ALA:O	13:a:97:TYR:OH	1.90	0.86
9:I:1:THR:HG22	9:I:129:SER:CB	2.06	0.86
14:N:16:PHE:HE1	14:N:166:ARG:N	1.34	0.86
9:W:1:THR:HG22	9:W:129:SER:CB	2.06	0.86
10:J:137:VAL:HG22	10:J:146:TYR:CE1	2.11	0.86
14:b:25:ASP:O	14:b:41:ARG:NH1	2.07	0.86
2:B:140:GLU:CG	2:B:141:GLY:H	1.89	0.86
11:Y:78:THR:HG22	11:Y:116:TYR:OH	1.74	0.86
10:X:134:ASP:OD1	10:X:135:PHE:N	2.07	0.86
1:A:13:ILE:O	1:A:15:ILE:HG12	1.75	0.86
11:K:44:LEU:HB3	11:K:102:LEU:HD11	1.57	0.86
2:P:181:LEU:HD21	2:P:185:ASP:C	2.01	0.86
6:T:13:TRP:CD1	7:U:22:GLN:NE2	2.43	0.86
8:V:98:ILE:CG2	8:V:100:ILE:HG13	2.05	0.86
14:b:9:THR:HG22	14:b:10:SER:H	1.38	0.86
13:M:100:ARG:HH11	13:M:127:VAL:HB	1.40	0.86
2:P:140:GLU:OE2	2:P:144:TYR:OH	1.94	0.86
3:Q:157:GLY:O	3:Q:159:TRP:HD1	1.56	0.86
11:K:44:LEU:HG	11:K:102:LEU:HD21	1.57	0.85
2:P:172:PHE:CE2	2:P:196:GLU:CD	2.54	0.85
8:V:20:THR:CG2	15:V:300:KNM:C20	2.49	0.85
12:Z:45:MET:SD	15:Z:300:KNM:H36	2.14	0.85
8:H:1:THR:OG1	15:H:300:KNM:O5	1.88	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:THR:CG2	15:H:300:KNM:C20	2.49	0.85
9:I:1:THR:HG22	9:I:129:SER:HB2	1.57	0.85
12:Z:45:MET:SD	15:Z:300:KNM:H38	2.15	0.85
14:b:16:PHE:CD1	14:b:165:ALA:HB3	2.10	0.85
15:L:300:KNM:H18	15:L:300:KNM:H29	1.59	0.85
7:U:181:MET:O	7:U:184:MET:N	2.09	0.85
10:X:137:VAL:HG22	10:X:146:TYR:CE1	2.11	0.85
11:Y:44:LEU:HB3	11:Y:102:LEU:HD11	1.57	0.85
7:G:190:VAL:CB	7:G:215:TRP:CE2	2.56	0.85
9:I:202:TYR:CE2	13:a:152:GLN:HG3	2.11	0.85
1:O:13:ILE:O	1:O:15:ILE:HG12	1.76	0.85
7:G:181:MET:O	7:G:184:MET:N	2.09	0.85
13:M:174:LEU:CD1	9:W:202:TYR:CE2	2.59	0.85
2:P:216:GLY:O	2:P:218:ARG:HG3	1.77	0.85
2:P:39:ALA:HB2	2:P:186:ALA:CB	2.07	0.85
2:P:140:GLU:CG	2:P:141:GLY:H	1.89	0.85
2:P:51:GLN:HG3	2:P:54:ILE:HA	1.59	0.85
2:B:181:LEU:HD21	2:B:185:ASP:C	2.01	0.85
13:M:16:ALA:CB	13:M:119:GLY:HA3	2.07	0.84
13:a:16:ALA:CB	13:a:119:GLY:HA3	2.07	0.84
14:N:91:TRP:CE3	14:N:94:ARG:HG3	2.11	0.84
8:H:98:ILE:CG2	8:H:100:ILE:HG13	2.05	0.84
15:I:300:KNM:H13	15:I:300:KNM:C1	2.08	0.84
8:V:45:ARG:NE	15:V:300:KNM:H33	1.92	0.84
15:Z:300:KNM:H18	15:Z:300:KNM:H29	1.59	0.84
8:H:17:ASP:OD2	8:H:170:SER:CB	2.24	0.84
2:B:181:LEU:CD2	2:B:185:ASP:O	2.25	0.84
14:N:91:TRP:CE3	14:N:94:ARG:CG	2.60	0.84
8:V:17:ASP:OD2	8:V:170:SER:CB	2.24	0.84
12:Z:149:VAL:O	12:Z:153:TYR:CD1	2.31	0.84
4:D:184:ASP:O	4:D:188:ILE:HD13	1.75	0.84
5:S:42:THR:HG23	5:S:194:ALA:CB	2.08	0.84
11:Y:85:ARG:HH22	11:Y:86:ARG:HH22	1.18	0.84
14:b:91:TRP:CE3	14:b:94:ARG:CG	2.60	0.84
14:b:91:TRP:CE3	14:b:94:ARG:HG3	2.11	0.84
2:B:140:GLU:OE2	2:B:144:TYR:OH	1.94	0.84
8:H:22:THR:HB	15:H:300:KNM:H13	1.58	0.84
8:H:45:ARG:HE	15:H:300:KNM:H33	1.41	0.84
10:J:64:GLN:HE21	11:K:85:ARG:NH2	1.75	0.84
14:N:16:PHE:HZ	14:N:166:ARG:CA	1.87	0.84
9:I:36:PHE:CE1	9:I:38:SER:CA	2.61	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:47:GLY:O	15:H:300:KNM:C13	2.25	0.84
8:V:9:ASP:OD2	8:V:149:LYS:HB2	1.78	0.84
9:W:36:PHE:CE1	9:W:38:SER:CA	2.61	0.84
1:A:161:CYS:SG	1:A:163:PHE:CE1	2.69	0.84
12:L:45:MET:SD	15:L:300:KNM:H38	2.15	0.84
4:R:184:ASP:O	4:R:188:ILE:HD13	1.75	0.84
11:Y:44:LEU:HG	11:Y:102:LEU:HD21	1.57	0.84
2:B:39:ALA:HB2	2:B:186:ALA:CB	2.07	0.83
2:B:216:GLY:O	2:B:218:ARG:HG3	1.77	0.83
9:I:129:SER:OG	15:I:300:KNM:C22	2.26	0.83
1:A:165:ALA:HB3	2:B:55:LEU:HD23	1.59	0.83
12:L:149:VAL:O	12:L:153:TYR:CD1	2.31	0.83
2:B:181:LEU:CD2	2:B:185:ASP:C	2.52	0.83
8:V:22:THR:HB	15:V:300:KNM:H13	1.58	0.83
10:X:157:MET:HG2	10:X:161:HIS:HD2	0.67	0.83
2:P:181:LEU:CD2	2:P:185:ASP:C	2.52	0.83
9:W:129:SER:OG	15:W:300:KNM:C22	2.26	0.83
2:B:138:TRP:CE2	2:B:143:PRO:HD3	2.14	0.83
3:C:205:LYS:HA	3:C:240:HIS:NE2	1.94	0.83
5:E:42:THR:HG23	5:E:194:ALA:CB	2.07	0.83
6:F:13:TRP:HB2	7:G:22:GLN:NE2	1.94	0.83
9:I:202:TYR:CE2	13:a:174:LEU:CD1	2.59	0.83
8:V:45:ARG:HE	15:V:300:KNM:H33	1.41	0.83
15:W:300:KNM:H13	15:W:300:KNM:C1	2.08	0.83
2:B:172:PHE:HE2	2:B:196:GLU:CD	1.87	0.83
6:T:13:TRP:HB2	7:U:22:GLN:NE2	1.94	0.83
1:A:161:CYS:HG	1:A:163:PHE:HE1	1.19	0.82
8:H:45:ARG:NE	15:H:300:KNM:H33	1.92	0.82
8:V:10:GLY:O	8:V:103:TRP:NE1	2.12	0.82
14:N:16:PHE:CE1	14:N:165:ALA:CB	2.62	0.82
14:N:26:MET:HB2	14:N:186:ARG:CZ	2.08	0.82
8:V:47:GLY:O	15:V:300:KNM:C13	2.25	0.82
2:B:51:GLN:HG3	2:B:54:ILE:HA	1.59	0.82
1:O:161:CYS:SG	1:O:163:PHE:CE1	2.69	0.82
2:P:138:TRP:CE2	2:P:143:PRO:HD3	2.14	0.82
3:Q:205:LYS:HA	3:Q:240:HIS:NE2	1.94	0.82
5:S:218:ALA:HB1	5:S:226:PHE:CZ	2.14	0.82
10:J:157:MET:HG2	10:J:161:HIS:HD2	0.67	0.82
14:N:59:ASP:CB	14:N:108:ASN:HD21	1.91	0.82
2:P:181:LEU:CD2	2:P:185:ASP:O	2.25	0.82
8:V:88:TYR:OH	14:b:62:TYR:CD2	2.32	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:26:MET:HB2	14:b:186:ARG:CZ	2.08	0.82
4:D:36:ARG:CG	4:D:142:PRO:HB2	2.10	0.82
6:F:49:LEU:HB2	6:F:195:LEU:HD11	1.62	0.82
11:Y:44:LEU:HD23	11:Y:102:LEU:HD13	1.61	0.82
14:b:59:ASP:CB	14:b:108:ASN:HD21	1.91	0.82
8:H:88:TYR:OH	14:N:62:TYR:CD2	2.32	0.82
13:M:152:GLN:HG3	9:W:202:TYR:CE2	2.11	0.82
1:O:165:ALA:HB3	2:P:55:LEU:HD23	1.59	0.82
2:P:183:LEU:HD13	2:P:213:ASN:OD1	1.80	0.82
10:X:64:GLN:HE21	11:Y:85:ARG:NH2	1.75	0.82
13:M:152:GLN:CD	9:W:202:TYR:CD2	2.57	0.82
1:A:103:TYR:O	9:I:81:ARG:NE	2.13	0.81
4:R:36:ARG:CG	4:R:142:PRO:HB2	2.10	0.81
8:V:115:PRO:HG3	14:b:36:PHE:HZ	1.44	0.81
9:I:122:LEU:HG	9:I:123:PRO:HD2	1.61	0.81
9:I:202:TYR:CD2	13:a:152:GLN:CD	2.57	0.81
6:T:49:LEU:HB2	6:T:195:LEU:HD11	1.62	0.81
6:T:77:LEU:CD1	6:T:80:ASP:H	1.93	0.81
14:N:26:MET:HE1	14:N:186:ARG:NH1	1.85	0.81
14:b:16:PHE:CE1	14:b:165:ALA:CB	2.62	0.81
12:L:50:ALA:O	13:M:97:TYR:OH	1.90	0.81
5:S:147:ASP:O	5:S:150:GLY:N	2.12	0.81
5:E:218:ALA:HB1	5:E:226:PHE:CZ	2.14	0.81
4:R:192:ILE:HG13	4:R:228:TYR:CE1	2.16	0.81
2:B:183:LEU:HD13	2:B:213:ASN:OD1	1.80	0.81
8:H:10:GLY:O	8:H:103:TRP:NE1	2.14	0.81
6:F:77:LEU:CD1	6:F:80:ASP:H	1.93	0.81
2:P:39:ALA:HB1	2:P:181:LEU:O	1.81	0.81
7:G:75:MET:CG	7:G:137:LEU:HD21	2.11	0.81
1:O:103:TYR:O	9:W:81:ARG:NE	2.13	0.81
2:P:172:PHE:HE2	2:P:196:GLU:CD	1.87	0.81
5:E:147:ASP:O	5:E:150:GLY:N	2.12	0.80
8:H:9:ASP:OD2	8:H:149:LYS:HB2	1.79	0.80
5:S:42:THR:CG2	5:S:194:ALA:HB1	2.11	0.80
9:W:70:THR:HG23	9:W:72:ARG:N	1.96	0.80
9:I:70:THR:HG23	9:I:72:ARG:N	1.96	0.80
9:W:122:LEU:HG	9:W:123:PRO:HD2	1.61	0.80
2:B:51:GLN:O	2:B:51:GLN:NE2	2.14	0.80
4:D:192:ILE:HG13	4:D:228:TYR:CE1	2.15	0.80
14:N:59:ASP:HB3	14:N:108:ASN:ND2	1.96	0.80
2:P:51:GLN:CD	2:P:54:ILE:HA	2.07	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:59:ASP:C	14:b:108:ASN:ND2	2.40	0.80
14:b:91:TRP:HE3	14:b:94:ARG:CG	1.95	0.80
8:H:115:PRO:HG3	14:N:36:PHE:HZ	1.44	0.80
10:J:26:ARG:HD2	10:J:33:MET:HG3	1.64	0.80
14:N:21:VAL:HG23	14:N:191:THR:HG22	1.63	0.80
14:N:91:TRP:HE3	14:N:94:ARG:CG	1.95	0.80
12:Z:42:LEU:HD11	12:Z:184:TRP:CD2	2.16	0.80
13:a:27:THR:HG22	13:a:40:SER:O	1.82	0.80
13:a:100:ARG:HH11	13:a:127:VAL:HB	1.40	0.80
11:K:44:LEU:HD23	11:K:102:LEU:HD13	1.61	0.80
11:K:67:TYR:CE1	11:K:75:LEU:HG	2.17	0.80
12:L:42:LEU:HD11	12:L:184:TRP:CD2	2.16	0.80
13:a:36:HIS:HB3	14:b:132:TYR:CZ	2.17	0.80
13:M:17:GLY:C	13:M:166:LEU:HD13	2.06	0.80
14:b:16:PHE:HZ	14:b:166:ARG:CA	1.87	0.80
13:M:27:THR:HG22	13:M:40:SER:O	1.82	0.80
13:M:46:LEU:HD23	13:M:72:LEU:HD21	1.64	0.80
2:P:51:GLN:NE2	2:P:51:GLN:O	2.14	0.80
5:S:229:PHE:HZ	5:S:233:GLU:HG2	1.39	0.80
12:Z:105:ASP:HB2	12:Z:108:GLY:O	1.82	0.80
2:B:51:GLN:HE22	2:B:56:TYR:HB2	1.47	0.79
8:H:45:ARG:NE	15:H:300:KNM:C19	2.45	0.79
12:L:141:ARG:HB3	11:Y:146:TYR:OH	1.82	0.79
8:V:45:ARG:NE	15:V:300:KNM:C19	2.45	0.79
13:a:17:GLY:C	13:a:166:LEU:HD13	2.06	0.79
14:b:26:MET:HE1	14:b:186:ARG:NH1	1.85	0.79
14:b:59:ASP:HB3	14:b:108:ASN:ND2	1.96	0.79
9:I:43:CYS:SG	9:I:98:LEU:HD22	2.22	0.79
1:A:103:TYR:HA	9:I:81:ARG:HH21	1.15	0.79
5:E:229:PHE:HZ	5:E:233:GLU:HG2	1.39	0.79
7:G:190:VAL:CG2	7:G:215:TRP:CE2	2.65	0.79
9:I:1:THR:HG21	9:I:129:SER:OG	1.83	0.79
11:K:146:TYR:OH	12:Z:141:ARG:HB3	1.82	0.79
13:M:36:HIS:HB3	14:N:132:TYR:CZ	2.17	0.79
7:U:75:MET:CG	7:U:137:LEU:HD21	2.11	0.79
11:Y:67:TYR:CE1	11:Y:75:LEU:HG	2.17	0.79
14:b:21:VAL:HG23	14:b:191:THR:HG22	1.63	0.79
14:b:115:TYR:OH	14:b:118:GLY:HA2	1.83	0.79
2:P:51:GLN:HE22	2:P:56:TYR:HB2	1.47	0.79
11:Y:46:CYS:SG	11:Y:100:VAL:HB	2.23	0.79
2:B:39:ALA:HB1	2:B:181:LEU:O	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:154:GLU:OE2	10:J:161:HIS:NE2	2.16	0.79
7:U:94:GLU:OE1	7:U:115:VAL:HG23	1.82	0.79
9:W:1:THR:CG2	15:W:300:KNM:H42	2.11	0.79
10:X:55:LEU:O	10:X:59:VAL:HG23	1.83	0.79
6:F:152:ASN:HA	7:G:85:ARG:HH12	1.48	0.79
5:S:70:ILE:HD11	5:S:76:CYS:HB3	1.64	0.79
6:T:152:ASN:HA	7:U:85:ARG:HH12	1.48	0.79
9:W:1:THR:HG21	9:W:129:SER:OG	1.83	0.79
14:b:16:PHE:CZ	14:b:166:ARG:HA	2.18	0.79
13:M:174:LEU:HD13	9:W:202:TYR:HE2	1.46	0.79
2:P:42:GLY:N	2:P:183:LEU:HD12	1.98	0.79
7:U:181:MET:O	7:U:183:GLU:N	2.16	0.79
10:X:26:ARG:HD2	10:X:33:MET:HG3	1.64	0.79
10:X:154:GLU:OE2	10:X:161:HIS:NE2	2.16	0.79
2:B:42:GLY:N	2:B:183:LEU:HD12	1.98	0.78
12:L:105:ASP:HB2	12:L:108:GLY:O	1.82	0.78
8:V:32:ASP:CG	8:V:186:ARG:NH2	2.41	0.78
9:I:1:THR:CG2	9:I:129:SER:OG	2.31	0.78
14:N:59:ASP:C	14:N:108:ASN:ND2	2.40	0.78
14:N:115:TYR:OH	14:N:118:GLY:HA2	1.83	0.78
7:U:190:VAL:CG2	7:U:215:TRP:CE2	2.65	0.78
9:W:43:CYS:SG	9:W:98:LEU:HD22	2.22	0.78
13:a:46:LEU:HD23	13:a:72:LEU:HD21	1.64	0.78
9:I:1:THR:CG2	15:I:300:KNM:H42	2.11	0.78
9:I:202:TYR:CZ	13:a:174:LEU:HD13	2.18	0.78
9:W:1:THR:CG2	9:W:129:SER:OG	2.31	0.78
11:Y:55:GLN:CG	12:Z:88:TYR:CD2	2.66	0.78
13:a:54:CYS:SG	13:a:108:ASN:ND2	2.57	0.78
12:L:19:ARG:CB	12:L:171:GLY:O	2.31	0.78
12:Z:36:GLU:HA	12:Z:42:LEU:HD22	1.66	0.78
11:K:46:CYS:SG	11:K:100:VAL:HB	2.23	0.78
10:X:137:VAL:HG23	10:X:146:TYR:CD2	2.19	0.78
12:Z:55:TRP:HD1	12:Z:97:MET:SD	2.07	0.78
7:G:94:GLU:OE1	7:G:115:VAL:HG23	1.82	0.78
7:G:190:VAL:HB	7:G:215:TRP:CZ2	2.14	0.78
13:M:47:THR:O	13:M:203:ILE:HD11	1.84	0.78
2:P:39:ALA:HB2	2:P:186:ALA:HB3	1.66	0.78
5:S:224:GLN:NE2	5:S:227:HIS:CE1	2.46	0.78
7:G:181:MET:O	7:G:183:GLU:N	2.16	0.78
8:H:32:ASP:CG	8:H:186:ARG:NH2	2.41	0.78
10:J:137:VAL:CG2	10:J:146:TYR:CD1	2.68	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:MET:CB	14:N:186:ARG:NH2	2.46	0.78
5:S:169:ALA:O	5:S:174:SER:OG	2.02	0.78
8:V:27:ALA:O	8:V:28:ASN:HB3	1.84	0.78
12:Z:19:ARG:CB	12:Z:171:GLY:O	2.31	0.78
2:B:51:GLN:CD	2:B:54:ILE:HA	2.07	0.77
2:B:147:GLN:NE2	2:B:162:MET:SD	2.57	0.77
9:I:202:TYR:HE2	13:a:174:LEU:HD13	1.46	0.77
9:W:172:ASN:HD21	9:W:191:VAL:HG22	1.49	0.77
6:F:15:PRO:HD2	6:F:16:GLN:OE1	1.83	0.77
11:Y:8:GLN:OE1	11:Y:115:LEU:CD2	2.32	0.77
10:J:55:LEU:O	10:J:59:VAL:HG23	1.83	0.77
13:M:174:LEU:HD13	9:W:202:TYR:CZ	2.18	0.77
13:M:54:CYS:SG	13:M:108:ASN:ND2	2.57	0.77
3:Q:24:ALA:O	3:Q:28:ILE:HD11	1.85	0.77
8:H:27:ALA:O	8:H:28:ASN:HB3	1.84	0.77
13:M:106:VAL:CG1	13:M:108:ASN:HD21	1.97	0.77
13:M:152:GLN:CG	9:W:202:TYR:CE2	2.67	0.77
14:N:91:TRP:HE3	14:N:94:ARG:HG3	1.47	0.77
13:a:106:VAL:CG1	13:a:108:ASN:HD21	1.97	0.77
12:L:36:GLU:HA	12:L:42:LEU:HD22	1.66	0.77
5:E:70:ILE:HD11	5:E:76:CYS:HB3	1.64	0.77
8:H:119:MET:HE3	14:N:57:TYR:HD2	0.69	0.77
2:B:39:ALA:HB2	2:B:186:ALA:HB3	1.66	0.77
4:D:192:ILE:CG1	4:D:228:TYR:CE1	2.68	0.77
5:E:169:ALA:O	5:E:174:SER:OG	2.02	0.77
8:H:98:ILE:HG21	8:H:100:ILE:HG13	1.67	0.77
10:J:137:VAL:HG23	10:J:146:TYR:CD2	2.19	0.77
14:N:4:PRO:CA	14:N:56:ASP:OD2	2.32	0.77
14:N:16:PHE:CZ	14:N:166:ARG:HA	2.18	0.77
6:T:103:LEU:CD2	6:T:104:PRO:O	2.33	0.77
14:b:16:PHE:HB3	14:b:162:GLN:HA	1.67	0.77
2:P:133:LEU:HD12	2:P:135:ILE:HG12	1.66	0.76
5:E:42:THR:CG2	5:E:194:ALA:HB1	2.11	0.76
14:N:162:GLN:HG2	14:N:166:ARG:HH21	1.49	0.76
2:P:133:LEU:HD11	2:P:135:ILE:HD11	1.67	0.76
9:W:80:ASN:ND2	9:W:111:TYR:CD1	2.53	0.76
13:a:106:VAL:CG1	13:a:108:ASN:OD1	2.33	0.76
14:N:46:ASN:O	14:N:47:ASN:C	2.27	0.76
3:Q:147:LEU:HD23	3:Q:159:TRP:O	1.86	0.76
5:S:186:HIS:H	5:S:189:MET:HE3	1.51	0.76
8:V:98:ILE:HG21	8:V:100:ILE:HG13	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:218:ALA:CB	5:E:226:PHE:CE1	2.69	0.76
12:L:42:LEU:HD11	12:L:184:TRP:CE2	2.21	0.76
12:L:55:TRP:HD1	12:L:97:MET:SD	2.07	0.76
4:R:192:ILE:CG1	4:R:228:TYR:CE1	2.68	0.76
5:S:229:PHE:CE2	5:S:233:GLU:HG3	2.20	0.76
9:W:36:PHE:CD1	9:W:38:SER:C	2.64	0.76
9:W:129:SER:OG	15:W:300:KNM:H41	1.85	0.76
14:b:162:GLN:HG2	14:b:166:ARG:HH21	1.49	0.76
8:H:178:ALA:O	8:H:184:VAL:HA	1.86	0.76
11:K:55:GLN:CG	12:L:88:TYR:CD2	2.66	0.76
13:a:17:GLY:HA3	13:a:166:LEU:HD21	1.66	0.76
14:b:26:MET:CB	14:b:186:ARG:NH2	2.46	0.76
8:H:18:SER:HB3	8:H:172:GLY:HA3	1.67	0.76
11:K:8:GLN:OE1	11:K:115:LEU:CD2	2.32	0.76
11:K:78:THR:CG2	11:K:116:TYR:OH	2.34	0.76
8:V:43:CYS:SG	8:V:98:ILE:HD12	2.26	0.76
6:F:103:LEU:CD2	6:F:104:PRO:O	2.33	0.76
10:X:137:VAL:CG2	10:X:146:TYR:CD1	2.68	0.76
6:F:13:TRP:HB2	7:G:22:GLN:HE22	1.49	0.76
8:H:33:LYS:HE2	15:H:300:KNM:C20	2.16	0.76
2:P:147:GLN:NE2	2:P:162:MET:SD	2.57	0.76
10:X:137:VAL:HG23	10:X:146:TYR:CE1	2.18	0.76
1:A:120:ASP:OD2	2:B:87:HIS:HE1	1.68	0.76
7:G:75:MET:HB2	7:G:137:LEU:HD22	1.67	0.76
9:I:172:ASN:HD21	9:I:191:VAL:HG22	1.49	0.76
12:Z:1:THR:HG23	15:Z:300:KNM:H30	1.68	0.76
12:Z:42:LEU:HD11	12:Z:184:TRP:CE2	2.21	0.76
14:b:26:MET:HE2	14:b:186:ARG:CZ	2.15	0.76
14:b:46:ASN:O	14:b:47:ASN:C	2.27	0.76
9:I:36:PHE:CD1	9:I:38:SER:C	2.64	0.76
9:I:80:ASN:ND2	9:I:111:TYR:CD1	2.53	0.76
5:E:186:HIS:H	5:E:189:MET:HE3	1.51	0.75
13:M:106:VAL:CG1	13:M:108:ASN:OD1	2.33	0.75
14:N:16:PHE:HB3	14:N:162:GLN:HA	1.67	0.75
14:N:26:MET:HE2	14:N:186:ARG:CZ	2.15	0.75
6:T:14:SER:O	6:T:17:GLY:HA3	1.86	0.75
6:F:43:HIS:CD2	6:F:184:LEU:HD22	2.22	0.75
7:U:75:MET:CG	7:U:137:LEU:CD2	2.64	0.75
13:a:47:THR:O	13:a:203:ILE:HD11	1.84	0.75
10:J:137:VAL:HG22	10:J:146:TYR:CD1	2.22	0.75
1:O:120:ASP:OD2	2:P:87:HIS:HE1	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:205:LYS:CB	3:Q:240:HIS:CD2	2.69	0.75
11:Y:78:THR:CG2	11:Y:116:TYR:OH	2.34	0.75
14:b:4:PRO:CA	14:b:56:ASP:OD2	2.32	0.75
14:b:91:TRP:CZ3	14:b:94:ARG:HB3	2.21	0.75
3:C:205:LYS:CB	3:C:240:HIS:CD2	2.69	0.75
8:H:1:THR:HG22	8:H:2:THR:N	2.01	0.75
8:H:43:CYS:SG	8:H:98:ILE:HD12	2.26	0.75
1:O:109:ILE:HG23	1:O:114:LEU:CG	2.17	0.75
2:P:49:LYS:O	2:P:206:ASN:HB3	1.87	0.75
2:P:140:GLU:HG2	2:P:141:GLY:N	2.00	0.75
11:Y:85:ARG:HD3	11:Y:124:LEU:HB2	1.69	0.75
1:A:109:ILE:HG23	1:A:114:LEU:CG	2.17	0.75
9:I:129:SER:OG	15:I:300:KNM:H41	1.85	0.75
13:M:152:GLN:CB	9:W:202:TYR:CD2	2.69	0.75
2:B:133:LEU:HD11	2:B:135:ILE:HD11	1.67	0.75
3:C:147:LEU:HD23	3:C:159:TRP:O	1.86	0.75
11:K:85:ARG:HD3	11:K:124:LEU:CB	2.17	0.75
9:W:146:MET:HE1	9:W:154:LEU:CD2	2.17	0.75
12:Z:153:TYR:CE2	12:Z:187:VAL:CG1	2.70	0.75
12:L:1:THR:HG23	15:L:300:KNM:H30	1.68	0.75
14:b:9:THR:HG22	14:b:10:SER:N	2.02	0.75
2:B:133:LEU:HD12	2:B:135:ILE:HG12	1.67	0.75
10:X:26:ARG:HD2	10:X:182:MET:HE3	1.69	0.75
11:Y:85:ARG:HD3	11:Y:124:LEU:CB	2.17	0.75
2:B:212:CYS:HG	2:B:217:PHE:HD2	1.32	0.75
3:C:24:ALA:O	3:C:28:ILE:HD11	1.84	0.75
9:I:146:MET:HE1	9:I:154:LEU:CD2	2.17	0.75
9:I:202:TYR:CE2	13:a:152:GLN:CG	2.67	0.75
11:K:147:TYR:HD1	11:K:159:LEU:HD21	1.52	0.75
12:L:153:TYR:CE2	12:L:187:VAL:CG1	2.70	0.75
2:P:138:TRP:CD1	2:P:143:PRO:HD3	2.21	0.75
2:B:138:TRP:CD1	2:B:143:PRO:HD3	2.21	0.74
9:I:1:THR:CG2	9:I:129:SER:CB	2.66	0.74
13:M:13:LEU:HD11	13:M:149:LEU:HD11	1.69	0.74
6:T:43:HIS:CD2	6:T:184:LEU:HD22	2.22	0.74
8:V:1:THR:HG22	8:V:2:THR:N	2.01	0.74
8:V:33:LYS:HE2	15:V:300:KNM:C20	2.16	0.74
2:B:181:LEU:HD23	2:B:186:ALA:CA	2.17	0.74
11:K:44:LEU:HD23	11:K:102:LEU:HD11	1.69	0.74
8:V:178:ALA:O	8:V:184:VAL:HA	1.86	0.74
2:B:49:LYS:O	2:B:206:ASN:HB3	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:TRP:HD1	7:G:22:GLN:NE2	1.83	0.74
9:I:41:ILE:HG12	9:I:102:GLY:HA3	1.69	0.74
2:P:138:TRP:HE1	2:P:143:PRO:HD3	1.52	0.74
8:V:18:SER:HB3	8:V:172:GLY:HA3	1.67	0.74
10:X:137:VAL:HG22	10:X:146:TYR:CD1	2.22	0.74
13:a:13:LEU:HD11	13:a:149:LEU:CD1	2.17	0.74
4:D:196:LEU:HD22	4:D:232:ILE:HD13	1.69	0.74
9:I:40:ASN:HB3	9:I:73:LEU:HD21	1.69	0.74
5:S:218:ALA:CB	5:S:226:PHE:CE1	2.69	0.74
6:T:13:TRP:HD1	7:U:22:GLN:NE2	1.83	0.74
11:Y:147:TYR:HD1	11:Y:159:LEU:HD21	1.52	0.74
6:T:13:TRP:HB2	7:U:22:GLN:HE22	1.50	0.74
10:X:26:ARG:CD	10:X:182:MET:HE3	2.18	0.74
9:I:49:ALA:HA	9:I:52:THR:HG22	1.70	0.74
14:N:9:THR:HG22	14:N:10:SER:N	2.02	0.74
6:T:7:ASP:OD2	6:T:14:SER:HA	1.88	0.74
2:B:39:ALA:O	2:B:40:ALA:CB	2.36	0.74
5:E:42:THR:HG23	5:E:194:ALA:HB1	1.70	0.74
5:E:229:PHE:CE2	5:E:233:GLU:HG3	2.20	0.74
9:I:202:TYR:HE2	13:a:174:LEU:CD1	1.99	0.74
13:M:13:LEU:HD11	13:M:149:LEU:CD1	2.17	0.74
5:S:35:SER:HB2	5:S:66:LYS:HZ2	1.53	0.74
1:A:103:TYR:O	9:I:81:ARG:CZ	2.36	0.74
9:W:41:ILE:HG12	9:W:102:GLY:HA3	1.69	0.74
11:Y:29:LYS:HD2	12:Z:122:SER:O	1.88	0.74
15:Z:300:KNM:H8	15:Z:300:KNM:N2	2.03	0.74
14:b:91:TRP:HE3	14:b:94:ARG:HG3	1.48	0.74
10:J:26:ARG:HD2	10:J:182:MET:HE3	1.69	0.73
6:T:69:HIS:ND1	6:T:96:ARG:NH2	2.36	0.73
8:V:84:LYS:O	8:V:88:TYR:HB2	1.88	0.73
2:B:140:GLU:HG2	2:B:141:GLY:N	2.00	0.73
6:T:195:LEU:CD2	6:T:210:VAL:HG12	2.18	0.73
13:a:99:ARG:HB3	13:a:104:TYR:CE2	2.23	0.73
1:A:103:TYR:CA	9:I:81:ARG:HH22	1.72	0.73
15:L:300:KNM:H8	15:L:300:KNM:N2	2.03	0.73
14:N:4:PRO:HB2	14:N:56:ASP:CG	2.14	0.73
3:Q:76:VAL:HG13	3:Q:134:LEU:CD2	2.18	0.73
9:W:1:THR:CG2	9:W:129:SER:CB	2.66	0.73
9:W:80:ASN:ND2	9:W:111:TYR:CE1	2.56	0.73
7:G:75:MET:CG	7:G:137:LEU:CD2	2.64	0.73
8:H:84:LYS:O	8:H:88:TYR:HB2	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:ARG:CD	10:J:182:MET:HE3	2.18	0.73
13:a:13:LEU:HD11	13:a:149:LEU:HD11	1.69	0.73
9:I:80:ASN:ND2	9:I:111:TYR:CE1	2.56	0.73
11:K:29:LYS:HD2	12:L:122:SER:O	1.88	0.73
13:M:174:LEU:CD1	9:W:202:TYR:HE2	1.99	0.73
4:R:196:LEU:HD22	4:R:232:ILE:HD13	1.69	0.73
8:V:119:MET:HE3	14:b:57:TYR:HD2	0.69	0.73
1:A:109:ILE:HG23	1:A:114:LEU:HD11	1.71	0.73
3:C:48:GLU:HA	3:C:210:LYS:O	1.89	0.73
10:J:18:CYS:SG	10:J:162:LEU:HD22	2.28	0.73
13:M:99:ARG:HB3	13:M:104:TYR:CE2	2.23	0.73
7:U:190:VAL:HB	7:U:215:TRP:CZ2	2.14	0.73
8:V:115:PRO:HG3	14:b:36:PHE:CZ	2.23	0.73
10:X:97:LYS:HB3	10:X:100:GLY:O	1.88	0.73
2:B:138:TRP:HE1	2:B:143:PRO:HD3	1.52	0.73
8:H:88:TYR:OH	14:N:62:TYR:HB3	1.87	0.73
10:J:27:PHE:CE2	10:J:35:THR:OG1	2.42	0.73
11:K:10:PRO:HD3	11:K:151:ILE:CG2	2.18	0.73
6:F:195:LEU:CD2	6:F:210:VAL:HG12	2.18	0.73
10:J:97:LYS:HB3	10:J:100:GLY:O	1.88	0.73
11:K:85:ARG:HD3	11:K:124:LEU:HB2	1.68	0.73
1:O:103:TYR:O	9:W:81:ARG:CZ	2.36	0.73
2:P:181:LEU:HD23	2:P:186:ALA:CA	2.17	0.73
15:Z:300:KNM:H21	15:Z:300:KNM:N2	2.04	0.73
14:N:21:VAL:HG22	14:N:191:THR:CG2	2.19	0.73
3:Q:48:GLU:HA	3:Q:210:LYS:O	1.89	0.73
6:T:184:LEU:HD21	6:T:214:ILE:CG2	2.17	0.73
9:W:40:ASN:HB3	9:W:73:LEU:HD21	1.69	0.73
9:W:49:ALA:HA	9:W:52:THR:HG22	1.70	0.73
10:X:18:CYS:SG	10:X:162:LEU:HD22	2.28	0.73
12:Z:55:TRP:CD1	12:Z:97:MET:SD	2.82	0.73
6:F:69:HIS:ND1	6:F:96:ARG:NH2	2.36	0.73
9:I:39:PRO:O	9:I:183:LEU:HD21	1.88	0.73
4:R:172:LEU:HD22	4:R:190:LEU:HD21	1.71	0.73
9:W:59:ILE:CG2	9:W:63:LEU:HD13	2.19	0.73
10:X:26:ARG:CD	10:X:33:MET:HG3	2.19	0.73
9:I:202:TYR:CD2	13:a:152:GLN:CB	2.69	0.72
10:J:26:ARG:CD	10:J:33:MET:HG3	2.19	0.72
5:S:120:ALA:O	5:S:121:LEU:HD23	1.89	0.72
2:B:172:PHE:CZ	2:B:196:GLU:OE1	2.42	0.72
5:S:218:ALA:CB	5:S:226:PHE:CZ	2.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:27:PHE:CE2	10:X:35:THR:OG1	2.42	0.72
1:A:109:ILE:CG2	1:A:114:LEU:CG	2.67	0.72
2:B:133:LEU:CD1	2:B:135:ILE:CG1	2.67	0.72
3:C:76:VAL:HG13	3:C:134:LEU:CD2	2.18	0.72
8:H:51:ASP:HB3	8:H:94:LEU:HD12	1.71	0.72
13:M:174:LEU:CB	9:W:202:TYR:OH	2.35	0.72
14:N:21:VAL:HG22	14:N:191:THR:HG22	1.71	0.72
2:P:133:LEU:CD1	2:P:135:ILE:CG1	2.66	0.72
5:E:218:ALA:CB	5:E:226:PHE:CZ	2.72	0.72
9:I:21:THR:O	15:I:300:KNM:H7	1.89	0.72
14:N:91:TRP:CZ3	14:N:94:ARG:HB3	2.21	0.72
2:P:39:ALA:O	2:P:40:ALA:CB	2.36	0.72
11:Y:55:GLN:CG	12:Z:88:TYR:CE2	2.71	0.72
9:I:202:TYR:OH	13:a:174:LEU:CD2	2.38	0.72
12:L:55:TRP:CD1	12:L:97:MET:SD	2.82	0.72
12:L:178:HIS:CB	12:L:187:VAL:HG21	2.20	0.72
13:M:17:GLY:HA3	13:M:166:LEU:HD21	1.66	0.72
8:V:51:ASP:HB3	8:V:94:LEU:HD12	1.71	0.72
9:W:39:PRO:O	9:W:183:LEU:HD21	1.88	0.72
11:Y:10:PRO:HD3	11:Y:151:ILE:CG2	2.18	0.72
11:Y:44:LEU:HD23	11:Y:102:LEU:HD11	1.69	0.72
9:I:59:ILE:CG2	9:I:63:LEU:HD13	2.19	0.72
1:O:102:LYS:O	9:W:81:ARG:NH1	2.22	0.72
12:Z:178:HIS:CB	12:Z:187:VAL:HG21	2.20	0.72
7:G:72:HIS:HB2	7:G:105:ASN:ND2	2.05	0.72
14:N:16:PHE:HD1	14:N:161:SER:O	1.73	0.72
8:V:88:TYR:OH	14:b:62:TYR:HB3	1.87	0.72
7:U:161:TRP:O	7:U:181:MET:SD	2.48	0.72
4:D:172:LEU:HD22	4:D:190:LEU:HD21	1.71	0.72
5:E:120:ALA:O	5:E:121:LEU:HD23	1.89	0.72
6:F:184:LEU:HD21	6:F:214:ILE:CG2	2.17	0.72
10:J:137:VAL:HG23	10:J:146:TYR:CE1	2.18	0.72
1:O:109:ILE:HG23	1:O:114:LEU:HD11	1.71	0.72
2:P:172:PHE:CZ	2:P:196:GLU:OE1	2.42	0.72
9:W:21:THR:O	15:W:300:KNM:H7	1.89	0.72
11:Y:8:GLN:O	11:Y:147:TYR:OH	2.05	0.72
13:a:106:VAL:CG1	13:a:108:ASN:ND2	2.53	0.72
5:E:70:ILE:HD11	5:E:76:CYS:HB2	1.72	0.71
8:H:115:PRO:HG3	14:N:36:PHE:CZ	2.23	0.71
15:I:300:KNM:H6	15:I:300:KNM:C2	2.20	0.71
14:N:16:PHE:CE2	14:N:21:VAL:CG2	2.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:120:ALA:C	5:S:121:LEU:HD23	2.15	0.71
14:b:4:PRO:HB2	14:b:56:ASP:CG	2.14	0.71
14:b:16:PHE:HZ	14:b:165:ALA:C	1.72	0.71
3:C:136:TYR:O	3:C:147:LEU:HA	1.90	0.71
14:b:21:VAL:HG22	14:b:191:THR:CG2	2.19	0.71
14:b:21:VAL:HG22	14:b:191:THR:HG22	1.71	0.71
4:D:31:THR:HG23	4:D:165:ALA:HB2	1.71	0.71
7:U:190:VAL:HG21	7:U:215:TRP:CE2	2.25	0.71
14:b:16:PHE:CE2	14:b:21:VAL:CG2	2.73	0.71
1:A:102:LYS:O	9:I:81:ARG:NH1	2.22	0.71
2:B:132:SER:OG	2:B:149:ASP:OD1	2.08	0.71
10:J:154:GLU:CD	10:J:161:HIS:NE2	2.48	0.71
15:L:300:KNM:H21	15:L:300:KNM:N2	2.04	0.71
9:W:63:LEU:HD11	9:W:82:MET:SD	2.31	0.71
6:F:13:TRP:CB	7:G:22:GLN:HE22	2.03	0.71
13:M:174:LEU:CD2	9:W:202:TYR:OH	2.38	0.71
9:W:39:PRO:O	9:W:183:LEU:CD2	2.39	0.71
1:A:102:LYS:O	9:I:81:ARG:CZ	2.39	0.71
5:E:35:SER:HB2	5:E:66:LYS:HZ2	1.53	0.71
7:G:161:TRP:O	7:G:181:MET:SD	2.48	0.71
13:M:16:ALA:HB2	13:M:21:ALA:HA	1.71	0.71
13:M:106:VAL:CG1	13:M:108:ASN:ND2	2.53	0.71
3:Q:198:ASN:OD1	3:Q:240:HIS:ND1	2.22	0.71
2:P:132:SER:OG	2:P:149:ASP:OD1	2.08	0.71
4:R:31:THR:HG23	4:R:165:ALA:HB2	1.71	0.71
5:S:42:THR:HG23	5:S:194:ALA:HB1	1.70	0.71
5:S:70:ILE:HD11	5:S:76:CYS:HB2	1.72	0.71
15:W:300:KNM:H6	15:W:300:KNM:C2	2.20	0.71
14:b:16:PHE:HD1	14:b:161:SER:O	1.73	0.71
13:M:18:GLU:O	13:M:20:PHE:N	2.24	0.71
3:Q:136:TYR:O	3:Q:147:LEU:HA	1.90	0.71
1:A:109:ILE:CG1	1:A:114:LEU:HD23	2.21	0.71
3:C:198:ASN:OD1	3:C:240:HIS:ND1	2.22	0.71
9:I:63:LEU:HD11	9:I:82:MET:SD	2.31	0.71
12:L:178:HIS:HB2	12:L:187:VAL:HG21	1.73	0.71
1:O:109:ILE:CG2	1:O:114:LEU:CG	2.67	0.71
6:T:13:TRP:CB	7:U:22:GLN:HE22	2.03	0.71
9:W:1:THR:CG2	9:W:129:SER:N	2.49	0.71
13:a:16:ALA:HB2	13:a:21:ALA:HA	1.71	0.71
8:H:47:GLY:C	15:H:300:KNM:H24	2.15	0.70
12:Z:178:HIS:HB2	12:Z:187:VAL:HG21	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:18:GLU:O	13:a:20:PHE:N	2.23	0.70
3:C:183:GLU:HG2	3:C:183:GLU:O	1.91	0.70
5:E:120:ALA:C	5:E:121:LEU:HD23	2.15	0.70
1:O:102:LYS:O	9:W:81:ARG:CZ	2.39	0.70
9:I:1:THR:CG2	9:I:129:SER:N	2.49	0.70
11:K:55:GLN:NE2	12:L:88:TYR:HD2	1.90	0.70
1:O:103:TYR:HA	9:W:81:ARG:HH21	1.15	0.70
9:I:1:THR:HG21	15:I:300:KNM:S1	2.32	0.70
11:Y:44:LEU:HG	11:Y:102:LEU:CD2	2.22	0.70
9:I:39:PRO:O	9:I:183:LEU:CD2	2.39	0.70
4:D:8:THR:O	5:E:135:ARG:HD3	1.92	0.70
11:K:55:GLN:CG	12:L:88:TYR:CE2	2.71	0.70
4:R:196:LEU:HD13	4:R:232:ILE:HG21	1.73	0.70
9:W:1:THR:HG21	15:W:300:KNM:S1	2.32	0.70
11:Y:23:SER:O	11:Y:24:ASN:OD1	0.70	0.70
14:b:26:MET:O	14:b:186:ARG:NH2	2.24	0.70
11:K:23:SER:O	11:K:24:ASN:OD1	0.70	0.70
14:N:26:MET:O	14:N:186:ARG:NH2	2.24	0.70
6:T:69:HIS:CE1	6:T:96:ARG:HH21	2.10	0.70
10:X:49:TYR:CD2	10:X:189:ILE:HD11	2.26	0.70
9:I:128:GLY:HA2	15:I:300:KNM:O4	1.92	0.70
4:R:8:THR:O	5:S:135:ARG:HD3	1.91	0.70
8:V:47:GLY:C	15:V:300:KNM:H24	2.15	0.70
11:Y:55:GLN:NE2	12:Z:88:TYR:HD2	1.90	0.70
2:B:44:VAL:HG23	2:B:211:ILE:HG23	1.73	0.69
15:L:300:KNM:H34	15:L:300:KNM:O2	1.92	0.69
1:O:109:ILE:CG1	1:O:114:LEU:CD2	2.70	0.69
3:Q:183:GLU:O	3:Q:183:GLU:HG2	1.91	0.69
6:T:14:SER:C	6:T:17:GLY:HA3	2.17	0.69
9:W:49:ALA:HA	15:W:300:KNM:H36	1.73	0.69
10:X:154:GLU:CD	10:X:161:HIS:NE2	2.48	0.69
14:b:59:ASP:HB2	14:b:108:ASN:ND2	2.05	0.69
7:U:72:HIS:HB2	7:U:105:ASN:ND2	2.05	0.69
15:Z:300:KNM:H34	15:Z:300:KNM:O2	1.92	0.69
13:a:15:ILE:HD11	13:a:175:VAL:HG22	1.74	0.69
14:N:59:ASP:HB2	14:N:108:ASN:ND2	2.05	0.69
9:W:129:SER:OG	15:W:300:KNM:H42	1.92	0.69
6:F:69:HIS:CE1	6:F:96:ARG:HH21	2.10	0.69
9:I:202:TYR:OH	13:a:174:LEU:CB	2.35	0.69
13:M:19:ASP:OD1	13:M:113:LEU:HD11	1.92	0.69
9:W:1:THR:O	9:W:128:GLY:HA3	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:16:LYS:O	10:X:17:ASN:C	2.36	0.69
13:a:19:ASP:OD1	13:a:113:LEU:HD11	1.92	0.69
14:b:173:MET:HB3	14:b:187:PHE:CE2	2.28	0.69
1:A:109:ILE:CG1	1:A:114:LEU:CD2	2.70	0.69
5:E:43:SER:HA	5:E:151:PRO:HG3	1.75	0.69
6:F:92:CYS:HA	6:F:103:LEU:HD13	1.75	0.69
7:G:75:MET:HE3	7:G:137:LEU:HD21	1.74	0.69
9:I:1:THR:O	9:I:128:GLY:HA3	1.93	0.69
13:M:15:ILE:HD11	13:M:175:VAL:HG22	1.74	0.69
1:O:161:CYS:HG	1:O:163:PHE:HE1	1.17	0.69
2:P:133:LEU:HD12	2:P:135:ILE:CG1	2.23	0.69
2:P:138:TRP:CD1	2:P:143:PRO:CD	2.76	0.69
13:a:106:VAL:HG13	13:a:108:ASN:ND2	2.08	0.69
8:H:117:GLY:CA	14:N:5:MET:HG3	2.23	0.69
9:W:128:GLY:HA2	15:W:300:KNM:O4	1.92	0.69
13:a:19:ASP:OD2	13:a:200:LYS:HG3	1.93	0.69
5:E:168:ARG:NH1	5:E:178:GLN:OE1	2.24	0.69
8:H:88:TYR:OH	14:N:62:TYR:CG	2.32	0.69
11:K:8:GLN:O	11:K:147:TYR:OH	2.05	0.69
13:M:106:VAL:HG13	13:M:108:ASN:HD21	1.57	0.69
14:b:16:PHE:HZ	14:b:166:ARG:HA	1.57	0.69
9:I:47:GLY:N	15:I:300:KNM:H29	2.04	0.68
9:W:63:LEU:CD1	9:W:82:MET:SD	2.81	0.68
13:a:100:ARG:NH1	13:a:127:VAL:CB	2.54	0.68
13:a:106:VAL:HG13	13:a:108:ASN:HD21	1.57	0.68
4:D:196:LEU:HD13	4:D:232:ILE:HG21	1.73	0.68
8:H:1:THR:HB	15:H:300:KNM:O5	1.91	0.68
9:I:63:LEU:CD1	9:I:82:MET:SD	2.81	0.68
1:O:109:ILE:CG1	1:O:114:LEU:HD23	2.21	0.68
6:T:13:TRP:H	7:U:22:GLN:HE22	1.40	0.68
11:Y:151:ILE:HG13	11:Y:152:SER:N	2.08	0.68
14:N:60:PHE:N	14:N:108:ASN:HD21	1.91	0.68
14:N:173:MET:HB3	14:N:187:PHE:CE2	2.28	0.68
5:S:147:ASP:O	5:S:149:LYS:N	2.27	0.68
6:T:92:CYS:HA	6:T:103:LEU:HD13	1.75	0.68
1:A:109:ILE:CD1	1:A:114:LEU:CD2	2.31	0.68
4:D:211:MET:CB	4:D:217:LEU:HD13	2.20	0.68
6:F:98:VAL:HG13	14:N:91:TRP:CE3	2.29	0.68
9:I:129:SER:OG	15:I:300:KNM:H42	1.92	0.68
11:K:151:ILE:HG13	11:K:152:SER:N	2.08	0.68
5:E:147:ASP:O	5:E:149:LYS:N	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:83:PHE:CD2	8:H:100:ILE:CD1	2.77	0.68
11:K:44:LEU:HG	11:K:102:LEU:CD2	2.22	0.68
5:S:43:SER:HA	5:S:151:PRO:HG3	1.75	0.68
7:U:104:TYR:OH	8:V:70:LEU:CD2	2.41	0.68
7:G:104:TYR:OH	8:H:70:LEU:CD2	2.41	0.68
9:I:49:ALA:HA	15:I:300:KNM:H36	1.73	0.68
2:P:44:VAL:HG23	2:P:211:ILE:HG23	1.73	0.68
7:U:75:MET:HE3	7:U:137:LEU:HD21	1.74	0.68
8:V:1:THR:HB	15:V:300:KNM:O5	1.91	0.68
14:b:9:THR:C	14:b:10:SER:HG	2.00	0.68
7:G:190:VAL:HG21	7:G:215:TRP:CE2	2.25	0.68
2:B:133:LEU:HD12	2:B:135:ILE:CG1	2.23	0.68
10:J:16:LYS:O	10:J:17:ASN:C	2.36	0.68
11:K:85:ARG:HH22	11:K:86:ARG:NH2	1.82	0.68
13:M:19:ASP:OD2	13:M:200:LYS:HG3	1.93	0.68
9:W:47:GLY:N	15:W:300:KNM:H29	2.03	0.68
6:F:13:TRP:H	7:G:22:GLN:HE22	1.40	0.68
13:M:16:ALA:HB1	13:M:119:GLY:CA	2.15	0.68
3:Q:111:VAL:HG13	3:Q:136:TYR:CE2	2.29	0.68
8:V:83:PHE:CD2	8:V:100:ILE:CD1	2.77	0.68
13:M:106:VAL:HG13	13:M:108:ASN:ND2	2.08	0.67
11:Y:85:ARG:HH22	11:Y:86:ARG:NH2	1.82	0.67
2:B:138:TRP:CD1	2:B:143:PRO:CD	2.76	0.67
2:B:140:GLU:CG	2:B:141:GLY:N	2.55	0.67
12:Z:178:HIS:O	12:Z:184:TRP:HA	1.95	0.67
12:L:178:HIS:O	12:L:184:TRP:HA	1.95	0.67
13:a:47:THR:O	13:a:203:ILE:CD1	2.42	0.67
9:I:144:PRO:O	9:I:145:ASP:HB3	1.95	0.67
14:N:16:PHE:HE2	14:N:21:VAL:CG2	2.06	0.67
6:T:98:VAL:HG13	14:b:91:TRP:CE3	2.29	0.67
8:V:117:GLY:CA	14:b:5:MET:HG3	2.23	0.67
14:b:60:PHE:N	14:b:108:ASN:HD21	1.91	0.67
3:C:111:VAL:HG13	3:C:136:TYR:CE2	2.29	0.67
2:P:140:GLU:CG	2:P:141:GLY:N	2.55	0.67
14:b:21:VAL:CG2	14:b:191:THR:CG2	2.73	0.67
2:B:138:TRP:CD1	2:B:143:PRO:CG	2.78	0.67
6:F:77:LEU:HD11	6:F:80:ASP:OD2	1.95	0.67
10:J:49:TYR:CD2	10:J:189:ILE:HD11	2.30	0.66
3:Q:157:GLY:O	3:Q:159:TRP:CD1	2.46	0.66
10:X:64:GLN:CD	11:Y:85:ARG:HH22	2.03	0.66
11:Y:46:CYS:CB	11:Y:102:LEU:HD12	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:16:PHE:HZ	14:N:166:ARG:HA	1.57	0.66
5:S:42:THR:OG1	5:S:45:GLY:O	2.11	0.66
12:Z:55:TRP:CZ2	12:Z:95:LEU:HD12	2.30	0.66
2:B:181:LEU:CD1	2:B:185:ASP:HB3	2.25	0.66
1:O:109:ILE:HG23	1:O:114:LEU:CD1	2.26	0.66
6:T:77:LEU:HD11	6:T:80:ASP:OD2	1.94	0.66
8:H:115:PRO:O	8:H:118:GLY:N	2.29	0.66
13:M:47:THR:O	13:M:203:ILE:CD1	2.42	0.66
14:N:46:ASN:C	14:N:48:SER:N	2.51	0.66
2:P:138:TRP:CD1	2:P:143:PRO:CG	2.78	0.66
8:V:115:PRO:O	8:V:118:GLY:N	2.29	0.66
9:W:49:ALA:CB	15:W:300:KNM:H36	2.26	0.66
3:Q:186:LEU:HD23	3:Q:186:LEU:O	1.95	0.66
9:W:36:PHE:HB2	9:W:42:TYR:HE1	1.60	0.66
6:T:13:TRP:CB	7:U:22:GLN:NE2	2.59	0.66
7:U:75:MET:CE	7:U:137:LEU:HD21	2.26	0.66
5:E:227:HIS:HE2	5:E:229:PHE:HD1	1.44	0.66
9:I:36:PHE:HB2	9:I:42:TYR:HE1	1.60	0.66
5:S:35:SER:CB	5:S:66:LYS:NZ	2.59	0.66
9:W:144:PRO:O	9:W:145:ASP:HB3	1.95	0.66
9:I:49:ALA:CB	15:I:300:KNM:H36	2.26	0.66
14:N:91:TRP:HZ3	14:N:94:ARG:CB	2.07	0.65
8:V:130:SER:OG	15:V:300:KNM:H41	1.97	0.65
14:b:16:PHE:HE2	14:b:21:VAL:CG2	2.06	0.65
14:b:193:THR:O	14:b:194:GLU:C	2.39	0.65
5:E:224:GLN:NE2	5:E:227:HIS:CE1	2.46	0.65
8:H:1:THR:CA	15:H:300:KNM:O5	2.44	0.65
11:K:85:ARG:CZ	11:K:86:ARG:HH22	2.09	0.65
2:P:39:ALA:O	2:P:40:ALA:HB2	1.96	0.65
1:O:109:ILE:CB	1:O:114:LEU:HD21	2.20	0.65
1:A:109:ILE:HG23	1:A:114:LEU:CD1	2.26	0.65
9:I:1:THR:N	9:I:169:SER:CB	2.59	0.65
9:I:47:GLY:O	15:I:300:KNM:N3	2.28	0.65
13:M:46:LEU:HD13	13:M:52:ILE:HG22	1.78	0.65
4:R:211:MET:CB	4:R:217:LEU:HD13	2.19	0.65
3:C:157:GLY:O	3:C:159:TRP:CD1	2.46	0.65
5:E:168:ARG:HD3	5:E:178:GLN:HE22	1.62	0.65
12:L:55:TRP:CZ2	12:L:95:LEU:HD12	2.30	0.65
11:Y:147:TYR:HD1	11:Y:159:LEU:CD2	2.09	0.65
5:E:188:SER:O	5:E:189:MET:HB2	1.95	0.65
6:F:13:TRP:CB	7:G:22:GLN:NE2	2.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ILE:CD1	1:O:114:LEU:CD2	2.31	0.65
10:X:137:VAL:CG2	10:X:146:TYR:CG	2.80	0.65
1:A:103:TYR:HA	9:I:81:ARG:HH22	0.82	0.65
3:C:186:LEU:HD23	3:C:186:LEU:O	1.95	0.65
4:D:31:THR:HG23	4:D:165:ALA:CB	2.26	0.65
7:G:75:MET:HG3	7:G:137:LEU:CD2	2.27	0.65
10:J:122:SER:CB	10:J:136:VAL:HG11	2.25	0.65
14:N:193:THR:O	14:N:194:GLU:C	2.39	0.65
2:P:51:GLN:HG3	2:P:54:ILE:CA	2.27	0.65
6:T:100:ASP:OD1	14:b:94:ARG:NH2	2.29	0.65
4:R:31:THR:HG23	4:R:165:ALA:CB	2.26	0.65
7:U:75:MET:HB2	7:U:137:LEU:HD22	1.67	0.65
10:X:122:SER:CB	10:X:136:VAL:HG11	2.25	0.65
14:b:59:ASP:CA	14:b:108:ASN:HD21	2.10	0.65
8:H:130:SER:OG	15:H:300:KNM:H41	1.97	0.65
10:J:176:ARG:HH22	13:a:146:GLN:CB	2.02	0.65
2:P:172:PHE:HE2	2:P:196:GLU:CG	2.09	0.65
9:W:1:THR:N	9:W:169:SER:CB	2.59	0.65
9:W:122:LEU:CG	9:W:123:PRO:HD2	2.26	0.65
2:B:51:GLN:HG3	2:B:54:ILE:CA	2.27	0.65
2:B:172:PHE:HE2	2:B:196:GLU:CG	2.09	0.65
5:E:35:SER:CB	5:E:66:LYS:NZ	2.59	0.65
6:F:100:ASP:OD1	14:N:94:ARG:NH2	2.29	0.65
10:J:57:THR:HG22	11:K:122:ALA:O	1.97	0.65
5:S:35:SER:CB	5:S:66:LYS:HZ2	2.10	0.65
6:T:77:LEU:HD11	6:T:80:ASP:CG	2.21	0.65
14:b:48:SER:CB	14:b:196:GLY:HA3	2.27	0.65
7:G:75:MET:CE	7:G:137:LEU:HD21	2.26	0.64
11:K:46:CYS:CB	11:K:102:LEU:HD12	2.26	0.64
1:O:103:TYR:HA	9:W:81:ARG:HH22	0.82	0.64
2:P:172:PHE:CE2	2:P:196:GLU:OE1	2.50	0.64
5:S:188:SER:O	5:S:189:MET:HB2	1.95	0.64
12:Z:55:TRP:CD1	12:Z:97:MET:HE1	2.32	0.64
13:a:46:LEU:HD13	13:a:52:ILE:HG22	1.78	0.64
3:C:203:VAL:HG11	3:C:210:LYS:NZ	2.11	0.64
5:E:35:SER:CB	5:E:66:LYS:HZ2	2.09	0.64
10:J:137:VAL:CG2	10:J:146:TYR:CG	2.80	0.64
13:M:146:GLN:CB	10:X:176:ARG:HH22	2.02	0.64
14:N:48:SER:CB	14:N:196:GLY:HA3	2.27	0.64
2:P:134:LEU:CD2	2:P:162:MET:SD	2.85	0.64
11:Y:120:TYR:CE1	11:Y:121:LEU:CD2	2.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:VAL:HG22	3:C:136:TYR:CD2	2.32	0.64
12:L:55:TRP:NE1	12:L:97:MET:HE1	2.12	0.64
14:N:16:PHE:HE1	14:N:166:ARG:H	0.71	0.64
3:Q:111:VAL:HG22	3:Q:136:TYR:CD2	2.32	0.64
3:Q:203:VAL:HG11	3:Q:210:LYS:NZ	2.11	0.64
5:S:168:ARG:NH1	5:S:178:GLN:OE1	2.24	0.64
6:T:195:LEU:HD23	6:T:210:VAL:HG12	1.79	0.64
8:V:45:ARG:HG3	15:V:300:KNM:H34	1.79	0.64
13:a:16:ALA:HB1	13:a:119:GLY:CA	2.15	0.64
6:F:77:LEU:HD11	6:F:80:ASP:CG	2.21	0.64
9:I:36:PHE:CD1	9:I:38:SER:O	2.51	0.64
5:S:50:VAL:CG2	5:S:66:LYS:HD3	2.27	0.64
2:B:134:LEU:CD2	2:B:162:MET:SD	2.85	0.64
11:K:170:ARG:NH2	12:Z:136:TYR:CG	2.66	0.64
13:M:100:ARG:NH1	13:M:127:VAL:CB	2.54	0.64
14:N:59:ASP:CA	14:N:108:ASN:HD21	2.10	0.64
8:V:1:THR:CA	15:V:300:KNM:O5	2.44	0.64
13:a:99:ARG:HD3	13:a:104:TYR:CE1	2.28	0.64
14:b:91:TRP:HZ3	14:b:94:ARG:HB3	1.63	0.64
8:H:47:GLY:C	15:H:300:KNM:C13	2.71	0.64
10:J:64:GLN:CD	11:K:85:ARG:HH22	2.03	0.64
11:K:147:TYR:HD1	11:K:159:LEU:CD2	2.09	0.64
12:L:55:TRP:CD1	12:L:97:MET:HE1	2.32	0.64
14:N:9:THR:HG22	14:N:140:GLY:O	1.97	0.64
14:N:21:VAL:CG2	14:N:191:THR:CG2	2.73	0.64
10:X:17:ASN:OD1	10:X:18:CYS:N	2.31	0.64
8:H:45:ARG:HG3	15:H:300:KNM:H34	1.79	0.64
1:O:13:ILE:O	1:O:13:ILE:HG13	1.97	0.64
2:P:181:LEU:CD1	2:P:185:ASP:HB3	2.25	0.64
10:X:57:THR:HG22	11:Y:122:ALA:O	1.97	0.64
11:Y:5:ILE:HD11	11:Y:143:LEU:HD22	1.80	0.64
2:B:39:ALA:O	2:B:40:ALA:HB2	1.96	0.64
2:B:172:PHE:CE2	2:B:196:GLU:OE1	2.50	0.64
10:J:17:ASN:OD1	10:J:18:CYS:N	2.31	0.64
14:N:16:PHE:CE1	14:N:165:ALA:N	2.66	0.64
9:W:36:PHE:CD1	9:W:38:SER:O	2.51	0.64
3:C:76:VAL:HA	3:C:134:LEU:HD23	1.79	0.64
5:E:50:VAL:CG2	5:E:66:LYS:HD3	2.27	0.64
1:O:120:ASP:OD2	2:P:87:HIS:CE1	2.51	0.64
6:T:184:LEU:CD2	6:T:214:ILE:HG21	2.22	0.64
8:V:32:ASP:CG	8:V:186:ARG:HH21	2.06	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:16:PHE:CE1	14:b:165:ALA:N	2.66	0.64
11:K:5:ILE:HD11	11:K:143:LEU:HD22	1.80	0.64
14:N:56:ASP:O	14:N:108:ASN:OD1	2.16	0.64
2:P:133:LEU:HD11	2:P:135:ILE:CD1	2.28	0.64
5:S:168:ARG:HD3	5:S:178:GLN:HE22	1.62	0.64
11:Y:85:ARG:CZ	11:Y:86:ARG:HH22	2.09	0.64
14:b:9:THR:HG22	14:b:140:GLY:O	1.97	0.64
2:B:133:LEU:HD11	2:B:135:ILE:CD1	2.28	0.63
9:I:104:ASP:O	9:I:105:VAL:C	2.42	0.63
15:V:300:KNM:O2	15:V:300:KNM:H37	1.98	0.63
2:B:42:GLY:CA	2:B:183:LEU:HD12	2.29	0.63
15:H:300:KNM:O2	15:H:300:KNM:H37	1.98	0.63
11:K:120:TYR:CE1	11:K:121:LEU:CD2	2.80	0.63
12:L:136:TYR:CG	11:Y:170:ARG:NH2	2.66	0.63
14:N:16:PHE:CD1	14:N:162:GLN:O	2.51	0.63
2:P:42:GLY:CA	2:P:183:LEU:HD12	2.29	0.63
5:S:227:HIS:HE2	5:S:229:PHE:HD1	1.44	0.63
7:U:75:MET:HG3	7:U:137:LEU:CD2	2.27	0.63
9:W:47:GLY:O	15:W:300:KNM:N3	2.28	0.63
12:Z:55:TRP:NE1	12:Z:97:MET:HE1	2.12	0.63
12:Z:153:TYR:CE2	12:Z:187:VAL:HG13	2.33	0.63
14:b:16:PHE:HE1	14:b:166:ARG:H	0.71	0.63
1:A:13:ILE:O	1:A:13:ILE:HG13	1.97	0.63
2:B:183:LEU:O	2:B:187:ILE:HG13	1.99	0.63
7:G:190:VAL:CG2	7:G:215:TRP:NE1	2.61	0.63
14:N:145:LEU:HG	9:W:136:ALA:HB2	1.80	0.63
3:Q:76:VAL:HA	3:Q:134:LEU:HD23	1.79	0.63
7:U:181:MET:O	7:U:182:LYS:C	2.41	0.63
8:V:47:GLY:C	15:V:300:KNM:C13	2.71	0.63
11:Y:24:ASN:HD21	11:Y:26:VAL:HG23	1.64	0.63
11:Y:24:ASN:ND2	11:Y:26:VAL:CG2	2.61	0.63
