



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:21 AM UTC

PDB ID : 8YIY / pdb_00008yiy
EMDB ID : EMD-39333
Title : Cryo-EM structure of human proteasome assembly intermediate preholo-1
Authors : Han, Y.; Han, Q.; Tang, Q.; Zhang, Y.; Liu, K.
Deposited on : 2024-02-29
Resolution : 3.41 Å(reported)

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:

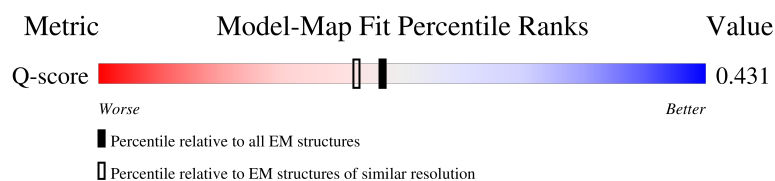
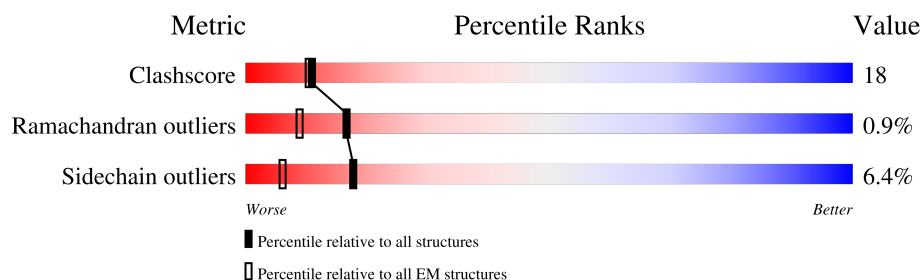
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.41 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.



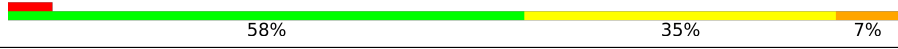
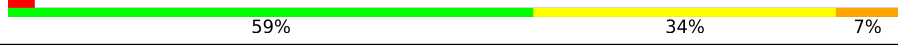
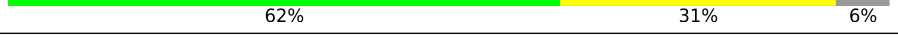
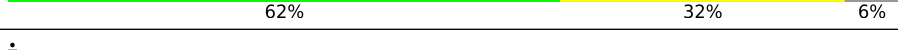
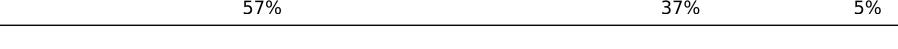
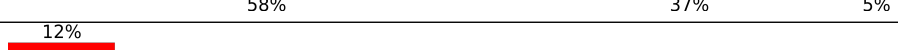
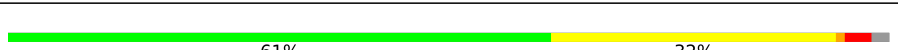
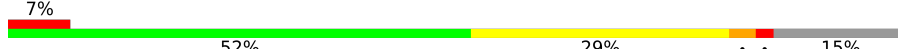
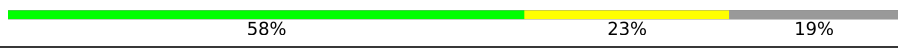
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13997 (2.91 - 3.91)

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	234	
1	O	234	
2	B	261	
2	P	261	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	253	
13	a	253	
14	N	239	
14	b	239	
15	c	288	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	f	288	22% 67% 29%
16	d	264	58% 48% 41% 10%
16	g	264	9% 47% 41% 10%
17	e	141	66% 43% 30% 20%
17	h	141	50% 43% 28% 7% 20%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 59560 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	228	Total	C	N	O	S	0	0
			1760	1124	296	334	6		
1	A	228	Total	C	N	O	S	0	0
			1760	1124	296	334	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	245	Total	C	N	O	S	0	0
			1894	1196	321	367	10		
2	B	245	Total	C	N	O	S	0	0
			1894	1196	321	367	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	239	Total	C	N	O	S	0	0
			1849	1159	325	360	5		
3	C	239	Total	C	N	O	S	0	0
			1849	1159	325	360	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	241	Total	C	N	O	S	0	0
			1840	1159	305	364	12		
4	D	241	Total	C	N	O	S	0	0
			1840	1159	305	364	12		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	238	Total	C	N	O	S	1	0
			1859	1165	335	348	11		
5	E	238	Total	C	N	O	S	1	0
			1859	1165	335	348	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	239	Total	C	N	O	S	1	0
			1858	1180	318	348	12		
6	F	239	Total	C	N	O	S	1	0
			1858	1180	318	348	12		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	245	Total	C	N	O	S	0	0
			1893	1201	317	361	14		
7	G	245	Total	C	N	O	S	0	0
			1893	1201	317	361	14		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	263	Total	C	N	O	S	2	0
			1984	1252	339	378	15		
8	H	263	Total	C	N	O	S	2	0
			1984	1252	339	378	15		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	200	Total	C	N	O	S	2	0
			1576	1004	265	289	18		
9	I	200	Total	C	N	O	S	2	0
			1576	1004	265	289	18		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	2	0
			1581	1013	269	289	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	2	0
			1581	1013	269	289	10		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	224	Total	C	N	O	S	3	0
			1737	1097	302	327	11		
11	K	224	Total	C	N	O	S	3	0
			1737	1097	302	327	11		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	213	Total	C	N	O	S	1	0
			1644	1043	281	309	11		
12	L	213	Total	C	N	O	S	1	0
			1644	1043	281	309	11		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	206	Total	C	N	O	S	1	0
			1605	1012	277	305	11		
13	M	206	Total	C	N	O	S	1	0
			1605	1012	277	305	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	200	Total	C	N	O	S	1	0
			1504	943	256	292	13		
14	N	200	Total	C	N	O	S	1	0
			1504	943	256	292	13		

- Molecule 15 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	280	Total	C	N	O	S	0	0
			2230	1421	374	416	19		
15	c	280	Total	C	N	O	S	0	0
			2230	1421	374	416	19		

- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	264	Total	C	N	O	S	0	0
			2062	1323	336	388	15		
16	d	264	Total	C	N	O	S	0	0
			2062	1323	336	388	15		

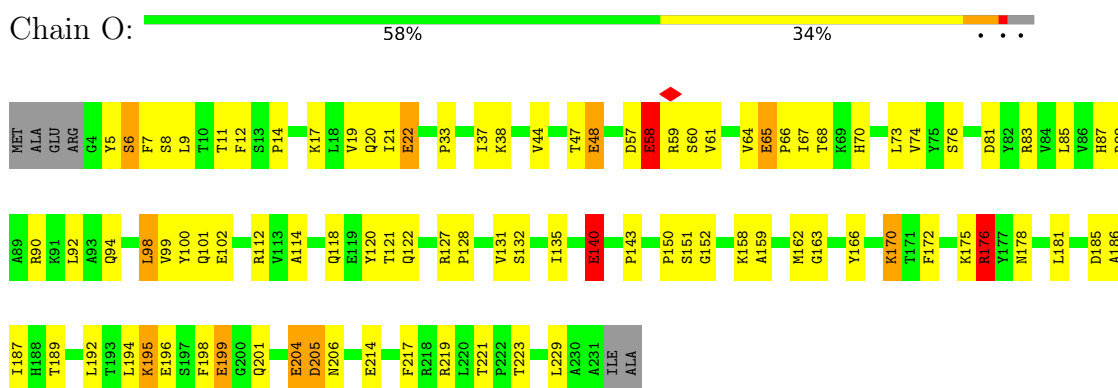
- Molecule 17 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	113	Total	C	N	O	S	0	0
			904	574	152	173	5		
17	e	113	Total	C	N	O	S	0	0
			904	574	152	173	5		

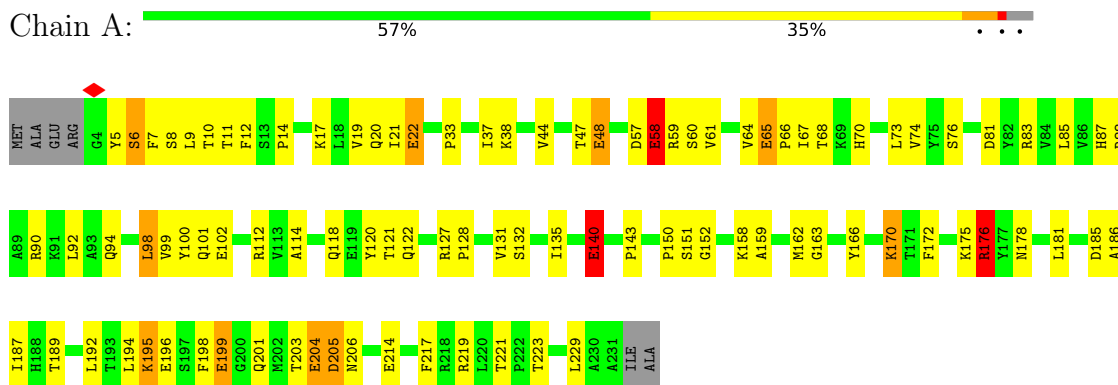
3 Residue-property plots

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.

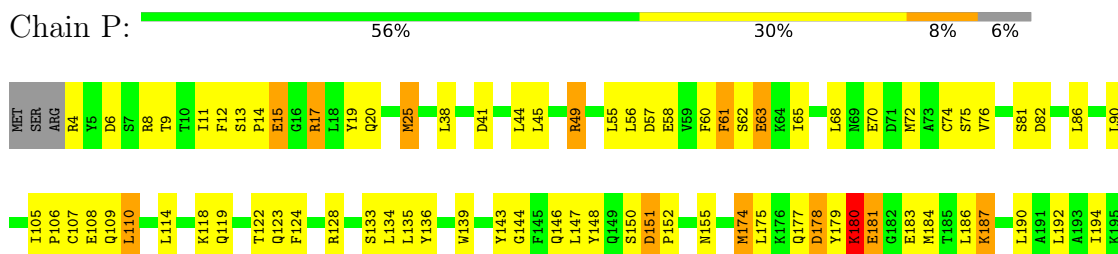
- Molecule 1: Proteasome subunit alpha type-2



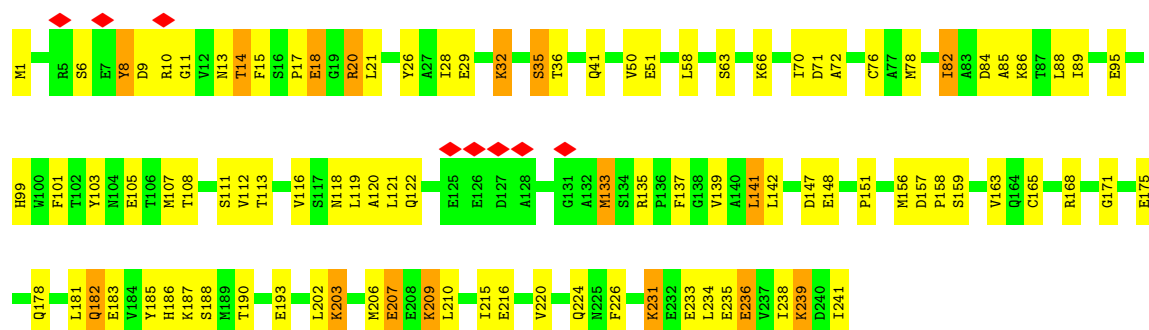
- Molecule 1: Proteasome subunit alpha type-2



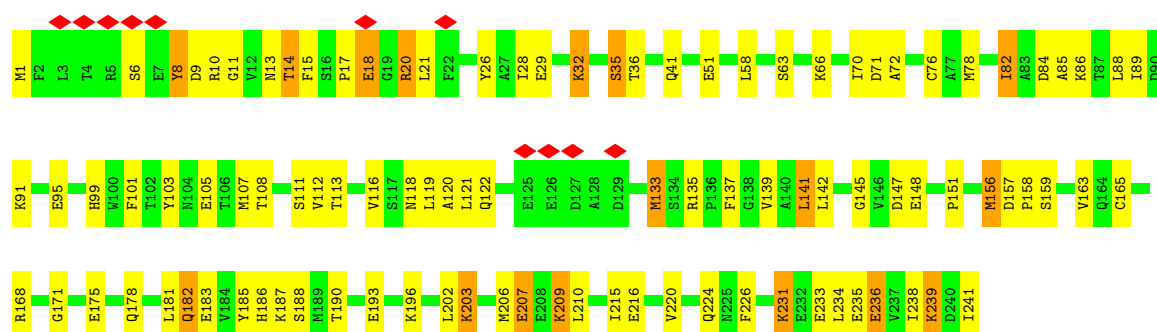
- Molecule 2: Proteasome subunit alpha type-4



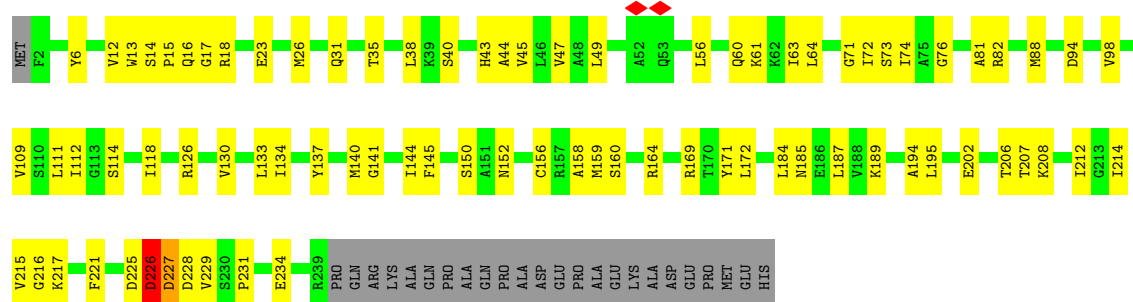




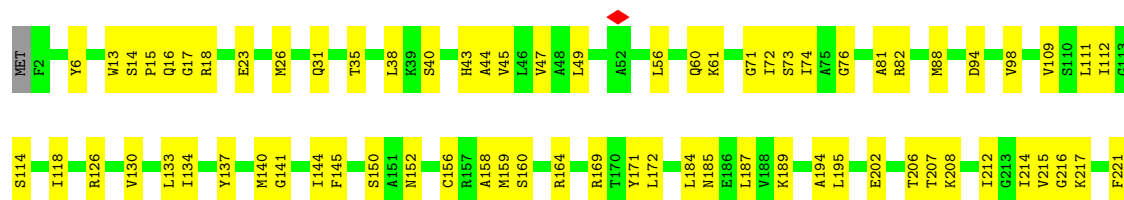
• Molecule 4: Proteasome subunit alpha type-5

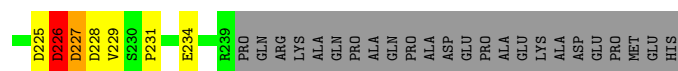


• Molecule 5: Proteasome subunit alpha type-1



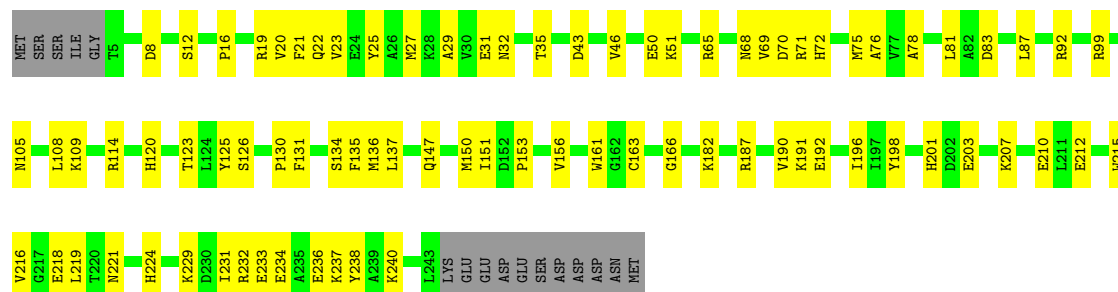
• Molecule 5: Proteasome subunit alpha type-1





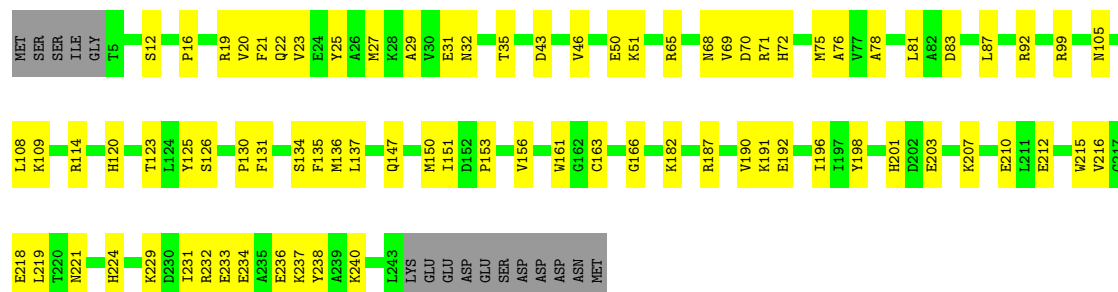
• Molecule 6: Proteasome subunit alpha type-3

Chain T: 62% 32% 6%



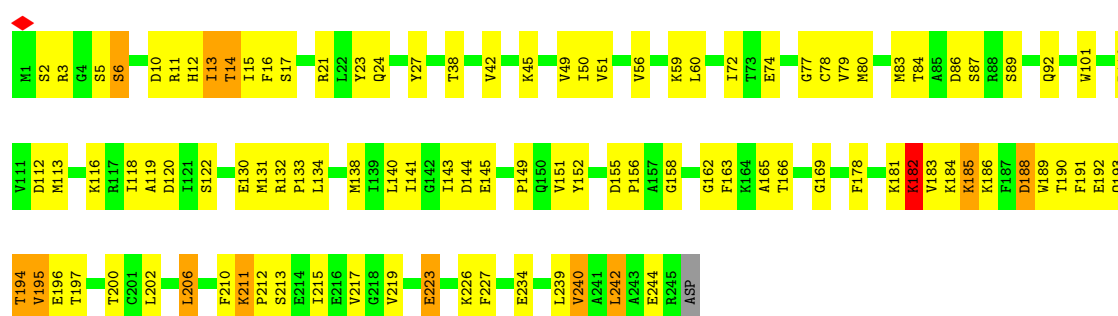
• Molecule 6: Proteasome subunit alpha type-3

Chain F: 62% 31% 6%



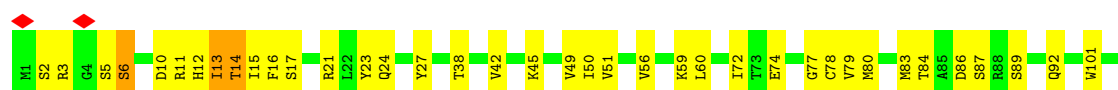
• Molecule 7: Proteasome subunit alpha type-6

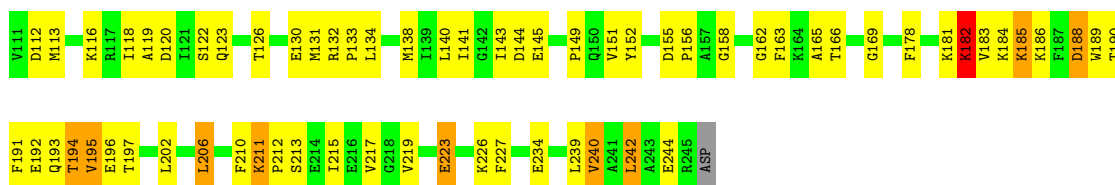
Chain U: 58% 37% 5%



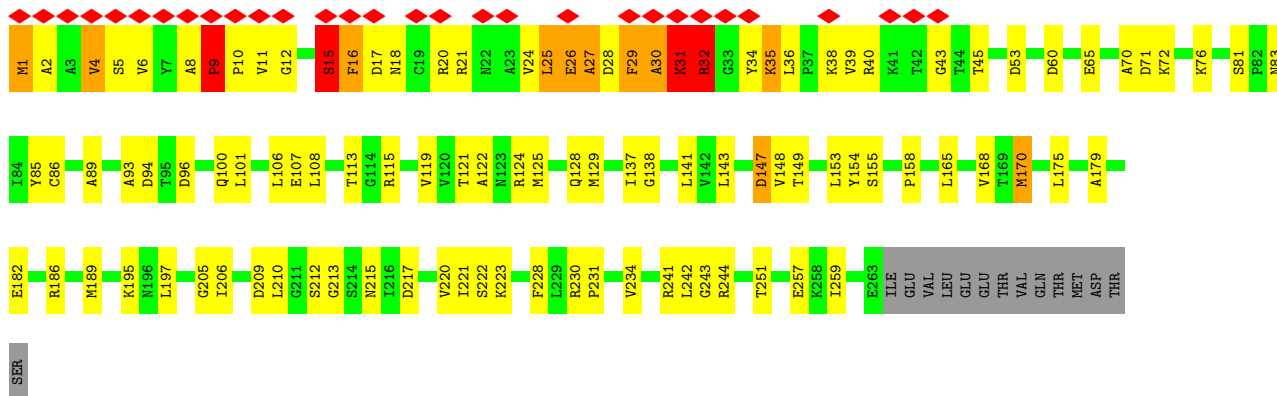
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 57% 37% 5%

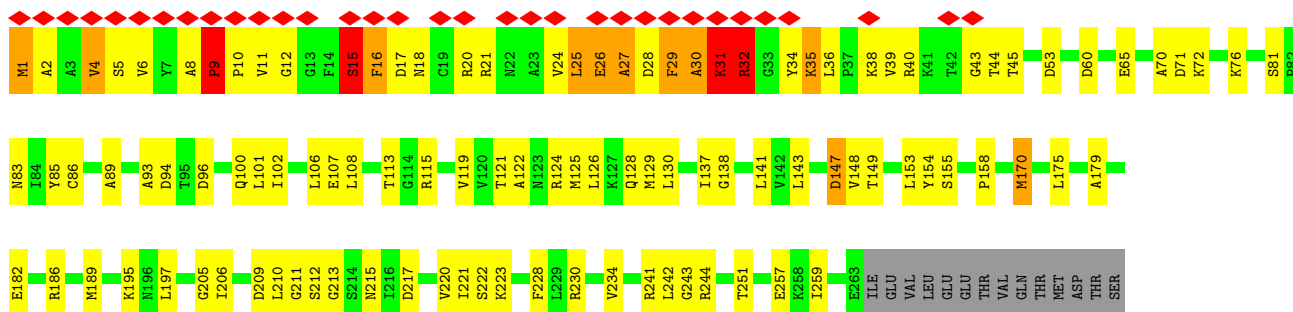




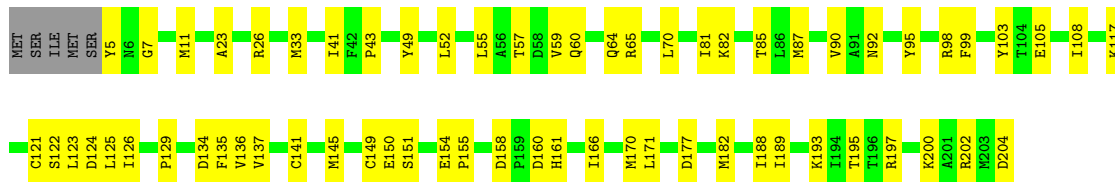
• Molecule 8: Proteasome subunit beta type-7



• Molecule 8: Proteasome subunit beta type-7

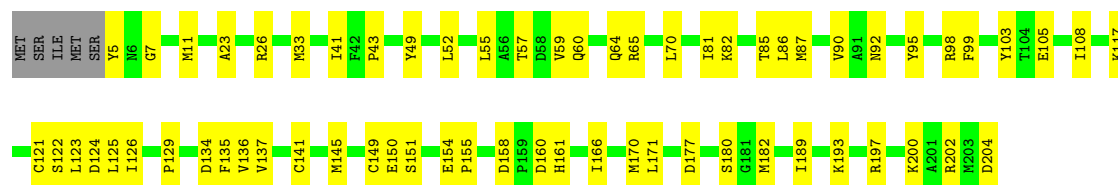


• Molecule 9: Proteasome subunit beta type-3



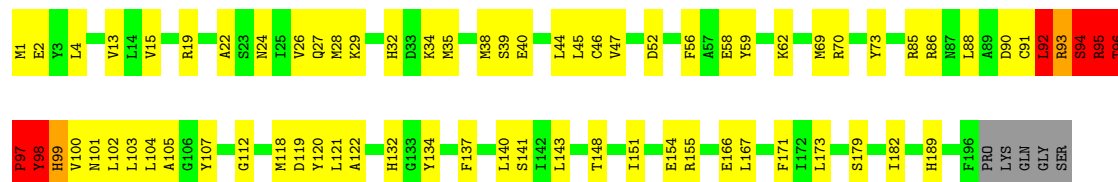
• Molecule 9: Proteasome subunit beta type-3





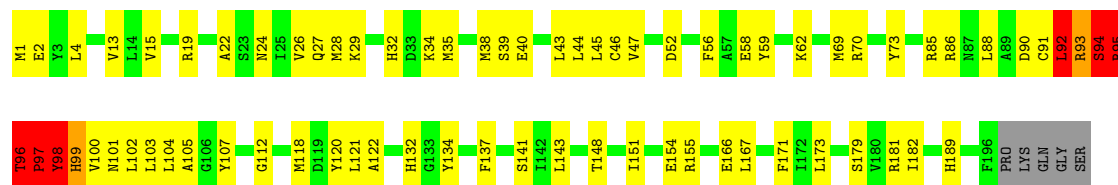
• Molecule 10: Proteasome subunit beta type-2

Chain X: 61% 32% . . .



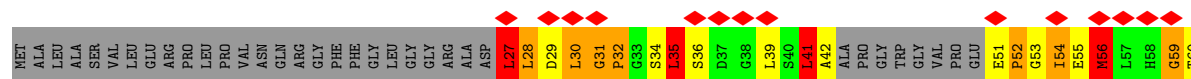
• Molecule 10: Proteasome subunit beta type-2

Chain J: 61% 32% . . .



• Molecule 11: Proteasome subunit beta type-5

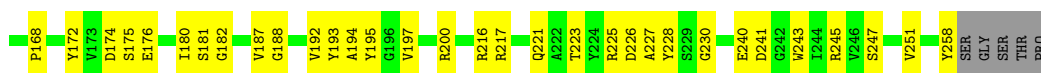
Chain Y: 5% 51% 29% . . 15%



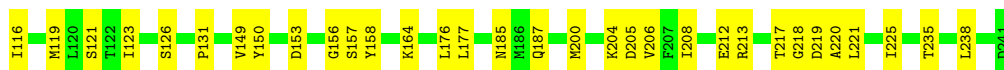
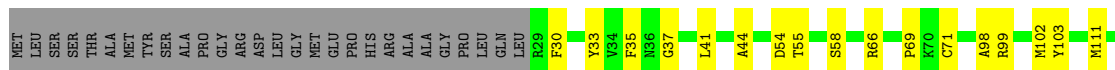
• Molecule 11: Proteasome subunit beta type-5

Chain K: 7% 52% 29% . . 15%

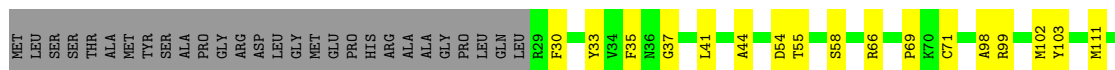




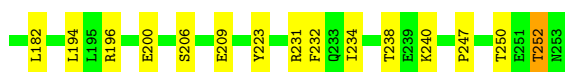
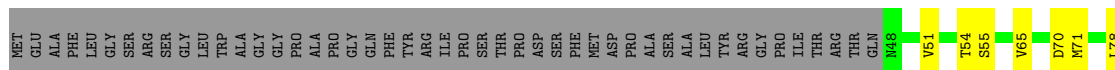
• Molecule 12: Proteasome subunit beta type-1



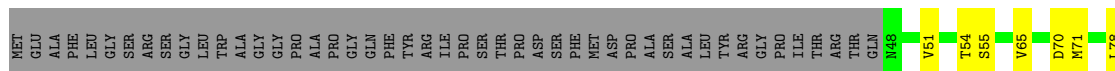
• Molecule 12: Proteasome subunit beta type-1



• Molecule 13: Proteasome subunit beta type-4

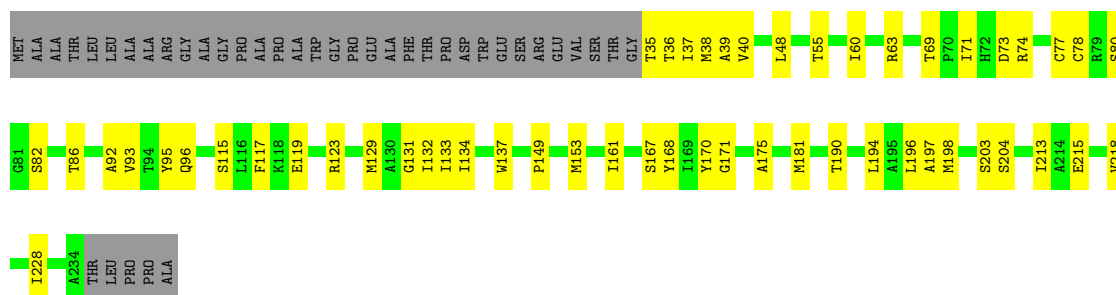


• Molecule 13: Proteasome subunit beta type-4



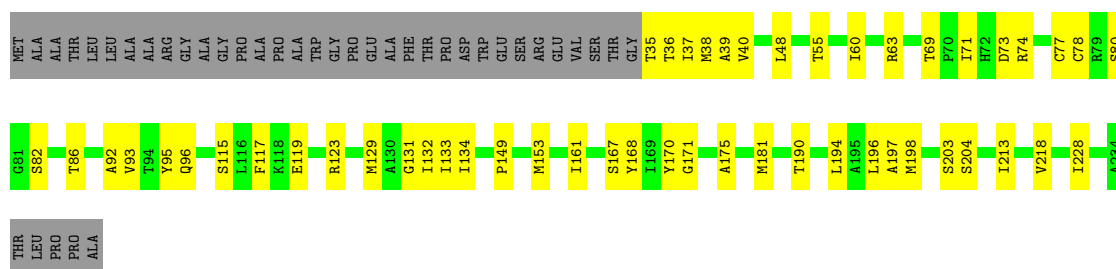
- Molecule 14: Proteasome subunit beta type-6

Chain b: 



- Molecule 14: Proteasome subunit beta type-6

Chain N: 



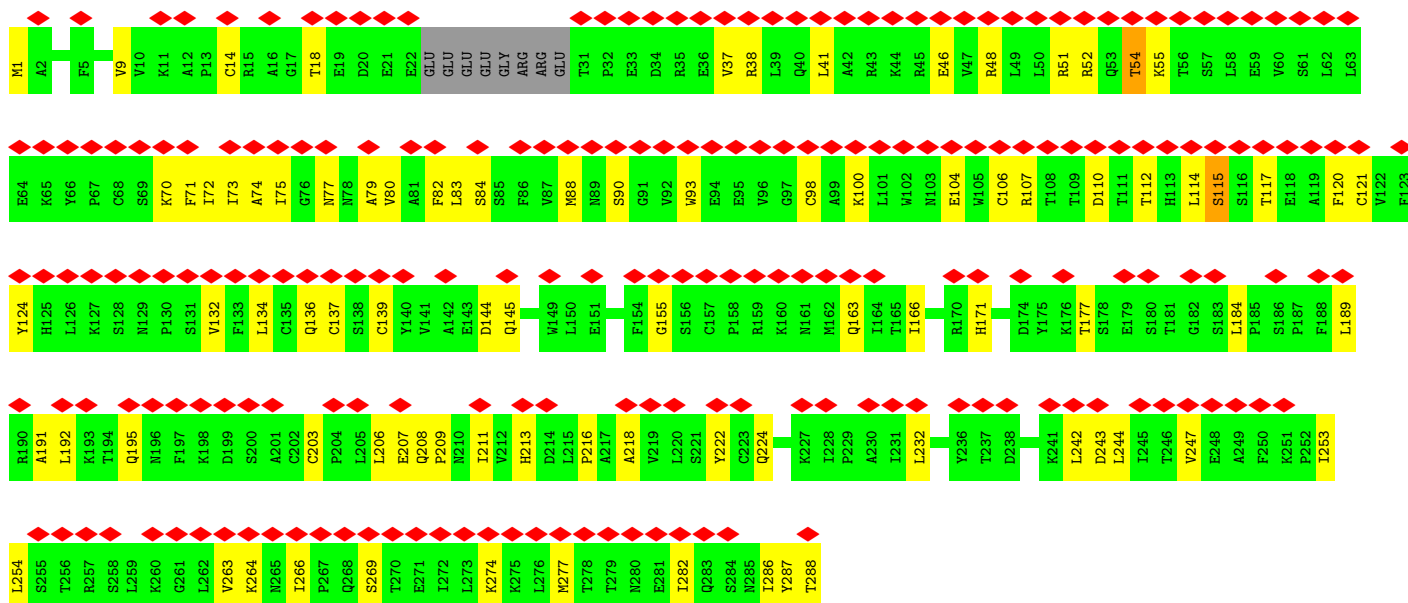
- Molecule 15: Proteasome assembly chaperone 1

Chain f: 

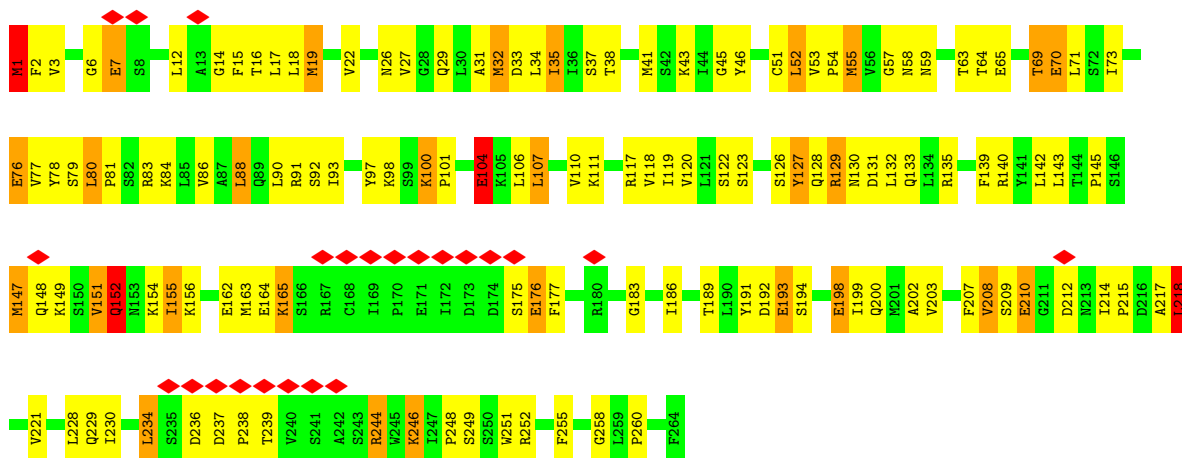


- Molecule 15: Proteasome assembly chaperone 1

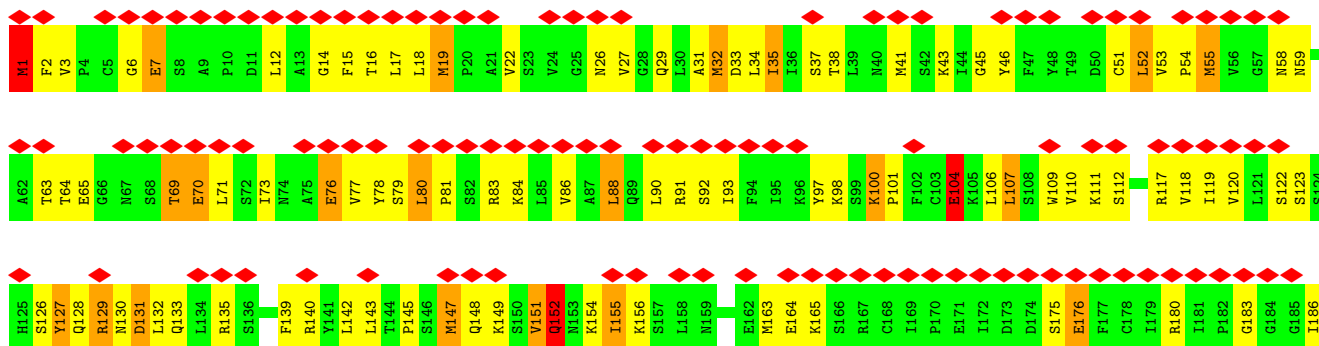
Chain c: 

