Full wwPDB EM Validation Report

Nov 3, 2022 – 02:48 PM EDT

PDB ID	:	5VF3
EMDB ID	:	EMD-8661
Title	:	Bacteriophage T4 isometric capsid
Authors	:	Chen, Z.; Sun, L.; Zhang, Z.; Fokine, A.; Padilla-Sanchez, V.; Hanein, D.; Jiang, W.; Rossmann, M.G.; Rao, V.B.
Deposited on	:	2017-04-06
Resolution	:	3.30 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:

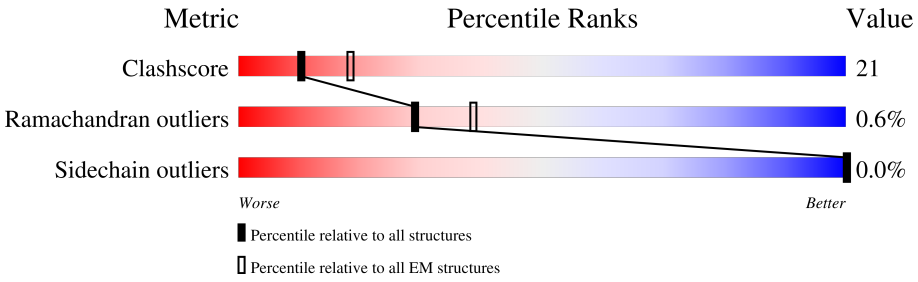
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



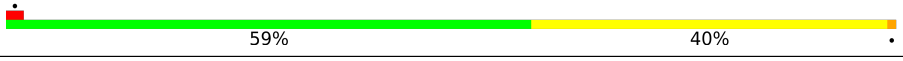
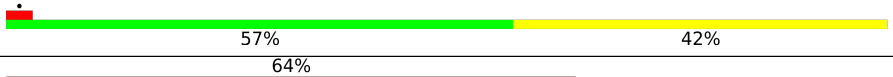
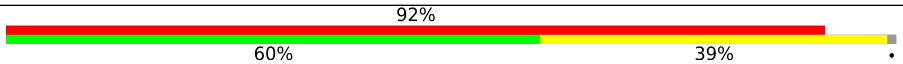
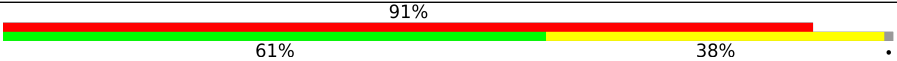
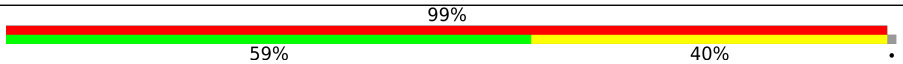
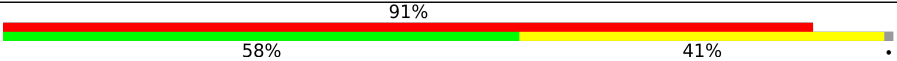
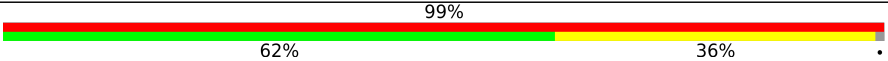
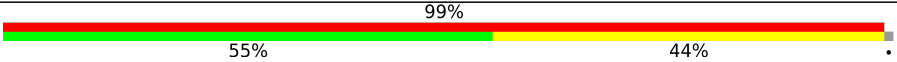
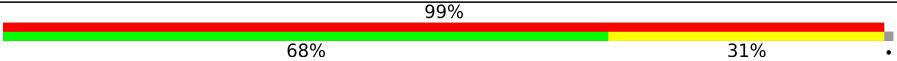
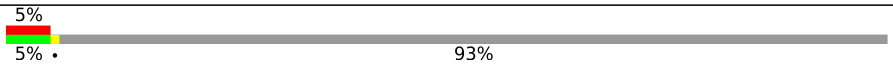
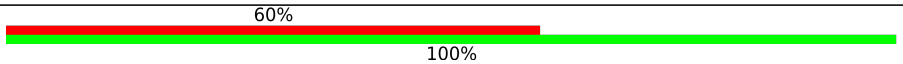
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	417	14% 98%
2	A	456	59% 40%
2	B	456	53% 47%
2	C	456	57% 43%
2	D	456	55% 44%
2	E	456	53% 47%
2	F	456	57% 43%
2	G	456	60% 39%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	456	
2	I	456	
2	J	456	
2	K	456	
2	L	456	
3	O	80	
3	P	80	
3	Q	80	
3	R	80	
3	S	80	
3	T	80	
3	U	80	
3	V	80	
3	W	80	
3	X	80	
3	Y	80	
4	Z	376	
5	z	15	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 51584 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 Capsid vertex protein gp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	415	3208	2039	521	640	8	0	0

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	456	3427	2168	584	660	15	0	0
2	B	456	3427	2168	584	660	15	0	0
2	C	456	3427	2168	584	660	15	0	0
2	D	456	3427	2168	584	660	15	0	0
2	E	456	3427	2168	584	660	15	0	0
2	F	456	3427	2168	584	660	15	0	0
2	G	456	3427	2168	584	660	15	0	0
2	H	456	3427	2168	584	660	15	0	0
2	I	456	3427	2168	584	660	15	0	0
2	J	456	3427	2168	584	660	15	0	0
2	K	456	3427	2168	584	660	15	0	0
2	L	456	3427	2168	584	660	15	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	THR	ALA	conflict	UNP P04535
B	275	THR	ALA	conflict	UNP P04535
C	275	THR	ALA	conflict	UNP P04535
D	275	THR	ALA	conflict	UNP P04535
E	275	THR	ALA	conflict	UNP P04535
F	275	THR	ALA	conflict	UNP P04535
G	275	THR	ALA	conflict	UNP P04535
H	275	THR	ALA	conflict	UNP P04535
I	275	THR	ALA	conflict	UNP P04535
J	275	THR	ALA	conflict	UNP P04535
K	275	THR	ALA	conflict	UNP P04535
L	275	THR	ALA	conflict	UNP P04535

- Molecule 3 is a protein called Small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	79	Total	C	N	O	0	0
			633	403	106	124		
3	P	79	Total	C	N	O	0	0
			633	403	106	124		
3	Q	79	Total	C	N	O	0	0
			633	403	106	124		
3	R	79	Total	C	N	O	0	0
			633	403	106	124		
3	S	79	Total	C	N	O	0	0
			633	403	106	124		
3	T	79	Total	C	N	O	0	0
			633	403	106	124		
3	U	79	Total	C	N	O	0	0
			633	403	106	124		
3	V	79	Total	C	N	O	0	0
			633	403	106	124		
3	W	79	Total	C	N	O	0	0
			633	403	106	124		
3	X	79	Total	C	N	O	0	0
			633	403	106	124		
3	Y	79	Total	C	N	O	0	0
			633	403	106	124		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	4	ALA	THR	conflict	UNP P03715

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	28	VAL	ILE	conflict	UNP P03715
P	4	ALA	THR	conflict	UNP P03715
P	28	VAL	ILE	conflict	UNP P03715
Q	4	ALA	THR	conflict	UNP P03715
Q	28	VAL	ILE	conflict	UNP P03715
R	4	ALA	THR	conflict	UNP P03715
R	28	VAL	ILE	conflict	UNP P03715
S	4	ALA	THR	conflict	UNP P03715
S	28	VAL	ILE	conflict	UNP P03715
T	4	ALA	THR	conflict	UNP P03715
T	28	VAL	ILE	conflict	UNP P03715
U	4	ALA	THR	conflict	UNP P03715
U	28	VAL	ILE	conflict	UNP P03715
V	4	ALA	THR	conflict	UNP P03715
V	28	VAL	ILE	conflict	UNP P03715
W	4	ALA	THR	conflict	UNP P03715
W	28	VAL	ILE	conflict	UNP P03715
X	4	ALA	THR	conflict	UNP P03715
X	28	VAL	ILE	conflict	UNP P03715
Y	4	ALA	THR	conflict	UNP P03715
Y	28	VAL	ILE	conflict	UNP P03715

- Molecule 4 is a protein called Highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	25	Total	C	N	O	S	0	0
			214	140	32	39	3		

- Molecule 5 is a protein called Highly immunogenic outer capsid protein.

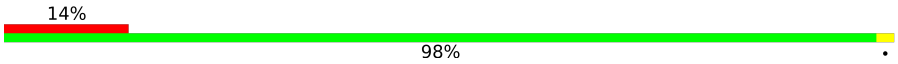
Mol	Chain	Residues	Atoms				AltConf	Trace
5	z	15	Total	C	N	O	0	0
			75	45	15	15		

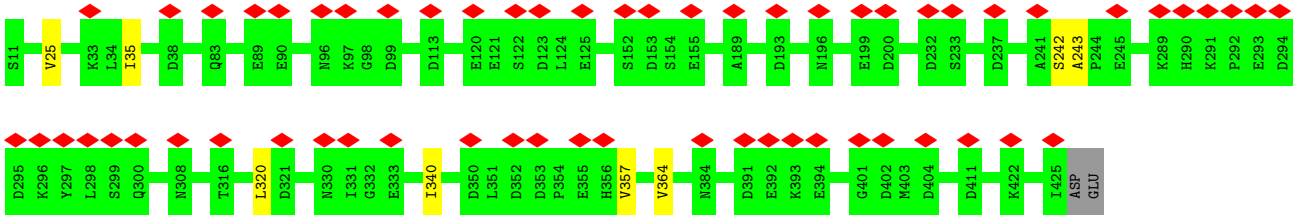
3 Residue-property plots (i)

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: Capsid vertex protein gp24

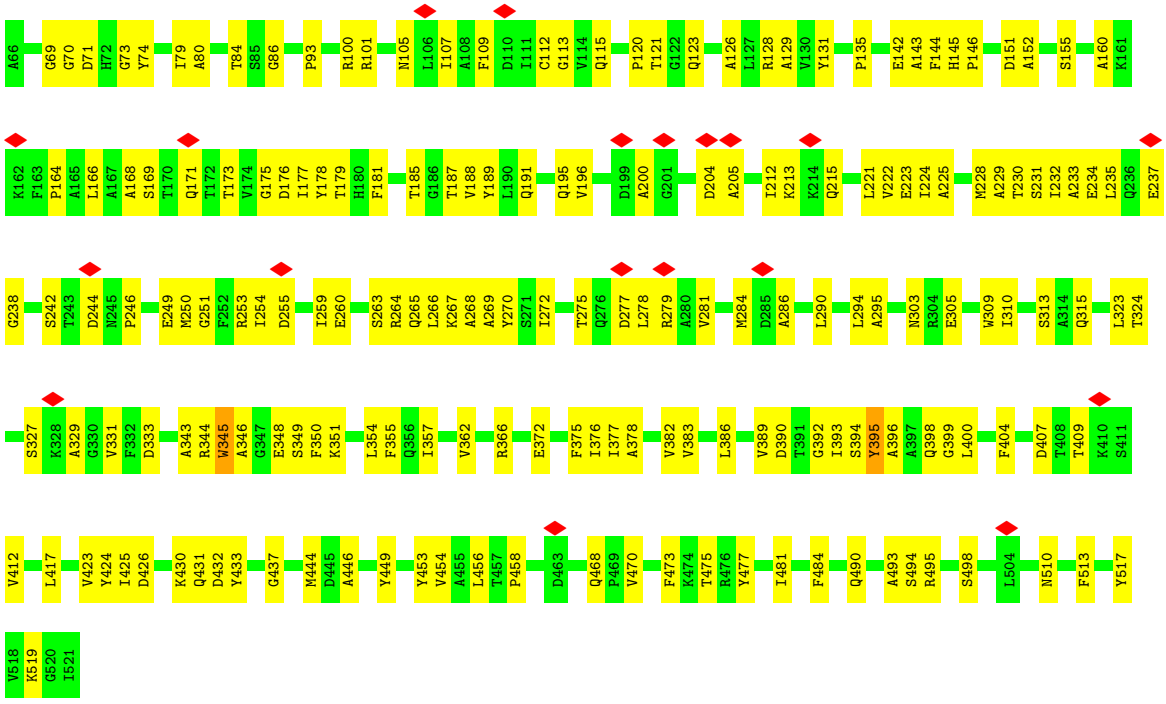
Chain a:





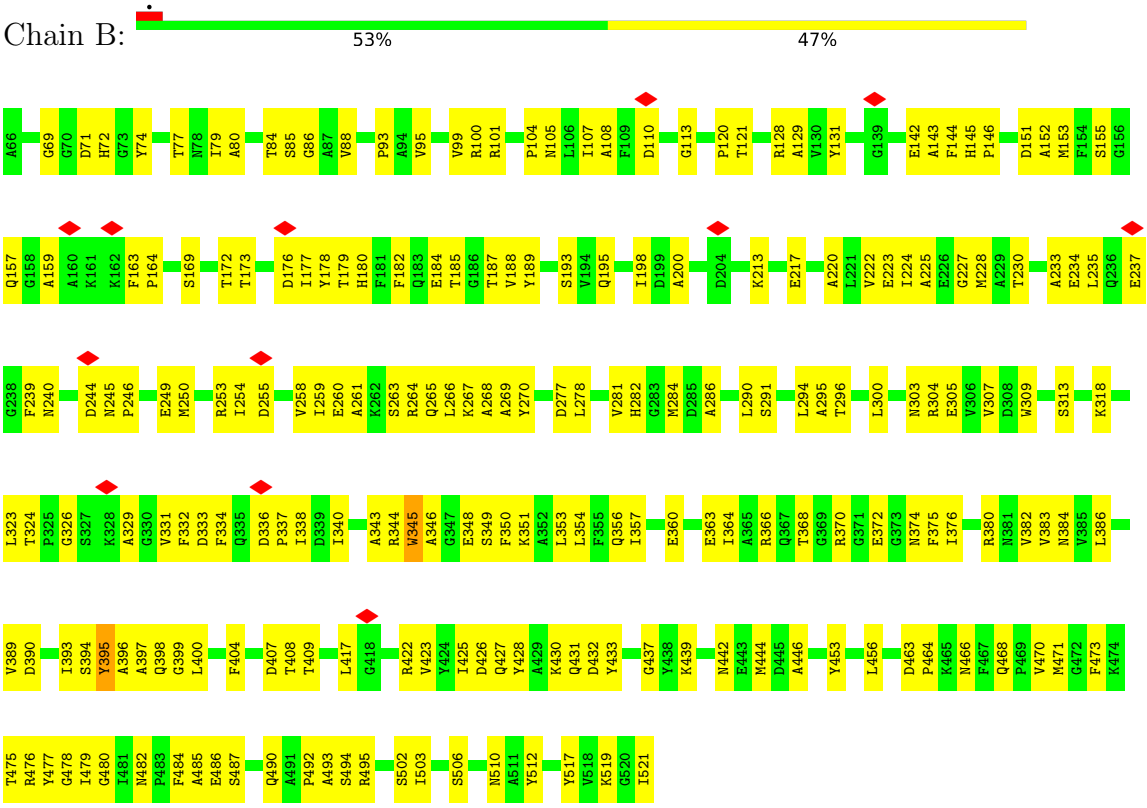
• Molecule 2: Major capsid protein

Chain A:



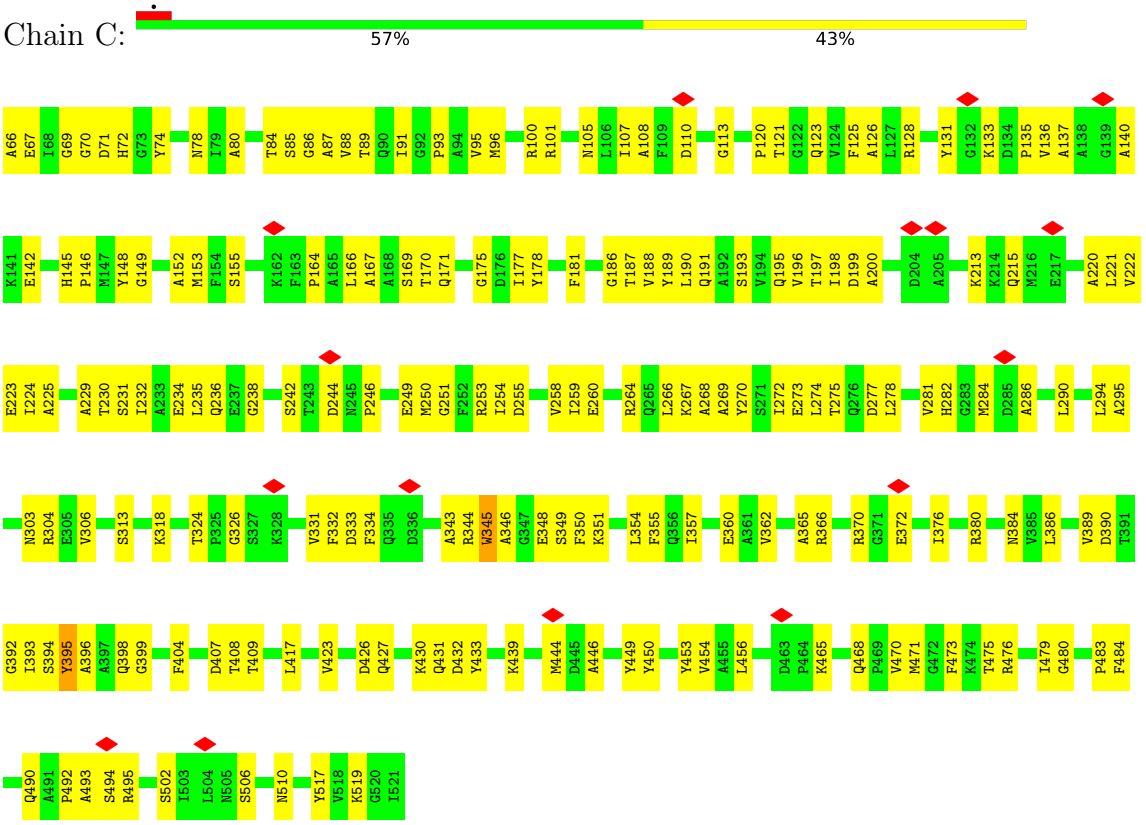
• Molecule 2: Major capsid protein

Chain B:



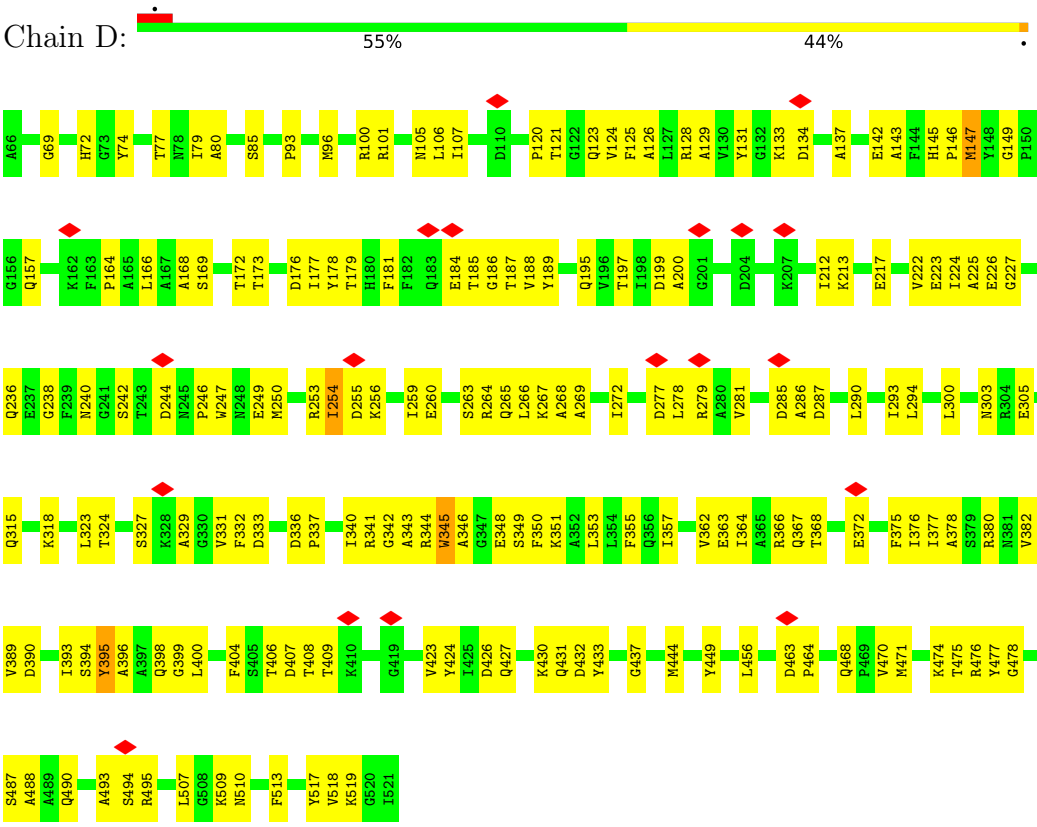
• Molecule 2: Major capsid protein

Chain C:



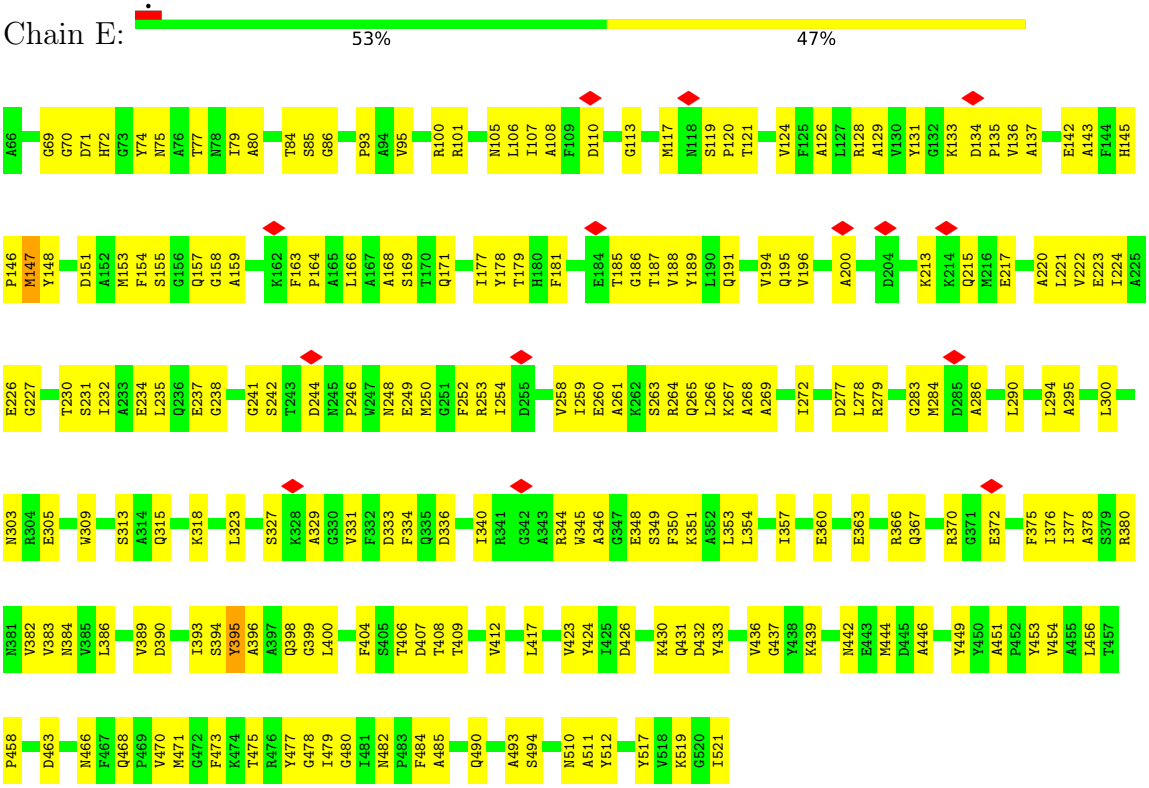
• Molecule 2: Major capsid protein

Chain D:



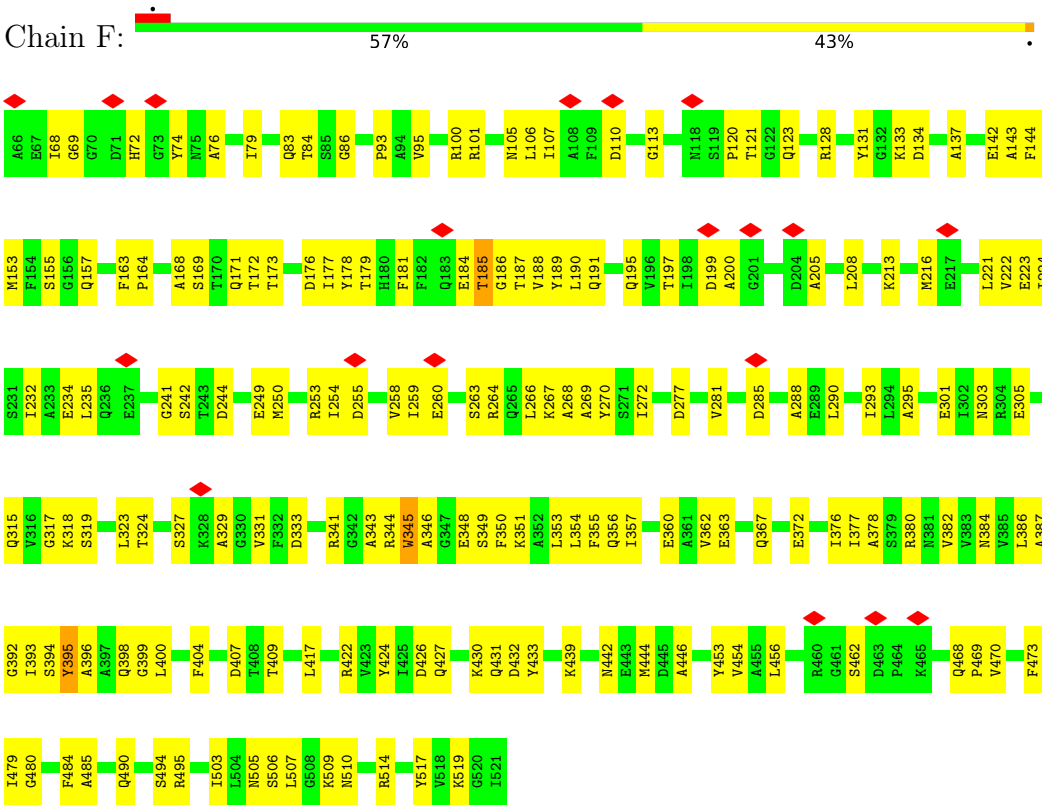
• Molecule 2: Major capsid protein

Chain E:



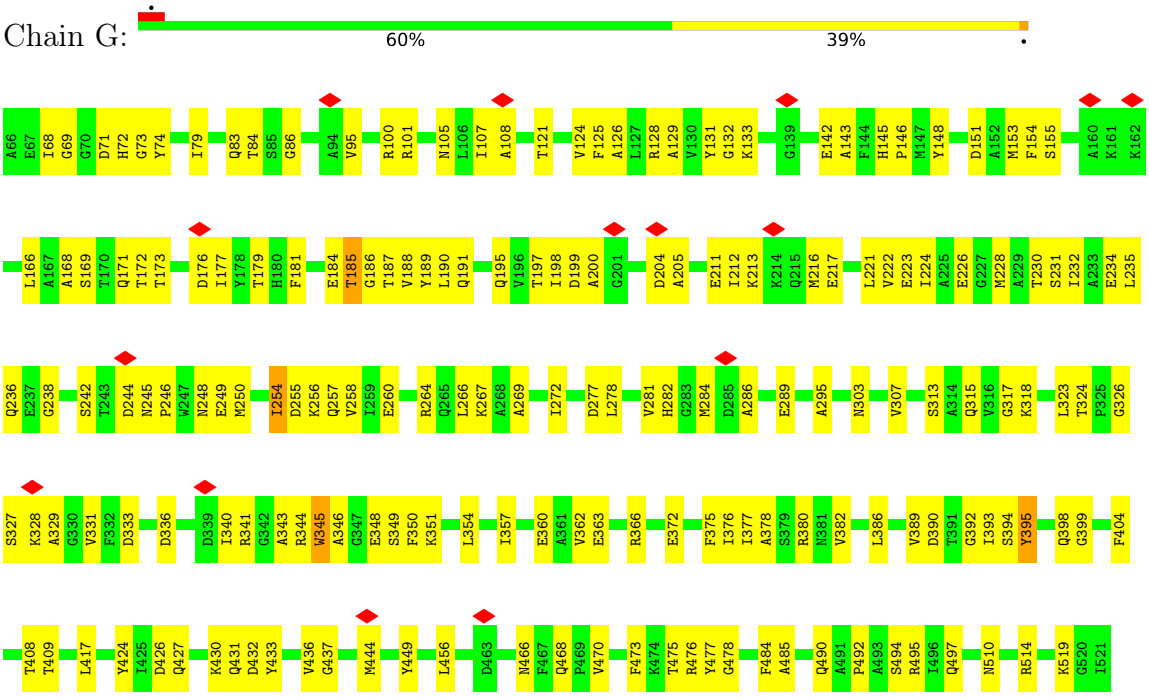
• Molecule 2: Major capsid protein

Chain F:



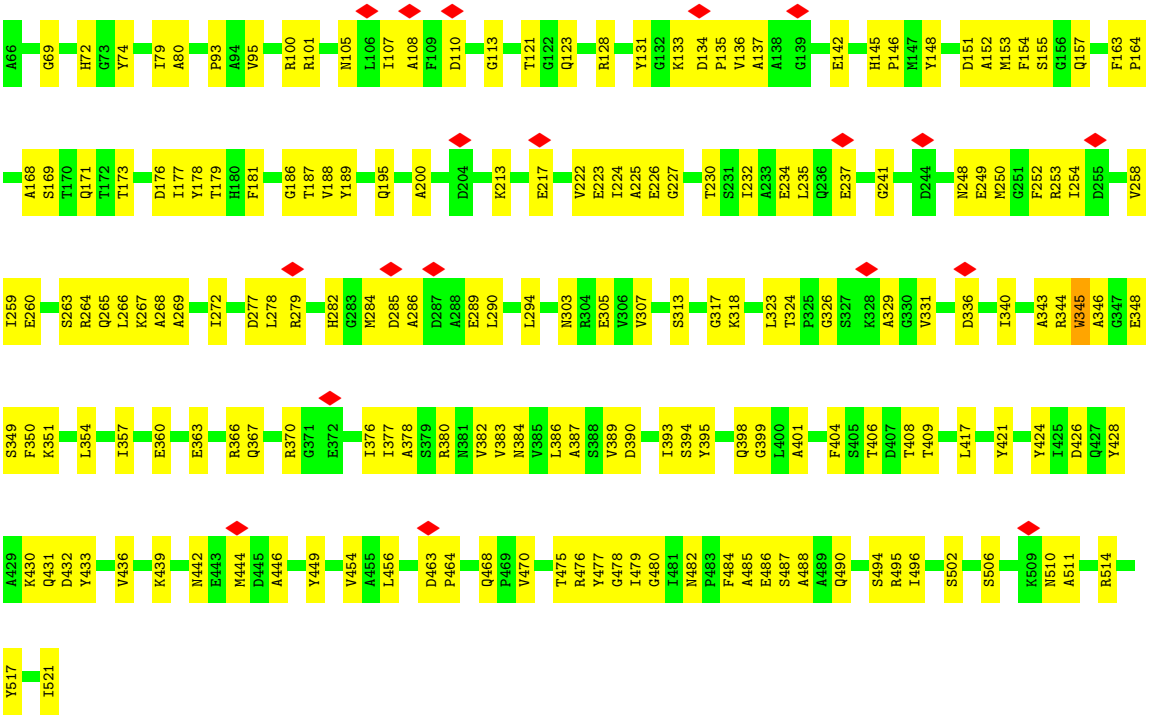
• Molecule 2: Major capsid protein

Chain G:



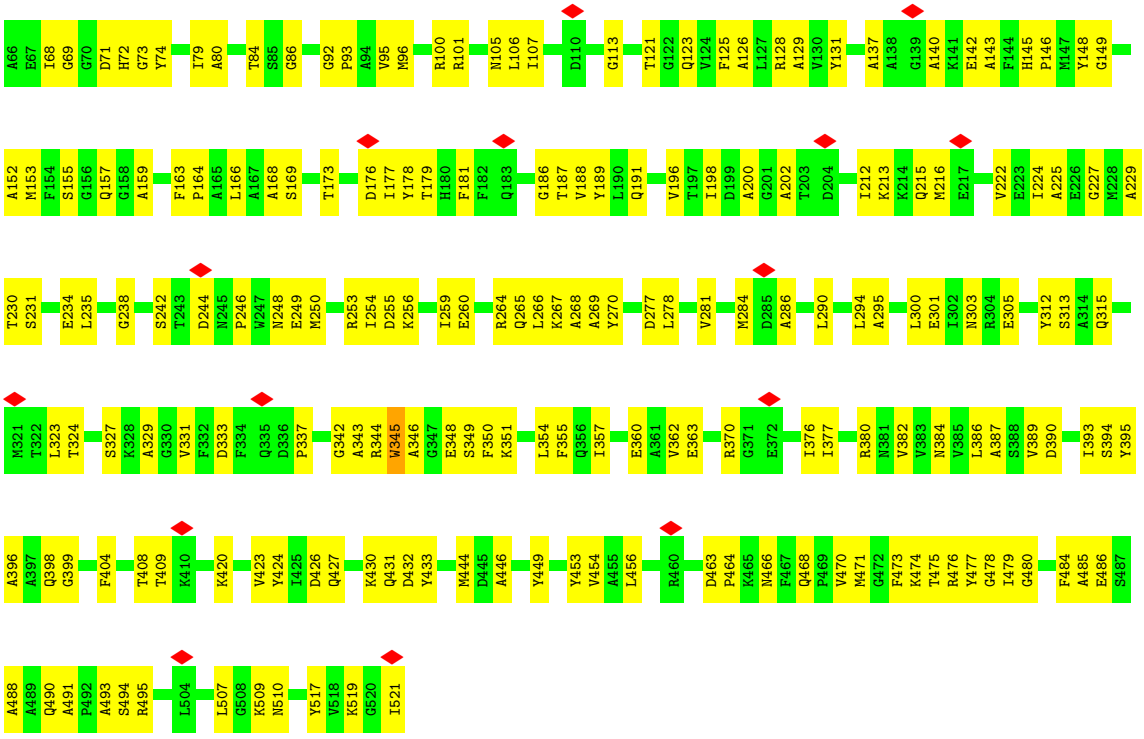
• Molecule 2: Major capsid protein

Chain H:



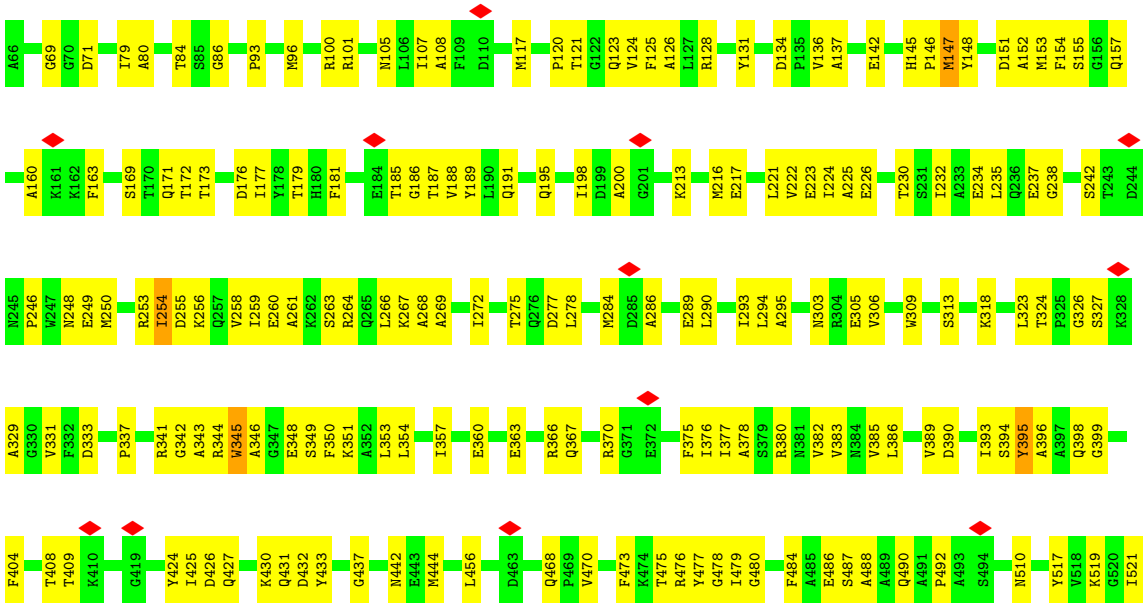
• Molecule 2: Major capsid protein

Chain I:



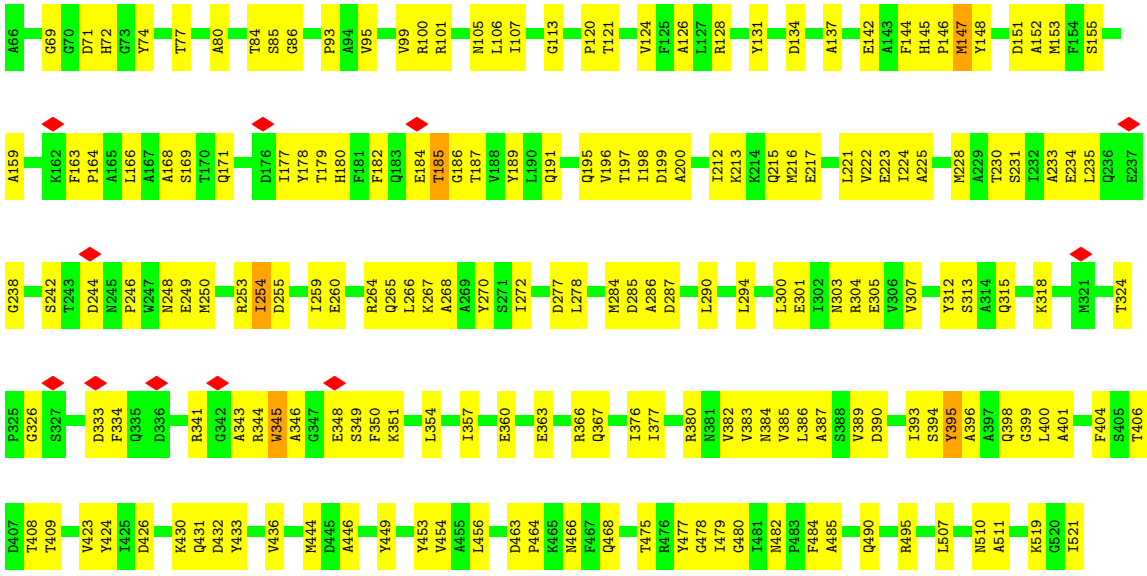
• Molecule 2: Major capsid protein

Chain J:



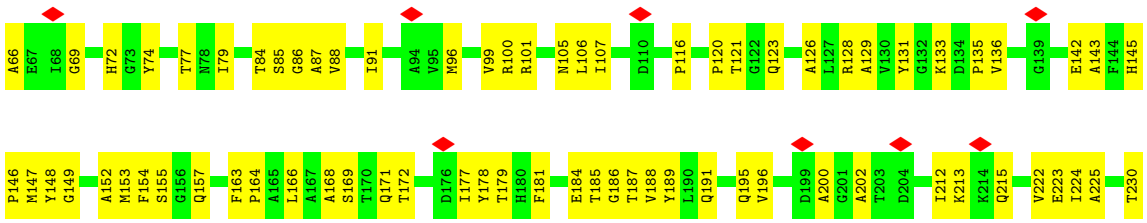
• Molecule 2: Major capsid protein

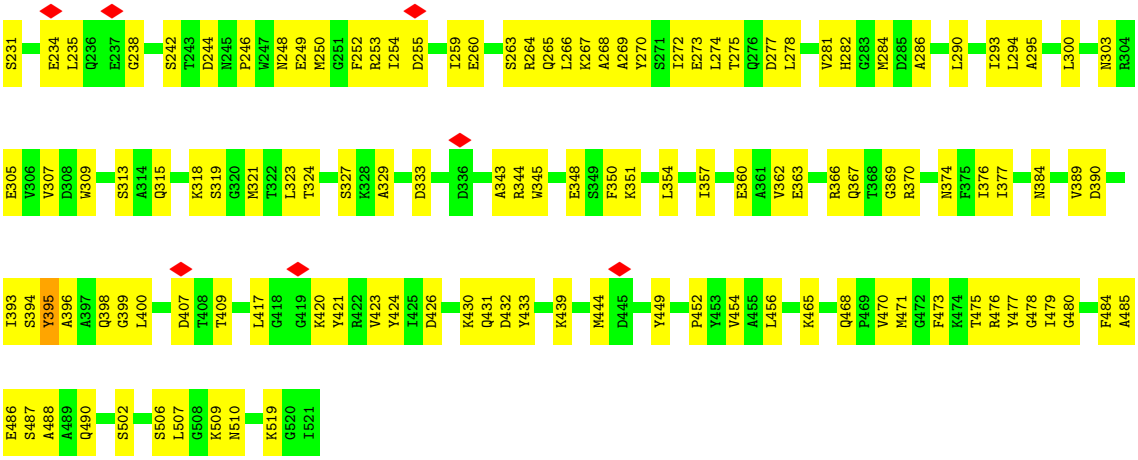
Chain K:



• Molecule 2: Major capsid protein

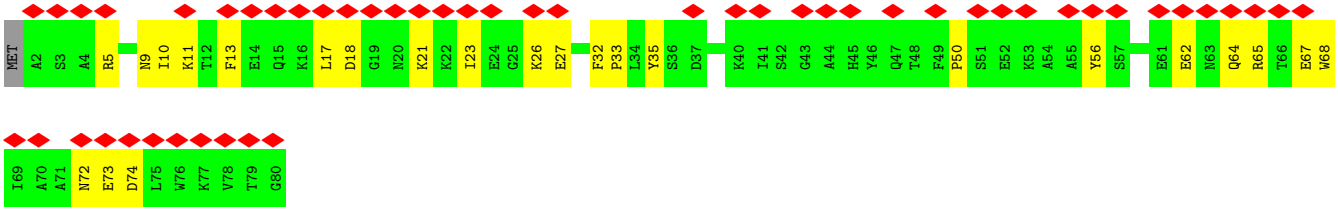
Chain L:





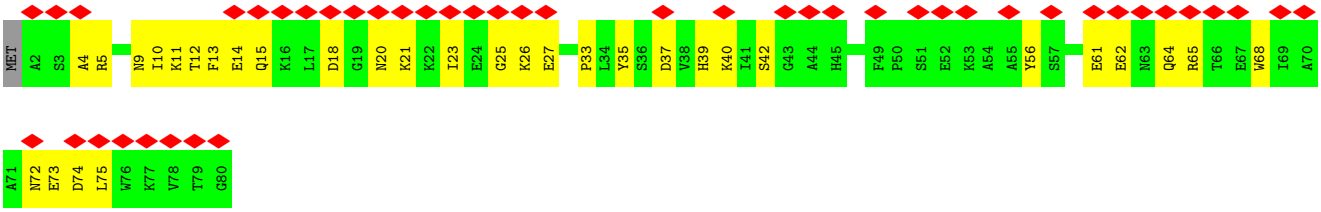
• Molecule 3: Small outer capsid protein

Chain O:



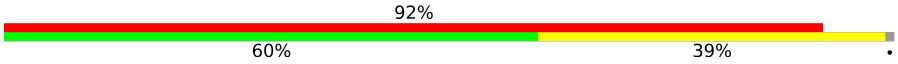
• Molecule 3: Small outer capsid protein

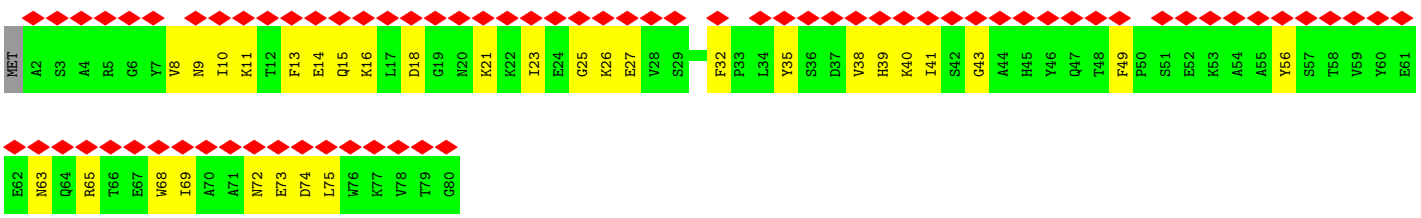
Chain P:



• Molecule 3: Small outer capsid protein

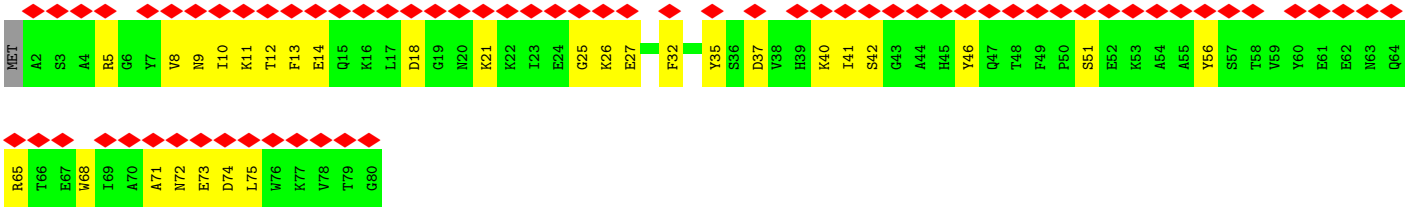
Chain Q:





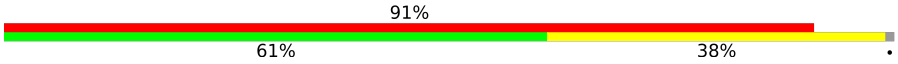
• Molecule 3: Small outer capsid protein

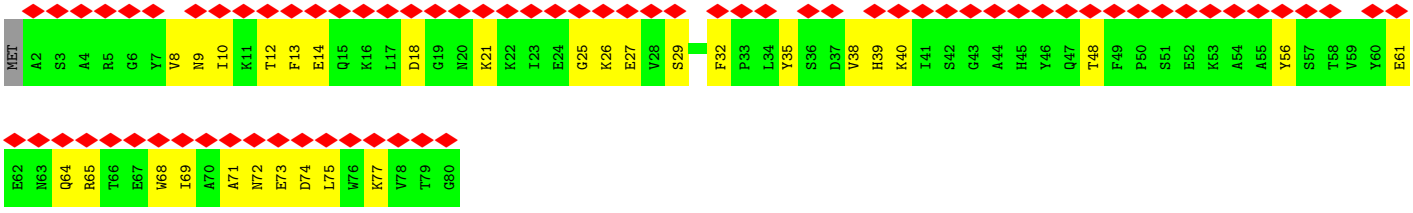
Chain R:



• Molecule 3: Small outer capsid protein

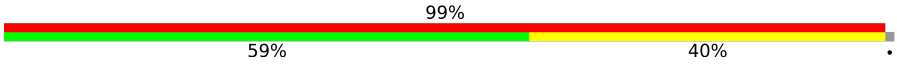
Chain S:

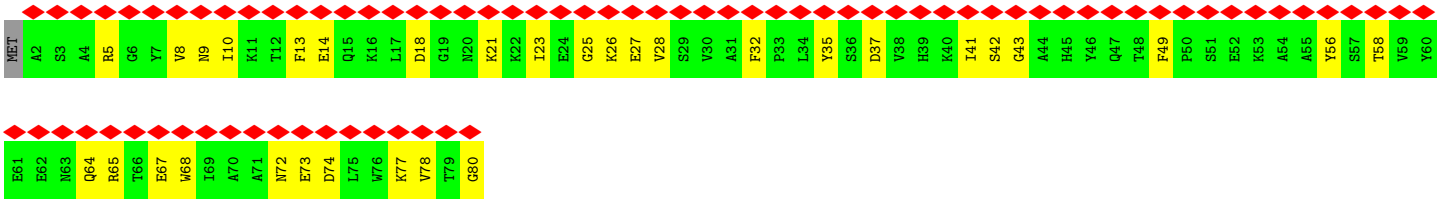




• Molecule 3: Small outer capsid protein

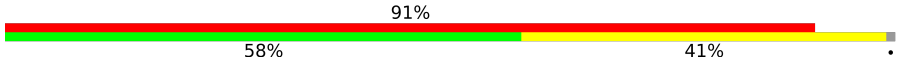
Chain T:

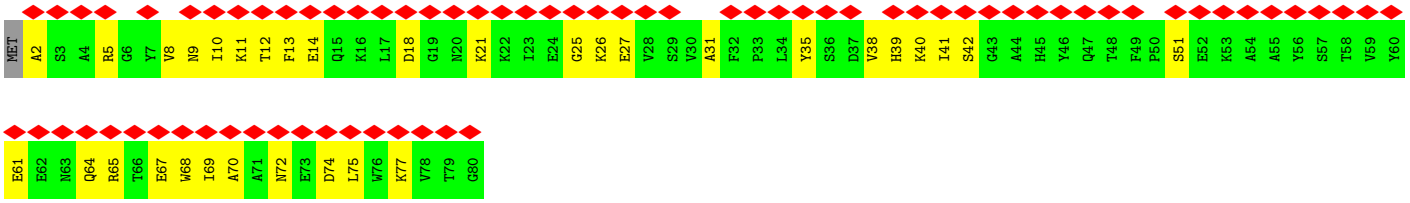




• Molecule 3: Small outer capsid protein

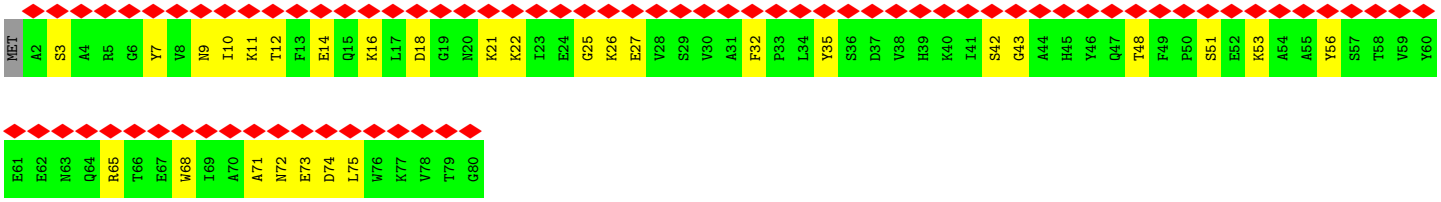
Chain U:





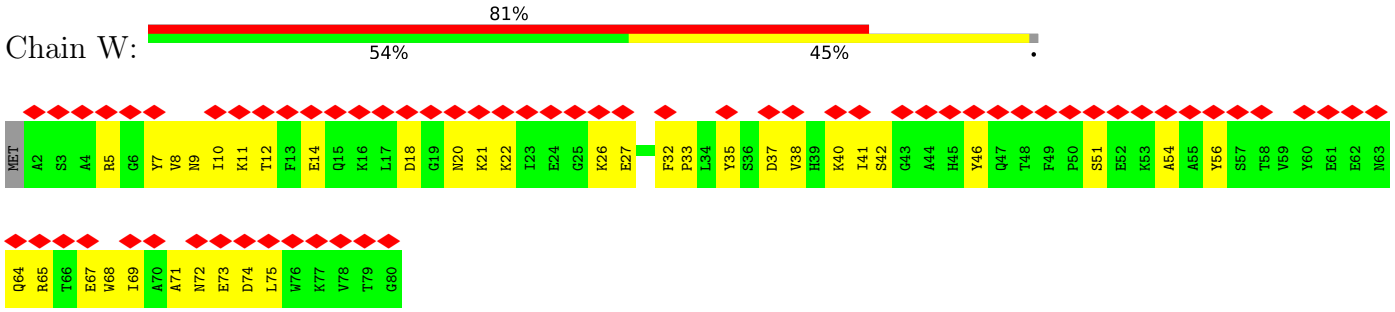
• Molecule 3: Small outer capsid protein

Chain V:



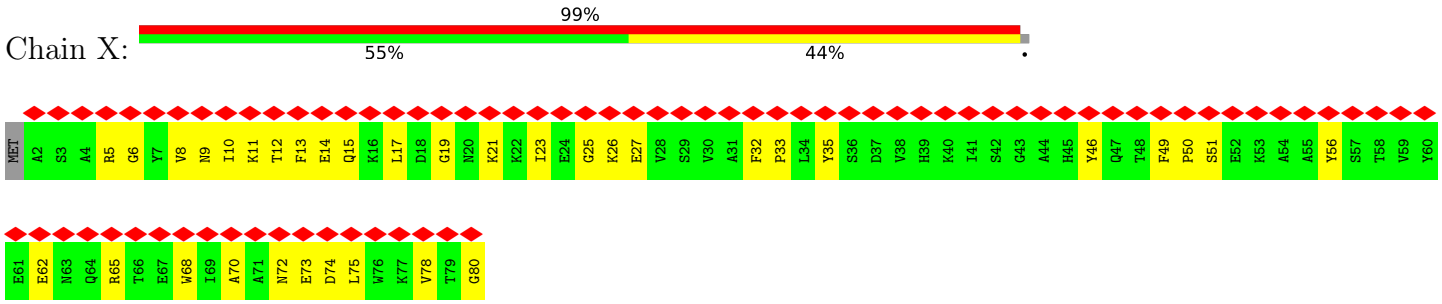
• Molecule 3: Small outer capsid protein

Chain W:



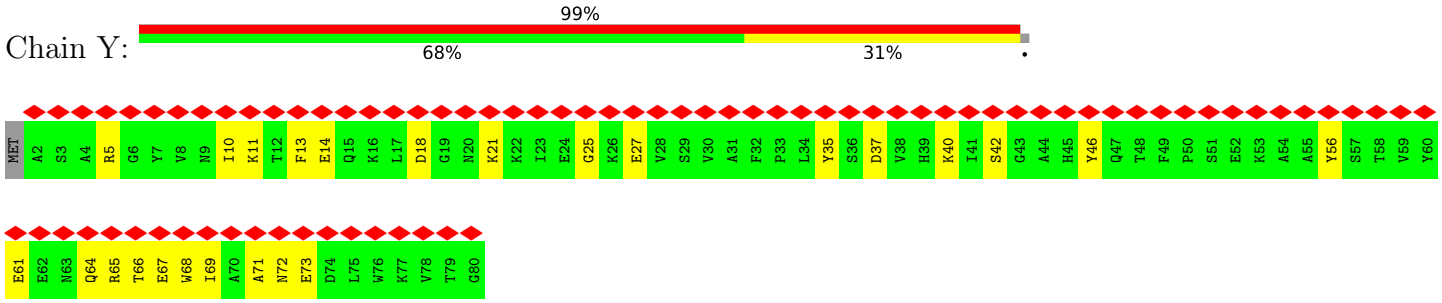
• Molecule 3: Small outer capsid protein

Chain X:



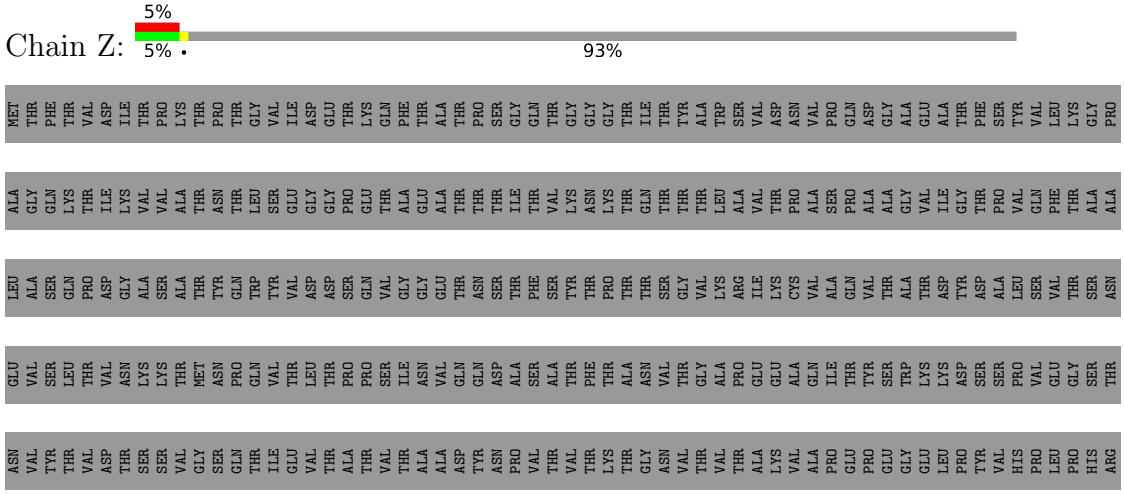
• Molecule 3: Small outer capsid protein

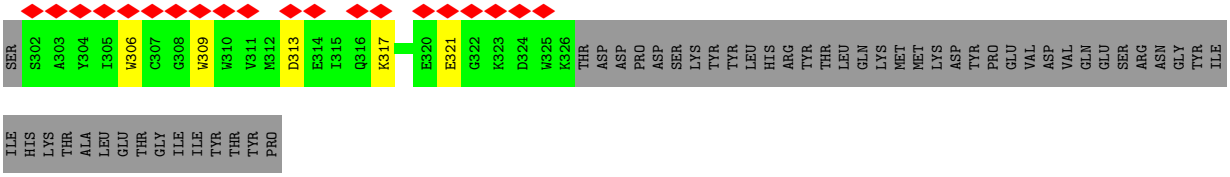
Chain Y:



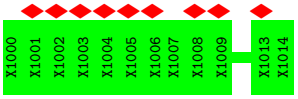
• Molecule 4: Highly immunogenic outer capsid protein

Chain Z:





• Molecule 5: Highly immunogenic outer capsid protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed during 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	26	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.346	Depositor
Minimum map value	-31.033	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.708	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	1244.16, 1244.16, 1244.16	wwPDB
Map dimensions	1536, 1536, 1536	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	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	0.56	0/3263	0.62	0/4430
2	A	0.61	0/3495	0.64	1/4734 (0.0%)
2	B	0.62	0/3495	0.64	1/4734 (0.0%)
2	C	0.63	0/3495	0.64	1/4734 (0.0%)
2	D	0.61	0/3495	0.64	1/4734 (0.0%)
2	E	0.63	0/3495	0.64	0/4734
2	F	0.62	0/3495	0.64	1/4734 (0.0%)
2	G	0.61	0/3495	0.64	1/4734 (0.0%)
2	H	0.61	0/3495	0.64	1/4734 (0.0%)
2	I	0.61	0/3495	0.64	1/4734 (0.0%)
2	J	0.61	0/3495	0.64	1/4734 (0.0%)
2	K	0.61	0/3495	0.64	1/4734 (0.0%)
2	L	0.61	0/3495	0.64	0/4734
3	O	0.41	0/648	0.49	0/876
3	P	0.41	0/648	0.51	0/876
3	Q	0.37	0/648	0.49	0/876
3	R	0.37	0/648	0.52	0/876
3	S	0.36	0/648	0.49	0/876
3	T	0.32	0/648	0.48	0/876
3	U	0.34	0/648	0.48	0/876
3	V	0.29	0/648	0.47	0/876
3	W	0.36	0/648	0.51	0/876
3	X	0.32	0/648	0.48	0/876
3	Y	0.33	0/648	0.47	0/876
4	Z	0.27	0/222	0.43	0/301
All	All	0.58	0/52553	0.62	10/71175 (0.0%)

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

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
2	E	0	1
2	F	0	1
2	G	0	1
2	K	0	1
3	Q	0	1
All	All	0	8

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	345	TRP	CA-CB-CG	5.85	124.81	113.70
2	H	345	TRP	CA-CB-CG	5.79	124.71	113.70
2	C	345	TRP	CA-CB-CG	5.67	124.48	113.70
2	D	345	TRP	CA-CB-CG	5.59	124.32	113.70
2	F	345	TRP	CA-CB-CG	5.58	124.30	113.70
2	I	345	TRP	CA-CB-CG	5.58	124.31	113.70
2	B	345	TRP	CA-CB-CG	5.56	124.27	113.70
2	J	345	TRP	CA-CB-CG	5.49	124.13	113.70
2	A	345	TRP	CA-CB-CG	5.35	123.87	113.70
2	G	345	TRP	CA-CB-CG	5.09	123.37	113.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	185	THR	Peptide
2	F	185	THR	Peptide
2	G	185	THR	Peptide
2	K	185	THR	Peptide
3	Q	63	ASN	Peptide
1	a	242	SER	Peptide
1	a	320	LEU	Peptide
1	a	35	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3208	0	3205	0	0
2	A	3427	0	3373	174	0
2	B	3427	0	3373	195	0
2	C	3427	0	3373	194	0
2	D	3427	0	3373	191	0
2	E	3427	0	3373	201	0
2	F	3427	0	3373	183	0
2	G	3427	0	3373	174	0
2	H	3427	0	3373	158	0
2	I	3427	0	3373	177	0
2	J	3427	0	3373	166	0
2	K	3427	0	3373	174	0
2	L	3427	0	3373	186	0
3	O	633	0	608	22	0
3	P	633	0	608	26	0
3	Q	633	0	608	28	0
3	R	633	0	608	25	0
3	S	633	0	608	29	0
3	T	633	0	608	33	0
3	U	633	0	608	24	0
3	V	633	0	608	23	0
3	W	633	0	608	28	0
3	X	633	0	608	30	0
3	Y	633	0	608	22	0
4	Z	214	0	187	3	0
5	z	75	0	19	0	0
All	All	51584	0	50575	2035	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 21.