14:b:16:PHE:CD1	14:b:162:GLN:O	2.51	0.63
9:I:122:LEU:CG	9:I:123:PRO:HD2	2.26	0.63
11:K:24:ASN:ND2	11:K:26:VAL:CG2	2.61	0.63
6:F:195:LEU:HD23	6:F:210:VAL:HG12	1.79	0.63
8:H:177:ALA:HA	8:H:186:ARG:HG3	1.80	0.63
11:K:67:TYR:CE2	11:K:75:LEU:HD21	2.33	0.63
13:M:104:TYR:HE1	14:N:97:TYR:OH	1.82	0.63
2:P:183:LEU:O	2:P:187:ILE:HG13	1.99	0.63
5:S:42:THR:CG2	5:S:194:ALA:HB3	2.00	0.63
14:b:16:PHE:CE2	14:b:21:VAL:CB	2.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:56:ASP:O	14:b:108:ASN:OD1	2.16	0.63
1:A:120:ASP:OD2	2:B:87:HIS:CE1	2.51	0.63
7:G:181:MET:O	7:G:182:LYS:C	2.41	0.63
15:V:300:KNM:O3	15:V:300:KNM:H18	1.98	0.63
5:E:42:THR:OG1	5:E:45:GLY:O	2.11	0.63
1:O:103:TYR:HB2	8:V:61:TYR:CD1	2.33	0.63
8:H:83:PHE:CD2	8:H:100:ILE:HD11	2.34	0.63
12:L:149:VAL:HG12	12:L:153:TYR:CZ	2.34	0.63
1:A:69:LEU:CD1	1:A:229:ILE:HG13	2.30	0.62
9:I:136:ALA:HB2	14:b:145:LEU:HG	1.80	0.62
13:M:106:VAL:CG1	13:M:108:ASN:CG	2.72	0.62
8:V:135:ILE:HG12	8:V:163:ALA:HB2	1.80	0.62
9:W:22:GLU:HA	15:W:300:KNM:H6	1.81	0.62
9:W:36:PHE:HA	9:W:42:TYR:HD1	1.64	0.62
11:Y:24:ASN:ND2	11:Y:26:VAL:HG22	2.15	0.62
14:b:16:PHE:CE1	14:b:166:ARG:CA	2.76	0.62
8:H:1:THR:C	8:H:2:THR:CA	2.72	0.62
8:H:135:ILE:HG12	8:H:163:ALA:HB2	1.80	0.62
11:K:56:PHE:HZ	11:K:84:THR:OG1	1.81	0.62
2:P:41:ASN:OD1	2:P:182:GLU:HA	2.00	0.62
8:V:83:PHE:CD2	8:V:100:ILE:HD11	2.34	0.62
11:Y:67:TYR:CE2	11:Y:75:LEU:HD21	2.33	0.62
14:b:46:ASN:C	14:b:48:SER:N	2.51	0.62
4:D:6:ALA:HB2	5:E:134:SER:OG	2.00	0.62
8:H:98:ILE:HG21	8:H:100:ILE:CG1	2.29	0.62
8:V:177:ALA:HA	8:V:186:ARG:HG3	1.80	0.62
9:I:46:ALA:HA	15:I:300:KNM:H31	1.81	0.62
11:K:24:ASN:HD21	11:K:26:VAL:HG23	1.64	0.62
6:T:210:VAL:O	6:T:210:VAL:HG23	1.99	0.62
9:W:104:ASP:O	9:W:105:VAL:C	2.42	0.62
10:X:137:VAL:CG2	10:X:146:TYR:CD2	2.82	0.62
1:A:103:TYR:HB2	8:H:61:TYR:CD1	2.33	0.62
6:F:210:VAL:HG23	6:F:210:VAL:O	1.99	0.62
15:L:300:KNM:H29	15:L:300:KNM:C10	2.29	0.62
12:Z:1:THR:CG2	15:Z:300:KNM:H30	2.30	0.62
13:a:17:GLY:CA	13:a:166:LEU:CD2	2.61	0.62
1:A:103:TYR:C	9:I:81:ARG:CZ	2.73	0.62
15:H:300:KNM:O3	15:H:300:KNM:H18	1.98	0.62
9:I:104:ASP:O	9:I:106:THR:N	2.32	0.62
10:J:137:VAL:CG2	10:J:146:TYR:CD2	2.82	0.62
7:U:190:VAL:CG2	7:U:215:TRP:NE1	2.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ALA:HA	15:I:300:KNM:C20	2.30	0.62
10:X:55:LEU:HD13	10:X:103:TYR:HB2	1.82	0.62
13:a:106:VAL:CG1	13:a:108:ASN:CG	2.72	0.62
3:C:28:ILE:HD12	3:C:28:ILE:H	1.65	0.62
8:H:32:ASP:CG	8:H:186:ARG:HH21	2.06	0.62
9:I:36:PHE:HA	9:I:42:TYR:HD1	1.64	0.62
12:L:1:THR:CG2	15:L:300:KNM:H30	2.30	0.62
12:L:153:TYR:CE2	12:L:187:VAL:HG13	2.33	0.62
12:L:153:TYR:CE2	12:L:187:VAL:HG11	2.35	0.62
9:W:46:ALA:HA	15:W:300:KNM:H31	1.81	0.62
9:W:104:ASP:O	9:W:106:THR:N	2.32	0.62
11:Y:55:GLN:CD	12:Z:88:TYR:HD2	2.08	0.62
1:A:109:ILE:CB	1:A:114:LEU:HD21	2.20	0.61
2:B:41:ASN:OD1	2:B:182:GLU:HA	2.00	0.61
11:K:55:GLN:CD	12:L:88:TYR:HD2	2.08	0.61
8:V:28:ASN:OD1	8:V:30:VAL:N	2.21	0.61
9:W:46:ALA:HB1	15:W:300:KNM:H29	1.82	0.61
12:Z:149:VAL:HG12	12:Z:153:TYR:CZ	2.34	0.61
1:O:69:LEU:HD12	1:O:229:ILE:HG13	1.82	0.61
14:N:91:TRP:HZ3	14:N:94:ARG:HB3	1.63	0.61
2:P:138:TRP:CD1	2:P:143:PRO:HG3	2.35	0.61
3:Q:12:PHE:HD2	4:R:21:TYR:CB	2.14	0.61
3:Q:79:ILE:HG22	3:Q:80:THR:N	2.15	0.61
4:R:6:ALA:HB2	5:S:134:SER:OG	2.00	0.61
6:T:13:TRP:N	7:U:22:GLN:HE22	1.99	0.61
12:Z:153:TYR:CE2	12:Z:187:VAL:HG11	2.35	0.61
13:a:48:ASP:O	13:a:203:ILE:CG1	2.34	0.61
13:a:104:TYR:HE1	14:b:97:TYR:OH	1.82	0.61
2:B:138:TRP:CD1	2:B:143:PRO:HG3	2.35	0.61
3:C:12:PHE:HD2	4:D:21:TYR:CB	2.14	0.61
5:E:191:LEU:HD13	5:E:221:GLN:HG2	1.82	0.61
6:F:13:TRP:N	7:G:22:GLN:HE22	1.99	0.61
3:Q:198:ASN:CG	3:Q:240:HIS:CE1	2.78	0.61
13:a:49:LYS:CD	13:a:113:LEU:HB3	2.30	0.61
3:C:79:ILE:HG22	3:C:80:THR:N	2.15	0.61
7:G:75:MET:CA	7:G:137:LEU:CD2	2.68	0.61
11:Y:56:PHE:HZ	11:Y:84:THR:OG1	1.81	0.61
6:F:121:GLN:HG3	7:G:122:TYR:HE2	1.66	0.61
8:H:175:ARG:HG2	8:H:188:VAL:HG22	1.81	0.61
13:M:48:ASP:O	13:M:203:ILE:CG1	2.34	0.61
13:M:49:LYS:CD	13:M:113:LEU:HB3	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:LEU:CD1	1:O:229:ILE:HG13	2.30	0.61
14:N:16:PHE:CE2	14:N:21:VAL:CB	2.45	0.61
14:N:197:VAL:O	14:N:197:VAL:HG12	2.00	0.61
8:V:175:ARG:HG2	8:V:188:VAL:HG22	1.81	0.61
15:Z:300:KNM:H29	15:Z:300:KNM:C10	2.29	0.61
14:b:197:VAL:HG12	14:b:197:VAL:O	2.00	0.61
3:C:198:ASN:CG	3:C:240:HIS:CE1	2.78	0.61
6:F:43:HIS:HB2	6:F:184:LEU:HD13	1.82	0.61
9:I:22:GLU:HA	15:I:300:KNM:H6	1.81	0.61
9:I:46:ALA:HB1	15:I:300:KNM:H29	1.82	0.61
5:S:166:ASP:CB	5:S:185:TYR:CZ	2.73	0.61
6:T:43:HIS:HB2	6:T:184:LEU:HD13	1.82	0.61
4:D:172:LEU:CD2	4:D:190:LEU:HD21	2.31	0.61
6:F:7:ASP:OD2	6:F:14:SER:HA	2.01	0.61
1:A:229:ILE:HD12	1:A:229:ILE:N	2.16	0.60
5:E:211:ASN:O	5:E:214:ASN:N	2.31	0.60
11:K:24:ASN:ND2	11:K:26:VAL:HG22	2.15	0.60
14:b:38:ASN:HA	14:b:186:ARG:NH2	2.16	0.60
14:b:145:LEU:HD21	14:b:175:VAL:CG1	2.27	0.60
1:A:43:ARG:HD2	1:A:149:PRO:O	2.01	0.60
1:O:103:TYR:CA	9:W:81:ARG:HH22	1.72	0.60
3:Q:28:ILE:HD12	3:Q:28:ILE:H	1.65	0.60
7:U:104:TYR:OH	8:V:70:LEU:HD21	2.02	0.60
8:V:98:ILE:HG21	8:V:100:ILE:CG1	2.29	0.60
5:E:191:LEU:CD1	5:E:221:GLN:HG2	2.31	0.60
10:J:176:ARG:CZ	13:a:146:GLN:HB3	2.31	0.60
12:L:21:THR:O	15:L:300:KNM:H25	2.00	0.60
9:W:36:PHE:CE1	9:W:38:SER:HA	2.36	0.60
12:Z:1:THR:O	12:Z:1:THR:HG22	2.01	0.60
2:B:68:THR:CG2	2:B:71:ILE:HB	2.27	0.60
7:G:46:VAL:HG22	7:G:215:TRP:CD1	2.36	0.60
9:I:36:PHE:CE1	9:I:38:SER:HA	2.36	0.60
9:I:172:ASN:OD1	9:I:190:THR:O	2.18	0.60
10:J:134:ASP:CG	10:J:135:PHE:H	2.07	0.60
11:K:55:GLN:NE2	12:L:88:TYR:CD2	2.69	0.60
14:N:38:ASN:HA	14:N:186:ARG:NH2	2.16	0.60
1:O:103:TYR:C	9:W:81:ARG:CZ	2.73	0.60
4:R:172:LEU:CD2	4:R:190:LEU:HD21	2.31	0.60
10:J:122:SER:HB3	10:J:136:VAL:CG1	2.29	0.60
13:a:15:ILE:HG22	13:a:135:PHE:CB	2.22	0.60
11:K:48:GLY:O	11:K:53:THR:HG21	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1:THR:HG22	12:L:1:THR:O	2.01	0.60
13:M:146:GLN:HB3	10:X:176:ARG:CZ	2.31	0.60
1:O:159:TYR:CD1	2:P:83:ARG:NH2	2.70	0.60
5:S:191:LEU:HD13	5:S:221:GLN:HG2	1.82	0.60
9:W:49:ALA:HA	15:W:300:KNM:C20	2.30	0.60
12:Z:21:THR:O	15:Z:300:KNM:H25	2.00	0.60
1:A:69:LEU:HD12	1:A:229:ILE:HG13	1.82	0.60
2:B:212:CYS:C	2:B:213:ASN:HD22	2.10	0.60
8:H:119:MET:SD	14:N:57:TYR:HB3	2.40	0.60
12:L:111:LEU:HD23	12:L:124:ALA:O	2.02	0.60
1:O:43:ARG:HD2	1:O:149:PRO:O	2.01	0.60
1:O:229:ILE:N	1:O:229:ILE:HD12	2.16	0.60
5:E:166:ASP:CB	5:E:185:TYR:CZ	2.73	0.60
7:G:104:TYR:OH	8:H:70:LEU:HD21	2.02	0.60
10:J:55:LEU:HD13	10:J:103:TYR:HB2	1.82	0.60
13:M:46:LEU:HD23	13:M:72:LEU:CD2	2.31	0.60
7:U:46:VAL:HG22	7:U:215:TRP:CD1	2.36	0.60
9:W:172:ASN:OD1	9:W:190:THR:O	2.18	0.60
10:X:122:SER:HB3	10:X:136:VAL:CG1	2.29	0.60
15:I:300:KNM:H18	15:I:300:KNM:H5	1.84	0.59
5:S:191:LEU:CD1	5:S:221:GLN:HG2	2.31	0.59
14:b:41:ARG:HG3	14:b:41:ARG:HH11	1.68	0.59
14:b:173:MET:CB	14:b:187:PHE:CE2	2.85	0.59
2:P:38:LYS:CA	2:P:43:VAL:HG22	2.28	0.59
3:Q:139:TRP:NE1	3:Q:144:GLY:HA2	2.18	0.59
8:V:4:MET:HB2	8:V:160:LEU:HD21	1.82	0.59
13:M:152:GLN:CB	9:W:202:TYR:HE2	2.13	0.59
6:T:121:GLN:HG3	7:U:122:TYR:HE2	1.66	0.59
8:V:119:MET:SD	14:b:57:TYR:HB3	2.40	0.59
11:Y:147:TYR:CD1	11:Y:159:LEU:HD21	2.36	0.59
12:Z:1:THR:HG22	12:Z:46:ALA:HA	1.84	0.59
8:H:8:PHE:HE2	8:H:143:TYR:CZ	2.20	0.59
12:Z:115:ASP:HB3	12:Z:119:ASN:HB2	1.84	0.59
3:C:139:TRP:NE1	3:C:144:GLY:HA2	2.18	0.59
8:H:117:GLY:HA3	14:N:5:MET:HG3	1.84	0.59
11:K:19:ARG:O	11:K:20:VAL:CG2	2.50	0.59
12:L:115:ASP:HB3	12:L:119:ASN:HB2	1.84	0.59
14:N:16:PHE:CZ	14:N:165:ALA:CB	2.86	0.59
11:Y:19:ARG:O	11:Y:20:VAL:CG2	2.50	0.59
1:A:109:ILE:HD13	1:A:114:LEU:HD23	0.66	0.59
13:M:99:ARG:CB	13:M:104:TYR:CE2	2.86	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:212:CYS:C	2:P:213:ASN:HD22	2.10	0.59
6:T:77:LEU:HD11	6:T:80:ASP:CB	2.33	0.59
11:Y:48:GLY:O	11:Y:53:THR:HG21	2.02	0.59
11:Y:67:TYR:CZ	11:Y:75:LEU:HD21	2.38	0.59
13:a:19:ASP:OD1	13:a:113:LEU:CD1	2.50	0.59
12:L:1:THR:HG22	12:L:46:ALA:HA	1.84	0.59
13:M:99:ARG:HB3	13:M:104:TYR:HE2	1.66	0.59
2:P:212:CYS:HG	2:P:217:PHE:HD2	1.46	0.59
15:W:300:KNM:H18	15:W:300:KNM:H5	1.84	0.59
12:Z:111:LEU:HD23	12:Z:124:ALA:O	2.02	0.59
3:C:8:ARG:C	3:C:10:THR:H	2.10	0.59
11:K:67:TYR:CZ	11:K:75:LEU:HD21	2.38	0.59
14:N:16:PHE:CZ	14:N:165:ALA:HB3	2.38	0.59
1:O:109:ILE:CG2	1:O:114:LEU:HD11	2.32	0.59
2:P:68:THR:CG2	2:P:71:ILE:HB	2.27	0.59
3:Q:76:VAL:HG12	3:Q:132:VAL:HG11	1.84	0.59
11:Y:10:PRO:HD3	11:Y:151:ILE:HG22	1.85	0.59
2:P:71:ILE:HG22	2:P:72:GLY:N	2.18	0.59
6:T:152:ASN:HD21	7:U:81:LEU:HD12	1.68	0.59
11:Y:184:ASP:O	11:Y:185:LYS:C	2.46	0.59
5:E:50:VAL:HG22	5:E:66:LYS:HD3	1.85	0.58
6:F:77:LEU:HD11	6:F:80:ASP:CB	2.33	0.58
7:G:120:HIS:CE1	7:G:124:LEU:HD21	2.38	0.58
11:K:147:TYR:CD1	11:K:159:LEU:HD21	2.36	0.58
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.83	0.58
13:a:99:ARG:CB	13:a:104:TYR:CE2	2.86	0.58
1:A:159:TYR:CD1	2:B:83:ARG:NH2	2.70	0.58
13:M:19:ASP:OD1	13:M:113:LEU:CD1	2.51	0.58
11:Y:55:GLN:NE2	12:Z:88:TYR:CD2	2.69	0.58
3:C:76:VAL:HG12	3:C:132:VAL:HG11	1.84	0.58
7:U:120:HIS:CE1	7:U:124:LEU:HD21	2.38	0.58
14:b:16:PHE:CZ	14:b:165:ALA:CB	2.86	0.58
14:N:41:ARG:HH11	14:N:41:ARG:HG3	1.68	0.58
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.83	0.58
13:M:15:ILE:HG22	13:M:135:PHE:CB	2.22	0.58
13:M:174:LEU:HD22	9:W:202:TYR:CZ	2.38	0.58
2:P:41:ASN:CB	2:P:183:LEU:HB2	2.19	0.58
7:U:122:TYR:CD1	7:U:131:PHE:CE1	2.92	0.58
13:M:99:ARG:CD	13:M:104:TYR:OH	2.52	0.58
2:B:71:ILE:HD11	2:B:106:THR:HA	1.86	0.58
3:Q:8:ARG:C	3:Q:10:THR:H	2.10	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:83:PHE:CE2	8:V:100:ILE:HG12	2.39	0.58
9:W:49:ALA:CA	15:W:300:KNM:H36	2.34	0.58
14:b:16:PHE:CZ	14:b:165:ALA:HB3	2.38	0.58
14:N:173:MET:CB	14:N:187:PHE:CE2	2.85	0.58
2:P:39:ALA:CB	2:P:186:ALA:CB	2.82	0.58
2:P:71:ILE:HD11	2:P:106:THR:HA	1.86	0.58
8:V:3:ILE:CG2	8:V:99:ILE:HD12	2.33	0.58
8:V:117:GLY:HA3	14:b:5:MET:HG3	1.84	0.58
14:b:89:HIS:NE2	14:b:131:ALA:HB1	2.19	0.58
6:F:14:SER:HB2	6:F:17:GLY:H	1.69	0.58
6:F:152:ASN:HD21	7:G:81:LEU:HD12	1.68	0.58
7:G:122:TYR:CD1	7:G:131:PHE:CE1	2.92	0.58
8:H:28:ASN:OD1	8:H:30:VAL:N	2.21	0.58
8:V:175:ARG:HG2	8:V:188:VAL:HG13	1.86	0.58
14:b:91:TRP:HZ3	14:b:94:ARG:CB	2.07	0.58
3:C:237:ILE:O	3:C:240:HIS:HB3	2.04	0.58
9:I:47:GLY:CA	15:I:300:KNM:H28	2.33	0.58
11:K:19:ARG:O	11:K:20:VAL:HG23	2.04	0.58
14:N:145:LEU:HD21	14:N:175:VAL:CG1	2.27	0.58
5:S:221:GLN:HB3	5:S:222:PRO:HD2	1.86	0.58
11:Y:19:ARG:O	11:Y:20:VAL:HG23	2.04	0.58
13:a:36:HIS:CB	14:b:132:TYR:OH	2.50	0.58
5:E:221:GLN:HB3	5:E:222:PRO:HD2	1.86	0.57
9:I:49:ALA:CA	15:I:300:KNM:H36	2.34	0.57
9:I:202:TYR:CZ	13:a:174:LEU:HD22	2.38	0.57
9:I:202:TYR:HE2	13:a:152:GLN:CB	2.13	0.57
9:I:202:TYR:HB2	13:a:152:GLN:CD	2.29	0.57
11:K:10:PRO:HD3	11:K:151:ILE:HG22	1.85	0.57
13:M:146:GLN:HB3	10:X:176:ARG:HH12	1.69	0.57
1:O:109:ILE:HD13	1:O:114:LEU:HD23	0.66	0.57
1:A:109:ILE:CG2	1:A:114:LEU:HD11	2.32	0.57
2:B:71:ILE:HG22	2:B:72:GLY:N	2.18	0.57
6:F:14:SER:HB2	6:F:17:GLY:O	2.04	0.57
11:K:44:LEU:CB	11:K:102:LEU:HD11	2.32	0.57
3:Q:237:ILE:O	3:Q:240:HIS:HB3	2.04	0.57
11:Y:45:LEU:O	11:Y:102:LEU:HG	2.05	0.57
1:A:102:LYS:O	9:I:81:ARG:NH2	2.38	0.57
8:H:1:THR:CG2	8:H:2:THR:N	2.67	0.57
13:M:152:GLN:CD	9:W:202:TYR:HB2	2.29	0.57
8:V:38:HIS:CD2	8:V:40:ARG:H	2.22	0.57
4:D:40:ILE:HG13	4:D:212:ARG:NH1	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:36:PHE:HA	9:I:42:TYR:CD1	2.38	0.57
11:K:121:LEU:O	11:K:122:ALA:CB	2.52	0.57
12:L:34:VAL:HG13	12:L:43:GLY:O	2.03	0.57
5:S:229:PHE:HZ	5:S:233:GLU:CG	2.04	0.57
9:W:36:PHE:HA	9:W:42:TYR:CD1	2.38	0.57
11:Y:8:GLN:HB2	11:Y:115:LEU:CD2	2.35	0.57
11:Y:121:LEU:O	11:Y:122:ALA:CB	2.52	0.57
12:Z:34:VAL:HG13	12:Z:43:GLY:O	2.03	0.57
13:a:46:LEU:HD23	13:a:72:LEU:CD2	2.31	0.57
13:a:99:ARG:CD	13:a:104:TYR:OH	2.52	0.57
9:I:186:LEU:O	9:I:189:TYR:HB2	2.05	0.57
14:N:9:THR:CG2	14:N:10:SER:H	2.15	0.57
4:R:40:ILE:HG13	4:R:212:ARG:NH1	2.19	0.57
8:V:1:THR:C	8:V:2:THR:CA	2.72	0.57
8:H:83:PHE:CE2	8:H:100:ILE:HG12	2.39	0.57
11:K:184:ASP:O	11:K:185:LYS:C	2.46	0.57
8:H:3:ILE:CG2	8:H:99:ILE:HD12	2.33	0.57
10:J:176:ARG:HH12	13:a:146:GLN:HB3	1.69	0.57
11:K:8:GLN:HB2	11:K:115:LEU:CD2	2.35	0.57
11:K:101:ASN:ND2	11:K:132:HIS:ND1	2.53	0.57
2:P:212:CYS:SG	2:P:217:PHE:CD2	2.98	0.57
6:T:14:SER:HB2	6:T:17:GLY:CA	2.34	0.57
14:b:91:TRP:CZ3	14:b:94:ARG:CG	2.86	0.57
6:F:69:HIS:CE1	6:F:102:PRO:HB2	2.40	0.57
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.45	0.57
15:I:300:KNM:H5	15:I:300:KNM:C10	2.34	0.57
6:T:19:ILE:H	6:T:19:ILE:HD12	1.69	0.57
13:a:99:ARG:HB3	13:a:104:TYR:HE2	1.66	0.57
5:E:218:ALA:HB1	5:E:226:PHE:HE1	1.66	0.57
8:H:175:ARG:HG2	8:H:188:VAL:HG13	1.86	0.57
9:I:60:SER:OG	9:I:64:GLU:OE2	2.23	0.57
8:V:7:GLN:HG2	8:V:8:PHE:N	2.19	0.57
11:Y:55:GLN:CD	12:Z:88:TYR:CD2	2.83	0.57
12:Z:11:GLY:HA3	12:Z:178:HIS:NE2	2.19	0.57
9:W:47:GLY:CA	15:W:300:KNM:H28	2.33	0.57
15:W:300:KNM:H5	15:W:300:KNM:C10	2.34	0.57
10:X:141:CYS:HB2	10:X:145:MET:HE2	1.87	0.57
15:I:300:KNM:C7	10:J:124:ASP:OD2	2.53	0.56
12:L:11:GLY:HA3	12:L:178:HIS:NE2	2.19	0.56
12:L:44:THR:HG22	12:L:45:MET:N	2.20	0.56
1:O:102:LYS:O	9:W:81:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:50:VAL:HG22	5:S:66:LYS:HD3	1.85	0.56
8:V:33:LYS:HE2	15:V:300:KNM:H36	1.87	0.56
15:Z:300:KNM:H25	15:Z:300:KNM:H15	1.70	0.56
14:b:16:PHE:O	14:b:19:GLY:O	2.22	0.56
2:B:39:ALA:CB	2:B:186:ALA:CB	2.82	0.56
9:I:129:SER:N	15:I:300:KNM:O4	2.38	0.56
14:N:89:HIS:CE1	14:N:125:VAL:HG22	2.40	0.56
14:N:89:HIS:NE2	14:N:131:ALA:HB1	2.19	0.56
9:W:60:SER:OG	9:W:64:GLU:OE2	2.23	0.56
11:Y:101:ASN:ND2	11:Y:132:HIS:ND1	2.53	0.56
12:Z:42:LEU:HD11	12:Z:184:TRP:CG	2.40	0.56
14:b:89:HIS:CE1	14:b:125:VAL:HG22	2.40	0.56
6:F:184:LEU:CD2	6:F:214:ILE:HG21	2.22	0.56
8:H:4:MET:HB2	8:H:160:LEU:HD21	1.82	0.56
8:H:38:HIS:CD2	8:H:40:ARG:H	2.22	0.56
9:I:170:GLY:O	9:I:171:SER:HB2	2.05	0.56
10:J:73:TYR:CZ	10:J:77:GLU:OE2	2.58	0.56
10:J:134:ASP:CG	10:J:135:PHE:N	2.63	0.56
15:L:300:KNM:H25	15:L:300:KNM:H15	1.70	0.56
14:N:16:PHE:O	14:N:19:GLY:O	2.22	0.56
9:W:186:LEU:O	9:W:189:TYR:HB2	2.05	0.56
10:X:73:TYR:CZ	10:X:77:GLU:OE2	2.58	0.56
11:Y:44:LEU:CB	11:Y:102:LEU:HD11	2.32	0.56
2:B:51:GLN:NE2	2:B:56:TYR:HB2	2.18	0.56
4:D:66:ASP:CB	4:D:68:ASN:OD1	2.54	0.56
6:F:14:SER:HB2	6:F:17:GLY:C	2.29	0.56
10:J:141:CYS:HB2	10:J:145:MET:HE2	1.87	0.56
12:L:42:LEU:HD11	12:L:184:TRP:CG	2.40	0.56
12:L:49:ALA:HB2	15:L:300:KNM:H32	1.88	0.56
14:N:115:TYR:CZ	14:N:118:GLY:HA2	2.41	0.56
6:T:13:TRP:CG	7:U:22:GLN:NE2	2.73	0.56
6:F:13:TRP:CG	7:G:22:GLN:NE2	2.73	0.56
13:M:99:ARG:HD3	13:M:104:TYR:CE1	2.28	0.56
2:P:38:LYS:HA	2:P:43:VAL:CG2	2.31	0.56
9:W:129:SER:N	15:W:300:KNM:O4	2.38	0.56
15:W:300:KNM:C7	10:X:124:ASP:OD2	2.53	0.56
9:W:170:GLY:O	9:W:171:SER:HB2	2.05	0.56
12:Z:44:THR:HG22	12:Z:45:MET:N	2.20	0.56
13:a:13:LEU:CD1	13:a:149:LEU:HD13	2.35	0.56
2:B:118:GLN:NE2	3:C:82:ASP:OD1	2.39	0.56
11:K:55:GLN:CD	12:L:88:TYR:CD2	2.83	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:49:ALA:HB2	15:Z:300:KNM:H32	1.88	0.56
11:K:45:LEU:O	11:K:102:LEU:HG	2.05	0.56
2:P:118:GLN:NE2	3:Q:82:ASP:OD1	2.39	0.56
6:T:69:HIS:CE1	6:T:102:PRO:HB2	2.40	0.56
8:V:98:ILE:HG22	8:V:100:ILE:HG13	1.88	0.56
3:C:99:LEU:HD12	10:J:64:GLN:HB3	1.88	0.56
11:K:14:LEU:HD22	11:K:156:ALA:HB1	1.88	0.56
13:M:17:GLY:HA3	13:M:166:LEU:CD1	2.36	0.56
13:M:17:GLY:CA	13:M:166:LEU:CD2	2.61	0.56
4:R:66:ASP:CB	4:R:68:ASN:OD1	2.54	0.56
14:b:115:TYR:CZ	14:b:118:GLY:HA2	2.41	0.56
7:G:122:TYR:CE1	7:G:131:PHE:CZ	2.94	0.56
9:I:202:TYR:CD2	13:a:152:GLN:NE2	2.74	0.56
14:N:4:PRO:HB2	14:N:56:ASP:OD1	2.06	0.56
5:S:211:ASN:O	5:S:214:ASN:N	2.31	0.56
8:V:1:THR:CG2	8:V:2:THR:N	2.67	0.56
8:V:3:ILE:O	8:V:127:ILE:HA	2.06	0.56
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.45	0.56
8:H:20:THR:HG22	15:H:300:KNM:H38	1.75	0.55
9:I:49:ALA:HB2	15:I:300:KNM:H33	1.87	0.55
13:M:36:HIS:CB	14:N:132:TYR:OH	2.50	0.55
13:M:146:GLN:HB3	10:X:176:ARG:NH1	2.20	0.55
2:P:172:PHE:HE2	2:P:196:GLU:HG2	1.71	0.55
6:T:14:SER:HB2	6:T:17:GLY:HA2	1.88	0.55
11:Y:14:LEU:HD22	11:Y:156:ALA:HB1	1.88	0.55
2:B:62:HIS:ND1	2:B:219:ARG:NH1	2.53	0.55
4:D:196:LEU:O	4:D:196:LEU:HD23	2.05	0.55
12:L:178:HIS:HB3	12:L:187:VAL:HG21	1.88	0.55
13:M:13:LEU:CD1	13:M:149:LEU:HD13	2.35	0.55
9:W:49:ALA:HB2	15:W:300:KNM:H33	1.87	0.55
10:X:10:VAL:HG23	10:X:53:ALA:HB3	1.88	0.55
13:a:113:LEU:HD23	13:a:114:ASP:O	2.06	0.55
2:B:44:VAL:HG23	2:B:211:ILE:CG2	2.37	0.55
2:B:172:PHE:HE2	2:B:196:GLU:HG2	1.71	0.55
6:F:19:ILE:HD12	6:F:19:ILE:H	1.70	0.55
11:K:170:ARG:HD3	12:Z:140:ASP:CG	2.23	0.55
13:M:113:LEU:HD23	13:M:114:ASP:O	2.06	0.55
13:M:152:GLN:NE2	9:W:202:TYR:CD2	2.74	0.55
2:P:62:HIS:ND1	2:P:219:ARG:NH1	2.53	0.55
4:R:196:LEU:O	4:R:196:LEU:HD23	2.05	0.55
14:b:59:ASP:HB2	14:b:108:ASN:CG	2.31	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:91:TRP:CZ3	14:b:94:ARG:HG3	2.40	0.55
2:B:38:LYS:CA	2:B:43:VAL:HG22	2.28	0.55
3:C:41:ASP:N	3:C:41:ASP:OD1	2.40	0.55
8:H:32:ASP:OD1	8:H:186:ARG:NH2	2.40	0.55
2:P:51:GLN:NE2	2:P:56:TYR:HB2	2.18	0.55
13:a:15:ILE:HD11	13:a:175:VAL:HG23	1.86	0.55
13:a:17:GLY:HA3	13:a:166:LEU:CD1	2.36	0.55
8:H:33:LYS:HE2	15:H:300:KNM:H36	1.87	0.55
10:J:10:VAL:HG23	10:J:53:ALA:HB3	1.88	0.55
10:J:176:ARG:NH1	13:a:146:GLN:HB3	2.20	0.55
13:M:19:ASP:OD2	13:M:200:LYS:N	2.40	0.55
13:M:152:GLN:NE2	9:W:202:TYR:CG	2.74	0.55
6:T:16:GLN:H	6:T:16:GLN:CD	2.15	0.55
8:V:4:MET:CB	8:V:160:LEU:CD2	2.81	0.55
11:Y:120:TYR:CE1	11:Y:121:LEU:HG	2.41	0.55
13:a:91:MET:HE3	13:a:95:ILE:HD12	1.89	0.55
11:K:19:ARG:C	11:K:20:VAL:HG23	2.32	0.55
11:K:120:TYR:CE1	11:K:121:LEU:HG	2.41	0.55
13:M:97:TYR:CE2	13:M:127:VAL:O	2.59	0.55
14:N:16:PHE:HE1	14:N:165:ALA:N	2.04	0.55
14:N:59:ASP:HB2	14:N:108:ASN:CG	2.31	0.55
9:W:59:ILE:CG2	9:W:63:LEU:CD1	2.85	0.55
14:b:16:PHE:HE1	14:b:165:ALA:N	2.04	0.55
12:L:21:THR:HG23	15:L:300:KNM:H24	1.89	0.55
14:N:91:TRP:CZ3	14:N:94:ARG:HG3	2.40	0.55
11:Y:19:ARG:C	11:Y:20:VAL:HG23	2.32	0.55
13:a:19:ASP:OD2	13:a:200:LYS:N	2.40	0.55
14:b:4:PRO:HB2	14:b:56:ASP:OD1	2.06	0.55
9:I:202:TYR:CG	13:a:152:GLN:NE2	2.74	0.55
13:M:15:ILE:CG2	13:M:135:PHE:CB	2.78	0.55
13:a:97:TYR:CE2	13:a:127:VAL:O	2.59	0.55
8:H:3:ILE:O	8:H:127:ILE:HA	2.06	0.55
15:H:300:KNM:H24	15:H:300:KNM:H28	1.89	0.55
13:M:13:LEU:CD1	13:M:149:LEU:CD1	2.85	0.55
7:U:122:TYR:CE1	7:U:131:PHE:CZ	2.94	0.55
10:X:134:ASP:CG	10:X:135:PHE:H	2.07	0.55
10:X:134:ASP:CG	10:X:135:PHE:N	2.63	0.55
2:B:51:GLN:HE21	2:B:51:GLN:C	2.13	0.55
12:Z:21:THR:HG23	15:Z:300:KNM:H24	1.89	0.55
3:Q:41:ASP:OD1	3:Q:41:ASP:N	2.40	0.54
6:T:43:HIS:CB	6:T:184:LEU:HD13	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:144:PRO:O	9:W:145:ASP:CB	2.55	0.54
2:B:38:LYS:HA	2:B:43:VAL:CG2	2.31	0.54
13:M:15:ILE:HD11	13:M:175:VAL:HG23	1.86	0.54
2:P:51:GLN:HE21	2:P:51:GLN:C	2.13	0.54
8:V:7:GLN:O	8:V:8:PHE:HB2	2.06	0.54
12:L:1:THR:CG2	15:L:300:KNM:C17	2.85	0.54
8:V:7:GLN:O	8:V:8:PHE:CB	2.55	0.54
8:V:28:ASN:OD1	8:V:29:ARG:N	2.41	0.54
3:Q:99:LEU:HD12	10:X:64:GLN:HB3	1.88	0.54
15:V:300:KNM:H24	15:V:300:KNM:H28	1.89	0.54
11:Y:29:LYS:HD3	12:Z:121:ILE:HB	1.89	0.54
11:Y:102:LEU:HD23	11:Y:103:LEU:C	2.33	0.54
13:a:106:VAL:HG11	13:a:108:ASN:HD21	1.73	0.54
14:b:193:THR:O	14:b:195:LYS:N	2.41	0.54
3:C:115:CYS:HB3	4:D:81:ARG:NH2	2.22	0.54
10:J:64:GLN:HE22	11:K:85:ARG:NH2	1.97	0.54
13:M:91:MET:HE3	13:M:95:ILE:HD12	1.89	0.54
2:P:44:VAL:HG23	2:P:211:ILE:CG2	2.37	0.54
2:P:212:CYS:SG	2:P:217:PHE:HD2	2.30	0.54
3:C:12:PHE:CZ	4:D:25:ALA:HB2	2.43	0.54
13:M:16:ALA:HA	13:M:20:PHE:O	2.07	0.54
14:N:91:TRP:CZ3	14:N:94:ARG:CG	2.86	0.54
3:Q:139:TRP:CD1	3:Q:144:GLY:C	2.86	0.54
5:S:220:VAL:HG22	5:S:226:PHE:HD1	1.73	0.54
8:V:51:ASP:HB3	8:V:94:LEU:CD1	2.38	0.54
8:V:127:ILE:HD11	8:V:136:TYR:CE1	2.43	0.54
3:C:139:TRP:CD1	3:C:144:GLY:C	2.86	0.54
7:G:190:VAL:CG2	7:G:215:TRP:HZ2	2.06	0.54
8:H:127:ILE:HD11	8:H:136:TYR:CE1	2.43	0.54
9:I:42:TYR:CD2	9:I:178:ILE:HD11	2.43	0.54
9:I:59:ILE:CG2	9:I:63:LEU:CD1	2.85	0.54
9:I:144:PRO:O	9:I:145:ASP:CB	2.55	0.54
11:K:102:LEU:HD23	11:K:103:LEU:C	2.33	0.54
11:K:170:ARG:CZ	12:Z:136:TYR:CD1	2.88	0.54
13:M:152:GLN:HG3	9:W:202:TYR:HD2	0.51	0.54
11:Y:121:LEU:O	11:Y:122:ALA:HB3	2.08	0.54
12:Z:178:HIS:HB3	12:Z:187:VAL:HG21	1.88	0.54
14:b:9:THR:CG2	14:b:10:SER:H	2.15	0.54
2:B:212:CYS:SG	2:B:217:PHE:HD2	2.30	0.54
12:L:44:THR:HB	12:L:100:MET:H	1.72	0.54
9:W:42:TYR:CD2	9:W:178:ILE:HD11	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:300:KNM:H12	10:X:124:ASP:OD2	2.08	0.54
3:Q:115:CYS:HB3	4:R:81:ARG:NH2	2.22	0.54
11:K:102:LEU:HD23	11:K:103:LEU:N	2.23	0.54
8:V:32:ASP:OD1	8:V:186:ARG:NH2	2.40	0.54
9:W:49:ALA:CA	9:W:52:THR:HG22	2.38	0.54
2:B:41:ASN:CB	2:B:183:LEU:HB2	2.20	0.53
2:B:172:PHE:CE2	2:B:196:GLU:CG	2.90	0.53
9:I:63:LEU:HD12	9:I:82:MET:SD	2.49	0.53
2:P:133:LEU:HD13	2:P:135:ILE:HG12	1.87	0.53
3:Q:12:PHE:CZ	4:R:25:ALA:HB2	2.43	0.53
13:a:135:PHE:CZ	13:a:150:ASP:HA	2.43	0.53
7:G:44:GLY:H	7:G:146:ALA:HB2	1.73	0.53
13:M:38:ARG:HH21	14:N:151:ARG:HD3	1.74	0.53
9:W:49:ALA:HA	9:W:52:THR:CG2	2.38	0.53
12:Z:44:THR:HB	12:Z:100:MET:H	1.72	0.53
13:a:13:LEU:CD1	13:a:149:LEU:CD1	2.85	0.53
5:E:220:VAL:HG22	5:E:226:PHE:HD1	1.73	0.53
6:F:43:HIS:CB	6:F:184:LEU:HD13	2.38	0.53
9:I:22:GLU:HA	15:I:300:KNM:C4	2.38	0.53
9:I:52:THR:HG21	15:I:300:KNM:H38	1.91	0.53
9:I:202:TYR:OH	13:a:174:LEU:CG	2.56	0.53
11:K:29:LYS:HD3	12:L:121:ILE:HB	1.89	0.53
12:L:44:THR:CG2	12:L:45:MET:N	2.71	0.53
14:N:193:THR:O	14:N:195:LYS:N	2.41	0.53
6:T:7:ASP:OD2	6:T:14:SER:OG	2.22	0.53
9:W:22:GLU:HA	15:W:300:KNM:C4	2.38	0.53
8:H:20:THR:HG22	15:H:300:KNM:H37	1.75	0.53
13:M:20:PHE:HZ	13:M:166:LEU:O	1.91	0.53
3:Q:12:PHE:HD2	4:R:21:TYR:HB2	1.74	0.53
5:S:37:ALA:O	5:S:170:ILE:N	2.38	0.53
11:Y:102:LEU:HD23	11:Y:103:LEU:N	2.23	0.53
12:Z:36:GLU:HA	12:Z:42:LEU:CD2	2.38	0.53
13:a:16:ALA:HA	13:a:20:PHE:O	2.07	0.53
2:B:70:HIS:HD2	2:B:217:PHE:N	2.07	0.53
12:L:21:THR:C	15:L:300:KNM:H11	2.34	0.53
12:L:136:TYR:CD1	11:Y:170:ARG:CZ	2.88	0.53
8:H:28:ASN:OD1	8:H:29:ARG:N	2.41	0.53
9:W:70:THR:CG2	9:W:72:ARG:H	2.04	0.53
12:Z:44:THR:CG2	12:Z:45:MET:N	2.71	0.53
11:K:121:LEU:O	11:K:122:ALA:HB3	2.08	0.53
14:N:16:PHE:CE1	14:N:166:ARG:CA	2.76	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:134:LEU:CD2	7:U:124:LEU:HD22	2.39	0.53
2:P:134:LEU:HD23	2:P:162:MET:SD	2.48	0.53
9:W:104:ASP:C	9:W:106:THR:N	2.65	0.53
12:Z:1:THR:CG2	15:Z:300:KNM:C17	2.85	0.53
13:a:20:PHE:HZ	13:a:166:LEU:O	1.91	0.53
3:C:31:ALA:HB1	3:C:77:ALA:O	2.09	0.53
3:C:111:VAL:HG22	3:C:136:TYR:CE2	2.44	0.53
6:F:15:PRO:O	7:G:28:LYS:HE3	2.08	0.53
9:I:70:THR:CG2	9:I:72:ARG:H	2.04	0.53
12:L:39:PRO:O	12:L:184:TRP:NE1	2.42	0.53
14:N:4:PRO:HA	14:N:56:ASP:OD2	2.09	0.53
9:W:63:LEU:HD12	9:W:82:MET:SD	2.48	0.53
12:Z:39:PRO:O	12:Z:184:TRP:NE1	2.42	0.53
8:H:51:ASP:HB3	8:H:94:LEU:CD1	2.38	0.53
8:H:103:TRP:CZ2	8:H:181:GLU:HB3	2.44	0.53
9:I:202:TYR:HD2	13:a:152:GLN:HG3	0.51	0.53
12:L:136:TYR:CZ	11:Y:170:ARG:NH2	2.76	0.53
13:M:13:LEU:HD11	13:M:149:LEU:HD13	1.91	0.53
13:M:174:LEU:CG	9:W:202:TYR:OH	2.56	0.53
6:T:77:LEU:HD11	6:T:80:ASP:HB2	1.90	0.53
14:b:4:PRO:HA	14:b:56:ASP:OD2	2.09	0.53
6:F:15:PRO:HA	7:G:25:TYR:CD1	2.44	0.53
11:K:8:GLN:HB2	11:K:115:LEU:HD21	1.91	0.53
7:U:75:MET:CA	7:U:137:LEU:CD2	2.68	0.53
8:V:103:TRP:CZ2	8:V:181:GLU:HB3	2.44	0.53
2:B:134:LEU:HD23	2:B:162:MET:SD	2.48	0.52
3:C:111:VAL:CG2	3:C:136:TYR:CD2	2.92	0.52
7:G:190:VAL:HG11	7:G:215:TRP:CH2	2.37	0.52
11:Y:120:TYR:HE1	11:Y:121:LEU:CD2	2.21	0.52
12:Z:21:THR:C	15:Z:300:KNM:H11	2.34	0.52
13:a:38:ARG:HH21	14:b:151:ARG:HD3	1.74	0.52
5:E:37:ALA:HB3	5:E:170:ILE:CG1	2.39	0.52
7:U:44:GLY:H	7:U:146:ALA:HB2	1.73	0.52
9:I:1:THR:HG22	9:I:129:SER:OG	2.04	0.52
9:I:36:PHE:HE1	9:I:39:PRO:CA	2.19	0.52
13:M:135:PHE:CZ	13:M:150:ASP:HA	2.44	0.52
3:Q:139:TRP:HD1	3:Q:145:PHE:N	2.08	0.52
5:S:37:ALA:HB3	5:S:170:ILE:HG13	1.92	0.52
8:V:27:ALA:O	8:V:28:ASN:CB	2.57	0.52
10:X:17:ASN:O	10:X:118:PRO:HG3	2.10	0.52
5:E:166:ASP:CG	5:E:185:TYR:OH	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:300:KNM:C7	10:J:124:ASP:CG	2.77	0.52
13:a:99:ARG:HD2	13:a:104:TYR:OH	2.09	0.52
1:A:134:LEU:CD2	7:G:124:LEU:HD22	2.39	0.52
12:L:149:VAL:CG1	12:L:153:TYR:CZ	2.93	0.52
5:E:32:LYS:O	5:E:172:SER:HB3	2.10	0.52
6:F:77:LEU:HD11	6:F:80:ASP:HB2	1.90	0.52
14:N:41:ARG:NH1	14:N:41:ARG:HG3	2.25	0.52
7:U:75:MET:CG	7:U:137:LEU:HD23	2.35	0.52
3:C:79:ILE:CG2	3:C:80:THR:N	2.73	0.52
4:D:36:ARG:HG2	4:D:142:PRO:HB2	1.89	0.52
5:E:100:TRP:C	5:E:100:TRP:CE3	2.88	0.52
7:G:90:ILE:O	7:G:94:GLU:HG3	2.09	0.52
10:J:17:ASN:O	10:J:118:PRO:HG3	2.10	0.52
1:O:229:ILE:N	1:O:229:ILE:CD1	2.73	0.52
5:S:37:ALA:HB3	5:S:170:ILE:CG1	2.39	0.52
9:W:45:GLY:HA3	9:W:52:THR:OG1	2.10	0.52
11:Y:8:GLN:HB2	11:Y:115:LEU:HD21	1.91	0.52
13:a:15:ILE:CG2	13:a:135:PHE:CB	2.78	0.52
6:F:69:HIS:CE1	6:F:96:ARG:NH2	2.77	0.52
7:G:94:GLU:CD	7:G:115:VAL:HG22	2.34	0.52
10:J:16:LYS:O	10:J:18:CYS:O	2.27	0.52
11:K:120:TYR:HE1	11:K:121:LEU:CD2	2.21	0.52
3:Q:111:VAL:HG22	3:Q:136:TYR:CE2	2.44	0.52
5:S:42:THR:HG22	5:S:194:ALA:CB	2.02	0.52
10:X:16:LYS:O	10:X:18:CYS:O	2.27	0.52
3:Q:111:VAL:CG2	3:Q:136:TYR:CD2	2.92	0.52
8:V:20:THR:HG22	15:V:300:KNM:H37	1.75	0.52
9:W:52:THR:HG21	15:W:300:KNM:H38	1.91	0.52
12:Z:149:VAL:CG1	12:Z:153:TYR:CZ	2.93	0.52
3:C:139:TRP:HD1	3:C:145:PHE:N	2.08	0.51
8:H:96:ALA:O	8:H:116:MET:HA	2.10	0.51
11:K:85:ARG:HD3	11:K:124:LEU:HB3	1.92	0.51
2:P:70:HIS:HD2	2:P:217:PHE:N	2.07	0.51
11:Y:44:LEU:CD2	11:Y:102:LEU:HD11	2.39	0.51
9:I:45:GLY:HA3	9:I:52:THR:OG1	2.10	0.51
12:L:36:GLU:HA	12:L:42:LEU:CD2	2.37	0.51
2:P:51:GLN:HE22	2:P:56:TYR:H	1.58	0.51
13:a:17:GLY:C	13:a:166:LEU:CD1	2.79	0.51
4:D:192:ILE:HG12	4:D:228:TYR:CE1	2.44	0.51
9:I:172:ASN:ND2	9:I:191:VAL:HG22	2.21	0.51
3:Q:31:ALA:HB1	3:Q:77:ALA:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1:THR:HG22	9:W:129:SER:OG	2.04	0.51
9:W:172:ASN:ND2	9:W:191:VAL:HG22	2.21	0.51
4:D:36:ARG:HG2	4:D:142:PRO:CG	2.41	0.51
5:E:37:ALA:HB3	5:E:170:ILE:HG13	1.92	0.51
9:I:122:LEU:HG	9:I:123:PRO:CD	2.38	0.51
9:I:127:MET:HG2	9:I:128:GLY:H	1.75	0.51
2:P:172:PHE:CE2	2:P:196:GLU:CG	2.90	0.51
4:R:36:ARG:HG2	4:R:142:PRO:CG	2.41	0.51
14:b:9:THR:CG2	14:b:10:SER:N	2.73	0.51
2:P:211:ILE:HD13	2:P:220:LEU:HG	1.92	0.51
9:W:127:MET:HG2	9:W:128:GLY:H	1.75	0.51
13:a:164:VAL:HG13	13:a:166:LEU:H	1.76	0.51
9:I:49:ALA:CA	9:I:52:THR:HG22	2.38	0.51
13:M:146:GLN:CB	10:X:176:ARG:HH12	2.23	0.51
14:N:173:MET:HB3	14:N:187:PHE:CD2	2.46	0.51
1:O:165:ALA:HB3	2:P:55:LEU:HD22	1.88	0.51
3:Q:79:ILE:CG2	3:Q:80:THR:N	2.73	0.51
5:S:229:PHE:CZ	5:S:233:GLU:HG3	2.38	0.51
9:W:36:PHE:HE1	9:W:39:PRO:CA	2.19	0.51
3:C:12:PHE:HD2	4:D:21:TYR:HB2	1.74	0.51
15:I:300:KNM:H12	10:J:124:ASP:OD2	2.08	0.51
12:L:140:ASP:CG	11:Y:170:ARG:HD3	2.23	0.51
4:R:66:ASP:HB3	4:R:68:ASN:OD1	2.11	0.51
7:U:90:ILE:O	7:U:94:GLU:HG3	2.09	0.51
14:b:25:ASP:HA	14:b:187:PHE:HB3	1.93	0.51
8:H:8:PHE:CE2	8:H:143:TYR:CZ	2.98	0.51
3:Q:151:ASP:HB3	3:Q:155:ASN:HB3	1.93	0.51
5:S:100:TRP:C	5:S:100:TRP:CE3	2.88	0.51
13:a:49:LYS:HD2	13:a:113:LEU:HB3	1.93	0.51
1:A:229:ILE:N	1:A:229:ILE:CD1	2.73	0.51
2:B:133:LEU:HA	2:B:162:MET:HE1	1.93	0.51
9:I:104:ASP:C	9:I:106:THR:N	2.65	0.51
13:M:99:ARG:HD2	13:M:104:TYR:OH	2.09	0.51
14:N:26:MET:HB2	14:N:186:ARG:HH22	1.70	0.51
2:P:39:ALA:CB	2:P:186:ALA:HB3	2.39	0.51
8:V:96:ALA:O	8:V:116:MET:HA	2.10	0.51
9:W:148:GLU:O	9:W:152:LYS:NZ	2.44	0.51
9:W:173:ILE:HB	9:W:190:THR:HB	1.92	0.51
14:b:41:ARG:NH1	14:b:41:ARG:HG3	2.25	0.51
5:E:37:ALA:O	5:E:169:ALA:HA	2.11	0.51
5:E:218:ALA:CB	5:E:226:PHE:HE1	2.22	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:189:HIS:CD2	11:K:190:ASP:O	2.64	0.51
13:M:106:VAL:HG11	13:M:108:ASN:HD21	1.73	0.51
5:S:32:LYS:O	5:S:172:SER:HB3	2.10	0.51
1:A:13:ILE:HD11	1:A:15:ILE:HD13	1.93	0.50
2:B:51:GLN:HE22	2:B:56:TYR:H	1.58	0.50
2:B:133:LEU:HD13	2:B:135:ILE:HG12	1.87	0.50
6:F:77:LEU:HD12	6:F:80:ASP:H	1.74	0.50
8:H:98:ILE:HG22	8:H:100:ILE:HG13	1.88	0.50
14:N:25:ASP:HA	14:N:187:PHE:HB3	1.93	0.50
5:S:37:ALA:O	5:S:169:ALA:HA	2.11	0.50
7:U:216:VAL:O	7:U:216:VAL:HG12	2.11	0.50
4:D:208:LEU:HD21	4:D:228:TYR:HE1	1.77	0.50
6:F:103:LEU:HD21	6:F:108:LEU:HB2	1.93	0.50
6:F:188:VAL:HG13	6:F:212:ILE:HD13	1.92	0.50
15:L:300:KNM:N2	15:L:300:KNM:H25	2.26	0.50
13:M:164:VAL:HG13	13:M:166:LEU:H	1.76	0.50
3:Q:99:LEU:CD1	10:X:64:GLN:HB3	2.41	0.50
4:R:40:ILE:HG22	4:R:41:VAL:N	2.26	0.50
8:V:9:ASP:CB	8:V:149:LYS:HD2	2.41	0.50
15:W:300:KNM:C7	10:X:124:ASP:CG	2.77	0.50
14:b:50:MET:HE2	14:b:192:VAL:HG23	0.81	0.50
7:G:216:VAL:O	7:G:216:VAL:HG12	2.11	0.50
8:H:117:GLY:N	14:N:5:MET:HG3	2.26	0.50
9:I:49:ALA:HA	9:I:52:THR:CG2	2.38	0.50
1:O:221:THR:O	1:O:224:ASN:N	2.42	0.50
3:Q:10:THR:O	4:R:125:ARG:HD3	2.12	0.50
15:Z:300:KNM:N2	15:Z:300:KNM:H25	2.26	0.50
14:b:173:MET:HB3	14:b:187:PHE:CD2	2.46	0.50
5:E:169:ALA:C	5:E:174:SER:OG	2.55	0.50
10:J:176:ARG:HH12	13:a:146:GLN:CB	2.23	0.50
1:O:13:ILE:HD11	1:O:15:ILE:HD13	1.93	0.50
4:R:216:SER:O	4:R:217:LEU:C	2.54	0.50
6:T:96:ARG:HA	6:T:101:ARG:O	2.11	0.50
6:T:103:LEU:HD21	6:T:108:LEU:HB2	1.93	0.50
11:Y:85:ARG:HD3	11:Y:124:LEU:HB3	1.92	0.50
2:B:43:VAL:HG11	2:B:136:CYS:HB2	1.94	0.50
3:C:12:PHE:HD2	4:D:21:TYR:HB3	1.75	0.50
3:C:139:TRP:CD1	3:C:145:PHE:N	2.79	0.50
4:D:40:ILE:HG22	4:D:41:VAL:N	2.26	0.50
3:Q:111:VAL:HG22	3:Q:136:TYR:CG	2.47	0.50
7:U:161:TRP:C	7:U:181:MET:HE1	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HG23	1:A:114:LEU:HG	1.94	0.50
9:I:173:ILE:HB	9:I:190:THR:HB	1.92	0.50
10:J:163:PHE:HA	10:J:188:ILE:HD11	1.94	0.50
12:L:55:TRP:CD1	12:L:97:MET:CE	2.94	0.50
13:M:20:PHE:HA	13:M:198:VAL:O	2.11	0.50
1:O:217:VAL:O	1:O:229:ILE:HG23	2.12	0.50
2:P:133:LEU:CD1	2:P:135:ILE:CD1	2.89	0.50
9:W:113:ILE:HA	9:W:118:SER:O	2.11	0.50
2:B:211:ILE:HD13	2:B:220:LEU:HG	1.92	0.50
5:E:66:LYS:O	5:E:78:MET:HE3	2.12	0.50
8:H:4:MET:CB	8:H:160:LEU:CD2	2.81	0.50
12:L:39:PRO:O	12:L:184:TRP:HD1	1.86	0.50
1:O:175:SER:HA	1:O:205:VAL:HG21	1.94	0.50
6:T:188:VAL:HG13	6:T:212:ILE:HD13	1.92	0.50
12:Z:55:TRP:CD1	12:Z:97:MET:CE	2.94	0.50
2:B:71:ILE:CG2	2:B:72:GLY:N	2.75	0.50
4:D:36:ARG:CG	4:D:142:PRO:CB	2.88	0.50
12:L:149:VAL:HG12	12:L:153:TYR:CE1	2.47	0.50
5:S:169:ALA:C	5:S:174:SER:OG	2.55	0.50
8:V:117:GLY:N	14:b:5:MET:HG3	2.26	0.50
10:X:10:VAL:HG23	10:X:53:ALA:CB	2.41	0.50
11:Y:42:ILE:HD11	11:Y:75:LEU:O	2.12	0.50
13:a:20:PHE:HA	13:a:198:VAL:O	2.11	0.50
1:A:134:LEU:HD22	7:G:124:LEU:HD22	1.94	0.50
2:B:51:GLN:HE21	2:B:54:ILE:H	1.59	0.50
2:B:138:TRP:NE1	2:B:143:PRO:CG	2.74	0.50
3:C:99:LEU:CD1	10:J:64:GLN:HB3	2.41	0.50
4:D:34:GLY:O	4:D:35:VAL:HG13	2.12	0.50
9:I:113:ILE:HA	9:I:118:SER:O	2.12	0.50
11:K:67:TYR:CZ	11:K:75:LEU:CD2	2.95	0.50
12:L:26:ILE:CD1	10:X:176:ARG:O	2.38	0.50
3:Q:12:PHE:HD2	4:R:21:TYR:HB3	1.76	0.50
6:T:69:HIS:CE1	6:T:96:ARG:NH2	2.77	0.50
6:T:184:LEU:HA	6:T:187:LEU:HD12	1.94	0.50
7:U:213:LEU:O	7:U:226:ILE:HD12	2.11	0.50
11:Y:78:THR:HG22	11:Y:116:TYR:CZ	2.47	0.50
1:A:217:VAL:O	1:A:229:ILE:HG23	2.12	0.49
3:C:111:VAL:HG22	3:C:136:TYR:CG	2.47	0.49
3:C:205:LYS:CA	3:C:240:HIS:NE2	2.73	0.49
4:D:66:ASP:HB3	4:D:68:ASN:OD1	2.11	0.49
5:E:35:SER:HB2	5:E:66:LYS:HZ3	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:98:ILE:HG22	8:H:99:ILE:N	2.27	0.49
10:J:10:VAL:HG23	10:J:53:ALA:CB	2.41	0.49
2:P:133:LEU:HA	2:P:162:MET:HE1	1.93	0.49
4:R:36:ARG:CG	4:R:142:PRO:CB	2.88	0.49
7:U:190:VAL:HG11	7:U:215:TRP:CH2	2.37	0.49
8:V:9:ASP:CG	8:V:149:LYS:HB2	2.37	0.49
14:b:47:ASN:O	14:b:197:VAL:CG2	2.61	0.49
6:F:43:HIS:CD2	6:F:216:GLY:HA3	2.47	0.49
11:K:44:LEU:CD2	11:K:102:LEU:HD11	2.39	0.49
14:N:26:MET:HB3	14:N:39:ILE:O	2.12	0.49
14:N:45:VAL:HG12	14:N:46:ASN:OD1	2.12	0.49
2:P:34:SER:N	2:P:162:MET:O	2.31	0.49
2:P:106:THR:HG21	2:P:137:GLY:HA3	1.94	0.49
2:P:138:TRP:NE1	2:P:143:PRO:CG	2.74	0.49
3:Q:139:TRP:CD1	3:Q:145:PHE:N	2.79	0.49
4:R:192:ILE:HG12	4:R:228:TYR:CE1	2.44	0.49
4:R:208:LEU:HD21	4:R:228:TYR:HE1	1.77	0.49
7:U:94:GLU:CD	7:U:115:VAL:HG22	2.34	0.49
11:Y:189:HIS:CD2	11:Y:190:ASP:O	2.64	0.49
12:Z:1:THR:CG2	12:Z:46:ALA:HA	2.42	0.49
2:B:137:GLY:N	2:B:144:TYR:O	2.40	0.49
9:I:122:LEU:CD1	9:I:123:PRO:HD2	2.42	0.49
1:O:134:LEU:HD22	7:U:124:LEU:HD22	1.94	0.49
2:P:51:GLN:HE21	2:P:54:ILE:H	1.59	0.49
10:X:137:VAL:CG2	10:X:146:TYR:CE2	2.69	0.49
12:Z:149:VAL:HG12	12:Z:153:TYR:CE1	2.47	0.49
2:B:34:SER:N	2:B:162:MET:O	2.31	0.49
3:C:151:ASP:HB3	3:C:155:ASN:HB3	1.93	0.49
6:F:96:ARG:HA	6:F:101:ARG:O	2.11	0.49
6:F:184:LEU:HA	6:F:187:LEU:HD12	1.94	0.49
13:M:49:LYS:HD2	13:M:113:LEU:HB3	1.93	0.49
14:N:91:TRP:CE3	14:N:91:TRP:HA	2.47	0.49
8:V:20:THR:HG22	15:V:300:KNM:H38	1.75	0.49
2:B:106:THR:HG21	2:B:137:GLY:HA3	1.94	0.49
7:G:213:LEU:O	7:G:226:ILE:HD12	2.11	0.49
8:H:33:LYS:HE2	15:H:300:KNM:H32	1.94	0.49
11:K:15:VAL:HB	11:K:45:LEU:HD11	1.95	0.49
11:K:42:ILE:HD11	11:K:75:LEU:O	2.12	0.49
12:L:149:VAL:CG1	12:L:153:TYR:CE1	2.96	0.49
2:P:43:VAL:HG11	2:P:136:CYS:HB2	1.94	0.49
6:T:43:HIS:CD2	6:T:216:GLY:HA3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:92:CYS:HA	6:T:103:LEU:CD1	2.42	0.49
8:V:66:HIS:O	8:V:70:LEU:HD13	2.13	0.49
8:V:88:TYR:OH	14:b:62:TYR:CG	2.32	0.49
10:X:64:GLN:HE22	11:Y:85:ARG:NH2	1.97	0.49
12:Z:39:PRO:O	12:Z:184:TRP:HD1	1.86	0.49
2:B:133:LEU:CD1	2:B:135:ILE:CD1	2.89	0.49
3:C:10:THR:O	4:D:125:ARG:HD3	2.12	0.49
5:S:66:LYS:O	5:S:78:MET:HE3	2.12	0.49
10:X:10:VAL:CG2	10:X:53:ALA:CB	2.90	0.49
10:X:163:PHE:HA	10:X:188:ILE:HD11	1.94	0.49
11:Y:15:VAL:HB	11:Y:45:LEU:HD11	1.95	0.49
2:B:172:PHE:CZ	2:B:196:GLU:CD	2.88	0.49
4:D:216:SER:O	4:D:217:LEU:C	2.54	0.49
8:H:66:HIS:O	8:H:70:LEU:HD13	2.13	0.49
13:M:93:SER:O	13:M:97:TYR:HD2	1.95	0.49
8:V:98:ILE:HG22	8:V:99:ILE:N	2.27	0.49
9:W:122:LEU:CD1	9:W:123:PRO:HD2	2.42	0.49
5:E:177:ALA:HB2	5:E:205:VAL:HG11	1.95	0.49
10:J:10:VAL:CG2	10:J:53:ALA:CB	2.90	0.49
2:P:213:ASN:N	2:P:213:ASN:ND2	2.60	0.49
14:b:91:TRP:CE3	14:b:91:TRP:HA	2.47	0.49
13:M:27:THR:CG2	13:M:40:SER:O	2.58	0.49
12:Z:149:VAL:CG1	12:Z:153:TYR:CE1	2.96	0.49
2:B:54:ILE:O	2:B:54:ILE:HG22	2.13	0.49
5:E:37:ALA:O	5:E:170:ILE:N	2.38	0.49
9:I:59:ILE:O	9:I:63:LEU:HD13	2.12	0.49
11:K:5:ILE:HD11	11:K:143:LEU:CD2	2.43	0.49
14:N:26:MET:HE2	14:N:186:ARG:NH2	2.27	0.49
2:P:71:ILE:CG2	2:P:72:GLY:N	2.75	0.49
4:R:34:GLY:O	4:R:35:VAL:HG13	2.12	0.49
8:V:4:MET:HB2	8:V:160:LEU:CD2	2.43	0.49
9:I:148:GLU:O	9:I:152:LYS:NZ	2.44	0.48
11:K:170:ARG:NH2	12:Z:136:TYR:CZ	2.76	0.48
13:M:20:PHE:CZ	13:M:166:LEU:O	2.66	0.48
13:M:99:ARG:NH1	13:M:104:TYR:CD1	2.81	0.48
2:P:147:GLN:OE1	2:P:162:MET:SD	2.71	0.48
3:Q:76:VAL:HA	3:Q:134:LEU:CD2	2.43	0.48
9:W:59:ILE:O	9:W:63:LEU:HD13	2.12	0.48
13:a:93:SER:O	13:a:97:TYR:HD2	1.95	0.48
2:B:213:ASN:N	2:B:213:ASN:ND2	2.60	0.48
5:E:147:ASP:C	5:E:149:LYS:N	2.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:229:PHE:HZ	5:E:233:GLU:CG	2.04	0.48
6:F:92:CYS:HA	6:F:103:LEU:CD1	2.42	0.48
14:N:4:PRO:CB	14:N:56:ASP:CG	2.70	0.48
3:Q:8:ARG:C	3:Q:10:THR:N	2.71	0.48
13:a:99:ARG:NH1	13:a:104:TYR:CD1	2.81	0.48