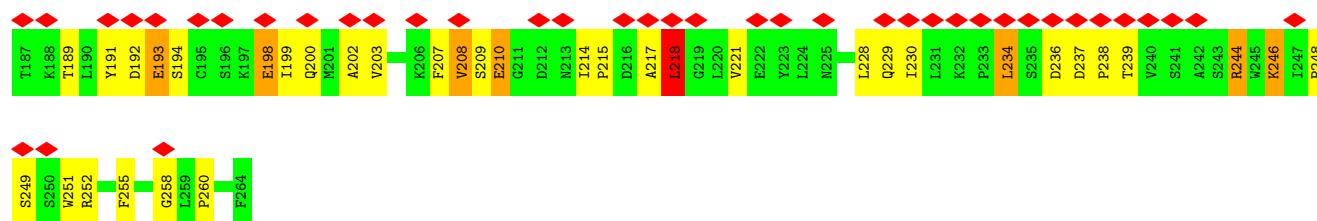


• Molecule 16: Proteasome assembly chaperone 2

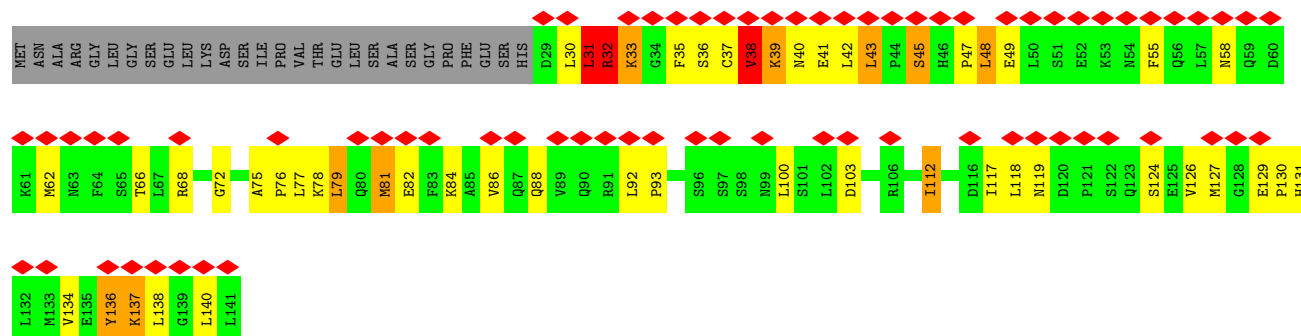


• Molecule 16: Proteasome assembly chaperone 2

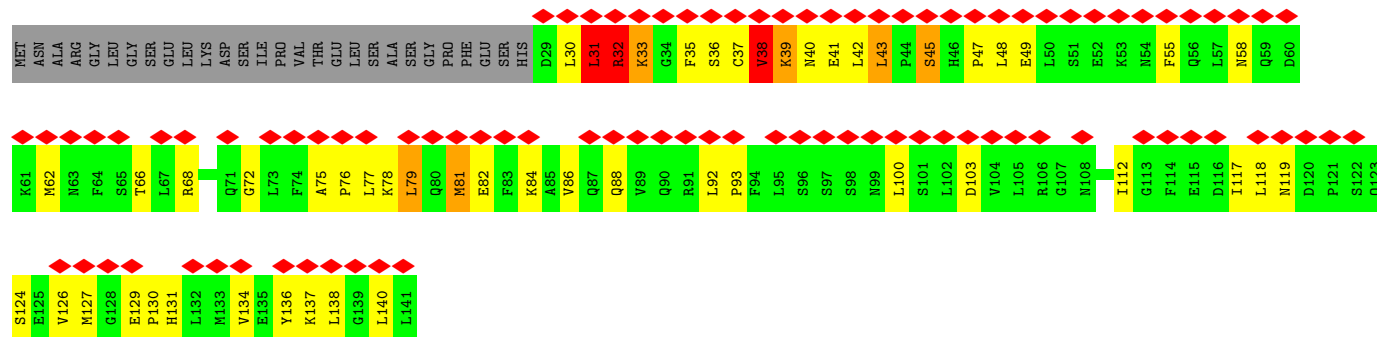
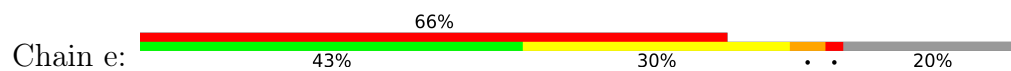




• Molecule 17: Proteasome maturation protein



• Molecule 17: Proteasome maturation protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.307	Depositor
Minimum map value	-1.388	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.237	Depositor
Map size (Å)	316.49997, 316.49997, 316.49997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.35	0/1799	0.64	4/2442 (0.2%)
1	O	0.35	0/1799	0.64	4/2442 (0.2%)
2	B	0.34	0/1924	0.67	2/2602 (0.1%)
2	P	0.34	0/1924	0.67	2/2602 (0.1%)
3	C	0.32	0/1875	0.67	1/2540 (0.0%)
3	Q	0.32	0/1875	0.67	1/2540 (0.0%)
4	D	0.31	0/1869	0.60	0/2523
4	R	0.31	0/1869	0.60	0/2523
5	E	0.31	0/1896	0.44	0/2563
5	S	0.31	0/1896	0.44	0/2563
6	F	0.30	0/1896	0.48	0/2556
6	T	0.29	0/1896	0.48	0/2556
7	G	0.34	0/1927	0.60	2/2606 (0.1%)
7	U	0.34	0/1927	0.60	2/2606 (0.1%)
8	H	0.42	0/2025	0.63	1/2742 (0.0%)
8	V	0.42	0/2025	0.63	1/2742 (0.0%)
9	I	0.36	0/1608	0.48	0/2168
9	W	0.36	0/1608	0.48	0/2168
10	J	0.54	2/1620 (0.1%)	0.70	6/2191 (0.3%)
10	X	0.53	2/1620 (0.1%)	0.70	6/2191 (0.3%)
11	K	0.47	0/1779	0.66	1/2401 (0.0%)
11	Y	0.47	0/1779	0.71	2/2401 (0.1%)
12	L	0.35	0/1677	0.46	0/2260
12	Z	0.35	0/1677	0.46	0/2260
13	M	0.35	0/1638	0.49	0/2216
13	a	0.34	0/1638	0.49	0/2216
14	N	0.33	0/1533	0.44	0/2074
14	b	0.33	0/1533	0.44	0/2074
15	c	0.21	0/2276	0.48	1/3085 (0.0%)
15	f	0.21	0/2276	0.48	1/3085 (0.0%)
16	d	0.27	0/2108	0.69	6/2858 (0.2%)
16	g	0.27	0/2108	0.69	6/2858 (0.2%)
17	e	0.50	0/919	0.83	2/1236 (0.2%)
17	h	0.49	0/919	0.84	2/1236 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	4/60738 (0.0%)	0.59	53/82126 (0.1%)

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
3	C	0	3
3	Q	0	3
5	E	0	1
5	S	0	1
8	H	0	5
8	V	0	5
10	J	0	2
10	X	0	2
11	K	0	1
11	Y	0	1
15	c	0	1
15	f	0	1
17	e	0	1
17	h	0	1
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	99[A]	HIS	C-O	9.41	1.35	1.24
10	J	99[B]	HIS	C-O	9.41	1.35	1.24
10	X	99[A]	HIS	C-O	9.38	1.35	1.24
10	X	99[B]	HIS	C-O	9.38	1.35	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	e	86	VAL	N-CA-C	-9.72	104.47	113.71
17	h	86	VAL	N-CA-C	-9.70	104.50	113.71
10	X	99[A]	HIS	CA-C-O	8.82	133.12	120.51
10	X	99[B]	HIS	CA-C-O	8.82	133.12	120.51
10	J	99[A]	HIS	CA-C-O	8.79	133.08	120.51
10	J	99[B]	HIS	CA-C-O	8.79	133.08	120.51
16	g	104	GLU	CA-CB-CG	8.12	130.34	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	d	104	GLU	CA-CB-CG	8.11	130.32	114.10
1	O	140	GLU	CA-CB-CG	8.10	130.29	114.10
1	A	140	GLU	CA-CB-CG	8.09	130.27	114.10
17	e	47	PRO	N-CA-C	-7.16	104.53	113.84
17	h	47	PRO	N-CA-C	-7.16	104.54	113.84
8	H	9	PRO	N-CA-C	-7.05	102.09	110.70
8	V	9	PRO	N-CA-C	-7.04	102.11	110.70
16	d	1	MET	CB-CG-SD	6.91	133.42	112.70
16	g	1	MET	CB-CG-SD	6.90	133.39	112.70
7	U	182	LYS	CB-CG-CD	6.88	127.14	111.30
7	G	182	LYS	CB-CG-CD	6.88	127.12	111.30
2	B	180	LYS	CB-CG-CD	6.85	127.05	111.30
2	P	180	LYS	CB-CG-CD	6.84	127.03	111.30
16	d	151	VAL	N-CA-C	-6.65	106.31	112.43
16	g	151	VAL	N-CA-C	-6.65	106.32	112.43
10	X	99[A]	HIS	O-C-N	-6.43	114.04	122.59
10	X	99[B]	HIS	O-C-N	-6.43	114.04	122.59
10	J	99[A]	HIS	O-C-N	-6.41	114.07	122.59
10	J	99[B]	HIS	O-C-N	-6.41	114.07	122.59
11	Y	78	ARG	CB-CA-C	-6.29	98.05	109.38
15	c	54	THR	N-CA-C	-6.29	106.57	114.56
15	f	54	THR	N-CA-C	-6.28	106.58	114.56
1	A	58	GLU	CA-CB-CG	6.27	126.64	114.10
1	O	58	GLU	CA-CB-CG	6.26	126.62	114.10
1	A	176	ARG	CG-CD-NE	6.18	125.61	112.00
1	O	176	ARG	CG-CD-NE	6.16	125.56	112.00
16	d	218	LEU	CA-CB-CG	6.09	137.63	116.30
16	g	218	LEU	CA-CB-CG	6.08	137.60	116.30
10	X	97	PRO	N-CA-CB	-6.02	96.93	103.25
10	J	97	PRO	N-CA-CB	-6.00	96.95	103.25
2	B	63	GLU	N-CA-C	-5.91	107.30	114.75
2	P	63	GLU	N-CA-C	-5.88	107.34	114.75
3	Q	233	GLU	CA-CB-CG	5.47	125.05	114.10
3	C	233	GLU	CA-CB-CG	5.46	125.02	114.10
16	d	155	ILE	CA-C-N	-5.34	113.96	122.66
16	d	155	ILE	C-N-CA	-5.34	113.96	122.66
7	G	191	PHE	N-CA-C	-5.33	108.03	114.75
7	U	191	PHE	N-CA-C	-5.32	108.04	114.75
16	g	155	ILE	CA-C-N	-5.32	113.99	122.66
16	g	155	ILE	C-N-CA	-5.32	113.99	122.66
1	A	58	GLU	CB-CG-CD	5.17	121.39	112.60
1	O	58	GLU	CB-CG-CD	5.17	121.38	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	92	LEU	N-CA-C	-5.13	106.23	113.20
10	J	92	LEU	N-CA-C	-5.11	106.25	113.20
11	Y	59	GLY	CA-C-O	-5.06	116.92	121.47
11	K	59	GLY	CA-C-O	-5.04	116.93	121.47

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	122	ASN	Peptide
3	C	16	LEU	Peptide
3	C	4	ASP	Peptide
5	E	226	ASP	Peptide
8	H	15	SER	Peptide
8	H	16	PHE	Peptide
8	H	32	ARG	Sidechain
8	H	35	LYS	Peptide
8	H	38	LYS	Peptide
10	J	93	ARG	Sidechain
10	J	95	ARG	Sidechain
11	K	76	ASP	Mainchain
3	Q	122	ASN	Peptide
3	Q	16	LEU	Peptide
3	Q	4	ASP	Peptide
5	S	226	ASP	Peptide
8	V	15	SER	Peptide
8	V	16	PHE	Peptide
8	V	32	ARG	Sidechain
8	V	35	LYS	Peptide
8	V	38	LYS	Peptide
10	X	93	ARG	Sidechain
10	X	95	ARG	Sidechain
11	Y	27	LEU	Mainchain
15	c	115	SER	Peptide
17	e	32	ARG	Sidechain
15	f	115	SER	Peptide
17	h	32	ARG	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	1760	0	1723	78	0
1	O	1760	0	1723	76	0
2	B	1894	0	1863	89	0
2	P	1894	0	1863	88	0
3	C	1849	0	1819	93	0
3	Q	1849	0	1819	92	0
4	D	1840	0	1828	81	0
4	R	1840	0	1828	82	0
5	E	1859	0	1842	60	0
5	S	1859	0	1842	64	0
6	F	1858	0	1834	61	0
6	T	1858	0	1834	64	0
7	G	1893	0	1893	84	0
7	U	1893	0	1893	84	0
8	H	1984	0	1997	136	0
8	V	1984	0	1997	129	0
9	I	1576	0	1593	56	0
9	W	1576	0	1593	54	0
10	J	1581	0	1585	91	0
10	X	1581	0	1585	88	0
11	K	1737	0	1708	87	0
11	Y	1737	0	1708	80	0
12	L	1644	0	1641	38	0
12	Z	1644	0	1641	36	0
13	M	1605	0	1586	63	0
13	a	1605	0	1586	59	0
14	N	1504	0	1475	45	0
14	b	1504	0	1475	46	0
15	c	2230	0	2250	68	0
15	f	2230	0	2250	68	0
16	d	2062	0	2092	110	0
16	g	2062	0	2092	109	0
17	e	904	0	911	70	0
17	h	904	0	911	72	0
All	All	59560	0	59280	2192	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 18.