All (2035) 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)
2:A:152:ALA:HB1	2:A:225:ALA:HB2	1.51	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:431:GLN:HE22	2:K:217:GLU:HB2	1.35	0.92
2:J:152:ALA:HB1	2:J:225:ALA:HB2	1.51	0.91
2:H:152:ALA:HB1	2:H:225:ALA:HB2	1.54	0.89
2:F:152:ALA:HB1	2:F:225:ALA:HB2	1.55	0.89
2:E:350:PHE:HB2	2:E:389:VAL:HG21	1.54	0.89
2:D:152:ALA:HB1	2:D:225:ALA:HB2	1.54	0.88
2:B:350:PHE:HB2	2:B:389:VAL:HG21	1.55	0.87
2:C:152:ALA:HB1	2:C:225:ALA:HB2	1.54	0.87
2:H:401:ALA:O	2:I:420:LYS:NZ	2.09	0.85
2:K:431:GLN:HE21	2:L:213:LYS:HB3	1.41	0.85
2:J:278:LEU:HD22	2:J:286:ALA:HB2	1.58	0.84
2:K:350:PHE:HB2	2:K:389:VAL:HG21	1.59	0.84
2:A:278:LEU:HD22	2:A:286:ALA:HB2	1.58	0.84
2:L:145:HIS:HD2	2:L:146:PRO:HD2	1.43	0.83
2:I:278:LEU:HD22	2:I:286:ALA:HB2	1.61	0.83
2:B:357:ILE:HD11	2:B:376:ILE:HG21	1.60	0.82
2:B:456:LEU:H	2:B:475:THR:HG22	1.43	0.82
3:T:14:GLU:HB3	3:T:25:GLY:H	1.43	0.82
2:D:350:PHE:HB2	2:D:389:VAL:HG21	1.61	0.82
2:G:278:LEU:HD22	2:G:286:ALA:HB2	1.62	0.82
2:C:357:ILE:HD11	2:C:376:ILE:HG21	1.60	0.82
2:C:456:LEU:H	2:C:475:THR:HG22	1.46	0.81
2:E:278:LEU:HD22	2:E:286:ALA:HB2	1.61	0.81
2:G:278:LEU:HD21	2:G:284:MET:HB2	1.60	0.81
2:F:145:HIS:HD2	2:F:146:PRO:HD2	1.43	0.81
2:F:350:PHE:HB2	2:F:389:VAL:HG21	1.61	0.81
2:I:350:PHE:HB2	2:I:389:VAL:HG21	1.63	0.81
2:I:107:ILE:H	2:I:303:ASN:HD21	1.29	0.81
2:J:264:ARG:NH1	2:K:155:SER:OG	2.14	0.81
2:A:372:GLU:HB2	2:F:407:ASP:HB3	1.61	0.80
2:J:107:ILE:H	2:J:303:ASN:HD21	1.29	0.80
2:H:456:LEU:H	2:H:475:THR:HG22	1.46	0.80
2:A:155:SER:HB3	2:F:266:LEU:HD11	1.64	0.80
2:G:105:ASN:ND2	2:G:409:THR:O	2.14	0.80
2:G:107:ILE:H	2:G:303:ASN:HD21	1.25	0.79
2:G:350:PHE:HB2	2:G:389:VAL:HG21	1.65	0.79
2:A:267:LYS:HB3	2:B:249:GLU:HG2	1.64	0.79
2:K:278:LEU:HD22	2:K:286:ALA:HB2	1.63	0.79
2:J:128:ARG:HE	2:J:484:PHE:HE1	1.31	0.79
2:J:351:LYS:NZ	2:J:390:ASP:O	2.15	0.79
2:L:357:ILE:HD11	2:L:376:ILE:HD13	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:278:LEU:HD21	2:K:284:MET:HB2	1.63	0.79
2:B:264:ARG:NH1	2:C:155:SER:OG	2.16	0.79
2:F:84:THR:HG22	2:F:86:GLY:H	1.48	0.78
2:F:426:ASP:OD2	2:F:433:TYR:OH	2.02	0.78
2:H:145:HIS:HD2	2:H:146:PRO:HD2	1.48	0.78
2:L:152:ALA:HB1	2:L:225:ALA:HB2	1.65	0.78
2:B:105:ASN:ND2	2:B:409:THR:O	2.15	0.78
2:D:357:ILE:HD11	2:D:376:ILE:HD13	1.64	0.78
2:E:145:HIS:HD2	2:E:146:PRO:HD2	1.49	0.78
2:A:278:LEU:HD21	2:A:284:MET:HB2	1.63	0.78
2:C:87:ALA:O	2:G:495:ARG:NH2	2.17	0.78
2:A:431:GLN:HE21	2:B:213:LYS:HB3	1.47	0.78
2:E:107:ILE:H	2:E:303:ASN:HD21	1.31	0.78
2:H:380:ARG:NH2	2:H:408:THR:OG1	2.15	0.78
2:G:264:ARG:NH1	2:H:155:SER:OG	2.17	0.78
2:J:431:GLN:HE21	2:K:213:LYS:HB3	1.49	0.78
2:A:264:ARG:NH1	2:B:155:SER:OG	2.17	0.77
2:E:267:LYS:HB3	2:F:249:GLU:HG2	1.65	0.77
2:K:267:LYS:HB3	2:L:249:GLU:HG2	1.66	0.77
2:D:495:ARG:NH2	2:L:87:ALA:O	2.17	0.77
2:H:107:ILE:H	2:H:303:ASN:HD21	1.31	0.77
2:B:278:LEU:HD21	2:B:284:MET:HB2	1.67	0.77
2:D:431:GLN:HE22	2:E:217:GLU:HB2	1.48	0.77
2:H:264:ARG:NH1	2:I:155:SER:OG	2.17	0.77
2:B:351:LYS:NZ	2:B:390:ASP:O	2.18	0.77
2:J:456:LEU:H	2:J:475:THR:HG22	1.50	0.76
2:G:84:THR:HG22	2:G:86:GLY:H	1.50	0.76
2:C:88:VAL:HG21	2:L:278:LEU:HD12	1.68	0.76
2:K:105:ASN:ND2	2:K:409:THR:O	2.19	0.76
2:C:278:LEU:HD22	2:C:286:ALA:HB2	1.68	0.76
2:E:168:ALA:HB1	2:E:200:ALA:HA	1.67	0.76
3:Y:14:GLU:HB3	3:Y:25:GLY:H	1.51	0.76
2:G:142:GLU:H	2:G:490:GLN:HG2	1.49	0.75
2:I:357:ILE:HD11	2:I:376:ILE:HD13	1.68	0.75
2:G:266:LEU:HD11	2:H:155:SER:HB3	1.68	0.75
2:B:128:ARG:HE	2:B:484:PHE:HE1	1.32	0.75
2:G:213:LYS:HB3	2:L:431:GLN:HE21	1.50	0.75
2:D:105:ASN:ND2	2:D:409:THR:O	2.19	0.75
2:H:426:ASP:OD2	2:H:433:TYR:OH	2.04	0.75
2:I:128:ARG:HE	2:I:484:PHE:HE1	1.33	0.75
2:I:266:LEU:HD11	2:J:155:SER:HB3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:431:GLN:HE21	2:J:213:LYS:HB3	1.49	0.75
2:B:313:SER:OG	2:B:510:ASN:ND2	2.19	0.75
2:C:431:GLN:HE21	2:D:213:LYS:HB3	1.50	0.75
2:I:152:ALA:HB1	2:I:225:ALA:HB2	1.67	0.74
2:B:234:GLU:OE2	2:F:69:GLY:N	2.17	0.74
2:B:380:ARG:NH2	2:B:408:THR:OG1	2.20	0.74
2:E:266:LEU:HD11	2:F:155:SER:HB3	1.69	0.74
2:C:431:GLN:HE22	2:D:217:GLU:HB2	1.52	0.74
2:D:151:ASP:HB2	2:D:189:TYR:HE1	1.52	0.74
2:A:426:ASP:OD2	2:A:433:TYR:OH	2.04	0.74
2:D:145:HIS:HD2	2:D:146:PRO:HD2	1.53	0.74
2:E:456:LEU:H	2:E:475:THR:HG22	1.52	0.74
2:G:277:ASP:OD1	2:G:278:LEU:N	2.20	0.74
2:D:398:GLN:HG2	2:D:399:GLY:H	1.52	0.74
2:F:333:ASP:HB3	2:F:519:LYS:HB2	1.70	0.74
2:G:155:SER:OG	2:L:264:ARG:NH1	2.21	0.74
2:L:177:ILE:HG12	2:L:224:ILE:HD11	1.70	0.74
2:C:268:ALA:HB2	2:C:294:LEU:HD11	1.69	0.73
2:G:398:GLN:HG2	2:G:399:GLY:H	1.52	0.73
2:L:456:LEU:H	2:L:475:THR:HG22	1.53	0.73
2:D:267:LYS:HB3	2:E:249:GLU:HG2	1.68	0.73
2:K:344:ARG:HH11	2:L:344:ARG:HH12	1.37	0.73
3:X:14:GLU:HB3	3:X:25:GLY:H	1.54	0.73
2:A:107:ILE:H	2:A:303:ASN:HD21	1.35	0.73
2:B:278:LEU:HD22	2:B:286:ALA:HB2	1.69	0.73
2:E:351:LYS:NZ	2:E:390:ASP:O	2.21	0.73
2:K:142:GLU:H	2:K:490:GLN:HG2	1.53	0.73
2:A:234:GLU:OE2	2:E:69:GLY:N	2.21	0.72
2:K:426:ASP:OD2	2:K:433:TYR:OH	2.07	0.72
2:B:145:HIS:HD2	2:B:146:PRO:HD2	1.53	0.72
2:H:278:LEU:HD21	2:H:284:MET:HB2	1.70	0.72
2:J:426:ASP:OD2	2:J:433:TYR:OH	2.07	0.72
2:I:313:SER:OG	2:I:510:ASN:ND2	2.22	0.72
2:G:456:LEU:H	2:G:475:THR:HG22	1.55	0.72
3:X:26:LYS:NZ	3:X:74:ASP:OD2	2.22	0.72
2:A:390:ASP:OD2	2:A:394:SER:OG	2.07	0.72
2:I:145:HIS:HD2	2:I:146:PRO:HD2	1.55	0.72
2:C:274:LEU:HD12	2:L:69:GLY:HA2	1.70	0.71
2:B:107:ILE:H	2:B:303:ASN:HD21	1.39	0.71
2:D:426:ASP:OD2	2:D:433:TYR:OH	2.08	0.71
2:G:431:GLN:HE22	2:H:217:GLU:HB2	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:390:ASP:OD2	2:L:394:SER:OG	2.07	0.71
2:C:145:HIS:HD2	2:C:146:PRO:HD2	1.54	0.71
2:F:128:ARG:HE	2:F:484:PHE:HE1	1.35	0.71
2:G:145:HIS:HD2	2:G:146:PRO:HD2	1.54	0.71
3:Q:38:VAL:HG11	3:Q:69:ILE:HG12	1.73	0.71
3:V:26:LYS:NZ	3:V:74:ASP:OD2	2.23	0.71
2:A:171:GLN:HE21	2:A:195:GLN:NE2	1.88	0.71
2:A:313:SER:OG	2:A:510:ASN:ND2	2.24	0.71
2:G:357:ILE:HD11	2:G:376:ILE:HD13	1.71	0.71
2:H:313:SER:OG	2:H:510:ASN:ND2	2.23	0.71
2:K:313:SER:OG	2:K:510:ASN:ND2	2.22	0.71
2:L:313:SER:OG	2:L:510:ASN:ND2	2.23	0.71
2:A:456:LEU:H	2:A:475:THR:HG22	1.55	0.71
3:Q:14:GLU:HB3	3:Q:25:GLY:N	2.06	0.71
2:A:128:ARG:HE	2:A:484:PHE:HE1	1.39	0.70
2:D:313:SER:OG	2:D:510:ASN:ND2	2.24	0.70
2:E:426:ASP:OD2	2:E:433:TYR:OH	2.08	0.70
2:I:398:GLN:HG2	2:I:399:GLY:H	1.56	0.70
2:K:145:HIS:HD2	2:K:146:PRO:HD2	1.55	0.70
3:U:26:LYS:NZ	3:U:74:ASP:OD2	2.24	0.70
2:C:264:ARG:NH1	2:D:155:SER:OG	2.24	0.70
2:D:107:ILE:H	2:D:303:ASN:HD21	1.37	0.70
2:J:267:LYS:HB3	2:K:249:GLU:HG2	1.74	0.70
2:K:253:ARG:NE	2:K:255:ASP:OD2	2.23	0.70
3:P:15:GLN:HE21	3:P:23:ILE:HD12	1.54	0.70
2:H:279:ARG:NH2	2:H:285:ASP:OD1	2.25	0.70
2:L:278:LEU:HD22	2:L:286:ALA:HB2	1.72	0.70
2:A:431:GLN:HE22	2:B:217:GLU:HB2	1.55	0.70
2:J:145:HIS:HD2	2:J:146:PRO:HD2	1.57	0.70
2:J:277:ASP:OD1	2:J:278:LEU:N	2.25	0.70
2:C:426:ASP:OD2	2:C:433:TYR:OH	2.10	0.70
2:E:277:ASP:OD1	2:E:278:LEU:N	2.25	0.69
2:A:151:ASP:HB2	2:A:189:TYR:HE1	1.57	0.69
2:B:152:ALA:HB1	2:B:225:ALA:HB2	1.74	0.69
2:C:398:GLN:HG2	2:C:399:GLY:H	1.55	0.69
2:A:145:HIS:HD2	2:A:146:PRO:HD2	1.57	0.69
2:L:268:ALA:HB2	2:L:294:LEU:HD11	1.74	0.69
2:B:426:ASP:OD2	2:B:433:TYR:OH	2.10	0.69
2:I:84:THR:HG22	2:I:86:GLY:H	1.57	0.69
2:K:363:GLU:OE2	2:K:366:ARG:NH2	2.25	0.69
2:D:351:LYS:NZ	2:D:390:ASP:O	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:398:GLN:HG2	2:J:399:GLY:H	1.57	0.69
2:E:151:ASP:HB2	2:E:189:TYR:HE1	1.56	0.69
2:C:333:ASP:HB3	2:C:519:LYS:HB2	1.74	0.69
2:F:456:LEU:H	2:F:475:THR:HG22	1.58	0.69
2:L:398:GLN:HG2	2:L:399:GLY:H	1.58	0.69
2:E:357:ILE:HD11	2:E:376:ILE:HG21	1.72	0.69
2:A:177:ILE:HG12	2:A:224:ILE:HD11	1.74	0.68
2:L:426:ASP:OD2	2:L:433:TYR:OH	2.10	0.68
2:C:84:THR:HG22	2:C:86:GLY:H	1.58	0.68
2:G:426:ASP:OD2	2:G:433:TYR:OH	2.12	0.68
2:E:398:GLN:HG2	2:E:399:GLY:H	1.58	0.68
2:H:390:ASP:OD2	2:H:394:SER:OG	2.12	0.68
2:C:380:ARG:NH2	2:C:408:THR:OG1	2.26	0.68
2:G:431:GLN:HE21	2:H:213:LYS:HB3	1.58	0.68
2:B:267:LYS:HB3	2:C:249:GLU:HG2	1.74	0.68
2:L:351:LYS:NZ	2:L:390:ASP:O	2.26	0.68
2:F:253:ARG:NE	2:F:255:ASP:OD2	2.26	0.68
2:A:69:GLY:N	2:C:234:GLU:OE2	2.27	0.68
2:G:166:LEU:HD22	2:G:212:ILE:HD11	1.76	0.68
2:E:431:GLN:HE21	2:F:213:LYS:HB3	1.58	0.68
2:A:351:LYS:NZ	2:A:390:ASP:O	2.23	0.68
2:I:278:LEU:HD21	2:I:284:MET:HB2	1.76	0.68
2:H:351:LYS:NZ	2:H:390:ASP:O	2.25	0.67
2:C:105:ASN:ND2	2:C:409:THR:O	2.27	0.67
2:D:431:GLN:NE2	2:E:213:LYS:O	2.27	0.67
2:H:267:LYS:HB3	2:I:249:GLU:HG2	1.76	0.67
2:G:476:ARG:HH21	2:H:230:THR:HG21	1.59	0.67
2:H:345:TRP:HB3	2:I:343:ALA:HA	1.75	0.67
2:L:107:ILE:H	2:L:303:ASN:HD21	1.41	0.67
2:F:268:ALA:HB1	2:F:290:LEU:HD13	1.75	0.67
2:I:277:ASP:OD1	2:I:278:LEU:N	2.27	0.67
2:J:84:THR:HG22	2:J:86:GLY:H	1.59	0.67
2:J:278:LEU:HD21	2:J:284:MET:HB2	1.75	0.67
2:G:177:ILE:HG12	2:G:224:ILE:HD11	1.77	0.67
2:C:351:LYS:NZ	2:C:390:ASP:O	2.27	0.67
2:J:142:GLU:H	2:J:490:GLN:HG2	1.59	0.67
2:F:357:ILE:HD11	2:F:376:ILE:HD13	1.77	0.67
2:L:323:LEU:HD21	2:L:329:ALA:HA	1.77	0.67
2:C:107:ILE:H	2:C:303:ASN:HD21	1.41	0.67
2:F:357:ILE:HD11	2:F:376:ILE:HG21	1.76	0.67
2:G:362:VAL:HG21	2:L:384:ASN:HD21	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:LEU:HD21	2:F:329:ALA:HA	1.77	0.66
2:F:398:GLN:HG2	2:F:399:GLY:H	1.60	0.66
2:I:177:ILE:HG12	2:I:224:ILE:HD11	1.78	0.66
3:T:26:LYS:NZ	3:T:74:ASP:OD2	2.28	0.66
2:A:268:ALA:HB2	2:A:294:LEU:HD11	1.76	0.66
2:C:278:LEU:HD12	2:L:88:VAL:HG21	1.76	0.66
2:B:384:ASN:HD21	2:C:362:VAL:HG21	1.59	0.66
2:G:213:LYS:O	2:L:431:GLN:NE2	2.28	0.66
2:K:266:LEU:HD11	2:L:155:SER:HB3	1.77	0.66
2:E:142:GLU:H	2:E:490:GLN:HG2	1.61	0.66
3:R:26:LYS:NZ	3:R:74:ASP:OD2	2.29	0.66
2:D:69:GLY:N	2:F:234:GLU:OE2	2.21	0.66
2:D:77:THR:OG1	3:R:5:ARG:NH2	2.28	0.66
2:K:168:ALA:HB1	2:K:200:ALA:HA	1.77	0.66
2:C:431:GLN:NE2	2:D:213:LYS:O	2.29	0.66
2:F:295:ALA:HB2	2:F:473:PHE:HE2	1.60	0.66
3:O:26:LYS:NZ	3:O:74:ASP:OD2	2.29	0.66
2:B:398:GLN:HG2	2:B:399:GLY:H	1.61	0.66
2:E:278:LEU:HD21	2:E:284:MET:HB2	1.76	0.66
2:G:234:GLU:OE2	2:K:69:GLY:N	2.24	0.66
2:A:398:GLN:HG2	2:A:399:GLY:H	1.60	0.66
2:B:333:ASP:HB3	2:B:519:LYS:HB2	1.78	0.66
2:F:331:VAL:HG12	2:F:517:TYR:HB2	1.78	0.66
2:H:430:LYS:HG2	2:I:216:MET:HE1	1.77	0.66
3:U:65:ARG:O	3:U:68:TRP:N	2.27	0.66
2:G:380:ARG:NH2	2:G:408:THR:OG1	2.29	0.65
2:K:398:GLN:HG2	2:K:399:GLY:H	1.61	0.65
3:X:17:LEU:HD22	3:X:23:ILE:HD11	1.77	0.65
2:F:222:VAL:HG22	2:F:223:GLU:H	1.61	0.65
2:I:74:TYR:CE2	2:J:260:GLU:HG2	2.32	0.65
2:I:269:ALA:HA	2:I:470:VAL:HA	1.78	0.65
2:I:426:ASP:OD2	2:I:433:TYR:OH	2.15	0.65
3:Y:18:ASP:HB3	3:Y:21:LYS:HD3	1.78	0.65
2:A:430:LYS:HE2	2:B:188:VAL:HG12	1.77	0.65
2:B:142:GLU:H	2:B:490:GLN:HG2	1.60	0.65
2:G:390:ASP:OD2	2:G:394:SER:OG	2.13	0.65
2:H:268:ALA:HB2	2:H:294:LEU:HD11	1.77	0.65
2:H:142:GLU:H	2:H:490:GLN:HG2	1.60	0.65
2:C:153:MET:HG2	2:C:189:TYR:CD2	2.32	0.65
2:D:222:VAL:HG22	2:D:223:GLU:H	1.62	0.65
2:H:128:ARG:HE	2:H:484:PHE:HE1	1.42	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:177:ILE:HG12	2:J:224:ILE:HD11	1.78	0.65
2:B:318:LYS:N	2:B:360:GLU:OE2	2.28	0.65
2:B:344:ARG:CZ	2:C:344:ARG:HH22	2.09	0.65
2:I:95:VAL:HG12	2:J:123:GLN:HE21	1.62	0.65
2:K:482:ASN:HB3	2:K:485:ALA:HB2	1.79	0.65
3:P:33:PRO:HG2	3:P:62:GLU:OE1	1.96	0.65
3:R:14:GLU:HB3	3:R:25:GLY:H	1.61	0.65
2:G:69:GLY:N	2:I:234:GLU:OE2	2.28	0.64
2:H:95:VAL:HG12	2:I:123:GLN:HE21	1.62	0.64
2:B:390:ASP:OD2	2:B:394:SER:OG	2.12	0.64
2:I:431:GLN:HE22	2:J:217:GLU:HB2	1.62	0.64
2:K:222:VAL:HG22	2:K:223:GLU:H	1.61	0.64
2:A:249:GLU:HG2	2:F:267:LYS:HB3	1.80	0.64
2:F:318:LYS:N	2:F:360:GLU:OE2	2.30	0.64
2:A:105:ASN:ND2	2:A:409:THR:O	2.19	0.64
2:G:333:ASP:HB3	2:G:519:LYS:HB2	1.78	0.64
2:K:351:LYS:NZ	2:K:390:ASP:O	2.29	0.64
2:K:401:ALA:O	2:L:420:LYS:NZ	2.29	0.64
2:D:266:LEU:HD11	2:E:155:SER:HB3	1.78	0.64
2:D:400:LEU:HD11	2:E:417:LEU:HB3	1.80	0.64
2:D:431:GLN:HE21	2:E:213:LYS:HB3	1.62	0.64
2:I:268:ALA:HB1	2:I:290:LEU:HD13	1.78	0.64
2:H:277:ASP:OD1	2:H:278:LEU:N	2.30	0.64
2:K:456:LEU:H	2:K:475:THR:HG22	1.61	0.64
3:X:5:ARG:HD2	3:X:33:PRO:HG3	1.80	0.64
2:G:351:LYS:NZ	2:G:390:ASP:O	2.30	0.64
3:U:2:ALA:N	3:U:61:GLU:OE2	2.31	0.64
3:X:23:ILE:HG12	3:X:78:VAL:HG22	1.80	0.64
2:E:398:GLN:HG2	2:E:399:GLY:N	2.14	0.63
3:R:11:LYS:HG3	3:R:27:GLU:HG2	1.79	0.63
2:B:268:ALA:HB1	2:B:290:LEU:HD13	1.80	0.63
2:K:101:ARG:HD2	2:L:146:PRO:HD3	1.80	0.63
2:L:166:LEU:HD22	2:L:212:ILE:HD11	1.80	0.63
2:B:345:TRP:HB3	2:C:343:ALA:HA	1.80	0.63
2:K:177:ILE:HG12	2:K:224:ILE:HD11	1.81	0.63
2:F:110:ASP:OD2	2:F:422:ARG:NH1	2.31	0.63
2:J:222:VAL:HG22	2:J:223:GLU:H	1.63	0.63
2:B:337:PRO:HB3	4:Z:306:TRP:HB3	1.81	0.63
2:A:131:TYR:HB3	2:A:250:MET:HG2	1.80	0.63
2:A:166:LEU:HD22	2:A:212:ILE:HD11	1.81	0.63
2:K:386:LEU:HB3	2:K:404:PHE:HE2	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:278:LEU:HD21	2:L:284:MET:HB2	1.79	0.63
3:Q:10:ILE:HD11	3:Q:35:TYR:HE1	1.61	0.63
2:G:222:VAL:HG22	2:G:223:GLU:H	1.64	0.63
2:I:142:GLU:H	2:I:490:GLN:HB3	1.63	0.63
2:J:121:THR:HA	2:J:259:ILE:O	1.99	0.63
2:A:357:ILE:HD11	2:A:376:ILE:HG21	1.81	0.63
2:B:235:LEU:HD23	2:F:68:ILE:HD13	1.80	0.62
2:H:266:LEU:HD11	2:I:155:SER:HB3	1.81	0.62
2:E:269:ALA:HA	2:E:470:VAL:HA	1.80	0.62
2:J:363:GLU:OE2	2:J:366:ARG:NH2	2.32	0.62
2:F:378:ALA:O	2:F:426:ASP:N	2.29	0.62
3:Q:26:LYS:HD2	3:Q:75:LEU:HD23	1.80	0.62
2:B:163:PHE:HB2	2:B:179:THR:HG23	1.80	0.62
2:G:350:PHE:CB	2:G:389:VAL:HG21	2.29	0.62
2:J:153:MET:HE2	2:J:226:GLU:H	1.63	0.62
2:A:333:ASP:HB3	2:A:519:LYS:HB2	1.82	0.62
2:E:84:THR:HG22	2:E:86:GLY:H	1.63	0.62
2:H:153:MET:HG2	2:H:189:TYR:CD2	2.34	0.62
2:K:264:ARG:NH1	2:L:155:SER:OG	2.33	0.62
3:W:11:LYS:HG3	3:W:27:GLU:HG2	1.81	0.62
2:E:121:THR:HA	2:E:259:ILE:O	1.99	0.62
2:E:345:TRP:HB3	2:F:343:ALA:HA	1.80	0.62
2:J:100:ARG:HG2	2:J:101:ARG:H	1.63	0.62
2:J:377:ILE:HG22	2:J:424:TYR:HB2	1.80	0.62
2:K:357:ILE:HD11	2:K:376:ILE:HG21	1.80	0.62
2:L:432:ASP:OD1	2:L:433:TYR:N	2.33	0.62
3:O:9:ASN:HB3	3:O:56:TYR:HE2	1.65	0.62
2:B:131:TYR:HB3	2:B:250:MET:HG2	1.82	0.62
2:C:343:ALA:HB1	2:C:348:GLU:HB3	1.82	0.62
2:I:80:ALA:HA	2:I:93:PRO:HG2	1.81	0.62
2:I:191:GLN:N	2:I:222:VAL:O	2.31	0.62
2:A:350:PHE:CB	2:A:389:VAL:HG21	2.29	0.62
2:C:350:PHE:CB	2:C:389:VAL:HG21	2.30	0.62
2:F:191:GLN:N	2:F:222:VAL:O	2.32	0.62
3:Y:11:LYS:HG3	3:Y:27:GLU:HG2	1.81	0.62
2:A:498:SER:HB3	2:F:76:ALA:HB2	1.82	0.62
2:B:84:THR:HG22	2:B:86:GLY:H	1.65	0.62
2:D:128:ARG:HE	2:D:484:PHE:HE1	1.47	0.62
2:C:266:LEU:HD11	2:D:155:SER:HB3	1.82	0.62
2:C:468:GLN:NE2	2:H:234:GLU:O	2.32	0.62
2:D:333:ASP:HB3	2:D:519:LYS:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:313:SER:OG	2:J:510:ASN:ND2	2.33	0.62
2:L:105:ASN:ND2	2:L:409:THR:O	2.33	0.62
2:B:266:LEU:HD11	2:C:155:SER:HB3	1.81	0.61
2:C:222:VAL:HG22	2:C:223:GLU:H	1.63	0.61
2:C:277:ASP:OD1	2:C:278:LEU:N	2.33	0.61
2:D:353:LEU:HD13	2:D:385:VAL:HG11	1.82	0.61
2:F:351:LYS:NZ	2:F:390:ASP:O	2.31	0.61
2:H:181:PHE:HD1	2:H:187:THR:HB	1.64	0.61
2:I:267:LYS:HB3	2:J:249:GLU:HG2	1.81	0.61
2:K:121:THR:HG22	2:K:260:GLU:OE1	2.01	0.61
3:P:26:LYS:NZ	3:P:74:ASP:OD2	2.32	0.61
2:E:95:VAL:HG12	2:F:123:GLN:HE21	1.65	0.61
2:K:277:ASP:OD1	2:K:278:LEU:N	2.33	0.61
2:L:222:VAL:HG22	2:L:223:GLU:H	1.64	0.61
2:A:266:LEU:HD11	2:B:155:SER:HB3	1.82	0.61
2:G:100:ARG:HG2	2:G:101:ARG:H	1.65	0.61
2:H:241:GLY:HA3	3:V:43:GLY:H	1.65	0.61
2:J:390:ASP:OD2	2:J:394:SER:OG	2.16	0.61
2:E:133:LYS:HE2	3:R:42:SER:HB2	1.83	0.61
2:G:155:SER:HB3	2:L:266:LEU:HD11	1.82	0.61
2:L:277:ASP:OD1	2:L:278:LEU:N	2.32	0.61
2:K:318:LYS:N	2:K:360:GLU:OE2	2.34	0.61
2:E:154:PHE:O	2:E:248:ASN:ND2	2.34	0.61
2:E:383:VAL:HG12	2:E:406:THR:HG22	1.81	0.61
2:F:244:ASP:HB2	3:Q:13:PHE:HE2	1.66	0.61
2:K:346:ALA:O	2:K:349:SER:N	2.34	0.61
2:A:222:VAL:HG22	2:A:223:GLU:H	1.66	0.61
2:D:430:LYS:HE2	2:E:188:VAL:CG1	2.30	0.61
2:I:350:PHE:CB	2:I:389:VAL:HG21	2.30	0.61
3:U:10:ILE:HD11	3:U:35:TYR:HE1	1.66	0.61
3:Y:14:GLU:HB3	3:Y:25:GLY:N	2.16	0.61
2:C:398:GLN:HG2	2:C:399:GLY:N	2.16	0.60
2:J:431:GLN:NE2	2:K:217:GLU:HB2	2.11	0.60
3:T:10:ILE:HD11	3:T:35:TYR:HE1	1.66	0.60
2:B:222:VAL:HG22	2:B:223:GLU:H	1.66	0.60
2:B:253:ARG:NE	2:B:255:ASP:OD2	2.33	0.60
2:D:145:HIS:NE2	2:D:487:SER:O	2.31	0.60
2:G:173:THR:OG1	2:G:176:ASP:OD2	2.18	0.60
2:J:269:ALA:HA	2:J:470:VAL:HA	1.82	0.60
2:A:400:LEU:HD11	2:B:417:LEU:HB3	1.82	0.60
2:B:69:GLY:N	2:D:234:GLU:OE2	2.23	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:380:ARG:NH1	2:J:427:GLN:O	2.32	0.60
2:B:331:VAL:HG12	2:B:517:TYR:HB2	1.82	0.60
2:D:431:GLN:NE2	2:E:217:GLU:HB2	2.16	0.60
2:E:222:VAL:HG22	2:E:223:GLU:H	1.66	0.60
2:I:253:ARG:NE	2:I:255:ASP:OD2	2.34	0.60
2:J:263:SER:HB2	2:K:230:THR:HG22	1.83	0.60
2:J:345:TRP:HB3	2:K:343:ALA:HA	1.82	0.60
2:K:166:LEU:HD11	2:K:221:LEU:HD21	1.83	0.60
3:R:12:THR:HG1	3:R:26:LYS:H	1.47	0.60
2:D:344:ARG:HD2	2:E:344:ARG:HH12	1.66	0.60
2:D:390:ASP:OD2	2:D:394:SER:OG	2.19	0.60
2:J:268:ALA:HB2	2:J:294:LEU:HD11	1.83	0.60
2:J:357:ILE:HD11	2:J:376:ILE:HD13	1.83	0.60
2:K:131:TYR:HB3	2:K:250:MET:HG2	1.82	0.60
2:D:173:THR:OG1	2:D:176:ASP:OD2	2.18	0.60
2:D:377:ILE:HG22	2:D:424:TYR:HB2	1.82	0.60
2:E:367:GLN:HB3	2:E:511:ALA:HB1	1.83	0.60
2:H:222:VAL:HG22	2:H:223:GLU:H	1.66	0.60
2:I:96:MET:HB2	2:J:124:VAL:HG22	1.84	0.60
2:J:268:ALA:HB1	2:J:290:LEU:HD13	1.82	0.60
2:C:66:ALA:N	2:G:249:GLU:OE1	2.35	0.60
2:C:148:TYR:HD1	2:C:186:GLY:H	1.50	0.60
2:D:80:ALA:HA	2:D:93:PRO:HG2	1.83	0.60
2:D:456:LEU:H	2:D:475:THR:HG22	1.65	0.60
2:F:107:ILE:H	2:F:303:ASN:HD21	1.48	0.60
2:F:142:GLU:H	2:F:490:GLN:HG2	1.66	0.60
2:H:398:GLN:HG2	2:H:399:GLY:H	1.65	0.60
2:L:128:ARG:HE	2:L:484:PHE:HE1	1.49	0.60
2:A:409:THR:HG21	2:B:370:ARG:O	2.02	0.59
2:B:363:GLU:OE2	2:B:366:ARG:NH2	2.35	0.59
2:C:177:ILE:HG12	2:C:224:ILE:HD11	1.84	0.59
2:D:268:ALA:HB1	2:D:290:LEU:HD13	1.83	0.59
2:I:333:ASP:HB3	2:I:519:LYS:HB2	1.84	0.59
2:L:145:HIS:NE2	2:L:487:SER:O	2.29	0.59
3:R:14:GLU:HB3	3:R:25:GLY:N	2.17	0.59
3:V:16:LYS:HZ3	3:W:20:ASN:H	1.48	0.59
2:H:357:ILE:HD11	2:H:376:ILE:HD13	1.83	0.59
3:P:65:ARG:O	3:P:68:TRP:N	2.35	0.59
2:E:105:ASN:ND2	2:E:409:THR:O	2.35	0.59
2:E:151:ASP:HB3	2:E:187:THR:HG23	1.85	0.59
2:E:313:SER:OG	2:E:510:ASN:ND2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:PRO:HG2	2:H:178:TYR:HD1	1.68	0.59
2:J:145:HIS:CD2	2:J:146:PRO:HD2	2.36	0.59
2:D:169:SER:OG	2:D:200:ALA:HB2	2.02	0.59
2:F:105:ASN:ND2	2:F:409:THR:O	2.23	0.59
2:I:105:ASN:ND2	2:I:409:THR:O	2.27	0.59
3:P:11:LYS:HG3	3:P:27:GLU:HG2	1.84	0.59
2:C:345:TRP:HB3	2:D:343:ALA:HA	1.84	0.59
2:C:357:ILE:HD11	2:C:376:ILE:HD13	1.84	0.59
2:E:430:LYS:HE2	2:F:188:VAL:HG11	1.84	0.59
2:H:357:ILE:HD11	2:H:376:ILE:HG21	1.83	0.59
2:H:398:GLN:HE21	2:I:355:PHE:HB2	1.67	0.59
2:L:318:LYS:N	2:L:360:GLU:OE2	2.35	0.59
2:E:390:ASP:OD2	2:E:394:SER:OG	2.20	0.59
2:D:264:ARG:NH1	2:E:155:SER:OG	2.34	0.59
3:R:18:ASP:HB3	3:R:21:LYS:HD3	1.84	0.59
2:E:432:ASP:OD1	2:E:433:TYR:N	2.36	0.59
2:G:431:GLN:NE2	2:H:217:GLU:HB2	2.18	0.59
2:K:377:ILE:HG22	2:K:424:TYR:HB2	1.84	0.59
2:B:110:ASP:OD2	2:B:422:ARG:NH2	2.36	0.58
2:B:157:GLN:N	2:B:227:GLY:O	2.34	0.58
2:K:100:ARG:HG2	2:K:101:ARG:H	1.68	0.58
2:C:269:ALA:HA	2:C:470:VAL:HA	1.84	0.58
2:D:177:ILE:HG12	2:D:224:ILE:HD11	1.85	0.58
2:H:145:HIS:CD2	2:H:146:PRO:HD2	2.35	0.58
2:A:376:ILE:HG12	2:A:423:VAL:HG22	1.85	0.58
2:D:85:SER:HB3	3:Q:32:PHE:HE1	1.68	0.58
2:J:151:ASP:HB2	2:J:189:TYR:HE1	1.68	0.58
3:Q:72:ASN:OD1	3:Q:73:GLU:N	2.36	0.58
2:B:153:MET:HG2	2:B:189:TYR:CD2	2.39	0.58
2:B:482:ASN:ND2	2:B:512:TYR:OH	2.35	0.58
2:D:272:ILE:HG22	2:D:468:GLN:HE21	1.69	0.58
2:D:380:ARG:NH2	2:D:408:THR:OG1	2.34	0.58
2:E:323:LEU:HD21	2:E:329:ALA:HA	1.84	0.58
2:H:485:ALA:HB1	2:H:510:ASN:OD1	2.03	0.58
2:J:266:LEU:HD11	2:K:155:SER:HB3	1.85	0.58
2:K:343:ALA:HB1	2:K:348:GLU:HB3	1.86	0.58
3:O:62:GLU:HG2	3:P:4:ALA:HB2	1.85	0.58
2:A:191:GLN:N	2:A:222:VAL:O	2.31	0.58
2:A:344:ARG:HH12	2:F:344:ARG:NH1	2.01	0.58
2:A:432:ASP:OD1	2:A:433:TYR:N	2.35	0.58
2:D:383:VAL:HG12	2:D:406:THR:HG22	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:9:ASN:HB3	3:W:56:TYR:HE2	1.69	0.58
2:G:377:ILE:HG22	2:G:424:TYR:HB2	1.84	0.58
2:I:323:LEU:HD21	2:I:329:ALA:HA	1.85	0.58
2:J:476:ARG:HH21	2:K:230:THR:HG21	1.68	0.58
2:L:253:ARG:NE	2:L:255:ASP:OD2	2.32	0.58
2:D:249:GLU:OE1	2:L:66:ALA:N	2.36	0.58
2:E:268:ALA:HB1	2:E:290:LEU:HD13	1.86	0.58
2:G:131:TYR:HB3	2:G:250:MET:HG2	1.85	0.58
2:I:331:VAL:HG12	2:I:517:TYR:HB2	1.85	0.58
2:I:386:LEU:HB3	2:I:404:PHE:HE2	1.68	0.58
2:K:398:GLN:HG2	2:K:399:GLY:N	2.18	0.58
2:B:375:PHE:CZ	2:B:437:GLY:HA3	2.39	0.58
2:G:249:GLU:HG2	2:L:267:LYS:HB3	1.85	0.58
2:H:177:ILE:HG12	2:H:224:ILE:HD11	1.84	0.58
2:A:168:ALA:HB1	2:A:200:ALA:HA	1.85	0.58
2:G:72:HIS:CD2	2:H:121:THR:HG21	2.38	0.58
2:H:278:LEU:HD22	2:H:286:ALA:HB2	1.86	0.58
2:I:346:ALA:O	2:I:349:SER:N	2.37	0.58
2:I:456:LEU:H	2:I:475:THR:HG22	1.69	0.58
2:B:431:GLN:HE21	2:C:213:LYS:HB3	1.67	0.58
2:E:232:ILE:HD11	3:T:49:PHE:HB3	1.86	0.58
2:J:80:ALA:HA	2:J:93:PRO:HG2	1.86	0.58
3:O:18:ASP:HB3	3:O:21:LYS:HD3	1.85	0.58
2:G:244:ASP:HB2	3:S:13:PHE:HE2	1.68	0.57
2:G:344:ARG:HH12	2:L:344:ARG:NH1	2.01	0.57
2:G:378:ALA:HB1	2:G:382:VAL:HG21	1.86	0.57
2:K:84:THR:HG22	2:K:86:GLY:H	1.68	0.57
2:K:264:ARG:HE	2:K:477:TYR:HE1	1.51	0.57
2:B:277:ASP:OD1	2:B:278:LEU:N	2.37	0.57
2:I:152:ALA:HB1	2:I:225:ALA:CB	2.34	0.57
2:L:121:THR:HA	2:L:259:ILE:O	2.03	0.57
2:D:407:ASP:HB3	2:E:372:GLU:HB2	1.86	0.57
2:E:101:ARG:HD2	2:F:146:PRO:HD3	1.86	0.57
2:G:100:ARG:NH2	2:G:289:GLU:OE1	2.37	0.57
2:L:363:GLU:OE2	2:L:366:ARG:NH2	2.37	0.57
3:Q:15:GLN:HE21	3:Q:23:ILE:HD12	1.69	0.57
3:Q:65:ARG:O	3:Q:68:TRP:N	2.38	0.57
3:S:9:ASN:HB3	3:S:56:TYR:CE2	2.40	0.57
2:B:269:ALA:HA	2:B:470:VAL:HA	1.87	0.57
2:G:191:GLN:N	2:G:222:VAL:O	2.37	0.57
3:S:10:ILE:HD11	3:S:35:TYR:CE1	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:GLN:HE21	2:D:355:PHE:HB2	1.69	0.57
2:D:323:LEU:HD21	2:D:329:ALA:HA	1.86	0.57
2:K:184:GLU:O	2:K:185:THR:OG1	2.21	0.57
2:C:390:ASP:OD2	2:C:394:SER:OG	2.18	0.57
2:D:344:ARG:HD2	2:E:344:ARG:NH1	2.20	0.57
2:H:145:HIS:NE2	2:H:487:SER:O	2.36	0.57
2:K:432:ASP:OD1	2:K:433:TYR:N	2.38	0.57
3:O:64:GLN:HB3	3:O:67:GLU:HB2	1.86	0.57
2:F:390:ASP:OD2	2:F:394:SER:OG	2.17	0.57
2:A:121:THR:HG21	2:F:72:HIS:NE2	2.20	0.57
2:A:305:GLU:HA	2:B:225:ALA:HB3	1.86	0.57
2:B:268:ALA:HB2	2:B:294:LEU:HD11	1.87	0.57
2:C:181:PHE:HD1	2:C:187:THR:HB	1.69	0.57
2:G:430:LYS:HE2	2:H:188:VAL:CG1	2.34	0.57
2:I:153:MET:HG2	2:I:189:TYR:CD2	2.39	0.57
2:L:398:GLN:HG2	2:L:399:GLY:N	2.18	0.57
3:P:11:LYS:HZ3	3:P:13:PHE:HE1	1.51	0.57
2:C:396:ALA:O	2:D:395:TYR:HA	2.05	0.57
2:E:100:ARG:HG2	2:E:101:ARG:H	1.70	0.57