1:A:165:ALA:HB3	2:B:55:LEU:HD22	1.88	0.48
2:B:106:THR:CG2	2:B:137:GLY:HA3	2.43	0.48
2:B:147:GLN:OE1	2:B:162:MET:SD	2.71	0.48
3:C:107:CYS:H	3:C:140:ASP:HB3	1.79	0.48
5:E:147:ASP:O	5:E:148:GLU:C	2.56	0.48
12:L:1:THR:CG2	12:L:46:ALA:HA	2.42	0.48
15:L:300:KNM:O5	15:L:300:KNM:H17	2.13	0.48
2:P:106:THR:CG2	2:P:137:GLY:HA3	2.43	0.48
3:Q:65:ILE:HD11	3:Q:73:ALA:HB1	1.95	0.48
14:b:45:VAL:HG12	14:b:46:ASN:OD1	2.12	0.48
14:b:47:ASN:O	14:b:197:VAL:HG23	2.13	0.48
3:C:12:PHE:HZ	4:D:25:ALA:HB2	1.78	0.48
8:H:27:ALA:O	8:H:28:ASN:CB	2.57	0.48
14:N:47:ASN:O	14:N:197:VAL:HG23	2.13	0.48
6:T:77:LEU:HD12	6:T:80:ASP:H	1.74	0.48
14:b:26:MET:HB3	14:b:39:ILE:O	2.12	0.48
14:b:60:PHE:N	14:b:108:ASN:ND2	2.61	0.48
1:A:175:SER:HA	1:A:205:VAL:HG21	1.94	0.48
7:G:75:MET:CG	7:G:137:LEU:HD23	2.35	0.48
9:I:52:THR:HG21	15:I:300:KNM:C20	2.43	0.48
15:Z:300:KNM:O5	15:Z:300:KNM:H17	2.14	0.48
13:a:18:GLU:O	13:a:19:ASP:C	2.57	0.48
14:b:26:MET:HE2	14:b:186:ARG:NH2	2.27	0.48
14:b:46:ASN:C	14:b:48:SER:H	2.21	0.48
3:C:45:LEU:CD2	3:C:65:ILE:HD13	2.44	0.48
5:E:50:VAL:HG21	5:E:66:LYS:HD3	1.93	0.48
5:E:229:PHE:CZ	5:E:233:GLU:HG3	2.38	0.48
8:H:32:ASP:OD2	8:H:35:THR:HG22	2.14	0.48
12:L:4:LEU:HA	12:L:127:SER:HA	1.95	0.48
12:L:91:LYS:HE2	12:L:117:GLU:HB3	1.95	0.48
14:N:47:ASN:O	14:N:197:VAL:CG2	2.61	0.48
2:B:70:HIS:NE2	2:B:212:CYS:O	2.46	0.48
3:C:65:ILE:HD11	3:C:73:ALA:HB1	1.95	0.48
8:H:7:GLN:O	8:H:8:PHE:HB2	2.12	0.48
8:H:176:LEU:HB3	8:H:187:GLN:HG2	1.95	0.48
9:I:128:GLY:CA	15:I:300:KNM:O4	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:THR:C	14:N:10:SER:HG	2.05	0.48
1:O:109:ILE:HG23	1:O:114:LEU:HG	1.94	0.48
9:W:52:THR:HG21	15:W:300:KNM:C20	2.43	0.48
11:Y:67:TYR:CZ	11:Y:75:LEU:CD2	2.95	0.48
15:Z:300:KNM:H8	15:Z:300:KNM:H15	1.77	0.48
5:E:42:THR:CG2	5:E:194:ALA:HB3	2.00	0.48
6:F:103:LEU:HD23	6:F:104:PRO:C	2.35	0.48
14:N:91:TRP:HE3	14:N:91:TRP:HA	1.79	0.48
6:T:7:ASP:OD2	6:T:14:SER:CA	2.58	0.48
8:V:176:LEU:HB3	8:V:187:GLN:HG2	1.95	0.48
12:Z:50:ALA:HB3	13:a:100:ARG:HH12	1.78	0.48
4:D:43:LEU:HD11	4:D:217:LEU:HD21	1.96	0.48
8:H:9:ASP:CB	8:H:149:LYS:HD2	2.44	0.48
15:L:300:KNM:H8	15:L:300:KNM:H15	1.77	0.48
2:P:54:ILE:HG22	2:P:54:ILE:O	2.13	0.48
3:Q:107:CYS:H	3:Q:140:ASP:HB3	1.79	0.48
5:S:147:ASP:O	5:S:148:GLU:C	2.56	0.48
8:V:33:LYS:HE2	15:V:300:KNM:H32	1.94	0.48
8:V:125:PHE:HB3	8:V:143:TYR:HE2	1.78	0.48
11:Y:24:ASN:HD21	11:Y:26:VAL:CG2	2.23	0.48
3:C:197:LEU:HD13	3:C:211:VAL:HG11	1.96	0.48
8:H:4:MET:HB2	8:H:160:LEU:CD2	2.43	0.48
12:L:22:ALA:HB2	15:L:300:KNM:H11	1.96	0.48
15:L:300:KNM:H29	15:L:300:KNM:C14	2.44	0.48
13:M:34:SER:O	13:M:34:SER:OG	2.30	0.48
1:O:179:LEU:HB3	2:P:55:LEU:HD21	1.95	0.48
6:T:15:PRO:C	6:T:17:GLY:H	2.09	0.48
11:Y:5:ILE:HD11	11:Y:143:LEU:CD2	2.43	0.48
12:Z:153:TYR:CZ	12:Z:187:VAL:HG11	2.49	0.48
14:b:91:TRP:HE3	14:b:91:TRP:HA	1.79	0.48
14:b:198:GLU:HG3	14:b:199:ILE:N	2.29	0.48
1:A:179:LEU:HB3	2:B:55:LEU:HD21	1.95	0.47
1:A:221:THR:O	1:A:224:ASN:N	2.42	0.47
11:K:78:THR:HG22	11:K:116:TYR:CZ	2.47	0.47
3:Q:205:LYS:CA	3:Q:240:HIS:NE2	2.73	0.47
11:Y:67:TYR:CG	11:Y:75:LEU:HD11	2.49	0.47
7:G:75:MET:HG3	7:G:137:LEU:HD23	1.96	0.47
3:Q:12:PHE:HZ	4:R:25:ALA:HB2	1.78	0.47
4:R:36:ARG:HG2	4:R:142:PRO:HB2	1.89	0.47
8:V:32:ASP:OD2	8:V:35:THR:HG22	2.14	0.47
3:C:8:ARG:C	3:C:10:THR:N	2.71	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:TRP:CD2	4:D:54:GLN:NE2	2.80	0.47
13:M:48:ASP:C	13:M:203:ILE:HG13	2.30	0.47
2:P:172:PHE:CZ	2:P:196:GLU:CD	2.88	0.47
5:E:188:SER:OG	5:E:189:MET:N	2.46	0.47
7:G:122:TYR:CE1	7:G:131:PHE:HZ	2.31	0.47
12:L:153:TYR:CZ	12:L:187:VAL:HG11	2.49	0.47
14:N:198:GLU:HG3	14:N:199:ILE:N	2.29	0.47
4:R:66:ASP:HB2	4:R:68:ASN:OD1	2.15	0.47
5:S:218:ALA:CB	5:S:226:PHE:HE1	2.22	0.47
7:U:122:TYR:CE1	7:U:131:PHE:HZ	2.31	0.47
8:V:125:PHE:HB3	8:V:143:TYR:CE2	2.49	0.47
9:W:122:LEU:HG	9:W:123:PRO:CD	2.38	0.47
2:B:179:GLU:HB3	2:B:180:ASP:H	1.34	0.47
13:M:20:PHE:HB2	13:M:197:ILE:HG23	1.96	0.47
13:M:54:CYS:SG	13:M:106:VAL:HG13	2.55	0.47
5:S:177:ALA:HB2	5:S:205:VAL:HG11	1.95	0.47
12:Z:22:ALA:HB2	15:Z:300:KNM:H11	1.96	0.47
12:Z:91:LYS:HE2	12:Z:117:GLU:HB3	1.95	0.47
13:a:20:PHE:HB2	13:a:197:ILE:HG23	1.96	0.47
13:a:20:PHE:CZ	13:a:166:LEU:O	2.67	0.47
15:H:300:KNM:H26	15:H:300:KNM:H17	1.60	0.47
11:K:67:TYR:CG	11:K:75:LEU:HD11	2.49	0.47
13:M:18:GLU:O	13:M:19:ASP:C	2.57	0.47
2:P:211:ILE:CD1	2:P:220:LEU:HG	2.45	0.47
5:S:147:ASP:C	5:S:149:LYS:N	2.70	0.47
13:a:48:ASP:C	13:a:203:ILE:HG13	2.30	0.47
14:b:9:THR:CG2	14:b:140:GLY:O	2.63	0.47
6:F:184:LEU:HD11	6:F:214:ILE:HD12	0.72	0.47
6:F:195:LEU:HD23	6:F:210:VAL:CG1	2.44	0.47
12:L:50:ALA:HB3	13:M:100:ARG:HH12	1.78	0.47
14:N:16:PHE:CZ	14:N:165:ALA:CA	2.92	0.47
3:Q:45:LEU:CD2	3:Q:65:ILE:HD13	2.44	0.47
5:S:50:VAL:HG21	5:S:66:LYS:HD3	1.93	0.47
5:S:218:ALA:HB1	5:S:226:PHE:HE1	1.66	0.47
6:T:152:ASN:ND2	7:U:81:LEU:HD12	2.30	0.47
11:Y:24:ASN:ND2	11:Y:26:VAL:HG23	2.26	0.47
12:Z:4:LEU:HA	12:Z:127:SER:HA	1.95	0.47
13:a:34:SER:O	13:a:34:SER:OG	2.30	0.47
2:B:133:LEU:HD12	2:B:133:LEU:O	2.14	0.47
3:C:76:VAL:HA	3:C:134:LEU:CD2	2.43	0.47
7:G:122:TYR:CD1	7:G:131:PHE:HE1	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:97:LYS:HB3	10:J:100:GLY:C	2.40	0.47
10:J:97:LYS:HB2	10:J:101:PRO:HA	1.97	0.47
12:L:55:TRP:HE1	12:L:97:MET:HE1	1.80	0.47
4:R:31:THR:HG23	4:R:165:ALA:CA	2.45	0.47
4:R:43:LEU:HD11	4:R:217:LEU:HD21	1.96	0.47
5:S:35:SER:HB2	5:S:66:LYS:HZ3	1.76	0.47
5:S:188:SER:OG	5:S:189:MET:N	2.46	0.47
4:D:66:ASP:HB2	4:D:68:ASN:OD1	2.15	0.47
4:D:155:ALA:HB3	5:E:63:SER:HB3	1.97	0.47
11:K:36:PHE:CE2	11:K:46:CYS:HB3	2.50	0.47
13:M:99:ARG:CG	13:M:104:TYR:CE2	2.98	0.47
1:O:76:ILE:HD12	1:O:114:LEU:CD1	2.26	0.47
3:C:159:TRP:CE2	4:D:54:GLN:NE2	2.68	0.47
14:N:26:MET:CB	14:N:186:ARG:HH22	2.26	0.47
2:P:138:TRP:NE1	2:P:143:PRO:HG3	2.30	0.47
9:W:172:ASN:OD1	9:W:191:VAL:CA	2.52	0.47
10:X:26:ARG:CG	10:X:33:MET:HG3	2.45	0.47
15:Z:300:KNM:H29	15:Z:300:KNM:C14	2.44	0.47
13:a:54:CYS:SG	13:a:106:VAL:HG13	2.55	0.47
9:I:1:THR:HG21	15:I:300:KNM:O4	2.15	0.46
13:M:17:GLY:C	13:M:166:LEU:CD1	2.79	0.46
13:M:49:LYS:HB3	13:M:113:LEU:N	2.21	0.46
13:a:20:PHE:CZ	13:a:166:LEU:HB3	2.50	0.46
2:B:211:ILE:CD1	2:B:220:LEU:HG	2.45	0.46
8:H:63:LEU:O	8:H:66:HIS:HB3	2.16	0.46
13:M:47:THR:HG1	13:M:50:THR:H	1.61	0.46
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.96	0.46
7:U:75:MET:HG3	7:U:137:LEU:HD21	1.93	0.46
13:a:27:THR:CG2	13:a:40:SER:O	2.58	0.46
15:I:300:KNM:C2	15:I:300:KNM:C4	2.86	0.46
12:L:51:ASP:O	12:L:55:TRP:CD1	2.69	0.46
14:N:50:MET:HE2	14:N:192:VAL:HG23	0.81	0.46
4:R:155:ALA:HB3	5:S:63:SER:HB3	1.97	0.46
12:Z:51:ASP:O	12:Z:55:TRP:CD1	2.69	0.46
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.96	0.46
2:P:133:LEU:CD1	2:P:135:ILE:HD11	2.44	0.46
2:P:133:LEU:HD12	2:P:133:LEU:O	2.14	0.46
4:R:40:ILE:HG22	4:R:211:MET:O	2.03	0.46
5:S:43:SER:CA	5:S:151:PRO:HG3	2.44	0.46
5:S:166:ASP:CG	5:S:185:TYR:OH	2.52	0.46
13:a:49:LYS:HD2	13:a:113:LEU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:137:VAL:CG2	10:J:146:TYR:CE2	2.69	0.46
11:K:120:TYR:HE1	11:K:121:LEU:HD21	1.80	0.46
2:P:157:TRP:NE1	3:Q:56:LEU:HD21	2.30	0.46
9:W:49:ALA:HB2	15:W:300:KNM:H36	1.98	0.46
14:b:48:SER:C	14:b:197:VAL:HG23	2.40	0.46
2:B:6:SER:O	3:C:127:LYS:HE3	2.16	0.46
2:B:212:CYS:SG	2:B:217:PHE:CD2	2.98	0.46
9:I:63:LEU:HD21	9:I:79:ALA:HB2	1.98	0.46
13:M:197:ILE:H	13:M:197:ILE:HD12	1.81	0.46
4:R:6:ALA:CB	5:S:134:SER:OG	2.64	0.46
6:T:14:SER:HB2	6:T:17:GLY:HA3	1.98	0.46
8:V:63:LEU:O	8:V:66:HIS:HB3	2.16	0.46
9:W:1:THR:HG21	15:W:300:KNM:O4	2.15	0.46
13:a:166:LEU:O	13:a:167:SER:C	2.58	0.46
2:B:157:TRP:NE1	3:C:56:LEU:HD21	2.30	0.46
3:Q:197:LEU:HD13	3:Q:211:VAL:HG11	1.96	0.46
2:B:70:HIS:CD2	2:B:217:PHE:N	2.84	0.46
8:H:9:ASP:HB2	8:H:149:LYS:HD2	1.98	0.46
10:J:57:THR:HG21	11:K:121:LEU:HB3	1.98	0.46
14:N:89:HIS:HB2	14:N:112:ILE:HD13	1.98	0.46
7:U:47:PHE:HE1	7:U:216:VAL:HG21	1.80	0.46
10:X:137:VAL:HB	10:X:145:MET:HE3	1.98	0.46
13:a:20:PHE:HZ	13:a:166:LEU:HB3	1.81	0.46
14:b:187:PHE:HE1	14:b:189:ILE:HD11	1.81	0.46
2:B:70:HIS:HE1	2:B:213:ASN:O	1.98	0.46
4:D:31:THR:HG23	4:D:165:ALA:CA	2.45	0.46
7:G:47:PHE:HE1	7:G:216:VAL:HG21	1.80	0.46
10:J:26:ARG:CG	10:J:33:MET:HG3	2.45	0.46
9:W:22:GLU:HG3	9:W:22:GLU:O	2.16	0.46
2:B:39:ALA:CB	2:B:186:ALA:HB3	2.39	0.46
2:B:138:TRP:NE1	2:B:143:PRO:HG3	2.30	0.46
6:F:152:ASN:ND2	7:G:81:LEU:HD12	2.30	0.46
7:G:46:VAL:HG22	7:G:215:TRP:HD1	1.79	0.46
14:N:46:ASN:C	14:N:48:SER:H	2.21	0.46
14:N:187:PHE:HE1	14:N:189:ILE:HD11	1.80	0.46
1:O:159:TYR:HD1	2:P:83:ARG:NH2	2.14	0.46
2:P:70:HIS:HE1	2:P:213:ASN:O	1.98	0.46
9:W:128:GLY:CA	15:W:300:KNM:O4	2.60	0.46
10:X:97:LYS:HB2	10:X:101:PRO:HA	1.97	0.46
11:Y:36:PHE:CE2	11:Y:46:CYS:HB3	2.50	0.46
4:D:199:VAL:HG12	4:D:200:GLN:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:184:ASP:O	11:K:187:GLY:N	2.37	0.45
13:M:49:LYS:HD2	13:M:113:LEU:O	2.16	0.45
4:R:199:VAL:HG12	4:R:200:GLN:H	1.81	0.45
6:T:195:LEU:HD23	6:T:210:VAL:CG1	2.44	0.45
7:U:122:TYR:CD1	7:U:131:PHE:HE1	2.31	0.45
8:V:33:LYS:HE2	15:V:300:KNM:C18	2.45	0.45
15:W:300:KNM:H42	15:W:300:KNM:H40	1.72	0.45
10:X:57:THR:HG21	11:Y:121:LEU:HB3	1.98	0.45
10:X:97:LYS:HB3	10:X:100:GLY:C	2.40	0.45
8:H:10:GLY:O	8:H:103:TRP:CD1	2.69	0.45
9:I:22:GLU:HG3	9:I:22:GLU:O	2.16	0.45
10:J:137:VAL:HB	10:J:145:MET:HE3	1.98	0.45
3:Q:76:VAL:HG11	3:Q:83:ALA:HB2	1.94	0.45
10:X:119:PHE:CD1	10:X:119:PHE:C	2.94	0.45
11:Y:20:VAL:HG12	11:Y:21:ALA:N	2.32	0.45
13:a:197:ILE:H	13:a:197:ILE:HD12	1.80	0.45
2:B:82:TYR:O	2:B:86:VAL:HG23	2.16	0.45
5:E:43:SER:CA	5:E:151:PRO:HG3	2.44	0.45
11:K:85:ARG:CZ	11:K:86:ARG:NH2	2.74	0.45
12:L:125:THR:OG1	12:L:143:TYR:CE2	2.70	0.45
2:P:181:LEU:CD1	2:P:185:ASP:CB	2.94	0.45
5:S:82:ILE:H	5:S:82:ILE:HD12	1.81	0.45
6:T:103:LEU:HD23	6:T:103:LEU:C	2.42	0.45
6:T:184:LEU:HD11	6:T:214:ILE:HD12	0.72	0.45
7:U:48:GLY:HA3	7:U:193:VAL:HG11	1.98	0.45
8:V:46:SER:N	8:V:97:GLY:O	2.49	0.45
9:W:36:PHE:HB2	9:W:42:TYR:CE1	2.47	0.45
8:H:33:LYS:HE2	15:H:300:KNM:C18	2.45	0.45
9:I:36:PHE:HB2	9:I:42:TYR:CE1	2.47	0.45
9:I:164:PHE:HB3	13:a:38:ARG:HH22	1.82	0.45
13:M:20:PHE:CZ	13:M:166:LEU:HB3	2.51	0.45
13:M:146:GLN:C	10:X:176:ARG:NH2	2.74	0.45
14:N:48:SER:C	14:N:197:VAL:HG23	2.40	0.45
2:P:70:HIS:CD2	2:P:217:PHE:N	2.84	0.45
2:P:82:TYR:O	2:P:86:VAL:HG23	2.16	0.45
2:P:96:TYR:CD1	2:P:104:ILE:HB	2.51	0.45
14:b:48:SER:HB3	14:b:196:GLY:HA3	1.99	0.45
15:H:300:KNM:H38	15:H:300:KNM:H27	1.77	0.45
10:J:119:PHE:CD1	10:J:119:PHE:C	2.94	0.45
13:M:99:ARG:CB	13:M:104:TYR:HE2	2.28	0.45
2:P:6:SER:O	3:Q:127:LYS:HE3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:14:SER:CA	6:T:17:GLY:HA3	2.47	0.45
7:U:75:MET:HG3	7:U:137:LEU:HD23	1.96	0.45
9:W:63:LEU:HD21	9:W:79:ALA:HB2	1.98	0.45
2:B:147:GLN:CD	2:B:162:MET:SD	2.99	0.45
2:B:151:SER:O	3:C:81:SER:CB	2.65	0.45
2:B:182:GLU:O	2:B:185:ASP:N	2.50	0.45
9:I:11:GLY:HA2	9:I:108:PRO:HB3	1.99	0.45
10:J:176:ARG:NH2	13:a:146:GLN:C	2.75	0.45
6:T:103:LEU:HD23	6:T:104:PRO:C	2.35	0.45
10:X:17:ASN:C	10:X:17:ASN:OD1	2.60	0.45
8:H:46:SER:N	8:H:97:GLY:O	2.49	0.45
10:J:26:ARG:HG3	10:J:33:MET:HG3	1.99	0.45
13:M:20:PHE:HZ	13:M:166:LEU:HB3	1.81	0.45
2:P:147:GLN:CD	2:P:162:MET:SD	2.99	0.45
11:Y:29:LYS:HD2	12:Z:122:SER:C	2.42	0.45
11:Y:120:TYR:HE1	11:Y:121:LEU:HD21	1.80	0.45
12:Z:49:ALA:CB	15:Z:300:KNM:H32	2.47	0.45
3:C:41:ASP:O	3:C:145:PHE:CE2	2.70	0.45
6:F:103:LEU:HD23	6:F:103:LEU:C	2.42	0.45
8:H:18:SER:CB	8:H:173:VAL:H	2.30	0.45
13:M:166:LEU:O	13:M:167:SER:C	2.58	0.45
14:N:11:VAL:HG23	14:N:54:SER:OG	2.17	0.45
7:U:75:MET:CE	7:U:137:LEU:HD11	2.47	0.45
9:W:11:GLY:HA2	9:W:108:PRO:HB3	1.99	0.45
2:B:51:GLN:NE2	2:B:51:GLN:C	2.74	0.45
2:B:68:THR:HG22	2:B:71:ILE:CB	2.32	0.45
11:K:44:LEU:CD2	11:K:102:LEU:CD1	2.86	0.45
11:K:120:TYR:CE1	11:K:121:LEU:HD21	2.52	0.45
12:L:19:ARG:HB3	12:L:171:GLY:H	1.82	0.45
12:L:49:ALA:CB	15:L:300:KNM:H32	2.47	0.45
14:N:190:ALA:HA	14:N:199:ILE:HA	1.98	0.45
4:R:34:GLY:O	4:R:35:VAL:CG1	2.65	0.45
10:X:116:PHE:O	10:X:116:PHE:CG	2.70	0.45
2:B:45:LEU:HD21	2:B:136:CYS:HB3	1.99	0.45
7:G:48:GLY:HA3	7:G:193:VAL:HG11	1.98	0.45
13:M:38:ARG:HH22	9:W:164:PHE:HB3	1.82	0.45
1:O:100:ASN:HA	8:V:61:TYR:HE1	1.82	0.45
5:S:40:ILE:HG21	5:S:194:ALA:HB1	1.98	0.45
8:V:42:PHE:HB2	8:V:179:ILE:HD11	2.00	0.45
9:W:36:PHE:HD1	9:W:38:SER:O	1.98	0.45
10:X:134:ASP:OD2	10:X:135:PHE:CE1	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:46:ASN:O	14:b:197:VAL:HG21	2.17	0.45
4:D:6:ALA:CB	5:E:134:SER:OG	2.64	0.44
5:E:227:HIS:O	5:E:227:HIS:CG	2.70	0.44
8:H:112:TYR:CZ	8:H:122:ARG:HD2	2.52	0.44
9:I:1:THR:H2	9:I:169:SER:CB	2.29	0.44
11:K:20:VAL:HG12	11:K:21:ALA:N	2.32	0.44
14:N:16:PHE:CD1	14:N:161:SER:O	2.61	0.44
14:N:187:PHE:O	14:N:187:PHE:CD1	2.70	0.44
1:O:109:ILE:CG2	1:O:114:LEU:CD1	2.92	0.44
2:P:85:LEU:HD22	2:P:133:LEU:CD2	2.47	0.44
2:P:151:SER:O	3:Q:81:SER:CB	2.65	0.44
8:V:135:ILE:HG22	8:V:139:VAL:HG23	2.00	0.44
12:Z:88:TYR:CD1	12:Z:88:TYR:O	2.70	0.44
3:C:8:ARG:O	3:C:10:THR:N	2.50	0.44
3:C:139:TRP:O	3:C:139:TRP:CE3	2.71	0.44
7:G:75:MET:CE	7:G:137:LEU:HD11	2.47	0.44
8:H:19:ARG:HH21	8:H:21:THR:HG21	1.82	0.44
14:N:46:ASN:O	14:N:197:VAL:HG21	2.17	0.44
6:T:77:LEU:HD13	6:T:80:ASP:H	1.80	0.44
2:B:96:TYR:CD1	2:B:104:ILE:HB	2.51	0.44
4:D:34:GLY:O	4:D:35:VAL:CG1	2.65	0.44
5:E:40:ILE:HG21	5:E:194:ALA:HB1	1.98	0.44
6:F:77:LEU:HD12	6:F:77:LEU:O	2.17	0.44
1:O:109:ILE:CB	1:O:114:LEU:CD2	2.89	0.44
3:Q:8:ARG:O	3:Q:10:THR:N	2.50	0.44
3:Q:33:THR:HG21	3:Q:200:THR:HG21	1.99	0.44
5:S:219:THR:O	5:S:227:HIS:ND1	2.51	0.44
14:b:190:ALA:HA	14:b:199:ILE:HA	1.98	0.44
2:B:214:GLU:HG3	2:B:214:GLU:O	2.18	0.44
3:C:45:LEU:HD21	3:C:75:SER:HB2	2.00	0.44
13:M:118:LYS:CG	13:M:119:GLY:N	2.80	0.44
3:Q:45:LEU:HD21	3:Q:75:SER:HB2	2.00	0.44
6:T:121:GLN:CG	7:U:122:TYR:HE2	2.30	0.44
8:V:125:PHE:CD1	8:V:143:TYR:CE2	3.05	0.44
10:X:10:VAL:CG2	10:X:53:ALA:HB3	2.47	0.44
10:X:116:PHE:O	10:X:116:PHE:CD2	2.70	0.44
13:a:99:ARG:CG	13:a:104:TYR:CE2	2.98	0.44
14:b:89:HIS:HB2	14:b:112:ILE:HD13	1.98	0.44
2:B:183:LEU:HD13	2:B:213:ASN:CG	2.42	0.44
3:C:76:VAL:HG12	3:C:132:VAL:CG1	2.48	0.44
5:E:218:ALA:CB	5:E:226:PHE:HZ	2.27	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:116:PHE:CD2	10:J:116:PHE:O	2.70	0.44
10:J:150:GLU:CB	13:a:185:ARG:HH21	2.31	0.44
12:L:88:TYR:CD1	12:L:88:TYR:O	2.70	0.44
2:P:182:GLU:O	2:P:185:ASP:N	2.50	0.44
2:P:219:ARG:O	2:P:220:LEU:C	2.61	0.44
3:Q:41:ASP:O	3:Q:145:PHE:CE2	2.70	0.44
6:T:13:TRP:HD1	7:U:22:GLN:HE21	1.45	0.44
6:T:77:LEU:HD12	6:T:77:LEU:O	2.18	0.44
11:Y:44:LEU:CG	11:Y:102:LEU:HD21	2.40	0.44
12:Z:19:ARG:HB3	12:Z:171:GLY:H	1.82	0.44
12:Z:125:THR:OG1	12:Z:143:TYR:CE2	2.70	0.44
14:b:187:PHE:CD1	14:b:187:PHE:O	2.70	0.44
1:A:100:ASN:HA	8:H:61:TYR:HE1	1.82	0.44
5:E:82:ILE:HD12	5:E:82:ILE:H	1.81	0.44
5:E:219:THR:O	5:E:227:HIS:ND1	2.51	0.44
6:F:15:PRO:HA	7:G:25:TYR:CE1	2.52	0.44
6:F:121:GLN:NE2	7:G:122:TYR:CE2	2.75	0.44
10:J:17:ASN:C	10:J:17:ASN:OD1	2.60	0.44
10:J:134:ASP:OD2	10:J:135:PHE:CE1	2.70	0.44
11:K:147:TYR:CD1	11:K:159:LEU:CD2	2.95	0.44
10:X:26:ARG:HG3	10:X:33:MET:HG3	1.99	0.44
13:a:37:THR:HG23	13:a:40:SER:OG	2.18	0.44
13:a:118:LYS:CG	13:a:119:GLY:N	2.80	0.44
14:b:11:VAL:HG23	14:b:54:SER:OG	2.17	0.44
2:B:51:GLN:NE2	2:B:54:ILE:H	2.15	0.44
10:J:64:GLN:HE21	11:K:85:ARG:HH22	1.38	0.44
13:M:54:CYS:CB	13:M:108:ASN:HD22	2.30	0.44
13:M:185:ARG:HH21	10:X:150:GLU:CB	2.31	0.44
2:P:61:VAL:HG21	2:P:83:ARG:HH21	1.83	0.44
5:S:100:TRP:CE3	5:S:100:TRP:O	2.71	0.44
5:S:227:HIS:O	5:S:227:HIS:CG	2.71	0.44
13:a:167:SER:O	13:a:171:ALA:HB2	2.18	0.44
2:B:51:GLN:CD	2:B:54:ILE:CA	2.86	0.44
2:B:85:LEU:HD22	2:B:133:LEU:CD2	2.47	0.44
2:B:181:LEU:CD1	2:B:185:ASP:CB	2.94	0.44
8:H:42:PHE:CE2	8:H:186:ARG:NH1	2.86	0.44
9:I:59:ILE:HG23	9:I:63:LEU:CD1	2.47	0.44
9:I:63:LEU:HD21	9:I:79:ALA:CB	2.47	0.44
2:P:45:LEU:HD21	2:P:136:CYS:HB3	1.99	0.44
2:P:51:GLN:NE2	2:P:54:ILE:H	2.15	0.44
2:P:53:SER:O	2:P:54:ILE:HB	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:53:SER:OG	2:P:56:TYR:CE1	2.70	0.44
8:V:18:SER:CB	8:V:173:VAL:H	2.30	0.44
8:V:112:TYR:CZ	8:V:122:ARG:HD2	2.52	0.44
11:Y:147:TYR:CD1	11:Y:159:LEU:CD2	2.95	0.44
11:Y:184:ASP:O	11:Y:186:ASN:N	2.51	0.44
14:b:47:ASN:C	14:b:197:VAL:HG23	2.43	0.44
8:H:42:PHE:HB2	8:H:179:ILE:HD11	2.00	0.44
11:K:184:ASP:O	11:K:186:ASN:N	2.51	0.44
14:N:9:THR:CG2	14:N:140:GLY:O	2.63	0.44
2:P:51:GLN:CD	2:P:54:ILE:CA	2.86	0.44
4:R:196:LEU:HB3	4:R:232:ILE:HD13	1.99	0.44
8:V:45:ARG:CG	15:V:300:KNM:H34	2.46	0.44
9:W:59:ILE:HG23	9:W:63:LEU:CD1	2.48	0.44
13:a:99:ARG:CB	13:a:104:TYR:HE2	2.28	0.44
5:E:100:TRP:CE3	5:E:100:TRP:O	2.71	0.43
8:H:135:ILE:HG22	8:H:139:VAL:HG23	2.00	0.43
11:K:29:LYS:HD2	12:L:122:SER:C	2.42	0.43
13:M:37:THR:HG23	13:M:40:SER:OG	2.18	0.43
13:M:104:TYR:CE1	14:N:97:TYR:OH	2.69	0.43
13:M:167:SER:O	13:M:171:ALA:HB2	2.18	0.43
14:N:9:THR:CG2	14:N:10:SER:N	2.73	0.43
14:N:142:GLY:HA2	14:N:146:ALA:H	1.83	0.43
3:Q:159:TRP:CD2	4:R:54:GLN:NE2	2.80	0.43
9:W:63:LEU:HD21	9:W:79:ALA:CB	2.47	0.43
13:a:20:PHE:O	13:a:20:PHE:CD1	2.71	0.43
14:b:142:GLY:HA2	14:b:146:ALA:H	1.83	0.43
4:D:40:ILE:HG22	4:D:211:MET:O	2.03	0.43
6:F:152:ASN:OD1	6:F:153:TYR:N	2.51	0.43
13:M:20:PHE:O	13:M:20:PHE:HD1	2.01	0.43
14:N:48:SER:HB3	14:N:196:GLY:HA3	1.99	0.43
5:S:227:HIS:O	5:S:227:HIS:CD2	2.71	0.43
6:T:152:ASN:OD1	6:T:153:TYR:N	2.51	0.43
8:V:42:PHE:CE2	8:V:186:ARG:NH1	2.86	0.43
8:V:98:ILE:CG2	8:V:99:ILE:N	2.81	0.43
8:V:119:MET:HE3	14:b:57:TYR:CB	2.20	0.43
15:W:300:KNM:C1	15:W:300:KNM:C7	2.89	0.43
15:W:300:KNM:C2	15:W:300:KNM:C4	2.86	0.43
10:X:10:VAL:CG2	10:X:53:ALA:HB2	2.48	0.43
10:J:6:ASN:HB3	10:J:7:GLY:H	1.59	0.43
12:L:103:GLY:HA2	12:L:179:VAL:HG11	2.00	0.43
1:O:43:ARG:CD	1:O:149:PRO:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:68:THR:HG22	2:P:71:ILE:CB	2.32	0.43
2:P:214:GLU:HG3	2:P:214:GLU:O	2.18	0.43
3:Q:139:TRP:O	3:Q:139:TRP:CE3	2.70	0.43
9:W:49:ALA:C	9:W:52:THR:HG22	2.44	0.43
12:Z:103:GLY:HA2	12:Z:179:VAL:HG11	2.00	0.43
14:b:16:PHE:CD1	14:b:161:SER:O	2.61	0.43
2:B:49:LYS:HB3	2:B:206:ASN:O	2.19	0.43
2:B:219:ARG:O	2:B:220:LEU:C	2.61	0.43
5:E:227:HIS:O	5:E:227:HIS:CD2	2.70	0.43
6:F:7:ASP:OD2	6:F:14:SER:CA	2.65	0.43
8:H:98:ILE:HG21	8:H:100:ILE:CD1	2.48	0.43
14:N:7:THR:OG1	14:N:56:ASP:OD1	2.36	0.43
2:P:53:SER:OG	2:P:56:TYR:CD1	2.71	0.43
3:Q:139:TRP:HB2	3:Q:145:PHE:CE1	2.53	0.43
5:S:211:ASN:H	5:S:214:ASN:HB3	1.83	0.43
8:V:18:SER:HB3	8:V:173:VAL:N	2.33	0.43
8:V:19:ARG:HH21	8:V:21:THR:HG21	1.82	0.43
2:B:53:SER:O	2:B:54:ILE:HB	2.18	0.43
2:B:133:LEU:CD1	2:B:135:ILE:HD11	2.44	0.43
3:C:157:GLY:C	3:C:159:TRP:CD1	2.96	0.43
7:G:216:VAL:O	7:G:216:VAL:CG1	2.66	0.43
8:H:98:ILE:CG2	8:H:99:ILE:N	2.81	0.43
9:I:172:ASN:OD1	9:I:191:VAL:CA	2.52	0.43
10:J:10:VAL:CG2	10:J:53:ALA:HB2	2.48	0.43
1:A:43:ARG:CD	1:A:149:PRO:O	2.66	0.43
1:A:109:ILE:CB	1:A:114:LEU:CD2	2.89	0.43
3:C:76:VAL:CG1	3:C:132:VAL:HG11	2.46	0.43
5:E:42:THR:HG22	5:E:194:ALA:CB	2.02	0.43
8:H:18:SER:HB3	8:H:173:VAL:H	1.84	0.43
3:Q:65:ILE:HD12	3:Q:74:CYS:O	2.19	0.43
3:Q:76:VAL:HG12	3:Q:132:VAL:CG1	2.48	0.43
12:Z:55:TRP:HE1	12:Z:97:MET:HE1	1.80	0.43
13:a:148:LEU:C	13:a:148:LEU:HD23	2.44	0.43
2:B:61:VAL:HG21	2:B:83:ARG:HH21	1.83	0.43
3:C:205:LYS:HA	3:C:240:HIS:CD2	2.54	0.43
6:F:14:SER:CB	6:F:17:GLY:O	2.67	0.43
6:F:121:GLN:CG	7:G:122:TYR:HE2	2.30	0.43
6:F:210:VAL:O	6:F:210:VAL:CG2	2.66	0.43
8:H:18:SER:HB3	8:H:173:VAL:N	2.33	0.43
8:H:160:LEU:O	8:H:163:ALA:HB3	2.18	0.43
9:I:202:TYR:CG	13:a:152:GLN:CD	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:300:KNM:H42	15:I:300:KNM:H40	1.72	0.43
10:J:10:VAL:CG2	10:J:53:ALA:HB3	2.47	0.43
13:M:63:THR:HG21	14:N:97:TYR:CE2	2.54	0.43
1:O:180:GLU:OE2	2:P:54:ILE:HG13	2.19	0.43
2:P:70:HIS:NE2	2:P:212:CYS:O	2.46	0.43
2:P:137:GLY:N	2:P:144:TYR:O	2.40	0.43
3:Q:186:LEU:HD23	3:Q:186:LEU:C	2.43	0.43
8:V:98:ILE:HG21	8:V:100:ILE:CD1	2.48	0.43
3:C:33:THR:HG21	3:C:200:THR:HG21	1.99	0.43
3:C:139:TRP:HB2	3:C:145:PHE:CE1	2.53	0.43
4:D:196:LEU:HB3	4:D:232:ILE:HD13	1.99	0.43
6:F:15:PRO:HG3	7:G:25:TYR:CZ	2.53	0.43
8:H:1:THR:HG21	15:H:300:KNM:H39	1.81	0.43
8:H:176:LEU:O	8:H:186:ARG:HA	2.19	0.43
11:K:56:PHE:CD1	11:K:56:PHE:C	2.97	0.43
14:N:47:ASN:C	14:N:197:VAL:HG23	2.43	0.43
2:P:49:LYS:HB3	2:P:206:ASN:O	2.19	0.43
7:U:46:VAL:HG22	7:U:215:TRP:HD1	1.79	0.43
11:Y:56:PHE:CD1	11:Y:56:PHE:C	2.97	0.43
14:b:193:THR:C	14:b:195:LYS:N	2.74	0.43
1:A:180:GLU:OE2	2:B:54:ILE:HG13	2.19	0.43
2:B:53:SER:OG	2:B:56:TYR:CD1	2.71	0.43
13:M:149:LEU:O	13:M:153:VAL:HG23	2.19	0.43
2:P:138:TRP:CE3	2:P:138:TRP:C	2.97	0.43
3:Q:76:VAL:CG1	3:Q:132:VAL:HG11	2.46	0.43
4:R:31:THR:HG23	4:R:165:ALA:HA	2.01	0.43
7:U:216:VAL:O	7:U:216:VAL:CG1	2.66	0.43
8:V:7:GLN:HG2	8:V:8:PHE:H	1.81	0.43
8:V:160:LEU:O	8:V:163:ALA:HB3	2.18	0.43
10:X:134:ASP:CG	10:X:135:PHE:CD1	2.97	0.43
11:Y:120:TYR:CE1	11:Y:121:LEU:HD21	2.52	0.43
13:a:54:CYS:CB	13:a:108:ASN:HD22	2.30	0.43
5:E:211:ASN:H	5:E:214:ASN:HB3	1.83	0.43
14:N:60:PHE:N	14:N:108:ASN:ND2	2.61	0.43
8:V:84:LYS:O	8:V:88:TYR:CB	2.63	0.43
13:a:149:LEU:O	13:a:153:VAL:HG23	2.19	0.43
14:b:26:MET:SD	14:b:186:ARG:O	2.77	0.43
3:C:65:ILE:HD12	3:C:74:CYS:O	2.19	0.42
4:D:36:ARG:HG2	4:D:142:PRO:CB	2.49	0.42
6:F:32:GLY:HA3	6:F:76:GLY:H	1.84	0.42
9:I:35:HIS:HB2	9:I:56:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10:PRO:HD2	11:K:12:TYR:CE1	2.53	0.42
13:M:148:LEU:HD23	13:M:148:LEU:C	2.44	0.42
14:N:26:MET:SD	14:N:186:ARG:O	2.77	0.42
8:V:10:GLY:O	8:V:103:TRP:CD1	2.70	0.42
13:a:17:GLY:CA	13:a:166:LEU:CD1	2.97	0.42
1:A:221:THR:HG22	1:A:222:VAL:N	2.34	0.42
2:B:138:TRP:CE3	2:B:138:TRP:C	2.97	0.42
8:H:18:SER:HB3	8:H:172:GLY:CA	2.44	0.42
11:K:24:ASN:HD21	11:K:26:VAL:CG2	2.22	0.42
13:M:20:PHE:O	13:M:20:PHE:CD1	2.71	0.42
14:N:25:ASP:HA	14:N:187:PHE:CB	2.49	0.42
14:b:25:ASP:HA	14:b:187:PHE:CB	2.49	0.42
3:C:186:LEU:HD23	3:C:186:LEU:C	2.43	0.42
9:I:36:PHE:CZ	9:I:38:SER:HA	2.54	0.42
13:M:17:GLY:CA	13:M:166:LEU:CD1	2.97	0.42
13:M:152:GLN:CD	9:W:202:TYR:CG	2.97	0.42
2:P:51:GLN:NE2	2:P:51:GLN:C	2.74	0.42
3:Q:157:GLY:C	3:Q:159:TRP:CD1	2.96	0.42
11:Y:15:VAL:HG11	11:Y:105:ALA:HB2	2.01	0.42
13:a:153:VAL:HG22	13:a:174:LEU:CD2	2.49	0.42
2:B:181:LEU:CD2	2:B:186:ALA:N	2.82	0.42
4:D:31:THR:HG23	4:D:165:ALA:HA	2.01	0.42
9:I:49:ALA:C	9:I:52:THR:HG22	2.44	0.42
10:J:134:ASP:CG	10:J:135:PHE:CD1	2.97	0.42
3:Q:7:SER:O	3:Q:8:ARG:HB2	2.20	0.42
8:V:18:SER:HB3	8:V:173:VAL:H	1.84	0.42
8:V:42:PHE:CD2	8:V:186:ARG:NH1	2.87	0.42
13:a:63:THR:HG21	14:b:97:TYR:CE2	2.53	0.42
11:K:166:GLU:OE1	11:K:170:ARG:HG3	2.19	0.42
13:M:36:HIS:CG	14:N:132:TYR:OH	2.73	0.42
13:M:153:VAL:HG22	13:M:174:LEU:CD2	2.49	0.42
14:N:193:THR:C	14:N:195:LYS:N	2.74	0.42
2:P:183:LEU:HD13	2:P:213:ASN:CG	2.42	0.42
9:W:35:HIS:HB2	9:W:56:THR:HG21	2.01	0.42
12:Z:19:ARG:HB2	12:Z:171:GLY:C	2.37	0.42
12:Z:19:ARG:CB	12:Z:171:GLY:H	2.33	0.42
13:a:17:GLY:HA3	13:a:166:LEU:CG	2.41	0.42
13:a:20:PHE:O	13:a:20:PHE:HD1	2.01	0.42
13:a:113:LEU:HB2	13:a:198:VAL:CG1	2.50	0.42
14:b:26:MET:CB	14:b:186:ARG:HH22	2.26	0.42
1:A:159:TYR:HD1	2:B:83:ARG:NH2	2.14	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:PHE:CD2	8:H:186:ARG:NH1	2.87	0.42
2:P:179:GLU:HB3	2:P:180:ASP:H	1.34	0.42
4:R:80:ALA:HA	4:R:129:ILE:HD13	2.01	0.42
4:R:209:ALA:O	4:R:217:LEU:HD11	2.20	0.42
6:T:121:GLN:HG3	7:U:122:TYR:CE2	2.52	0.42
8:V:45:ARG:CD	15:V:300:KNM:H34	2.50	0.42
8:V:176:LEU:O	8:V:186:ARG:HA	2.19	0.42
9:I:129:SER:HG	15:I:300:KNM:H41	1.82	0.42
10:J:116:PHE:O	10:J:116:PHE:CG	2.70	0.42
11:K:120:TYR:CE1	11:K:121:LEU:HD23	2.55	0.42
1:O:159:TYR:CE1	2:P:83:ARG:NH2	2.88	0.42
9:W:80:ASN:CG	9:W:111:TYR:CD1	2.98	0.42
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.55	0.42
11:Y:20:VAL:CG1	11:Y:21:ALA:N	2.83	0.42
11:Y:166:GLU:OE1	11:Y:170:ARG:HG3	2.19	0.42
13:a:148:LEU:HD22	13:a:178:VAL:HG12	2.02	0.42
7:G:69:VAL:HG21	7:G:137:LEU:CD2	2.50	0.42
13:M:113:LEU:HB2	13:M:198:VAL:CG1	2.50	0.42
13:M:148:LEU:HD22	13:M:178:VAL:HG12	2.02	0.42
1:O:13:ILE:HG22	3:Q:5:TYR:CE2	2.55	0.42
12:Z:21:THR:C	15:Z:300:KNM:C6	2.93	0.42
3:C:7:SER:O	3:C:8:ARG:HB2	2.20	0.42
3:C:33:THR:HG22	3:C:34:CYS:N	2.35	0.42
4:D:80:ALA:HA	4:D:129:ILE:HD13	2.01	0.42
4:D:209:ALA:O	4:D:217:LEU:HD11	2.20	0.42
6:F:40:SER:HB2	6:F:187:LEU:HD11	2.02	0.42
8:H:7:GLN:O	8:H:8:PHE:CD2	2.73	0.42
9:I:49:ALA:HB2	15:I:300:KNM:H36	1.98	0.42
9:I:97:ALA:HB3	9:I:127:MET:SD	2.59	0.42
13:M:17:GLY:CA	13:M:166:LEU:HD13	2.49	0.42
14:N:36:PHE:C	14:N:38:ASN:H	2.28	0.42
2:P:181:LEU:HD23	2:P:186:ALA:N	2.34	0.42
4:R:46:GLU:HG2	4:R:47:LYS:H	1.85	0.42
5:S:227:HIS:NE2	5:S:229:PHE:HD1	2.16	0.42
6:T:40:SER:HB2	6:T:187:LEU:HD11	2.02	0.42
9:W:36:PHE:CZ	9:W:38:SER:HA	2.54	0.42
9:W:97:ALA:HB3	9:W:127:MET:SD	2.59	0.42
9:W:128:GLY:C	15:W:300:KNM:O4	2.63	0.42
10:X:19:VAL:HG22	10:X:118:PRO:HG3	2.02	0.42
14:b:36:PHE:C	14:b:38:ASN:H	2.28	0.42
4:D:196:LEU:HD13	4:D:232:ILE:CG2	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:SER:C	5:E:151:PRO:HG3	2.45	0.42
8:H:83:PHE:CG	8:H:100:ILE:HD11	2.54	0.42
10:J:58:ASP:OD1	10:J:102:TYR:HB3	2.20	0.42
2:P:68:THR:CG2	2:P:71:ILE:HG13	2.50	0.42
3:Q:33:THR:HG22	3:Q:34:CYS:N	2.35	0.42
7:U:119:VAL:HA	7:U:131:PHE:CE1	2.55	0.42
7:U:169:ARG:O	7:U:173:LYS:HG2	2.20	0.42
2:B:181:LEU:HD23	2:B:186:ALA:N	2.34	0.41
7:G:119:VAL:HA	7:G:131:PHE:CE1	2.55	0.41
8:H:8:PHE:HB3	8:H:9:ASP:OD1	2.20	0.41
9:I:37:ILE:HG21	9:I:63:LEU:HD22	2.02	0.41
9:I:64:GLU:O	9:I:68:LEU:HB2	2.20	0.41
11:K:15:VAL:HG11	11:K:105:ALA:HB2	2.01	0.41
11:K:56:PHE:CE2	11:K:88:LEU:HD21	2.55	0.41
12:L:19:ARG:CB	12:L:171:GLY:H	2.33	0.41
2:P:151:SER:O	3:Q:81:SER:HB3	2.20	0.41
2:P:181:LEU:CD2	2:P:186:ALA:N	2.82	0.41
6:T:32:GLY:HA3	6:T:76:GLY:H	1.84	0.41
10:X:163:PHE:CA	10:X:188:ILE:HD11	2.50	0.41
11:Y:10:PRO:HD2	11:Y:12:TYR:CE1	2.53	0.41
13:a:13:LEU:HD13	13:a:149:LEU:HD13	2.01	0.41
5:E:43:SER:HA	5:E:151:PRO:CG	2.48	0.41
9:I:1:THR:HG23	9:I:1:THR:O	2.19	0.41
9:I:36:PHE:HD1	9:I:38:SER:O	1.98	0.41
9:I:80:ASN:CG	9:I:111:TYR:CD1	2.98	0.41
3:Q:154:GLY:O	4:R:78:ALA:HB2	2.20	0.41
4:R:36:ARG:HG2	4:R:142:PRO:CB	2.49	0.41
5:S:43:SER:C	5:S:151:PRO:HG3	2.45	0.41
8:V:38:HIS:CG	8:V:39:ASP:N	2.89	0.41
12:Z:21:THR:O	15:Z:300:KNM:H11	2.20	0.41
1:A:13:ILE:HG22	3:C:5:TYR:CE2	2.55	0.41
2:B:151:SER:O	3:C:81:SER:HB3	2.20	0.41
7:G:47:PHE:HE1	7:G:216:VAL:CG2	2.33	0.41
8:H:47:GLY:C	15:H:300:KNM:H23	2.45	0.41
9:I:185:PHE:HE2	9:I:187:ARG:HD3	1.85	0.41
10:J:19:VAL:HG22	10:J:118:PRO:HG3	2.02	0.41
11:K:24:ASN:ND2	11:K:26:VAL:HG23	2.26	0.41
12:L:21:THR:O	15:L:300:KNM:H11	2.20	0.41
1:O:221:THR:HG22	1:O:222:VAL:N	2.34	0.41
2:P:147:GLN:OE1	2:P:162:MET:HG2	2.21	0.41
9:W:1:THR:HG23	9:W:1:THR:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:64:GLN:HE21	11:Y:85:ARG:HH22	1.38	0.41
13:a:13:LEU:HD11	13:a:149:LEU:HD13	1.91	0.41
13:a:17:GLY:CA	13:a:166:LEU:HD13	2.49	0.41
13:a:36:HIS:CG	14:b:132:TYR:OH	2.73	0.41
14:b:26:MET:SD	14:b:186:ARG:HG2	2.61	0.41
2:B:68:THR:CG2	2:B:71:ILE:HG13	2.50	0.41
4:D:70:CYS:SG	4:D:217:LEU:HD22	2.60	0.41
4:D:196:LEU:HD22	4:D:232:ILE:HG21	2.03	0.41
5:E:186:HIS:N	5:E:189:MET:HE3	2.27	0.41
7:G:161:TRP:C	7:G:181:MET:HE1	2.32	0.41
7:G:169:ARG:O	7:G:173:LYS:HG2	2.20	0.41
10:J:150:GLU:HB3	13:a:185:ARG:HH21	1.85	0.41
11:K:9:GLY:HA3	11:K:12:TYR:CE1	2.55	0.41
2:P:210:GLY:HA2	2:P:219:ARG:HA	2.02	0.41
8:V:83:PHE:CG	8:V:100:ILE:HD11	2.54	0.41
1:A:109:ILE:CG2	1:A:114:LEU:CD1	2.92	0.41
1:A:159:TYR:CE1	2:B:83:ARG:NH2	2.88	0.41
7:G:181:MET:C	7:G:183:GLU:N	2.71	0.41
11:K:44:LEU:CG	11:K:102:LEU:HD11	2.51	0.41
12:L:88:TYR:CD1	12:L:88:TYR:C	2.97	0.41
2:P:138:TRP:HE1	2:P:143:PRO:CD	2.19	0.41
10:X:27:PHE:CD2	10:X:38:PHE:CG	3.09	0.41
11:Y:85:ARG:CZ	11:Y:86:ARG:NH2	2.74	0.41
8:H:45:ARG:CD	15:H:300:KNM:H34	2.50	0.41
8:H:45:ARG:CG	15:H:300:KNM:H34	2.46	0.41
11:K:19:ARG:C	11:K:20:VAL:CG2	2.93	0.41
12:L:21:THR:O	15:L:300:KNM:C6	2.69	0.41
12:L:178:HIS:HB3	12:L:187:VAL:CG2	2.50	0.41
13:M:13:LEU:HD13	13:M:149:LEU:HD13	2.01	0.41
14:N:187:PHE:CD1	14:N:187:PHE:C	2.98	0.41
3:Q:205:LYS:HA	3:Q:240:HIS:CD2	2.54	0.41
5:S:218:ALA:CB	5:S:226:PHE:HZ	2.27	0.41
8:V:18:SER:HB3	8:V:172:GLY:CA	2.44	0.41
12:Z:21:THR:O	15:Z:300:KNM:C6	2.69	0.41
2:B:53:SER:OG	2:B:56:TYR:CE1	2.70	0.41
5:E:202:LEU:HA	5:E:205:VAL:HG22	2.03	0.41
5:E:220:VAL:HG22	5:E:226:PHE:CD1	2.55	0.41
7:G:41:CYS:SG	7:G:42:LYS:N	2.94	0.41
9:I:37:ILE:CG2	9:I:63:LEU:HD22	2.50	0.41
9:I:128:GLY:C	15:I:300:KNM:O4	2.63	0.41
9:I:151:ALA:HA	9:I:154:LEU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:44:LEU:CG	11:K:102:LEU:HD21	2.40	0.41
3:Q:159:TRP:CE2	4:R:54:GLN:NE2	2.68	0.41
4:R:102:VAL:HG11	4:R:107:ILE:HD11	2.03	0.41
10:X:138:SER:O	10:X:145:MET:HE1	2.21	0.41
11:Y:9:GLY:HA3	11:Y:12:TYR:CZ	2.56	0.41
11:Y:19:ARG:C	11:Y:20:VAL:CG2	2.93	0.41
12:Z:49:ALA:CA	15:Z:300:KNM:H32	2.51	0.41
14:b:7:THR:OG1	14:b:56:ASP:OD1	2.36	0.41
14:b:187:PHE:CD1	14:b:187:PHE:C	2.98	0.41
10:J:27:PHE:CD2	10:J:38:PHE:CG	3.09	0.41
11:K:20:VAL:CG1	11:K:21:ALA:N	2.83	0.41
11:K:120:TYR:CE1	11:K:121:LEU:CG	3.04	0.41
4:R:70:CYS:SG	4:R:217:LEU:HD22	2.60	0.41
8:V:127:ILE:HD12	8:V:132:SER:O	2.21	0.41
2:B:151:SER:O	3:C:81:SER:OG	2.39	0.41
3:C:154:GLY:O	4:D:78:ALA:HB2	2.21	0.41
4:D:46:GLU:HG2	4:D:47:LYS:H	1.85	0.41
8:H:38:HIS:CG	8:H:39:ASP:N	2.89	0.41
15:I:300:KNM:C1	15:I:300:KNM:C7	2.89	0.41
10:J:163:PHE:CA	10:J:188:ILE:HD11	2.50	0.41
11:K:120:TYR:CD1	11:K:121:LEU:N	2.89	0.41
12:L:21:THR:C	15:L:300:KNM:C6	2.93	0.41
13:M:100:ARG:HH12	13:M:127:VAL:HB	1.74	0.41
13:M:185:ARG:HH21	10:X:150:GLU:HB3	1.85	0.41
14:N:26:MET:SD	14:N:186:ARG:HG2	2.61	0.41
1:O:109:ILE:HG12	1:O:114:LEU:HG	2.02	0.41
2:P:70:HIS:HA	2:P:217:PHE:HB2	2.03	0.41
2:P:151:SER:O	3:Q:81:SER:OG	2.39	0.41
2:P:217:PHE:CD1	2:P:218:ARG:N	2.89	0.41
4:R:144:LEU:HD23	4:R:144:LEU:O	2.21	0.41
5:S:202:LEU:HA	5:S:205:VAL:HG22	2.03	0.41
5:S:206:MET:HE3	5:S:208:GLU:H	1.86	0.41
9:W:37:ILE:CG2	9:W:63:LEU:HD22	2.50	0.41
9:W:185:PHE:CE2	9:W:187:ARG:HB2	2.56	0.41
9:W:185:PHE:HE2	9:W:187:ARG:HD3	1.85	0.41
10:X:58:ASP:OD1	10:X:102:TYR:HB3	2.20	0.41
11:Y:44:LEU:CG	11:Y:102:LEU:HD11	2.51	0.41
2:B:217:PHE:CD1	2:B:218:ARG:N	2.89	0.41
4:D:36:ARG:HD2	4:D:142:PRO:O	2.21	0.41
4:D:65:LEU:HD11	4:D:71:MET:HB2	2.03	0.41
9:I:185:PHE:CE2	9:I:187:ARG:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:184:ASP:OD2	11:K:186:ASN:OD1	2.39	0.41
4:R:196:LEU:HD22	4:R:232:ILE:HG21	2.03	0.41
8:V:178:ALA:HB3	8:V:185:GLU:H	1.86	0.41
9:W:8:TYR:CE1	9:W:13:VAL:HG23	2.56	0.41
10:X:154:GLU:OE2	10:X:161:HIS:CE1	2.74	0.41
13:a:43:CYS:O	13:a:43:CYS:SG	2.79	0.41
1:A:77:GLY:HA3	1:A:227:PHE:CE1	2.56	0.40
5:E:206:MET:HE3	5:E:208:GLU:H	1.86	0.40
6:F:137:TYR:CD1	6:F:216:GLY:HA2	2.56	0.40
8:H:127:ILE:HD12	8:H:132:SER:O	2.21	0.40
9:I:8:TYR:CE1	9:I:13:VAL:HG23	2.56	0.40
9:I:49:ALA:O	9:I:52:THR:HG22	2.21	0.40
12:L:20:ALA:CB	15:L:300:KNM:C19	2.99	0.40
12:L:49:ALA:CA	15:L:300:KNM:H32	2.51	0.40
14:N:46:ASN:O	14:N:197:VAL:CG2	2.69	0.40
2:P:43:VAL:CG1	2:P:44:VAL:N	2.84	0.40
2:P:83:ARG:O	2:P:87:HIS:CE1	2.75	0.40
7:U:41:CYS:SG	7:U:42:LYS:N	2.94	0.40
8:V:43:CYS:SG	8:V:98:ILE:CD1	3.06	0.40
15:V:300:KNM:H26	15:V:300:KNM:H17	1.60	0.40
9:W:151:ALA:HA	9:W:154:LEU:HB3	2.02	0.40
2:B:210:GLY:HA2	2:B:219:ARG:HA	2.02	0.40
4:D:144:LEU:HD23	4:D:144:LEU:O	2.21	0.40
5:E:227:HIS:NE2	5:E:229:PHE:HD1	2.16	0.40
7:G:87:LEU:HD13	7:G:135:PHE:CE1	2.57	0.40
8:H:84:LYS:O	8:H:88:TYR:CB	2.63	0.40
12:L:42:LEU:HD11	12:L:184:TRP:CD1	2.56	0.40
13:M:17:GLY:HA3	13:M:166:LEU:CG	2.41	0.40
1:O:180:GLU:OE2	2:P:54:ILE:HD12	2.22	0.40
3:Q:25:MET:HA	3:Q:28:ILE:HD13	2.02	0.40
7:U:47:PHE:HE1	7:U:216:VAL:CG2	2.33	0.40
12:Z:178:HIS:HB3	12:Z:187:VAL:CG2	2.50	0.40
1:A:13:ILE:CG2	3:C:5:TYR:CE2	3.05	0.40
2:B:85:LEU:CD2	2:B:133:LEU:HD21	2.51	0.40
2:B:147:GLN:OE1	2:B:162:MET:HG2	2.21	0.40
3:C:21:VAL:HG13	3:C:153:SER:HB3	2.04	0.40
3:C:115:CYS:CB	4:D:81:ARG:NH2	2.85	0.40
6:F:147:THR:HG22	6:F:153:TYR:HB3	2.04	0.40
9:I:8:TYR:CD1	9:I:13:VAL:HG23	2.57	0.40
11:K:9:GLY:HA3	11:K:12:TYR:CZ	2.56	0.40
12:L:1:THR:HG23	15:L:300:KNM:C17	2.45	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:149:VAL:O	12:L:153:TYR:CE1	2.74	0.40
13:M:43:CYS:O	13:M:43:CYS:SG	2.79	0.40
14:N:147:GLN:HB3	14:N:148:PRO:HD3	2.03	0.40
2:P:138:TRP:C	2:P:138:TRP:HE3	2.29	0.40
3:Q:140:ASP:OD1	3:Q:143:TYR:HB2	2.21	0.40
4:R:39:ASP:O	4:R:40:ILE:HD13	2.22	0.40
4:R:196:LEU:HD22	4:R:232:ILE:CG2	2.51	0.40
5:S:70:ILE:CD1	5:S:76:CYS:HB2	2.48	0.40
7:U:69:VAL:HG21	7:U:137:LEU:CD2	2.50	0.40
8:V:47:GLY:C	15:V:300:KNM:H23	2.45	0.40
12:Z:20:ALA:CB	15:Z:300:KNM:C19	2.99	0.40
1:A:76:ILE:HD12	1:A:114:LEU:CD1	2.26	0.40
2:B:83:ARG:O	2:B:87:HIS:CE1	2.75	0.40
2:B:213:ASN:HD22	2:B:213:ASN:N	2.19	0.40
11:K:3:TYR:CE2	11:K:167:LEU:HD11	2.57	0.40
4:R:208:LEU:HD11	4:R:228:TYR:OH	2.22	0.40
8:V:13:VAL:HG13	8:V:176:LEU:HD21	2.04	0.40
11:Y:115:LEU:HD23	11:Y:115:LEU:H	1.86	0.40
2:B:70:HIS:HA	2:B:217:PHE:HB2	2.03	0.40
2:B:134:LEU:HG	2:B:162:MET:CE	2.52	0.40
8:H:13:VAL:HG13	8:H:176:LEU:HD21	2.04	0.40
14:N:6:VAL:CG1	14:N:28:GLY:O	2.70	0.40
1:O:13:ILE:CG2	3:Q:5:TYR:CE2	3.05	0.40
3:Q:12:PHE:HZ	4:R:25:ALA:CB	2.33	0.40
5:S:220:VAL:HG22	5:S:226:PHE:CD1	2.55	0.40
9:W:37:ILE:HG21	9:W:63:LEU:HD22	2.02	0.40
11:Y:3:TYR:CE2	11:Y:167:LEU:HD11	2.57	0.40
11:Y:120:TYR:CD1	11:Y:121:LEU:N	2.89	0.40
12:Z:55:TRP:HA	12:Z:55:TRP:CE3	2.57	0.40
14:b:46:ASN:O	14:b:197:VAL:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	186/246 (76%)	178 (96%)	8 (4%)	0	100	100
1	O	186/246 (76%)	178 (96%)	8 (4%)	0	100	100
2	B	210/234 (90%)	198 (94%)	10 (5%)	2 (1%)	12	44
2	P	210/234 (90%)	198 (94%)	10 (5%)	2 (1%)	12	44
3	C	233/261 (89%)	225 (97%)	8 (3%)	0	100	100
3	Q	233/261 (89%)	225 (97%)	8 (3%)	0	100	100
4	D	206/248 (83%)	201 (98%)	5 (2%)	0	100	100
4	R	206/248 (83%)	201 (98%)	5 (2%)	0	100	100
5	E	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	24	57
5	S	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	24	57
6	F	187/263 (71%)	184 (98%)	3 (2%)	0	100	100
6	T	187/263 (71%)	185 (99%)	2 (1%)	0	100	100
7	G	203/255 (80%)	196 (97%)	7 (3%)	0	100	100
7	U	203/255 (80%)	196 (97%)	7 (3%)	0	100	100
8	H	179/205 (87%)	164 (92%)	13 (7%)	2 (1%)	11	43
8	V	179/205 (87%)	165 (92%)	12 (7%)	2 (1%)	11	43
9	I	194/234 (83%)	187 (96%)	6 (3%)	1 (0%)	24	57
9	W	194/234 (83%)	187 (96%)	6 (3%)	1 (0%)	24	57
10	J	168/204 (82%)	158 (94%)	10 (6%)	0	100	100
10	X	168/204 (82%)	158 (94%)	10 (6%)	0	100	100
11	K	187/201 (93%)	173 (92%)	10 (5%)	4 (2%)	5	31
11	Y	187/201 (93%)	173 (92%)	10 (5%)	4 (2%)	5	31
12	L	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
12	Z	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
13	M	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	24	57
13	a	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	24	57
14	N	178/219 (81%)	161 (90%)	17 (10%)	0	100	100
14	b	178/219 (81%)	161 (90%)	17 (10%)	0	100	100
All	All	5432/6456 (84%)	5168 (95%)	242 (4%)	22 (0%)	31	62