All (2192) 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)
8:H:9:PRO:CG	17:e:126:VAL:CG2	1.92	1.46
8:V:9:PRO:CG	17:h:126:VAL:CG2	1.93	1.44
8:V:9:PRO:HG3	17:h:126:VAL:CG2	0.97	1.44
8:H:9:PRO:HG3	17:e:126:VAL:CG2	0.97	1.42
10:J:92:LEU:HA	10:J:97:PRO:CG	1.50	1.41
10:X:92:LEU:HA	10:X:97:PRO:CG	1.50	1.40
8:V:9:PRO:CG	17:h:126:VAL:HG22	1.55	1.33
10:J:92:LEU:CA	10:J:97:PRO:HG3	1.62	1.30
8:V:9:PRO:HD3	17:h:126:VAL:O	1.29	1.28
10:X:92:LEU:CA	10:X:97:PRO:HG3	1.62	1.27
8:H:9:PRO:HD3	17:e:126:VAL:O	1.29	1.25
8:H:9:PRO:CG	17:e:126:VAL:HG23	1.61	1.24
11:Y:228:TYR:OH	8:H:32:ARG:HD3	1.38	1.24
8:V:32:ARG:HD3	11:K:228:TYR:OH	1.37	1.22
10:X:91:CYS:O	10:X:97:PRO:HD3	1.40	1.21
8:H:9:PRO:CG	17:e:126:VAL:HG22	1.55	1.21
10:J:91:CYS:O	10:J:97:PRO:HD3	1.40	1.21
11:Y:228:TYR:OH	8:H:32:ARG:CD	1.91	1.18
8:V:32:ARG:CD	11:K:228:TYR:OH	1.91	1.16
8:V:28:ASP:HA	8:V:34:TYR:HA	1.19	1.15
8:H:28:ASP:HA	8:H:34:TYR:HA	1.19	1.15
5:E:94:ASP:OD2	11:K:32:PRO:O	1.65	1.13
5:S:94:ASP:OD2	11:Y:32:PRO:O	1.65	1.13
8:V:9:PRO:CG	17:h:126:VAL:HG23	1.61	1.13
8:H:28:ASP:HA	8:H:34:TYR:CA	1.83	1.08
8:V:28:ASP:HA	8:V:34:TYR:CA	1.84	1.07
8:H:9:PRO:CD	17:e:126:VAL:O	2.05	1.04
8:V:9:PRO:CD	17:h:126:VAL:O	2.05	1.04
10:X:46[A]:CYS:SG	10:X:100:VAL:CG1	2.46	1.03
10:J:46[A]:CYS:SG	10:J:100:VAL:CG1	2.47	1.03
2:B:174:MET:O	2:B:178:ASP:HB2	1.60	1.02
2:B:201:MET:HE1	2:B:206:LEU:HB3	1.42	1.00
2:P:174:MET:O	2:P:178:ASP:HB2	1.60	0.99
2:P:201:MET:HE1	2:P:206:LEU:HB3	1.42	0.99
10:J:91:CYS:O	10:J:97:PRO:CD	2.10	0.99
10:X:91:CYS:O	10:X:97:PRO:CD	2.10	0.98
8:V:9:PRO:HG3	17:h:126:VAL:HG23	0.98	0.97
12:Z:212:GLU:OE2	8:H:72:LYS:CD	2.13	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:152:GLN:OE1	16:d:156:LYS:NZ	1.99	0.96
11:Y:28:LEU:HD11	13:a:144:ARG:HD3	1.47	0.96
8:H:9:PRO:CD	17:e:126:VAL:HG23	1.95	0.95
8:V:9:PRO:HG2	17:h:124:SER:O	1.66	0.95
8:V:72:LYS:CD	12:L:212:GLU:OE2	2.14	0.95
3:C:7:ILE:HD12	3:C:18:GLN:HB2	1.48	0.95
3:Q:7:ILE:HD12	3:Q:18:GLN:HB2	1.48	0.95
8:V:9:PRO:CD	17:h:126:VAL:HG23	1.95	0.95
14:N:35:THR:N	14:N:204:SER:HG	1.63	0.95
8:H:9:PRO:HG3	17:e:126:VAL:HG23	0.98	0.94
16:g:152:GLN:OE1	16:g:156:LYS:NZ	1.99	0.94
8:H:9:PRO:HG2	17:e:124:SER:O	1.66	0.94
8:V:28:ASP:CA	8:V:34:TYR:HA	1.99	0.92
14:b:35:THR:N	14:b:204:SER:HG	1.66	0.92
8:H:28:ASP:CA	8:H:34:TYR:HA	1.99	0.92
16:d:32:MET:HA	16:d:35:ILE:HG23	1.53	0.90
1:A:38:LYS:NZ	2:B:57:ASP:OD2	2.05	0.90
1:O:38:LYS:NZ	2:P:57:ASP:OD2	2.05	0.89
10:J:46[A]:CYS:SG	10:J:100:VAL:HG11	2.13	0.88
10:X:46[A]:CYS:SG	10:X:100:VAL:HG11	2.13	0.88
12:Z:212:GLU:OE2	8:H:72:LYS:HD2	1.74	0.88
11:K:29:ASP:HB2	13:M:147:LYS:NZ	1.88	0.88
15:f:195:GLN:OE1	15:f:224:GLN:NE2	2.07	0.87
16:g:32:MET:HA	16:g:35:ILE:HG23	1.53	0.87
1:O:58:GLU:OE1	1:O:58:GLU:N	2.07	0.87
13:a:194:LEU:CD1	8:H:179:ALA:HB1	2.05	0.87
1:A:58:GLU:OE1	1:A:58:GLU:N	2.07	0.86
15:c:195:GLN:OE1	15:c:224:GLN:NE2	2.07	0.86
8:V:32:ARG:HD2	11:K:228:TYR:OH	1.75	0.86
8:V:179:ALA:HB1	13:M:194:LEU:CD1	2.06	0.85
11:Y:28:LEU:HD11	13:a:144:ARG:HH11	1.39	0.85
8:V:72:LYS:HD2	12:L:212:GLU:OE2	1.75	0.85
3:Q:7:ILE:HD11	3:Q:19:VAL:HG23	1.58	0.84
14:b:196:LEU:HD11	14:N:175:ALA:HB2	1.57	0.84
3:C:7:ILE:HD11	3:C:19:VAL:HG23	1.58	0.84
10:J:59:TYR:HD1	17:e:31:LEU:HD22	1.42	0.84
16:d:104:GLU:N	16:d:104:GLU:OE1	2.10	0.84
10:X:98:TYR:HB2	10:X:100:VAL:HG23	1.59	0.84
1:O:94:GLN:NE2	8:V:107:GLU:OE2	2.11	0.84
11:Y:228:TYR:OH	8:H:32:ARG:HD2	1.75	0.84
14:b:175:ALA:HB2	14:N:196:LEU:HD11	1.57	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLN:NE2	8:H:107:GLU:OE2	2.11	0.83
16:g:104:GLU:N	16:g:104:GLU:OE1	2.10	0.83
11:Y:28:LEU:HD22	13:a:107:TYR:HE2	1.44	0.83
8:H:35:LYS:HD3	9:I:7:GLY:H	1.43	0.83
6:F:70:ASP:OD1	6:F:71:ARG:N	2.12	0.83
10:X:59:TYR:HD1	17:h:31:LEU:HD22	1.42	0.83
8:V:35:LYS:HG3	8:V:36:LEU:H	1.44	0.82
2:B:218:ARG:NH1	2:B:223:THR:OG1	2.11	0.82
2:P:218:ARG:NH1	2:P:223:THR:OG1	2.12	0.82
8:V:72:LYS:HD3	12:L:212:GLU:OE2	1.79	0.82
7:U:189:TRP:HA	7:U:193:GLN:HB2	1.61	0.82
1:A:11:THR:HA	2:B:20:GLN:HE22	1.45	0.82
10:J:98:TYR:HB2	10:J:100:VAL:HG23	1.59	0.82
3:Q:124:ARG:HH12	17:h:140:LEU:HD22	1.45	0.82
3:C:124:ARG:HH12	17:e:140:LEU:HD22	1.45	0.82
10:X:52:ASP:HB3	10:X:98:TYR:HB3	1.61	0.82
3:C:231:GLU:HA	3:C:234:LYS:HB2	1.62	0.82
8:V:35:LYS:HD3	9:W:7:GLY:H	1.43	0.82
12:Z:212:GLU:OE2	8:H:72:LYS:HD3	1.77	0.82
10:J:46[A]:CYS:SG	10:J:100:VAL:HG13	2.20	0.81
3:Q:220:LEU:HD22	3:Q:227:LYS:HD2	1.63	0.81
10:J:52:ASP:HB3	10:J:98:TYR:HB3	1.61	0.81
6:T:70:ASP:OD1	6:T:71:ARG:N	2.12	0.81
8:H:35:LYS:HG3	8:H:36:LEU:H	1.44	0.81
13:a:223:TYR:CD2	8:H:182:GLU:OE2	2.34	0.80
3:Q:231:GLU:HA	3:Q:234:LYS:HB2	1.62	0.80
7:G:189:TRP:HA	7:G:193:GLN:HB2	1.61	0.80
16:d:3:VAL:HG23	16:d:46:TYR:HB2	1.64	0.80
8:V:9:PRO:HG3	17:h:126:VAL:HG22	0.80	0.80
1:O:11:THR:HA	2:P:20:GLN:HE22	1.45	0.80
3:C:220:LEU:HD22	3:C:227:LYS:HD2	1.63	0.80
8:H:9:PRO:HG3	17:e:126:VAL:HG22	0.80	0.80
11:K:29:ASP:HB2	13:M:147:LYS:HZ3	1.46	0.79
16:g:3:VAL:HG23	16:g:46:TYR:HB2	1.64	0.79
8:H:20:ARG:HH12	17:e:41:GLU:HG2	1.47	0.79
10:X:44:LEU:HD11	10:X:102:LEU:HD23	1.64	0.79
8:V:182:GLU:OE2	13:M:223:TYR:CD2	2.35	0.79
10:X:46[A]:CYS:SG	10:X:100:VAL:HG13	2.20	0.79
6:F:50:GLU:OE2	6:F:201:HIS:ND1	2.16	0.79
2:P:143:TYR:HB2	2:P:146:GLN:HE21	1.47	0.78
8:V:20:ARG:HH12	17:h:41:GLU:HG2	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:180:LYS:HA	2:P:180:LYS:HE3	1.66	0.78
4:R:236:GLU:HA	4:R:239:LYS:HE3	1.65	0.78
2:P:8:ARG:HD2	2:P:11:ILE:HD11	1.66	0.78
3:Q:185:ASP:OD1	3:Q:234:LYS:NZ	2.17	0.78
6:T:50:GLU:OE2	6:T:201:HIS:ND1	2.16	0.78
7:U:240:VAL:O	7:U:244:GLU:N	2.13	0.78
1:A:204:GLU:HB3	1:A:205:ASP:OD1	1.83	0.78
1:O:7:PHE:HB3	15:f:9:VAL:HG11	1.66	0.78
16:g:130:ASN:OD1	16:g:133:GLN:NE2	2.17	0.78
8:H:259:ILE:HD11	9:I:193:LYS:HD2	1.65	0.78
1:A:7:PHE:HB3	15:c:9:VAL:HG11	1.66	0.78
8:V:32:ARG:HD3	11:K:228:TYR:HH	1.47	0.78
8:V:241:ARG:NH1	9:W:151:SER:O	2.17	0.78
10:J:44:LEU:HD11	10:J:102:LEU:HD23	1.64	0.77
5:S:226:ASP:O	5:S:228:ASP:N	2.18	0.77
13:a:194:LEU:HD13	8:H:179:ALA:HB1	1.65	0.77
5:E:226:ASP:O	5:E:228:ASP:N	2.18	0.77
16:d:130:ASN:OD1	16:d:133:GLN:NE2	2.17	0.77
2:B:180:LYS:HA	2:B:180:LYS:HE3	1.66	0.77
3:C:185:ASP:OD1	3:C:234:LYS:NZ	2.17	0.77
11:Y:30:LEU:HD21	13:a:136:TRP:CD1	2.20	0.77
8:V:101:LEU:HD22	8:V:129:MET:HE1	1.66	0.77
1:O:204:GLU:HB3	1:O:205:ASP:OD1	1.83	0.77
8:V:259:ILE:HD11	9:W:193:LYS:HD2	1.65	0.77
10:J:59:TYR:CD1	17:e:31:LEU:CD2	2.68	0.77
8:V:179:ALA:HB1	13:M:194:LEU:HD13	1.66	0.76
8:H:101:LEU:HD22	8:H:129:MET:HE1	1.66	0.76
2:P:4:ARG:HG2	3:Q:5:ARG:HE	1.49	0.76
7:U:112:ASP:OD2	8:V:115:ARG:NH2	2.17	0.76
10:X:59:TYR:CD1	17:h:31:LEU:CD2	2.68	0.76
7:G:112:ASP:OD2	8:H:115:ARG:NH2	2.17	0.76
8:H:241:ARG:NH1	9:I:151:SER:O	2.17	0.76
2:B:143:TYR:HB2	2:B:146:GLN:HE21	1.47	0.76
4:R:20:ARG:HB3	15:f:288:THR:HG23	1.68	0.75
16:d:143:LEU:HB3	16:d:147:MET:HB3	1.67	0.75
4:D:20:ARG:HB3	15:c:288:THR:HG23	1.68	0.75
2:B:8:ARG:HD2	2:B:11:ILE:HD11	1.66	0.75
12:Z:185:ASN:ND2	9:I:171:LEU:HB3	2.02	0.75
11:K:28:LEU:HD21	13:M:144:ARG:HH11	1.51	0.75
7:G:182:LYS:HE2	7:G:182:LYS:HA	1.69	0.75
4:R:118:ASN:OD1	5:S:82:ARG:NH2	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:GLU:HA	4:D:239:LYS:HE3	1.66	0.75
5:S:140:MET:HE1	13:a:125:GLY:HA3	1.68	0.74
8:H:40:ARG:NE	8:H:65:GLU:OE2	2.19	0.74
10:X:59:TYR:HD1	17:h:31:LEU:CD2	2.00	0.74
6:F:108:LEU:HD23	6:F:147:GLN:HB2	1.69	0.74
1:O:140:GLU:OE1	1:O:140:GLU:N	2.21	0.74
8:V:40:ARG:NE	8:V:65:GLU:OE2	2.19	0.74
2:B:4:ARG:HG2	3:C:5:ARG:HE	1.49	0.74
4:D:118:ASN:OD1	5:E:82:ARG:NH2	2.19	0.74
9:W:65:ARG:NH1	10:X:86:ARG:HH22	1.86	0.74
16:g:143:LEU:HB3	16:g:147:MET:HB3	1.67	0.74
7:U:6:SER:HB3	7:U:11:ARG:HB3	1.68	0.74
1:A:140:GLU:OE1	1:A:140:GLU:N	2.21	0.74
16:d:63:THR:HG23	16:d:64:THR:HG23	1.70	0.74
8:V:257:GLU:OE1	9:W:197:ARG:NH1	2.20	0.74
9:W:171:LEU:HB3	12:L:185:ASN:ND2	2.03	0.74
10:X:92:LEU:HA	10:X:97:PRO:HG3	0.77	0.74
5:E:140:MET:HE1	13:M:125:GLY:HA3	1.68	0.74
7:G:6:SER:HB3	7:G:11:ARG:HB3	1.68	0.73
15:c:192:LEU:HD21	15:c:206:LEU:HB3	1.70	0.73
15:f:192:LEU:HD21	15:f:206:LEU:HB3	1.71	0.73
8:H:257:GLU:OE1	9:I:197:ARG:NH1	2.20	0.73
16:g:63:THR:HG23	16:g:64:THR:HG23	1.70	0.73
7:U:182:LYS:HE2	7:U:182:LYS:HA	1.69	0.73
11:Y:59:GLY:HA2	11:Y:92:LYS:HZ2	1.52	0.73
3:C:36:ARG:HH21	3:C:157:LYS:HG2	1.54	0.73
10:J:92:LEU:HA	10:J:97:PRO:HG3	0.77	0.72
4:R:178:GLN:HG2	15:f:282:ILE:HG13	1.71	0.72
9:I:65:ARG:NH1	10:J:86:ARG:HH22	1.86	0.72
6:T:108:LEU:HD23	6:T:147:GLN:HB2	1.69	0.72
8:H:186:ARG:H	8:H:189:MET:HE3	1.54	0.72
1:O:88:ARG:NH1	17:h:103:ASP:OD2	2.23	0.72
7:U:141:ILE:HG22	7:U:151:VAL:HG22	1.72	0.72
1:A:88:ARG:NH1	17:e:103:ASP:OD2	2.23	0.72
11:Y:29:ASP:HB3	13:a:143:SER:OG	1.89	0.72
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.72	0.72
11:K:59:GLY:HA2	11:K:92:LYS:NZ	2.05	0.72
11:K:59:GLY:HA2	11:K:92:LYS:HZ1	1.54	0.71
14:b:161:ILE:HD11	14:b:170:TYR:CD1	2.25	0.71
14:N:161:ILE:HD11	14:N:170:TYR:CD1	2.25	0.71
6:T:120:HIS:NE2	7:U:86:ASP:OD1	2.17	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:GLU:O	4:D:239:LYS:NZ	2.22	0.71
10:J:59:TYR:HD1	17:e:31:LEU:CD2	2.00	0.71
16:d:77:VAL:HG22	16:d:88:LEU:HD12	1.72	0.71
3:Q:36:ARG:HH21	3:Q:157:LYS:HG2	1.54	0.71
16:g:77:VAL:HG22	16:g:88:LEU:HD12	1.73	0.71
7:U:49:VAL:HG22	7:U:219:VAL:HG12	1.73	0.71
8:V:186:ARG:H	8:V:189:MET:HE3	1.54	0.70
7:G:49:VAL:HG22	7:G:219:VAL:HG12	1.73	0.70
16:g:38:THR:HA	16:g:246:LYS:HB2	1.72	0.70
14:N:38:MET:HE2	14:N:190:THR:HG23	1.74	0.70
7:U:49:VAL:HG11	7:U:195:VAL:HG12	1.73	0.70
4:D:178:GLN:HG2	15:c:282:ILE:HG13	1.71	0.70
14:b:38:MET:HE2	14:b:190:THR:HG23	1.73	0.70
13:M:117:ILE:HA	13:M:120:GLU:HG2	1.72	0.70
3:Q:124:ARG:NH1	17:h:140:LEU:HD22	2.07	0.70
8:V:243:GLY:N	12:L:205:ASP:OD2	2.17	0.70
10:J:95:ARG:O	10:J:96:THR:C	2.35	0.70
11:Y:59:GLY:HA2	11:Y:92:LYS:NZ	2.05	0.70
3:C:124:ARG:NH1	17:e:140:LEU:HD22	2.07	0.69
6:F:120:HIS:NE2	7:G:86:ASP:OD1	2.17	0.69
10:X:95:ARG:O	10:X:96:THR:C	2.35	0.69
16:d:38:THR:HA	16:d:246:LYS:HB2	1.72	0.69
14:N:213:ILE:HG12	14:N:218:VAL:HG12	1.74	0.69
2:P:151:ASP:OD1	2:P:151:ASP:N	2.25	0.69
5:S:18:ARG:NH1	16:g:258:GLY:O	2.26	0.69
15:c:155:GLY:O	15:c:222:TYR:OH	2.10	0.69
13:M:131:ARG:NH1	13:M:178:GLU:OE2	2.25	0.69
2:B:124:PHE:HB2	3:C:124:ARG:HG3	1.75	0.69
2:B:200:THR:O	2:B:200:THR:OG1	2.11	0.69
16:d:228:LEU:HB3	16:d:230:ILE:HG23	1.75	0.69
9:W:33:MET:O	11:K:225:ARG:NH1	2.26	0.69
13:a:131:ARG:NH1	13:a:178:GLU:OE2	2.25	0.69
7:G:49:VAL:HG11	7:G:195:VAL:HG12	1.73	0.69
17:e:93:PRO:HD2	17:e:134:VAL:HG23	1.75	0.69
2:B:151:ASP:OD1	2:B:151:ASP:N	2.25	0.69
5:E:18:ARG:NH1	16:d:258:GLY:O	2.26	0.69
2:P:124:PHE:HB2	3:Q:124:ARG:HG3	1.75	0.68
14:b:213:ILE:HG12	14:b:218:VAL:HG12	1.74	0.68
16:g:228:LEU:HB3	16:g:230:ILE:HG23	1.75	0.68
14:b:161:ILE:HD11	14:b:170:TYR:HD1	1.57	0.68
16:g:215:PRO:HA	16:g:218:LEU:HD12	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD13	1:A:112:ARG:HB3	1.76	0.68
7:G:240:VAL:O	7:G:244:GLU:N	2.13	0.68
16:d:215:PRO:HA	16:d:218:LEU:HD12	1.75	0.68
1:O:205:ASP:OD1	1:O:205:ASP:N	2.26	0.68
3:Q:117:ARG:HE	17:h:140:LEU:HD21	1.59	0.68
11:Y:30:LEU:O	11:Y:31:GLY:C	2.37	0.68
12:Z:205:ASP:OD2	8:H:243:GLY:N	2.17	0.68
15:f:155:GLY:O	15:f:222:TYR:OH	2.10	0.68
13:a:117:ILE:HA	13:a:120:GLU:HG2	1.72	0.68
13:M:78:LEU:HD21	14:N:170:TYR:HE2	1.59	0.68
2:P:108:GLU:OE2	3:Q:57:ARG:NH1	2.22	0.68
5:E:189:LYS:NZ	5:E:234:GLU:O	2.27	0.68
8:V:43:GLY:HA3	8:V:89:ALA:HA	1.76	0.68
1:A:6:SER:HA	1:A:19:VAL:HG21	1.76	0.68
5:E:13:TRP:H	6:F:22:GLN:HE22	1.41	0.68
1:O:99:VAL:HA	9:W:92:ASN:ND2	2.09	0.68
16:d:111:LYS:HE3	16:d:199:ILE:HD11	1.75	0.68
4:R:236:GLU:O	4:R:239:LYS:NZ	2.22	0.68
16:g:111:LYS:HE3	16:g:199:ILE:HD11	1.75	0.68
2:P:61:PHE:O	2:P:61:PHE:HD1	1.77	0.67
11:Y:225:ARG:NH1	9:I:33:MET:O	2.27	0.67
4:R:220:VAL:HG12	4:R:226:PHE:HA	1.76	0.67
13:a:78:LEU:HD21	14:b:170:TYR:HE2	1.59	0.67
3:C:117:ARG:HE	17:e:140:LEU:HD21	1.59	0.67
4:R:17:PRO:O	4:R:18:GLU:HG3	1.95	0.67
2:B:118:LYS:NZ	2:B:150:SER:OG	2.27	0.67
4:D:220:VAL:HG12	4:D:226:PHE:HA	1.76	0.67
8:V:43:GLY:HA2	8:V:76:LYS:HD3	1.76	0.67
17:h:93:PRO:HD2	17:h:134:VAL:HG23	1.75	0.67
6:F:12:SER:HA	7:G:132:ARG:HD3	1.77	0.67
5:S:189:LYS:NZ	5:S:234:GLU:O	2.27	0.67
8:V:35:LYS:HE3	9:W:5:TYR:HB3	1.77	0.67
1:A:99:VAL:HA	9:I:92:ASN:ND2	2.09	0.67
8:H:35:LYS:HE3	9:I:5:TYR:HB3	1.77	0.67
14:N:161:ILE:HD11	14:N:170:TYR:HD1	1.57	0.67
17:e:77:LEU:O	17:e:81:MET:HB2	1.95	0.67
2:B:49:ARG:NH2	2:B:63:GLU:OE2	2.28	0.66
2:B:61:PHE:HD1	2:B:61:PHE:O	1.77	0.66
11:Y:67:PHE:HE2	11:Y:69:HIS:HB2	1.60	0.66
2:B:108:GLU:OE2	3:C:57:ARG:NH1	2.22	0.66
2:P:49:ARG:NH2	2:P:63:GLU:OE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:GLY:HA3	8:H:89:ALA:HA	1.76	0.66
1:O:92:LEU:HD13	1:O:112:ARG:HB3	1.76	0.66
4:R:231:LYS:NZ	4:R:235:GLU:OE2	2.29	0.66
5:S:13:TRP:H	6:T:22:GLN:HE22	1.41	0.66
6:T:12:SER:HA	7:U:132:ARG:HD3	1.77	0.66
8:V:39:VAL:HG23	8:V:40:ARG:H	1.59	0.66
17:h:77:LEU:O	17:h:81:MET:HB2	1.94	0.66
11:K:67:PHE:HE2	11:K:69:HIS:HB2	1.60	0.66
2:P:118:LYS:NZ	2:P:150:SER:OG	2.27	0.66
7:U:202:LEU:O	7:U:206:LEU:HB2	1.96	0.66
9:W:65:ARG:HH12	10:X:86:ARG:HH22	1.43	0.66
1:A:158:LYS:NZ	2:B:56:LEU:O	2.28	0.66
16:d:16:THR:HG23	16:d:117:ARG:HB2	1.78	0.66
1:O:6:SER:HA	1:O:19:VAL:HG21	1.76	0.66
4:D:17:PRO:O	4:D:18:GLU:HG3	1.95	0.66
4:D:207:GLU:HA	4:D:207:GLU:OE2	1.95	0.66
8:H:39:VAL:HG23	8:H:40:ARG:H	1.59	0.66
5:E:60:GLN:HG3	5:E:61:LYS:H	1.60	0.66
8:H:43:GLY:HA2	8:H:76:LYS:HD3	1.76	0.66
4:R:207:GLU:HA	4:R:207:GLU:OE2	1.95	0.65
7:G:89:SER:OG	17:e:78:LYS:NZ	2.29	0.65
10:J:13:VAL:HG11	10:J:105:ALA:HB1	1.78	0.65
5:S:60:GLN:HG3	5:S:61:LYS:H	1.60	0.65
4:D:231:LYS:NZ	4:D:235:GLU:OE2	2.29	0.65
11:K:172:TYR:CE1	11:K:187:VAL:HG11	2.31	0.65
17:e:45:SER:HB3	17:e:49:GLU:HG3	1.79	0.65
8:V:179:ALA:HB1	13:M:194:LEU:HD11	1.78	0.65
11:Y:172:TYR:CE1	11:Y:187:VAL:HG11	2.31	0.65
4:D:11:GLY:O	4:D:14:THR:OG1	2.14	0.65
4:D:41:GLN:NE2	4:D:151:PRO:O	2.29	0.65
1:O:158:LYS:NZ	2:P:56:LEU:O	2.28	0.65
1:A:205:ASP:OD1	1:A:205:ASP:N	2.26	0.65
4:R:11:GLY:O	4:R:14:THR:OG1	2.14	0.65
7:G:13:ILE:HD11	7:G:133:PRO:HD3	1.79	0.65
4:R:71:ASP:OD1	4:R:72:ALA:N	2.29	0.65
17:h:45:SER:HB3	17:h:49:GLU:HG3	1.79	0.65
15:c:77:ASN:HA	15:c:80:VAL:HG22	1.79	0.65
3:Q:170:GLU:HA	3:Q:173:GLU:HG2	1.79	0.65
7:U:13:ILE:HD11	7:U:133:PRO:HD3	1.78	0.65
5:E:26:MET:HE2	5:E:150:SER:HB3	1.79	0.65
9:I:65:ARG:HH12	10:J:86:ARG:HH22	1.43	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:41:GLN:NE2	4:R:151:PRO:O	2.29	0.65
8:V:28:ASP:HA	8:V:34:TYR:CB	2.26	0.64
2:B:86:LEU:HD22	2:B:114:LEU:HD11	1.79	0.64
10:X:92:LEU:HA	10:X:97:PRO:CD	2.27	0.64
16:g:16:THR:HG23	16:g:117:ARG:HB2	1.78	0.64
3:C:170:GLU:HA	3:C:173:GLU:HG2	1.79	0.64
10:J:29:LYS:HE2	11:K:180:ILE:HB	1.80	0.64
10:J:92:LEU:CA	10:J:97:PRO:CG	2.45	0.64
1:A:21:ILE:HG21	1:A:151:SER:HB3	1.78	0.64
4:D:71:ASP:OD1	4:D:72:ALA:N	2.29	0.64
7:U:89:SER:OG	17:h:78:LYS:NZ	2.29	0.64
7:G:202:LEU:O	7:G:206:LEU:HB2	1.96	0.64
11:Y:28:LEU:CD1	13:a:144:ARG:HH11	2.09	0.64
1:O:21:ILE:HG21	1:O:151:SER:HB3	1.78	0.64
8:V:206:ILE:HG12	8:V:213:GLY:HA2	1.79	0.64
8:H:28:ASP:HA	8:H:34:TYR:CB	2.26	0.64
8:H:206:ILE:HG12	8:H:213:GLY:HA2	1.79	0.64
1:O:176:ARG:HB3	1:O:176:ARG:NH1	2.13	0.64
12:Z:187:GLN:HG2	8:H:251:THR:O	1.98	0.64
8:V:96:ASP:O	8:V:100:GLN:HG3	1.97	0.64
8:H:96:ASP:O	8:H:100:GLN:HG3	1.97	0.64
11:K:61:THR:H	11:K:188:GLY:HA3	1.63	0.64
5:S:26:MET:HE2	5:S:150:SER:HB3	1.79	0.64
15:c:38:ARG:HD2	16:d:97:TYR:HE2	1.63	0.64
4:D:175:GLU:OE1	4:D:175:GLU:N	2.25	0.63
8:V:251:THR:O	12:L:187:GLN:HG2	1.98	0.63
11:Y:82:GLY:C	8:H:34:TYR:OH	2.42	0.63
13:a:70:ASP:HA	13:a:232:PHE:HA	1.80	0.63
15:f:38:ARG:HD2	16:g:97:TYR:HE2	1.63	0.63
2:B:4:ARG:HA	2:B:14:PRO:HD3	1.80	0.63
15:c:82:PHE:HB2	15:c:247:VAL:HG13	1.80	0.63
11:Y:61:THR:H	11:Y:188:GLY:HA3	1.63	0.63
14:b:194:LEU:O	14:b:198:MET:HG3	1.98	0.63
16:g:73:ILE:N	16:g:76:GLU:OE2	2.31	0.63
16:g:238:PRO:HG3	16:g:244:ARG:NH1	2.14	0.63
11:K:28:LEU:HD22	13:M:107:TYR:HE2	1.63	0.63
10:X:13:VAL:HG11	10:X:105:ALA:HB1	1.78	0.63
10:X:29:LYS:HE2	11:Y:180:ILE:HB	1.80	0.63
2:B:239:LYS:HA	2:B:242:GLU:OE2	1.99	0.63
6:F:237:LYS:HA	6:F:237:LYS:HE3	1.79	0.63
8:H:18:ASN:H	10:J:93:ARG:HB3	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:250:THR:HG22	13:M:252:THR:HG22	1.79	0.63
2:P:180:LYS:HA	2:P:180:LYS:CE	2.29	0.63
15:f:18:THR:HG21	16:g:183:GLY:HA2	1.80	0.63
16:d:248:PRO:HG2	16:d:251:TRP:CD1	2.34	0.63
2:P:86:LEU:HD22	2:P:114:LEU:HD11	1.79	0.63
6:T:198:TYR:OH	6:T:236:GLU:OE2	2.16	0.63
9:W:26:ARG:HG3	9:W:182:MET:HG3	1.81	0.63
2:B:241:GLU:OE1	2:B:241:GLU:HA	1.98	0.63
10:J:91:CYS:HB3	10:J:95:ARG:HH12	1.64	0.63
16:d:238:PRO:HG3	16:d:244:ARG:NH1	2.14	0.63
8:V:18:ASN:H	10:X:93:ARG:HB3	1.63	0.63
8:H:241:ARG:NH2	9:I:154:GLU:OE1	2.32	0.63
11:K:29:ASP:HB2	13:M:147:LYS:HZ1	1.64	0.63
2:P:239:LYS:HA	2:P:242:GLU:OE2	1.99	0.63
8:V:34:TYR:OH	11:K:82:GLY:C	2.42	0.63
13:a:238:THR:HG23	13:a:240:LYS:H	1.64	0.63
13:a:250:THR:HG22	13:a:252:THR:HG22	1.79	0.63
6:F:198:TYR:OH	6:F:236:GLU:OE2	2.16	0.63
8:V:241:ARG:NH2	9:W:154:GLU:OE1	2.32	0.62
12:L:153:ASP:OD1	12:L:157:SER:N	2.26	0.62
2:P:241:GLU:HA	2:P:241:GLU:OE1	1.98	0.62
11:Y:193:TYR:HB3	10:J:141:SER:OG	1.99	0.62
13:a:194:LEU:HD11	8:H:179:ALA:HB1	1.78	0.62
15:f:82:PHE:HB2	15:f:247:VAL:HG13	1.80	0.62
3:C:145:TYR:CE2	3:C:155:ALA:HB2	2.34	0.62
15:f:121:CYS:H	15:f:137:CYS:HA	1.65	0.62
15:c:18:THR:HG21	16:d:183:GLY:HA2	1.80	0.62
1:A:176:ARG:NH1	1:A:176:ARG:HB3	2.13	0.62
13:M:70:ASP:HA	13:M:232:PHE:HA	1.81	0.62
2:P:4:ARG:HA	2:P:14:PRO:HD3	1.80	0.62
15:f:77:ASN:HA	15:f:80:VAL:HG22	1.79	0.62
14:N:194:LEU:O	14:N:198:MET:HG3	1.98	0.62
16:d:73:ILE:N	16:d:76:GLU:OE2	2.31	0.62
15:f:218:ALA:HB2	16:g:54:PRO:HG3	1.82	0.62
3:Q:145:TYR:CE2	3:Q:155:ALA:HB2	2.34	0.62
5:S:160:SER:O	5:S:169:ARG:NH1	2.33	0.62
11:Y:63:LEU:HD12	11:Y:194:ALA:HB1	1.82	0.62
5:E:81:ALA:HB2	5:E:130:VAL:HG21	1.82	0.62
11:K:27:LEU:HD12	11:K:28:LEU:O	2.00	0.62
6:T:237:LYS:HA	6:T:237:LYS:HE3	1.79	0.62
2:P:200:THR:O	2:P:200:THR:OG1	2.11	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:224:GLN:OE1	4:R:224:GLN:N	2.33	0.61
12:Z:153:ASP:OD1	12:Z:157:SER:N	2.26	0.61
4:D:224:GLN:OE1	4:D:224:GLN:N	2.33	0.61
5:E:76:GLY:HA3	5:E:130:VAL:HA	1.82	0.61
11:K:63:LEU:HD12	11:K:194:ALA:HB1	1.82	0.61
16:g:248:PRO:HG2	16:g:251:TRP:CD1	2.34	0.61
10:J:92:LEU:HA	10:J:97:PRO:CD	2.27	0.61
5:E:160:SER:O	5:E:169:ARG:NH1	2.33	0.61
8:H:182:GLU:OE2	14:N:63:ARG:NH1	2.33	0.61
10:X:39:SER:OG	10:X:40:GLU:N	2.32	0.61
2:B:180:LYS:HA	2:B:180:LYS:CE	2.29	0.61
3:Q:103:THR:HG22	3:Q:105:GLU:H	1.65	0.61
5:E:184:LEU:HD11	5:E:214:ILE:HD13	1.83	0.61
6:F:161:TRP:CE2	6:F:182:LYS:HE3	2.36	0.61
13:M:238:THR:HG23	13:M:240:LYS:H	1.64	0.61
4:D:51:GLU:HA	4:D:215:ILE:HG22	1.83	0.61
15:c:218:ALA:HB2	16:d:54:PRO:HG3	1.82	0.61
4:R:51:GLU:HA	4:R:215:ILE:HG22	1.83	0.61
10:X:91:CYS:HB3	10:X:95:ARG:HH12	1.64	0.61
10:X:141:SER:OG	11:K:193:TYR:HB3	2.00	0.61
14:N:38:MET:HG3	14:N:161:ILE:HG22	1.81	0.61
16:d:31:ALA:HA	16:d:34:LEU:HD12	1.82	0.61
1:O:198:PHE:HZ	1:O:206:ASN:HD22	1.49	0.61
10:J:39:SER:OG	10:J:40:GLU:N	2.32	0.61
5:S:76:GLY:HA3	5:S:130:VAL:HA	1.82	0.61
6:T:161:TRP:CE2	6:T:182:LYS:HE3	2.36	0.61
8:V:182:GLU:OE2	14:b:63:ARG:NH1	2.33	0.61
14:b:38:MET:HG3	14:b:161:ILE:HG22	1.81	0.61
3:Q:115:LYS:NZ	3:Q:129:ILE:HG13	2.16	0.61
16:d:52:LEU:HD11	16:d:90:LEU:HD22	1.82	0.61
7:U:21:ARG:HH22	16:g:135:ARG:NH2	1.99	0.60
3:C:115:LYS:NZ	3:C:129:ILE:HG13	2.16	0.60
3:Q:96:LEU:CD2	17:h:31:LEU:HB3	2.31	0.60
9:W:11:MET:HG2	9:W:170:MET:HE3	1.82	0.60
14:b:73:ASP:OD1	14:b:74:ARG:N	2.34	0.60
3:C:103:THR:HG22	3:C:105:GLU:H	1.65	0.60
15:f:192:LEU:HB2	15:f:232:LEU:HB3	1.83	0.60
1:A:99:VAL:HA	9:I:92:ASN:HD22	1.65	0.60
3:C:96:LEU:CD2	17:e:31:LEU:HB3	2.31	0.60
9:I:26:ARG:HG3	9:I:182:MET:HG3	1.81	0.60
11:K:28:LEU:HD21	13:M:144:ARG:NH1	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:73:ASP:OD1	14:N:74:ARG:N	2.34	0.60
2:B:201:MET:HE1	2:B:206:LEU:CB	2.25	0.60
5:E:74:ILE:HG21	5:E:81:ALA:HB1	1.84	0.60
7:G:193:GLN:H	7:G:193:GLN:CD	2.10	0.60
15:c:192:LEU:HB2	15:c:232:LEU:HB3	1.83	0.60
7:U:193:GLN:H	7:U:193:GLN:CD	2.10	0.60
11:K:30:LEU:O	11:K:31:GLY:C	2.43	0.60
15:c:121:CYS:H	15:c:137:CYS:HA	1.65	0.60
4:R:157:ASP:O	4:R:159:SER:N	2.31	0.60
3:C:220:LEU:O	3:C:228:TYR:OH	2.14	0.60
4:D:163:VAL:HG23	4:D:165:CYS:HB3	1.83	0.60
16:g:31:ALA:HA	16:g:34:LEU:HD12	1.82	0.60
16:g:52:LEU:HD11	16:g:90:LEU:HD22	1.82	0.60
12:Z:55:THR:OG1	12:Z:220:ALA:HB3	2.02	0.60
15:f:286:ILE:HG23	15:f:288:THR:H	1.67	0.60
4:D:157:ASP:O	4:D:159:SER:N	2.31	0.60
4:R:6:SER:HG	4:R:8:TYR:HE1	1.50	0.60
4:R:76:CYS:SG	4:R:141:LEU:HD23	2.42	0.60
5:S:81:ALA:HB2	5:S:130:VAL:HG21	1.82	0.60
3:C:66:ASP:OD2	3:C:95:ARG:NH2	2.35	0.60
12:L:55:THR:OG1	12:L:220:ALA:HB3	2.02	0.60
9:W:160:ASP:OD1	9:W:161:HIS:N	2.35	0.59
8:H:31:LYS:O	8:H:32:ARG:C	2.45	0.59
1:O:99:VAL:HA	9:W:92:ASN:HD22	1.65	0.59
3:Q:94:HIS:ND1	3:Q:102:VAL:HG12	2.17	0.59
4:R:163:VAL:HG23	4:R:165:CYS:HB3	1.83	0.59
2:P:68:LEU:HD12	2:P:72:MET:HE2	1.84	0.59
7:U:186:LYS:HE2	7:U:188:ASP:HB2	1.83	0.59
3:C:94:HIS:ND1	3:C:102:VAL:HG12	2.17	0.59
7:G:186:LYS:HE2	7:G:188:ASP:HB2	1.83	0.59
2:P:201:MET:HE1	2:P:206:LEU:CB	2.25	0.59
3:Q:21:TYR:O	3:Q:25:ALA:N	2.36	0.59
3:Q:66:ASP:OD2	3:Q:95:ARG:NH2	2.35	0.59
5:S:184:LEU:HD11	5:S:214:ILE:HD13	1.83	0.59
8:V:9:PRO:CG	17:h:124:SER:O	2.46	0.59
14:b:38:MET:CG	14:b:161:ILE:HG22	2.33	0.59
4:D:76:CYS:SG	4:D:141:LEU:HD23	2.42	0.59
8:H:9:PRO:CG	17:e:124:SER:O	2.46	0.59
9:I:121:CYS:SG	9:I:122:SER:N	2.76	0.59
11:Y:83:ALA:O	9:I:177:ASP:OD1	2.20	0.59
1:A:198:PHE:HZ	1:A:206:ASN:HD22	1.49	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:LEU:HD11	2:B:237:ILE:HD12	1.85	0.59
5:E:98:VAL:HG11	11:K:30:LEU:HD11	1.85	0.59
9:I:11:MET:HG2	9:I:170:MET:HE3	1.82	0.59
11:K:28:LEU:O	11:K:29:ASP:C	2.45	0.59
8:V:31:LYS:O	8:V:32:ARG:C	2.45	0.59
5:S:74:ILE:HG21	5:S:81:ALA:HB1	1.84	0.59
8:H:9:PRO:CB	17:e:126:VAL:CG2	2.78	0.59
13:M:51:VAL:HG11	14:N:153:MET:HE1	1.84	0.59
7:U:10:ASP:O	7:U:24:GLN:NE2	2.35	0.59
8:H:15:SER:OG	8:H:17:ASP:O	2.21	0.59
8:H:9:PRO:CB	17:e:126:VAL:HG22	2.30	0.58
9:I:160:ASP:OD1	9:I:161:HIS:N	2.35	0.58
2:P:238:LYS:O	2:P:242:GLU:HG3	2.04	0.58
5:S:49:LEU:HB2	5:S:195:LEU:HD21	1.85	0.58
7:G:21:ARG:HH22	16:d:135:ARG:NH2	1.99	0.58
6:T:16:PRO:HA	7:U:27:TYR:CD1	2.38	0.58
9:W:121:CYS:SG	9:W:122:SER:N	2.76	0.58
13:a:51:VAL:HG11	14:b:153:MET:HE1	1.84	0.58
16:g:100:LYS:O	16:g:104:GLU:OE1	2.20	0.58
2:B:235:GLN:O	2:B:238:LYS:HG3	2.03	0.58
11:Y:200[A]:ARG:HD3	10:J:166:GLU:HB2	1.85	0.58
7:G:10:ASP:O	7:G:24:GLN:NE2	2.35	0.58
2:P:233:VAL:O	2:P:237:ILE:HG12	2.04	0.58
8:V:15:SER:OG	8:V:17:ASP:O	2.21	0.58
6:F:16:PRO:HA	7:G:27:TYR:CD1	2.38	0.58
14:N:38:MET:CG	14:N:161:ILE:HG22	2.33	0.58
3:Q:96:LEU:HD23	17:h:31:LEU:HB3	1.86	0.58
15:c:286:ILE:HG23	15:c:288:THR:H	1.67	0.58
2:P:198:ASN:HA	2:P:201:MET:SD	2.44	0.58
10:X:92:LEU:CA	10:X:97:PRO:CG	2.45	0.58
2:B:233:VAL:O	2:B:237:ILE:HG12	2.04	0.58
3:C:158:ALA:HB1	3:C:172:LEU:HD21	1.86	0.58
11:K:65:PHE:CZ	11:K:72:ILE:HD11	2.39	0.58
16:d:100:LYS:O	16:d:104:GLU:OE1	2.20	0.58
13:a:194:LEU:CD1	8:H:179:ALA:CB	2.82	0.58
13:M:78:LEU:HD21	14:N:170:TYR:CE2	2.39	0.58
1:O:38:LYS:HD2	1:O:143:PRO:HG2	1.86	0.58
8:V:9:PRO:HD3	17:h:126:VAL:HG23	1.86	0.58
8:V:30:ALA:O	8:V:31:LYS:C	2.46	0.58
9:W:177:ASP:OD1	11:K:83:ALA:O	2.21	0.58
11:Y:65:PHE:CZ	11:Y:72:ILE:HD11	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:141:MET:HE2	13:a:151:LEU:HB3	1.86	0.58
8:H:27:ALA:O	8:H:28:ASP:C	2.47	0.58
2:P:90:LEU:HD21	2:P:114:LEU:HD22	1.86	0.57
3:Q:220:LEU:O	3:Q:228:TYR:OH	2.14	0.57
2:B:68:LEU:HD11	2:B:74:CYS:HB2	1.86	0.57
3:C:21:TYR:O	3:C:25:ALA:N	2.36	0.57
4:D:203:LYS:HE2	4:D:241:ILE:HG23	1.86	0.57
8:V:35:LYS:HG3	8:V:36:LEU:N	2.16	0.57
2:B:198:ASN:HA	2:B:201:MET:SD	2.44	0.57
2:P:68:LEU:HD11	2:P:74:CYS:HB2	1.86	0.57
2:P:235:GLN:O	2:P:238:LYS:HG3	2.03	0.57
3:C:39:ASP:OD2	3:C:213:ARG:NH1	2.37	0.57
8:H:30:ALA:O	8:H:31:LYS:C	2.46	0.57
13:M:141:MET:HE2	13:M:151:LEU:HB3	1.86	0.57
3:Q:158:ALA:HB1	3:Q:172:LEU:HD21	1.86	0.57
3:Q:192:ILE:HD11	3:Q:208:LEU:HD22	1.87	0.57
8:V:9:PRO:CB	17:h:126:VAL:CG2	2.78	0.57
4:D:108:THR:OG1	4:D:147:ASP:OD2	2.20	0.57
5:E:49:LEU:HB2	5:E:195:LEU:HD21	1.85	0.57
10:X:166:GLU:HB2	11:K:200[A]:ARG:HD3	1.84	0.57
8:V:215:ASN:ND2	8:V:234:VAL:HG12	2.19	0.57
1:A:38:LYS:HD2	1:A:143:PRO:HG2	1.86	0.57
2:B:68:LEU:HD12	2:B:72:MET:HE2	1.84	0.57
2:P:206:LEU:HD11	2:P:237:ILE:HD12	1.85	0.57
3:Q:39:ASP:OD2	3:Q:213:ARG:NH1	2.37	0.57
4:R:9:ASP:HB2	4:R:26:TYR:CE2	2.40	0.57
4:R:175:GLU:OE1	4:R:175:GLU:N	2.25	0.57
5:S:137:TYR:OH	5:S:217:LYS:HD2	2.05	0.57
1:A:33:PRO:HD2	1:A:48:GLU:OE1	2.05	0.57
17:e:92:LEU:HD13	17:e:134:VAL:HG21	1.86	0.57
13:M:117:ILE:O	13:M:121:LEU:HG	2.05	0.57
16:d:237:ASP:OD1	16:d:239:THR:OG1	2.20	0.57
11:Y:28:LEU:CD1	13:a:144:ARG:HD3	2.30	0.56
17:h:92:LEU:HD13	17:h:134:VAL:HG21	1.86	0.56
2:B:90:LEU:HD21	2:B:114:LEU:HD22	1.86	0.56
16:d:238:PRO:HG3	16:d:244:ARG:HH12	1.70	0.56
1:O:33:PRO:HD2	1:O:48:GLU:OE1	2.05	0.56
2:B:238:LYS:O	2:B:242:GLU:HG3	2.03	0.56
16:d:215:PRO:HA	16:d:218:LEU:CD1	2.36	0.56
4:R:203:LYS:HE2	4:R:241:ILE:HG23	1.87	0.56
8:V:9:PRO:CB	17:h:126:VAL:HG22	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:27:ALA:O	8:V:28:ASP:C	2.47	0.56
10:X:19:ARG:HD3	10:X:179:SER:HB3	1.88	0.56
11:Y:98:PRO:HA	11:Y:243:TRP:NE1	2.20	0.56
13:a:78:LEU:HD21	14:b:170:TYR:CE2	2.39	0.56
13:a:117:ILE:O	13:a:121:LEU:HG	2.05	0.56
4:D:9:ASP:HB2	4:D:26:TYR:CE2	2.40	0.56
8:H:215:ASN:ND2	8:H:234:VAL:HG12	2.19	0.56
10:J:19:ARG:HD3	10:J:179:SER:HB3	1.88	0.56
10:J:94:SER:O	10:J:96:THR:N	2.38	0.56
14:N:119:GLU:O	14:N:123:ARG:HG2	2.05	0.56
7:U:196:GLU:O	7:U:200:THR:OG1	2.13	0.56
14:b:119:GLU:O	14:b:123:ARG:HG2	2.05	0.56
1:A:120:TYR:OH	17:e:100:LEU:HB3	2.06	0.56
15:c:93:TRP:HB3	15:c:124:TYR:HB3	1.88	0.56
4:D:18:GLU:O	5:E:31:GLN:NE2	2.39	0.56
7:U:11:ARG:HH12	16:g:126:SER:HB3	1.71	0.56
14:b:55:THR:HG22	14:b:60:ILE:HD13	1.88	0.56
16:g:215:PRO:HA	16:g:218:LEU:CD1	2.36	0.56
16:g:238:PRO:HG3	16:g:244:ARG:HH12	1.70	0.56
3:C:96:LEU:HD23	17:e:31:LEU:HB3	1.86	0.56
13:M:155:MET:SD	13:M:155:MET:N	2.79	0.56
10:J:59:TYR:CD1	17:e:31:LEU:HD22	2.29	0.56
11:K:98:PRO:HA	11:K:243:TRP:NE1	2.20	0.56
16:g:18:LEU:HD23	16:g:119:ILE:HB	1.88	0.56
16:g:234:LEU:HD23	16:g:236:ASP:HA	1.88	0.56
5:E:137:TYR:OH	5:E:217:LYS:HD2	2.05	0.56
11:K:29:ASP:HB3	13:M:143:SER:OG	2.05	0.56
16:d:234:LEU:HD23	16:d:236:ASP:HA	1.88	0.56
1:O:120:TYR:OH	17:h:100:LEU:HB3	2.05	0.56
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.41	0.56
6:T:192:GLU:O	6:T:196:ILE:HG12	2.06	0.56
10:X:141:SER:HB3	11:K:197:VAL:HG23	1.88	0.56
11:K:226:ASP:OD1	11:K:227:ALA:N	2.39	0.56
1:O:65:GLU:OE1	1:O:90:ARG:NH2	2.36	0.56
10:X:92:LEU:HD12	10:X:97:PRO:HG3	1.88	0.56
11:Y:51:GLU:O	11:Y:53:GLY:N	2.39	0.56
3:C:192:ILE:HD11	3:C:208:LEU:HD22	1.86	0.56
8:H:9:PRO:HG2	17:e:124:SER:C	2.31	0.56
11:Y:30:LEU:HG	13:a:136:TRP:HE1	1.70	0.55
15:f:177:THR:HG21	15:f:184:LEU:HD21	1.88	0.55
8:H:9:PRO:HD3	17:e:126:VAL:HG23	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:93:TRP:HB3	15:f:124:TYR:HB3	1.88	0.55
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.41	0.55
8:V:35:LYS:HZ1	9:W:55:LEU:N	2.03	0.55
9:W:202:ARG:NH2	9:W:204:ASP:OD2	2.34	0.55
10:X:94:SER:O	10:X:96:THR:N	2.38	0.55
8:H:209:ASP:OD1	8:H:210:LEU:N	2.39	0.55
11:K:51:GLU:O	11:K:53:GLY:N	2.39	0.55
16:d:59:ASN:HB2	16:d:70:GLU:HB3	1.89	0.55
1:O:172:PHE:CZ	1:O:176:ARG:HD3	2.42	0.55
4:R:18:GLU:O	5:S:31:GLN:NE2	2.39	0.55
8:V:9:PRO:HG2	17:h:126:VAL:H	1.72	0.55
11:Y:226:ASP:OD1	11:Y:227:ALA:N	2.39	0.55
13:a:155:MET:N	13:a:155:MET:SD	2.79	0.55
3:C:146:GLN:HB2	3:C:159:ASN:ND2	2.21	0.55
10:J:92:LEU:HD12	10:J:97:PRO:HG3	1.88	0.55
2:P:41:ASP:OD1	2:P:186:LEU:HB2	2.06	0.55
3:Q:36:ARG:HG3	3:Q:142:PRO:HB2	1.89	0.55
3:Q:146:GLN:HB2	3:Q:159:ASN:ND2	2.21	0.55
3:C:36:ARG:HG3	3:C:142:PRO:HB2	1.89	0.55
4:D:70:ILE:HD11	4:D:89:ILE:HD12	1.88	0.55
7:G:130:GLU:OE1	7:G:130:GLU:N	2.40	0.55
11:K:163:TRP:CZ3	11:K:168:PRO:HG3	2.42	0.55
14:N:55:THR:HG22	14:N:60:ILE:HD13	1.88	0.55
1:O:198:PHE:O	1:O:199:GLU:HG2	2.07	0.55
7:U:38:THR:HA	7:U:169:GLY:HA3	1.89	0.55
8:V:209:ASP:OD1	8:V:210:LEU:N	2.39	0.55
1:A:20:GLN:HE22	7:G:16:PHE:H	1.55	0.55
3:C:215:GLN:NE2	3:C:216:SER:O	2.40	0.55
6:F:192:GLU:O	6:F:196:ILE:HG12	2.06	0.55
13:M:152:TRP:CD2	13:M:172:MET:HE1	2.42	0.55
3:Q:215:GLN:NE2	3:Q:216:SER:O	2.40	0.55
12:Z:176:LEU:HD23	12:Z:206:VAL:HG12	1.88	0.55
16:g:192:ASP:OD1	16:g:193:GLU:N	2.40	0.55
1:A:198:PHE:O	1:A:199:GLU:HG2	2.07	0.55
6:F:108:LEU:HD11	6:F:137:LEU:HB3	1.89	0.55
9:I:202:ARG:NH2	9:I:204:ASP:OD2	2.34	0.55
15:c:177:THR:HG21	15:c:184:LEU:HD21	1.88	0.55
16:d:129:ARG:HD3	16:d:207:PHE:HB3	1.88	0.55
4:R:70:ILE:HD11	4:R:89:ILE:HD12	1.88	0.55
7:U:118:ILE:HD12	7:U:138:MET:HE1	1.89	0.55
11:Y:67:PHE:CE2	11:Y:69:HIS:HB2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:200[B]:ARG:HD3	10:J:166:GLU:HB2	1.89	0.55
1:A:65:GLU:OE1	1:A:90:ARG:NH2	2.36	0.55
2:B:41:ASP:OD1	2:B:186:LEU:HB2	2.06	0.55
10:J:92:LEU:HD12	10:J:97:PRO:HB3	1.89	0.55
15:c:209:PRO:HD3	16:d:252:ARG:NH2	2.22	0.55
11:Y:163:TRP:CZ3	11:Y:168:PRO:HG3	2.42	0.55
11:Y:197:VAL:HG23	10:J:141:SER:HB3	1.88	0.55
1:A:172:PHE:CZ	1:A:176:ARG:HD3	2.42	0.55
16:d:192:ASP:OD1	16:d:193:GLU:N	2.39	0.55
4:R:107:MET:HG2	4:R:112:VAL:HG23	1.89	0.55
7:G:118:ILE:HD12	7:G:138:MET:HE1	1.89	0.55
16:d:1:MET:CE	16:d:1:MET:HA	2.37	0.55
6:T:83:ASP:HB3	6:T:131:PHE:HD1	1.72	0.54
7:U:80:MET:HB3	7:U:87:SER:HB2	1.90	0.54
8:V:9:PRO:HG2	17:h:124:SER:C	2.31	0.54
15:f:209:PRO:HD3	16:g:252:ARG:NH2	2.22	0.54
4:D:6:SER:HG	4:D:8:TYR:HE1	1.55	0.54
10:J:92:LEU:HD12	10:J:97:PRO:CG	2.37	0.54
4:D:202:LEU:O	4:D:206:MET:HG2	2.07	0.54
6:F:35:THR:HA	6:F:166:GLY:HA3	1.89	0.54
7:U:130:GLU:N	7:U:130:GLU:OE1	2.40	0.54
10:X:166:GLU:HB2	11:K:200[B]:ARG:HD3	1.88	0.54
16:g:129:ARG:HD3	16:g:207:PHE:HB3	1.89	0.54
2:B:143:TYR:HB2	2:B:146:GLN:NE2	2.21	0.54
8:H:9:PRO:HG2	17:e:126:VAL:H	1.72	0.54
9:I:141:CYS:HB2	9:I:145:MET:HE1	1.90	0.54
16:d:18:LEU:HD23	16:d:119:ILE:HB	1.88	0.54
2:P:82:ASP:OD2	2:P:128:ARG:NH1	2.24	0.54
10:X:29:LYS:HD3	11:Y:181:SER:O	2.08	0.54
10:X:59:TYR:CD1	17:h:31:LEU:HD22	2.29	0.54
10:J:2:GLU:OE1	10:J:47:VAL:HB	2.07	0.54
11:K:67:PHE:CE2	11:K:69:HIS:HB2	2.41	0.54
15:c:73:ILE:CG2	15:c:166:ILE:HG22	2.38	0.54
10:X:92:LEU:HD12	10:X:97:PRO:CG	2.37	0.54
13:a:152:TRP:CD2	13:a:172:MET:HE1	2.42	0.54
16:g:12:LEU:HA	16:g:15:PHE:HD2	1.73	0.54
7:G:11:ARG:HH12	16:d:126:SER:HB3	1.71	0.54
12:L:176:LEU:HD23	12:L:206:VAL:HG12	1.88	0.54
6:T:108:LEU:HD11	6:T:137:LEU:HB3	1.89	0.54
15:f:213:HIS:ND1	15:f:213:HIS:O	2.40	0.54
16:g:59:ASN:HB2	16:g:70:GLU:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:53:ASP:N	8:H:53:ASP:OD1	2.39	0.54
11:K:123:ARG:NH1	11:K:126:GLU:OE1	2.41	0.54
15:c:213:HIS:ND1	15:c:213:HIS:O	2.40	0.54
1:O:20:GLN:HE22	7:U:16:PHE:H	1.55	0.54
8:V:53:ASP:N	8:V:53:ASP:OD1	2.39	0.54
16:g:1:MET:CE	16:g:1:MET:HA	2.37	0.54
16:g:17:LEU:HD23	16:g:118:VAL:HG13	1.90	0.54
4:D:107:MET:HG2	4:D:112:VAL:HG23	1.89	0.54
15:c:73:ILE:HG23	15:c:166:ILE:HG22	1.90	0.54
16:d:79:SER:HB2	16:d:86:VAL:HG22	1.90	0.54
4:R:202:LEU:O	4:R:206:MET:HG2	2.07	0.54
8:V:257:GLU:HG3	9:W:197:ARG:HG2	1.90	0.54
3:C:57:ARG:HG3	3:C:60:ARG:HH12	1.73	0.54
8:H:26:GLU:O	8:H:27:ALA:C	2.50	0.54
8:H:257:GLU:HG3	9:I:197:ARG:HG2	1.90	0.54
11:Y:28:LEU:HD22	13:a:107:TYR:CE2	2.35	0.54
11:Y:123:ARG:NH1	11:Y:126:GLU:OE1	2.41	0.54
2:B:13:SER:C	2:B:15:GLU:H	2.16	0.54
4:D:84:ASP:OD1	4:D:135:ARG:NH2	2.41	0.54
8:H:244:ARG:HG3	8:H:244:ARG:O	2.08	0.54
10:X:2:GLU:OE1	10:X:47:VAL:HB	2.07	0.53
13:a:137:LEU:HD23	13:a:157:ILE:HD11	1.90	0.53
16:g:69:THR:O	16:g:69:THR:OG1	2.26	0.53
4:R:84:ASP:OD1	4:R:135:ARG:NH2	2.41	0.53
9:W:141:CYS:HB2	9:W:145:MET:HE1	1.90	0.53
16:g:145:PRO:HA	16:g:148:GLN:HB2	1.90	0.53
3:C:200:GLN:NE2	3:C:204:LYS:O	2.41	0.53
6:F:216:VAL:HB	6:F:224:HIS:HA	1.90	0.53
7:G:38:THR:HA	7:G:169:GLY:HA3	1.89	0.53
3:Q:200:GLN:NE2	3:Q:204:LYS:O	2.41	0.53
6:T:35:THR:HA	6:T:166:GLY:HA3	1.89	0.53
15:f:73:ILE:CG2	15:f:166:ILE:HG22	2.38	0.53
4:R:108:THR:OG1	4:R:147:ASP:OD2	2.20	0.53
6:T:216:VAL:HB	6:T:224:HIS:HA	1.90	0.53
8:V:26:GLU:O	8:V:27:ALA:C	2.50	0.53
8:V:179:ALA:CB	13:M:194:LEU:CD1	2.83	0.53
10:X:96:THR:O	10:X:97:PRO:C	2.51	0.53
15:f:73:ILE:HG23	15:f:166:ILE:HG22	1.90	0.53
10:J:29:LYS:HD3	11:K:181:SER:O	2.08	0.53
7:U:152:TYR:CE1	7:U:162:GLY:HA2	2.44	0.53
16:g:41:MET:HG2	16:g:80:LEU:HD12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:57:ARG:HG3	3:Q:60:ARG:HH12	1.73	0.53
10:X:92:LEU:HD12	10:X:97:PRO:HB3	1.89	0.53
1:A:88:ARG:HD3	17:e:100:LEU:HD12	1.90	0.53
10:J:95:ARG:HA	17:e:40:ASN:HD21	1.74	0.53
11:K:181:SER:OG	11:K:182:GLY:N	2.42	0.53
13:M:86:ARG:NH1	13:M:98:ALA:O	2.42	0.53
15:c:266:ILE:O	15:c:269:SER:OG	2.23	0.53
16:d:218:LEU:HA	16:d:221:VAL:HG22	1.91	0.53
7:U:42:VAL:HG12	7:U:165:ALA:HB1	1.91	0.53
9:W:134:ASP:OD1	9:W:135:PHE:N	2.42	0.53
11:Y:181:SER:OG	11:Y:182:GLY:N	2.42	0.53
15:f:266:ILE:O	15:f:269:SER:OG	2.23	0.53
16:d:145:PRO:HA	16:d:148:GLN:HB2	1.90	0.53
11:Y:60:THR:HG21	11:Y:228:TYR:O	2.09	0.53
6:F:83:ASP:HB3	6:F:131:PHE:HD1	1.72	0.53
7:G:80:MET:HB3	7:G:87:SER:HB2	1.90	0.53
10:J:96:THR:O	10:J:97:PRO:C	2.51	0.53
11:K:76:ASP:OD1	11:K:77:SER:N	2.41	0.53
15:c:72:ILE:O	15:c:134:LEU:HA	2.09	0.53
16:d:12:LEU:HA	16:d:15:PHE:HD2	1.73	0.53
2:P:143:TYR:HB2	2:P:146:GLN:NE2	2.21	0.53
7:U:113:MET:HA	7:U:113:MET:HE3	1.91	0.53
6:F:16:PRO:HA	7:G:27:TYR:CE1	2.44	0.53
6:F:72:HIS:CE1	6:F:105:ASN:HB3	2.44	0.53
8:H:9:PRO:HD2	17:e:124:SER:HB2	1.91	0.53
8:H:9:PRO:HD2	17:e:127:MET:HE2	1.91	0.53
11:K:28:LEU:HD22	13:M:107:TYR:CE2	2.44	0.53
16:d:69:THR:O	16:d:69:THR:OG1	2.26	0.53
16:d:83:ARG:O	16:d:83:ARG:HG2	2.09	0.53
2:P:38:LEU:O	2:P:179:TYR:OH	2.27	0.53
7:U:51:VAL:HG22	7:U:217:VAL:HG22	1.91	0.53
8:V:244:ARG:O	8:V:244:ARG:HG3	2.08	0.53
10:J:58:GLU:O	10:J:62:LYS:HG2	2.09	0.53
14:N:115:SER:O	14:N:119:GLU:HG2	2.08	0.53
2:P:13:SER:C	2:P:15:GLU:H	2.16	0.52
4:D:8:TYR:N	4:D:8:TYR:CD1	2.77	0.52
5:E:88:MET:HE3	5:E:112:ILE:HD11	1.91	0.52
6:F:123:THR:HG22	6:F:130:PRO:HB3	1.91	0.52
7:G:110:PRO:HB2	7:G:112:ASP:OD1	2.10	0.52
8:H:9:PRO:CD	17:e:127:MET:HE2	2.39	0.52
4:R:8:TYR:N	4:R:8:TYR:CD1	2.77	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:110:PRO:HB2	7:U:112:ASP:OD1	2.10	0.52
7:G:113:MET:HA	7:G:113:MET:HE3	1.91	0.52
11:K:60:THR:HG21	11:K:228:TYR:O	2.09	0.52
17:e:84:LYS:O	17:e:88:GLN:HG3	2.09	0.52
2:P:17:ARG:HE	2:P:19:TYR:HE1	1.58	0.52
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	1.90	0.52
6:T:72:HIS:CE1	6:T:105:ASN:HB3	2.44	0.52
10:X:58:GLU:O	10:X:62:LYS:HG2	2.09	0.52
14:b:93:VAL:HG11	14:b:117:PHE:CE2	2.43	0.52
16:g:147:MET:CE	16:g:200:GLN:HB3	2.40	0.52
16:g:218:LEU:HA	16:g:221:VAL:HG22	1.91	0.52
1:A:101:GLN:NE2	8:H:100:GLN:OE1	2.42	0.52
7:G:152:TYR:CE1	7:G:162:GLY:HA2	2.44	0.52
9:I:57:THR:OG1	10:J:121:LEU:O	2.23	0.52
11:K:86:ALA:O	12:L:164:LYS:NZ	2.37	0.52
1:O:94:GLN:HG3	8:V:108:LEU:HG	1.91	0.52
4:R:10:ARG:HB2	15:f:1:MET:SD	2.50	0.52
8:V:9:PRO:CD	17:h:127:MET:HE2	2.39	0.52
16:g:98:LYS:HD3	16:g:101:PRO:HG2	1.91	0.52
16:g:107:LEU:HG	16:g:193:GLU:OE2	2.09	0.52
17:h:84:LYS:O	17:h:88:GLN:HG3	2.09	0.52
2:B:38:LEU:O	2:B:179:TYR:OH	2.27	0.52
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.90	0.52
3:C:4:ASP:HB3	3:C:21:TYR:HE2	1.74	0.52
14:N:93:VAL:HG11	14:N:117:PHE:CE2	2.43	0.52
15:c:14:CYS:HA	16:d:210:GLU:OE2	2.09	0.52
16:d:107:LEU:HG	16:d:193:GLU:OE2	2.09	0.52
1:O:88:ARG:HD3	17:h:100:LEU:HD12	1.90	0.52
3:Q:4:ASP:HB3	3:Q:21:TYR:HE2	1.74	0.52
6:T:16:PRO:HA	7:U:27:TYR:CE1	2.44	0.52
7:U:194:THR:O	7:U:197:THR:N	2.31	0.52
15:f:72:ILE:O	15:f:134:LEU:HA	2.09	0.52
16:g:79:SER:HB2	16:g:86:VAL:HG22	1.90	0.52
10:J:99[A]:HIS:HA	10:J:120:TYR:HB2	1.92	0.52
13:M:137:LEU:HD23	13:M:157:ILE:HD11	1.90	0.52
17:e:68:ARG:HG3	17:e:76:PRO:HG2	1.90	0.52
1:O:8:SER:O	1:O:9:LEU:HB3	2.09	0.52
6:T:123:THR:HG22	6:T:130:PRO:HB3	1.91	0.52
7:U:78:CYS:HB3	7:U:140:LEU:HD23	1.92	0.52
8:V:9:PRO:HD2	17:h:127:MET:HE2	1.91	0.52
13:a:86:ARG:NH1	13:a:98:ALA:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:115:SER:O	14:b:119:GLU:HG2	2.08	0.52
4:D:107:MET:HE2	4:D:112:VAL:HA	1.92	0.52
10:J:99[B]:HIS:HA	10:J:120:TYR:HB2	1.92	0.52
5:S:73[A]:SER:HB3	5:S:133:LEU:HB2	1.92	0.52
11:K:156[A]:MET:H	11:K:175:SER:HB3	1.75	0.52
11:K:156[B]:MET:H	11:K:175:SER:HB3	1.75	0.52
16:d:147:MET:CE	16:d:200:GLN:HB3	2.40	0.52
1:O:9:LEU:HB2	1:O:20:GLN:HG3	1.91	0.52
6:T:51:LYS:HB3	6:T:210:GLU:O	2.10	0.52
7:U:178:PHE:HA	7:U:181:LYS:HE2	1.91	0.52
7:U:194:THR:O	7:U:196:GLU:N	2.43	0.52
10:X:99[A]:HIS:HA	10:X:120:TYR:HB2	1.92	0.52
14:b:168:TYR:HA	14:N:167:SER:O	2.10	0.52
15:f:14:CYS:HA	16:g:210:GLU:OE2	2.09	0.52
16:g:237:ASP:OD1	16:g:239:THR:OG1	2.20	0.52
17:h:68:ARG:HG3	17:h:76:PRO:HG2	1.90	0.52
2:B:4:ARG:HG2	3:C:5:ARG:NE	2.23	0.52
3:C:46:GLU:OE2	3:C:163:ARG:NH2	2.43	0.52
4:D:6:SER:OG	4:D:8:TYR:HE1	1.92	0.52
4:D:10:ARG:HB2	15:c:1:MET:SD	2.50	0.52
7:G:77:GLY:HA3	7:G:227:PHE:CD1	2.45	0.52
9:I:158:ASP:OD1	9:I:161:HIS:ND1	2.32	0.52
12:L:123:ILE:O	12:L:126:SER:OG	2.28	0.52
2:P:198:ASN:ND2	2:P:201:MET:SD	2.81	0.52
3:Q:62:ILE:HG21	3:Q:209:ALA:HB3	1.92	0.52
7:U:77:GLY:HA3	7:U:227:PHE:CD1	2.45	0.52
1:A:8:SER:O	1:A:9:LEU:HB3	2.09	0.52
1:A:9:LEU:HB2	1:A:20:GLN:HG3	1.91	0.52
7:G:42:VAL:HG12	7:G:165:ALA:HB1	1.91	0.52
16:d:27:VAL:HG21	16:d:208:VAL:HG11	1.92	0.52
2:P:119:GLN:NE2	2:P:123:GLN:OE1	2.33	0.52
3:Q:46:GLU:OE2	3:Q:163:ARG:NH2	2.43	0.52
3:Q:80:ALA:HA	3:Q:129:ILE:HD13	1.92	0.52
6:T:23:VAL:O	6:T:27:MET:HG3	2.10	0.52
7:U:182:LYS:HA	7:U:182:LYS:CE	2.39	0.52
10:X:99[B]:HIS:HA	10:X:120:TYR:HB2	1.92	0.52
12:Z:123:ILE:O	12:Z:126:SER:OG	2.28	0.52
7:G:194:THR:O	7:G:196:GLU:N	2.43	0.52
10:J:107:TYR:HE1	10:J:112:GLY:HA2	1.75	0.52
4:R:107:MET:HE2	4:R:112:VAL:HA	1.92	0.51
5:S:215:VAL:HB	5:S:221:PHE:HD1	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:5:SER:O	15:f:9:VAL:HA	2.10	0.51
7:U:131:MET:SD	17:h:82:GLU:HG2	2.50	0.51
10:X:95:ARG:HA	17:h:40:ASN:HD21	1.74	0.51
14:b:48:LEU:HD12	14:b:78:CYS:SG	2.50	0.51
16:g:78:TYR:OH	16:g:91:ARG:NH2	2.43	0.51
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.29	0.51
3:C:192:ILE:O	3:C:196:LEU:HG	2.11	0.51
8:H:217:ASP:OD2	8:H:230:ARG:HD2	2.10	0.51
10:J:101:ASN:HB3	10:J:132:HIS:CD2	2.45	0.51
1:O:101:GLN:NE2	8:V:100:GLN:OE1	2.42	0.51
2:P:139:TRP:NE1	2:P:144:GLY:HA2	2.25	0.51
5:S:156:CYS:SG	5:S:159:MET:HG3	2.50	0.51
3:C:80:ALA:HA	3:C:129:ILE:HD13	1.92	0.51
5:E:156:CYS:SG	5:E:159:MET:HG3	2.50	0.51
7:G:50:ILE:HD12	7:G:79:VAL:HB	1.93	0.51
3:Q:4:ASP:OD1	3:Q:21:TYR:OH	2.26	0.51
8:V:217:ASP:OD2	8:V:230:ARG:HD2	2.10	0.51
15:f:208:GLN:NE2	16:g:58:ASN:O	2.32	0.51
1:A:94:GLN:HG3	8:H:108:LEU:HG	1.91	0.51
3:C:4:ASP:OD1	3:C:21:TYR:OH	2.26	0.51
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.76	0.51
7:G:178:PHE:HA	7:G:181:LYS:HE2	1.91	0.51
8:H:26:GLU:HG3	8:H:31:LYS:HE3	1.93	0.51
16:d:41:MET:HG2	16:d:80:LEU:HD12	1.91	0.51
16:d:78:TYR:OH	16:d:91:ARG:NH2	2.43	0.51
4:R:13:ASN:HB3	5:S:126:ARG:HB3	1.92	0.51
7:U:211:LYS:O	7:U:213:SER:N	2.43	0.51
4:D:13:ASN:HB3	5:E:126:ARG:HB3	1.92	0.51
5:E:6:TYR:CD2	5:E:15:PRO:HD3	2.46	0.51
7:G:211:LYS:O	7:G:213:SER:N	2.43	0.51
16:d:98:LYS:HD3	16:d:101:PRO:HG2	1.91	0.51
5:S:6:TYR:CD2	5:S:15:PRO:HD3	2.46	0.51
8:V:9:PRO:HD2	17:h:124:SER:HB2	1.91	0.51
11:Y:27:LEU:O	11:Y:28:LEU:HB3	2.10	0.51
11:Y:223:THR:HG21	11:Y:251:VAL:HG11	1.92	0.51
16:g:83:ARG:HG2	16:g:83:ARG:O	2.09	0.51
16:g:151:VAL:HG13	16:g:155:ILE:HD11	1.92	0.51
6:F:51:LYS:HB3	6:F:210:GLU:O	2.10	0.51
8:H:189:MET:HE1	8:H:197:LEU:HD22	1.93	0.51
3:Q:192:ILE:O	3:Q:196:LEU:HG	2.11	0.51
10:X:101:ASN:HB3	10:X:132:HIS:CD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:107:TYR:HE1	10:X:112:GLY:HA2	1.75	0.51
12:Z:111:MET:HE3	12:Z:116:ILE:HG12	1.93	0.51
2:B:139:TRP:NE1	2:B:144:GLY:HA2	2.25	0.51
4:D:235:GLU:HA	4:D:238:ILE:HG12	1.93	0.51
7:G:182:LYS:HA	7:G:182:LYS:CE	2.39	0.51
1:O:64:VAL:HG12	1:O:217:PHE:HZ	1.75	0.51
4:R:6:SER:OG	4:R:8:TYR:HE1	1.92	0.51
4:R:107:MET:HG2	4:R:112:VAL:CG2	2.41	0.51
5:E:158:ALA:HB1	5:E:172:LEU:HD13	1.93	0.51
7:G:78:CYS:HB3	7:G:140:LEU:HD23	1.92	0.51
10:J:28:MET:SD	11:K:195:TYR:OH	2.65	0.51
16:d:17:LEU:HD23	16:d:118:VAL:HG13	1.90	0.51
16:d:19:MET:SD	16:d:106:LEU:HD21	2.51	0.51
16:d:33:ASP:OD2	16:d:251:TRP:NE1	2.44	0.51
3:Q:196:LEU:HA	3:Q:199:VAL:HB	1.93	0.51
5:S:158:ALA:HB1	5:S:172:LEU:HD13	1.93	0.51
8:V:16:PHE:O	8:V:16:PHE:HD1	1.93	0.51
1:A:19:VAL:HA	1:A:22:GLU:HB2	1.93	0.51
4:D:107:MET:HG2	4:D:112:VAL:CG2	2.41	0.51
8:H:16:PHE:O	8:H:16:PHE:HD1	1.93	0.51
9:I:134:ASP:OD1	9:I:135:PHE:N	2.42	0.51
11:K:216:ARG:NH1	11:K:247:SER:OG	2.38	0.51
12:L:33:TYR:OH	12:L:131:PRO:O	2.20	0.51
14:N:48:LEU:HD12	14:N:78:CYS:SG	2.50	0.51
5:S:88:MET:HE3	5:S:112:ILE:HD11	1.91	0.51
8:V:189:MET:HE1	8:V:197:LEU:HD22	1.93	0.51
11:Y:156[A]:MET:H	11:Y:175:SER:HB3	1.75	0.51
14:b:167:SER:O	14:N:168:TYR:HA	2.10	0.51
15:f:206:LEU:HD23	15:f:207:GLU:O	2.11	0.51
15:f:208:GLN:HB2	16:g:252:ARG:NH2	2.26	0.51
2:B:82:ASP:OD2	2:B:128:ARG:NH1	2.24	0.51
4:D:107:MET:HE3	4:D:111:SER:OG	2.11	0.51
7:G:51:VAL:HG22	7:G:217:VAL:HG22	1.91	0.51
7:G:194:THR:O	7:G:197:THR:N	2.31	0.51
10:J:182:ILE:HG22	10:J:189:HIS:HB2	1.93	0.51
14:N:80:SER:OG	14:N:131:GLY:O	2.29	0.51
16:d:151:VAL:HG13	16:d:155:ILE:HD11	1.92	0.51
4:R:107:MET:HE3	4:R:111:SER:OG	2.11	0.51
7:U:50:ILE:HD12	7:U:79:VAL:HB	1.93	0.51
11:Y:156[B]:MET:H	11:Y:175:SER:HB3	1.75	0.51
1:A:64:VAL:HG12	1:A:217:PHE:HZ	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:ARG:NE	17:e:140:LEU:HD21	2.25	0.51
15:c:206:LEU:HD23	15:c:207:GLU:O	2.11	0.51
1:O:19:VAL:HA	1:O:22:GLU:HB2	1.93	0.50
8:V:26:GLU:HG3	8:V:31:LYS:HE3	1.93	0.50
13:a:71:MET:HB3	13:a:84:ILE:O	2.12	0.50
16:g:27:VAL:HG21	16:g:208:VAL:HG11	1.92	0.50
1:A:192:LEU:O	1:A:196:GLU:HG2	2.11	0.50
2:B:216:LEU:HD12	2:B:225:ILE:HG13	1.94	0.50
7:G:5:SER:O	15:c:9:VAL:HA	2.10	0.50
12:L:111:MET:HE3	12:L:116:ILE:HG12	1.93	0.50
2:P:194:ILE:HG13	2:P:236:LEU:HG	1.94	0.50
10:X:29:LYS:NZ	10:X:32:HIS:HA	2.27	0.50
2:B:107:CYS:HB2	2:B:146:GLN:OE1	2.12	0.50
11:Y:192:VAL:HG21	10:J:137:PHE:HB3	1.94	0.50
15:c:208:GLN:HB2	16:d:252:ARG:NH2	2.26	0.50
16:d:147:MET:HE2	16:d:200:GLN:HB3	1.93	0.50
5:S:40:SER:HB3	5:S:187:LEU:HD13	1.93	0.50
5:S:137:TYR:CE2	5:S:141:GLY:HA2	2.46	0.50
12:Z:33:TYR:OH	12:Z:131:PRO:O	2.20	0.50
3:C:196:LEU:HA	3:C:199:VAL:HB	1.93	0.50
5:E:73[A]:SER:HB3	5:E:133:LEU:HB2	1.91	0.50
12:L:54:ASP:OD2	12:L:217:THR:HA	2.11	0.50
3:Q:115:LYS:HZ3	3:Q:129:ILE:HG13	1.77	0.50
6:T:68:ASN:OD1	6:T:224:HIS:ND1	2.38	0.50
6:T:237:LYS:O	6:T:240:LYS:N	2.45	0.50
13:a:206:SER:OG	13:a:209:GLU:OE2	2.28	0.50
16:g:147:MET:HE2	16:g:200:GLN:HB3	1.93	0.50
3:C:62:ILE:HG21	3:C:209:ALA:HB3	1.92	0.50
5:E:14:SER:C	5:E:16:GLN:H	2.20	0.50
6:F:23:VAL:O	6:F:27:MET:HG3	2.10	0.50
6:F:125:TYR:CE2	17:e:81:MET:HG3	2.47	0.50
7:G:131:MET:SD	17:e:82:GLU:HG2	2.50	0.50
13:M:71:MET:HB3	13:M:84:ILE:O	2.12	0.50
1:O:192:LEU:O	1:O:196:GLU:HG2	2.11	0.50
2:P:119:GLN:HA	2:P:122:THR:HG22	1.94	0.50
7:U:13:ILE:HG22	7:U:14:THR:HG22	1.94	0.50
10:X:91:CYS:O	10:X:97:PRO:CA	2.60	0.50
16:g:19:MET:SD	16:g:106:LEU:HD21	2.51	0.50
16:g:189:THR:O	16:g:193:GLU:HB3	2.12	0.50
2:B:17:ARG:HE	2:B:19:TYR:HE1	1.58	0.50
5:E:137:TYR:CE2	5:E:141:GLY:HA2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:95:TYR:CE1	9:I:98:ARG:HD3	2.47	0.50
13:M:196:ARG:O	13:M:200:GLU:HG2	2.12	0.50
14:N:71:ILE:HD11	14:N:77:CYS:SG	2.52	0.50
9:W:95:TYR:CE1	9:W:98:ARG:HD3	2.47	0.50
10:X:85:ARG:HA	10:X:118:MET:HE1	1.94	0.50
11:Y:78:ARG:HG3	11:Y:79:ALA:N	2.27	0.50
14:b:196:LEU:HD13	14:N:171:GLY:O	2.11	0.50
8:H:35:LYS:HG3	8:H:36:LEU:N	2.16	0.50
10:J:1:MET:HG2	10:J:134:TYR:CE2	2.47	0.50
11:K:29:ASP:OD2	13:M:143:SER:HB2	2.10	0.50
1:O:9:LEU:HD22	1:O:128:PRO:HD3	1.94	0.50
3:Q:7:ILE:HD12	3:Q:18:GLN:CB	2.34	0.50
8:V:155:SER:HB2	8:V:170[A]:MET:HE2	1.94	0.50
12:Z:54:ASP:OD2	12:Z:217:THR:HA	2.11	0.50
14:b:71:ILE:HD11	14:b:77:CYS:SG	2.52	0.50
14:b:171:GLY:O	14:N:196:LEU:HD13	2.11	0.50
6:F:191:LYS:HB3	6:F:238:TYR:CD2	2.47	0.50
17:e:37:CYS:SG	17:e:38:VAL:N	2.84	0.50
2:P:107:CYS:HB2	2:P:146:GLN:OE1	2.12	0.50
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.29	0.50
9:W:57:THR:OG1	10:X:121:LEU:O	2.23	0.50
12:Z:213:ARG:NH1	8:H:70:ALA:O	2.45	0.50
8:V:124:ARG:O	8:V:128:GLN:HG3	2.11	0.49
9:W:49:TYR:HD2	9:W:189:ILE:HD11	1.77	0.49
10:X:182:ILE:HG22	10:X:189:HIS:HB2	1.93	0.49
11:Y:61:THR:HB	11:Y:76:ASP:OD2	2.12	0.49
15:f:144:ASP:OD1	15:f:145:GLN:HG2	2.12	0.49
2:B:119:GLN:NE2	2:B:123:GLN:OE1	2.33	0.49
3:C:124:ARG:HH12	17:e:140:LEU:CD2	2.22	0.49
10:J:29:LYS:NZ	10:J:32:HIS:HA	2.27	0.49
11:K:94:ILE:HD11	11:K:104:MET:HE2	1.94	0.49
11:K:223:THR:HG21	11:K:251:VAL:HG11	1.92	0.49
15:c:208:GLN:NE2	16:d:58:ASN:O	2.32	0.49
16:d:194:SER:O	16:d:198:GLU:N	2.45	0.49
6:T:125:TYR:CE2	17:h:81:MET:HG3	2.47	0.49
5:E:40:SER:HB3	5:E:187:LEU:HD13	1.93	0.49
6:F:229:LYS:O	6:F:232:ARG:N	2.45	0.49
16:d:189:THR:O	16:d:193:GLU:HB3	2.12	0.49
1:O:67:ILE:HD11	1:O:73:LEU:HD11	1.94	0.49
6:T:236:GLU:OE1	6:T:240:LYS:NZ	2.32	0.49
10:X:1:MET:HG2	10:X:134:TYR:CE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:212:ILE:H	5:E:212:ILE:HD12	1.77	0.49
6:F:114:ARG:NE	17:e:72:GLY:HA2	2.28	0.49
12:L:66:ARG:HB3	12:L:219:ASP:HB3	1.95	0.49
12:Z:44:ALA:HB2	12:Z:149:VAL:HG23	1.95	0.49
15:f:112:THR:C	15:f:114:LEU:H	2.21	0.49
3:Q:124:ARG:HD3	3:Q:124:ARG:N	2.28	0.49
4:R:8:TYR:N	4:R:8:TYR:HD1	2.10	0.49
4:R:103:TYR:O	4:R:105:GLU:N	2.44	0.49
4:R:235:GLU:HA	4:R:238:ILE:HG12	1.93	0.49
6:T:191:LYS:HB3	6:T:238:TYR:CD2	2.47	0.49
7:U:155:ASP:HB2	7:U:156:PRO:HD2	1.95	0.49
9:W:43:PRO:HA	9:W:49:TYR:CD1	2.48	0.49
9:W:158:ASP:OD1	9:W:161:HIS:ND1	2.32	0.49
10:X:28:MET:SD	11:Y:195:TYR:OH	2.65	0.49
10:X:137:PHE:HB3	11:K:192:VAL:HG21	1.94	0.49
16:g:194:SER:O	16:g:198:GLU:N	2.45	0.49
3:C:8:THR:OG1	4:D:135:ARG:HB3	2.12	0.49
3:C:124:ARG:HD3	3:C:124:ARG:N	2.28	0.49
4:D:8:TYR:N	4:D:8:TYR:HD1	2.10	0.49
5:E:45:VAL:HG12	5:E:214:ILE:HG12	1.95	0.49
7:U:141:ILE:HD11	7:U:227:PHE:HE1	1.77	0.49
8:V:16:PHE:O	8:V:16:PHE:CD1	2.65	0.49
13:a:196:ARG:O	13:a:200:GLU:HG2	2.12	0.49
9:I:43:PRO:HA	9:I:49:TYR:CD1	2.48	0.49
10:J:85:ARG:HA	10:J:118:MET:HE1	1.94	0.49
10:J:91:CYS:O	10:J:97:PRO:CA	2.60	0.49
1:O:88:ARG:HD3	17:h:100:LEU:CD1	2.43	0.49
3:Q:8:THR:OG1	4:R:135:ARG:HB3	2.12	0.49
3:Q:155:ALA:HB3	4:R:63:SER:OG	2.13	0.49
4:R:233:GLU:HA	4:R:236:GLU:HB2	1.95	0.49
8:V:28:ASP:HB2	8:V:36:LEU:CB	2.42	0.49
11:Y:94:ILE:HD11	11:Y:104:MET:HE2	1.95	0.49
16:g:33:ASP:OD2	16:g:251:TRP:NE1	2.44	0.49
1:A:21:ILE:HD11	1:A:121:THR:HB	1.95	0.49
2:B:4:ARG:CA	2:B:14:PRO:HD3	2.42	0.49
8:H:124:ARG:O	8:H:128:GLN:HG3	2.11	0.49
2:P:4:ARG:CA	2:P:14:PRO:HD3	2.42	0.49
3:Q:221:ASN:O	3:Q:223:GLU:N	2.46	0.49
4:R:1:MET:O	16:g:91:ARG:HB3	2.13	0.49
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.95	0.49
16:g:186:ILE:HA	16:g:189:THR:HG22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PRO:HG2	16:d:255:PHE:CE1	2.48	0.49
16:d:37:SER:OG	16:d:246:LYS:HB3	2.13	0.49
6:T:229:LYS:O	6:T:232:ARG:N	2.45	0.49
11:Y:217:ARG:HD2	11:Y:258:TYR:CZ	2.48	0.49
1:A:67:ILE:HD11	1:A:73:LEU:HD11	1.95	0.49
1:A:122:GLN:HB2	2:B:128:ARG:NH2	2.28	0.49
4:D:233:GLU:HA	4:D:236:GLU:HB2	1.95	0.49
9:I:90:VAL:HG21	9:I:108:ILE:HD11	1.95	0.49
15:c:112:THR:C	15:c:114:LEU:H	2.21	0.49
2:P:90:LEU:HD21	2:P:114:LEU:HB2	1.95	0.49
2:P:216:LEU:HD12	2:P:225:ILE:HG13	1.94	0.49
5:S:14:SER:C	5:S:16:GLN:H	2.20	0.49
5:S:212:ILE:HD12	5:S:212:ILE:H	1.77	0.49
8:V:70:ALA:O	12:L:213:ARG:NH1	2.45	0.49
15:f:84:SER:HA	15:f:88:MET:HB2	1.95	0.49
4:D:17:PRO:C	4:D:18:GLU:HG3	2.37	0.49
7:G:13:ILE:HG22	7:G:14:THR:HG22	1.94	0.49
7:G:13:ILE:HG13	7:G:24:GLN:HB2	1.94	0.49
7:G:141:ILE:HD11	7:G:227:PHE:HE1	1.77	0.49
8:H:155:SER:HB2	8:H:170[A]:MET:HE2	1.94	0.49
1:O:122:GLN:HB2	2:P:128:ARG:NH2	2.28	0.48
11:Y:216:ARG:NH1	11:Y:247:SER:OG	2.38	0.48
2:B:194:ILE:HG13	2:B:236:LEU:HG	1.94	0.48
4:D:1:MET:O	16:d:91:ARG:HB3	2.13	0.48
12:L:103:TYR:CD1	12:L:111:MET:HG2	2.48	0.48
17:e:126:VAL:O	17:e:127:MET:HE2	2.13	0.48
5:S:45:VAL:HG12	5:S:214:ILE:HG12	1.94	0.48
12:Z:103:TYR:CD1	12:Z:111:MET:HG2	2.48	0.48
3:C:155:ALA:HB3	4:D:63:SER:OG	2.13	0.48
3:C:221:ASN:O	3:C:223:GLU:N	2.46	0.48
7:G:155:ASP:HB2	7:G:156:PRO:HD2	1.95	0.48
8:H:16:PHE:O	8:H:16:PHE:CD1	2.65	0.48
9:I:49:TYR:HD2	9:I:189:ILE:HD11	1.77	0.48
13:M:65:VAL:HG23	13:M:165:SER:HB3	1.95	0.48
15:c:84:SER:HA	15:c:88:MET:HB2	1.95	0.48
3:Q:117:ARG:NE	17:h:140:LEU:HD21	2.25	0.48
15:f:80:VAL:HA	15:f:136:GLN:OE1	2.14	0.48
16:g:37:SER:OG	16:g:246:LYS:HB3	2.13	0.48
5:E:185:ASN:O	5:E:189:LYS:HG2	2.13	0.48
10:J:38:MET:HE3	10:J:44:LEU:HB3	1.94	0.48
13:M:231:ARG:HH21	13:M:247:PRO:HG3	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:21:ILE:HD11	1:O:121:THR:HB	1.95	0.48
4:R:209:LYS:HD3	4:R:210:LEU:H	1.78	0.48
5:S:15:PRO:HG2	16:g:255:PHE:CE1	2.48	0.48
6:T:114:ARG:NE	17:h:72:GLY:HA2	2.27	0.48
8:V:86:CYS:SG	8:V:141:LEU:HB3	2.54	0.48
16:g:26:ASN:ND2	16:g:29:GLN:OE1	2.46	0.48
17:h:37:CYS:SG	17:h:38:VAL:N	2.84	0.48