2:I:456:LEU:HD12	2:I:475:THR:HG21	1.86	0.57
2:L:133:LYS:HE2	3:U:42:SER:HB2	1.86	0.57
2:L:313:SER:O	2:L:510:ASN:HB2	2.05	0.57
2:A:357:ILE:HD11	2:A:376:ILE:HD13	1.86	0.56
2:C:267:LYS:HB3	2:D:249:GLU:HG2	1.86	0.56
2:G:343:ALA:HB1	2:G:348:GLU:HB3	1.85	0.56
2:L:374:ASN:ND2	2:L:439:LYS:O	2.39	0.56
3:Q:10:ILE:HD11	3:Q:35:TYR:CE1	2.40	0.56
2:A:145:HIS:CD2	2:A:146:PRO:HD2	2.39	0.56
2:C:136:VAL:HG11	2:C:495:ARG:NH2	2.20	0.56
2:D:232:ILE:HD11	3:X:49:PHE:HB3	1.87	0.56
2:G:168:ALA:HB1	2:G:200:ALA:HA	1.87	0.56
2:J:131:TYR:HB3	2:J:250:MET:HG2	1.87	0.56
2:J:148:TYR:HD1	2:J:186:GLY:H	1.54	0.56
2:K:121:THR:HA	2:K:259:ILE:O	2.06	0.56
3:T:14:GLU:HB3	3:T:25:GLY:N	2.17	0.56
3:X:15:GLN:HE21	3:X:23:ILE:HD12	1.70	0.56
2:A:315:GLN:HG3	2:A:510:ASN:O	2.05	0.56
2:D:142:GLU:H	2:D:490:GLN:HG2	1.70	0.56
2:D:149:GLY:H	2:D:186:GLY:HA2	1.70	0.56
2:K:153:MET:HG2	2:K:189:TYR:CD2	2.41	0.56
2:K:357:ILE:HD11	2:K:376:ILE:HD13	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:354:LEU:HA	2:L:357:ILE:HG22	1.88	0.56
3:P:14:GLU:HB3	3:P:25:GLY:N	2.21	0.56
2:A:269:ALA:HA	2:A:470:VAL:HA	1.88	0.56
2:C:69:GLY:HA2	2:L:274:LEU:HD13	1.87	0.56
2:C:238:GLY:HA2	2:C:242:SER:O	2.05	0.56
2:E:153:MET:HE2	2:E:226:GLU:H	1.70	0.56
2:G:188:VAL:CG1	2:L:430:LYS:HE2	2.35	0.56
2:H:171:GLN:NE2	2:H:195:GLN:HE21	2.03	0.56
2:H:432:ASP:OD1	2:H:433:TYR:N	2.37	0.56
2:K:164:PRO:HG2	2:K:178:TYR:HD1	1.70	0.56
2:C:380:ARG:NH1	2:C:427:GLN:O	2.35	0.56
2:D:168:ALA:HB1	2:D:200:ALA:HA	1.88	0.56
2:J:191:GLN:N	2:J:222:VAL:O	2.38	0.56
2:K:354:LEU:HA	2:K:357:ILE:HG22	1.86	0.56
3:O:9:ASN:HB3	3:O:56:TYR:CE2	2.40	0.56
2:A:268:ALA:HB1	2:A:290:LEU:HD13	1.87	0.56
2:F:179:THR:HG22	2:F:189:TYR:CD2	2.41	0.56
2:I:301:GLU:OE1	2:J:155:SER:OG	2.21	0.56
2:A:129:ALA:O	2:A:143:ALA:N	2.31	0.56
2:D:153:MET:HE2	2:D:226:GLU:H	1.70	0.56
2:E:235:LEU:HD12	2:E:235:LEU:O	2.05	0.56
2:I:101:ARG:HH12	2:J:145:HIS:CD2	2.24	0.56
2:K:80:ALA:HA	2:K:93:PRO:HG2	1.88	0.56
2:L:152:ALA:HB1	2:L:225:ALA:CB	2.36	0.56
2:A:74:TYR:CE2	2:B:260:GLU:HG2	2.41	0.56
2:B:430:LYS:HE2	2:C:188:VAL:HG11	1.86	0.56
2:G:393:ILE:HA	2:L:398:GLN:O	2.05	0.56
2:H:80:ALA:HA	2:H:93:PRO:HG2	1.87	0.56
2:A:155:SER:HB3	2:F:266:LEU:CD1	2.35	0.56
2:B:177:ILE:HG12	2:B:224:ILE:HD11	1.87	0.56
2:C:95:VAL:HG12	2:D:123:GLN:HE21	1.71	0.56
2:E:163:PHE:HB2	2:E:179:THR:HG23	1.87	0.56
2:I:100:ARG:HG2	2:I:101:ARG:H	1.71	0.56
2:L:269:ALA:HA	2:L:470:VAL:HA	1.86	0.56
2:A:185:THR:O	2:F:430:LYS:HE3	2.06	0.55
2:B:398:GLN:HG2	2:B:399:GLY:N	2.21	0.55
2:H:105:ASN:HD21	2:H:409:THR:C	2.09	0.55
2:I:344:ARG:O	2:I:348:GLU:HB2	2.06	0.55
2:I:398:GLN:HG2	2:I:399:GLY:N	2.21	0.55
2:C:384:ASN:HD21	2:D:362:VAL:HG21	1.72	0.55
2:E:234:GLU:O	2:L:468:GLN:NE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:380:ARG:NH2	2:E:408:THR:OG1	2.37	0.55
2:K:409:THR:HG21	2:L:370:ARG:O	2.06	0.55
3:W:65:ARG:O	3:W:68:TRP:N	2.39	0.55
2:A:323:LEU:HD21	2:A:329:ALA:HA	1.87	0.55
2:A:362:VAL:HG21	2:F:384:ASN:HD21	1.71	0.55
2:E:177:ILE:HG12	2:E:224:ILE:HD11	1.87	0.55
2:E:237:GLU:HG3	2:L:465:LYS:HB3	1.88	0.55
2:E:398:GLN:HE21	2:F:355:PHE:HB2	1.70	0.55
3:P:5:ARG:HD2	3:P:33:PRO:HG3	1.87	0.55
3:Y:65:ARG:O	3:Y:68:TRP:N	2.39	0.55
2:D:151:ASP:HB2	2:D:189:TYR:CE1	2.39	0.55
2:L:350:PHE:HB3	2:L:389:VAL:HG21	1.89	0.55
2:A:146:PRO:HB2	2:A:366:ARG:O	2.06	0.55
2:A:230:THR:HG22	2:F:263:SER:HB2	1.89	0.55
2:A:263:SER:HB2	2:B:230:THR:HG22	1.89	0.55
2:F:184:GLU:O	2:F:185:THR:OG1	2.22	0.55
2:G:313:SER:OG	2:G:510:ASN:ND2	2.40	0.55
2:H:121:THR:HA	2:H:259:ILE:O	2.06	0.55
2:K:344:ARG:CZ	2:L:344:ARG:HH22	2.18	0.55
2:L:145:HIS:CD2	2:L:146:PRO:HD2	2.33	0.55
3:P:20:ASN:H	3:Q:16:LYS:NZ	2.04	0.55
3:V:18:ASP:HB3	3:V:21:LYS:HD3	1.89	0.55
3:X:9:ASN:ND2	3:X:51:SER:OG	2.40	0.55
2:A:135:PRO:HG3	2:A:251:GLY:HA3	1.89	0.55
2:B:263:SER:HB2	2:C:230:THR:HG22	1.89	0.55
2:G:344:ARG:O	2:G:348:GLU:HB2	2.07	0.55
2:H:323:LEU:HD21	2:H:329:ALA:HA	1.89	0.55
2:J:169:SER:OG	2:J:200:ALA:HB2	2.07	0.55
2:L:116:PRO:HA	2:L:452:PRO:HD2	1.88	0.55
2:G:432:ASP:OD1	2:G:433:TYR:N	2.39	0.55
2:G:456:LEU:HD12	2:G:475:THR:CG2	2.37	0.55
2:H:101:ARG:HH12	2:I:145:HIS:CD2	2.25	0.55
2:L:275:THR:HG22	2:L:286:ALA:HB3	1.88	0.55
2:A:386:LEU:HB3	2:A:404:PHE:HE2	1.72	0.55
2:C:191:GLN:N	2:C:222:VAL:O	2.35	0.55
2:D:197:THR:HG22	2:D:199:ASP:H	1.72	0.55
2:D:398:GLN:HG2	2:D:399:GLY:N	2.21	0.55
2:I:129:ALA:O	2:I:143:ALA:N	2.37	0.55
2:I:264:ARG:NH1	2:J:155:SER:OG	2.40	0.55
2:A:115:GLN:NE2	2:A:444:MET:SD	2.79	0.55
2:A:175:GLY:HA2	2:F:503:ILE:HD11	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:431:GLN:NE2	2:B:217:GLU:HB2	2.20	0.55
2:C:169:SER:OG	2:C:200:ALA:HB2	2.07	0.55
2:G:129:ALA:O	2:G:143:ALA:N	2.27	0.55
2:I:244:ASP:O	2:I:246:PRO:HD3	2.07	0.55
2:J:396:ALA:O	2:K:395:TYR:HA	2.07	0.55
2:K:333:ASP:HB3	2:K:519:LYS:HB2	1.88	0.55
2:E:74:TYR:CE2	2:F:260:GLU:HG2	2.42	0.54
2:G:188:VAL:HG11	2:L:430:LYS:HE2	1.89	0.54
2:K:106:LEU:HB3	2:K:303:ASN:ND2	2.22	0.54
2:K:430:LYS:HE2	2:L:188:VAL:CG1	2.37	0.54
3:U:11:LYS:HZ2	3:U:13:PHE:HE1	1.55	0.54
2:D:346:ALA:O	2:D:349:SER:N	2.40	0.54
2:J:331:VAL:HG12	2:J:517:TYR:HB2	1.89	0.54
3:W:9:ASN:HB3	3:W:56:TYR:CE2	2.42	0.54
2:A:213:LYS:HB3	2:F:431:GLN:HE21	1.71	0.54
2:A:244:ASP:HB2	3:O:13:PHE:HE2	1.71	0.54
2:G:74:TYR:CE2	2:H:260:GLU:HG2	2.42	0.54
2:I:169:SER:OG	2:I:200:ALA:HB2	2.07	0.54
2:L:343:ALA:HB1	2:L:348:GLU:HB3	1.90	0.54
2:K:166:LEU:HD22	2:K:212:ILE:HD11	1.89	0.54
2:C:502:SER:O	2:C:506:SER:OG	2.25	0.54
2:G:267:LYS:HB3	2:H:249:GLU:HG2	1.89	0.54
2:I:235:LEU:HD12	2:I:235:LEU:O	2.07	0.54
2:K:235:LEU:HD12	2:K:235:LEU:O	2.08	0.54
2:G:125:PHE:CE2	2:L:282:HIS:HE1	2.25	0.54
2:H:135:PRO:HB3	2:H:252:PHE:O	2.08	0.54
2:H:169:SER:OG	2:H:200:ALA:HB2	2.08	0.54
2:I:166:LEU:HD22	2:I:212:ILE:HD11	1.90	0.54
2:L:168:ALA:HB2	2:L:202:ALA:O	2.07	0.54
2:A:350:PHE:HB3	2:A:389:VAL:HG21	1.88	0.54
2:C:101:ARG:HH12	2:D:145:HIS:CD2	2.26	0.54
2:D:430:LYS:HE2	2:E:188:VAL:HG12	1.90	0.54
2:F:295:ALA:HB2	2:F:473:PHE:CE2	2.43	0.54
2:H:107:ILE:HG21	2:H:307:VAL:HG21	1.88	0.54
2:I:181:PHE:HD1	2:I:187:THR:HB	1.73	0.54
2:L:169:SER:OG	2:L:200:ALA:HB2	2.08	0.54
3:T:65:ARG:O	3:T:68:TRP:N	2.41	0.54
3:Y:68:TRP:O	3:Y:72:ASN:N	2.40	0.54
2:E:264:ARG:NH1	2:F:155:SER:OG	2.39	0.54
2:E:272:ILE:HG22	2:E:468:GLN:HE21	1.73	0.54
2:F:173:THR:OG1	2:F:176:ASP:OD2	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:ILE:HG12	2:F:224:ILE:HD11	1.88	0.54
2:F:235:LEU:HD12	2:F:235:LEU:O	2.08	0.54
2:F:353:LEU:O	2:F:356:GLN:N	2.41	0.54
2:I:444:MET:O	2:I:449:TYR:OH	2.26	0.54
3:S:26:LYS:NZ	3:S:74:ASP:O	2.40	0.54
2:A:121:THR:O	2:F:93:PRO:HB3	2.08	0.54
2:A:142:GLU:H	2:A:490:GLN:HG2	1.72	0.54
2:C:398:GLN:NE2	2:D:355:PHE:HB2	2.23	0.54
2:D:179:THR:HG22	2:D:189:TYR:CE2	2.42	0.54
2:E:485:ALA:HB1	2:E:510:ASN:OD1	2.08	0.54
2:F:398:GLN:HG2	2:F:399:GLY:N	2.21	0.54
2:G:121:THR:HG21	2:L:72:HIS:CD2	2.42	0.54
2:H:383:VAL:HG12	2:H:406:THR:HG22	1.89	0.54
2:J:179:THR:HG22	2:J:189:TYR:CE2	2.43	0.54
3:T:10:ILE:HD13	3:T:41:ILE:HG21	1.90	0.54
3:V:11:LYS:HG3	3:V:27:GLU:HG2	1.90	0.54
2:H:350:PHE:CB	2:H:389:VAL:HG21	2.37	0.54
2:H:377:ILE:HG22	2:H:424:TYR:HB2	1.90	0.54
3:O:65:ARG:O	3:O:68:TRP:N	2.41	0.54
2:A:378:ALA:HB1	2:A:382:VAL:CG2	2.39	0.53
2:C:268:ALA:HB1	2:C:290:LEU:HD13	1.89	0.53
2:F:153:MET:HE2	2:F:226:GLU:H	1.73	0.53
2:F:277:ASP:O	2:F:281:VAL:HG12	2.08	0.53
2:H:133:LYS:HE2	3:W:42:SER:HB2	1.90	0.53
2:H:235:LEU:HD12	2:H:235:LEU:O	2.08	0.53
2:H:272:ILE:HG22	2:H:468:GLN:HG2	1.90	0.53
3:S:9:ASN:HB3	3:S:56:TYR:HE2	1.72	0.53
3:U:10:ILE:HD11	3:U:35:TYR:CE1	2.43	0.53
3:X:10:ILE:HD11	3:X:35:TYR:CE1	2.43	0.53
2:A:398:GLN:HG2	2:A:399:GLY:N	2.23	0.53
2:B:396:ALA:O	2:C:395:TYR:HA	2.08	0.53
2:E:128:ARG:HE	2:E:484:PHE:HE1	1.56	0.53
2:E:494:SER:HA	3:R:37:ASP:CG	2.28	0.53
2:G:100:ARG:HG2	2:G:101:ARG:N	2.22	0.53
2:G:128:ARG:HE	2:G:484:PHE:HE1	1.56	0.53
2:G:238:GLY:HA2	2:G:242:SER:O	2.09	0.53
2:I:268:ALA:HB2	2:I:294:LEU:HD11	1.89	0.53
2:J:398:GLN:HG2	2:J:399:GLY:N	2.23	0.53
2:J:398:GLN:O	2:K:393:ILE:HA	2.08	0.53
2:K:128:ARG:HE	2:K:484:PHE:HE1	1.55	0.53
2:E:354:LEU:HA	2:E:357:ILE:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:181:PHE:HD1	2:G:187:THR:HB	1.73	0.53
2:K:184:GLU:HG3	2:K:366:ARG:HH12	1.73	0.53
3:W:68:TRP:CZ2	3:W:72:ASN:HB3	2.43	0.53
2:B:486:GLU:O	2:B:487:SER:OG	2.25	0.53
2:C:69:GLY:N	2:E:234:GLU:OE2	2.22	0.53
2:C:133:LYS:HE2	3:Y:42:SER:HB2	1.89	0.53
2:D:129:ALA:O	2:D:143:ALA:N	2.30	0.53
2:F:172:THR:O	2:F:195:GLN:HA	2.09	0.53
2:F:430:LYS:N	2:F:430:LYS:HD2	2.24	0.53
2:G:318:LYS:N	2:G:360:GLU:OE2	2.41	0.53
2:H:367:GLN:HB3	2:H:511:ALA:HB1	1.91	0.53
2:G:266:LEU:CD1	2:H:155:SER:HB3	2.38	0.53
2:I:164:PRO:HG2	2:I:178:TYR:HD1	1.72	0.53
2:L:106:LEU:HD21	2:L:300:LEU:HD23	1.90	0.53
2:B:344:ARG:HH11	2:C:344:ARG:HH12	1.57	0.53
2:C:80:ALA:HA	2:C:93:PRO:HG2	1.90	0.53
2:C:431:GLN:NE2	2:D:217:GLU:HB2	2.21	0.53
2:J:442:ASN:HB3	2:J:444:MET:H	1.73	0.53
3:V:16:LYS:HZ3	3:V:22:LYS:HD3	1.74	0.53
2:A:70:GLY:N	2:C:234:GLU:OE1	2.42	0.53
2:B:376:ILE:HG12	2:B:423:VAL:HG22	1.91	0.53
2:C:85:SER:HB3	3:T:32:PHE:CE1	2.43	0.53
2:H:163:PHE:HB2	2:H:179:THR:HG23	1.89	0.53
2:J:272:ILE:O	2:J:275:THR:HG22	2.09	0.53
2:L:85:SER:HB3	3:V:32:PHE:CE1	2.44	0.53
3:O:17:LEU:HD13	3:O:23:ILE:HD11	1.91	0.53
2:B:172:THR:O	2:B:195:GLN:HA	2.08	0.53
3:X:9:ASN:HB3	3:X:56:TYR:CE2	2.44	0.53
2:A:395:TYR:HA	2:F:396:ALA:O	2.08	0.53
2:B:374:ASN:ND2	2:B:439:LYS:O	2.42	0.53
2:D:238:GLY:HA2	2:D:242:SER:O	2.09	0.53
2:D:318:LYS:HE3	2:D:327:SER:HB3	1.90	0.53
2:E:244:ASP:HB2	3:T:13:PHE:HE2	1.74	0.53
2:G:431:GLN:NE2	2:H:213:LYS:O	2.41	0.53
2:J:476:ARG:NH2	2:K:230:THR:HG21	2.23	0.53
2:A:235:LEU:HD12	2:A:235:LEU:O	2.09	0.53
2:C:164:PRO:HG2	2:C:178:TYR:HD1	1.74	0.53
2:F:387:ALA:HB2	2:F:404:PHE:HB2	1.90	0.53
2:G:398:GLN:HG2	2:G:399:GLY:N	2.22	0.53
2:I:69:GLY:N	2:K:234:GLU:OE2	2.19	0.53
2:I:380:ARG:NH2	2:I:408:THR:OG1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:ILE:HD12	2:L:88:VAL:HG22	1.90	0.52
2:E:145:HIS:CD2	2:E:146:PRO:HD2	2.37	0.52
2:F:72:HIS:ND1	2:F:83:GLN:O	2.39	0.52
2:G:258:VAL:HG11	2:L:79:ILE:HB	1.91	0.52
2:H:363:GLU:OE2	2:H:366:ARG:NH2	2.41	0.52
2:I:164:PRO:HG2	2:I:178:TYR:CD1	2.44	0.52
2:L:153:MET:HG2	2:L:189:TYR:CD2	2.44	0.52
3:P:12:THR:HG21	3:P:75:LEU:HD13	1.91	0.52
3:V:65:ARG:O	3:V:68:TRP:N	2.42	0.52
2:A:417:LEU:HB3	2:F:400:LEU:HD11	1.91	0.52
2:B:95:VAL:HG12	2:C:123:GLN:HE21	1.74	0.52
2:B:386:LEU:HB3	2:B:404:PHE:HE2	1.74	0.52
2:E:268:ALA:HB2	2:E:294:LEU:HD11	1.90	0.52
2:H:331:VAL:HG12	2:H:517:TYR:HB2	1.91	0.52
2:L:244:ASP:O	2:L:246:PRO:HD3	2.10	0.52
3:P:10:ILE:HD11	3:P:35:TYR:CE1	2.44	0.52
2:A:237:GLU:HB2	2:A:246:PRO:HA	1.92	0.52
2:B:120:PRO:O	2:B:121:THR:OG1	2.28	0.52
2:B:346:ALA:O	2:B:349:SER:N	2.43	0.52
2:C:100:ARG:HG2	2:C:101:ARG:H	1.74	0.52
2:D:181:PHE:HZ	2:D:490:GLN:HE22	1.56	0.52
2:D:350:PHE:CB	2:D:389:VAL:HG21	2.36	0.52
2:E:377:ILE:HG22	2:E:424:TYR:HB2	1.91	0.52
2:E:400:LEU:HD11	2:F:417:LEU:HB3	1.91	0.52
2:G:315:GLN:HG3	2:G:510:ASN:O	2.10	0.52
2:H:318:LYS:N	2:H:360:GLU:OE2	2.41	0.52
2:J:318:LYS:N	2:J:360:GLU:OE2	2.40	0.52
2:K:272:ILE:HG22	2:K:468:GLN:HG2	1.90	0.52
2:C:135:PRO:HG3	2:C:251:GLY:HA3	1.91	0.52
2:F:113:GLY:HA2	2:F:439:LYS:HE2	1.92	0.52
2:I:305:GLU:HA	2:J:225:ALA:HB3	1.92	0.52
2:K:100:ARG:HG2	2:K:101:ARG:N	2.25	0.52
3:O:68:TRP:CZ2	3:O:72:ASN:HB3	2.45	0.52
2:L:131:TYR:HB3	2:L:250:MET:HG2	1.92	0.52
3:V:12:THR:HG21	3:V:75:LEU:HD13	1.90	0.52
2:B:100:ARG:HG2	2:B:101:ARG:N	2.25	0.52
2:F:153:MET:HE2	2:F:226:GLU:N	2.25	0.52
2:G:95:VAL:HG12	2:H:123:GLN:HE21	1.75	0.52
2:I:337:PRO:O	2:I:342:GLY:N	2.40	0.52
2:I:463:ASP:OD1	2:I:464:PRO:HD2	2.10	0.52
2:A:354:LEU:HA	2:A:357:ILE:HG22	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:GLU:N	2:B:245:ASN:O	2.40	0.52
2:D:85:SER:HB3	3:Q:32:PHE:CE1	2.45	0.52
2:E:384:ASN:HD21	2:F:362:VAL:HG21	1.74	0.52
2:F:145:HIS:CD2	2:F:146:PRO:HD2	2.34	0.52
2:F:241:GLY:HA3	3:Q:43:GLY:HA2	1.90	0.52
2:F:313:SER:O	2:F:510:ASN:HB2	2.09	0.52
2:G:230:THR:HG22	2:L:263:SER:HB2	1.91	0.52
2:H:346:ALA:O	2:H:349:SER:N	2.42	0.52
3:O:11:LYS:HG3	3:O:27:GLU:HG2	1.92	0.52
3:X:11:LYS:HG3	3:X:27:GLU:HG2	1.91	0.52
2:C:266:LEU:CD1	2:D:155:SER:HB3	2.39	0.52
2:D:244:ASP:HB2	3:X:13:PHE:HE2	1.75	0.52
2:K:376:ILE:HG12	2:K:423:VAL:HG22	1.92	0.52
2:L:344:ARG:O	2:L:348:GLU:HB2	2.10	0.52
2:A:179:THR:HG22	2:A:189:TYR:CE2	2.44	0.52
2:B:400:LEU:HD11	2:C:417:LEU:HB3	1.92	0.52
2:D:133:LYS:HE2	3:V:42:SER:HB2	1.92	0.52
2:D:244:ASP:O	2:D:246:PRO:HD3	2.10	0.52
2:F:100:ARG:HG2	2:F:101:ARG:N	2.25	0.52
2:G:357:ILE:HD11	2:G:376:ILE:HG21	1.91	0.52
2:J:101:ARG:HH12	2:K:145:HIS:CD2	2.28	0.52
2:K:444:MET:O	2:K:449:TYR:OH	2.28	0.52
2:L:181:PHE:HD1	2:L:187:THR:HB	1.75	0.52
2:D:279:ARG:HH21	2:D:285:ASP:HA	1.76	0.52
2:E:80:ALA:HA	2:E:93:PRO:HG2	1.91	0.52
2:H:72:HIS:CD2	2:I:121:THR:HG21	2.45	0.52
2:H:164:PRO:HG2	2:H:178:TYR:CD1	2.45	0.52
2:J:333:ASP:HB3	2:J:519:LYS:HB2	1.91	0.52
2:J:382:VAL:O	2:J:386:LEU:HD13	2.09	0.52
2:L:235:LEU:HD12	2:L:235:LEU:O	2.10	0.52
2:A:100:ARG:HG2	2:A:101:ARG:H	1.74	0.51
2:B:428:TYR:CZ	2:C:149:GLY:HA2	2.45	0.51
2:D:147:MET:SD	2:D:367:GLN:HG2	2.50	0.51
2:E:164:PRO:HG2	2:E:178:TYR:CD1	2.46	0.51
2:I:266:LEU:CD1	2:J:155:SER:HB3	2.38	0.51
2:K:72:HIS:CD2	2:L:121:THR:HG21	2.45	0.51
3:S:72:ASN:OD1	3:S:73:GLU:N	2.43	0.51
3:W:40:LYS:H	3:W:72:ASN:ND2	2.09	0.51
4:Z:309:TRP:O	4:Z:313:ASP:N	2.40	0.51
2:A:277:ASP:O	2:A:281:VAL:HG12	2.10	0.51
2:A:396:ALA:O	2:B:395:TYR:HA	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:GLN:O	2:E:393:ILE:HA	2.09	0.51
2:F:380:ARG:NH1	2:F:427:GLN:O	2.44	0.51
2:G:153:MET:HG2	2:G:189:TYR:CD2	2.45	0.51
2:J:100:ARG:HG2	2:J:101:ARG:N	2.25	0.51
2:K:164:PRO:HG2	2:K:178:TYR:CD1	2.45	0.51
3:Y:72:ASN:OD1	3:Y:73:GLU:N	2.43	0.51
2:A:100:ARG:HG2	2:A:101:ARG:N	2.25	0.51
2:A:155:SER:OG	2:F:264:ARG:NH1	2.40	0.51
2:B:235:LEU:HD12	2:B:235:LEU:O	2.10	0.51
2:B:305:GLU:HG2	2:B:309:TRP:CD1	2.45	0.51
2:C:235:LEU:HD12	2:C:235:LEU:O	2.10	0.51
2:C:344:ARG:O	2:C:348:GLU:HB2	2.10	0.51
2:F:113:GLY:H	2:F:446:ALA:HB1	1.75	0.51
2:G:197:THR:HG22	2:G:199:ASP:H	1.75	0.51
2:J:346:ALA:O	2:J:349:SER:N	2.43	0.51
3:O:11:LYS:HZ2	3:O:13:PHE:HE1	1.56	0.51
2:F:74:TYR:HA	2:F:79:ILE:HD11	1.93	0.51
2:I:377:ILE:HG22	2:I:424:TYR:HB2	1.93	0.51
2:J:380:ARG:NH2	2:J:408:THR:OG1	2.44	0.51
2:D:485:ALA:HB1	2:D:510:ASN:OD1	2.11	0.51
2:E:100:ARG:HG2	2:E:101:ARG:N	2.25	0.51
2:E:117:MET:HE1	2:E:261:ALA:HB2	1.93	0.51
2:E:121:THR:HG22	2:E:260:GLU:OE1	2.11	0.51
2:F:131:TYR:CE2	2:F:143:ALA:HA	2.45	0.51
2:I:101:ARG:NH1	2:J:145:HIS:HD2	2.08	0.51
2:J:131:TYR:CB	2:J:250:MET:HG2	2.41	0.51
2:K:180:HIS:HD2	2:K:182:PHE:CE1	2.29	0.51
2:L:107:ILE:HG21	2:L:307:VAL:HG21	1.92	0.51
2:B:180:HIS:HD2	2:B:182:PHE:CD1	2.29	0.51
2:C:350:PHE:HB3	2:C:389:VAL:HG21	1.93	0.51
2:F:354:LEU:HA	2:F:357:ILE:HG22	1.93	0.51
2:H:263:SER:HB2	2:I:230:THR:HG22	1.92	0.51
2:L:148:TYR:HD1	2:L:186:GLY:H	1.57	0.51
2:L:333:ASP:HB3	2:L:519:LYS:HB2	1.93	0.51
3:P:72:ASN:OD1	3:P:73:GLU:N	2.43	0.51
3:Q:9:ASN:HB3	3:Q:56:TYR:CE2	2.46	0.51
3:V:14:GLU:HB3	3:V:25:GLY:H	1.75	0.51
2:A:71:ASP:CG	2:C:231:SER:HB2	2.30	0.51
2:A:253:ARG:NE	2:A:255:ASP:OD2	2.44	0.51
2:C:197:THR:HG22	2:C:199:ASP:H	1.75	0.51
2:E:357:ILE:HD11	2:E:376:ILE:HD13	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:398:GLN:HG2	2:H:399:GLY:N	2.25	0.51
2:K:384:ASN:HD21	2:L:362:VAL:HG21	1.74	0.51
2:K:453:TYR:CD2	2:K:454:VAL:HG13	2.46	0.51
2:K:463:ASP:OD1	2:K:464:PRO:HD2	2.09	0.51
3:S:65:ARG:O	3:S:68:TRP:N	2.44	0.51
2:E:85:SER:HB3	3:O:32:PHE:CE1	2.46	0.51
2:K:238:GLY:HA2	2:K:242:SER:O	2.11	0.51
3:Q:26:LYS:NZ	3:Q:74:ASP:O	2.40	0.51
2:B:173:THR:OG1	2:B:176:ASP:OD2	2.28	0.51
2:B:493:ALA:O	2:B:494:SER:OG	2.28	0.51
2:C:502:SER:N	2:C:506:SER:OG	2.40	0.51
2:D:278:LEU:HD12	2:D:286:ALA:HB2	1.93	0.51
2:H:168:ALA:HB1	2:H:200:ALA:HA	1.93	0.51
3:R:9:ASN:ND2	3:R:51:SER:OG	2.44	0.51
2:B:383:VAL:HG21	2:B:425:ILE:HG12	1.93	0.51
2:C:126:ALA:N	2:C:255:ASP:O	2.44	0.51
2:G:315:GLN:OE1	2:G:514:ARG:NH1	2.44	0.51
2:H:409:THR:HG21	2:I:370:ARG:O	2.11	0.51
2:K:131:TYR:CB	2:K:250:MET:HG2	2.41	0.51
2:K:344:ARG:HD2	2:L:344:ARG:NH1	2.26	0.51
3:O:10:ILE:HD11	3:O:35:TYR:CE1	2.46	0.51
3:X:10:ILE:HD11	3:X:35:TYR:HE1	1.76	0.51
2:A:188:VAL:CG1	2:F:430:LYS:HE2	2.41	0.50
2:B:323:LEU:HD21	2:B:329:ALA:HA	1.92	0.50
2:E:181:PHE:HD1	2:E:187:THR:HB	1.75	0.50
2:K:305:GLU:HA	2:L:225:ALA:HB3	1.93	0.50
3:S:18:ASP:HB3	3:S:21:LYS:HD3	1.92	0.50
3:V:72:ASN:OD1	3:V:73:GLU:N	2.44	0.50
3:X:27:GLU:HB3	3:X:56:TYR:CD1	2.46	0.50
2:A:120:PRO:HB2	2:A:121:THR:HG23	1.93	0.50
2:D:121:THR:HA	2:D:259:ILE:O	2.12	0.50
2:D:313:SER:O	2:D:510:ASN:HB2	2.11	0.50
2:G:363:GLU:OE2	2:G:366:ARG:NH2	2.44	0.50
2:H:179:THR:HG22	2:H:189:TYR:CD1	2.47	0.50
2:I:72:HIS:CD2	2:J:121:THR:HG21	2.46	0.50
2:L:131:TYR:CB	2:L:250:MET:HG2	2.41	0.50
2:B:79:ILE:HB	2:C:258:VAL:HG11	1.92	0.50
2:C:128:ARG:CZ	2:C:492:PRO:HD3	2.41	0.50
2:D:235:LEU:HD12	2:D:235:LEU:O	2.11	0.50
2:D:344:ARG:CZ	2:E:344:ARG:HH22	2.23	0.50
2:E:134:ASP:HB3	2:E:137:ALA:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:442:ASN:HB3	2:E:444:MET:H	1.76	0.50
2:G:380:ARG:NH1	2:G:427:GLN:O	2.38	0.50
2:J:69:GLY:N	2:L:234:GLU:OE2	2.44	0.50
2:L:485:ALA:HB1	2:L:510:ASN:OD1	2.11	0.50
2:B:456:LEU:HD12	2:B:475:THR:HG21	1.94	0.50
2:C:430:LYS:HE2	2:D:188:VAL:CG1	2.41	0.50
2:F:244:ASP:HB2	3:Q:13:PHE:CE2	2.45	0.50
2:G:151:ASP:HB2	2:G:189:TYR:CE2	2.47	0.50
2:G:235:LEU:O	2:G:235:LEU:HD12	2.12	0.50
2:H:456:LEU:HD12	2:H:475:THR:HG21	1.93	0.50
3:R:68:TRP:CZ2	3:R:72:ASN:HB3	2.46	0.50
3:W:64:GLN:HB3	3:W:67:GLU:HB2	1.93	0.50
2:A:151:ASP:HB2	2:A:189:TYR:CE1	2.43	0.50
2:B:100:ARG:HG2	2:B:101:ARG:H	1.74	0.50
2:C:164:PRO:HG2	2:C:178:TYR:CD1	2.47	0.50
2:D:164:PRO:HG2	2:D:178:TYR:HD1	1.77	0.50
2:E:120:PRO:O	2:E:121:THR:OG1	2.28	0.50
2:J:71:ASP:CG	2:L:231:SER:HB2	2.32	0.50
2:L:430:LYS:N	2:L:430:LYS:HD2	2.26	0.50
3:U:38:VAL:HG11	3:U:69:ILE:HG12	1.94	0.50
2:B:104:PRO:HB2	2:B:427:GLN:HE22	1.77	0.50
2:B:354:LEU:HA	2:B:357:ILE:HG22	1.93	0.50
2:C:345:TRP:HA	2:D:341:ARG:O	2.11	0.50
2:C:346:ALA:O	2:C:349:SER:N	2.45	0.50
2:D:181:PHE:HD1	2:D:187:THR:HB	1.76	0.50
2:D:269:ALA:HA	2:D:470:VAL:HA	1.92	0.50
2:E:75:ASN:ND2	3:O:5:ARG:HA	2.27	0.50
2:J:353:LEU:HD13	2:J:385:VAL:HG11	1.93	0.50
2:J:386:LEU:HB3	2:J:404:PHE:HE2	1.77	0.50
2:K:131:TYR:HB3	2:K:250:MET:HE2	1.93	0.50
2:C:96:MET:HB2	2:D:124:VAL:HG22	1.92	0.50
2:C:295:ALA:HB2	2:C:473:PHE:HE2	1.77	0.50
2:D:378:ALA:HB1	2:D:382:VAL:HG23	1.93	0.50
2:E:376:ILE:HG22	2:E:436:VAL:HG22	1.92	0.50
2:G:362:VAL:HG21	2:L:384:ASN:ND2	2.25	0.50
2:H:344:ARG:NH1	2:I:344:ARG:HH12	2.08	0.50
2:I:344:ARG:CZ	2:J:344:ARG:HH12	2.25	0.50
2:L:444:MET:O	2:L:449:TYR:OH	2.13	0.50
3:T:72:ASN:OD1	3:T:73:GLU:N	2.44	0.50
3:V:51:SER:OG	3:V:53:LYS:O	2.18	0.50
2:A:310:ILE:HG23	2:A:513:PHE:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:HG2	2:B:178:TYR:CD1	2.46	0.50
2:C:270:TYR:HB3	2:C:290:LEU:HD12	1.93	0.50
2:F:153:MET:SD	2:F:157:GLN:HB3	2.52	0.50
2:G:260:GLU:HG2	2:L:74:TYR:CE2	2.47	0.50
2:H:148:TYR:HB3	2:H:186:GLY:HA2	1.94	0.50
2:H:444:MET:O	2:H:449:TYR:OH	2.30	0.50
2:J:134:ASP:HB3	2:J:137:ALA:HB2	1.93	0.50
2:J:153:MET:HE2	2:J:226:GLU:N	2.26	0.50
2:J:350:PHE:HB3	2:J:389:VAL:HG21	1.94	0.50
3:V:3:SER:N	3:V:7:TYR:OH	2.38	0.50
3:X:9:ASN:HB3	3:X:56:TYR:HE2	1.76	0.50
2:A:481:ILE:HD11	2:A:510:ASN:HD21	1.77	0.50
2:B:360:GLU:O	2:B:363:GLU:N	2.45	0.50
2:D:331:VAL:HG12	2:D:517:TYR:HB2	1.94	0.50
2:H:343:ALA:HB1	2:H:348:GLU:HB3	1.94	0.50
2:J:323:LEU:HD21	2:J:329:ALA:HA	1.93	0.50
2:J:432:ASP:OD1	2:J:433:TYR:N	2.45	0.50
2:L:100:ARG:HG2	2:L:101:ARG:H	1.77	0.50
2:L:172:THR:O	2:L:195:GLN:HA	2.12	0.50
3:S:26:LYS:NZ	3:S:74:ASP:OD2	2.34	0.50
2:C:275:THR:HG22	2:C:286:ALA:HB3	1.94	0.49
2:C:324:THR:O	2:C:326:GLY:N	2.45	0.49
2:C:350:PHE:HB2	2:C:389:VAL:HG21	1.94	0.49
2:D:145:HIS:CD2	2:D:146:PRO:HD2	2.41	0.49
2:E:166:LEU:HD11	2:E:221:LEU:HD21	1.94	0.49
2:J:235:LEU:O	2:J:235:LEU:HD12	2.12	0.49
2:J:521:ILE:HA	2:K:341:ARG:NH2	2.27	0.49
3:U:14:GLU:HB3	3:U:25:GLY:H	1.76	0.49
3:W:38:VAL:HG11	3:W:69:ILE:HG12	1.94	0.49
2:A:121:THR:HG22	2:A:260:GLU:OE1	2.12	0.49
2:D:476:ARG:HH21	2:E:230:THR:HG21	1.77	0.49
2:I:493:ALA:O	2:I:494:SER:OG	2.30	0.49
2:K:113:GLY:H	2:K:446:ALA:HB1	1.77	0.49
2:K:344:ARG:NH1	2:L:344:ARG:HH12	2.05	0.49
2:K:380:ARG:NH2	2:K:408:THR:OG1	2.44	0.49
2:A:173:THR:OG1	2:A:176:ASP:OD2	2.29	0.49
2:C:89:THR:HG23	2:G:495:ARG:NH2	2.27	0.49
2:E:129:ALA:O	2:E:143:ALA:N	2.34	0.49
2:F:285:ASP:HB3	2:F:288:ALA:HB3	1.93	0.49
2:G:71:ASP:CG	2:I:231:SER:HB2	2.33	0.49
2:K:171:GLN:HE21	2:K:195:GLN:HE21	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:74:ASP:OD1	3:U:77:LYS:HE3	2.12	0.49
2:A:430:LYS:HE2	2:B:188:VAL:CG1	2.42	0.49
2:B:77:THR:HG21	3:Y:5:ARG:NH2	2.27	0.49
2:J:179:THR:HG22	2:J:189:TYR:CD2	2.47	0.49
2:K:191:GLN:N	2:K:222:VAL:O	2.45	0.49
3:Q:8:VAL:HG23	3:Q:32:PHE:HD1	1.78	0.49
3:Y:11:LYS:O	3:Y:46:TYR:HA	2.12	0.49
2:B:113:GLY:H	2:B:446:ALA:HB1	1.77	0.49
2:B:121:THR:HG22	2:B:260:GLU:HA	1.93	0.49
2:C:100:ARG:HG2	2:C:101:ARG:N	2.28	0.49
2:D:268:ALA:HB2	2:D:294:LEU:HD11	1.93	0.49
2:D:277:ASP:O	2:D:281:VAL:HG12	2.13	0.49
2:F:100:ARG:HG2	2:F:101:ARG:H	1.77	0.49
2:G:336:ASP:O	2:G:340:ILE:HG12	2.13	0.49
2:A:80:ALA:HA	2:A:93:PRO:HG2	1.94	0.49
2:A:181:PHE:HD1	2:A:187:THR:HB	1.77	0.49
2:A:375:PHE:CZ	2:A:437:GLY:HA3	2.47	0.49
2:A:383:VAL:HG21	2:A:425:ILE:HG12	1.95	0.49
2:C:88:VAL:HG22	2:G:254:ILE:HD12	1.95	0.49
2:C:407:ASP:HB3	2:D:372:GLU:HB2	1.94	0.49
2:D:253:ARG:NE	2:D:255:ASP:OD2	2.43	0.49
2:G:101:ARG:HD2	2:H:146:PRO:HD3	1.94	0.49
2:H:269:ALA:HA	2:H:470:VAL:HA	1.95	0.49
2:J:383:VAL:HG21	2:J:425:ILE:HG12	1.95	0.49
2:K:344:ARG:HD2	2:L:344:ARG:CZ	2.42	0.49
2:B:169:SER:OG	2:B:200:ALA:HB2	2.12	0.49
2:B:398:GLN:O	2:C:393:ILE:HA	2.12	0.49
2:E:147:MET:HE2	2:E:366:ARG:HG2	1.94	0.49
2:G:313:SER:O	2:G:510:ASN:HB2	2.12	0.49
2:A:348:GLU:OE1	2:A:348:GLU:N	2.45	0.49
2:B:344:ARG:HD2	2:C:344:ARG:NH1	2.27	0.49
2:B:345:TRP:CD2	2:C:348:GLU:HG3	2.48	0.49
2:B:398:GLN:HE21	2:C:355:PHE:HB2	1.78	0.49
2:B:398:GLN:NE2	2:C:355:PHE:HB2	2.28	0.49
2:G:444:MET:O	2:G:449:TYR:OH	2.21	0.49
2:H:171:GLN:HE21	2:H:195:GLN:HE21	1.58	0.49
2:C:145:HIS:CD2	2:C:146:PRO:HD2	2.42	0.49
2:E:396:ALA:O	2:F:395:TYR:HA	2.12	0.49
2:G:131:TYR:CB	2:G:250:MET:HG2	2.43	0.49
2:J:71:ASP:HB3	2:L:230:THR:HG23	1.95	0.49
2:J:345:TRP:HA	2:K:341:ARG:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:466:ASN:O	2:K:468:GLN:HG3	2.13	0.49
3:W:72:ASN:OD1	3:W:73:GLU:N	2.46	0.49
2:A:378:ALA:HB1	2:A:382:VAL:HG21	1.93	0.49
2:B:163:PHE:HB2	2:B:179:THR:CG2	2.43	0.49