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ALA
2	B	54	ILE
5	E	189	MET
8	H	8	PHE
11	K	122	ALA
11	K	151	ILE
2	P	40	ALA
2	P	54	ILE
5	S	189	MET
8	V	8	PHE
11	Y	122	ALA
11	Y	151	ILE
8	H	28	ASN
11	K	176	PRO
8	V	28	ASN
11	Y	176	PRO
13	M	41	PRO
13	a	41	PRO
9	I	188	PRO
11	K	97	PRO
9	W	188	PRO
11	Y	97	PRO

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	A	166/210 (79%)	162 (98%)	4 (2%)	43	64
1	O	166/210 (79%)	162 (98%)	4 (2%)	43	64
2	B	177/191 (93%)	167 (94%)	10 (6%)	19	46
2	P	177/191 (93%)	167 (94%)	10 (6%)	19	46
3	C	199/221 (90%)	195 (98%)	4 (2%)	48	67
3	Q	199/221 (90%)	195 (98%)	4 (2%)	48	67
4	D	179/211 (85%)	175 (98%)	4 (2%)	45	65
4	R	179/211 (85%)	175 (98%)	4 (2%)	45	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	181/203 (89%)	179 (99%)	2 (1%)	65	74
5	S	181/203 (89%)	179 (99%)	2 (1%)	65	74
6	F	166/224 (74%)	163 (98%)	3 (2%)	51	69
6	T	166/224 (74%)	163 (98%)	3 (2%)	51	69
7	G	170/212 (80%)	168 (99%)	2 (1%)	63	73
7	U	170/212 (80%)	168 (99%)	2 (1%)	63	73
8	H	142/159 (89%)	139 (98%)	3 (2%)	47	66
8	V	142/159 (89%)	139 (98%)	3 (2%)	47	66
9	I	162/195 (83%)	160 (99%)	2 (1%)	63	73
9	W	162/195 (83%)	160 (99%)	2 (1%)	63	73
10	J	149/173 (86%)	148 (99%)	1 (1%)	76	78
10	X	149/173 (86%)	148 (99%)	1 (1%)	76	78
11	K	160/171 (94%)	159 (99%)	1 (1%)	78	79
11	Y	160/171 (94%)	159 (99%)	1 (1%)	78	79
12	L	148/159 (93%)	143 (97%)	5 (3%)	32	57
12	Z	148/159 (93%)	143 (97%)	5 (3%)	32	57
13	M	155/178 (87%)	152 (98%)	3 (2%)	50	68
13	a	155/178 (87%)	152 (98%)	3 (2%)	50	68
14	N	152/181 (84%)	150 (99%)	2 (1%)	61	72
14	b	152/181 (84%)	150 (99%)	2 (1%)	61	72
All	All	4612/5376 (86%)	4520 (98%)	92 (2%)	48	67