17:h:43:LEU:H	17:h:43:LEU:HG	1.41	0.48
2:B:12:PHE:N	3:C:18:GLN:OE1	2.44	0.48
2:B:119:GLN:HA	2:B:122:THR:HG22	1.94	0.48
4:D:103:TYR:O	4:D:105:GLU:N	2.44	0.48
7:G:77:GLY:HA3	7:G:227:PHE:CE1	2.48	0.48
8:H:86:CYS:SG	8:H:141:LEU:HB3	2.54	0.48
4:R:28:ILE:HD13	4:R:158:PRO:HD2	1.95	0.48
11:Y:98:PRO:HA	11:Y:243:TRP:HE1	1.78	0.48
2:B:90:LEU:HD21	2:B:114:LEU:HB2	1.95	0.48
2:B:187:LYS:HA	2:B:190:LEU:HB2	1.94	0.48
3:C:227:LYS:HA	3:C:230:ALA:HB3	1.96	0.48
6:F:203:GLU:HB2	6:F:207:LYS:NZ	2.27	0.48
11:K:217:ARG:HD2	11:K:258:TYR:CZ	2.48	0.48
2:P:187:LYS:HA	2:P:190:LEU:HB2	1.94	0.48
7:U:13:ILE:HG13	7:U:24:GLN:HB2	1.94	0.48
16:g:2:PHE:CZ	16:g:45:GLY:HA3	2.49	0.48
17:h:126:VAL:O	17:h:127:MET:HE2	2.13	0.48
1:A:9:LEU:HD22	1:A:128:PRO:HD3	1.94	0.48
4:D:120:ALA:O	4:D:121:LEU:HG	2.14	0.48
12:L:200:MET:HE2	12:L:225:ILE:HD11	1.96	0.48
2:P:192:LEU:O	2:P:196:VAL:HG23	2.14	0.48
1:A:88:ARG:HD3	17:e:100:LEU:CD1	2.43	0.48
9:I:11:MET:SD	9:I:166:ILE:HG13	2.54	0.48
11:K:61:THR:HB	11:K:76:ASP:OD2	2.12	0.48
15:c:144:ASP:OD1	15:c:145:GLN:HG2	2.13	0.48
16:d:26:ASN:ND2	16:d:29:GLN:OE1	2.46	0.48
1:O:175:LYS:O	1:O:176:ARG:HG2	2.14	0.48
4:R:18:GLU:HB3	15:f:171:HIS:NE2	2.29	0.48
6:T:203:GLU:HB2	6:T:207:LYS:NZ	2.28	0.48
7:U:77:GLY:HA3	7:U:227:PHE:CE1	2.48	0.48
7:U:239:LEU:O	7:U:242:LEU:HB2	2.14	0.48
9:W:11:MET:SD	9:W:166:ILE:HG13	2.54	0.48
9:W:125:LEU:HD23	9:W:125:LEU:H	1.79	0.48
12:Z:66:ARG:HB3	12:Z:219:ASP:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LYS:HZ3	3:C:129:ILE:HG13	1.79	0.48
3:C:228:TYR:O	3:C:232:ILE:HG13	2.14	0.48
4:D:28:ILE:HD13	4:D:158:PRO:HD2	1.95	0.48
6:F:237:LYS:O	6:F:240:LYS:N	2.45	0.48
7:G:239:LEU:O	7:G:242:LEU:HB2	2.14	0.48
5:S:17:GLY:HA3	6:T:29:ALA:HA	1.96	0.48
5:S:44:ALA:HB1	5:S:144:ILE:HD11	1.96	0.48
4:D:18:GLU:HB3	15:c:171:HIS:NE2	2.29	0.48
6:F:22:GLN:O	6:F:130:PRO:HG2	2.14	0.48
6:F:65:ARG:HH21	6:F:78:ALA:HA	1.79	0.48
9:I:137:VAL:HG11	9:I:145:MET:HB3	1.95	0.48
11:K:30:LEU:HD21	13:M:136:TRP:CD1	2.49	0.48
16:d:15:PHE:CZ	16:d:81:PRO:HA	2.49	0.48
1:O:83:ARG:O	1:O:87:HIS:ND1	2.43	0.48
4:R:17:PRO:C	4:R:18:GLU:HG3	2.37	0.48
8:V:93:ALA:HB3	9:W:126:ILE:HD12	1.96	0.48
16:g:151:VAL:HG13	16:g:155:ILE:CD1	2.44	0.48
15:c:80:VAL:HA	15:c:136:GLN:OE1	2.14	0.48
16:d:15:PHE:CD1	16:d:84:LYS:HA	2.49	0.48
3:Q:227:LYS:HA	3:Q:230:ALA:HB3	1.96	0.47
10:X:22:ALA:HA	10:X:27:GLN:HA	1.96	0.47
10:X:38:MET:HE3	10:X:44:LEU:HB3	1.94	0.47
12:Z:200:MET:HE2	12:Z:225:ILE:HD11	1.96	0.47
1:A:175:LYS:O	1:A:176:ARG:HG2	2.14	0.47
5:E:44:ALA:HB1	5:E:144:ILE:HD11	1.96	0.47
13:M:206:SER:OG	13:M:209:GLU:OE2	2.28	0.47
16:d:139:PHE:O	16:d:140:ARG:NH1	2.44	0.47
3:Q:228:TYR:O	3:Q:232:ILE:HG13	2.14	0.47
5:S:185:ASN:O	5:S:189:LYS:HG2	2.13	0.47
9:W:90:VAL:HG21	9:W:108:ILE:HD11	1.95	0.47
10:X:35:MET:HE3	10:X:45:LEU:HD21	1.96	0.47
10:X:56:PHE:HE2	10:X:102:LEU:HD21	1.78	0.47
16:g:15:PHE:CZ	16:g:81:PRO:HA	2.49	0.47
2:B:49:ARG:HG3	2:B:49:ARG:O	2.14	0.47
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.95	0.47
8:H:28:ASP:HB2	8:H:36:LEU:CB	2.42	0.47
8:H:35:LYS:HZ1	9:I:55:LEU:HG	1.77	0.47
12:L:44:ALA:HB2	12:L:149:VAL:HG23	1.95	0.47
16:d:133:GLN:HG3	16:d:140:ARG:HH21	1.79	0.47
2:P:4:ARG:HG2	3:Q:5:ARG:NE	2.23	0.47
4:R:120:ALA:O	4:R:121:LEU:HG	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:137:VAL:HG11	9:W:145:MET:HB3	1.95	0.47
15:f:51:ARG:O	15:f:55:LYS:N	2.45	0.47
9:I:125:LEU:HD23	9:I:125:LEU:H	1.79	0.47
10:J:56:PHE:HE2	10:J:102:LEU:HD21	1.78	0.47
4:R:36:THR:HA	4:R:171:GLY:HA3	1.97	0.47
4:R:82:ILE:H	4:R:82:ILE:HG13	1.24	0.47
4:D:209:LYS:HD3	4:D:210:LEU:H	1.78	0.47
11:K:217:ARG:NH2	11:K:221:GLN:OE1	2.47	0.47
15:c:71:PHE:N	15:c:163:GLN:O	2.42	0.47
1:O:70:HIS:HA	1:O:217:PHE:H	1.79	0.47
3:Q:83:VAL:HG11	3:Q:129:ILE:HD11	1.96	0.47
11:Y:28:LEU:HD11	13:a:144:ARG:NH1	2.20	0.47
16:g:15:PHE:CD1	16:g:84:LYS:HA	2.49	0.47
2:B:123:GLN:HG2	2:B:124:PHE:H	1.80	0.47
8:H:9:PRO:CG	17:e:126:VAL:O	2.62	0.47
15:c:48:ARG:NH2	15:c:100:LYS:HD2	2.30	0.47
3:Q:124:ARG:HD3	3:Q:124:ARG:H	1.79	0.47
6:T:22:GLN:O	6:T:130:PRO:HG2	2.14	0.47
16:g:142:LEU:HB2	16:g:203:VAL:HB	1.96	0.47
3:C:98:VAL:O	3:C:98:VAL:HG12	2.14	0.47
11:K:34:SER:O	11:K:35:LEU:C	2.57	0.47
15:c:38:ARG:HD2	16:d:97:TYR:CE2	2.47	0.47
16:d:151:VAL:HG13	16:d:155:ILE:CD1	2.44	0.47
16:d:186:ILE:HA	16:d:189:THR:HG22	1.95	0.47
2:P:12:PHE:N	3:Q:18:GLN:OE1	2.44	0.47
6:T:75:MET:HE2	6:T:135:PHE:CD2	2.50	0.47
7:U:190:THR:N	7:U:193:GLN:OE1	2.40	0.47
7:U:223:GLU:H	7:U:223:GLU:CD	2.23	0.47
9:W:117:LYS:HE2	9:W:117:LYS:HB2	1.65	0.47
15:f:88:MET:HE1	15:f:124:TYR:HB2	1.97	0.47
16:g:27:VAL:HG21	16:g:208:VAL:HG21	1.97	0.47
16:g:133:GLN:HG3	16:g:140:ARG:HH21	1.79	0.47
1:A:70:HIS:HA	1:A:217:PHE:H	1.79	0.47
1:A:73:LEU:HD23	1:A:135:ILE:HG12	1.96	0.47
2:B:192:LEU:O	2:B:196:VAL:HG23	2.14	0.47
2:B:198:ASN:ND2	2:B:201:MET:SD	2.81	0.47
4:D:88:LEU:HA	4:D:88:LEU:HD23	1.77	0.47
6:F:75:MET:HE2	6:F:135:PHE:CD2	2.50	0.47
10:J:4:LEU:HD22	10:J:45:LEU:HB3	1.97	0.47
15:c:243:ASP:OD1	15:c:244:LEU:N	2.46	0.47
16:d:2:PHE:CZ	16:d:45:GLY:HA3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:142:LEU:HB2	16:d:203:VAL:HB	1.96	0.47
4:R:15:PHE:HE1	4:R:21:LEU:HG	1.80	0.47
4:R:35:SER:OG	4:R:66:LYS:HE2	2.14	0.47
6:T:135:PHE:CE2	6:T:151:ILE:HD13	2.50	0.47
13:a:231:ARG:HH21	13:a:247:PRO:HG3	1.79	0.47
1:A:94:GLN:O	1:A:98:LEU:HD12	2.14	0.47
3:C:124:ARG:HD3	3:C:124:ARG:H	1.79	0.47
3:C:231:GLU:HG2	3:C:234:LYS:HD3	1.97	0.47
5:E:13:TRP:N	6:F:22:GLN:HE22	2.11	0.47
7:G:21:ARG:NH2	16:d:135:ARG:NH2	2.62	0.47
10:J:15:VAL:HB	10:J:45:LEU:HD11	1.97	0.47
11:K:98:PRO:HA	11:K:243:TRP:HE1	1.78	0.47
1:O:76:SER:OG	1:O:162:MET:HE2	2.15	0.47
8:V:170[B]:MET:HB3	8:V:170[B]:MET:HE2	1.59	0.47
8:V:182:GLU:OE2	13:M:223:TYR:HD2	1.95	0.47
10:X:91:CYS:O	10:X:97:PRO:HA	2.15	0.47
10:X:154:GLU:HG2	10:X:155:ARG:N	2.29	0.47
11:Y:34:SER:O	11:Y:35:LEU:C	2.57	0.47
11:Y:135:VAL:HG23	11:Y:164:ASP:HB3	1.97	0.47
13:a:65:VAL:HG23	13:a:165:SER:HB3	1.96	0.47
16:g:139:PHE:O	16:g:140:ARG:NH1	2.44	0.47
3:C:41:VAL:HG22	3:C:136:PHE:HE1	1.79	0.47
8:H:8:ALA:O	8:H:10:PRO:HD3	2.15	0.47
16:d:229:GLN:N	16:d:229:GLN:OE1	2.48	0.47
1:O:118:GLN:HG3	2:P:81:SER:HB2	1.97	0.47
2:P:231:LYS:HA	2:P:234:GLU:OE1	2.15	0.47
6:T:65:ARG:HH21	6:T:78:ALA:HA	1.79	0.47
10:X:35:MET:HG2	10:X:45:LEU:CD2	2.45	0.47
16:g:53:VAL:HG22	16:g:93:ILE:O	2.15	0.47
10:J:91:CYS:O	10:J:97:PRO:HA	2.15	0.47
1:O:5:TYR:CD2	1:O:14:PRO:HD3	2.50	0.46
1:O:94:GLN:O	1:O:98:LEU:HD12	2.15	0.46
1:O:100:TYR:HB3	9:W:85:THR:HG23	1.97	0.46
4:R:103:TYR:HE1	12:Z:119:MET:HG3	1.80	0.46
7:U:21:ARG:NH2	16:g:135:ARG:NH2	2.62	0.46
4:D:35:SER:OG	4:D:66:LYS:HE2	2.14	0.46
5:E:17:GLY:HA3	6:F:29:ALA:HA	1.96	0.46
6:F:135:PHE:CE2	6:F:151:ILE:HD13	2.50	0.46
7:G:118:ILE:CD1	7:G:138:MET:HE1	2.45	0.46
8:H:8:ALA:HB1	17:e:127:MET:HE1	1.97	0.46
10:J:35:MET:HE3	10:J:45:LEU:HD21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:154:GLU:HG2	10:J:155:ARG:N	2.29	0.46
14:N:38:MET:HE3	14:N:40:VAL:HG23	1.98	0.46
14:N:132:ILE:O	14:N:133:ILE:HD13	2.15	0.46
16:d:19:MET:HE3	16:d:19:MET:HB2	1.64	0.46
16:d:51:CYS:HA	16:d:98:LYS:HG2	1.97	0.46
16:d:53:VAL:HG22	16:d:93:ILE:O	2.15	0.46
1:O:176:ARG:NH1	1:O:176:ARG:CB	2.78	0.46
3:Q:98:VAL:HG12	3:Q:98:VAL:O	2.14	0.46
6:T:69:VAL:HA	6:T:92:ARG:HG2	1.97	0.46
8:V:175:LEU:H	8:V:175:LEU:HD12	1.80	0.46
8:V:222:SER:OG	8:V:223:LYS:N	2.48	0.46
10:X:4:LEU:HD22	10:X:45:LEU:HB3	1.97	0.46
15:f:48:ARG:NH2	15:f:100:LYS:HD2	2.30	0.46
15:f:170:ARG:NH2	15:f:214:ASP:OD2	2.39	0.46
16:g:229:GLN:OE1	16:g:229:GLN:N	2.48	0.46
4:D:190:THR:O	4:D:193:GLU:HG2	2.15	0.46
10:J:22:ALA:HA	10:J:27:GLN:HA	1.96	0.46
15:c:166:ILE:HG13	15:c:232:LEU:HA	1.97	0.46
3:Q:229:VAL:O	3:Q:232:ILE:N	2.49	0.46
3:Q:231:GLU:HG2	3:Q:234:LYS:HD3	1.97	0.46
7:U:112:ASP:HB3	7:U:152:TYR:HE2	1.80	0.46
7:U:118:ILE:CD1	7:U:138:MET:HE1	2.45	0.46
10:X:15:VAL:HB	10:X:45:LEU:HD11	1.97	0.46
15:f:243:ASP:OD1	15:f:244:LEU:N	2.46	0.46
3:C:229:VAL:O	3:C:232:ILE:N	2.49	0.46
4:D:103:TYR:HE1	12:L:119:MET:HG3	1.80	0.46
6:F:69:VAL:HA	6:F:92:ARG:HG2	1.97	0.46
8:H:18:ASN:N	10:J:93:ARG:HB3	2.29	0.46
8:H:175:LEU:HD12	8:H:175:LEU:H	1.80	0.46
16:d:43:LYS:HA	16:d:78:TYR:HD1	1.81	0.46
3:Q:41:VAL:HG22	3:Q:136:PHE:HE1	1.79	0.46
4:R:190:THR:O	4:R:193:GLU:HG2	2.15	0.46
4:R:234:LEU:O	4:R:238:ILE:HG12	2.16	0.46
8:V:18:ASN:N	10:X:93:ARG:HB3	2.29	0.46
1:A:118:GLN:O	1:A:121:THR:OG1	2.31	0.46
2:B:231:LYS:HA	2:B:234:GLU:OE1	2.15	0.46
5:E:225:ASP:O	5:E:229:VAL:HG13	2.16	0.46
6:F:68:ASN:OD1	6:F:224:HIS:ND1	2.38	0.46
7:G:23:TYR:HB3	7:G:27:TYR:CE2	2.50	0.46
7:G:144:ASP:OD1	7:G:144:ASP:N	2.49	0.46
11:K:30:LEU:HG	13:M:136:TRP:HE1	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:141:MET:SD	13:M:155:MET:HE1	2.55	0.46
3:Q:116:GLN:NE2	3:Q:120:GLN:HE22	2.14	0.46
4:R:119:LEU:HD12	4:R:119:LEU:HA	1.73	0.46
13:a:155:MET:HE2	13:a:155:MET:HB2	1.74	0.46
1:A:5:TYR:CD2	1:A:14:PRO:HD3	2.50	0.46
1:A:176:ARG:NH1	1:A:176:ARG:CB	2.78	0.46
6:F:114:ARG:HE	17:e:72:GLY:HA2	1.80	0.46
7:G:123:GLN:O	7:G:126:THR:OG1	2.31	0.46
8:H:93:ALA:HB3	9:I:126:ILE:HD12	1.96	0.46
10:J:45:LEU:HD12	10:J:103:LEU:HD23	1.98	0.46
11:K:135:VAL:HG23	11:K:164:ASP:HB3	1.97	0.46
16:d:27:VAL:HG21	16:d:208:VAL:HG21	1.97	0.46
1:O:73:LEU:HD23	1:O:135:ILE:HG12	1.96	0.46
3:Q:12:PRO:HB2	15:f:104:GLU:CG	2.46	0.46
6:T:114:ARG:HE	17:h:72:GLY:HA2	1.80	0.46
9:W:11:MET:HE1	9:W:149:CYS:SG	2.56	0.46
10:X:91:CYS:HB3	10:X:95:ARG:NH1	2.30	0.46
4:D:36:THR:HA	4:D:171:GLY:HA3	1.96	0.46
10:J:34:LYS:HD3	10:J:47:VAL:HG12	1.98	0.46
10:J:92:LEU:HD12	10:J:97:PRO:CB	2.45	0.46
15:c:115:SER:O	15:c:117:THR:N	2.48	0.46
4:R:101:PHE:CD1	11:Y:116:ARG:HG2	2.51	0.46
5:S:225:ASP:O	5:S:229:VAL:HG13	2.16	0.46
7:U:23:TYR:HB3	7:U:27:TYR:CE2	2.50	0.46
14:b:132:ILE:O	14:b:133:ILE:HD13	2.16	0.46
16:g:119:ILE:HG23	16:g:202:ALA:HB3	1.96	0.46
3:C:221:ASN:C	3:C:221:ASN:OD1	2.58	0.46
4:D:15:PHE:HE1	4:D:21:LEU:HG	1.80	0.46
4:D:209:LYS:HD3	4:D:209:LYS:HA	1.67	0.46
8:H:28:ASP:CB	8:H:34:TYR:HA	2.45	0.46
15:c:88:MET:HE1	15:c:124:TYR:HB2	1.96	0.46
16:d:175:SER:OG	16:d:176:GLU:N	2.49	0.46
13:a:54:THR:HG23	13:a:55:SER:N	2.30	0.46
14:b:95:TYR:HE2	17:h:66:THR:HG21	1.80	0.46
15:f:115:SER:O	15:f:117:THR:N	2.48	0.46
1:A:118:GLN:HG3	2:B:81:SER:HB2	1.97	0.46
2:B:136:TYR:O	2:B:147:LEU:HD12	2.15	0.46
6:F:231:ILE:HA	6:F:234:GLU:HG2	1.97	0.46
7:G:112:ASP:HB3	7:G:152:TYR:HE2	1.80	0.46
8:H:28:ASP:HA	8:H:34:TYR:HB3	1.98	0.46
8:H:94:ASP:HB3	8:H:137:ILE:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:222:SER:OG	8:H:223:LYS:N	2.49	0.46
9:I:11:MET:HE1	9:I:149:CYS:SG	2.56	0.46
13:M:152:TRP:CE3	13:M:172:MET:HE1	2.51	0.46
2:P:49:ARG:HG3	2:P:49:ARG:O	2.15	0.46
2:P:201:MET:HB2	2:P:202:ASP:O	2.16	0.46
8:V:8:ALA:HB1	17:h:127:MET:HE1	1.97	0.46
8:V:28:ASP:CB	8:V:34:TYR:HA	2.45	0.46
13:M:88:MET:SD	13:M:109:LYS:HG2	2.56	0.46
9:W:122:SER:HB2	9:W:136:VAL:HB	1.98	0.46
1:A:76:SER:OG	1:A:162:MET:HE2	2.15	0.46
3:C:83:VAL:HG11	3:C:129:ILE:HD11	1.96	0.46
3:C:146:GLN:HB2	3:C:159:ASN:HD21	1.80	0.46
4:D:234:LEU:O	4:D:238:ILE:HG12	2.16	0.46
7:G:50:ILE:HG23	7:G:141:ILE:HD13	1.97	0.46
10:J:35:MET:HG2	10:J:45:LEU:CD2	2.45	0.46
2:P:106:PRO:HG2	10:X:73:TYR:OH	2.16	0.45
7:U:144:ASP:OD1	7:U:144:ASP:N	2.49	0.45
13:a:88:MET:SD	13:a:109:LYS:HG2	2.56	0.45
13:a:141:MET:SD	13:a:155:MET:HE1	2.55	0.45
15:f:166:ILE:HG13	15:f:232:LEU:HA	1.97	0.45
16:g:176:GLU:H	16:g:176:GLU:HG3	1.45	0.45
3:C:157:LYS:HE2	3:C:157:LYS:HB2	1.51	0.45
6:F:150:MET:HG3	6:F:163:CYS:SG	2.56	0.45
11:K:240:GLU:O	11:K:241:ASP:C	2.59	0.45
11:K:245[A]:ARG:HE	11:K:245[A]:ARG:HB2	1.52	0.45
12:L:41:LEU:HD11	12:L:177:LEU:HD11	1.98	0.45
12:L:218:GLY:HA2	12:L:238:LEU:HD12	1.98	0.45
13:M:155:MET:HE2	13:M:155:MET:HB2	1.75	0.45
13:M:169:TYR:HB2	13:M:182:LEU:HD13	1.98	0.45
16:d:53:VAL:HG23	16:d:92:SER:HB2	1.98	0.45
3:Q:157:LYS:HE2	3:Q:157:LYS:HB2	1.51	0.45
4:R:175:GLU:H	4:R:175:GLU:CD	2.21	0.45
10:X:140:LEU:HA	10:X:140:LEU:HD23	1.78	0.45
15:f:48:ARG:HH11	15:f:48:ARG:HG3	1.81	0.45
16:g:19:MET:HG2	16:g:120:VAL:HG22	1.98	0.45
16:g:43:LYS:HA	16:g:78:TYR:HD1	1.80	0.45
16:g:175:SER:OG	16:g:176:GLU:N	2.49	0.45
2:B:106:PRO:HG2	10:J:73:TYR:OH	2.16	0.45
5:E:114:SER:O	5:E:118:ILE:HG12	2.16	0.45
13:M:54:THR:HG23	13:M:55:SER:N	2.30	0.45
15:c:48:ARG:HH11	15:c:48:ARG:HG3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:119:ILE:HG23	16:d:202:ALA:HB3	1.96	0.45
17:e:39:LYS:HB3	17:e:39:LYS:HE3	1.48	0.45
3:Q:221:ASN:OD1	3:Q:221:ASN:C	2.58	0.45
5:S:114:SER:O	5:S:118:ILE:HG12	2.16	0.45
7:U:86:ASP:HB3	7:U:134:LEU:HB3	1.98	0.45
8:V:28:ASP:HA	8:V:34:TYR:HB3	1.98	0.45
10:X:93:ARG:HB2	10:X:94:SER:H	1.55	0.45
14:b:134:ILE:H	14:b:134:ILE:HD12	1.81	0.45
15:f:82:PHE:HD2	15:f:83:LEU:HD22	1.82	0.45
16:g:53:VAL:HG23	16:g:92:SER:HB2	1.98	0.45
3:C:116:GLN:NE2	3:C:120:GLN:HE22	2.14	0.45
7:G:223:GLU:H	7:G:223:GLU:CD	2.23	0.45
10:J:69:MET:HE3	10:J:69:MET:HB3	1.69	0.45
16:d:176:GLU:H	16:d:176:GLU:HG3	1.45	0.45
1:O:57:ASP:OD1	1:O:58:GLU:N	2.50	0.45
4:R:26:TYR:O	4:R:29:GLU:HB2	2.17	0.45
6:T:76:ALA:HB3	6:T:136:MET:HE3	1.99	0.45
6:T:134:SER:OG	6:T:153:PRO:HD3	2.17	0.45
6:T:150:MET:HG3	6:T:163:CYS:SG	2.56	0.45
6:T:190:VAL:HG21	6:T:215:TRP:CZ3	2.51	0.45
6:T:231:ILE:HA	6:T:234:GLU:HG2	1.97	0.45
10:X:45:LEU:HD12	10:X:103:LEU:HD23	1.98	0.45
11:Y:245[A]:ARG:HE	11:Y:245[A]:ARG:HB2	1.52	0.45
12:Z:218:GLY:HA2	12:Z:238:LEU:HD12	1.98	0.45
16:g:51:CYS:HA	16:g:98:LYS:HG2	1.97	0.45
3:C:12:PRO:HB2	15:c:104:GLU:CG	2.46	0.45
3:C:96:LEU:HD21	17:e:31:LEU:HB3	1.98	0.45
16:d:143:LEU:O	16:d:191:TYR:OH	2.30	0.45
3:Q:99:GLU:OE1	11:Y:140:LYS:HE2	2.16	0.45
3:Q:146:GLN:HB2	3:Q:159:ASN:HD21	1.80	0.45
5:S:13:TRP:N	6:T:22:GLN:HE22	2.11	0.45
6:T:25:TYR:O	6:T:29:ALA:N	2.50	0.45
7:U:12:HIS:CG	7:U:13:ILE:H	2.35	0.45
8:V:9:PRO:CG	17:h:126:VAL:O	2.62	0.45
9:W:204:ASP:OD2	11:K:251:VAL:HG21	2.17	0.45
10:X:92:LEU:HD12	10:X:97:PRO:CB	2.45	0.45
12:Z:41:LEU:HD11	12:Z:177:LEU:HD11	1.98	0.45
13:a:169:TYR:HB2	13:a:182:LEU:HD13	1.98	0.45
1:A:176:ARG:CB	1:A:176:ARG:HH11	2.29	0.45
2:B:201:MET:H	2:B:201:MET:HG2	1.55	0.45
8:H:138:GLY:HA2	8:H:158:PRO:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:23:ALA:HB2	9:I:41:ILE:HD11	1.99	0.45
6:T:156:VAL:HG22	7:U:84:THR:HB	1.98	0.45
8:V:8:ALA:O	8:V:10:PRO:HD3	2.15	0.45
10:X:91:CYS:CB	10:X:95:ARG:HH12	2.29	0.45
13:a:141:MET:CE	13:a:155:MET:HE1	2.46	0.45
1:A:100:TYR:HB3	9:I:85:THR:HG23	1.98	0.45
3:C:99:GLU:OE1	11:K:140:LYS:HE2	2.16	0.45
5:E:206:THR:HG23	5:E:208:LYS:H	1.81	0.45
6:F:190:VAL:HG21	6:F:215:TRP:CZ3	2.51	0.45
8:H:60:ASP:OD1	8:H:76:LYS:NZ	2.47	0.45
8:H:119:VAL:HG23	8:H:147[A]:ASP:OD1	2.17	0.45
10:J:94:SER:HB2	10:J:95:ARG:H	1.70	0.45
12:L:121:SER:OG	12:L:156:GLY:O	2.25	0.45
15:c:82:PHE:HD2	15:c:83:LEU:HD22	1.82	0.45
17:e:43:LEU:H	17:e:43:LEU:HG	1.41	0.45
8:V:30:ALA:O	8:V:32:ARG:N	2.50	0.45
17:h:117:ILE:HG13	17:h:118:LEU:HG	1.99	0.45
3:C:4:ASP:HA	3:C:17:PHE:CB	2.47	0.45
4:D:32:LYS:HB2	15:c:107:ARG:NH1	2.32	0.45
4:D:101:PHE:CD1	11:K:116:ARG:HG2	2.51	0.45
6:F:134:SER:OG	6:F:153:PRO:HD3	2.17	0.45
13:M:141:MET:CE	13:M:155:MET:HE1	2.46	0.45
14:N:95:TYR:HE2	17:e:66:THR:HG21	1.80	0.45
3:Q:11:SER:O	3:Q:14:GLY:N	2.50	0.45
3:Q:229:VAL:HA	3:Q:232:ILE:HD12	1.99	0.45
4:R:32:LYS:HB2	15:f:107:ARG:NH1	2.32	0.45
4:R:142:LEU:HD23	4:R:142:LEU:HA	1.80	0.45
14:b:129:MET:HE2	14:b:129:MET:HB3	1.87	0.45
2:B:201:MET:HB2	2:B:202:ASP:O	2.16	0.45
4:D:26:TYR:O	4:D:29:GLU:HB2	2.17	0.45
4:D:133:MET:HE2	4:D:137:PHE:CZ	2.52	0.45
4:D:185:TYR:CD2	5:E:56:LEU:HD11	2.52	0.45
7:G:12:HIS:CG	7:G:13:ILE:H	2.35	0.45
1:O:81:ASP:CG	1:O:127:ARG:HH22	2.24	0.45
2:P:136:TYR:O	2:P:147:LEU:HD12	2.15	0.45
3:Q:4:ASP:HA	3:Q:17:PHE:CB	2.47	0.45
10:X:34:LYS:HD3	10:X:47:VAL:HG12	1.98	0.45
13:a:124:ASP:OD1	13:a:124:ASP:N	2.50	0.45
13:a:152:TRP:CE3	13:a:172:MET:HE1	2.51	0.45
15:f:82:PHE:CD2	15:f:83:LEU:HD22	2.52	0.45
16:g:106:LEU:O	16:g:110:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:h:31:LEU:HG	17:h:35:PHE:HB3	1.98	0.45
1:A:81:ASP:CG	1:A:127:ARG:HH22	2.24	0.45
6:F:25:TYR:O	6:F:29:ALA:N	2.50	0.45
6:F:76:ALA:HB3	6:F:136:MET:HE3	1.99	0.45
6:F:156:VAL:HG22	7:G:84:THR:HB	1.98	0.45
16:d:246:LYS:HD3	16:d:246:LYS:HA	1.80	0.45
17:e:31:LEU:HG	17:e:35:PHE:HB3	1.98	0.45
1:O:194:LEU:HD23	1:O:194:LEU:HA	1.79	0.45
2:P:123:GLN:HG2	2:P:124:PHE:H	1.80	0.45
3:Q:96:LEU:HD21	17:h:31:LEU:HB3	1.98	0.45
7:U:50:ILE:HG23	7:U:141:ILE:HD13	1.98	0.45
8:V:179:ALA:CB	13:M:194:LEU:HD11	2.45	0.45
9:W:23:ALA:HB2	9:W:41:ILE:HD11	1.99	0.45
15:f:71:PHE:N	15:f:163:GLN:O	2.42	0.45
4:D:15:PHE:CZ	5:E:126:ARG:HD2	2.52	0.45
5:E:60:GLN:HG3	5:E:61:LYS:N	2.31	0.45
7:G:86:ASP:HB3	7:G:134:LEU:HB3	1.98	0.45
8:H:4:VAL:HG13	17:e:32:ARG:NH1	2.32	0.45
8:H:30:ALA:O	8:H:32:ARG:N	2.50	0.45
9:I:122:SER:HB2	9:I:136:VAL:HB	1.98	0.45
10:J:91:CYS:HB3	10:J:95:ARG:NH1	2.30	0.45
15:c:51:ARG:O	15:c:55:LYS:N	2.45	0.45
16:d:19:MET:HG2	16:d:120:VAL:HG22	1.98	0.45
4:R:185:TYR:CD2	5:S:56:LEU:HD11	2.52	0.44
5:S:98:VAL:HG11	11:Y:30:LEU:HD11	1.99	0.44
8:V:119:VAL:HG23	8:V:147[A]:ASP:OD1	2.17	0.44
3:C:11:SER:O	3:C:14:GLY:N	2.50	0.44
4:D:82:ILE:H	4:D:82:ILE:HG13	1.24	0.44
8:H:15:SER:O	8:H:16:PHE:CD2	2.70	0.44
10:J:44:LEU:HD13	10:J:104:LEU:HD12	1.99	0.44
13:M:98:ALA:HB2	13:M:155:MET:HG3	1.99	0.44
14:N:134:ILE:H	14:N:134:ILE:HD12	1.81	0.44
17:e:55:PHE:HA	17:e:58:ASN:HB2	1.99	0.44
17:e:75:ALA:O	17:e:79:LEU:HD22	2.17	0.44
8:V:94:ASP:HB3	8:V:137:ILE:HG23	1.98	0.44
9:W:87:MET:SD	9:W:129:PRO:HB3	2.58	0.44
12:Z:121:SER:OG	12:Z:156:GLY:O	2.25	0.44
14:b:37:ILE:HD12	14:b:133:ILE:HG12	1.99	0.44
14:b:132:ILE:C	14:b:133:ILE:HD13	2.42	0.44
15:f:38:ARG:HD2	16:g:97:TYR:CE2	2.47	0.44
4:D:182:GLN:HG2	4:D:183:GLU:N	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:132:ILE:C	14:N:133:ILE:HD13	2.42	0.44
1:O:176:ARG:CB	1:O:176:ARG:HH11	2.29	0.44
3:Q:16:LEU:HD12	3:Q:16:LEU:O	2.17	0.44
4:R:84:ASP:HB3	4:R:137:PHE:HD2	1.83	0.44
4:R:133:MET:HE2	4:R:137:PHE:CZ	2.52	0.44
5:S:43:HIS:CD2	5:S:216:GLY:HA3	2.52	0.44
5:S:206:THR:HG23	5:S:208:LYS:H	1.81	0.44
8:V:4:VAL:HG13	17:h:32:ARG:NH1	2.32	0.44
1:A:203:THR:OG1	1:A:204:GLU:N	2.49	0.44
3:C:16:LEU:HD12	3:C:16:LEU:O	2.17	0.44
5:E:111:LEU:HD23	5:E:111:LEU:HA	1.78	0.44
9:I:11:MET:CG	9:I:170:MET:HE3	2.48	0.44
10:J:35:MET:HG2	10:J:45:LEU:HD22	2.00	0.44
2:P:235:GLN:HG2	2:P:238:LYS:HE3	2.00	0.44
8:V:138:GLY:HA2	8:V:158:PRO:HB3	1.99	0.44
14:b:38:MET:HE3	14:b:40:VAL:HG23	1.98	0.44
15:f:211:ILE:HD11	16:g:55:MET:HG3	2.00	0.44
17:h:32:ARG:HA	17:h:32:ARG:HD2	1.48	0.44
1:A:83:ARG:HH12	7:G:120:ASP:CG	2.26	0.44
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.72	0.44
3:C:15:HIS:O	3:C:16:LEU:C	2.60	0.44
4:D:84:ASP:HB3	4:D:137:PHE:HD2	1.83	0.44
5:E:152:ASN:HD21	6:F:81:LEU:HD12	1.83	0.44
6:F:70:ASP:CG	6:F:99:ARG:HH22	2.26	0.44
7:G:72:ILE:HD11	7:G:78:CYS:SG	2.58	0.44
13:M:102:TYR:HD2	14:N:153:MET:HG3	1.82	0.44
15:c:189:LEU:HD21	15:c:253:ILE:HD11	1.99	0.44
15:c:242:LEU:HB3	15:c:277:MET:SD	2.57	0.44
4:R:15:PHE:CZ	5:S:126:ARG:HD2	2.52	0.44
7:U:194:THR:C	7:U:197:THR:HG22	2.43	0.44
10:X:44:LEU:HD13	10:X:104:LEU:HD12	1.99	0.44
11:Y:86:ALA:O	12:Z:164:LYS:NZ	2.37	0.44
13:a:102:TYR:HD2	14:b:153:MET:HG3	1.82	0.44
13:a:194:LEU:HD11	8:H:179:ALA:CB	2.44	0.44
16:g:151:VAL:O	16:g:155:ILE:HD12	2.18	0.44
3:C:160:ALA:O	3:C:169:ARG:NH2	2.51	0.44
5:E:43:HIS:CD2	5:E:216:GLY:HA3	2.52	0.44
9:I:117:LYS:HE2	9:I:117:LYS:HB2	1.65	0.44
15:c:82:PHE:CD2	15:c:83:LEU:HD22	2.52	0.44
6:T:70:ASP:CG	6:T:99:ARG:HH22	2.26	0.44
6:T:187:ARG:NH1	6:T:231:ILE:HG12	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:221:ASN:O	6:T:221:ASN:CG	2.61	0.44
7:U:17:SER:OG	7:U:21:ARG:N	2.48	0.44
7:U:101:TRP:CD1	7:U:101:TRP:C	2.96	0.44
10:X:171:PHE:CE2	10:X:173:LEU:HB2	2.53	0.44
11:Y:240:GLU:O	11:Y:241:ASP:C	2.60	0.44
15:f:90:SER:HB3	15:f:264:LYS:HE2	2.00	0.44
16:g:143:LEU:C	16:g:191:TYR:HH	2.23	0.44
17:h:75:ALA:O	17:h:79:LEU:HD22	2.17	0.44
3:C:153:TYR:CD1	3:C:153:TYR:C	2.96	0.44
3:C:204:LYS:HA	3:C:204:LYS:HD3	1.81	0.44
8:H:45:THR:HG21	8:H:205:GLY:HA3	1.99	0.44
10:J:43:LEU:HD23	10:J:43:LEU:HA	1.77	0.44
6:T:231:ILE:O	6:T:234:GLU:HG2	2.18	0.44
11:Y:174:ASP:OD1	11:Y:176:GLU:HG2	2.18	0.44
11:Y:217:ARG:NH2	11:Y:221:GLN:OE1	2.47	0.44
12:Z:58:SER:HB3	8:H:210:LEU:HD11	2.00	0.44
1:A:83:ARG:O	1:A:87:HIS:ND1	2.42	0.44
2:B:235:GLN:HG2	2:B:238:LYS:HE3	2.00	0.44
4:D:99:HIS:CD2	4:D:103:TYR:CD2	3.06	0.44
11:K:35:LEU:HD22	11:K:35:LEU:HA	1.80	0.44
11:K:111:CYS:O	11:K:112:SER:C	2.61	0.44
1:O:83:ARG:HH12	7:U:120:ASP:CG	2.26	0.44
4:R:202:LEU:HD12	4:R:202:LEU:HA	1.84	0.44
3:C:7:ILE:HD12	3:C:18:GLN:CB	2.34	0.44
3:C:66:ASP:CG	3:C:67:ASP:H	2.26	0.44
8:H:121:THR:O	8:H:125:MET:HG3	2.18	0.44
3:Q:200:GLN:NE2	3:Q:204:LYS:HB2	2.33	0.44
4:R:99:HIS:CD2	4:R:103:TYR:CD2	3.06	0.44
5:S:88:MET:HE1	5:S:134:ILE:HG12	2.00	0.44
5:S:164:ARG:HG2	5:S:164:ARG:HH11	1.82	0.44
8:V:15:SER:O	8:V:16:PHE:CD2	2.70	0.44
15:f:242:LEU:HB3	15:f:277:MET:SD	2.57	0.44
17:h:55:PHE:HA	17:h:58:ASN:HB2	1.99	0.44
10:J:86:ARG:NH1	10:J:90:ASP:OD1	2.50	0.44
11:K:28:LEU:CD2	13:M:144:ARG:HH11	2.27	0.44
11:K:174:ASP:OD1	11:K:176:GLU:HG2	2.18	0.44
14:N:37:ILE:HD12	14:N:133:ILE:HG12	1.99	0.44
15:c:211:ILE:HD11	16:d:55:MET:HG3	2.00	0.44
1:O:5:TYR:OH	2:P:6:ASP:OD2	2.36	0.43
1:O:132:SER:OG	1:O:150:PRO:HD3	2.18	0.43
7:U:192:GLU:C	7:U:194:THR:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:45:THR:HG21	8:V:205:GLY:HA3	1.99	0.43
13:a:98:ALA:HB2	13:a:155:MET:HG3	1.99	0.43
15:f:37:VAL:O	15:f:41:LEU:HD23	2.18	0.43
1:A:57:ASP:OD1	1:A:58:GLU:N	2.50	0.43
5:E:164:ARG:HG2	5:E:164:ARG:HH11	1.82	0.43
6:F:221:ASN:CG	6:F:221:ASN:O	2.61	0.43
7:G:143:ILE:HD13	7:G:149:PRO:HA	2.00	0.43
11:K:56:MET:HE2	11:K:56:MET:HB2	1.52	0.43
12:L:221:LEU:O	12:L:235:THR:HA	2.18	0.43
15:c:90:SER:HB3	15:c:264:LYS:HE2	2.00	0.43
16:d:22:VAL:HG22	16:d:29:GLN:NE2	2.33	0.43
16:d:106:LEU:O	16:d:110:VAL:HG23	2.17	0.43
17:e:32:ARG:HA	17:e:32:ARG:HD2	1.48	0.43
3:Q:3:TYR:C	3:Q:5:ARG:H	2.26	0.43
3:Q:15:HIS:O	3:Q:16:LEU:C	2.60	0.43
3:Q:153:TYR:C	3:Q:153:TYR:CD1	2.96	0.43
3:Q:160:ALA:O	3:Q:169:ARG:NH2	2.51	0.43
3:Q:188:ILE:O	3:Q:192:ILE:HG12	2.18	0.43
7:U:112:ASP:OD1	7:U:113:MET:N	2.51	0.43
10:X:86:ARG:NH1	10:X:90:ASP:OD1	2.50	0.43
11:Y:35:LEU:HB3	11:Y:36:SER:H	1.58	0.43
12:Z:98:ALA:O	12:Z:102:MET:HG3	2.18	0.43
3:C:185:ASP:OD1	3:C:185:ASP:C	2.61	0.43
4:D:175:GLU:H	4:D:175:GLU:CD	2.21	0.43
6:F:19:ARG:HE	6:F:21:PHE:HE1	1.66	0.43
16:d:180:ARG:HA	16:d:180:ARG:HD2	1.82	0.43
3:Q:97:THR:HG23	11:Y:144:ASN:HD22	1.83	0.43
3:Q:185:ASP:OD1	3:Q:185:ASP:C	2.61	0.43
4:R:88:LEU:HD22	4:R:116:VAL:HG13	1.99	0.43
8:V:228:PHE:CE2	8:V:230:ARG:HD3	2.54	0.43
15:f:213:HIS:O	15:f:213:HIS:CG	2.71	0.43
4:D:88:LEU:HD22	4:D:116:VAL:HG13	1.99	0.43
5:E:38:LEU:HD23	5:E:38:LEU:H	1.83	0.43
6:F:20:VAL:O	6:F:23:VAL:HG12	2.18	0.43
7:G:112:ASP:OD1	7:G:113:MET:N	2.51	0.43
7:G:185:LYS:C	7:G:185:LYS:HE2	2.44	0.43
7:G:194:THR:C	7:G:197:THR:HG22	2.42	0.43
8:H:106:LEU:HD22	8:H:122:ALA:HB2	2.00	0.43
9:I:87:MET:SD	9:I:129:PRO:HB3	2.58	0.43
15:c:75:ILE:HD13	15:c:216:PRO:HD3	2.00	0.43
17:e:117:ILE:HG13	17:e:118:LEU:HG	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:152:ASN:HD21	6:T:81:LEU:HD12	1.83	0.43
8:V:16:PHE:HE2	9:W:99:PHE:CD2	2.37	0.43
9:W:43:PRO:HA	9:W:49:TYR:HD1	1.83	0.43
10:X:24:ASN:C	10:X:26:VAL:N	2.76	0.43
10:X:94:SER:HB2	10:X:95:ARG:H	1.70	0.43
12:Z:221:LEU:O	12:Z:235:THR:HA	2.18	0.43
15:f:189:LEU:HD21	15:f:253:ILE:HD11	1.99	0.43
16:g:79:SER:HA	16:g:86:VAL:HA	2.00	0.43
3:C:229:VAL:HA	3:C:232:ILE:HD12	1.99	0.43
6:F:187:ARG:NH1	6:F:231:ILE:HG12	2.33	0.43
7:G:101:TRP:CD1	7:G:101:TRP:C	2.96	0.43
9:I:43:PRO:HA	9:I:49:TYR:HD1	1.83	0.43
15:c:213:HIS:O	15:c:213:HIS:CG	2.71	0.43
16:d:12:LEU:HA	16:d:15:PHE:CD2	2.53	0.43
2:P:123:GLN:O	2:P:124:PHE:C	2.62	0.43
5:S:35:THR:HG23	5:S:133:LEU:HD12	2.01	0.43
6:T:229:LYS:HG2	6:T:233:GLU:OE1	2.19	0.43
7:U:72:ILE:HD11	7:U:78:CYS:SG	2.58	0.43
11:Y:251:VAL:HG21	9:I:204:ASP:OD2	2.18	0.43
2:B:139:TRP:CG	2:B:218:ARG:HD3	2.54	0.43
3:C:200:GLN:NE2	3:C:204:LYS:HB2	2.33	0.43
6:F:229:LYS:HG2	6:F:233:GLU:OE1	2.19	0.43
9:I:105:GLU:HG2	9:I:124:ASP:HA	2.00	0.43
15:c:52:ARG:HD2	15:c:98:CYS:SG	2.59	0.43
1:O:67:ILE:HD11	1:O:73:LEU:CD1	2.48	0.43
2:P:8:ARG:O	2:P:9:THR:HG22	2.19	0.43
2:P:60:PHE:O	2:P:62:SER:N	2.52	0.43
3:Q:66:ASP:CG	3:Q:67:ASP:H	2.26	0.43
6:T:20:VAL:O	6:T:23:VAL:HG12	2.18	0.43
6:T:43:ASP:HB2	6:T:218:GLU:HB3	2.01	0.43
8:V:85:TYR:HB2	8:V:221:ILE:HD11	2.01	0.43
1:A:132:SER:OG	1:A:150:PRO:HD3	2.18	0.43
1:A:170:LYS:HE2	1:A:170:LYS:HB3	1.43	0.43
3:C:97:THR:HG23	11:K:144:ASN:HD22	1.83	0.43
6:F:201:HIS:NE2	6:F:203:GLU:HA	2.34	0.43
8:H:16:PHE:HE2	9:I:99:PHE:CD2	2.37	0.43
8:H:81:SER:O	8:H:83:ASN:N	2.52	0.43
8:H:130:LEU:HD23	8:H:130:LEU:HA	1.86	0.43
10:J:143:LEU:HA	10:J:143:LEU:HD23	1.81	0.43
12:L:98:ALA:O	12:L:102:MET:HG3	2.18	0.43
3:Q:172:LEU:HD23	4:R:58:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:219:LEU:HD23	6:T:219:LEU:H	1.84	0.43
7:U:143:ILE:HD13	7:U:149:PRO:HA	2.00	0.43
8:V:4:VAL:HB	17:h:129:GLU:HG3	2.00	0.43
10:X:29:LYS:HE3	10:X:29:LYS:HB3	1.73	0.43
1:A:195:LYS:HA	1:A:198:PHE:HB2	2.01	0.43
5:E:228:ASP:O	5:E:231:PRO:HD2	2.19	0.43
7:G:17:SER:OG	7:G:21:ARG:N	2.48	0.43
8:H:35:LYS:HZ1	9:I:55:LEU:N	2.15	0.43
15:c:286:ILE:HG23	15:c:288:THR:N	2.32	0.43
2:P:74:CYS:SG	2:P:75:SER:N	2.92	0.43
2:P:139:TRP:HE1	2:P:144:GLY:HA2	1.83	0.43
5:S:38:LEU:HD23	5:S:38:LEU:H	1.83	0.43
5:S:133:LEU:HD23	5:S:133:LEU:HA	1.83	0.43
9:W:11:MET:CG	9:W:170:MET:HE3	2.48	0.43
15:f:52:ARG:HD2	15:f:98:CYS:SG	2.59	0.43
16:g:15:PHE:HD1	16:g:84:LYS:HA	1.83	0.43
3:C:3:TYR:C	3:C:5:ARG:H	2.26	0.43
5:E:35:THR:HG23	5:E:133:LEU:HD12	2.01	0.43
6:F:231:ILE:O	6:F:234:GLU:HG2	2.18	0.43
8:H:4:VAL:HB	17:e:129:GLU:HG3	2.00	0.43
10:J:171:PHE:CE2	10:J:173:LEU:HB2	2.53	0.43
13:M:169:TYR:O	13:M:176:ALA:HA	2.19	0.43
15:c:37:VAL:O	15:c:41:LEU:HD23	2.19	0.43
3:Q:68:ASN:HA	3:Q:211:MET:HE1	2.01	0.43
3:Q:124:ARG:HH12	17:h:140:LEU:CD2	2.22	0.43
7:U:185:LYS:C	7:U:185:LYS:HE2	2.44	0.43
10:X:69:MET:HE3	10:X:69:MET:HB3	1.69	0.43
15:f:120:PHE:HD1	15:f:139:CYS:HB3	1.84	0.43
16:g:129:ARG:HB3	16:g:133:GLN:HB2	2.01	0.43
16:g:212:ASP:OD1	16:g:212:ASP:N	2.52	0.43
1:A:114:ALA:HB1	1:A:152:GLY:O	2.19	0.43
1:A:159:ALA:O	2:B:55:LEU:HD13	2.19	0.43
2:B:76:VAL:HA	2:B:134:LEU:HD23	2.01	0.43
6:F:43:ASP:HB2	6:F:218:GLU:HB3	2.01	0.43
8:H:143:LEU:HB3	8:H:154:TYR:HB2	2.01	0.43
16:d:151:VAL:O	16:d:155:ILE:HD12	2.18	0.43
1:O:159:ALA:O	2:P:55:LEU:HD13	2.19	0.43
2:P:76:VAL:HA	2:P:134:LEU:HD23	2.01	0.43
3:Q:229:VAL:O	3:Q:230:ALA:C	2.62	0.43
7:U:152:TYR:CD1	7:U:162:GLY:HA2	2.54	0.43
11:Y:35:LEU:HD22	11:Y:35:LEU:HA	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:55:THR:HG22	12:Z:69:PRO:HA	2.01	0.43
1:A:178:ASN:H	1:A:181:LEU:HD12	1.84	0.43
2:B:60:PHE:O	2:B:62:SER:N	2.52	0.43
3:C:188:ILE:O	3:C:192:ILE:HG12	2.18	0.43
5:E:171:TYR:HD2	5:E:194:ALA:HA	1.84	0.43
5:E:202:GLU:HB3	15:c:274:LYS:HE3	2.00	0.43
8:H:28:ASP:HB2	8:H:36:LEU:HB2	2.01	0.43
8:H:108:LEU:HD23	8:H:108:LEU:HA	1.86	0.43
16:d:129:ARG:HB3	16:d:133:GLN:HB2	2.01	0.43
17:e:39:LYS:H	17:e:39:LYS:HG2	1.52	0.43
2:P:201:MET:H	2:P:201:MET:HG2	1.55	0.42
6:T:19:ARG:HE	6:T:21:PHE:HE1	1.66	0.42
8:V:1:MET:HE1	10:X:70:ARG:HD2	2.01	0.42
8:V:210:LEU:HD11	12:L:58:SER:HB3	2.01	0.42
10:X:119:ASP:OD1	10:X:121:LEU:N	2.48	0.42
1:A:44:VAL:HG21	1:A:187:ILE:HD13	2.01	0.42
1:A:67:ILE:HD11	1:A:73:LEU:CD1	2.48	0.42
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.79	0.42
2:B:123:GLN:O	2:B:124:PHE:C	2.62	0.42
2:B:139:TRP:HE1	2:B:144:GLY:HA2	1.83	0.42
4:D:85:ALA:HB2	4:D:139:VAL:HG21	2.01	0.42
7:G:152:TYR:CD1	7:G:162:GLY:HA2	2.54	0.42
8:H:85:TYR:HB2	8:H:221:ILE:HD11	2.01	0.42
10:J:91:CYS:O	10:J:97:PRO:CG	2.66	0.42
14:N:69:THR:HB	14:N:77:CYS:SG	2.59	0.42
16:d:79:SER:HA	16:d:86:VAL:HA	2.00	0.42
1:O:12:PHE:CZ	2:P:128:ARG:HD2	2.54	0.42
2:P:135:LEU:HD23	2:P:135:LEU:HA	1.83	0.42
5:S:72:ILE:HG21	5:S:88:MET:SD	2.59	0.42
7:U:144:ASP:CG	7:U:145:GLU:H	2.27	0.42
8:V:20:ARG:O	8:V:24:VAL:HG22	2.19	0.42
8:V:106:LEU:HD22	8:V:122:ALA:HB2	2.00	0.42
11:Y:66:LYS:O	11:Y:66:LYS:HG2	2.19	0.42
11:Y:111:CYS:O	11:Y:112:SER:C	2.61	0.42
17:h:48:LEU:HD23	17:h:48:LEU:HA	1.80	0.42
2:B:74:CYS:SG	2:B:75:SER:N	2.92	0.42
2:B:198:ASN:HA	2:B:198:ASN:HD22	1.69	0.42
3:C:68:ASN:HA	3:C:211:MET:HE1	2.01	0.42
4:D:95:GLU:OE2	4:D:95:GLU:HA	2.19	0.42
12:L:55:THR:HG22	12:L:69:PRO:HA	2.01	0.42
1:O:44:VAL:HG21	1:O:187:ILE:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:61:PHE:CD1	2:P:61:PHE:C	2.98	0.42
2:P:136:TYR:HB2	2:P:148:TYR:HB2	2.01	0.42
7:U:163:PHE:CD2	7:U:166:THR:HB	2.54	0.42
10:X:95:ARG:O	10:X:97:PRO:N	2.52	0.42
11:Y:83:ALA:N	8:H:34:TYR:OH	2.52	0.42
14:b:161:ILE:HD13	14:b:161:ILE:HG21	1.73	0.42
2:B:90:LEU:HD22	2:B:110:LEU:HD21	2.02	0.42
5:E:88:MET:HE1	5:E:134:ILE:HG12	2.00	0.42
6:F:219:LEU:H	6:F:219:LEU:HD23	1.83	0.42
8:H:228:PHE:CE2	8:H:230:ARG:HD3	2.54	0.42
10:J:95:ARG:O	10:J:97:PRO:N	2.52	0.42
2:P:58:GLU:C	2:P:60:PHE:H	2.27	0.42
5:S:109:VAL:HG21	5:S:145:PHE:CD2	2.54	0.42
6:T:201:HIS:NE2	6:T:203:GLU:HA	2.34	0.42
7:U:2:SER:OG	7:U:3:ARG:N	2.52	0.42
8:V:71:ASP:OD1	8:V:72:LYS:N	2.53	0.42
8:V:195:LYS:HD2	8:V:220:VAL:HG21	2.01	0.42
9:W:105:GLU:HG2	9:W:124:ASP:HA	2.00	0.42
14:b:39:ALA:HB2	14:b:48:LEU:HD13	2.02	0.42
14:b:69:THR:HB	14:b:77:CYS:SG	2.59	0.42
15:f:75:ILE:HD13	15:f:216:PRO:HD3	2.00	0.42
16:g:22:VAL:HG22	16:g:29:GLN:NE2	2.33	0.42
17:h:39:LYS:HB3	17:h:39:LYS:HE3	1.48	0.42
6:F:70:ASP:OD2	6:F:99:ARG:NH2	2.49	0.42
7:G:113:MET:SD	8:H:113:THR:HA	2.60	0.42
7:G:144:ASP:CG	7:G:145:GLU:H	2.27	0.42
7:G:215:ILE:HD13	7:G:215:ILE:HA	1.90	0.42
9:I:154:GLU:OE2	9:I:155:PRO:HD2	2.20	0.42
12:L:176:LEU:CD2	12:L:206:VAL:HG12	2.50	0.42
16:d:127:TYR:CD1	16:d:127:TYR:C	2.97	0.42
1:O:87:HIS:CE1	7:U:116:LYS:HE2	2.54	0.42
1:O:114:ALA:HB1	1:O:152:GLY:O	2.19	0.42
3:Q:204:LYS:HD3	3:Q:204:LYS:HA	1.81	0.42
4:R:168:ARG:HD3	4:R:178:GLN:HE22	1.85	0.42
5:S:228:ASP:O	5:S:231:PRO:HD2	2.19	0.42
6:T:31:GLU:OE1	6:T:31:GLU:N	2.52	0.42
6:T:70:ASP:OD2	6:T:99:ARG:NH2	2.49	0.42
8:V:60:ASP:OD2	8:V:212:SER:OG	2.24	0.42
9:W:55:LEU:HD12	9:W:103:TYR:HB2	2.02	0.42
10:X:35:MET:HG2	10:X:45:LEU:HD22	2.00	0.42
12:Z:213:ARG:CG	9:I:150:GLU:HG3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:149:PRO:HG2	14:b:153:MET:HE3	2.02	0.42
16:g:19:MET:HE3	16:g:19:MET:HB2	1.64	0.42
17:h:68:ARG:HA	17:h:72:GLY:O	2.20	0.42
1:A:12:PHE:CZ	2:B:128:ARG:HD2	2.54	0.42
2:B:136:TYR:HB2	2:B:148:TYR:HB2	2.01	0.42
4:D:168:ARG:HD3	4:D:178:GLN:HE22	1.85	0.42
5:E:72:ILE:HG21	5:E:88:MET:SD	2.59	0.42
11:K:56:MET:HE1	11:K:110:ASP:H	1.84	0.42
1:O:60:SER:OG	1:O:61:VAL:N	2.53	0.42
2:P:61:PHE:HD1	2:P:61:PHE:C	2.27	0.42
3:Q:47:LYS:C	3:Q:49:SER:H	2.28	0.42
3:Q:124:ARG:HH12	17:h:140:LEU:HD13	1.85	0.42
4:R:99:HIS:CD2	4:R:103:TYR:HD2	2.38	0.42
5:S:202:GLU:HB3	15:f:274:LYS:HE3	2.00	0.42
8:V:81:SER:O	8:V:83:ASN:N	2.52	0.42
8:V:143:LEU:HB3	8:V:154:TYR:HB2	2.01	0.42
11:Y:30:LEU:HD23	11:Y:30:LEU:HA	1.58	0.42
13:a:223:TYR:HD2	8:H:182:GLU:OE2	1.94	0.42
14:b:82:SER:O	14:b:86:THR:HG23	2.19	0.42
1:A:60:SER:OG	1:A:61:VAL:N	2.53	0.42
5:E:49:LEU:HB2	5:E:195:LEU:HD11	2.02	0.42
6:F:46:VAL:HG21	6:F:190:VAL:HG22	2.02	0.42
11:K:66:LYS:O	11:K:66:LYS:HG2	2.20	0.42
1:O:163:GLY:O	1:O:166:TYR:HB3	2.20	0.42
2:P:139:TRP:CG	2:P:218:ARG:HD3	2.54	0.42
3:Q:41:VAL:HG13	3:Q:136:PHE:CE1	2.55	0.42
8:V:34:TYR:OH	11:K:83:ALA:N	2.53	0.42
8:V:121:THR:O	8:V:125:MET:HG3	2.18	0.42
8:V:143:LEU:O	8:V:153:LEU:HD12	2.19	0.42
13:a:167:LEU:HG	13:a:182:LEU:HD12	2.01	0.42
15:f:46:GLU:HG2	15:f:48:ARG:HG3	2.01	0.42
16:g:165:LYS:HA	16:g:165:LYS:HD2	1.79	0.42
16:g:214:ILE:HB	16:g:215:PRO:HD3	2.02	0.42
16:g:234:LEU:O	16:g:238:PRO:HD3	2.20	0.42
1:A:66:PRO:HD3	1:A:219:ARG:HH21	1.85	0.42
1:A:163:GLY:O	1:A:166:TYR:HB3	2.20	0.42
2:B:61:PHE:CD1	2:B:61:PHE:C	2.97	0.42
3:C:45:VAL:HG23	3:C:62:ILE:HD11	2.01	0.42
6:F:31:GLU:OE1	6:F:31:GLU:N	2.52	0.42
7:G:2:SER:OG	7:G:3:ARG:N	2.52	0.42
7:G:163:PHE:CD2	7:G:166:THR:HB	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:LEU:O	8:H:153:LEU:HD12	2.19	0.42
10:J:91:CYS:CB	10:J:95:ARG:HH12	2.29	0.42
11:K:28:LEU:HD11	13:M:144:ARG:HH11	1.84	0.42
14:N:161:ILE:HD13	14:N:161:ILE:HG21	1.73	0.42
16:d:34:LEU:HD11	16:d:217:ALA:HB1	2.02	0.42
16:d:109:TRP:O	16:d:112:SER:OG	2.27	0.42
16:d:214:ILE:HB	16:d:215:PRO:HD3	2.02	0.42
17:e:68:ARG:HA	17:e:72:GLY:O	2.20	0.42
4:R:181:LEU:O	4:R:185:TYR:N	2.45	0.42
4:R:209:LYS:HD3	4:R:209:LYS:HA	1.67	0.42
7:U:185:LYS:HE2	7:U:185:LYS:HB3	1.68	0.42
14:b:161:ILE:HD11	14:b:170:TYR:CE1	2.55	0.42
15:f:254:LEU:HD22	15:f:263:VAL:HG21	2.01	0.42
17:h:75:ALA:HB3	17:h:76:PRO:HD3	2.02	0.42
4:D:120:ALA:C	4:D:122:GLN:H	2.28	0.42
5:E:88:MET:CE	5:E:112:ILE:HD11	2.49	0.42
12:L:150:TYR:HD2	12:L:158:TYR:HD2	1.66	0.42
12:L:204:LYS:O	12:L:208:ILE:HG12	2.20	0.42
13:M:104:ASP:HB3	13:M:151:LEU:HD22	2.02	0.42
14:N:198:MET:HE1	14:N:228:ILE:HD13	2.02	0.42
15:c:286:ILE:O	15:c:287:TYR:HB2	2.20	0.42
1:O:195:LYS:HA	1:O:198:PHE:HB2	2.01	0.42
4:R:120:ALA:C	4:R:122:GLN:H	2.27	0.42
7:U:92:GLN:HA	7:U:92:GLN:OE1	2.20	0.42
9:W:81:ILE:HG12	9:W:82:LYS:O	2.20	0.42
10:X:91:CYS:O	10:X:97:PRO:CG	2.66	0.42
11:Y:118:LEU:HD22	11:Y:142:LEU:HB2	2.01	0.42
12:Z:111:MET:HE1	12:Z:119:MET:CE	2.50	0.42
12:Z:205:ASP:CG	8:H:242:LEU:H	2.28	0.42
2:B:8:ARG:O	2:B:9:THR:HG22	2.19	0.42
3:C:229:VAL:O	3:C:230:ALA:C	2.62	0.42
6:F:126:SER:H	7:G:130:GLU:HB2	1.85	0.42
7:G:119:ALA:HB1	7:G:158:GLY:O	2.20	0.42
8:H:148:VAL:HG13	8:H:149:THR:HG23	2.01	0.42
9:I:122:SER:C	9:I:123:LEU:HD12	2.45	0.42
12:L:30:PHE:CZ	13:M:145:ARG:HG2	2.55	0.42
13:M:145:ARG:HG3	13:M:173:LEU:HD23	2.01	0.42
15:c:120:PHE:HD1	15:c:139:CYS:HB3	1.84	0.42
16:d:100:LYS:O	16:d:101:PRO:C	2.63	0.42
1:O:85:LEU:HD23	1:O:85:LEU:HA	1.71	0.42
7:U:113:MET:SD	8:V:113:THR:HA	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:21:ARG:O	8:V:25:LEU:HB2	2.20	0.42
9:W:154:GLU:OE2	9:W:155:PRO:HD2	2.20	0.42
12:Z:30:PHE:CZ	13:a:145:ARG:HG2	2.55	0.42
12:Z:150:TYR:HD2	12:Z:158:TYR:HD2	1.66	0.42
15:f:106:CYS:O	15:f:110:ASP:HB3	2.20	0.42
16:g:143:LEU:O	16:g:191:TYR:OH	2.30	0.42
16:g:234:LEU:HD12	16:g:244:ARG:NH1	2.35	0.42
1:A:186:ALA:HA	1:A:189:THR:HG22	2.02	0.42
3:C:41:VAL:HG13	3:C:136:PHE:CE1	2.55	0.42
3:C:172:LEU:HD23	4:D:58:LEU:HD13	2.01	0.42
4:D:181:LEU:HA	4:D:181:LEU:HD23	1.84	0.42
5:E:109:VAL:HG21	5:E:145:PHE:CD2	2.54	0.42
7:G:211:LYS:HB2	7:G:212:PRO:HD2	2.02	0.42
9:I:55:LEU:HD12	9:I:103:TYR:HB2	2.01	0.42
9:I:141:CYS:SG	9:I:180:SER:OG	2.62	0.42
12:L:111:MET:HE1	12:L:119:MET:CE	2.50	0.42
14:N:36:THR:HG21	14:N:197:ALA:CB	2.50	0.42
14:N:129:MET:HE2	14:N:129:MET:HB3	1.87	0.42
16:d:55:MET:HE1	16:d:91:ARG:HD2	2.02	0.42
3:Q:223:GLU:HG2	3:Q:224:GLU:H	1.84	0.41
4:R:85:ALA:HB2	4:R:139:VAL:HG21	2.01	0.41
10:X:29:LYS:HZ1	10:X:32:HIS:HA	1.85	0.41
11:Y:223:THR:OG1	11:Y:230:GLY:HA2	2.20	0.41
12:Z:35:PHE:CZ	12:Z:37:GLY:HA2	2.55	0.41
13:a:145:ARG:HG3	13:a:173:LEU:HD23	2.01	0.41
14:b:36:THR:HG21	14:b:197:ALA:CB	2.50	0.41
14:b:198:MET:HE1	14:b:228:ILE:HD13	2.02	0.41
1:A:47:THR:HB	1:A:74:VAL:HG21	2.02	0.41
4:D:99:HIS:CD2	4:D:103:TYR:HD2	2.38	0.41
4:D:186:HIS:CD2	4:D:188:SER:H	2.38	0.41
8:H:21:ARG:O	8:H:25:LEU:HB2	2.20	0.41
8:H:195:LYS:HD2	8:H:220:VAL:HG21	2.01	0.41
9:I:52:LEU:HB2	9:I:59:VAL:HG13	2.02	0.41
12:L:35:PHE:CZ	12:L:37:GLY:HA2	2.55	0.41
13:M:167:LEU:HD12	13:M:167:LEU:HA	1.90	0.41
13:M:232:PHE:HE2	13:M:234:ILE:HD11	1.85	0.41
2:P:45:LEU:HD21	2:P:75:SER:HB2	2.01	0.41
2:P:235:GLN:HA	2:P:238:LYS:HG2	2.02	0.41
4:R:234:LEU:HA	4:R:234:LEU:HD23	1.81	0.41
7:U:211:LYS:HB2	7:U:212:PRO:HD2	2.02	0.41
9:W:52:LEU:HB2	9:W:59:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:41:LEU:O	11:Y:42:ALA:C	2.63	0.41
11:Y:56:MET:HE1	11:Y:110:ASP:H	1.84	0.41
16:g:34:LEU:HD11	16:g:217:ALA:HB1	2.02	0.41
3:C:158:ALA:CB	3:C:172:LEU:HD21	2.50	0.41
7:G:56:VAL:HG13	7:G:56:VAL:O	2.20	0.41
8:H:86:CYS:SG	8:H:141:LEU:HD23	2.60	0.41
10:J:88:LEU:HG	10:J:122:ALA:HB2	2.02	0.41
11:K:97:ASN:C	11:K:99:TYR:H	2.28	0.41
14:N:82:SER:O	14:N:86:THR:HG23	2.19	0.41
15:c:106:CYS:O	15:c:110:ASP:HB3	2.20	0.41
16:d:15:PHE:HD1	16:d:84:LYS:HA	1.83	0.41
16:d:119:ILE:H	16:d:119:ILE:HG13	1.69	0.41
1:O:178:ASN:H	1:O:181:LEU:HD12	1.84	0.41
2:P:60:PHE:C	2:P:62:SER:H	2.28	0.41
5:S:111:LEU:HD23	5:S:111:LEU:HA	1.78	0.41
8:V:86:CYS:SG	8:V:141:LEU:HD23	2.60	0.41
10:X:167:LEU:HD12	10:X:171:PHE:HB2	2.02	0.41
13:a:167:LEU:HD12	13:a:167:LEU:HA	1.90	0.41
1:A:87:HIS:CE1	7:G:116:LYS:HE2	2.54	0.41
2:B:25:MET:HG3	2:B:152:PRO:HD2	2.03	0.41
2:B:45:LEU:HD21	2:B:75:SER:HB2	2.01	0.41
2:B:61:PHE:HD1	2:B:61:PHE:C	2.27	0.41
9:I:81:ILE:HG12	9:I:82:LYS:O	2.20	0.41
11:K:223:THR:OG1	11:K:230:GLY:HA2	2.20	0.41
16:d:234:LEU:HD12	16:d:244:ARG:NH1	2.35	0.41
2:P:133:SER:OG	2:P:150:SER:O	2.28	0.41
4:R:182:GLN:HG2	4:R:183:GLU:N	2.26	0.41
5:S:171:TYR:HD2	5:S:194:ALA:HA	1.85	0.41
7:U:119:ALA:HB1	7:U:158:GLY:O	2.20	0.41
8:V:1:MET:O	8:V:2:ALA:C	2.63	0.41
11:Y:97:ASN:C	11:Y:99:TYR:H	2.28	0.41
13:a:169:TYR:O	13:a:176:ALA:HA	2.19	0.41
15:f:74:ALA:HB1	15:f:79:ALA:HB1	2.02	0.41
1:A:58:GLU:HG2	1:A:59:ARG:NH2	2.35	0.41
2:B:60:PHE:C	2:B:62:SER:H	2.28	0.41
2:B:179:TYR:CE2	2:B:181:GLU:HA	2.56	0.41
7:G:210:PHE:CD2	7:G:215:ILE:HD11	2.56	0.41
8:H:4:VAL:HG13	17:e:32:ARG:HH12	1.85	0.41
8:H:20:ARG:O	8:H:24:VAL:HG22	2.19	0.41
10:J:52:ASP:HB3	10:J:98:TYR:CB	2.42	0.41
10:J:91:CYS:C	10:J:93:ARG:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:108:LEU:HD11	13:M:141:MET:HE3	2.03	0.41
14:N:39:ALA:HB2	14:N:48:LEU:HD13	2.02	0.41
15:c:46:GLU:HG2	15:c:48:ARG:HG3	2.01	0.41
16:d:6:GLY:O	16:d:7:GLU:HG2	2.21	0.41
1:O:58:GLU:HG2	1:O:59:ARG:NH2	2.35	0.41
1:O:66:PRO:HD3	1:O:219:ARG:HH21	1.85	0.41
5:S:23:GLU:HG2	16:g:260:PRO:HG2	2.02	0.41
6:T:126:SER:H	7:U:130:GLU:HB2	1.85	0.41
7:U:186:LYS:HZ3	7:U:188:ASP:H	1.67	0.41
8:V:165:LEU:HD12	8:V:168:VAL:HG12	2.03	0.41
8:V:242:LEU:H	12:L:205:ASP:CG	2.28	0.41
10:X:91:CYS:C	10:X:93:ARG:H	2.28	0.41
13:a:104:ASP:HB3	13:a:151:LEU:HD22	2.02	0.41
16:g:165:LYS:HB3	16:g:177:PHE:HB3	2.02	0.41
3:C:124:ARG:HH12	17:e:140:LEU:HD13	1.85	0.41
3:C:156:TRP:CD1	3:C:156:TRP:N	2.89	0.41
4:D:156:MET:HE3	4:D:156:MET:HB3	1.97	0.41
5:E:23:GLU:HG2	16:d:260:PRO:HG2	2.02	0.41
7:G:101:TRP:CH2	7:G:113:MET:HG3	2.56	0.41
8:H:12:GLY:HA3	17:e:119:ASN:HB3	2.03	0.41
10:J:43:LEU:HD11	10:J:181:ARG:HD2	2.03	0.41
10:J:93:ARG:HB2	10:J:94:SER:H	1.55	0.41
10:J:148:THR:O	10:J:151:ILE:HG13	2.21	0.41
11:K:156[B]:MET:HE3	11:K:158:THR:HG23	2.02	0.41
13:M:167:LEU:HG	13:M:182:LEU:HD12	2.01	0.41
15:c:52:ARG:C	15:c:54:THR:H	2.29	0.41
15:c:74:ALA:HB1	15:c:79:ALA:HB1	2.02	0.41
15:c:254:LEU:HD22	15:c:263:VAL:HG21	2.01	0.41
1:O:170:LYS:HE2	1:O:170:LYS:HB3	1.43	0.41
3:Q:90:GLU:HG2	3:Q:110:TYR:CG	2.56	0.41
3:Q:156:TRP:CD1	3:Q:156:TRP:N	2.89	0.41
5:S:88:MET:CE	5:S:112:ILE:HD11	2.49	0.41
6:T:87:LEU:HD23	6:T:87:LEU:HA	1.92	0.41
8:V:28:ASP:HB2	8:V:36:LEU:HB2	2.01	0.41
9:W:122:SER:C	9:W:123:LEU:HD12	2.45	0.41
9:W:150:GLU:HG3	12:L:213:ARG:CG	2.50	0.41
10:X:88:LEU:HG	10:X:122:ALA:HB2	2.02	0.41
12:Z:176:LEU:CD2	12:Z:206:VAL:HG12	2.50	0.41
13:a:112:LEU:HD12	13:a:112:LEU:O	2.20	0.41
16:g:246:LYS:HD3	16:g:246:LYS:HA	1.80	0.41
3:C:208:LEU:HB3	3:C:228:TYR:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:92:GLN:OE1	7:G:92:GLN:HA	2.20	0.41
8:H:1:MET:HE1	10:J:70:ARG:HD2	2.01	0.41
8:H:35:LYS:CG	8:H:36:LEU:H	2.24	0.41
8:H:71:ASP:OD1	8:H:72:LYS:N	2.53	0.41
11:K:240:GLU:OE2	11:K:241:ASP:N	2.54	0.41
14:N:149:PRO:HG2	14:N:153:MET:HE3	2.02	0.41
1:O:100:TYR:O	1:O:102:GLU:N	2.54	0.41
8:V:148:VAL:HG13	8:V:149:THR:HG23	2.01	0.41
10:X:148:THR:O	10:X:151:ILE:HG13	2.21	0.41
14:b:80:SER:OG	14:b:131:GLY:O	2.29	0.41
15:f:286:ILE:HG23	15:f:288:THR:N	2.32	0.41
16:g:55:MET:HE1	16:g:91:ARG:HD2	2.02	0.41
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.83	0.41
2:B:185:THR:OG1	2:B:186:LEU:N	2.54	0.41
3:C:223:GLU:HG2	3:C:224:GLU:H	1.84	0.41
7:G:13:ILE:HG22	7:G:14:THR:N	2.35	0.41
7:G:190:THR:N	7:G:193:GLN:OE1	2.40	0.41
10:J:167:LEU:HD12	10:J:171:PHE:HB2	2.02	0.41
14:N:35:THR:N	14:N:203:SER:O	2.54	0.41
14:N:161:ILE:HD11	14:N:170:TYR:CE1	2.55	0.41
15:c:77:ASN:O	15:c:80:VAL:HG22	2.21	0.41
15:c:191:ALA:HB2	15:c:203:CYS:SG	2.61	0.41
17:e:75:ALA:HB3	17:e:76:PRO:HD3	2.02	0.41
1:O:47:THR:HB	1:O:74:VAL:HG21	2.02	0.41
2:P:86:LEU:HD23	2:P:86:LEU:HA	1.77	0.41
3:Q:208:LEU:HB3	3:Q:228:TYR:CE1	2.56	0.41
4:R:186:HIS:CD2	4:R:188:SER:H	2.38	0.41
5:S:17:GLY:O	6:T:32:ASN:ND2	2.54	0.41
7:U:13:ILE:HG22	7:U:14:THR:N	2.35	0.41
7:U:152:TYR:HE1	7:U:162:GLY:HA2	1.86	0.41
9:W:200:LYS:HB2	9:W:200:LYS:HE3	1.74	0.41
11:Y:165:LYS:HA	11:Y:165:LYS:HE3	2.03	0.41
13:a:81:PHE:HZ	14:b:149:PRO:HG3	1.86	0.41
13:a:166:PHE:HE1	13:a:178:GLU:OE2	2.04	0.41
14:b:35:THR:N	14:b:203:SER:O	2.54	0.41
15:f:191:ALA:HB2	15:f:203:CYS:SG	2.61	0.41
16:g:127:TYR:C	16:g:127:TYR:CD1	2.97	0.41
1:A:6:SER:HA	1:A:19:VAL:CG2	2.49	0.41
4:D:234:LEU:HA	4:D:234:LEU:HD23	1.81	0.41
5:E:17:GLY:O	6:F:32:ASN:ND2	2.54	0.41
8:H:215:ASN:HD22	8:H:234:VAL:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:ASN:C	10:J:26:VAL:H	2.29	0.41
12:L:177:LEU:HD23	12:L:177:LEU:HA	1.87	0.41
13:M:166:PHE:HE1	13:M:178:GLU:OE2	2.04	0.41
1:O:186:ALA:HA	1:O:189:THR:HG22	2.02	0.41
2:P:25:MET:HG3	2:P:152:PRO:HD2	2.03	0.41
2:P:179:TYR:CE2	2:P:181:GLU:HA	2.56	0.41
3:Q:4:ASP:HA	3:Q:17:PHE:HB2	2.02	0.41
3:Q:45:VAL:HG23	3:Q:62:ILE:HD11	2.02	0.41
5:S:171:TYR:CD2	5:S:194:ALA:HA	2.56	0.41
5:S:207:THR:HG21	5:S:227:ASP:HA	2.03	0.41
7:U:56:VAL:HG13	7:U:56:VAL:O	2.20	0.41
8:V:4:VAL:HG13	17:h:32:ARG:HH12	1.85	0.41
9:W:188:ILE:HB	9:W:195:THR:OG1	2.21	0.41
10:X:143:LEU:HD23	10:X:143:LEU:HA	1.81	0.41
11:Y:156[B]:MET:HE3	11:Y:158:THR:HG23	2.02	0.41
13:a:232:PHE:HE2	13:a:234:ILE:HD11	1.85	0.41
15:f:286:ILE:O	15:f:287:TYR:HB2	2.20	0.41
16:g:6:GLY:O	16:g:7:GLU:HG2	2.21	0.41
16:g:162:GLU:HG3	16:g:163:MET:N	2.36	0.41
1:A:8:SER:C	1:A:10:THR:H	2.29	0.41
2:B:57:ASP:CG	2:B:58:GLU:H	2.29	0.41
2:B:58:GLU:C	2:B:60:PHE:H	2.27	0.41
2:B:86:LEU:HD23	2:B:86:LEU:HA	1.77	0.41
2:B:235:GLN:HA	2:B:238:LYS:HG2	2.02	0.41
3:C:4:ASP:HA	3:C:17:PHE:HB2	2.02	0.41
3:C:47:LYS:C	3:C:49:SER:H	2.28	0.41
3:C:90:GLU:HG2	3:C:110:TYR:CG	2.56	0.41
6:F:51:LYS:HD2	6:F:212:GLU:OE1	2.21	0.41
7:G:152:TYR:HE1	7:G:162:GLY:HA2	1.86	0.41
8:H:60:ASP:OD2	8:H:212:SER:OG	2.24	0.41
10:J:29:LYS:HZ1	10:J:32:HIS:HA	1.84	0.41
11:K:41:LEU:O	11:K:42:ALA:C	2.63	0.41
11:K:87:SER:CB	12:L:159:GLN:HE22	2.34	0.41
11:K:175:SER:OG	11:K:176:GLU:OE1	2.39	0.41
12:L:99:ARG:HD2	12:L:102:MET:SD	2.61	0.41
13:M:153:ASN:HB3	13:M:155:MET:SD	2.61	0.41
15:c:224:GLN:OE1	16:d:71:LEU:HD23	2.21	0.41
16:d:234:LEU:O	16:d:238:PRO:HD3	2.20	0.41
1:O:20:GLN:OE1	1:O:20:GLN:HA	2.21	0.41
1:O:121:THR:HG21	1:O:151:SER:HA	2.03	0.41
6:T:51:LYS:HD2	6:T:212:GLU:OE1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:109:LYS:HE3	6:T:109:LYS:HB3	1.84	0.41
7:U:210:PHE:CD2	7:U:215:ILE:HD11	2.56	0.41
9:W:11:MET:SD	9:W:170:MET:HE3	2.61	0.41
12:Z:99:ARG:HD2	12:Z:102:MET:SD	2.61	0.41
12:Z:204:LYS:O	12:Z:208:ILE:HG12	2.20	0.41
16:g:38:THR:CA	16:g:246:LYS:HB2	2.48	0.41
16:g:100:LYS:O	16:g:101:PRO:C	2.63	0.41
17:h:31:LEU:HB3	17:h:32:ARG:H	1.64	0.41
4:D:8:TYR:CE2	4:D:17:PRO:HD3	2.56	0.41
5:E:207:THR:HG21	5:E:227:ASP:HA	2.03	0.41
6:F:109:LYS:HE3	6:F:109:LYS:HB3	1.84	0.41
8:H:1:MET:HE3	8:H:1:MET:HB3	1.73	0.41
8:H:39:VAL:O	8:H:40:ARG:HB2	2.21	0.41
8:H:170[B]:MET:HB3	8:H:170[B]:MET:HE2	1.59	0.41
9:I:60:GLN:O	9:I:64:GLN:HG3	2.21	0.41
9:I:70:LEU:HD11	9:I:81:ILE:HG21	2.02	0.41
11:K:148:GLN:HG2	17:e:37:CYS:HB3	2.03	0.41
14:N:92:ALA:O	14:N:96:GLN:HG3	2.20	0.41
15:c:70:LYS:HB2	15:c:132:VAL:HG22	2.03	0.41
1:O:92:LEU:HD23	1:O:92:LEU:HA	1.89	0.40
1:O:94:GLN:OE1	1:O:94:GLN:HA	2.21	0.40
7:U:101:TRP:CH2	7:U:113:MET:HG3	2.56	0.40
13:a:153:ASN:HB3	13:a:155:MET:SD	2.61	0.40
14:b:137:TRP:CH2	14:b:215:GLU:HG2	2.56	0.40
15:f:224:GLN:OE1	16:g:71:LEU:HD23	2.21	0.40
3:C:199:VAL:HG13	3:C:201:SER:H	1.86	0.40
4:D:142:LEU:HD23	4:D:142:LEU:HA	1.80	0.40
8:H:102:ILE:HG13	8:H:126:LEU:CD2	2.52	0.40
9:I:86:LEU:O	9:I:90:VAL:HG23	2.21	0.40
11:K:35:LEU:HB3	11:K:36:SER:H	1.58	0.40
13:M:65:VAL:HG21	13:M:166:PHE:O	2.21	0.40
2:P:105:ILE:HG12	2:P:109:GLN:HB2	2.03	0.40
4:R:78:MET:HG2	4:R:85:ALA:HB1	2.03	0.40
4:R:95:GLU:OE2	4:R:95:GLU:HA	2.19	0.40
5:S:49:LEU:HB2	5:S:195:LEU:HD11	2.02	0.40
6:T:8:ASP:HB3	6:T:21:PHE:HD2	1.86	0.40
8:V:12:GLY:HA3	17:h:119:ASN:HB3	2.03	0.40
9:W:60:GLN:O	9:W:64:GLN:HG3	2.21	0.40
11:Y:164:ASP:OD1	11:Y:166:ARG:N	2.50	0.40
14:b:92:ALA:O	14:b:96:GLN:HG3	2.20	0.40
15:f:114:LEU:O	15:f:115:SER:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	1:A:151:SER:HA	2.03	0.40
2:B:51:ASN:HB3	2:B:56:LEU:CD1	2.51	0.40
11:K:29:ASP:CB	13:M:147:LYS:HZ1	2.32	0.40
11:K:165:LYS:HA	11:K:165:LYS:HE3	2.03	0.40
17:e:38:VAL:HG22	17:e:41:GLU:HB3	2.03	0.40
2:P:175:LEU:HD12	2:P:175:LEU:HA	1.95	0.40
3:Q:19:VAL:O	3:Q:23:GLN:HB2	2.22	0.40
4:R:8:TYR:CE2	4:R:17:PRO:HD3	2.56	0.40
4:R:50:VAL:HG22	4:R:51:GLU:O	2.22	0.40
6:T:46:VAL:HG21	6:T:190:VAL:HG22	2.02	0.40
8:V:215:ASN:HD22	8:V:234:VAL:HA	1.86	0.40
11:Y:240:GLU:OE2	11:Y:241:ASP:N	2.54	0.40
17:h:136:TYR:O	17:h:137:LYS:C	2.64	0.40
1:A:5:TYR:OH	2:B:6:ASP:OD2	2.36	0.40
1:A:20:GLN:HA	1:A:20:GLN:OE1	2.21	0.40
4:D:91:LYS:HB2	4:D:119:LEU:HD22	2.04	0.40
4:D:145:GLY:HA2	4:D:220:VAL:HG21	2.03	0.40
7:G:21:ARG:NH2	16:d:131:ASP:OD2	2.55	0.40
8:H:1:MET:O	8:H:2:ALA:C	2.63	0.40
8:H:44:THR:HG21	8:H:211:GLY:O	2.21	0.40
9:I:200:LYS:HE3	9:I:200:LYS:HB2	1.74	0.40
10:J:29:LYS:HE3	10:J:29:LYS:HB3	1.74	0.40
10:J:35:MET:HE1	10:J:181:ARG:HG3	2.03	0.40
13:M:112:LEU:O	13:M:112:LEU:HD12	2.20	0.40
15:c:114:LEU:O	15:c:115:SER:C	2.65	0.40
16:d:14:GLY:O	16:d:84:LYS:HE2	2.21	0.40
2:P:90:LEU:HD22	2:P:110:LEU:HD21	2.01	0.40
2:P:241:GLU:O	2:P:244:GLU:HG3	2.21	0.40
5:S:12:VAL:HA	6:T:22:GLN:HE22	1.86	0.40
9:W:70:LEU:HD11	9:W:81:ILE:HG21	2.02	0.40
15:f:52:ARG:C	15:f:54:THR:H	2.29	0.40
15:f:77:ASN:O	15:f:80:VAL:HG22	2.21	0.40
16:g:14:GLY:O	16:g:84:LYS:HE2	2.21	0.40
1:A:100:TYR:O	1:A:102:GLU:N	2.54	0.40
4:D:78:MET:HG2	4:D:85:ALA:HB1	2.03	0.40
8:H:106:LEU:HD12	8:H:106:LEU:HA	1.85	0.40
10:J:24:ASN:C	10:J:26:VAL:N	2.76	0.40
11:K:118:LEU:HD22	11:K:142:LEU:HB2	2.01	0.40
16:d:214:ILE:HD12	16:d:251:TRP:CZ3	2.57	0.40
1:O:98:LEU:HD13	17:h:112:ILE:HD11	2.03	0.40
3:Q:6:ALA:O	3:Q:9:VAL:HG23	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:99:HIS:ND1	4:R:107:MET:HB2	2.36	0.40
4:R:101:PHE:HD1	11:Y:116:ARG:HG2	1.86	0.40
5:S:63:ILE:O	5:S:64:LEU:HD23	2.22	0.40
5:S:71:GLY:HA3	5:S:221:PHE:CE1	2.56	0.40
8:V:230:ARG:HA	8:V:231:PRO:HA	1.90	0.40
11:Y:146:VAL:HG21	11:Y:156[A]:MET:HE1	2.04	0.40
13:a:108:LEU:HD11	13:a:141:MET:HE3	2.03	0.40
16:g:57:GLY:O	16:g:71:LEU:HD12	2.22	0.40
17:h:92:LEU:HD22	17:h:134:VAL:CG2	2.52	0.40
1:A:118:GLN:HB2	1:A:152:GLY:HA3	2.03	0.40
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.81	0.40
3:C:6:ALA:O	3:C:9:VAL:HG23	2.22	0.40
6:F:87:LEU:HA	6:F:87:LEU:HD23	1.92	0.40
7:G:192:GLU:C	7:G:194:THR:N	2.76	0.40
9:I:11:MET:SD	9:I:170:MET:HE3	2.61	0.40
11:K:156[A]:MET:HE2	11:K:156[A]:MET:HB3	1.90	0.40
13:M:124:ASP:OD1	13:M:124:ASP:N	2.50	0.40
14:N:123:ARG:HG2	14:N:123:ARG:H	1.73	0.40
16:d:1:MET:HA	16:d:1:MET:HE2	2.04	0.40
16:d:142:LEU:HD11	16:d:163:MET:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/234 (97%)	204 (90%)	21 (9%)	1 (0%)	30	59
1	O	226/234 (97%)	204 (90%)	21 (9%)	1 (0%)	30	59
2	B	243/261 (93%)	220 (90%)	23 (10%)	0	100	100
2	P	243/261 (93%)	220 (90%)	23 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	237/248 (96%)	198 (84%)	38 (16%)	1 (0%)	30	59
3	Q	237/248 (96%)	198 (84%)	38 (16%)	1 (0%)	30	59
4	D	239/241 (99%)	217 (91%)	22 (9%)	0	100	100
4	R	239/241 (99%)	217 (91%)	22 (9%)	0	100	100
5	E	237/263 (90%)	214 (90%)	21 (9%)	2 (1%)	16	44
5	S	237/263 (90%)	214 (90%)	21 (9%)	2 (1%)	16	44
6	F	238/255 (93%)	226 (95%)	12 (5%)	0	100	100
6	T	238/255 (93%)	226 (95%)	12 (5%)	0	100	100
7	G	243/246 (99%)	216 (89%)	25 (10%)	2 (1%)	16	44
7	U	243/246 (99%)	216 (89%)	25 (10%)	2 (1%)	16	44
8	H	263/277 (95%)	223 (85%)	32 (12%)	8 (3%)	3	18
8	V	263/277 (95%)	223 (85%)	32 (12%)	8 (3%)	3	18
9	I	200/205 (98%)	190 (95%)	10 (5%)	0	100	100
9	W	200/205 (98%)	190 (95%)	10 (5%)	0	100	100
10	J	196/201 (98%)	178 (91%)	13 (7%)	5 (3%)	4	21
10	X	196/201 (98%)	178 (91%)	13 (7%)	5 (3%)	4	21
11	K	223/263 (85%)	187 (84%)	28 (13%)	8 (4%)	2	16
11	Y	223/263 (85%)	190 (85%)	26 (12%)	7 (3%)	3	18
12	L	212/241 (88%)	204 (96%)	8 (4%)	0	100	100
12	Z	212/241 (88%)	204 (96%)	8 (4%)	0	100	100
13	M	205/253 (81%)	196 (96%)	9 (4%)	0	100	100
13	a	205/253 (81%)	196 (96%)	9 (4%)	0	100	100
14	N	199/239 (83%)	189 (95%)	10 (5%)	0	100	100
14	b	199/239 (83%)	188 (94%)	11 (6%)	0	100	100
15	c	276/288 (96%)	242 (88%)	34 (12%)	0	100	100
15	f	276/288 (96%)	242 (88%)	34 (12%)	0	100	100
16	d	262/264 (99%)	230 (88%)	31 (12%)	1 (0%)	30	59
16	g	262/264 (99%)	230 (88%)	31 (12%)	1 (0%)	30	59
17	e	111/141 (79%)	88 (79%)	17 (15%)	6 (5%)	1	10
17	h	111/141 (79%)	89 (80%)	16 (14%)	6 (5%)	1	10
All	All	7620/8240 (92%)	6847 (90%)	706 (9%)	67 (1%)	16	41