2:C:74:TYR:CE2	2:D:260:GLU:HG2	2.48	0.49
2:E:331:VAL:HG12	2:E:517:TYR:HB2	1.95	0.49
2:F:148:TYR:HB3	2:F:186:GLY:HA2	1.95	0.49
2:F:432:ASP:OD1	2:F:433:TYR:N	2.45	0.49
2:J:272:ILE:HG22	2:J:468:GLN:HE21	1.78	0.49
2:K:106:LEU:HD21	2:K:300:LEU:HD23	1.95	0.49
2:K:431:GLN:NE2	2:L:213:LYS:O	2.46	0.49
2:A:392:GLY:O	2:F:399:GLY:HA3	2.13	0.48
2:C:273:GLU:HG3	2:H:234:GLU:HA	1.94	0.48
2:D:396:ALA:O	2:E:395:TYR:HA	2.13	0.48
2:F:269:ALA:HA	2:F:470:VAL:HA	1.93	0.48
2:G:395:TYR:HA	2:L:396:ALA:O	2.13	0.48
2:H:100:ARG:HG2	2:H:101:ARG:H	1.77	0.48
2:K:244:ASP:O	2:K:246:PRO:HD3	2.13	0.48
2:K:382:VAL:HG12	2:K:521:ILE:HD11	1.96	0.48
2:K:384:ASN:O	2:K:387:ALA:N	2.45	0.48
2:A:279:ARG:HD2	2:A:284:MET:O	2.12	0.48
2:A:398:GLN:O	2:B:393:ILE:HA	2.14	0.48
2:C:244:ASP:O	2:C:246:PRO:HD3	2.13	0.48
2:D:430:LYS:N	2:D:430:LYS:HD2	2.28	0.48
2:E:101:ARG:HG2	2:F:144:PHE:O	2.14	0.48
2:F:181:PHE:HD1	2:F:187:THR:HB	1.78	0.48
2:G:345:TRP:NE1	2:G:348:GLU:OE1	2.47	0.48
2:G:375:PHE:CZ	2:G:437:GLY:HA3	2.48	0.48
2:H:313:SER:O	2:H:510:ASN:HB2	2.13	0.48
2:L:181:PHE:HZ	2:L:490:GLN:HE22	1.62	0.48
2:D:164:PRO:HG2	2:D:178:TYR:CD1	2.48	0.48
2:D:476:ARG:NH2	2:E:230:THR:HG21	2.27	0.48
2:F:313:SER:OG	2:F:510:ASN:ND2	2.45	0.48
2:G:184:GLU:O	2:G:185:THR:OG1	2.32	0.48
2:G:341:ARG:O	2:L:345:TRP:HA	2.14	0.48
3:R:11:LYS:HD2	3:R:56:TYR:OH	2.13	0.48
3:U:68:TRP:CE2	3:U:72:ASN:HB3	2.48	0.48
3:X:12:THR:HG21	3:X:75:LEU:HD13	1.94	0.48
2:B:128:ARG:NE	2:B:484:PHE:HE1	2.07	0.48
2:B:344:ARG:NH1	2:C:344:ARG:HH22	2.11	0.48
2:D:364:ILE:O	2:D:368:THR:OG1	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:TYR:HB3	2:E:186:GLY:HA2	1.94	0.48
3:Q:26:LYS:NZ	3:Q:74:ASP:OD2	2.45	0.48
2:A:80:ALA:HA	2:A:93:PRO:CG	2.44	0.48
2:C:121:THR:HA	2:C:259:ILE:O	2.13	0.48
2:D:377:ILE:HA	2:D:424:TYR:O	2.13	0.48
2:D:486:GLU:C	2:D:488:ALA:H	2.17	0.48
2:E:135:PRO:HB3	2:E:252:PHE:O	2.13	0.48
2:E:263:SER:HB2	2:F:230:THR:HG22	1.96	0.48
2:E:346:ALA:O	2:E:349:SER:N	2.46	0.48
2:E:456:LEU:HD12	2:E:475:THR:CG2	2.43	0.48
2:G:346:ALA:O	2:G:349:SER:N	2.47	0.48
2:H:428:TYR:CZ	2:I:149:GLY:HA2	2.49	0.48
2:L:142:GLU:H	2:L:490:GLN:HG2	1.78	0.48
2:L:238:GLY:HA2	2:L:242:SER:O	2.13	0.48
3:X:8:VAL:HG11	3:X:35:TYR:CE2	2.49	0.48
2:F:157:GLN:N	2:F:227:GLY:O	2.46	0.48
2:F:360:GLU:O	2:F:363:GLU:N	2.46	0.48
2:G:79:ILE:CG2	2:H:121:THR:HB	2.43	0.48
2:H:152:ALA:HB1	2:H:225:ALA:CB	2.35	0.48
2:I:476:ARG:NH2	2:J:230:THR:HG21	2.29	0.48
3:W:9:ASN:ND2	3:W:51:SER:OG	2.45	0.48
2:B:184:GLU:O	2:B:185:THR:OG1	2.27	0.48
2:E:345:TRP:NE1	2:E:348:GLU:OE1	2.46	0.48
2:E:444:MET:O	2:E:449:TYR:OH	2.32	0.48
2:G:477:TYR:CD2	2:G:478:GLY:N	2.81	0.48
2:H:494:SER:HA	3:W:37:ASP:CG	2.33	0.48
2:I:101:ARG:NH1	2:J:145:HIS:CD2	2.81	0.48
2:I:101:ARG:HD2	2:J:146:PRO:HD3	1.96	0.48
2:B:71:ASP:OD2	3:X:50:PRO:HG3	2.14	0.48
2:C:313:SER:OG	2:C:510:ASN:HB2	2.14	0.48
2:D:179:THR:HG22	2:D:189:TYR:CD2	2.48	0.48
2:F:377:ILE:HG22	2:F:424:TYR:HB2	1.96	0.48
2:G:272:ILE:HG22	2:G:468:GLN:HE21	1.79	0.48
2:H:153:MET:SD	2:H:157:GLN:HB3	2.53	0.48
2:K:313:SER:O	2:K:510:ASN:HB2	2.13	0.48
2:L:295:ALA:HB2	2:L:473:PHE:HE2	1.78	0.48
2:B:159:ALA:HB3	2:B:228:MET:CE	2.43	0.48
2:C:196:VAL:HG21	2:C:215:GLN:OE1	2.14	0.48
2:C:376:ILE:HG12	2:C:423:VAL:HG22	1.95	0.48
2:E:295:ALA:HB2	2:E:473:PHE:CE2	2.49	0.48
2:E:482:ASN:O	2:E:485:ALA:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:305:GLU:HA	2:I:225:ALA:HB3	1.95	0.48
2:H:378:ALA:O	2:H:426:ASP:N	2.46	0.48
2:I:71:ASP:CG	2:K:231:SER:HB2	2.33	0.48
2:K:120:PRO:O	2:K:121:THR:OG1	2.31	0.48
3:W:26:LYS:HD2	3:W:75:LEU:HD23	1.95	0.48
3:W:68:TRP:O	3:W:71:ALA:N	2.47	0.48
3:X:21:LYS:HG2	3:X:80:GLY:HA2	1.95	0.48
2:A:260:GLU:HG2	2:F:74:TYR:CE2	2.49	0.48
2:D:172:THR:O	2:D:195:GLN:HA	2.14	0.48
2:D:348:GLU:OE1	2:D:348:GLU:N	2.45	0.48
2:F:171:GLN:NE2	2:F:195:GLN:HE21	2.11	0.48
2:F:505:ASN:OD1	2:F:506:SER:N	2.46	0.48
2:I:295:ALA:HB2	2:I:473:PHE:HE2	1.77	0.48
2:K:74:TYR:CE2	2:L:260:GLU:HG2	2.49	0.48
3:S:40:LYS:H	3:S:72:ASN:ND2	2.12	0.48
2:B:313:SER:O	2:B:510:ASN:HB2	2.14	0.47
2:C:193:SER:OG	2:C:220:ALA:O	2.23	0.47
2:D:153:MET:HE2	2:D:226:GLU:N	2.29	0.47
2:E:72:HIS:CD2	2:F:121:THR:HG21	2.48	0.47
2:E:407:ASP:HB3	2:F:372:GLU:HB2	1.95	0.47
2:G:345:TRP:HB3	2:H:343:ALA:HA	1.96	0.47
2:A:160:ALA:HB1	2:A:232:ILE:HG21	1.95	0.47
2:A:204:ASP:OD1	2:A:205:ALA:N	2.47	0.47
2:B:407:ASP:HB3	2:C:372:GLU:HB2	1.95	0.47
2:C:304:ARG:NH1	2:C:426:ASP:OD1	2.46	0.47
2:E:105:ASN:HB2	2:E:412:VAL:HG23	1.96	0.47
2:E:323:LEU:HD22	2:E:327:SER:HB2	1.95	0.47
2:I:270:TYR:HB3	2:I:290:LEU:HD12	1.95	0.47
3:T:28:VAL:HG21	3:T:68:TRP:HZ3	1.78	0.47
2:A:266:LEU:CD1	2:B:155:SER:HB3	2.44	0.47
2:C:331:VAL:HG11	2:C:519:LYS:HE3	1.96	0.47
2:H:134:ASP:HB3	2:H:137:ALA:HB2	1.97	0.47
2:H:234:GLU:OE2	2:L:69:GLY:N	2.31	0.47
2:H:324:THR:O	2:H:326:GLY:N	2.47	0.47
2:I:396:ALA:O	2:J:395:TYR:HA	2.15	0.47
2:C:432:ASP:OD1	2:C:433:TYR:N	2.47	0.47
2:D:240:ASN:ND2	3:X:46:TYR:OH	2.48	0.47
2:E:318:LYS:N	2:E:360:GLU:OE2	2.47	0.47
2:E:386:LEU:HB3	2:E:404:PHE:HE2	1.79	0.47
2:F:152:ALA:HB1	2:F:225:ALA:CB	2.36	0.47
2:H:348:GLU:OE1	2:H:348:GLU:N	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:PHE:HB2	2:H:389:VAL:HG21	1.95	0.47
2:I:354:LEU:HA	2:I:357:ILE:HG22	1.97	0.47
2:J:125:PHE:HA	2:J:256:LYS:HA	1.96	0.47
2:J:348:GLU:OE1	2:J:348:GLU:N	2.47	0.47
2:J:389:VAL:HG12	2:J:390:ASP:N	2.29	0.47
2:K:196:VAL:HG21	2:K:215:GLN:OE1	2.13	0.47
2:K:398:GLN:O	2:L:393:ILE:HA	2.14	0.47
3:W:26:LYS:NZ	3:W:74:ASP:OD2	2.47	0.47
2:B:384:ASN:ND2	2:C:362:VAL:HG21	2.28	0.47
2:I:128:ARG:NH1	2:I:490:GLN:O	2.44	0.47
2:I:345:TRP:HA	2:J:341:ARG:O	2.14	0.47
2:I:376:ILE:HG12	2:I:423:VAL:HG22	1.95	0.47
2:I:431:GLN:NE2	2:J:213:LYS:O	2.47	0.47
2:I:477:TYR:CD2	2:I:478:GLY:N	2.82	0.47
2:L:377:ILE:HG22	2:L:424:TYR:HB2	1.95	0.47
2:C:295:ALA:HB2	2:C:473:PHE:CE2	2.49	0.47
2:D:134:ASP:HB3	2:D:137:ALA:HB2	1.97	0.47
2:D:432:ASP:OD1	2:D:433:TYR:N	2.47	0.47
2:F:290:LEU:HD23	2:F:293:ILE:HD11	1.95	0.47
2:L:272:ILE:HG22	2:L:468:GLN:HG2	1.97	0.47
3:O:72:ASN:OD1	3:O:73:GLU:N	2.48	0.47
3:Q:14:GLU:HB3	3:Q:25:GLY:H	1.75	0.47
2:A:84:THR:HG22	2:A:86:GLY:H	1.78	0.47
2:B:152:ALA:HB1	2:B:225:ALA:CB	2.44	0.47
2:E:158:GLY:HA2	2:E:163:PHE:HE2	1.78	0.47
2:F:147:MET:SD	2:F:367:GLN:HG2	2.55	0.47
2:F:357:ILE:CD1	2:F:376:ILE:HD13	2.43	0.47
2:G:190:LEU:HB3	2:G:221:LEU:HG	1.96	0.47
2:I:168:ALA:HB1	2:I:200:ALA:HA	1.97	0.47
2:I:430:LYS:O	2:J:213:LYS:HE2	2.15	0.47
2:K:344:ARG:O	2:K:348:GLU:HB2	2.13	0.47
2:K:477:TYR:CD2	2:K:478:GLY:N	2.83	0.47
3:P:9:ASN:HB3	3:P:56:TYR:CE2	2.50	0.47
2:C:277:ASP:O	2:C:281:VAL:HG12	2.15	0.47
2:E:151:ASP:HB3	2:E:187:THR:CG2	2.44	0.47
2:I:79:ILE:HB	2:J:258:VAL:HG11	1.96	0.47
2:I:432:ASP:OD1	2:I:433:TYR:N	2.48	0.47
2:J:146:PRO:HB2	2:J:366:ARG:O	2.15	0.47
2:J:378:ALA:HB1	2:J:382:VAL:CG2	2.45	0.47
2:K:163:PHE:HB2	2:K:179:THR:HG23	1.95	0.47
2:L:129:ALA:O	2:L:143:ALA:N	2.36	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:27:GLU:HB3	3:R:56:TYR:CD1	2.49	0.47
3:X:68:TRP:CE2	3:X:72:ASN:HB3	2.49	0.47
2:B:380:ARG:HH22	2:B:427:GLN:HB2	1.79	0.47
2:B:430:LYS:N	2:B:430:LYS:HD2	2.30	0.47
2:D:101:ARG:HH12	2:E:145:HIS:CD2	2.33	0.47
2:F:169:SER:OG	2:F:200:ALA:HB2	2.15	0.47
2:G:378:ALA:HB1	2:G:382:VAL:CG2	2.44	0.47
2:I:384:ASN:O	2:I:387:ALA:N	2.48	0.47
3:S:40:LYS:H	3:S:72:ASN:HD22	1.63	0.47
2:A:444:MET:O	2:A:449:TYR:OH	2.33	0.47
2:E:179:THR:HG22	2:E:189:TYR:CD2	2.50	0.47
2:E:521:ILE:HA	2:F:341:ARG:HH22	1.80	0.47
2:F:134:ASP:HB3	2:F:137:ALA:HB2	1.97	0.47
2:H:163:PHE:HB2	2:H:179:THR:CG2	2.45	0.47
2:H:384:ASN:HD21	2:I:362:VAL:HG21	1.80	0.47
2:J:318:LYS:HE3	2:J:327:SER:HB3	1.97	0.47
2:J:477:TYR:CD2	2:J:478:GLY:N	2.83	0.47
3:P:40:LYS:H	3:P:72:ASN:HD22	1.62	0.47
3:R:68:TRP:O	3:R:71:ALA:N	2.47	0.47
2:C:137:ALA:HB3	2:C:140:ALA:HB2	1.97	0.46
2:E:272:ILE:HG22	2:E:468:GLN:NE2	2.30	0.46
2:G:257:GLN:HG2	2:G:497:GLN:HG3	1.97	0.46
3:Q:27:GLU:HB3	3:Q:56:TYR:CD1	2.50	0.46
3:Y:27:GLU:HB3	3:Y:56:TYR:CD1	2.50	0.46
2:A:164:PRO:HG2	2:A:178:TYR:HD1	1.80	0.46
2:B:466:ASN:O	2:B:468:GLN:HG3	2.15	0.46
2:D:126:ALA:N	2:D:255:ASP:O	2.46	0.46
2:D:263:SER:HB2	2:E:230:THR:HG22	1.97	0.46
2:D:375:PHE:CE1	2:D:437:GLY:HA3	2.49	0.46
2:J:337:PRO:O	2:J:342:GLY:N	2.36	0.46
2:L:136:VAL:HG12	2:L:253:ARG:NE	2.30	0.46
2:A:79:ILE:HB	2:B:258:VAL:HG11	1.97	0.46
2:A:238:GLY:HA2	2:A:242:SER:O	2.15	0.46
2:A:458:PRO:HA	2:A:473:PHE:HD1	1.79	0.46
2:B:84:THR:HB	2:B:88:VAL:O	2.15	0.46
2:D:120:PRO:O	2:D:121:THR:OG1	2.33	0.46
2:E:131:TYR:CB	2:E:250:MET:HG2	2.45	0.46
2:G:386:LEU:HB3	2:G:404:PHE:HE2	1.79	0.46
2:G:409:THR:HG21	2:H:370:ARG:O	2.16	0.46
2:G:417:LEU:HB3	2:L:400:LEU:HD11	1.95	0.46
2:H:398:GLN:O	2:I:393:ILE:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:345:TRP:HB3	2:J:343:ALA:HA	1.98	0.46
2:I:398:GLN:O	2:J:393:ILE:HA	2.15	0.46
2:K:107:ILE:HG21	2:K:307:VAL:HG21	1.98	0.46
2:A:179:THR:HG22	2:A:189:TYR:CD2	2.51	0.46
2:E:164:PRO:HG2	2:E:178:TYR:HD1	1.78	0.46
2:E:241:GLY:HA3	3:T:43:GLY:HA2	1.97	0.46
2:E:431:GLN:NE2	2:F:213:LYS:HB3	2.28	0.46
2:F:121:THR:HA	2:F:259:ILE:O	2.14	0.46
2:G:216:MET:HA	2:G:221:LEU:O	2.15	0.46
2:G:348:GLU:HG3	2:L:345:TRP:CD2	2.50	0.46
2:I:343:ALA:HB1	2:I:348:GLU:HB3	1.97	0.46
2:K:390:ASP:OD2	2:K:394:SER:OG	2.30	0.46
2:L:149:GLY:H	2:L:186:GLY:HA2	1.81	0.46
3:V:16:LYS:NZ	3:W:20:ASN:H	2.12	0.46
2:B:397:ALA:HB1	2:C:393:ILE:HG22	1.97	0.46
2:C:145:HIS:HD2	2:C:146:PRO:CD	2.27	0.46
2:C:331:VAL:HG12	2:C:517:TYR:HB2	1.97	0.46
2:E:179:THR:HG22	2:E:189:TYR:CE2	2.51	0.46
2:F:106:LEU:HA	2:F:303:ASN:ND2	2.30	0.46
2:G:328:LYS:HD3	2:G:331:VAL:HG21	1.96	0.46
2:G:430:LYS:N	2:G:430:LYS:HD2	2.30	0.46
2:I:453:TYR:HB3	2:I:476:ARG:O	2.16	0.46
2:K:179:THR:HG22	2:K:189:TYR:CE1	2.51	0.46
3:O:10:ILE:HD11	3:O:35:TYR:HE1	1.80	0.46
3:W:5:ARG:NH1	3:W:33:PRO:HB3	2.29	0.46
2:C:78:ASN:OD1	3:T:5:ARG:HD3	2.15	0.46
2:D:100:ARG:HG2	2:D:101:ARG:H	1.80	0.46
2:E:334:PHE:CZ	2:E:353:LEU:HD12	2.50	0.46
2:G:79:ILE:HB	2:H:258:VAL:HG11	1.97	0.46
2:G:145:HIS:CD2	2:G:146:PRO:HD2	2.43	0.46
2:G:244:ASP:O	2:G:246:PRO:HD3	2.15	0.46
2:G:372:GLU:HB2	2:L:407:ASP:HB3	1.96	0.46
2:H:131:TYR:HB3	2:H:250:MET:HG2	1.97	0.46
2:H:502:SER:N	2:H:506:SER:OG	2.48	0.46
2:J:136:VAL:HG12	2:J:253:ARG:NE	2.30	0.46
2:L:309:TRP:O	2:L:313:SER:N	2.44	0.46
2:E:344:ARG:O	2:E:348:GLU:HB2	2.16	0.46
2:E:360:GLU:O	2:E:363:GLU:N	2.46	0.46
2:G:231:SER:HB2	2:K:71:ASP:CG	2.36	0.46
2:L:100:ARG:HG2	2:L:101:ARG:N	2.31	0.46
3:O:27:GLU:HB3	3:O:56:TYR:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:27:GLU:HB3	3:S:56:TYR:CD1	2.51	0.46
2:A:272:ILE:HG22	2:A:468:GLN:HG2	1.97	0.46
2:C:171:GLN:HE21	2:C:195:GLN:NE2	2.13	0.46
2:C:432:ASP:O	2:C:433:TYR:HB3	2.16	0.46
2:C:465:LYS:HB3	2:H:237:GLU:HG3	1.98	0.46
2:D:337:PRO:O	2:D:342:GLY:N	2.33	0.46
2:F:377:ILE:HA	2:F:424:TYR:O	2.15	0.46
2:I:431:GLN:NE2	2:J:217:GLU:HB2	2.30	0.46
2:K:169:SER:OG	2:K:200:ALA:HB2	2.16	0.46
3:S:14:GLU:HB3	3:S:25:GLY:N	2.31	0.46
3:T:8:VAL:HG11	3:T:35:TYR:CE2	2.50	0.46
2:A:324:THR:HB	2:A:327:SER:HG	1.81	0.46
2:C:281:VAL:HG21	2:L:91:ILE:H	1.81	0.46
2:H:354:LEU:HA	2:H:357:ILE:HG22	1.98	0.46
2:I:126:ALA:N	2:I:255:ASP:O	2.46	0.46
2:K:265:GLN:C	2:K:266:LEU:HD12	2.36	0.46
2:K:270:TYR:HB3	2:K:290:LEU:HD12	1.98	0.46
2:L:348:GLU:OE1	2:L:348:GLU:N	2.44	0.46
3:P:9:ASN:HB3	3:P:56:TYR:HE2	1.81	0.46
2:A:101:ARG:HD2	2:B:146:PRO:HD3	1.98	0.46
2:B:131:TYR:CB	2:B:250:MET:HG2	2.46	0.46
2:D:107:ILE:HG22	2:D:303:ASN:HD21	1.81	0.46
2:E:106:LEU:HD21	2:E:300:LEU:HD23	1.98	0.46
2:F:163:PHE:HB2	2:F:179:THR:HG23	1.97	0.46
2:F:190:LEU:HB3	2:F:221:LEU:HG	1.97	0.46
2:G:244:ASP:HB2	3:S:13:PHE:CE2	2.49	0.46
2:H:69:GLY:N	2:J:234:GLU:OE2	2.46	0.46
2:H:241:GLY:HA3	3:V:43:GLY:N	2.31	0.46
2:I:137:ALA:HB3	2:I:140:ALA:HB2	1.97	0.46
2:L:184:GLU:O	2:L:185:THR:OG1	2.30	0.46
3:X:33:PRO:HG2	3:X:62:GLU:OE1	2.16	0.46
2:A:196:VAL:HG21	2:A:215:GLN:OE1	2.16	0.45
2:B:334:PHE:CZ	2:B:353:LEU:HD12	2.51	0.45
2:E:477:TYR:CD2	2:E:478:GLY:N	2.83	0.45
2:I:100:ARG:HG2	2:I:101:ARG:N	2.30	0.45
2:K:77:THR:HG21	3:U:5:ARG:NH2	2.31	0.45
2:L:389:VAL:HG12	2:L:390:ASP:N	2.31	0.45
3:T:28:VAL:HA	3:T:58:THR:HB	1.98	0.45
3:X:6:GLY:O	3:X:32:PHE:N	2.40	0.45
2:C:454:VAL:HG22	2:C:476:ARG:HB2	1.99	0.45
2:C:493:ALA:O	2:C:494:SER:OG	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:GLN:OE1	2:D:474:LYS:HE2	2.16	0.45
2:F:324:THR:HB	2:F:327:SER:OG	2.17	0.45
2:F:343:ALA:HB1	2:F:348:GLU:HB3	1.98	0.45
2:G:169:SER:OG	2:G:200:ALA:HB2	2.16	0.45
2:G:269:ALA:HA	2:G:470:VAL:HA	1.97	0.45
2:H:173:THR:OG1	2:H:176:ASP:OD2	2.32	0.45
2:K:396:ALA:O	2:L:395:TYR:HA	2.16	0.45
2:L:270:TYR:HB3	2:L:290:LEU:CD1	2.46	0.45
3:U:10:ILE:HD13	3:U:41:ILE:HG21	1.96	0.45
3:W:10:ILE:HD11	3:W:35:TYR:HE1	1.80	0.45
2:A:270:TYR:HB3	2:A:290:LEU:CD1	2.46	0.45
2:B:72:HIS:CD2	2:C:121:THR:HG21	2.51	0.45
2:B:270:TYR:HB3	2:B:290:LEU:CD1	2.47	0.45
2:B:432:ASP:O	2:B:433:TYR:HB3	2.17	0.45
2:C:171:GLN:HE21	2:C:195:GLN:HE21	1.63	0.45
2:E:305:GLU:OE1	2:E:477:TYR:OH	2.25	0.45
2:F:312:TYR:CE1	2:F:507:LEU:HD12	2.51	0.45
2:F:453:TYR:CD2	2:F:454:VAL:HG13	2.52	0.45
2:H:74:TYR:CE2	2:I:260:GLU:HG2	2.51	0.45
2:H:100:ARG:NH1	2:H:289:GLU:OE1	2.48	0.45
2:H:107:ILE:HG21	2:H:307:VAL:CG2	2.46	0.45
2:J:430:LYS:N	2:J:430:LYS:HD2	2.32	0.45
2:K:152:ALA:HB1	2:K:225:ALA:HB2	1.98	0.45
2:K:430:LYS:HE2	2:L:188:VAL:HG11	1.98	0.45
3:P:20:ASN:H	3:Q:16:LYS:HZ3	1.63	0.45
3:V:14:GLU:HB3	3:V:25:GLY:N	2.31	0.45
2:B:244:ASP:O	2:B:246:PRO:HD3	2.16	0.45
2:D:336:ASP:O	2:D:340:ILE:HG12	2.16	0.45
2:F:168:ALA:HB1	2:F:200:ALA:HA	1.97	0.45
2:J:354:LEU:HA	2:J:357:ILE:HG22	1.97	0.45
3:W:18:ASP:HB3	3:W:21:LYS:HD3	1.97	0.45
2:A:265:GLN:O	2:A:266:LEU:HD12	2.17	0.45
2:A:431:GLN:NE2	2:B:213:LYS:O	2.49	0.45
2:B:277:ASP:O	2:B:281:VAL:HG12	2.17	0.45
2:B:334:PHE:HZ	2:B:353:LEU:HD12	1.80	0.45
2:C:268:ALA:HB3	2:C:471:MET:CG	2.46	0.45
2:E:399:GLY:HA3	2:F:392:GLY:O	2.16	0.45
2:I:507:LEU:O	2:I:509:LYS:HG3	2.16	0.45
2:J:96:MET:HB2	2:K:124:VAL:HG22	1.98	0.45
2:J:181:PHE:HD1	2:J:187:THR:HB	1.82	0.45
2:J:216:MET:HA	2:J:221:LEU:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:196:VAL:HG21	2:L:215:GLN:OE1	2.16	0.45
3:S:61:GLU:N	3:S:64:GLN:OE1	2.49	0.45
2:A:109:PHE:HD1	2:A:112:CYS:SG	2.39	0.45
2:A:144:PHE:O	2:F:101:ARG:HG2	2.15	0.45
2:B:146:PRO:HB2	2:B:366:ARG:O	2.15	0.45
2:B:353:LEU:O	2:B:356:GLN:N	2.49	0.45
2:B:485:ALA:HB1	2:B:510:ASN:OD1	2.16	0.45
2:D:376:ILE:HG12	2:D:423:VAL:HG22	1.99	0.45
2:E:244:ASP:HB2	3:T:13:PHE:CE2	2.51	0.45
2:E:375:PHE:CZ	2:E:437:GLY:HA3	2.52	0.45
2:G:217:GLU:HB2	2:L:431:GLN:HE22	1.81	0.45
2:J:305:GLU:HG2	2:J:309:TRP:CD1	2.52	0.45
2:K:334:PHE:CZ	2:K:385:VAL:HG11	2.51	0.45
2:L:477:TYR:CD2	2:L:478:GLY:N	2.85	0.45
3:Q:18:ASP:HB3	3:Q:21:LYS:HD3	1.98	0.45
2:B:324:THR:O	2:B:326:GLY:N	2.49	0.45
2:C:494:SER:HA	3:Y:37:ASP:CG	2.36	0.45
2:E:131:TYR:HB3	2:E:250:MET:HG2	1.99	0.45
2:E:456:LEU:HD12	2:E:475:THR:HG21	1.98	0.45
2:F:378:ALA:HB1	2:F:382:VAL:CG2	2.46	0.45
2:F:432:ASP:O	2:F:433:TYR:HB3	2.17	0.45
2:G:146:PRO:HB2	2:G:366:ARG:O	2.17	0.45
2:G:272:ILE:HG22	2:G:468:GLN:HG2	1.99	0.45
2:G:456:LEU:HD12	2:G:475:THR:HG21	1.96	0.45
2:I:148:TYR:HD1	2:I:186:GLY:H	1.65	0.45
2:I:168:ALA:HB2	2:I:202:ALA:O	2.17	0.45
2:J:105:ASN:ND2	2:J:409:THR:O	2.24	0.45
3:W:41:ILE:HD13	3:W:46:TYR:CZ	2.52	0.45
3:X:72:ASN:OD1	3:X:73:GLU:N	2.50	0.45
2:C:72:HIS:CD2	2:D:121:THR:HG21	2.52	0.45
2:D:100:ARG:HG2	2:D:101:ARG:N	2.32	0.45
2:D:477:TYR:CD2	2:D:478:GLY:N	2.84	0.45
2:E:194:VAL:HG12	2:E:220:ALA:HA	1.99	0.45
2:F:477:TYR:CD2	2:F:478:GLY:N	2.85	0.45
2:G:124:VAL:HG22	2:L:96:MET:HB2	1.99	0.45
2:H:482:ASN:O	2:H:485:ALA:HB2	2.15	0.45
3:O:5:ARG:NH1	3:O:33:PRO:HB3	2.31	0.45
3:S:71:ALA:O	3:S:74:ASP:HB3	2.16	0.45
3:U:64:GLN:HB3	3:U:67:GLU:HB2	1.98	0.45
3:X:14:GLU:HB3	3:X:25:GLY:N	2.27	0.45
3:X:65:ARG:O	3:X:68:TRP:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:61:GLU:N	3:Y:64:GLN:OE1	2.50	0.45
2:B:121:THR:HA	2:B:259:ILE:O	2.17	0.45
2:C:131:TYR:CB	2:C:250:MET:HG2	2.47	0.45
2:E:158:GLY:HA2	2:E:163:PHE:CE2	2.52	0.45
2:G:344:ARG:NH1	2:L:344:ARG:HD2	2.31	0.45
2:H:383:VAL:O	2:H:387:ALA:N	2.47	0.45
2:L:164:PRO:HG2	2:L:178:TYR:CD1	2.51	0.45
3:R:12:THR:HG21	3:R:75:LEU:HD22	1.97	0.45
2:A:393:ILE:HA	2:F:398:GLN:O	2.17	0.45
2:C:476:ARG:HH21	2:D:230:THR:HG21	1.81	0.45
2:E:333:ASP:HB3	2:E:519:LYS:HB2	1.98	0.45
2:E:430:LYS:HG2	2:F:216:MET:HE1	1.99	0.45
2:E:493:ALA:O	2:E:494:SER:OG	2.25	0.45
2:F:131:TYR:CB	2:F:250:MET:HG2	2.47	0.45
2:F:270:TYR:HB3	2:F:290:LEU:CD1	2.47	0.45
2:G:380:ARG:HH21	2:G:408:THR:HG1	1.63	0.45
2:H:486:GLU:C	2:H:488:ALA:H	2.21	0.45
2:I:121:THR:HA	2:I:259:ILE:O	2.17	0.45
2:I:479:ILE:HG22	2:I:480:GLY:N	2.32	0.45
2:J:145:HIS:NE2	2:J:487:SER:O	2.48	0.45
2:J:255:ASP:OD2	2:J:492:PRO:HG3	2.17	0.45
3:S:12:THR:HG21	3:S:75:LEU:HD13	1.99	0.45
2:B:228:MET:SD	2:B:233:ALA:HB2	2.57	0.44
2:B:237:GLU:HB2	2:B:246:PRO:HA	1.98	0.44
2:B:503:ILE:HD11	2:C:175:GLY:HA2	1.99	0.44
2:D:344:ARG:O	2:D:348:GLU:HB2	2.17	0.44
2:G:245:ASN:OD1	2:G:245:ASN:N	2.50	0.44
2:G:255:ASP:OD2	2:G:492:PRO:HG2	2.17	0.44
2:J:278:LEU:CD2	2:J:284:MET:HB2	2.45	0.44
2:L:191:GLN:N	2:L:222:VAL:O	2.47	0.44
3:Y:66:THR:HA	3:Y:69:ILE:HB	1.99	0.44
2:A:105:ASN:HB2	2:A:412:VAL:HG23	1.98	0.44
2:A:344:ARG:O	2:A:348:GLU:HB2	2.17	0.44
2:A:377:ILE:HA	2:A:424:TYR:O	2.16	0.44
2:B:179:THR:HG22	2:B:189:TYR:CE1	2.52	0.44
2:C:190:LEU:HB3	2:C:221:LEU:HG	1.99	0.44
2:C:456:LEU:N	2:C:475:THR:HG22	2.23	0.44
2:D:456:LEU:HD12	2:D:475:THR:HG21	1.99	0.44
2:E:398:GLN:NE2	2:F:355:PHE:HB2	2.32	0.44
2:F:350:PHE:CB	2:F:389:VAL:HG21	2.40	0.44
2:F:479:ILE:HG22	2:F:480:GLY:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:232:ILE:HG12	3:V:48:THR:O	2.17	0.44
2:H:454:VAL:HG22	2:H:476:ARG:HB2	1.97	0.44
2:I:253:ARG:NH1	2:I:491:ALA:HB1	2.33	0.44
2:K:350:PHE:CB	2:K:389:VAL:HG21	2.40	0.44
2:L:120:PRO:O	2:L:121:THR:OG1	2.34	0.44
3:R:11:LYS:HZ2	3:R:13:PHE:HE1	1.64	0.44
3:Y:11:LYS:HZ3	3:Y:13:PHE:HE1	1.66	0.44
2:A:345:TRP:NE1	2:A:348:GLU:OE1	2.50	0.44
2:D:157:GLN:N	2:D:227:GLY:O	2.49	0.44
2:E:345:TRP:CD2	2:F:348:GLU:HG3	2.53	0.44
2:E:458:PRO:HA	2:E:473:PHE:CD1	2.52	0.44
2:J:126:ALA:O	2:J:254:ILE:HA	2.17	0.44
2:L:290:LEU:HD23	2:L:293:ILE:HD11	1.99	0.44
2:L:345:TRP:NE1	2:L:348:GLU:OE1	2.50	0.44
3:U:8:VAL:HG11	3:U:35:TYR:CE2	2.52	0.44
3:U:14:GLU:HB3	3:U:25:GLY:N	2.32	0.44
3:V:9:ASN:HB3	3:V:56:TYR:CD2	2.53	0.44
2:C:272:ILE:HG22	2:C:468:GLN:HG2	1.99	0.44
2:C:282:HIS:HE1	2:D:125:PHE:CE2	2.35	0.44
2:D:444:MET:O	2:D:449:TYR:OH	2.12	0.44
2:G:148:TYR:HB3	2:G:186:GLY:HA2	2.00	0.44
2:G:171:GLN:NE2	2:G:195:GLN:HE21	2.15	0.44
2:G:217:GLU:HB2	2:L:431:GLN:NE2	2.33	0.44
2:H:456:LEU:HD12	2:H:475:THR:CG2	2.47	0.44
2:J:345:TRP:CD2	2:K:348:GLU:HG3	2.52	0.44
3:Q:39:HIS:ND1	3:Q:39:HIS:O	2.51	0.44
2:B:80:ALA:HA	2:B:93:PRO:CG	2.47	0.44
2:B:282:HIS:HE1	2:C:125:PHE:CE2	2.36	0.44
2:C:78:ASN:HD21	3:T:5:ARG:HB3	1.82	0.44
2:E:151:ASP:HB2	2:E:189:TYR:CE1	2.45	0.44
2:G:125:PHE:HA	2:G:256:LYS:HA	1.99	0.44
2:G:204:ASP:OD1	2:G:205:ALA:N	2.50	0.44
2:G:323:LEU:HD21	2:G:329:ALA:HA	2.00	0.44
2:G:324:THR:O	2:G:326:GLY:N	2.51	0.44
2:H:345:TRP:CD2	2:I:348:GLU:HG3	2.53	0.44
2:I:264:ARG:NH2	2:J:226:GLU:O	2.51	0.44
2:K:348:GLU:OE1	2:K:348:GLU:N	2.51	0.44
3:S:74:ASP:OD1	3:S:77:LYS:HE3	2.18	0.44
2:A:145:HIS:CD2	2:F:101:ARG:HH12	2.35	0.44
2:B:193:SER:OG	2:B:220:ALA:O	2.26	0.44
2:B:336:ASP:O	2:B:340:ILE:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:494:SER:O	2:C:495:ARG:HB2	2.16	0.44
2:D:474:LYS:HD3	2:L:273:GLU:OE2	2.18	0.44
2:F:232:ILE:HD11	3:Q:49:PHE:CB	2.48	0.44
2:G:295:ALA:HB2	2:G:473:PHE:HE2	1.83	0.44
2:J:100:ARG:NH1	2:J:289:GLU:OE1	2.51	0.44
2:K:376:ILE:HG22	2:K:436:VAL:HG22	2.00	0.44
2:L:477:TYR:CG	2:L:478:GLY:N	2.86	0.44
3:R:10:ILE:HD11	3:R:35:TYR:HE1	1.83	0.44
3:S:68:TRP:CZ2	3:S:72:ASN:HB3	2.53	0.44
3:T:74:ASP:OD1	3:T:77:LYS:HE3	2.17	0.44
3:W:14:GLU:OE1	3:W:22:LYS:HD2	2.17	0.44
2:B:291:SER:HA	2:B:471:MET:HE1	2.00	0.44
2:B:332:PHE:HE2	2:B:334:PHE:CE1	2.36	0.44
2:E:77:THR:HG21	3:P:5:ARG:NH2	2.33	0.44
2:E:265:GLN:C	2:E:266:LEU:HD12	2.38	0.44
2:I:345:TRP:NE1	2:I:348:GLU:OE1	2.50	0.44
2:J:306:VAL:O	2:J:309:TRP:N	2.51	0.44
2:J:456:LEU:HD12	2:J:475:THR:CG2	2.48	0.44
2:J:479:ILE:HG22	2:J:480:GLY:N	2.33	0.44
2:K:367:GLN:HB3	2:K:511:ALA:HB1	2.00	0.44
2:L:305:GLU:HG2	2:L:309:TRP:CD1	2.52	0.44
2:A:100:ARG:NH2	2:A:284:MET:HE2	2.32	0.44
2:A:164:PRO:HG2	2:A:178:TYR:CD1	2.52	0.44
2:B:151:ASP:HB3	2:B:187:THR:CG2	2.48	0.44
2:B:179:THR:HG22	2:B:189:TYR:CD1	2.52	0.44
2:D:72:HIS:HD2	2:E:260:GLU:OE2	2.01	0.44
2:E:171:GLN:HE21	2:E:195:GLN:HE21	1.65	0.44
2:E:171:GLN:NE2	2:E:195:GLN:HE21	2.16	0.44
2:E:196:VAL:HG21	2:E:215:GLN:OE1	2.18	0.44
2:F:266:LEU:HB3	2:F:267:LYS:H	1.65	0.44
2:F:305:GLU:HG2	2:F:309:TRP:CD1	2.52	0.44
2:G:73:GLY:O	2:G:74:TYR:HB2	2.17	0.44
2:G:133:LYS:HE2	3:T:42:SER:HB2	2.00	0.44
2:G:232:ILE:HG12	3:S:48:THR:O	2.18	0.44
2:H:100:ARG:HG2	2:H:101:ARG:N	2.32	0.44
2:J:145:HIS:ND1	2:J:148:TYR:CD2	2.86	0.44
2:J:238:GLY:HA2	2:J:242:SER:O	2.17	0.44
2:J:272:ILE:HG22	2:J:468:GLN:HG2	2.00	0.44
2:K:180:HIS:HD2	2:K:182:PHE:CD1	2.35	0.44
2:K:430:LYS:HD2	2:K:430:LYS:N	2.33	0.44
2:L:315:GLN:HG3	2:L:510:ASN:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:486:GLU:C	2:L:488:ALA:H	2.21	0.44
2:A:309:TRP:O	2:A:313:SER:N	2.47	0.44
2:A:493:ALA:O	2:A:494:SER:OG	2.34	0.44
2:E:71:ASP:OD2	3:O:50:PRO:HG3	2.18	0.44
2:E:163:PHE:HB2	2:E:179:THR:CG2	2.48	0.44
2:E:313:SER:O	2:E:510:ASN:HB2	2.17	0.44
2:F:164:PRO:HG2	2:F:178:TYR:CD1	2.53	0.44
2:I:73:GLY:O	2:I:74:TYR:HB2	2.18	0.44
2:I:456:LEU:HD12	2:I:475:THR:CG2	2.48	0.44
2:L:324:THR:HB	2:L:327:SER:OG	2.18	0.44
3:R:9:ASN:HB3	3:R:56:TYR:CE2	2.52	0.44
3:V:68:TRP:HA	3:V:71:ALA:HB3	1.99	0.44
3:W:7:TYR:CD1	3:W:54:ALA:HB2	2.53	0.44
3:Y:68:TRP:CE2	3:Y:72:ASN:HB3	2.53	0.44
2:A:453:TYR:CD2	2:A:454:VAL:HG13	2.53	0.43
2:B:432:ASP:OD1	2:B:433:TYR:N	2.51	0.43
2:C:153:MET:HG2	2:C:189:TYR:HD2	1.80	0.43
2:E:142:GLU:H	2:E:490:GLN:CG	2.31	0.43
2:F:319:SER:HA	2:F:323:LEU:HG	1.99	0.43
2:G:376:ILE:HG22	2:G:436:VAL:HA	1.99	0.43
2:G:398:GLN:O	2:H:393:ILE:HA	2.18	0.43
2:I:485:ALA:HB1	2:I:510:ASN:OD1	2.18	0.43
2:J:173:THR:OG1	2:J:176:ASP:OD2	2.35	0.43
2:K:197:THR:HG22	2:K:199:ASP:H	1.83	0.43
3:S:38:VAL:HG11	3:S:69:ILE:HG12	2.00	0.43
2:A:377:ILE:HG22	2:A:424:TYR:HB2	2.00	0.43
2:B:479:ILE:HG22	2:B:480:GLY:N	2.33	0.43
2:D:382:VAL:O	2:D:386:LEU:HD13	2.17	0.43
2:E:238:GLY:HA2	2:E:242:SER:O	2.18	0.43
2:F:317:GLY:HA2	2:F:514:ARG:NH2	2.34	0.43
2:F:346:ALA:O	2:F:349:SER:N	2.51	0.43
2:G:72:HIS:ND1	2:G:83:GLN:O	2.51	0.43
2:H:431:GLN:NE2	2:I:213:LYS:O	2.51	0.43
2:I:68:ILE:HD11	2:K:235:LEU:HD23	2.00	0.43