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	215	ILE
1	A	222	VAL
1	A	229	ILE
2	B	51	GLN
2	B	64	VAL
2	B	70	HIS
2	B	106	THR
2	B	140	GLU
2	B	207	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	211	ILE
2	B	212	CYS
2	B	213	ASN
2	B	222	PRO
3	C	41	ASP
3	C	76	VAL
3	C	151	ASP
3	C	203	VAL
4	D	8	THR
4	D	13	ASP
4	D	26	VAL
4	D	168	VAL
5	E	63	SER
5	E	70	ILE
6	F	66	VAL
6	F	132	LEU
6	F	178	GLU
7	G	165	ILE
7	G	197	ILE
8	H	6	VAL
8	H	121	VAL
8	H	186	ARG
9	I	37	ILE
9	I	76	VAL
10	J	19	VAL
11	K	100	VAL
12	L	58	LEU
12	L	174	VAL
12	L	179	VAL
12	L	185	ILE
12	L	192	VAL
13	M	15	ILE
13	M	18	GLU
13	M	106	VAL
14	N	21	VAL
14	N	112	ILE
1	O	51	VAL
1	O	215	ILE
1	O	222	VAL
1	O	229	ILE
2	P	51	GLN
2	P	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	70	HIS
2	P	106	THR
2	P	140	GLU
2	P	207	ILE
2	P	211	ILE
2	P	212	CYS
2	P	213	ASN
2	P	222	PRO
3	Q	41	ASP
3	Q	76	VAL
3	Q	151	ASP
3	Q	203	VAL
4	R	8	THR
4	R	13	ASP
4	R	26	VAL
4	R	168	VAL
5	S	63	SER
5	S	70	ILE
6	T	66	VAL
6	T	132	LEU
6	T	178	GLU
7	U	165	ILE
7	U	197	ILE
8	V	6	VAL
8	V	121	VAL
8	V	186	ARG
9	W	37	ILE
9	W	76	VAL
10	X	19	VAL
11	Y	100	VAL
12	Z	58	LEU
12	Z	174	VAL
12	Z	179	VAL
12	Z	185	ILE
12	Z	192	VAL
13	a	15	ILE
13	a	18	GLU
13	a	106	VAL
14	b	21	VAL
14	b	112	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
2	B	51	GLN
2	B	62	HIS
2	B	87	HIS
2	B	94	GLN
2	B	188	HIS
2	B	206	ASN
2	B	213	ASN
3	C	230	GLN
4	D	18	GLN
4	D	85	ASN
4	D	94	HIS
5	E	13	ASN
5	E	23	GLN
5	E	224	GLN
6	F	21	GLN
6	F	90	GLN
7	G	22	GLN
7	G	105	ASN
8	H	38	HIS
8	H	123	GLN
9	I	153	ASN
10	J	64	GLN
10	J	161	HIS
10	J	187	HIS
11	K	55	GLN
11	K	65	GLN
11	K	101	ASN
11	K	186	ASN
11	K	189	HIS
12	L	10	HIS
12	L	70	ASN
13	M	79	ASN
13	M	80	ASN
13	M	108	ASN
13	M	146	GLN
14	N	108	ASN
14	N	147	GLN
2	P	51	GLN
2	P	62	HIS
2	P	70	HIS
2	P	87	HIS
2	P	94	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	188	HIS
2	P	206	ASN
2	P	213	ASN
3	Q	69	ASN
3	Q	230	GLN
4	R	18	GLN
4	R	85	ASN
4	R	94	HIS
5	S	23	GLN
5	S	224	GLN
6	T	21	GLN
6	T	183	ASN
7	U	22	GLN
7	U	105	ASN
8	V	38	HIS
8	V	123	GLN
9	W	153	ASN
10	X	64	GLN
10	X	161	HIS
10	X	187	HIS
11	Y	55	GLN
11	Y	65	GLN
11	Y	101	ASN
11	Y	186	ASN
11	Y	189	HIS
12	Z	10	HIS
12	Z	70	ASN
13	a	79	ASN
13	a	80	ASN
13	a	108	ASN
13	a	146	GLN
14	b	108	ASN
14	b	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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$
15	KNM	H	300	8	30,30,68	1.84	2 (6%)	39,41,91	1.00	2 (5%)
15	KNM	Z	300	12	30,30,68	1.83	2 (6%)	39,41,91	0.97	2 (5%)
15	KNM	W	300	9	29,29,68	1.81	2 (6%)	36,39,91	1.26	2 (5%)
15	KNM	V	300	8	30,30,68	1.84	2 (6%)	39,41,91	1.00	2 (5%)
15	KNM	I	300	9	29,29,68	1.82	2 (6%)	36,39,91	1.27	2 (5%)
15	KNM	L	300	12	30,30,68	1.83	2 (6%)	39,41,91	0.98	2 (5%)