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	S	227	ASP
8	V	27	ALA
8	V	32	ARG
10	X	95	ARG
10	X	97	PRO
11	Y	52	PRO
11	Y	56	MET
17	h	31	LEU
5	E	227	ASP
8	H	27	ALA
8	H	32	ARG
10	J	95	ARG
10	J	97	PRO
11	K	52	PRO
11	K	56	MET
17	e	31	LEU
5	S	226	ASP
7	U	194	THR
7	U	195	VAL
8	V	29	PHE
8	V	31	LYS
10	X	94	SER
11	Y	31	GLY
17	h	36	SER
5	E	226	ASP
7	G	194	THR
7	G	195	VAL
8	H	29	PHE
8	H	31	LYS
10	J	94	SER
11	K	31	GLY
17	e	36	SER
1	O	140	GLU
10	X	98	TYR
11	Y	35	LEU
17	h	42	LEU
1	A	140	GLU
10	J	98	TYR
11	K	35	LEU
17	e	42	LEU
8	V	5	SER
8	V	30	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	54	ILE
16	g	152	GLN
17	h	33	LYS
17	h	38	VAL
8	H	5	SER
8	H	30	ALA
11	K	30	LEU
11	K	54	ILE
16	d	152	GLN
17	e	33	LYS
17	e	38	VAL
8	V	9	PRO
8	V	15	SER
10	X	96	THR
11	Y	41	LEU
8	H	9	PRO
8	H	15	SER
10	J	96	THR
11	K	41	LEU
3	Q	7	ILE
17	h	130	PRO
3	C	7	ILE
17	e	130	PRO
11	Y	32	PRO
11	K	32	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	182/191 (95%)	159 (87%)	23 (13%)	4	17
1	O	182/191 (95%)	159 (87%)	23 (13%)	4	17
2	B	197/221 (89%)	169 (86%)	28 (14%)	3	13
2	P	197/221 (89%)	169 (86%)	28 (14%)	3	13
3	C	193/211 (92%)	170 (88%)	23 (12%)	5	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	193/211 (92%)	170 (88%)	23 (12%)	5	19
4	D	200/203 (98%)	177 (88%)	23 (12%)	5	20
4	R	200/203 (98%)	178 (89%)	22 (11%)	6	21
5	E	200/224 (89%)	200 (100%)	0	100	100
5	S	200/224 (89%)	200 (100%)	0	100	100
6	F	193/212 (91%)	193 (100%)	0	100	100
6	T	193/212 (91%)	193 (100%)	0	100	100
7	G	205/210 (98%)	183 (89%)	22 (11%)	6	22
7	U	205/210 (98%)	183 (89%)	22 (11%)	6	22
8	H	213/228 (93%)	201 (94%)	12 (6%)	19	45
8	V	213/228 (93%)	201 (94%)	12 (6%)	19	45
9	I	170/174 (98%)	170 (100%)	0	100	100
9	W	170/174 (98%)	170 (100%)	0	100	100
10	J	169/171 (99%)	163 (96%)	6 (4%)	31	55
10	X	169/171 (99%)	163 (96%)	6 (4%)	31	55
11	K	176/202 (87%)	165 (94%)	11 (6%)	16	41
11	Y	176/202 (87%)	164 (93%)	12 (7%)	14	39
12	L	176/199 (88%)	174 (99%)	2 (1%)	65	73
12	Z	176/199 (88%)	174 (99%)	2 (1%)	65	73
13	M	170/206 (82%)	169 (99%)	1 (1%)	78	80
13	a	170/206 (82%)	169 (99%)	1 (1%)	78	80
14	N	156/181 (86%)	154 (99%)	2 (1%)	61	71
14	b	156/181 (86%)	154 (99%)	2 (1%)	61	71
15	c	255/262 (97%)	255 (100%)	0	100	100
15	f	255/262 (97%)	255 (100%)	0	100	100
16	d	237/237 (100%)	197 (83%)	40 (17%)	2	9
16	g	237/237 (100%)	197 (83%)	40 (17%)	2	9
17	e	105/128 (82%)	88 (84%)	17 (16%)	2	10
17	h	105/128 (82%)	88 (84%)	17 (16%)	2	10
All	All	6394/6920 (92%)	5974 (93%)	420 (7%)	18	40