2:I:409:THR:HG21	2:J:370:ARG:O	2.17	0.43
2:K:285:ASP:C	2:K:287:ASP:H	2.22	0.43
2:K:377:ILE:HA	2:K:424:TYR:O	2.17	0.43
2:L:171:GLN:NE2	2:L:195:GLN:HE21	2.16	0.43
2:L:350:PHE:CB	2:L:389:VAL:HG21	2.48	0.43
3:Y:10:ILE:HD11	3:Y:35:TYR:HE1	1.83	0.43
2:A:344:ARG:NH1	2:B:344:ARG:HH12	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:PHE:CB	2:B:389:VAL:HG21	2.36	0.43
2:E:159:ALA:HB2	2:E:248:ASN:ND2	2.33	0.43
2:I:131:TYR:CB	2:I:250:MET:HG2	2.48	0.43
2:I:145:HIS:CD2	2:I:146:PRO:HD2	2.45	0.43
2:J:305:GLU:HA	2:K:225:ALA:HB3	2.00	0.43
2:K:126:ALA:N	2:K:255:ASP:O	2.51	0.43
3:V:10:ILE:HD11	3:V:35:TYR:CE1	2.53	0.43
2:B:295:ALA:HB2	2:B:473:PHE:CE2	2.53	0.43
2:D:125:PHE:HA	2:D:256:LYS:HA	1.99	0.43
2:E:334:PHE:HZ	2:E:353:LEU:HD12	1.83	0.43
2:E:432:ASP:O	2:E:433:TYR:HB3	2.18	0.43
2:H:110:ASP:O	2:H:439:LYS:HG2	2.18	0.43
2:J:264:ARG:NH1	2:K:155:SER:HG	2.15	0.43
2:L:146:PRO:HB3	2:L:369:GLY:HA3	2.00	0.43
3:V:10:ILE:HD11	3:V:35:TYR:HE1	1.84	0.43
2:A:126:ALA:N	2:A:255:ASP:O	2.51	0.43
2:A:350:PHE:HB2	2:A:389:VAL:HG21	2.00	0.43
2:D:121:THR:HG22	2:D:260:GLU:OE1	2.18	0.43
2:D:324:THR:HB	2:D:327:SER:HG	1.83	0.43
2:F:255:ASP:OD2	2:F:495:ARG:HG2	2.19	0.43
2:F:494:SER:HA	3:P:37:ASP:CG	2.39	0.43
2:G:131:TYR:HB3	2:G:250:MET:HE2	2.00	0.43
2:L:360:GLU:O	2:L:363:GLU:N	2.51	0.43
2:L:376:ILE:HG12	2:L:423:VAL:HG22	2.01	0.43
3:Q:10:ILE:HD13	3:Q:41:ILE:HG21	2.00	0.43
2:D:184:GLU:O	2:D:185:THR:OG1	2.34	0.43
2:F:133:LYS:HE2	3:P:42:SER:HB2	2.01	0.43
2:F:442:ASN:HB3	2:F:444:MET:H	1.83	0.43
2:I:323:LEU:HD21	2:I:329:ALA:CA	2.48	0.43
2:K:128:ARG:NE	2:K:484:PHE:HE1	2.15	0.43
2:L:479:ILE:HG22	2:L:480:GLY:N	2.34	0.43
3:X:70:ALA:O	3:X:74:ASP:HB2	2.19	0.43
2:B:164:PRO:HG2	2:B:178:TYR:HD1	1.82	0.43
2:B:265:GLN:C	2:B:266:LEU:HD12	2.39	0.43
2:B:430:LYS:HE2	2:C:188:VAL:CG1	2.49	0.43
2:C:351:LYS:HE3	2:C:394:SER:O	2.19	0.43
2:C:479:ILE:HG22	2:C:480:GLY:N	2.34	0.43
2:D:74:TYR:CE2	2:E:260:GLU:HG2	2.53	0.43
2:D:305:GLU:HG2	2:D:309:TRP:CD1	2.54	0.43
2:E:378:ALA:HB1	2:E:382:VAL:HG21	2.00	0.43
2:G:145:HIS:HD2	2:G:146:PRO:CD	2.29	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:TYR:CB	2:H:250:MET:HG2	2.49	0.43
2:H:317:GLY:HA2	2:H:514:ARG:NH2	2.33	0.43
2:H:430:LYS:HE2	2:I:188:VAL:HG11	2.01	0.43
2:I:313:SER:O	2:I:510:ASN:HB2	2.18	0.43
3:O:33:PRO:HG2	3:O:62:GLU:OE1	2.18	0.43
2:A:351:LYS:HE3	2:A:394:SER:O	2.18	0.43
2:B:93:PRO:HB2	2:C:123:GLN:HB3	2.01	0.43
2:B:281:VAL:HG13	2:B:282:HIS:N	2.34	0.43
2:C:456:LEU:HD12	2:C:475:THR:HG21	2.01	0.43
2:D:79:ILE:HB	2:E:258:VAL:HG11	2.00	0.43
2:D:131:TYR:CB	2:D:250:MET:HG2	2.48	0.43
2:D:290:LEU:HD23	2:D:293:ILE:HD11	2.01	0.43
2:D:375:PHE:CZ	2:D:437:GLY:HA3	2.54	0.43
2:D:380:ARG:NH1	2:D:427:GLN:O	2.42	0.43
2:E:146:PRO:HB2	2:E:366:ARG:O	2.18	0.43
2:E:398:GLN:O	2:F:393:ILE:HA	2.18	0.43
2:G:333:ASP:OD1	2:G:333:ASP:N	2.52	0.43
2:G:354:LEU:HA	2:G:357:ILE:HG22	2.01	0.43
2:K:383:VAL:HG12	2:K:406:THR:HG22	2.01	0.43
2:L:454:VAL:HG22	2:L:476:ARG:HB2	2.01	0.43
3:P:14:GLU:HB3	3:P:25:GLY:H	1.82	0.43
3:U:40:LYS:HG3	3:U:40:LYS:O	2.19	0.43
2:B:99:VAL:HG12	2:C:484:PHE:CE2	2.54	0.43
2:C:354:LEU:HA	2:C:357:ILE:HG22	2.01	0.43
2:D:172:THR:HA	2:D:178:TYR:OH	2.19	0.43
2:D:305:GLU:OE1	2:D:477:TYR:OH	2.30	0.43
2:D:363:GLU:OE2	2:D:366:ARG:NH2	2.51	0.43
2:E:244:ASP:O	2:E:246:PRO:HD3	2.18	0.43
2:F:107:ILE:HG22	2:F:303:ASN:OD1	2.18	0.43
2:F:128:ARG:NE	2:F:484:PHE:HE1	2.11	0.43
2:K:134:ASP:HB3	2:K:137:ALA:HB2	2.01	0.43
2:K:268:ALA:HB2	2:K:294:LEU:HD11	2.01	0.43
3:W:12:THR:OG1	3:W:26:LYS:O	2.30	0.43
2:B:151:ASP:OD1	2:B:151:ASP:N	2.51	0.43
2:B:463:ASP:OD1	2:B:464:PRO:HD2	2.18	0.43
2:C:398:GLN:O	2:D:393:ILE:HA	2.18	0.43
2:C:444:MET:O	2:C:449:TYR:OH	2.23	0.43
2:F:345:TRP:NE1	2:F:348:GLU:OE1	2.51	0.43
2:J:172:THR:O	2:J:195:GLN:HA	2.19	0.43
2:A:305:GLU:OE1	2:A:477:TYR:OH	2.24	0.42
2:A:331:VAL:HG12	2:A:517:TYR:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:GLU:CD	2:F:69:GLY:H	2.13	0.42
2:B:296:THR:O	2:B:300:LEU:HG	2.19	0.42
2:D:493:ALA:O	2:D:494:SER:OG	2.25	0.42
2:E:113:GLY:H	2:E:446:ALA:HB1	1.83	0.42
2:F:179:THR:HG22	2:F:189:TYR:CE2	2.54	0.42
2:H:430:LYS:HD2	2:H:430:LYS:N	2.33	0.42
2:I:157:GLN:N	2:I:227:GLY:O	2.52	0.42
2:I:196:VAL:HG21	2:I:215:GLN:OE1	2.19	0.42
2:I:430:LYS:HE2	2:J:188:VAL:CG1	2.49	0.42
2:I:521:ILE:HA	2:J:341:ARG:NH2	2.34	0.42
2:K:147:MET:HE2	2:K:366:ARG:HG2	2.01	0.42
2:L:154:PHE:CZ	2:L:248:ASN:HB3	2.54	0.42
3:R:8:VAL:HG23	3:R:32:PHE:HD1	1.83	0.42
3:T:9:ASN:HB3	3:T:56:TYR:CE2	2.54	0.42
3:W:10:ILE:HD11	3:W:35:TYR:CE1	2.54	0.42
2:A:169:SER:OG	2:A:200:ALA:HB2	2.19	0.42
2:E:482:ASN:ND2	2:E:512:TYR:OH	2.52	0.42
2:G:74:TYR:OH	2:I:229:ALA:HA	2.19	0.42
2:H:479:ILE:HG22	2:H:480:GLY:N	2.33	0.42
2:I:290:LEU:HA	2:I:290:LEU:HD23	1.80	0.42
2:J:105:ASN:HD21	2:J:409:THR:C	2.16	0.42
2:L:107:ILE:HG21	2:L:307:VAL:CG2	2.49	0.42
3:P:40:LYS:O	3:P:40:LYS:HG3	2.19	0.42
3:T:27:GLU:HB3	3:T:56:TYR:CD1	2.54	0.42
3:Y:11:LYS:HD2	3:Y:56:TYR:OH	2.20	0.42
2:B:80:ALA:HA	2:B:93:PRO:HG2	2.00	0.42
2:B:129:ALA:O	2:B:143:ALA:N	2.47	0.42
2:C:71:ASP:CG	2:E:231:SER:HB2	2.39	0.42
2:D:310:ILE:HG12	2:D:513:PHE:CE2	2.54	0.42
2:D:324:THR:HB	2:D:327:SER:OG	2.19	0.42
2:D:432:ASP:O	2:D:433:TYR:HB3	2.19	0.42
2:I:324:THR:HB	2:I:327:SER:OG	2.19	0.42
2:J:154:PHE:CZ	2:J:248:ASN:HB3	2.55	0.42
2:K:324:THR:O	2:K:326:GLY:N	2.52	0.42
3:R:41:ILE:HD13	3:R:46:TYR:CZ	2.55	0.42
3:U:9:ASN:ND2	3:U:51:SER:OG	2.52	0.42
3:W:8:VAL:HG23	3:W:32:PHE:HD1	1.85	0.42
2:A:73:GLY:O	2:A:74:TYR:HB2	2.19	0.42
2:B:107:ILE:HG21	2:B:307:VAL:CG2	2.48	0.42
2:D:107:ILE:H	2:D:303:ASN:ND2	2.11	0.42
2:D:131:TYR:HB2	2:D:250:MET:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:GLN:HG3	2:D:510:ASN:O	2.18	0.42
2:E:305:GLU:HG2	2:E:309:TRP:CD1	2.54	0.42
2:E:453:TYR:CD2	2:E:454:VAL:HG13	2.55	0.42
2:H:386:LEU:HB3	2:H:404:PHE:HE2	1.83	0.42
2:K:270:TYR:HB3	2:K:290:LEU:CD1	2.49	0.42
2:L:268:ALA:HB3	2:L:471:MET:HG3	2.02	0.42
3:S:39:HIS:ND1	3:S:39:HIS:O	2.53	0.42
3:S:40:LYS:O	3:S:40:LYS:HG3	2.19	0.42
2:A:295:ALA:HB2	2:A:473:PHE:CE2	2.54	0.42
2:A:346:ALA:O	2:A:349:SER:N	2.53	0.42
2:B:180:HIS:HD2	2:B:182:PHE:CE1	2.38	0.42
2:C:107:ILE:HG22	2:C:303:ASN:OD1	2.19	0.42
2:E:119:SER:HA	2:E:453:TYR:HE1	1.85	0.42
2:F:120:PRO:O	2:F:121:THR:OG1	2.37	0.42
2:F:315:GLN:HG3	2:F:510:ASN:O	2.20	0.42
2:H:136:VAL:HG12	2:H:253:ARG:NE	2.35	0.42
2:H:153:MET:HE1	2:H:226:GLU:HG2	2.01	0.42
2:I:113:GLY:H	2:I:446:ALA:HB1	1.84	0.42
2:I:159:ALA:HB2	2:I:248:ASN:ND2	2.34	0.42
2:I:198:ILE:HD12	2:I:198:ILE:HG23	1.81	0.42
2:J:171:GLN:HG2	2:J:195:GLN:HE21	1.84	0.42
2:J:324:THR:O	2:J:326:GLY:N	2.52	0.42
2:A:128:ARG:NE	2:A:484:PHE:HE1	2.13	0.42
2:A:229:ALA:HA	2:E:74:TYR:OH	2.19	0.42
2:A:456:LEU:HD12	2:A:475:THR:CG2	2.50	0.42
2:C:101:ARG:NH1	2:D:145:HIS:CD2	2.87	0.42
2:C:120:PRO:O	2:C:121:THR:OG1	2.35	0.42
2:D:236:GLN:HG3	2:D:247:TRP:CD1	2.55	0.42
2:F:197:THR:HG22	2:F:199:ASP:H	1.85	0.42
2:G:126:ALA:HB1	2:G:484:PHE:CE1	2.55	0.42
2:J:293:ILE:HG22	2:K:144:PHE:HE2	1.85	0.42
2:J:456:LEU:N	2:J:475:THR:HG22	2.27	0.42
2:K:315:GLN:HG3	2:K:510:ASN:O	2.20	0.42
2:A:123:GLN:HE21	2:F:95:VAL:HG12	1.85	0.42
2:C:91:ILE:H	2:L:281:VAL:HG21	1.85	0.42
2:C:278:LEU:HD21	2:C:284:MET:HB2	2.02	0.42
2:C:345:TRP:NE1	2:C:348:GLU:OE1	2.52	0.42
2:D:166:LEU:HD22	2:D:212:ILE:HD11	2.02	0.42
2:E:295:ALA:HB2	2:E:473:PHE:HE2	1.84	0.42
2:G:485:ALA:HB1	2:G:510:ASN:OD1	2.19	0.42
2:H:477:TYR:CD2	2:H:478:GLY:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:348:GLU:OE1	2:I:348:GLU:N	2.52	0.42
2:I:390:ASP:OD2	2:I:394:SER:OG	2.38	0.42
2:J:295:ALA:HB2	2:J:473:PHE:HE2	1.85	0.42
2:K:479:ILE:HG22	2:K:480:GLY:N	2.34	0.42
2:L:270:TYR:HB3	2:L:290:LEU:HD12	2.01	0.42
2:L:295:ALA:HB2	2:L:473:PHE:CE2	2.54	0.42
3:P:61:GLU:N	3:P:64:GLN:OE1	2.52	0.42
3:U:18:ASP:HB3	3:U:21:LYS:HD3	2.01	0.42
3:U:39:HIS:ND1	3:U:39:HIS:O	2.52	0.42
2:D:278:LEU:HD23	2:D:278:LEU:HA	1.79	0.42
2:F:235:LEU:HD13	2:F:242:SER:HB3	2.01	0.42
2:F:341:ARG:HD3	2:F:341:ARG:HA	1.79	0.42
2:H:151:ASP:CG	2:H:154:PHE:HB2	2.40	0.42
2:I:106:LEU:HD21	2:I:300:LEU:HD23	2.01	0.42
2:I:270:TYR:HB3	2:I:290:LEU:CD1	2.49	0.42
2:J:237:GLU:OE1	2:J:246:PRO:HA	2.19	0.42
2:L:84:THR:HG22	2:L:86:GLY:H	1.84	0.42
2:L:135:PRO:HB3	2:L:252:PHE:O	2.19	0.42
3:T:8:VAL:HG23	3:T:32:PHE:HD1	1.85	0.42
3:W:65:ARG:O	3:W:69:ILE:N	2.41	0.42
2:A:121:THR:HA	2:A:259:ILE:O	2.19	0.42
2:A:155:SER:OG	2:F:301:GLU:OE1	2.24	0.42
2:A:228:MET:SD	2:A:233:ALA:HB2	2.59	0.42
2:A:234:GLU:OE1	2:E:70:GLY:N	2.43	0.42
2:B:255:ASP:HB2	2:B:492:PRO:HG3	2.00	0.42
2:B:364:ILE:O	2:B:368:THR:OG1	2.32	0.42
2:B:456:LEU:HD12	2:B:475:THR:CG2	2.50	0.42
2:C:85:SER:HB3	3:T:32:PHE:HE1	1.85	0.42
2:E:232:ILE:HD11	3:T:49:PHE:CB	2.49	0.42
2:F:164:PRO:HG2	2:F:178:TYR:HD1	1.85	0.42
2:F:386:LEU:HB3	2:F:404:PHE:HE2	1.84	0.42
2:I:253:ARG:HH21	2:I:495:ARG:CG	2.33	0.42
2:I:382:VAL:HG12	2:I:521:ILE:HD11	2.01	0.42
2:J:198:ILE:HD12	2:J:198:ILE:HG23	1.86	0.42
2:J:344:ARG:O	2:J:348:GLU:HB2	2.20	0.42
2:K:163:PHE:HB2	2:K:179:THR:CG2	2.49	0.42
2:L:77:THR:HG21	3:T:5:ARG:NH2	2.35	0.42
3:S:26:LYS:HD2	3:S:75:LEU:HD23	2.01	0.42
3:T:21:LYS:HA	3:T:80:GLY:HA2	2.02	0.42
2:A:101:ARG:HG2	2:B:144:PHE:O	2.20	0.42
2:A:101:ARG:HH12	2:B:145:HIS:CD2	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:SER:HB3	3:X:32:PHE:CE1	2.54	0.42
2:B:198:ILE:O	2:B:198:ILE:HG22	2.20	0.42
2:B:255:ASP:OD2	2:B:495:ARG:HG2	2.19	0.42
2:C:131:TYR:HB3	2:C:250:MET:HG2	2.01	0.42
2:C:167:ALA:H	2:C:170:THR:HG21	1.85	0.42
2:D:409:THR:HG21	2:E:370:ARG:O	2.19	0.42
2:F:131:TYR:HB3	2:F:250:MET:HG2	2.00	0.42
2:I:173:THR:OG1	2:I:176:ASP:OD2	2.38	0.42
2:I:265:GLN:C	2:I:266:LEU:HD12	2.40	0.42
3:Y:64:GLN:HB3	3:Y:67:GLU:HB2	2.01	0.42
3:Y:68:TRP:O	3:Y:71:ALA:N	2.53	0.42
2:B:345:TRP:NE1	2:B:348:GLU:OE1	2.53	0.41
2:B:409:THR:HG21	2:C:370:ARG:O	2.20	0.41
2:B:442:ASN:HB3	2:B:444:MET:H	1.84	0.41
2:D:268:ALA:HB3	2:D:471:MET:CG	2.50	0.41
2:D:333:ASP:N	2:D:333:ASP:OD1	2.52	0.41
2:D:345:TRP:CD2	2:E:348:GLU:HG3	2.54	0.41
2:E:107:ILE:H	2:E:303:ASN:ND2	2.08	0.41
2:E:117:MET:HB2	2:E:451:ALA:HB1	2.02	0.41
2:F:205:ALA:O	2:F:208:LEU:N	2.53	0.41
2:H:157:GLN:N	2:H:227:GLY:O	2.53	0.41
2:J:153:MET:SD	2:J:157:GLN:HB3	2.60	0.41
2:J:324:THR:O	2:J:327:SER:N	2.47	0.41
2:K:80:ALA:HA	2:K:93:PRO:CG	2.50	0.41
2:L:106:LEU:HD22	2:L:303:ASN:HD22	1.85	0.41
2:L:153:MET:SD	2:L:157:GLN:HB3	2.59	0.41
3:T:68:TRP:CZ2	3:T:72:ASN:HB3	2.55	0.41
3:V:27:GLU:HB3	3:V:56:TYR:CD1	2.55	0.41
2:A:244:ASP:HB2	3:O:13:PHE:CE2	2.54	0.41
2:A:275:THR:HG22	2:A:286:ALA:HB3	2.01	0.41
2:B:386:LEU:HB3	2:B:404:PHE:CE2	2.55	0.41
2:C:67:GLU:OE1	2:L:290:LEU:HD11	2.20	0.41
2:C:166:LEU:HB2	2:C:178:TYR:HB3	2.02	0.41
2:C:306:VAL:HG11	2:C:450:TYR:HB2	2.02	0.41
2:D:482:ASN:O	2:D:485:ALA:HB2	2.20	0.41
2:G:172:THR:O	2:G:195:GLN:HA	2.20	0.41
2:H:442:ASN:HB3	2:H:444:MET:H	1.84	0.41
2:I:454:VAL:HG22	2:I:476:ARG:HB2	2.02	0.41
2:K:171:GLN:NE2	2:K:195:GLN:HE21	2.18	0.41
2:K:432:ASP:O	2:K:433:TYR:HB3	2.20	0.41
3:S:18:ASP:HB3	3:S:21:LYS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:64:GLN:HB3	3:T:67:GLU:HB2	2.01	0.41
2:A:458:PRO:HA	2:A:473:PHE:CD1	2.55	0.41
2:B:331:VAL:HG11	2:B:519:LYS:HE3	2.02	0.41
2:B:502:SER:N	2:B:506:SER:OG	2.53	0.41
2:C:110:ASP:O	2:C:439:LYS:HG2	2.19	0.41
2:C:270:TYR:HB3	2:C:290:LEU:CD1	2.50	0.41
2:E:344:ARG:NH1	2:F:344:ARG:HH12	2.17	0.41
2:H:265:GLN:C	2:H:266:LEU:HD12	2.41	0.41
2:H:417:LEU:HD12	2:H:421:TYR:HD2	1.85	0.41
2:H:463:ASP:OD1	2:H:464:PRO:HD2	2.20	0.41
2:I:148:TYR:HB3	2:I:186:GLY:HA2	2.03	0.41
2:I:315:GLN:HG3	2:I:510:ASN:O	2.20	0.41
2:I:380:ARG:NH1	2:I:427:GLN:O	2.48	0.41
2:J:377:ILE:HA	2:J:424:TYR:O	2.19	0.41
2:K:305:GLU:HG3	2:L:225:ALA:O	2.19	0.41
3:P:40:LYS:H	3:P:72:ASN:ND2	2.18	0.41
3:R:65:ARG:O	3:R:68:TRP:N	2.53	0.41
2:C:146:PRO:HB2	2:C:366:ARG:O	2.21	0.41
2:C:232:ILE:HG22	2:C:236:GLN:HE22	1.85	0.41
2:D:232:ILE:HD11	3:X:49:PHE:CB	2.50	0.41
2:D:332:PHE:O	2:D:518:VAL:HA	2.21	0.41
2:E:268:ALA:HB3	2:E:471:MET:CG	2.51	0.41
2:F:133:LYS:HG3	2:F:249:GLU:OE1	2.20	0.41
2:F:272:ILE:HG22	2:F:468:GLN:HG2	2.02	0.41
2:G:68:ILE:HD11	2:I:235:LEU:HD23	2.03	0.41
2:G:198:ILE:O	2:G:211:GLU:HG2	2.20	0.41
2:G:344:ARG:HH12	2:L:344:ARG:HH11	1.67	0.41
2:G:431:GLN:OE1	2:H:217:GLU:HB2	2.21	0.41
2:H:154:PHE:CZ	2:H:248:ASN:HB3	2.56	0.41
2:H:476:ARG:HH21	2:I:230:THR:HG21	1.85	0.41
2:I:179:THR:HG22	2:I:189:TYR:CD1	2.54	0.41
2:J:79:ILE:CG2	2:K:121:THR:HB	2.51	0.41
3:R:40:LYS:HG3	3:R:40:LYS:O	2.20	0.41
3:R:40:LYS:H	3:R:72:ASN:HD22	1.68	0.41
2:B:348:GLU:OE1	2:B:348:GLU:N	2.50	0.41
2:C:269:ALA:O	2:L:66:ALA:HA	2.20	0.41
2:C:365:ALA:HB2	2:C:372:GLU:HA	2.03	0.41
2:D:382:VAL:HG21	2:D:433:TYR:O	2.20	0.41
2:D:456:LEU:N	2:D:475:THR:HG22	2.34	0.41
2:E:110:ASP:O	2:E:439:LYS:HG2	2.21	0.41
2:E:376:ILE:HG12	2:E:423:VAL:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:282:HIS:HE1	2:I:125:PHE:CE2	2.38	0.41
2:H:495:ARG:O	2:H:496:ILE:HD13	2.21	0.41
2:I:125:PHE:HA	2:I:256:LYS:HA	2.02	0.41
2:I:312:TYR:CE1	2:I:507:LEU:HD12	2.55	0.41
2:I:360:GLU:O	2:I:363:GLU:N	2.53	0.41
2:J:260:GLU:HG3	2:J:261:ALA:N	2.35	0.41
2:J:324:THR:HB	2:J:327:SER:OG	2.21	0.41
2:K:95:VAL:HG12	2:L:123:GLN:HE21	1.85	0.41
2:K:386:LEU:HB3	2:K:404:PHE:CE2	2.50	0.41
2:K:400:LEU:HD11	2:L:417:LEU:HB3	2.02	0.41
2:L:265:GLN:C	2:L:266:LEU:HD12	2.40	0.41
2:L:507:LEU:O	2:L:509:LYS:HG3	2.20	0.41
3:Q:11:LYS:HG3	3:Q:27:GLU:HG2	2.02	0.41
3:Y:10:ILE:HD11	3:Y:35:TYR:CE1	2.55	0.41
2:A:74:TYR:OH	2:C:229:ALA:HA	2.19	0.41
2:A:386:LEU:HB3	2:A:404:PHE:CE2	2.53	0.41
2:A:432:ASP:O	2:A:433:TYR:HB3	2.21	0.41
2:B:453:TYR:HB3	2:B:476:ARG:O	2.20	0.41
2:C:113:GLY:H	2:C:446:ALA:HB1	1.86	0.41
2:D:463:ASP:OD1	2:D:464:PRO:HD2	2.20	0.41
2:F:290:LEU:HD23	2:F:290:LEU:HA	1.91	0.41
2:G:494:SER:HA	3:T:37:ASP:OD2	2.21	0.41
2:I:238:GLY:HA2	2:I:242:SER:O	2.21	0.41
2:J:163:PHE:HB2	2:J:179:THR:HG23	2.03	0.41
2:J:360:GLU:O	2:J:363:GLU:N	2.53	0.41
2:K:145:HIS:CD2	2:K:146:PRO:HD2	2.43	0.41
2:K:228:MET:SD	2:K:233:ALA:HB2	2.60	0.41
2:A:231:SER:HB2	2:E:71:ASP:CG	2.41	0.41
2:A:255:ASP:OD2	2:A:495:ARG:HG2	2.21	0.41
2:A:355:PHE:HB2	2:F:398:GLN:HE21	1.84	0.41
2:B:337:PRO:CB	4:Z:306:TRP:HB3	2.50	0.41
2:C:70:GLY:HA3	2:C:86:GLY:HA3	2.02	0.41
2:C:128:ARG:HE	2:C:484:PHE:HE1	1.69	0.41
2:D:106:LEU:HD21	2:D:300:LEU:HD23	2.02	0.41
2:D:268:ALA:HB3	2:D:471:MET:HG2	2.02	0.41
2:E:126:ALA:HB1	2:E:484:PHE:CE1	2.55	0.41
2:F:290:LEU:HA	2:F:293:ILE:HG12	2.02	0.41
2:F:462:SER:HA	2:F:469:PRO:HA	2.02	0.41
2:I:179:THR:HG22	2:I:189:TYR:CE1	2.56	0.41
2:J:375:PHE:CZ	2:J:437:GLY:HA3	2.55	0.41
2:K:146:PRO:HB2	2:K:366:ARG:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:301:GLU:O	2:K:305:GLU:N	2.54	0.41
2:L:420:LYS:HD2	2:L:421:TYR:CE2	2.56	0.41
3:R:72:ASN:OD1	3:R:73:GLU:N	2.54	0.41
3:W:14:GLU:CD	3:X:19:GLY:HA2	2.40	0.41
2:A:345:TRP:HB3	2:B:343:ALA:HA	2.01	0.41
2:A:456:LEU:N	2:A:475:THR:HG22	2.30	0.41
2:B:304:ARG:HA	2:B:304:ARG:HD2	1.91	0.41
2:B:456:LEU:N	2:B:475:THR:HG22	2.22	0.41
2:D:285:ASP:C	2:D:287:ASP:H	2.24	0.41
2:D:507:LEU:O	2:D:509:LYS:HG3	2.21	0.41
2:E:136:VAL:HG12	2:E:253:ARG:NE	2.36	0.41
2:F:232:ILE:HD11	3:Q:49:PHE:HB3	2.03	0.41
2:H:268:ALA:HB1	2:H:290:LEU:HD13	2.01	0.41
2:K:198:ILE:HG23	2:K:198:ILE:HD12	1.76	0.41
2:K:312:TYR:CE1	2:K:507:LEU:HD12	2.55	0.41
2:L:163:PHE:HB2	2:L:179:THR:CG2	2.51	0.41
2:L:319:SER:HA	2:L:323:LEU:HG	2.03	0.41
2:L:502:SER:N	2:L:506:SER:OG	2.48	0.41
3:U:31:ALA:HB2	3:U:61:GLU:HA	2.02	0.41
2:A:71:ASP:OD1	2:C:231:SER:HB2	2.20	0.41
2:A:343:ALA:HA	2:F:345:TRP:HB3	2.03	0.41
2:B:74:TYR:CE2	2:C:260:GLU:HG2	2.56	0.41
2:B:399:GLY:HA3	2:C:392:GLY:O	2.20	0.41
2:B:477:TYR:CD2	2:B:478:GLY:N	2.88	0.41
2:C:453:TYR:HB3	2:C:476:ARG:O	2.21	0.41
2:D:265:GLN:C	2:D:266:LEU:HD12	2.42	0.41
2:D:323:LEU:HD22	2:D:327:SER:HB2	2.01	0.41
2:D:378:ALA:HB1	2:D:382:VAL:CG2	2.51	0.41
2:D:482:ASN:O	2:D:485:ALA:N	2.50	0.41
2:E:80:ALA:HA	2:E:93:PRO:CG	2.51	0.41
2:E:181:PHE:HA	2:E:187:THR:HA	2.03	0.41
2:E:191:GLN:N	2:E:222:VAL:O	2.51	0.41
2:F:333:ASP:OD1	2:F:333:ASP:N	2.54	0.41
2:F:348:GLU:OE1	2:F:348:GLU:N	2.51	0.41
2:G:125:PHE:HE1	2:G:256:LYS:HE3	1.85	0.41
2:G:281:VAL:HG13	2:G:282:HIS:N	2.36	0.41
2:G:456:LEU:HD12	2:G:475:THR:HG22	2.03	0.41
2:I:142:GLU:H	2:I:490:GLN:HG2	1.86	0.41
2:I:163:PHE:HB2	2:I:179:THR:CG2	2.50	0.41
2:I:265:GLN:OE1	2:I:474:LYS:HE2	2.21	0.41
2:I:268:ALA:HB3	2:I:471:MET:CG	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:486:GLU:C	2:I:488:ALA:H	2.24	0.41
2:J:71:ASP:OD1	2:L:231:SER:HB2	2.21	0.41
2:J:160:ALA:HB1	2:J:232:ILE:HG21	2.03	0.41
2:K:99:VAL:HG12	2:L:484:PHE:CE2	2.55	0.41
2:K:345:TRP:CD2	2:L:348:GLU:HG3	2.56	0.41
2:L:147:MET:SD	2:L:367:GLN:HG2	2.60	0.41
2:L:168:ALA:HB1	2:L:200:ALA:HA	2.02	0.41
3:P:18:ASP:HB3	3:P:21:LYS:HD3	2.03	0.41
3:P:39:HIS:ND1	3:P:39:HIS:O	2.54	0.41
3:T:8:VAL:HG11	3:T:35:TYR:CZ	2.56	0.41
3:T:9:ASN:HB3	3:T:56:TYR:CD2	2.55	0.41
3:T:18:ASP:HB3	3:T:21:LYS:HD3	2.02	0.41
2:A:113:GLY:H	2:A:446:ALA:HB1	1.86	0.41
2:A:166:LEU:HD11	2:A:221:LEU:HD21	2.03	0.41
2:B:239:PHE:CD2	2:B:240:ASN:HB2	2.56	0.41
2:E:157:GLN:HB2	2:E:227:GLY:O	2.20	0.41
2:G:132:GLY:O	2:G:133:LYS:HB3	2.20	0.41
2:G:476:ARG:NH2	2:H:230:THR:HG21	2.31	0.41
2:G:484:PHE:CE2	2:L:99:VAL:HG12	2.56	0.41
2:H:382:VAL:HG12	2:H:521:ILE:HD11	2.03	0.41
2:I:277:ASP:O	2:I:281:VAL:HG12	2.21	0.41
2:I:466:ASN:O	2:I:468:GLN:HG3	2.21	0.41
2:K:159:ALA:HB2	2:K:248:ASN:ND2	2.35	0.41
3:U:11:LYS:HG3	3:U:27:GLU:HG2	2.02	0.41
2:A:407:ASP:HB3	2:B:372:GLU:HB2	2.03	0.40
2:C:253:ARG:NE	2:C:255:ASP:OD2	2.55	0.40
2:C:318:LYS:N	2:C:360:GLU:OE2	2.54	0.40
2:D:269:ALA:CB	2:D:470:VAL:HG12	2.51	0.40
2:E:169:SER:OG	2:E:200:ALA:HB2	2.21	0.40
2:E:315:GLN:HG3	2:E:510:ASN:O	2.21	0.40
2:E:336:ASP:O	2:E:340:ILE:HG12	2.21	0.40
2:E:479:ILE:HG22	2:E:480:GLY:N	2.37	0.40
2:G:128:ARG:NE	2:G:484:PHE:HE1	2.18	0.40
2:G:317:GLY:HA2	2:G:514:ARG:NH2	2.36	0.40
2:G:318:LYS:HE3	2:G:327:SER:HB3	2.03	0.40
2:G:392:GLY:O	2:L:399:GLY:HA3	2.21	0.40
2:I:430:LYS:HE3	2:J:185:THR:O	2.20	0.40
2:J:120:PRO:O	2:J:121:THR:OG1	2.36	0.40
2:K:85:SER:HB3	3:S:32:PHE:CE1	2.55	0.40
2:K:244:ASP:C	2:K:246:PRO:HD3	2.42	0.40
2:K:255:ASP:OD2	2:K:495:ARG:HG2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:266:LEU:CD1	2:L:155:SER:HB3	2.49	0.40
2:K:272:ILE:HG22	2:K:468:GLN:HE21	1.86	0.40
2:K:290:LEU:HA	2:K:290:LEU:HD23	1.83	0.40
2:L:184:GLU:OE2	2:L:321:MET:HB2	2.20	0.40
3:S:68:TRP:HA	3:S:71:ALA:HB3	2.03	0.40
3:U:12:THR:HG21	3:U:75:LEU:HD13	2.03	0.40
3:U:70:ALA:O	3:U:74:ASP:HB2	2.21	0.40
2:A:188:VAL:HG11	2:F:430:LYS:HE2	2.03	0.40
2:D:96:MET:HB2	2:E:124:VAL:HG22	2.02	0.40
2:D:232:ILE:HG22	2:D:236:GLN:HE22	1.86	0.40
2:D:386:LEU:HB3	2:D:404:PHE:CE2	2.56	0.40
2:E:72:HIS:HD2	2:F:260:GLU:OE2	2.04	0.40
2:E:79:ILE:HB	2:F:258:VAL:HG11	2.03	0.40
2:F:344:ARG:O	2:F:348:GLU:HB2	2.22	0.40
2:F:507:LEU:O	2:F:509:LYS:HG3	2.21	0.40
2:G:107:ILE:HG21	2:G:307:VAL:CG2	2.51	0.40
2:G:153:MET:HE2	2:G:226:GLU:N	2.36	0.40
2:J:117:MET:HE1	2:J:261:ALA:HB2	2.03	0.40
2:K:148:TYR:HB3	2:K:186:GLY:HA2	2.03	0.40
2:K:151:ASP:HB3	2:K:187:THR:HG21	2.03	0.40
2:K:304:ARG:HA	2:K:304:ARG:HD2	1.89	0.40
3:S:8:VAL:HG11	3:S:35:TYR:CE2	2.57	0.40
3:Y:40:LYS:HG3	3:Y:40:LYS:O	2.21	0.40
2:A:345:TRP:CD2	2:B:348:GLU:HG3	2.56	0.40
2:B:326:GLY:HA3	2:B:338:ILE:HD13	2.02	0.40
2:E:521:ILE:HA	2:F:341:ARG:NH2	2.35	0.40
2:H:79:ILE:CG2	2:I:121:THR:HB	2.51	0.40
2:H:145:HIS:ND1	2:H:148:TYR:CD2	2.89	0.40
2:I:92:GLY:HA2	2:I:93:PRO:HD3	1.90	0.40
2:I:446:ALA:HB3	2:I:449:TYR:CE1	2.56	0.40
2:L:456:LEU:N	2:L:475:THR:HG22	2.29	0.40
3:R:10:ILE:HD11	3:R:35:TYR:CE1	2.57	0.40
3:T:23:ILE:HG12	3:T:78:VAL:HG22	2.02	0.40
2:A:266:LEU:HD23	2:B:250:MET:HG3	2.02	0.40
2:B:260:GLU:HG3	2:B:261:ALA:N	2.36	0.40
2:B:382:VAL:HG12	2:B:521:ILE:HD11	2.03	0.40
2:C:198:ILE:O	2:C:198:ILE:HG22	2.22	0.40
2:C:332:PHE:HE2	2:C:334:PHE:CE1	2.40	0.40
2:C:483:PRO:O	2:C:484:PHE:HB2	2.22	0.40
2:E:463:ASP:HB3	2:E:466:ASN:OD1	2.20	0.40
2:F:485:ALA:HB1	2:F:510:ASN:OD1	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:148:TYR:HD1	2:G:186:GLY:H	1.69	0.40
2:G:153:MET:HE2	2:G:226:GLU:H	1.87	0.40
2:G:228:MET:SD	2:G:236:GLN:NE2	2.95	0.40
2:G:466:ASN:O	2:G:468:GLN:HG3	2.22	0.40
2:H:336:ASP:O	2:H:340:ILE:HG12	2.22	0.40
2:I:345:TRP:HE1	2:J:344:ARG:HH21	1.69	0.40
2:I:351:LYS:NZ	2:I:390:ASP:O	2.42	0.40
2:I:357:ILE:HD11	2:I:376:ILE:HG21	2.04	0.40
2:K:126:ALA:O	2:K:254:ILE:HA	2.22	0.40
2:L:126:ALA:HB1	2:L:484:PHE:CE1	2.57	0.40
3:Q:40:LYS:O	3:Q:40:LYS:HG3	2.22	0.40
3:S:9:ASN:OD1	3:S:29:SER:OG	2.21	0.40
2:A:244:ASP:O	2:A:246:PRO:HD3	2.22	0.40
2:C:142:GLU:N	2:C:490:GLN:OE1	2.37	0.40
2:C:386:LEU:HB3	2:C:404:PHE:HE2	1.85	0.40
2:E:279:ARG:NH1	2:E:283:GLY:O	2.55	0.40
2:G:154:PHE:CZ	2:G:248:ASN:HB3	2.57	0.40
2:G:179:THR:HG22	2:G:189:TYR:CE1	2.56	0.40
2:H:113:GLY:H	2:H:446:ALA:HB1	1.86	0.40
2:H:376:ILE:HG22	2:H:436:VAL:HG22	2.04	0.40
2:H:477:TYR:CG	2:H:478:GLY:N	2.90	0.40
2:I:131:TYR:HB3	2:I:250:MET:HG2	2.03	0.40
2:J:147:MET:HE3	2:J:367:GLN:HG2	2.04	0.40
2:J:430:LYS:HG2	2:K:216:MET:HE1	2.03	0.40
2:J:486:GLU:C	2:J:488:ALA:H	2.24	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	413/417 (99%)	374 (91%)	34 (8%)	5 (1%)	13 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	454/456 (100%)	411 (90%)	41 (9%)	2 (0%)	34	66
2	B	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	22	54
2	C	454/456 (100%)	408 (90%)	43 (10%)	3 (1%)	22	54
2	D	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	22	54
2	E	454/456 (100%)	406 (89%)	44 (10%)	4 (1%)	17	48
2	F	454/456 (100%)	413 (91%)	39 (9%)	2 (0%)	34	66
2	G	454/456 (100%)	413 (91%)	38 (8%)	3 (1%)	22	54
2	H	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	22	54
2	I	454/456 (100%)	408 (90%)	44 (10%)	2 (0%)	34	66
2	J	454/456 (100%)	413 (91%)	37 (8%)	4 (1%)	17	48
2	K	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	22	54
2	L	454/456 (100%)	409 (90%)	43 (10%)	2 (0%)	34	66
3	O	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	P	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	Q	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	R	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	S	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	T	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
3	U	77/80 (96%)	72 (94%)	5 (6%)	0	100	100
3	V	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	W	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	X	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	Y	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
4	Z	23/376 (6%)	23 (100%)	0	0	100	100
All	All	6731/7145 (94%)	6083 (90%)	609 (9%)	39 (1%)	29	57