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
15	KNM	H	300	8	-	27/38/38/98	-
15	KNM	Z	300	12	-	12/38/38/98	-
15	KNM	W	300	9	-	19/37/37/98	-
15	KNM	V	300	8	-	27/38/38/98	-
15	KNM	I	300	9	-	19/37/37/98	-
15	KNM	L	300	12	-	11/38/38/98	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	300	KNM	C16-S1	-9.53	1.66	1.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	300	KNM	C16-S1	-9.53	1.66	1.78
15	L	300	KNM	C16-S1	-9.31	1.66	1.78
15	Z	300	KNM	C16-S1	-9.28	1.66	1.78
15	I	300	KNM	C16-S1	-8.98	1.66	1.78
15	W	300	KNM	C16-S1	-8.92	1.67	1.78
15	L	300	KNM	C22-S1	-2.77	1.66	1.75
15	Z	300	KNM	C22-S1	-2.77	1.66	1.75
15	H	300	KNM	C22-S1	-2.74	1.66	1.75
15	V	300	KNM	C22-S1	-2.74	1.66	1.75
15	W	300	KNM	C22-S1	-2.71	1.66	1.75
15	I	300	KNM	C22-S1	-2.69	1.66	1.75

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	300	KNM	C1-N1-C3	4.49	122.36	113.88
15	I	300	KNM	C1-N1-C3	4.48	122.34	113.88
15	W	300	KNM	O5-S1-O4	-4.43	108.90	117.22
15	I	300	KNM	O5-S1-O4	-4.43	108.90	117.22
15	H	300	KNM	O5-S1-O4	-4.17	109.40	117.22
15	V	300	KNM	O5-S1-O4	-4.17	109.40	117.22
15	L	300	KNM	O5-S1-O4	-4.15	109.42	117.22
15	Z	300	KNM	O5-S1-O4	-4.15	109.42	117.22
15	L	300	KNM	C15-N3-C14	-2.44	119.36	123.29
15	Z	300	KNM	C15-N3-C14	-2.40	119.42	123.29
15	H	300	KNM	O5-S1-C16	2.31	109.99	108.33
15	V	300	KNM	O5-S1-C16	2.31	109.99	108.33