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	6	SER
1	O	17	LYS
1	O	22	GLU
1	O	37	ILE
1	O	48	GLU
1	O	58	GLU
1	O	65	GLU
1	O	68	THR
1	O	98	LEU
1	O	131	VAL
1	O	140	GLU
1	O	170	LYS
1	O	176	ARG
1	O	185	ASP
1	O	195	LYS
1	O	199	GLU
1	O	201	GLN
1	O	204	GLU
1	O	205	ASP
1	O	214	GLU
1	O	221	THR
1	O	223	THR
1	O	229	LEU
2	P	15	GLU
2	P	17	ARG
2	P	25	MET
2	P	44	LEU
2	P	49	ARG
2	P	61	PHE
2	P	65	ILE
2	P	70	GLU
2	P	110	LEU
2	P	151	ASP
2	P	174	MET
2	P	177	GLN
2	P	178	ASP
2	P	180	LYS
2	P	181	GLU
2	P	183	GLU
2	P	184	MET
2	P	187	LYS
2	P	198	ASN
2	P	200	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	201	MET
2	P	216	LEU
2	P	218	ARG
2	P	234	GLU
2	P	238	LYS
2	P	241	GLU
2	P	242	GLU
2	P	246	LYS
3	Q	7	ILE
3	Q	23	GLN
3	Q	52	LYS
3	Q	56	GLU
3	Q	105	GLU
3	Q	113	SER
3	Q	150	SER
3	Q	153	TYR
3	Q	157	LYS
3	Q	166	LYS
3	Q	170	GLU
3	Q	172	LEU
3	Q	183	THR
3	Q	185	ASP
3	Q	214	ASP
3	Q	216	SER
3	Q	221	ASN
3	Q	226	GLU
3	Q	227	LYS
3	Q	233	GLU
3	Q	234	LYS
3	Q	235	GLU
3	Q	236	LYS
4	R	8	TYR
4	R	14	THR
4	R	18	GLU
4	R	20	ARG
4	R	32	LYS
4	R	35	SER
4	R	82	ILE
4	R	86	LYS
4	R	113	THR
4	R	133	MET
4	R	141	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	148	GLU
4	R	156	MET
4	R	182	GLN
4	R	187	LYS
4	R	203	LYS
4	R	207	GLU
4	R	209	LYS
4	R	216	GLU
4	R	231	LYS
4	R	236	GLU
4	R	239	LYS
7	U	6	SER
7	U	13	ILE
7	U	14	THR
7	U	15	ILE
7	U	45	LYS
7	U	59	LYS
7	U	60	LEU
7	U	74	GLU
7	U	83	MET
7	U	122	SER
7	U	182	LYS
7	U	183	VAL
7	U	184	LYS
7	U	185	LYS
7	U	188	ASP
7	U	206	LEU
7	U	211	LYS
7	U	223	GLU
7	U	226	LYS
7	U	234	GLU
7	U	240	VAL
7	U	242	LEU
8	V	1	MET
8	V	4	VAL
8	V	6	VAL
8	V	11	VAL
8	V	25	LEU
8	V	26	GLU
8	V	29	PHE
8	V	31	LYS
8	V	147[A]	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	147[B]	ASP
8	V	170[A]	MET
8	V	170[B]	MET
10	X	92	LEU
10	X	94	SER
10	X	95	ARG
10	X	96	THR
10	X	97	PRO
10	X	98	TYR
11	Y	27	LEU
11	Y	28	LEU
11	Y	30	LEU
11	Y	35	LEU
11	Y	39	LEU
11	Y	41	LEU
11	Y	52	PRO
11	Y	54	ILE
11	Y	55	GLU
11	Y	56	MET
11	Y	156[A]	MET
11	Y	156[B]	MET
12	Z	71[A]	CYS
12	Z	71[B]	CYS
13	a	252	THR
14	b	181[A]	MET
14	b	181[B]	MET
16	g	1	MET
16	g	7	GLU
16	g	19	MET
16	g	32	MET
16	g	35	ILE
16	g	52	LEU
16	g	55	MET
16	g	65	GLU
16	g	69	THR
16	g	70	GLU
16	g	76	GLU
16	g	80	LEU
16	g	88	LEU
16	g	100	LYS
16	g	104	GLU
16	g	107	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	g	122	SER
16	g	123	SER
16	g	127	TYR
16	g	128	GLN
16	g	129	ARG
16	g	131	ASP
16	g	132	LEU
16	g	147	MET
16	g	149	LYS
16	g	152	GLN
16	g	154	LYS
16	g	164	GLU
16	g	165	LYS
16	g	176	GLU
16	g	193	GLU
16	g	198	GLU
16	g	208	VAL
16	g	209	SER
16	g	210	GLU
16	g	218	LEU
16	g	234	LEU
16	g	244	ARG
16	g	246	LYS
16	g	249	SER
17	h	30	LEU
17	h	31	LEU
17	h	32	ARG
17	h	33	LYS
17	h	38	VAL
17	h	39	LYS
17	h	43	LEU
17	h	45	SER
17	h	48	LEU
17	h	62	MET
17	h	79	LEU
17	h	81	MET
17	h	112	ILE
17	h	131	HIS
17	h	136	TYR
17	h	137	LYS
17	h	138	LEU
1	A	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	17	LYS
1	A	22	GLU
1	A	37	ILE
1	A	48	GLU
1	A	58	GLU
1	A	65	GLU
1	A	68	THR
1	A	98	LEU
1	A	131	VAL
1	A	140	GLU
1	A	170	LYS
1	A	176	ARG
1	A	185	ASP
1	A	195	LYS
1	A	199	GLU
1	A	201	GLN
1	A	204	GLU
1	A	205	ASP
1	A	214	GLU
1	A	221	THR
1	A	223	THR
1	A	229	LEU
2	B	15	GLU
2	B	17	ARG
2	B	25	MET
2	B	44	LEU
2	B	49	ARG
2	B	61	PHE
2	B	65	ILE
2	B	70	GLU
2	B	110	LEU
2	B	151	ASP
2	B	174	MET
2	B	177	GLN
2	B	178	ASP
2	B	180	LYS
2	B	181	GLU
2	B	183	GLU
2	B	184	MET
2	B	187	LYS
2	B	198	ASN
2	B	200	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	201	MET
2	B	216	LEU
2	B	218	ARG
2	B	234	GLU
2	B	238	LYS
2	B	241	GLU
2	B	242	GLU
2	B	246	LYS
3	C	7	ILE
3	C	23	GLN
3	C	52	LYS
3	C	56	GLU
3	C	105	GLU
3	C	113	SER
3	C	150	SER
3	C	153	TYR
3	C	157	LYS
3	C	166	LYS
3	C	170	GLU
3	C	172	LEU
3	C	183	THR
3	C	185	ASP
3	C	214	ASP
3	C	216	SER
3	C	221	ASN
3	C	226	GLU
3	C	227	LYS
3	C	233	GLU
3	C	234	LYS
3	C	235	GLU
3	C	236	LYS
4	D	8	TYR
4	D	14	THR
4	D	18	GLU
4	D	20	ARG
4	D	32	LYS
4	D	35	SER
4	D	82	ILE
4	D	86	LYS
4	D	113	THR
4	D	133	MET
4	D	141	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	148	GLU
4	D	156	MET
4	D	182	GLN
4	D	187	LYS
4	D	196	LYS
4	D	203	LYS
4	D	207	GLU
4	D	209	LYS
4	D	216	GLU
4	D	231	LYS
4	D	236	GLU
4	D	239	LYS
7	G	6	SER
7	G	13	ILE
7	G	14	THR
7	G	15	ILE
7	G	45	LYS
7	G	59	LYS
7	G	60	LEU
7	G	74	GLU
7	G	83	MET
7	G	122	SER
7	G	182	LYS
7	G	183	VAL
7	G	184	LYS
7	G	185	LYS
7	G	188	ASP
7	G	206	LEU
7	G	211	LYS
7	G	223	GLU
7	G	226	LYS
7	G	234	GLU
7	G	240	VAL
7	G	242	LEU
8	H	1	MET
8	H	4	VAL
8	H	6	VAL
8	H	11	VAL
8	H	25	LEU
8	H	26	GLU
8	H	29	PHE
8	H	31	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	147[A]	ASP
8	H	147[B]	ASP
8	H	170[A]	MET
8	H	170[B]	MET
10	J	92	LEU
10	J	94	SER
10	J	95	ARG
10	J	96	THR
10	J	97	PRO
10	J	98	TYR
11	K	27	LEU
11	K	30	LEU
11	K	35	LEU
11	K	39	LEU
11	K	41	LEU
11	K	52	PRO
11	K	54	ILE
11	K	55	GLU
11	K	56	MET
11	K	156[A]	MET
11	K	156[B]	MET
12	L	71[A]	CYS
12	L	71[B]	CYS
13	M	252	THR
14	N	181[A]	MET
14	N	181[B]	MET
16	d	1	MET
16	d	7	GLU
16	d	19	MET
16	d	32	MET
16	d	35	ILE
16	d	52	LEU
16	d	55	MET
16	d	65	GLU
16	d	69	THR
16	d	70	GLU
16	d	76	GLU
16	d	80	LEU
16	d	88	LEU
16	d	100	LYS
16	d	104	GLU
16	d	107	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	d	122	SER
16	d	123	SER
16	d	127	TYR
16	d	128	GLN
16	d	129	ARG
16	d	131	ASP
16	d	132	LEU
16	d	147	MET
16	d	149	LYS
16	d	152	GLN
16	d	154	LYS
16	d	164	GLU
16	d	165	LYS
16	d	176	GLU
16	d	193	GLU
16	d	198	GLU
16	d	208	VAL
16	d	209	SER
16	d	210	GLU
16	d	218	LEU
16	d	234	LEU
16	d	244	ARG
16	d	246	LYS
16	d	249	SER
17	e	30	LEU
17	e	31	LEU
17	e	32	ARG
17	e	33	LYS
17	e	38	VAL
17	e	39	LYS
17	e	43	LEU
17	e	45	SER
17	e	48	LEU
17	e	62	MET
17	e	79	LEU
17	e	81	MET
17	e	112	ILE
17	e	131	HIS
17	e	136	TYR
17	e	137	LYS
17	e	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61)