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	395	TYR
2	H	395	TYR
2	I	395	TYR
2	J	395	TYR
2	L	395	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	25	VAL
2	A	395	TYR
2	B	395	TYR
2	E	395	TYR
2	F	395	TYR
2	G	395	TYR
2	H	108	ALA
2	K	395	TYR
2	B	108	ALA
2	C	108	ALA
2	D	147	MET
2	D	395	TYR
2	E	108	ALA
2	G	108	ALA
2	J	108	ALA
2	J	147	MET
2	E	147	MET
2	K	147	MET
1	a	243	ALA
1	a	364	VAL
1	a	340	ILE
2	A	254	ILE
2	C	254	ILE
2	D	254	ILE
2	J	254	ILE
2	E	254	ILE
2	F	254	ILE
2	G	254	ILE
2	H	254	ILE
2	I	254	ILE
2	K	254	ILE
2	B	254	ILE
2	L	254	ILE
1	a	357	VAL

5.3.2 Protein sidechains (i)

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	350/352 (99%)	350 (100%)	0	100	100
2	A	346/346 (100%)	346 (100%)	0	100	100
2	B	346/346 (100%)	346 (100%)	0	100	100
2	C	346/346 (100%)	346 (100%)	0	100	100
2	D	346/346 (100%)	346 (100%)	0	100	100
2	E	346/346 (100%)	346 (100%)	0	100	100
2	F	346/346 (100%)	346 (100%)	0	100	100
2	G	346/346 (100%)	346 (100%)	0	100	100
2	H	346/346 (100%)	346 (100%)	0	100	100
2	I	346/346 (100%)	346 (100%)	0	100	100
2	J	346/346 (100%)	346 (100%)	0	100	100
2	K	346/346 (100%)	346 (100%)	0	100	100
2	L	346/346 (100%)	346 (100%)	0	100	100
3	O	66/67 (98%)	66 (100%)	0	100	100
3	P	66/67 (98%)	66 (100%)	0	100	100
3	Q	66/67 (98%)	66 (100%)	0	100	100
3	R	66/67 (98%)	66 (100%)	0	100	100
3	S	66/67 (98%)	66 (100%)	0	100	100
3	T	66/67 (98%)	66 (100%)	0	100	100
3	U	66/67 (98%)	66 (100%)	0	100	100
3	V	66/67 (98%)	66 (100%)	0	100	100
3	W	66/67 (98%)	66 (100%)	0	100	100
3	X	66/67 (98%)	66 (100%)	0	100	100
3	Y	66/67 (98%)	66 (100%)	0	100	100
4	Z	21/319 (7%)	19 (90%)	2 (10%)	8	29
All	All	5249/5560 (94%)	5247 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Z	317	LYS
4	Z	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111)

such sidechains are listed below:

Mol	Chain	Res	Type
1	a	290	HIS
1	a	317	ASN
1	a	356	HIS
1	a	384	ASN
2	A	72	HIS
2	A	195	GLN
2	A	282	HIS
2	A	356	GLN
2	A	367	GLN
2	A	384	ASN
2	A	431	GLN
2	A	510	ASN
2	B	145	HIS
2	B	180	HIS
2	B	282	HIS
2	B	303	ASN
2	B	356	GLN
2	B	384	ASN
2	B	482	ASN
2	B	510	ASN
2	C	75	ASN
2	C	145	HIS
2	C	195	GLN
2	C	236	GLN
2	C	282	HIS
2	C	356	GLN
2	C	384	ASN
2	C	431	GLN
2	D	171	GLN
2	D	236	GLN
2	D	240	ASN
2	D	282	HIS
2	D	303	ASN
2	D	356	GLN
2	D	384	ASN
2	D	431	GLN
2	D	468	GLN
2	D	510	ASN
2	E	145	HIS
2	E	171	GLN
2	E	236	GLN
2	E	282	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	303	ASN
2	E	356	GLN
2	E	367	GLN
2	E	468	GLN
2	E	482	ASN
2	E	510	ASN
2	F	145	HIS
2	F	171	GLN
2	F	236	GLN
2	F	282	HIS
2	F	356	GLN
2	F	367	GLN
2	F	510	ASN
2	G	145	HIS
2	G	171	GLN
2	G	282	HIS
2	G	303	ASN
2	G	356	GLN
2	G	431	GLN
2	G	468	GLN
2	G	510	ASN
2	H	72	HIS
2	H	105	ASN
2	H	171	GLN
2	H	282	HIS
2	H	303	ASN
2	H	356	GLN
2	H	398	GLN
2	H	510	ASN
2	I	236	GLN
2	I	282	HIS
2	I	303	ASN
2	I	356	GLN
2	I	384	ASN
2	I	431	GLN
2	I	510	ASN
2	J	195	GLN
2	J	236	GLN
2	J	282	HIS
2	J	303	ASN
2	J	356	GLN
2	J	367	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	384	ASN
2	J	431	GLN
2	J	468	GLN
2	J	510	ASN
2	K	171	GLN
2	K	180	HIS
2	K	282	HIS
2	K	356	GLN
2	K	367	GLN
2	K	384	ASN
2	K	431	GLN
2	K	468	GLN
2	K	510	ASN
2	L	72	HIS
2	L	171	GLN
2	L	282	HIS
2	L	303	ASN
2	L	356	GLN
2	L	384	ASN
2	L	431	GLN
2	L	510	ASN
3	P	15	GLN
3	P	45	HIS
3	Q	15	GLN
3	Q	45	HIS
3	T	45	HIS
3	X	15	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

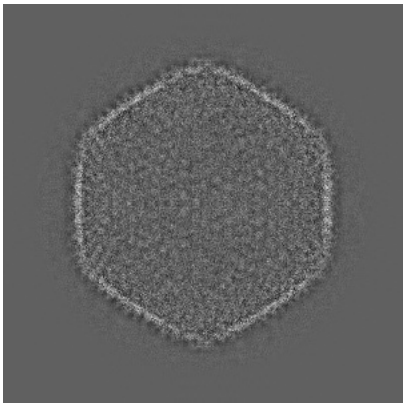
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8661. These allow visual inspection of the internal detail of the map and identification of artifacts.

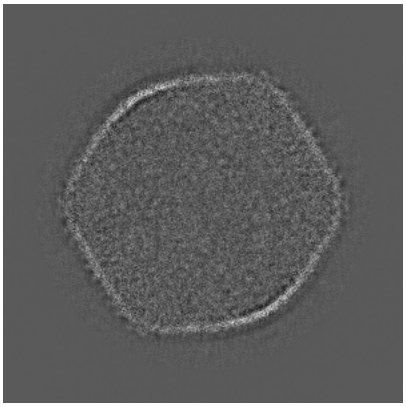
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

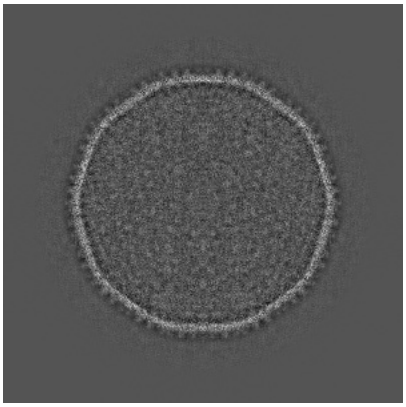
6.1.1 Primary map



X



Y

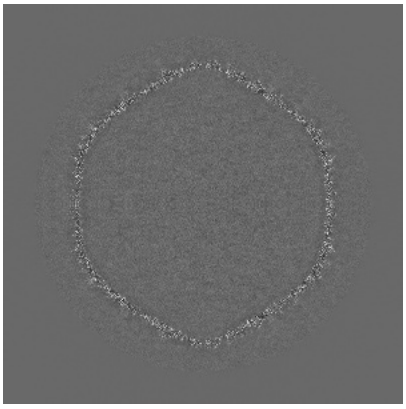


Z

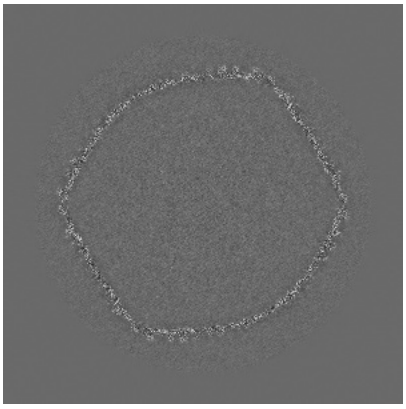
The images above show the map projected in three orthogonal directions.

6.2 Central slices

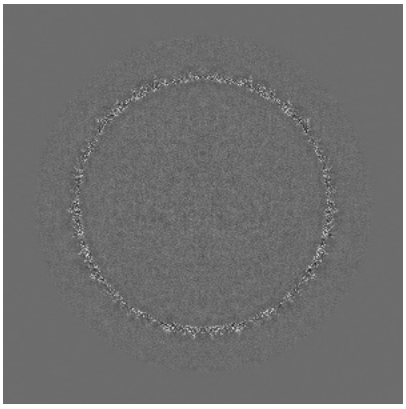
6.2.1 Primary map



X Index: 768



Y Index: 768

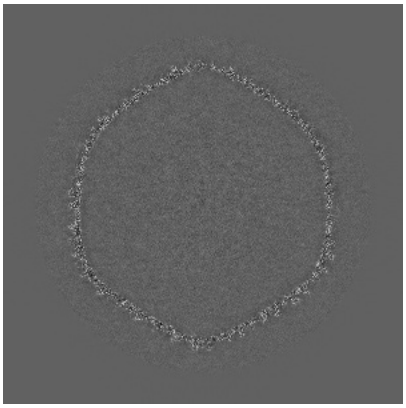


Z Index: 768

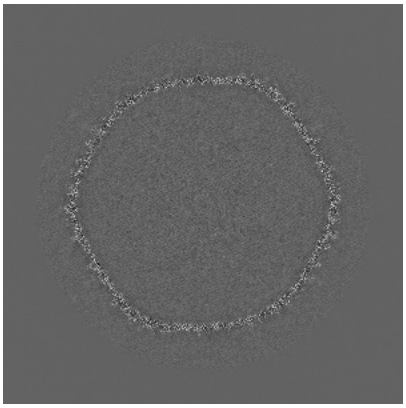
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

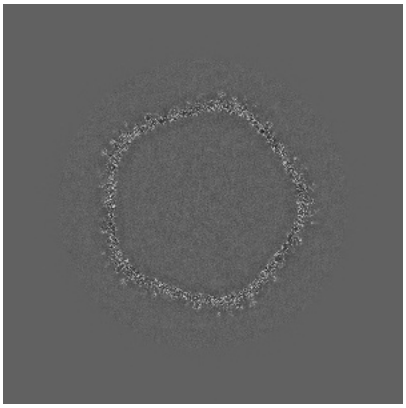
6.3.1 Primary map



X Index: 734



Y Index: 666



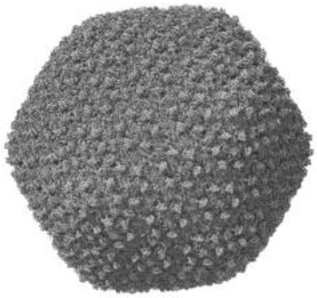
Z Index: 1095

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

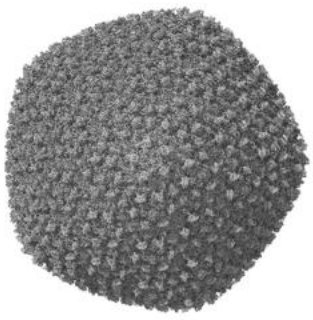
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

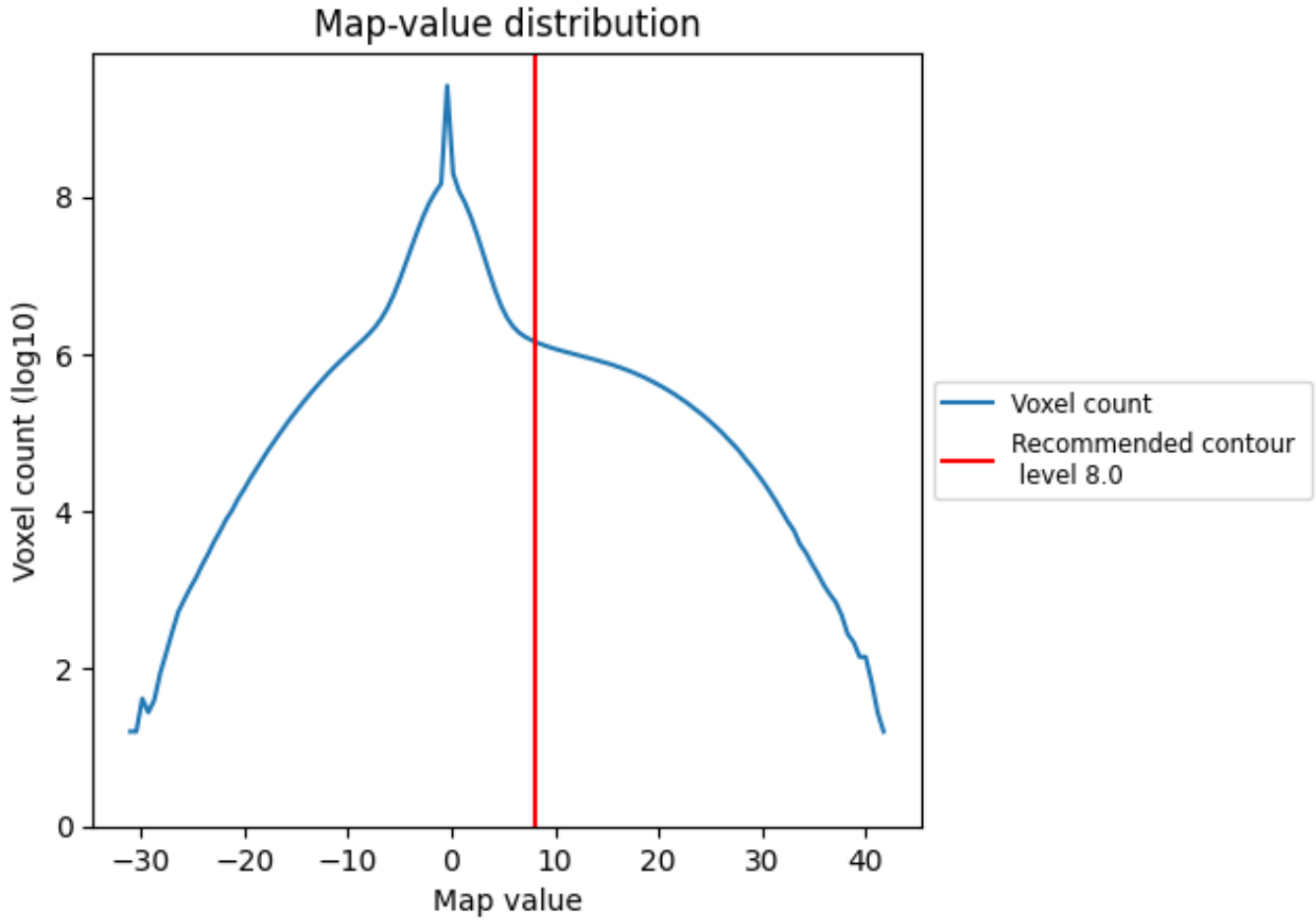
6.5 Mask visualisation (i)

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

7 Map analysis

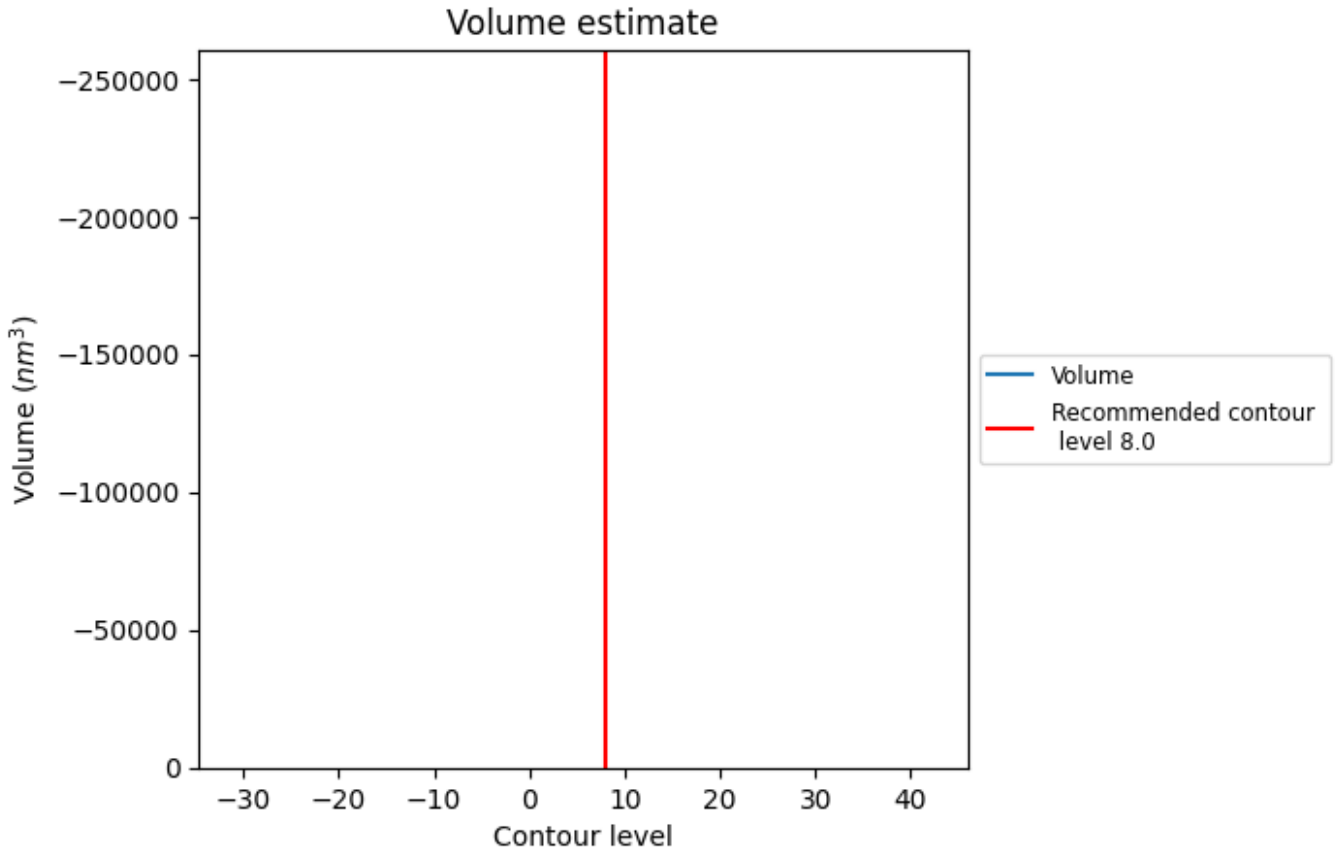
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

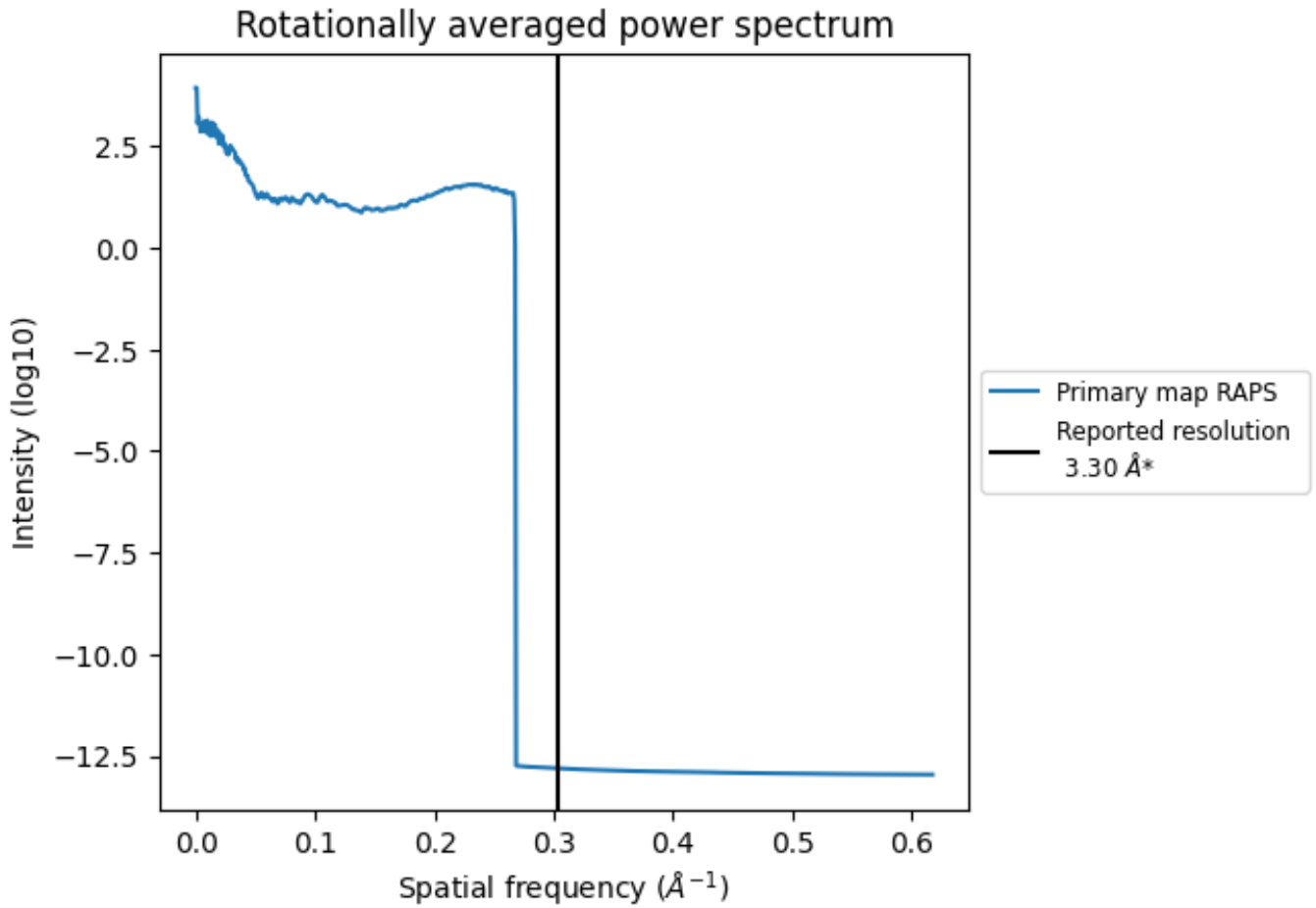
7.2 Volume estimate



The volume at the recommended contour level is -2271095 nm^3; this corresponds to an approximate mass of -2051540 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 (i)



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

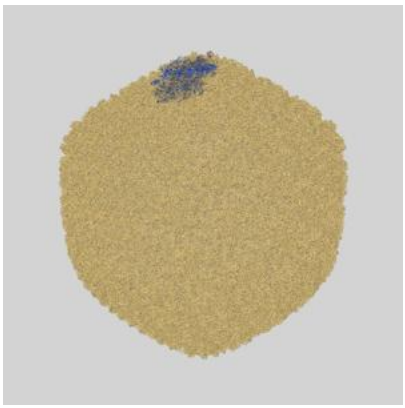
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

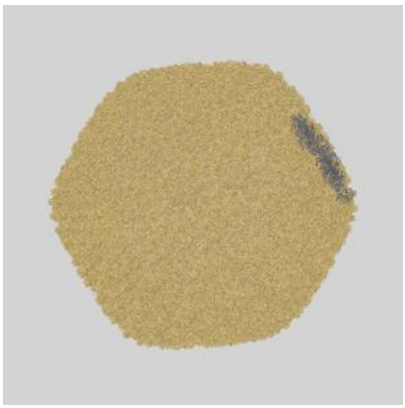
This section contains information regarding the fit between EMDB map EMD-8661 and PDB model 5VF3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

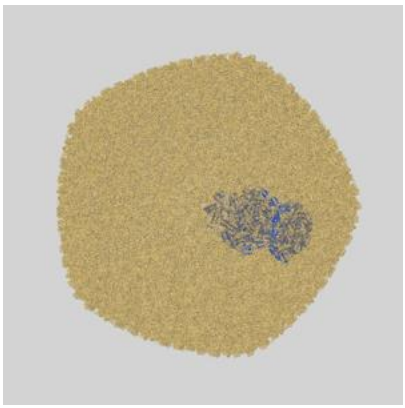
9.1.1 Map-model overlay



X

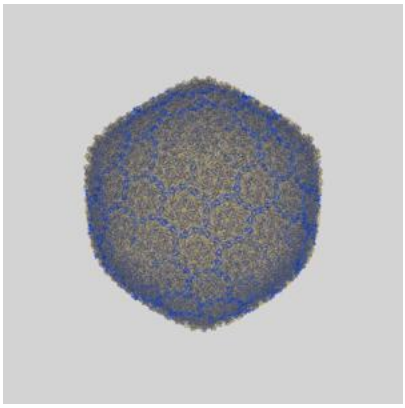


Y

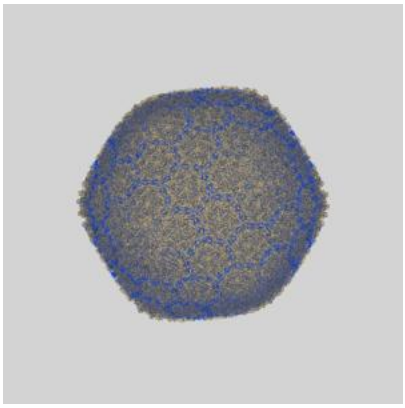


Z

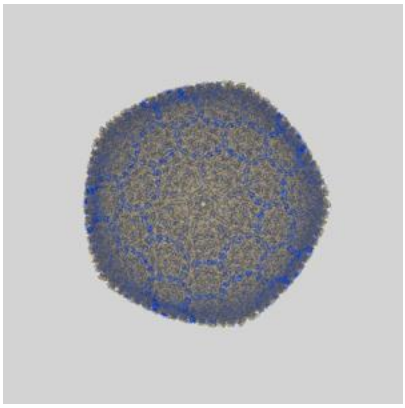
9.1.2 Map-model assembly overlay



X



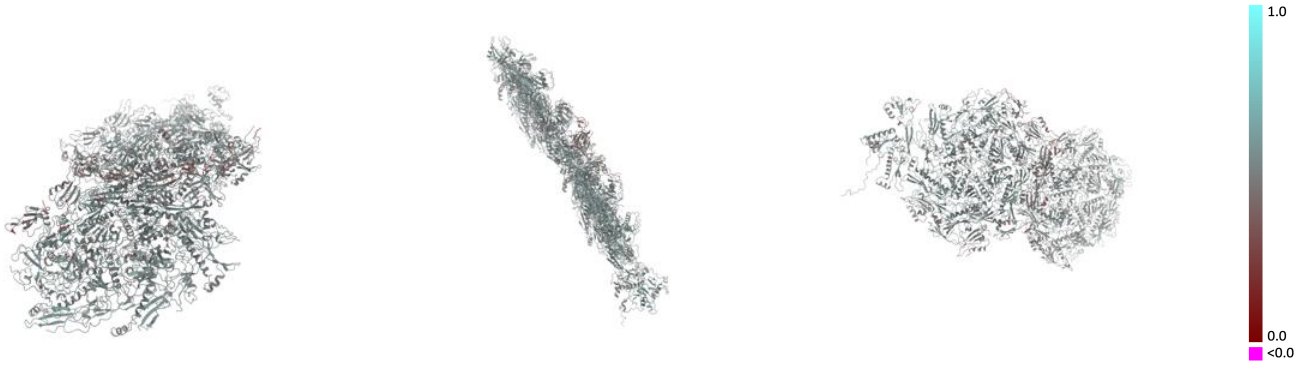
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

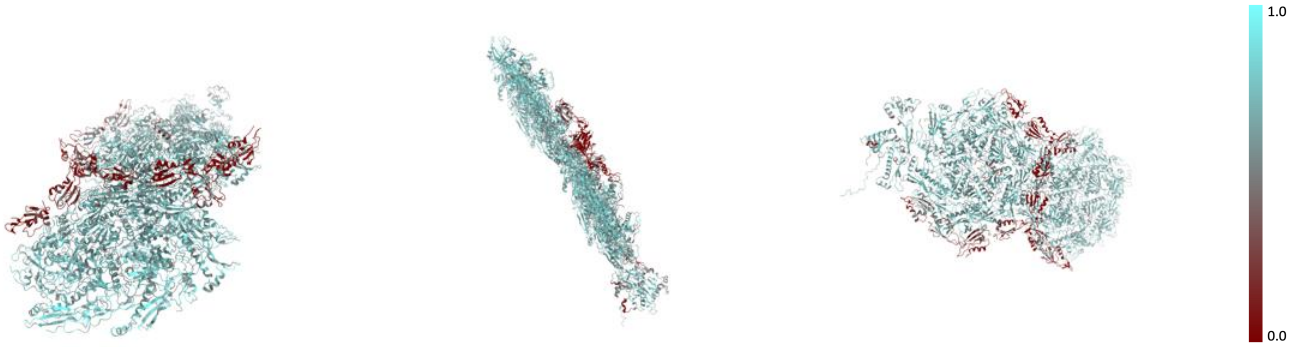
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

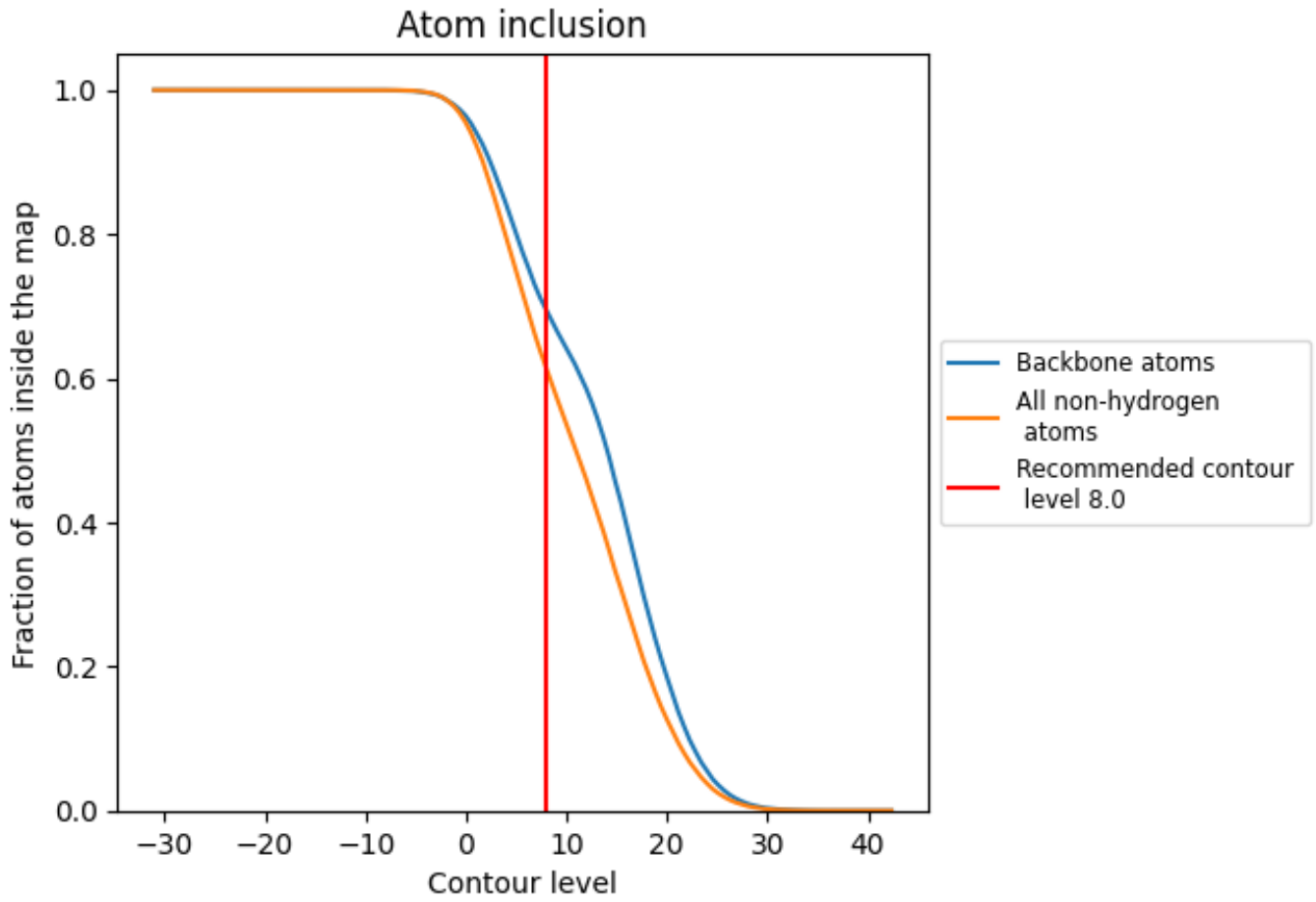
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.0).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 61% 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 (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6135	0.5050
A	0.6863	0.5210
B	0.7002	0.5190
C	0.6972	0.5160
D	0.6990	0.5160
E	0.7053	0.5180
F	0.6978	0.5180
G	0.6999	0.5170
H	0.6961	0.5160
I	0.6990	0.5120
J	0.7064	0.5150
K	0.7026	0.5150
L	0.7020	0.5170
O	0.2814	0.4740
P	0.3505	0.4830
Q	0.1174	0.4570
R	0.1527	0.4490
S	0.1367	0.4520
T	0.0145	0.4090
U	0.1254	0.4380
V	0.0032	0.3920
W	0.1768	0.4470
X	0.0177	0.4140
Y	0.0386	0.4050
Z	0.2392	0.4650
a	0.5942	0.5010
z	0.4267	0.4650