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	300	KNM	O1-C1-N1-C3
15	H	300	KNM	C2-C1-N1-C3
15	H	300	KNM	C3-C8-N2-C9
15	H	300	KNM	C17-C15-N3-C14
15	H	300	KNM	C21-C16-S1-O4
15	H	300	KNM	C21-C16-S1-O5
15	I	300	KNM	C2-C1-N1-C3
15	I	300	KNM	C4-C3-N1-C1
15	I	300	KNM	C8-C3-N1-C1
15	I	300	KNM	C3-C8-N2-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	I	300	KNM	O3-C8-N2-C9
15	I	300	KNM	C21-C16-S1-O4
15	I	300	KNM	C21-C16-S1-O5
15	I	300	KNM	C21-C16-S1-C22
15	L	300	KNM	C11-C10-C9-N2
15	L	300	KNM	C21-C16-S1-O5
15	V	300	KNM	O1-C1-N1-C3
15	V	300	KNM	C2-C1-N1-C3
15	V	300	KNM	C3-C8-N2-C9
15	V	300	KNM	C17-C15-N3-C14
15	V	300	KNM	C21-C16-S1-O4
15	V	300	KNM	C21-C16-S1-O5
15	W	300	KNM	C2-C1-N1-C3
15	W	300	KNM	C4-C3-N1-C1
15	W	300	KNM	C8-C3-N1-C1
15	W	300	KNM	C3-C8-N2-C9
15	W	300	KNM	O3-C8-N2-C9
15	W	300	KNM	C21-C16-S1-O4
15	W	300	KNM	C21-C16-S1-O5
15	W	300	KNM	C21-C16-S1-C22
15	Z	300	KNM	C11-C10-C9-N2
15	Z	300	KNM	C21-C16-S1-O5
15	H	300	KNM	O3-C8-N2-C9
15	V	300	KNM	O3-C8-N2-C9
15	I	300	KNM	C11-C10-C9-C14
15	W	300	KNM	C11-C10-C9-C14
15	I	300	KNM	C11-C10-C9-N2
15	W	300	KNM	C11-C10-C9-N2
15	H	300	KNM	C11-C10-C9-N2
15	V	300	KNM	C11-C10-C9-N2
15	H	300	KNM	C11-C10-C9-C14
15	V	300	KNM	C11-C10-C9-C14
15	H	300	KNM	N3-C15-C21-C16
15	V	300	KNM	N3-C15-C21-C16
15	H	300	KNM	C4-C3-C8-O3
15	V	300	KNM	C4-C3-C8-O3
15	H	300	KNM	C4-C3-C8-N2
15	V	300	KNM	C4-C3-C8-N2
15	H	300	KNM	O2-C14-C9-C10
15	V	300	KNM	O2-C14-C9-C10
15	H	300	KNM	N3-C14-C9-C10
15	V	300	KNM	N3-C14-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	H	300	KNM	C3-C4-C5-C7
15	V	300	KNM	C3-C4-C5-C7
15	H	300	KNM	C9-C10-C11-C13
15	V	300	KNM	C9-C10-C11-C13
15	H	300	KNM	C9-C10-C11-C12
15	V	300	KNM	C9-C10-C11-C12
15	H	300	KNM	C3-C4-C5-C6
15	V	300	KNM	C3-C4-C5-C6
15	L	300	KNM	C3-C4-C5-C7
15	Z	300	KNM	C3-C4-C5-C7
15	H	300	KNM	C17-C15-C21-C16
15	V	300	KNM	C17-C15-C21-C16
15	H	300	KNM	C10-C9-N2-C8
15	V	300	KNM	C10-C9-N2-C8
15	I	300	KNM	C3-C4-C5-C6
15	W	300	KNM	C3-C4-C5-C6
15	L	300	KNM	O2-C14-N3-C15
15	Z	300	KNM	O2-C14-N3-C15
15	L	300	KNM	C3-C4-C5-C6
15	Z	300	KNM	C3-C4-C5-C6
15	I	300	KNM	C3-C4-C5-C7
15	W	300	KNM	C3-C4-C5-C7
15	H	300	KNM	C21-C15-C17-C18
15	V	300	KNM	C21-C15-C17-C18
15	Z	300	KNM	C9-C14-N3-C15
15	L	300	KNM	C9-C14-N3-C15
15	I	300	KNM	O2-C14-N3-C15
15	W	300	KNM	O2-C14-N3-C15
15	H	300	KNM	N3-C15-C17-C18
15	V	300	KNM	N3-C15-C17-C18
15	L	300	KNM	C2-C1-N1-C3
15	Z	300	KNM	C2-C1-N1-C3
15	I	300	KNM	C9-C14-N3-C15
15	W	300	KNM	C9-C14-N3-C15
15	H	300	KNM	C14-C9-N2-C8
15	V	300	KNM	C14-C9-N2-C8
15	W	300	KNM	O2-C14-C9-N2
15	I	300	KNM	O2-C14-C9-N2
15	I	300	KNM	N3-C14-C9-N2
15	W	300	KNM	N3-C14-C9-N2
15	L	300	KNM	O1-C1-N1-C3
15	Z	300	KNM	O1-C1-N1-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	H	300	KNM	S1-C16-C21-C15
15	V	300	KNM	S1-C16-C21-C15
15	H	300	KNM	C21-C16-S1-C22
15	V	300	KNM	C21-C16-S1-C22
15	H	300	KNM	C21-C15-N3-C14
15	V	300	KNM	C21-C15-N3-C14
15	L	300	KNM	C15-C17-C18-C19
15	Z	300	KNM	C15-C17-C18-C19
15	I	300	KNM	C17-C15-N3-C14
15	W	300	KNM	C17-C15-N3-C14
15	L	300	KNM	C11-C10-C9-C14
15	Z	300	KNM	C11-C10-C9-C14
15	I	300	KNM	O2-C14-C9-C10
15	W	300	KNM	O2-C14-C9-C10
15	Z	300	KNM	O2-C14-C9-N2
15	H	300	KNM	O2-C14-N3-C15
15	V	300	KNM	O2-C14-N3-C15
15	L	300	KNM	O2-C14-C9-N2
15	I	300	KNM	C21-C15-N3-C14
15	W	300	KNM	C21-C15-N3-C14
15	Z	300	KNM	C9-C10-C11-C12

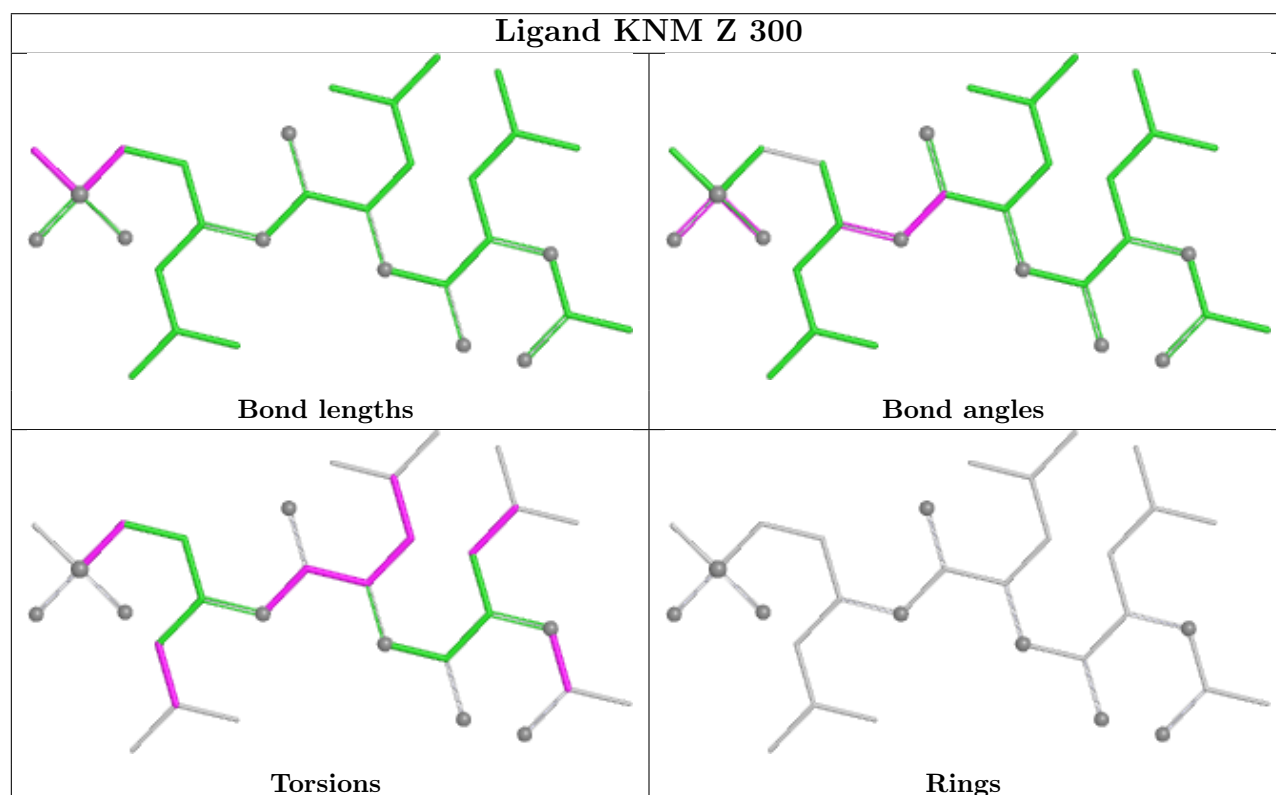
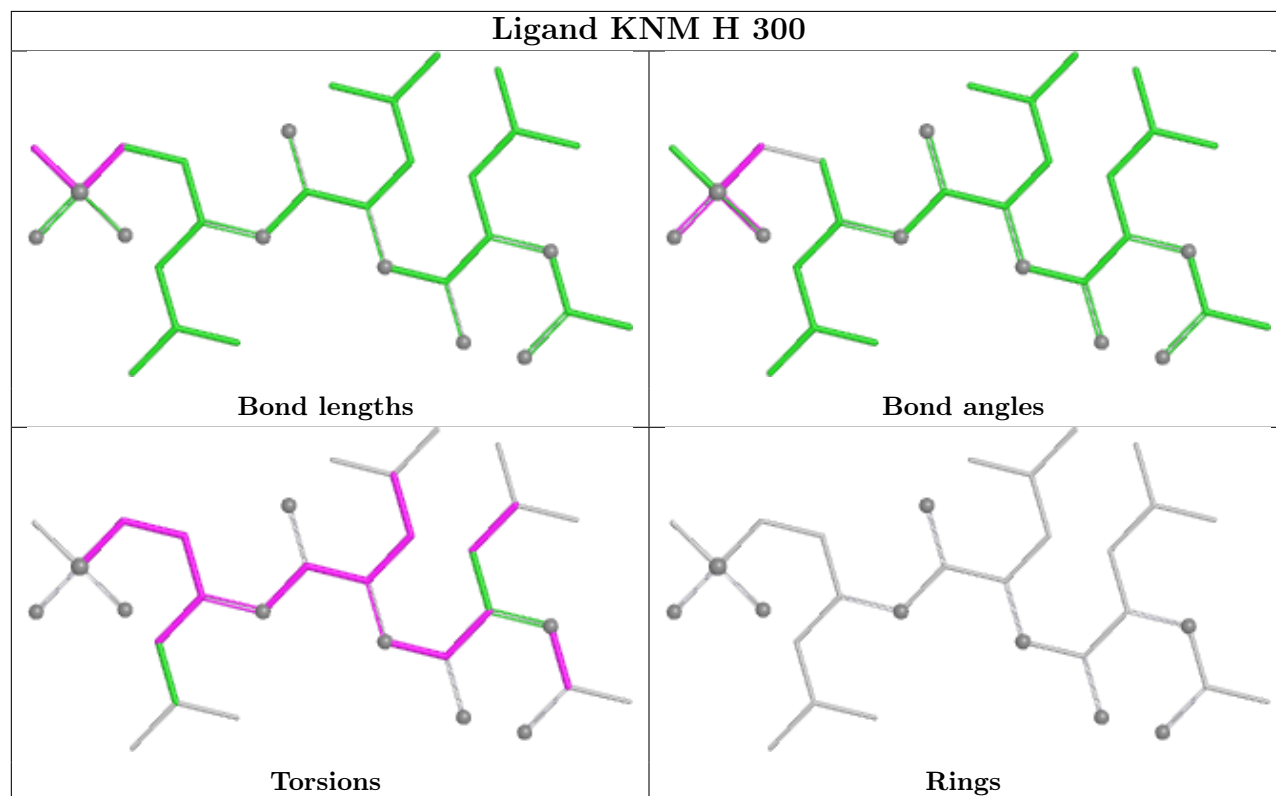
There are no ring outliers.

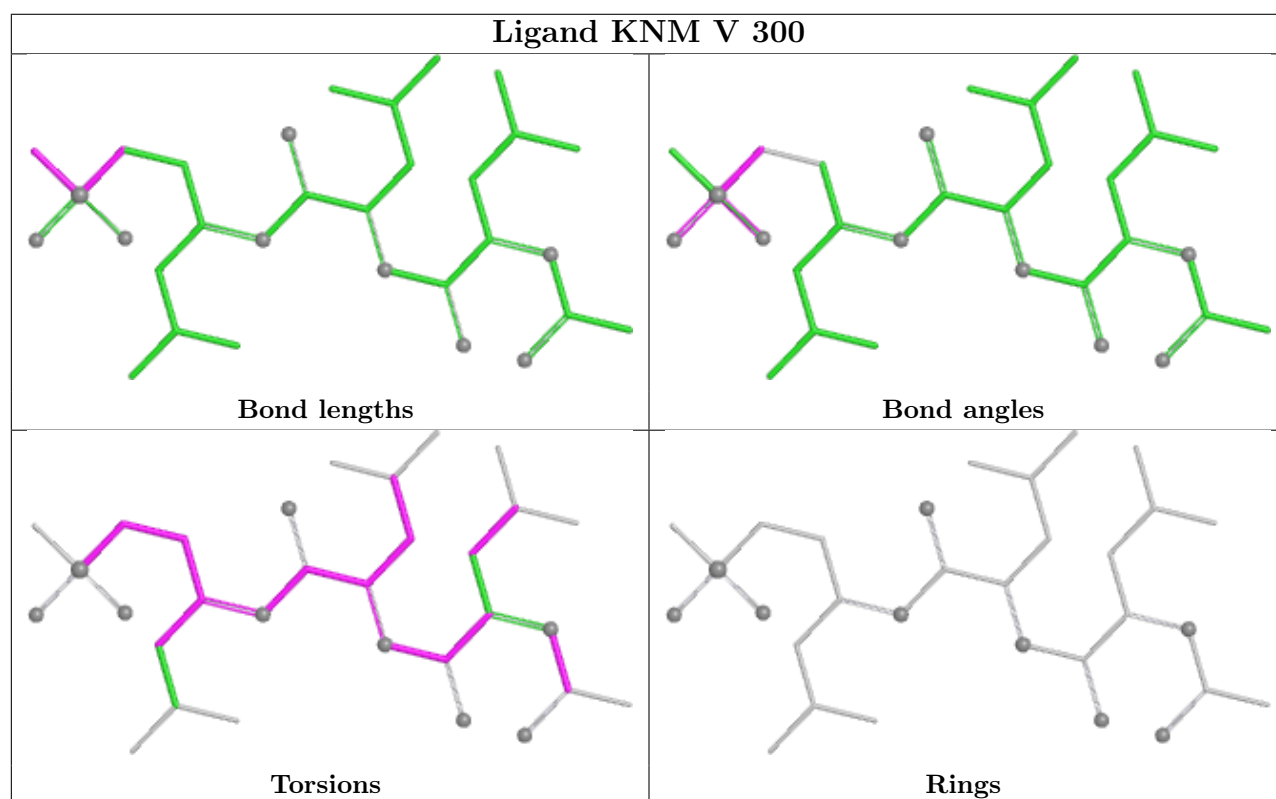
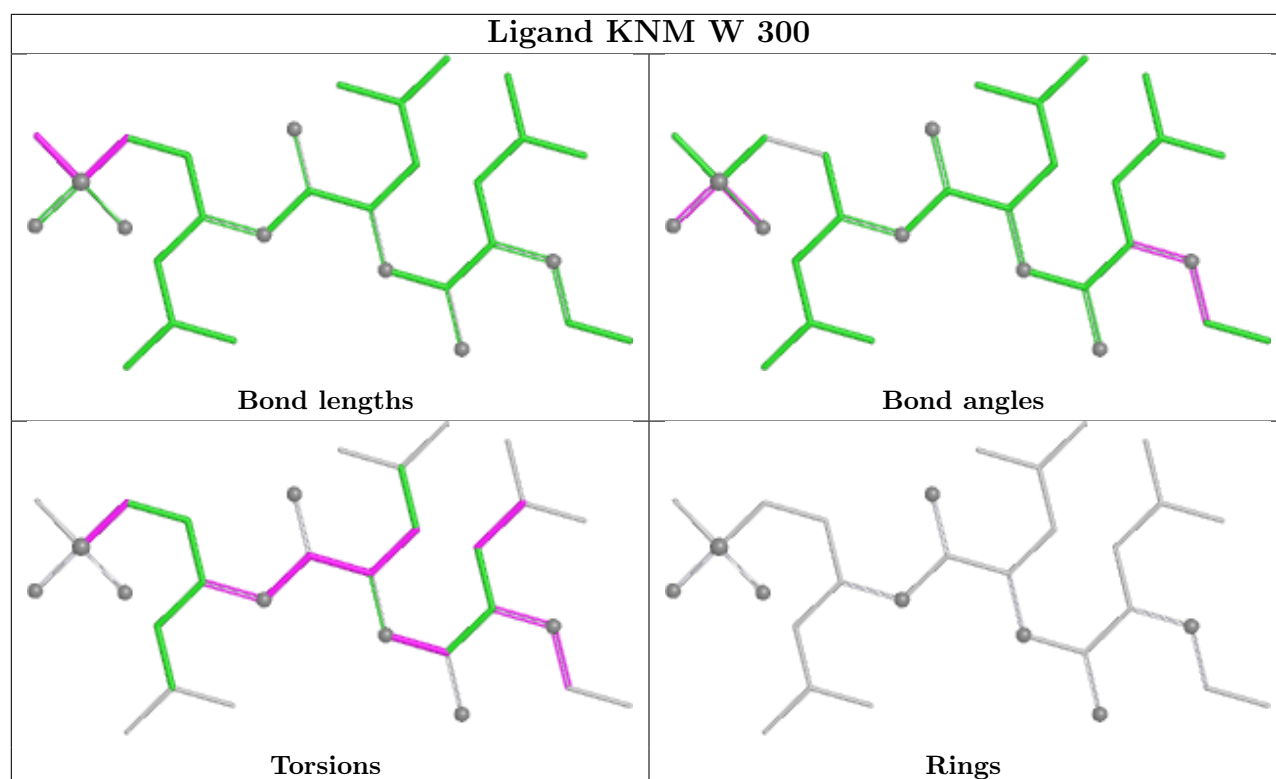
6 monomers are involved in 220 short contacts:

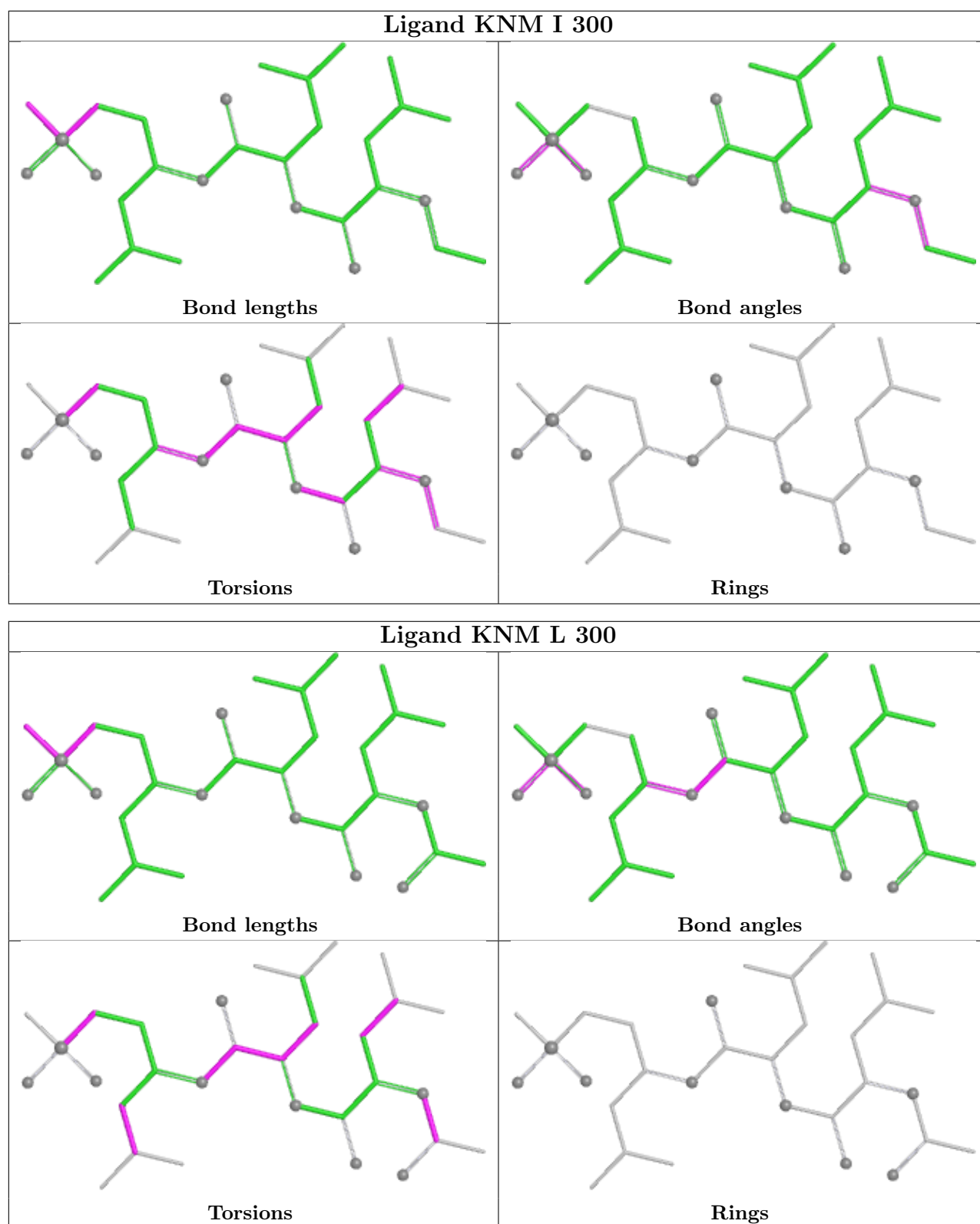
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	300	KNM	35	0
15	Z	300	KNM	30	0
15	W	300	KNM	45	0
15	V	300	KNM	33	0
15	I	300	KNM	46	0
15	L	300	KNM	31	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1
8	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1:THR	C	2:THR	N	1.78
1	V	1:THR	C	2:THR	N	1.78

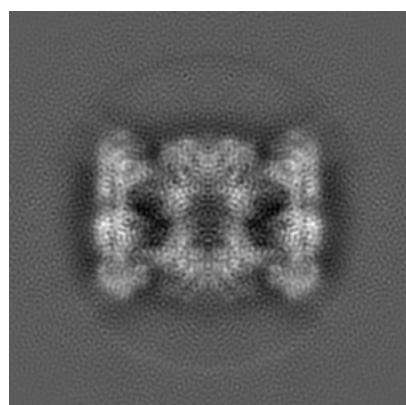
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2981. These allow visual inspection of the internal detail of the map and identification of artifacts.