such sidechains are listed below:

Mol	Chain	Res	Type
1	O	20	GLN
1	O	101	GLN
2	P	20	GLN
2	P	40	ASN
2	P	51	ASN
2	P	102	GLN
2	P	149	GLN
3	Q	116	GLN
4	R	114	GLN
4	R	182	GLN
4	R	227	HIS
5	S	60	GLN
5	S	152	ASN
6	T	22	GLN
8	V	18	ASN
8	V	123	ASN
8	V	159	HIS
8	V	208	ASN
8	V	215	ASN
9	W	32	GLN
9	W	92	ASN
10	X	63	ASN
10	X	71	ASN
10	X	101	ASN
10	X	132	HIS
10	X	174	ASN
12	Z	86	HIS
14	b	157	GLN
14	b	221	GLN
15	f	196	ASN
17	h	40	ASN
1	A	20	GLN
1	A	101	GLN
2	B	20	GLN
2	B	51	ASN
2	B	102	GLN
2	B	149	GLN
3	C	116	GLN
4	D	114	GLN
4	D	227	HIS
5	E	60	GLN
5	E	152	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	22	GLN
8	H	123	ASN
8	H	159	HIS
8	H	208	ASN
8	H	215	ASN
9	I	32	GLN
9	I	172	ASN
10	J	63	ASN
10	J	101	ASN
10	J	132	HIS
12	L	86	HIS
12	L	159	GLN
12	L	179	ASN
12	L	188	ASN
13	M	114	GLN
14	N	157	GLN
14	N	221	GLN
15	c	196	ASN
17	e	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

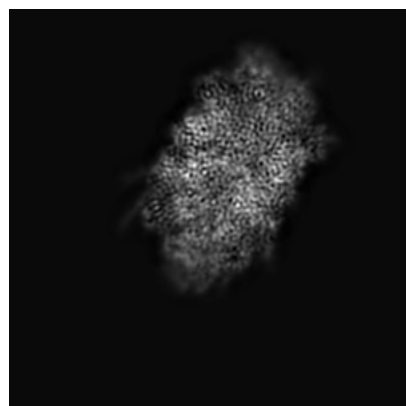
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39333. These allow visual inspection of the internal detail of the map and identification of artifacts.