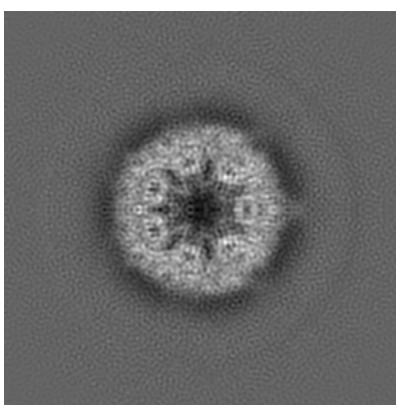
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

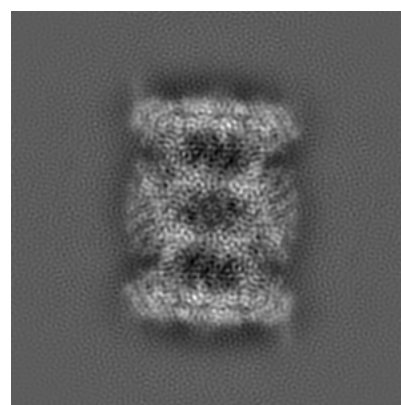
6.1.1 Primary map



X



Y

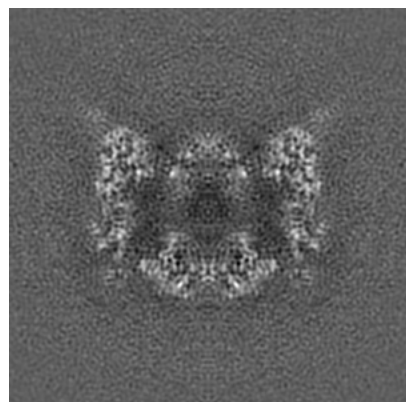


Z

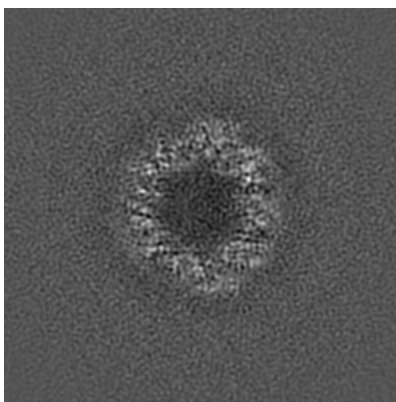
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

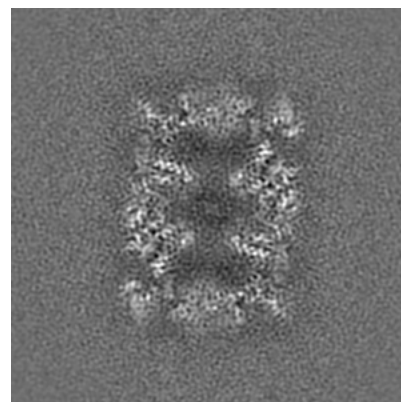
6.2.1 Primary map



X Index: 128



Y Index: 128

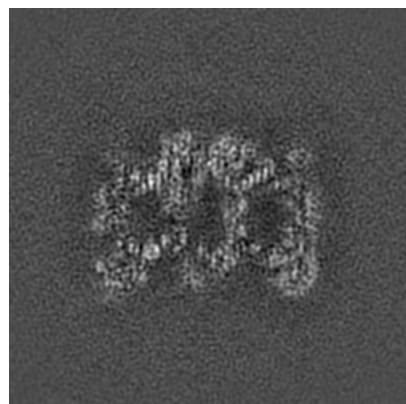


Z Index: 128

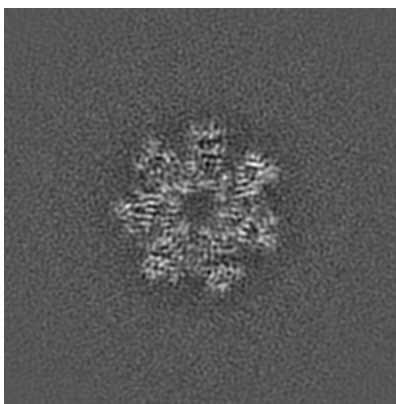
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

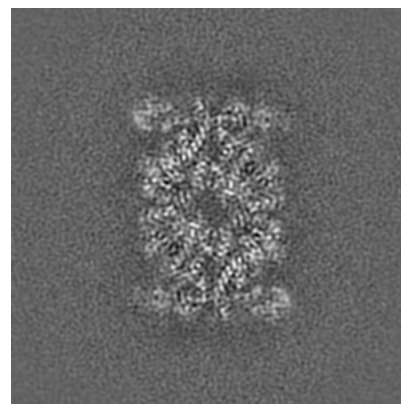
6.3.1 Primary map



X Index: 146



Y Index: 145

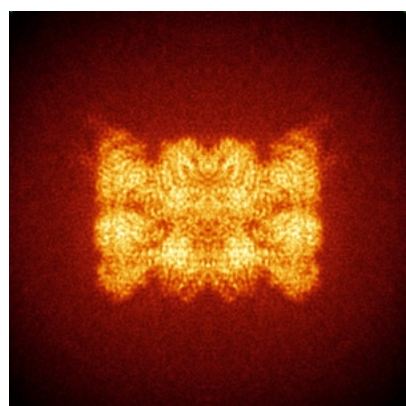


Z Index: 100

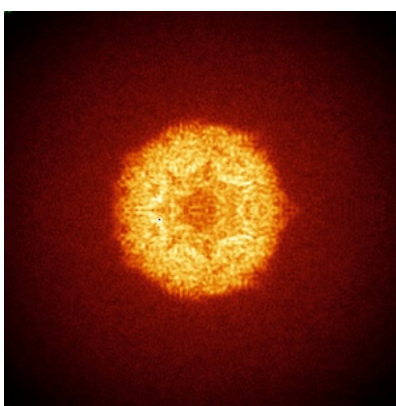
The images above show the largest variance slices of the map in three orthogonal directions.

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

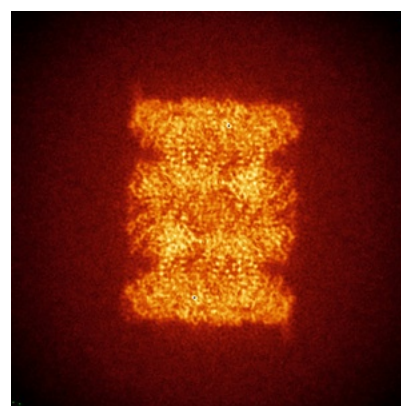
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

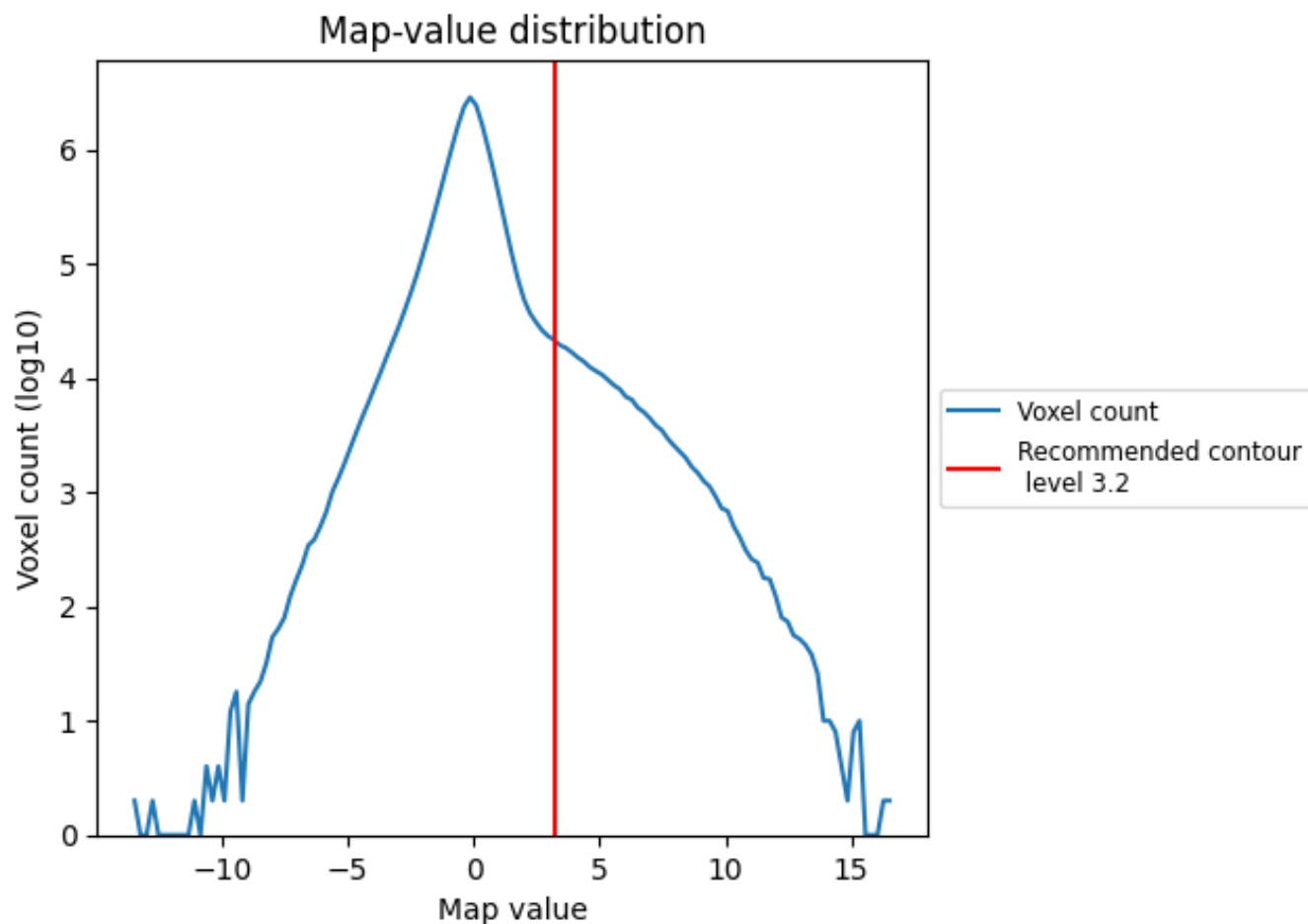
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

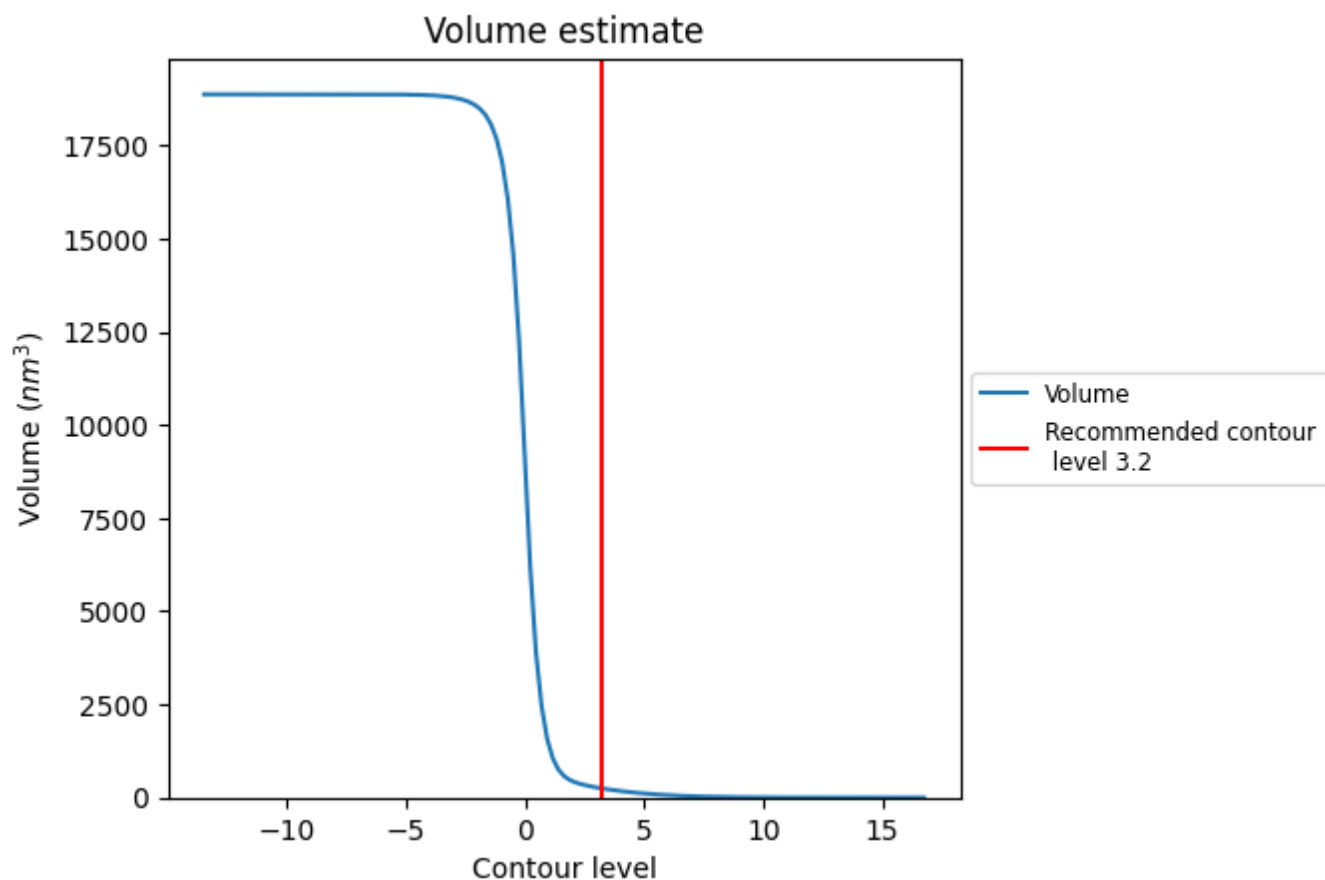
This section contains the results of statistical analysis of the map.

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.

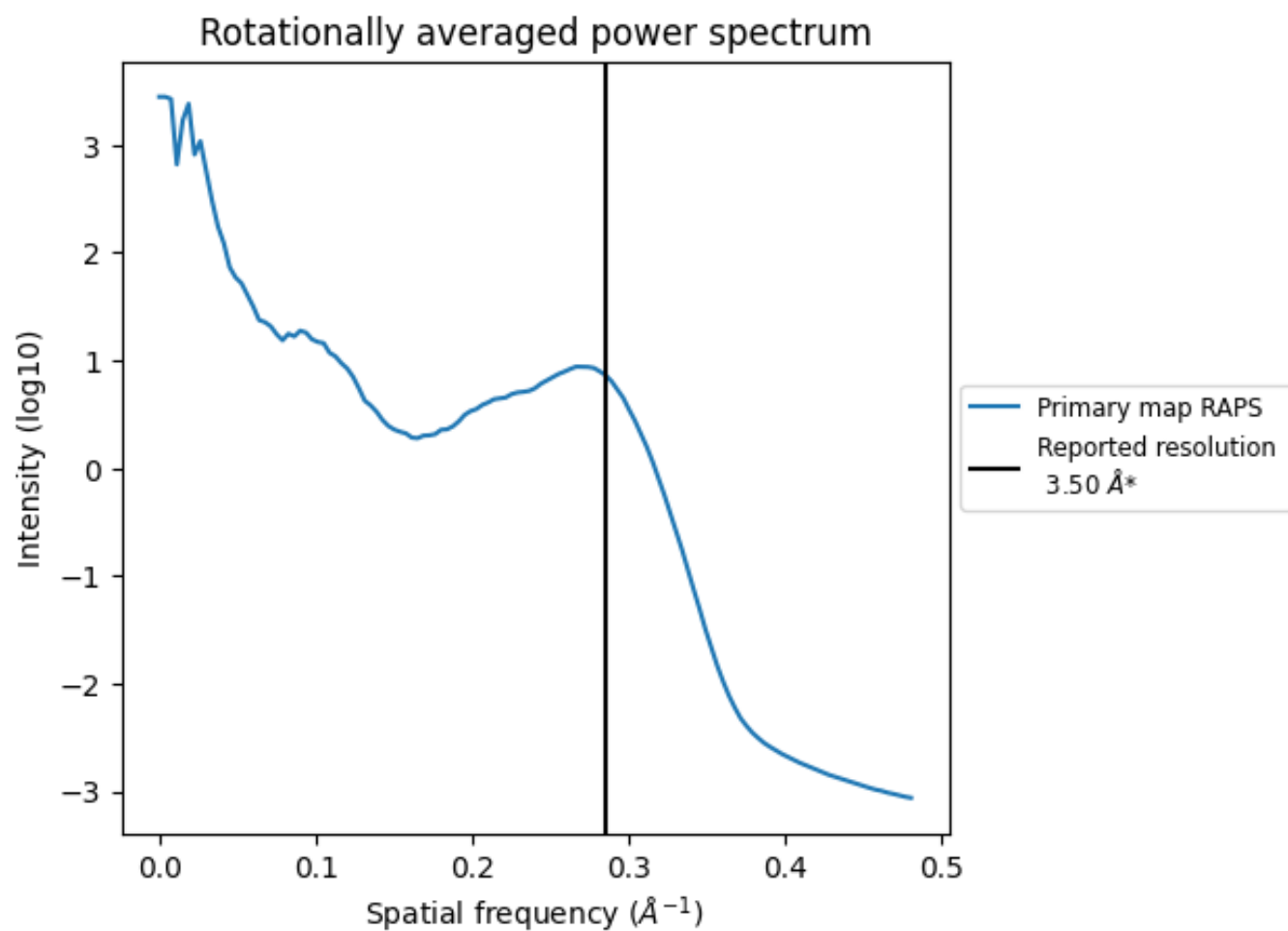
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 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 0.286 Å⁻¹

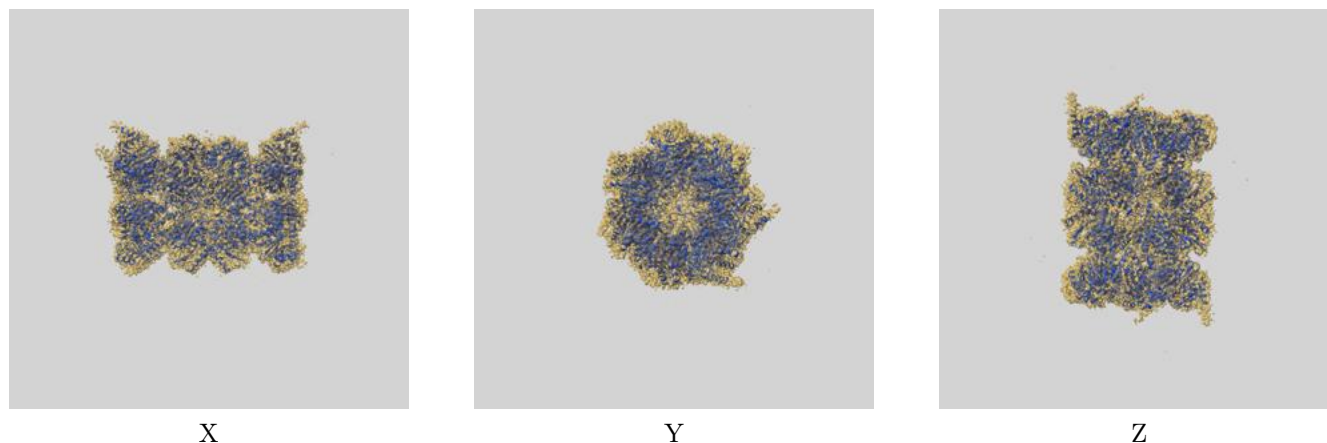
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

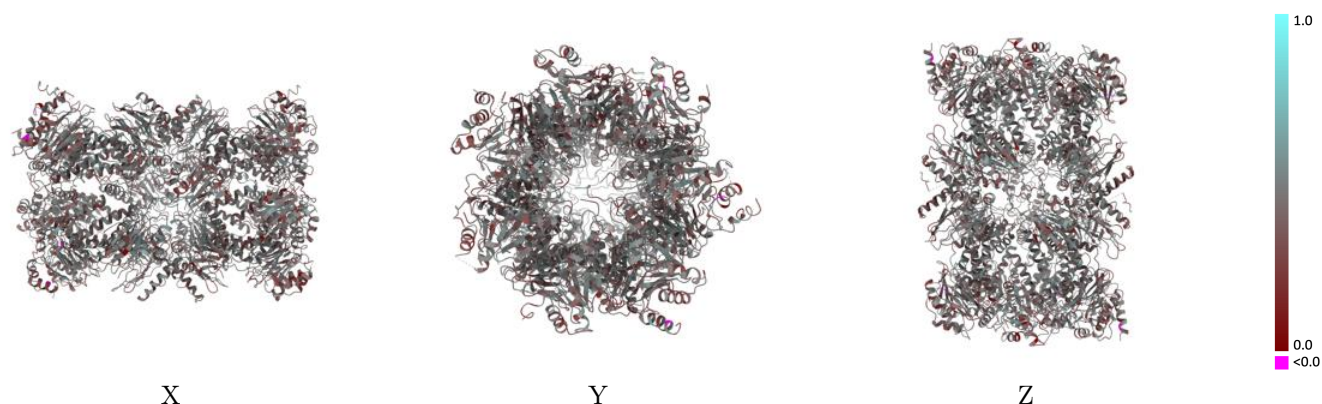
This section contains information regarding the fit between EMDB map EMD-2981 and PDB model 5A0Q. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



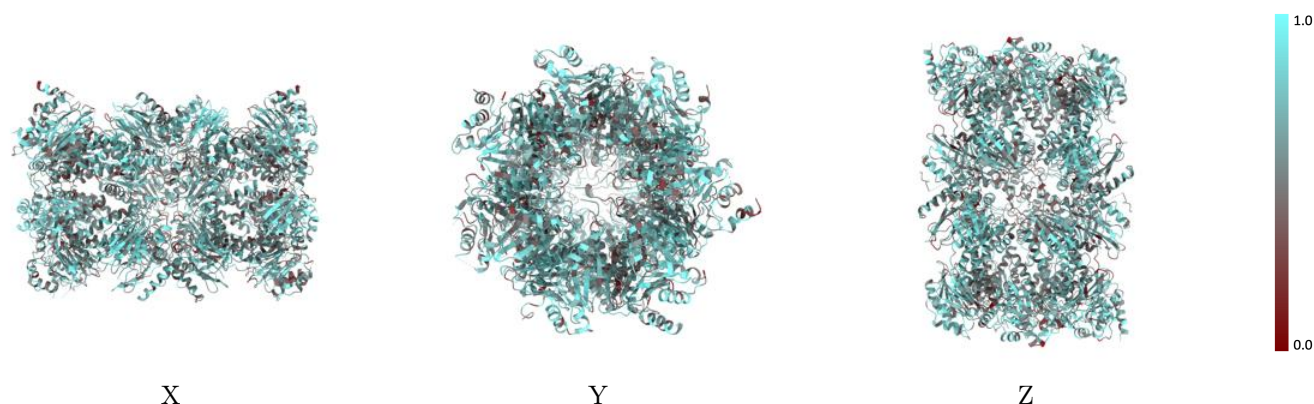
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



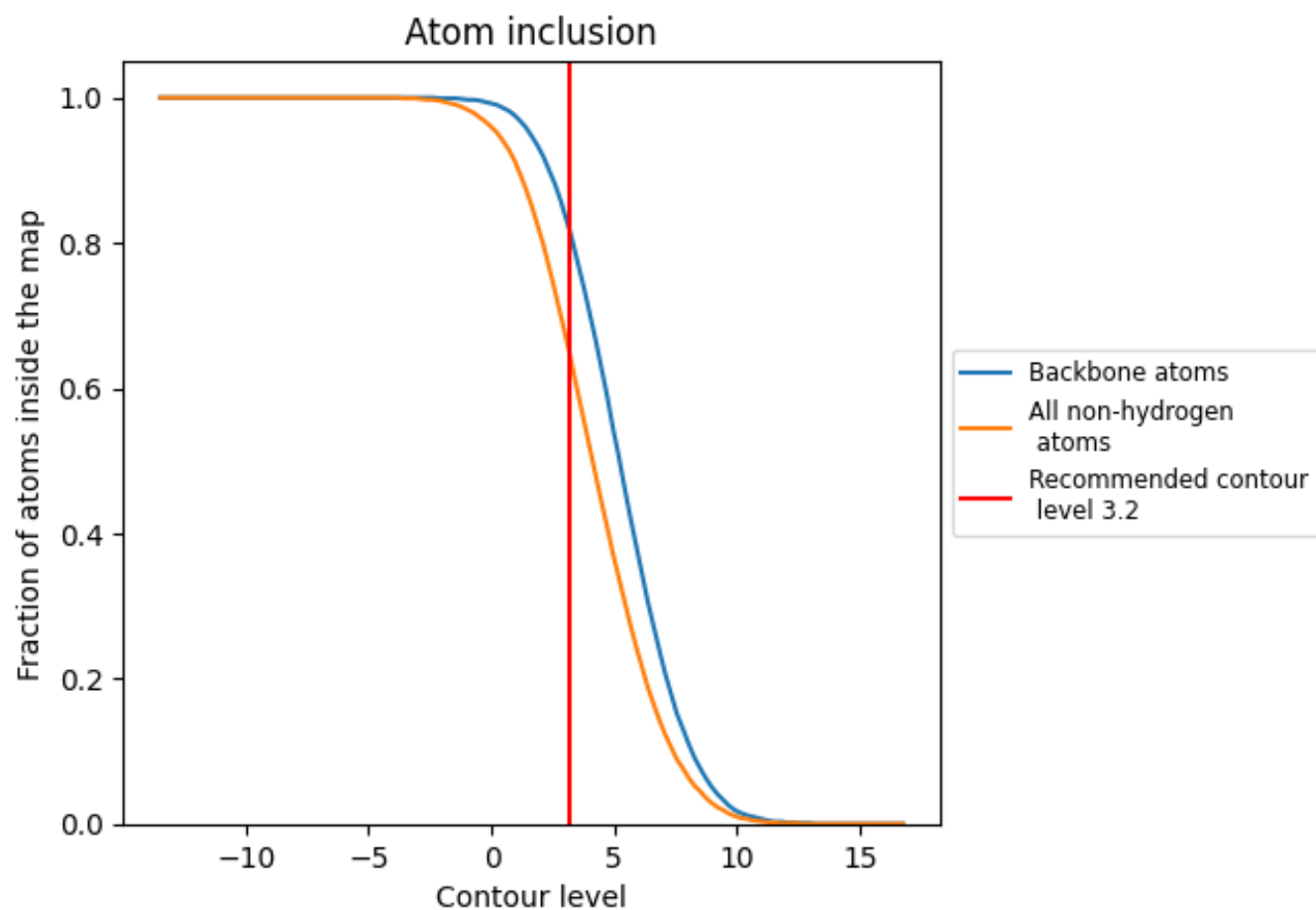
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 64% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.4260
A	 0.6340	 0.4310
B	 0.6690	 0.4240
C	 0.6450	 0.4180
D	 0.6260	 0.4200
E	 0.6460	 0.4120
F	 0.6400	 0.4210
G	 0.6330	 0.4180
H	 0.6440	 0.4290
I	 0.6710	 0.4400
J	 0.6060	 0.4300
K	 0.6340	 0.4310
L	 0.6980	 0.4420
M	 0.6280	 0.4300
N	 0.6470	 0.4250
O	 0.6350	 0.4290
P	 0.6690	 0.4240
Q	 0.6440	 0.4210
R	 0.6260	 0.4170
S	 0.6460	 0.4120
T	 0.6400	 0.4250
U	 0.6330	 0.4150
V	 0.6430	 0.4320
W	 0.6700	 0.4400
X	 0.6060	 0.4290
Y	 0.6350	 0.4300
Z	 0.6980	 0.4420
a	 0.6290	 0.4250
b	 0.6460	 0.4270