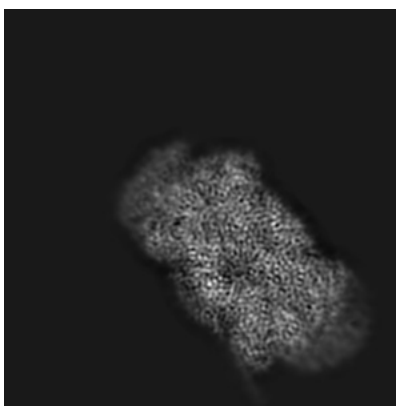
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

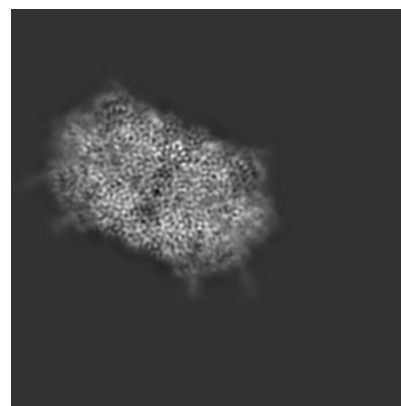
6.1.1 Primary map



X

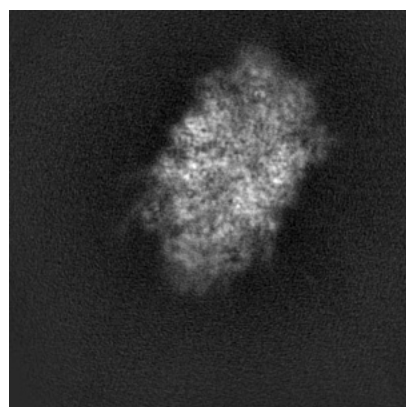


Y

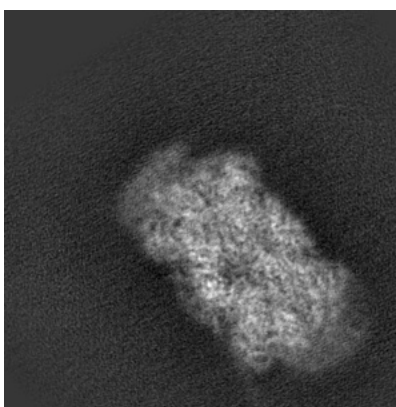


Z

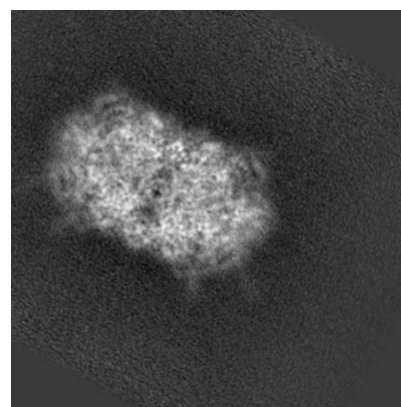
6.1.2 Raw map



X



Y

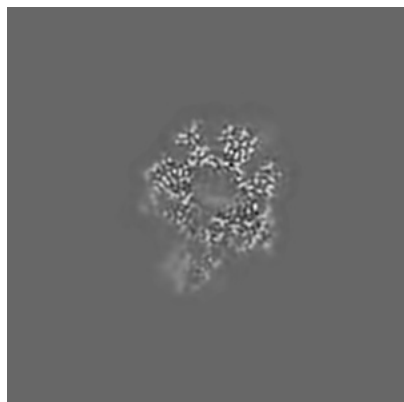


Z

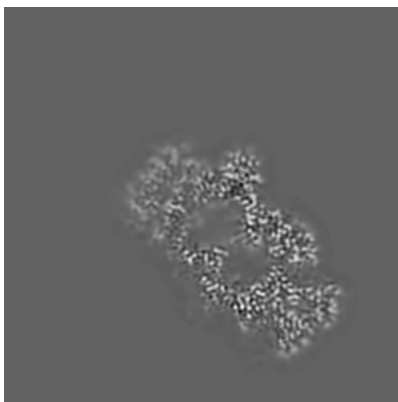
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

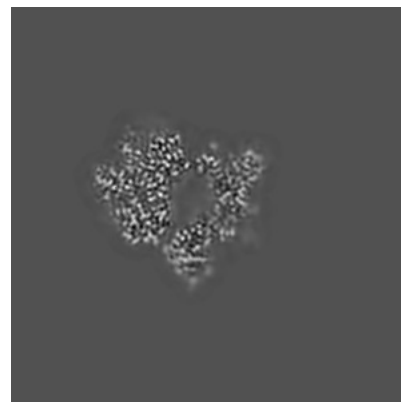
6.2.1 Primary map



X Index: 150

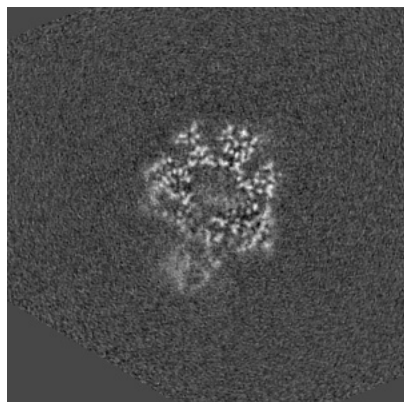


Y Index: 150

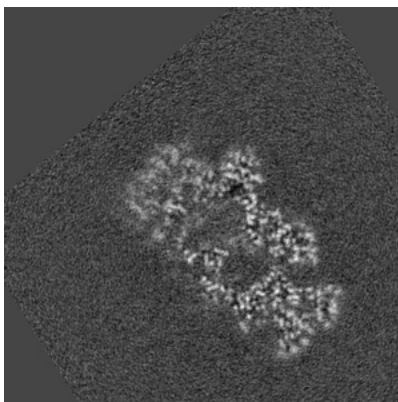


Z Index: 150

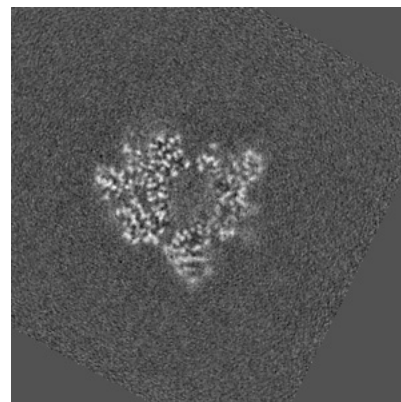
6.2.2 Raw map



X Index: 150



Y Index: 150

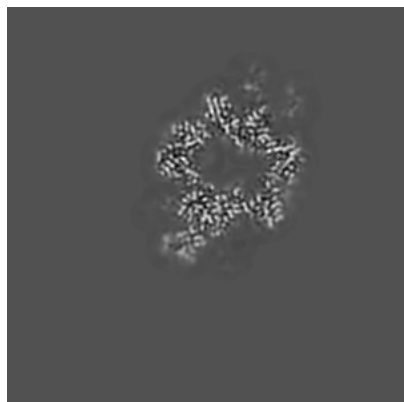


Z Index: 150

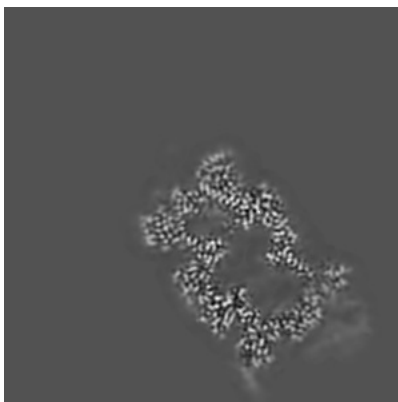
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

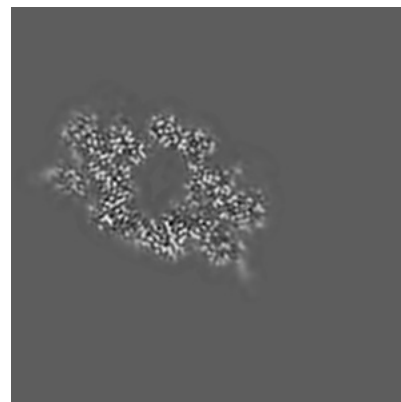
6.3.1 Primary map



X Index: 113

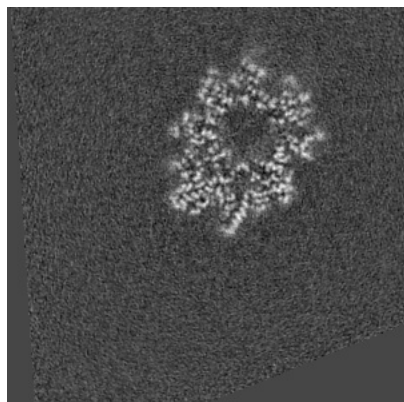


Y Index: 172

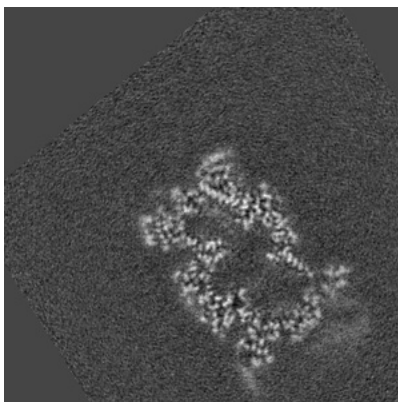


Z Index: 179

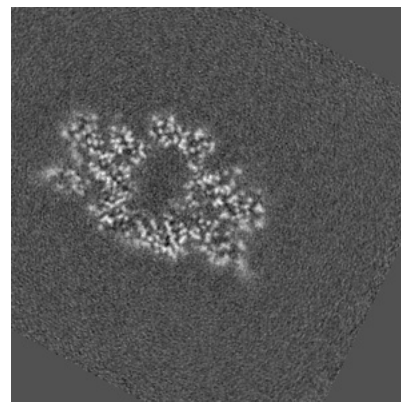
6.3.2 Raw map



X Index: 88



Y Index: 172

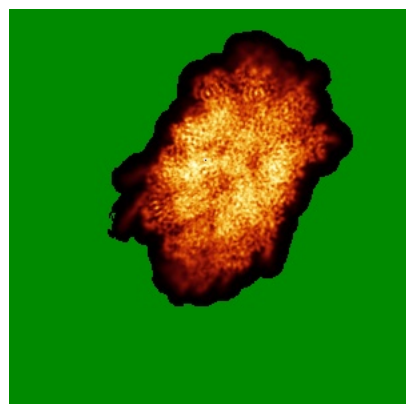


Z Index: 179

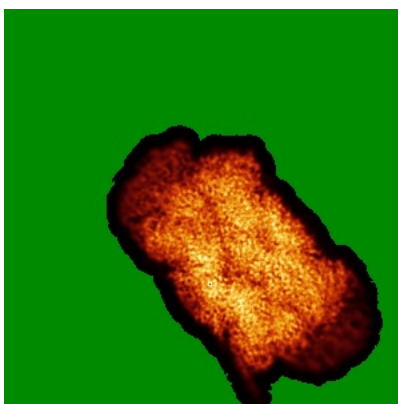
The images above show the largest variance slices of the map in three orthogonal directions.

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

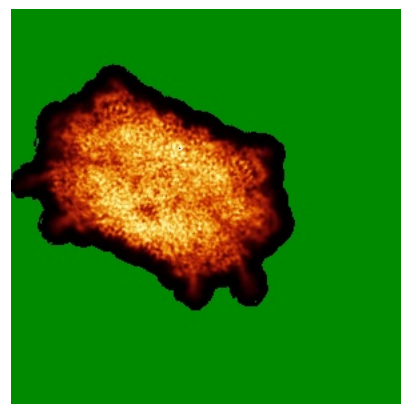
6.4.1 Primary map



X

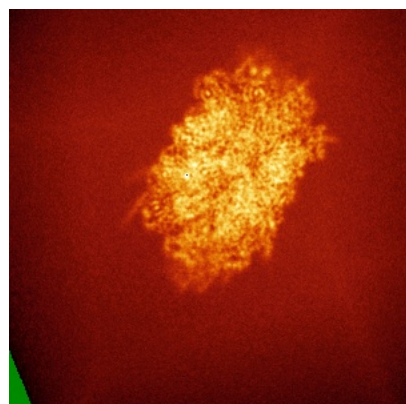


Y

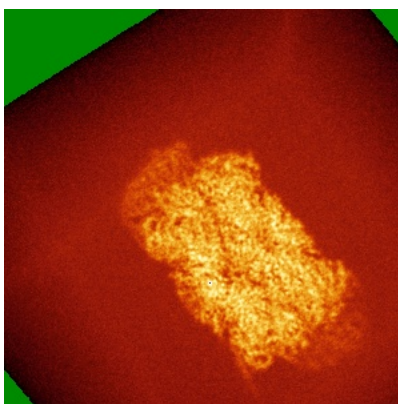


Z

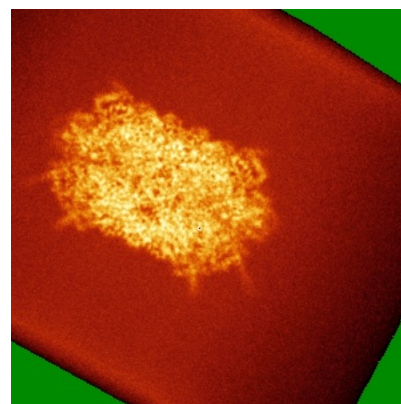
6.4.2 Raw map



X



Y

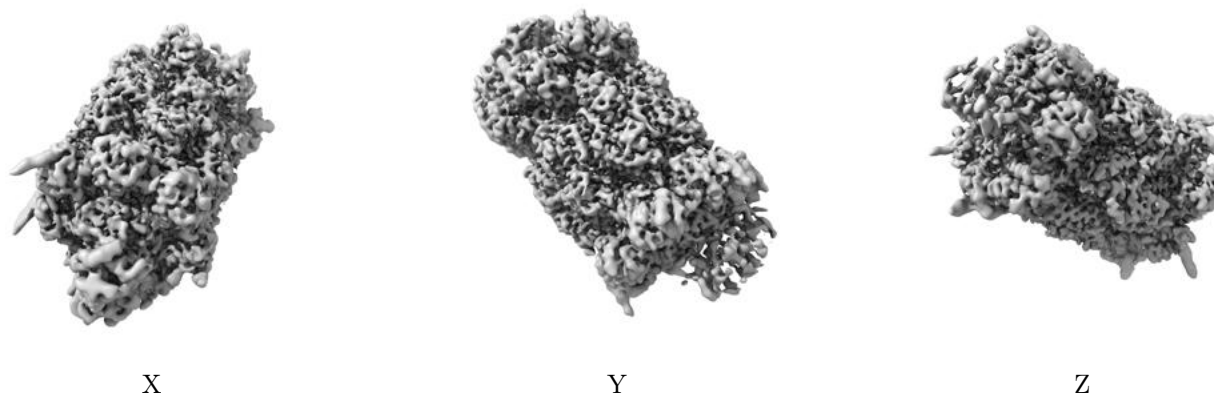


Z

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

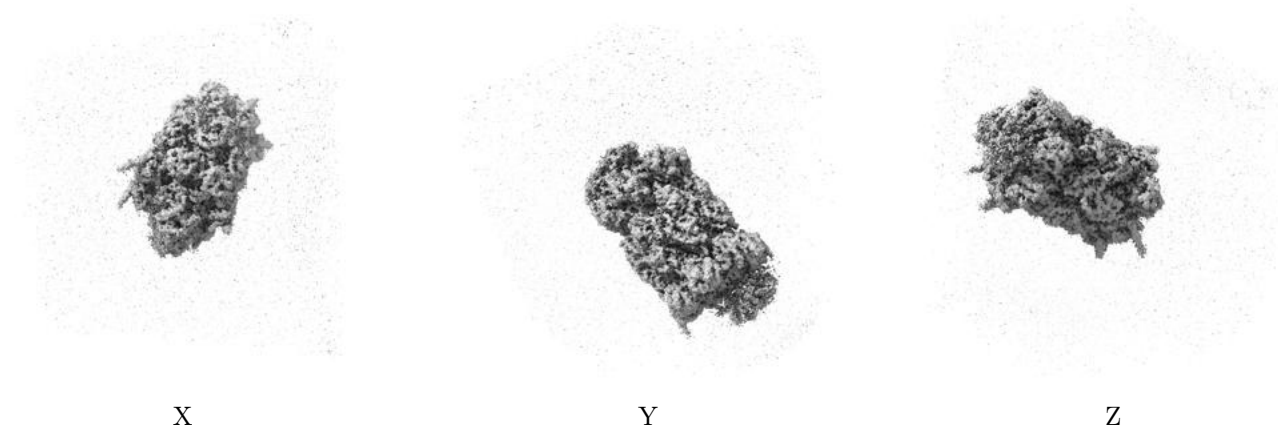
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.237. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

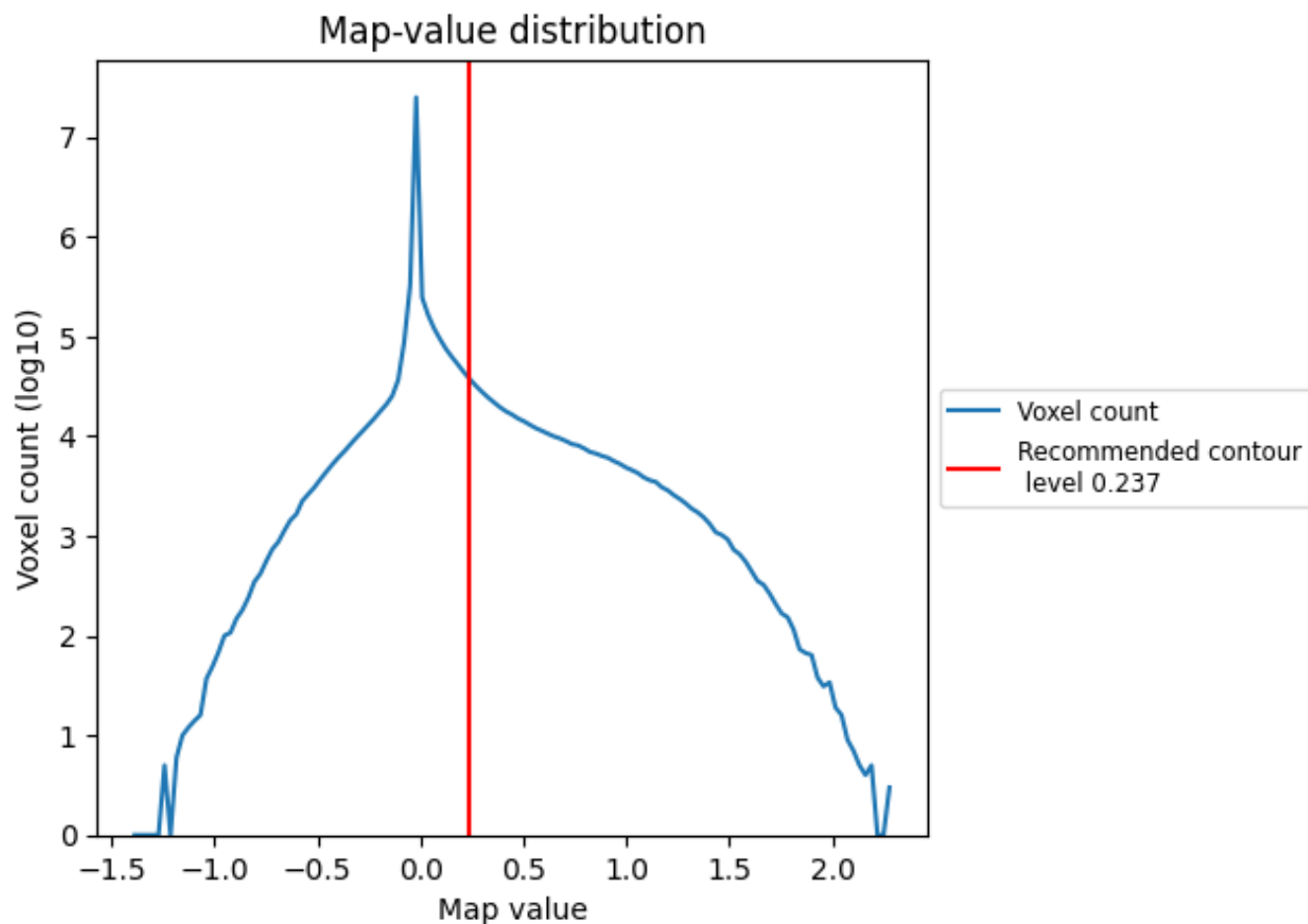
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

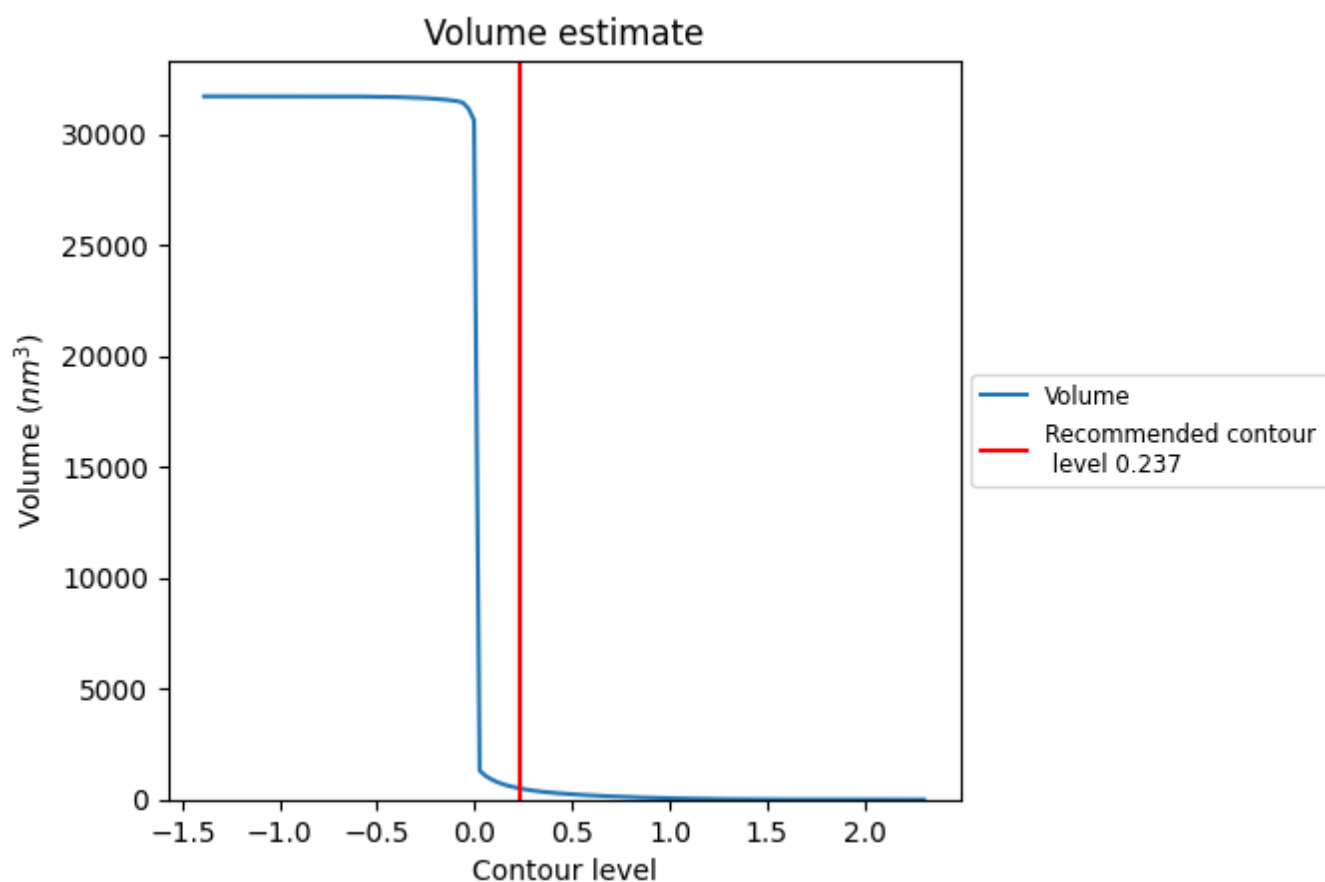
This section contains the results of statistical analysis of the map.

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.

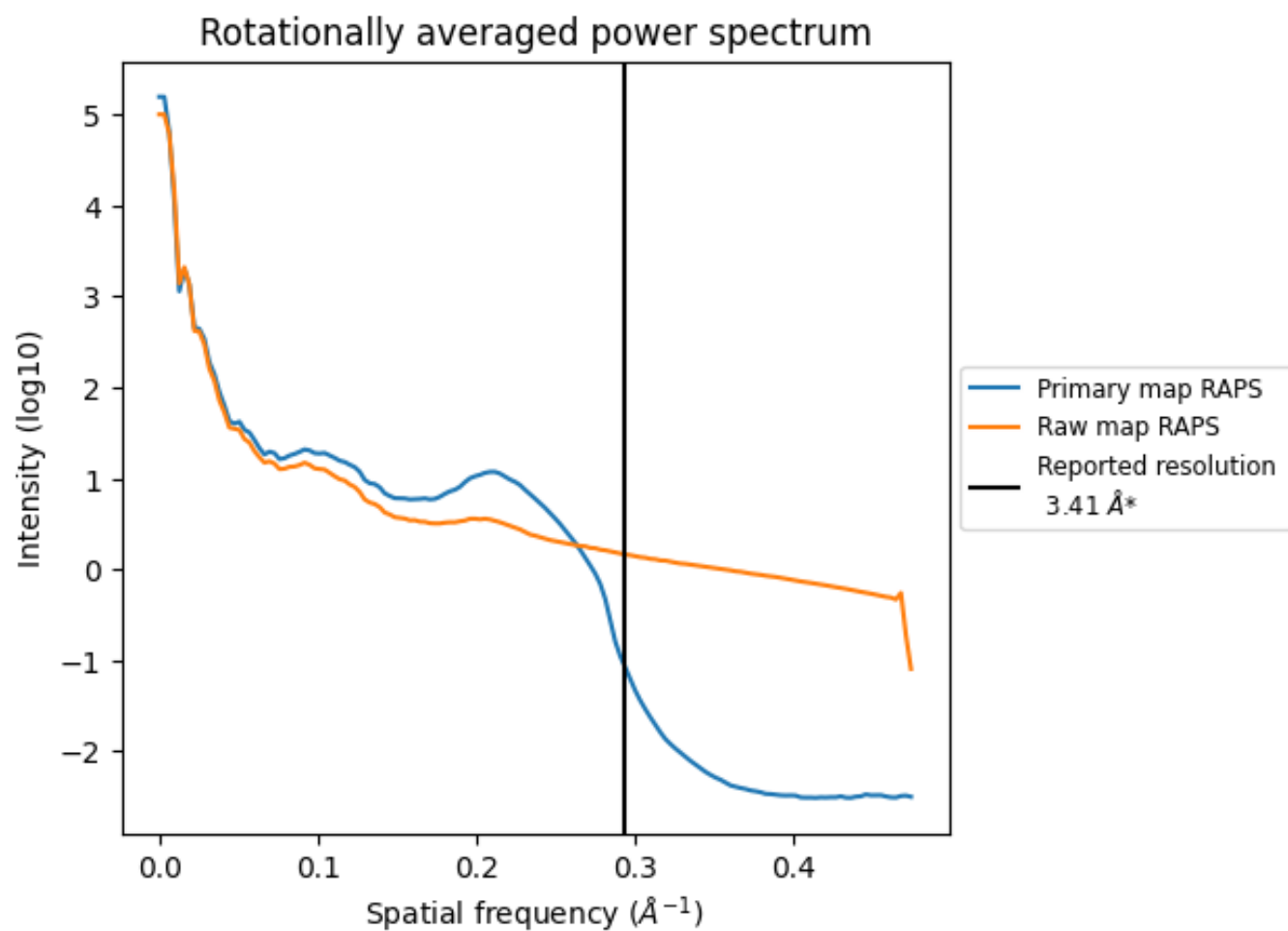
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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 ⓘ

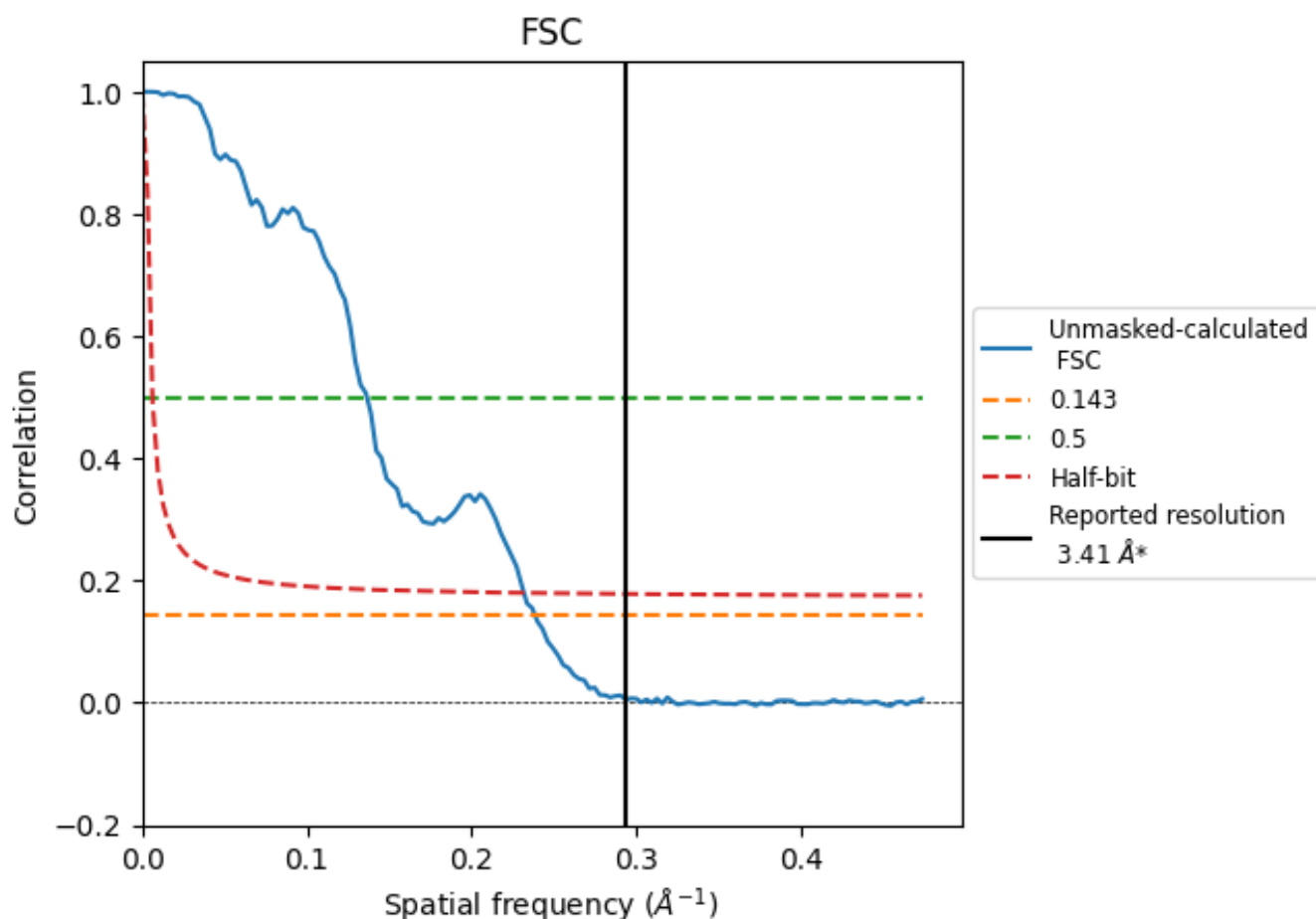


*Reported resolution corresponds to spatial frequency of $0.293 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

8.2 Resolution estimates [i](#)

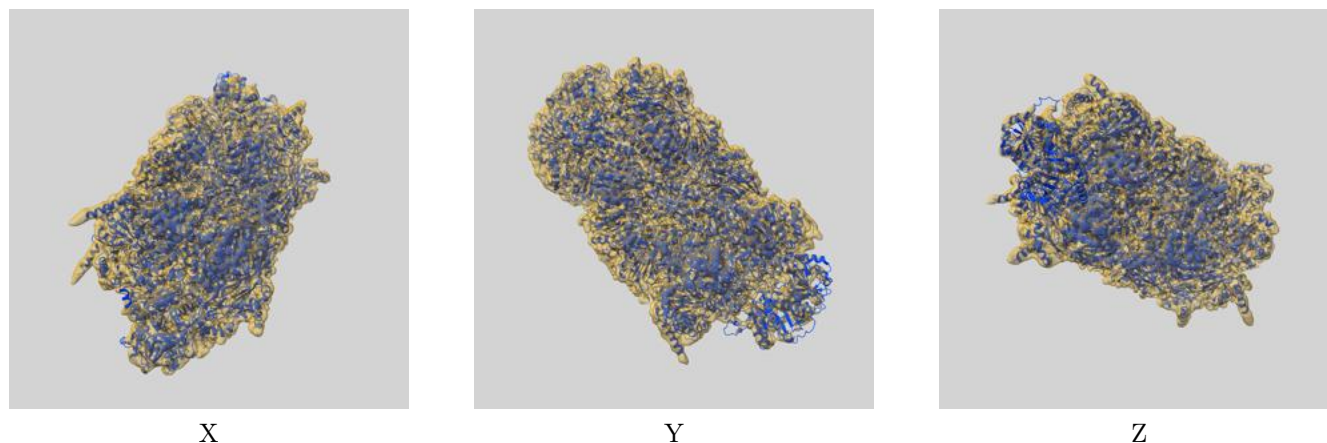
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.19	7.33	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.41 by more than 10 %

9 Map-model fit [i](#)

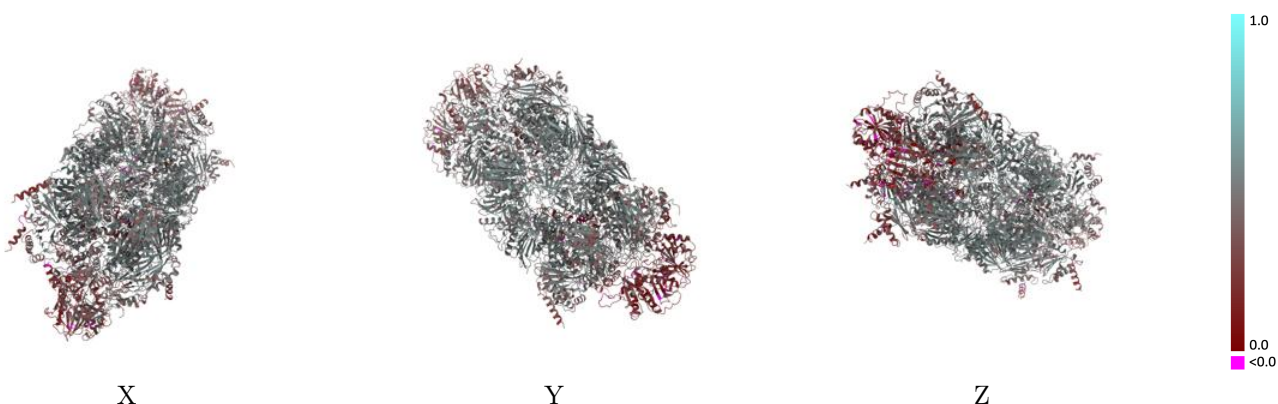
This section contains information regarding the fit between EMDB map EMD-39333 and PDB model 8YIY. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.237 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](#)

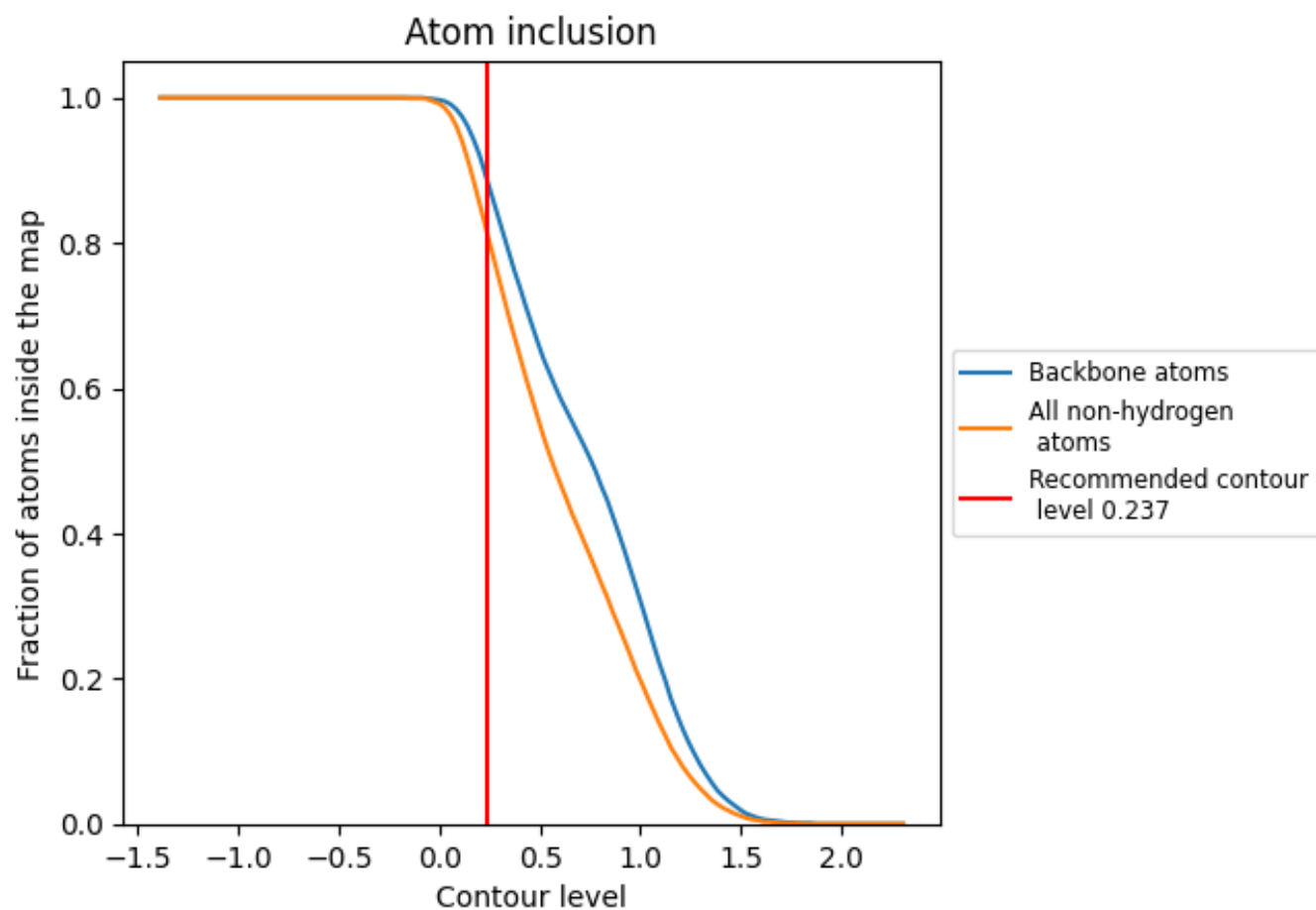


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.4310
A	 0.8940	 0.4540
B	 0.8830	 0.4470
C	 0.8470	 0.3920
D	 0.8430	 0.4320
E	 0.9070	 0.4530
F	 0.9030	 0.4590
G	 0.8990	 0.4510
H	 0.8080	 0.4380
I	 0.9310	 0.5010
J	 0.9150	 0.4960
K	 0.8600	 0.4690
L	 0.9270	 0.4990
M	 0.9230	 0.5000
N	 0.9300	 0.5000
O	 0.9070	 0.4630
P	 0.8820	 0.4390
Q	 0.8760	 0.4260
R	 0.8700	 0.4490
S	 0.9200	 0.4810
T	 0.9160	 0.4710
U	 0.9060	 0.4590
V	 0.8320	 0.4610
W	 0.9480	 0.5190
X	 0.9370	 0.5180
Y	 0.8970	 0.5000
Z	 0.9390	 0.5110
a	 0.9400	 0.5130
b	 0.9410	 0.5150
c	 0.2230	 0.1990
d	 0.3340	 0.2170
e	 0.1530	 0.2070
f	 0.5760	 0.2870
g	 0.6960	 0.3170
h	 0.3220	 0.2580

