



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:19 PM EST

PDB ID : 3IYW
EMDB ID : EMD-5190
Title : West Nile virus in complex with Fab fragments of MAb CR4354 (fitted coordinates of envelope proteins and Fab fragments of one icosahedral ASU)
Authors : Rossmann, M.G.; Kaufmann, B.
Deposited on : 2010-06-18
Resolution : 13.70 Å (reported)
Based on initial models : 2HG0, 3N9G

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.31.3

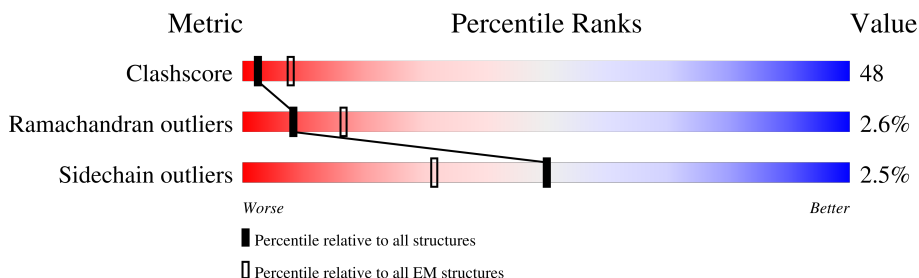
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.70 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	403	
1	B	403	
1	C	403	
2	H	230	
2	K	230	
3	L	220	
3	M	220	
4	D	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	3	<div><div></div><div>33%</div></div>
			<div><div></div><div>67%</div></div>
4	F	3	<div><div></div><div>33%</div></div>
			<div><div></div><div>67%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16202 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 Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3030	1908	519	581	22		
1	B	400	Total	C	N	O	S	0	0
			3030	1908	519	581	22		
1	C	400	Total	C	N	O	S	0	0
			3030	1908	519	581	22		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	NDG	-	expression tag	UNP Q9Q6P4
A	402	NDG	-	expression tag	UNP Q9Q6P4
A	403	FUL	-	expression tag	UNP Q9Q6P4
B	401	NDG	-	expression tag	UNP Q9Q6P4
B	402	NDG	-	expression tag	UNP Q9Q6P4
B	403	FUL	-	expression tag	UNP Q9Q6P4
C	401	NDG	-	expression tag	UNP Q9Q6P4
C	402	NDG	-	expression tag	UNP Q9Q6P4
C	403	FUL	-	expression tag	UNP Q9Q6P4

- Molecule 2 is a protein called CR4354 Fab fragment X1, heavy chain H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	230	Total	C	N	O	S	24	0
			1850	1172	309	356	13		
2	K	230	Total	C	N	O	S	24	0
			1850	1172	309	356	13		

- Molecule 3 is a protein called CR4354 Fab fragment X1, light chain L.

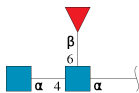
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	220	Total	C	N	O	S	9	0
			1649	1027	275	342	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	220	Total	C	N	O	S	9	0
			1649	1027	275	342	5		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose.

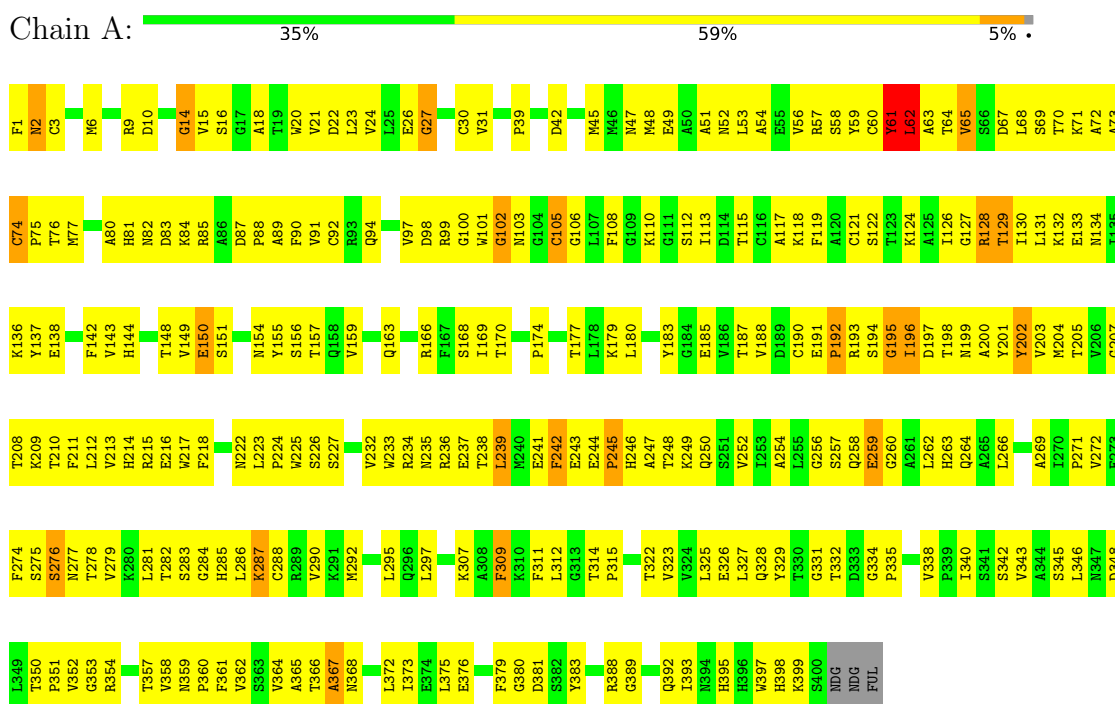


Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			38	22	2	14		
4	E	3	Total	C	N	O	0	0
			38	22	2	14		
4	F	3	Total	C	N	O	0	0
			38	22	2	14		

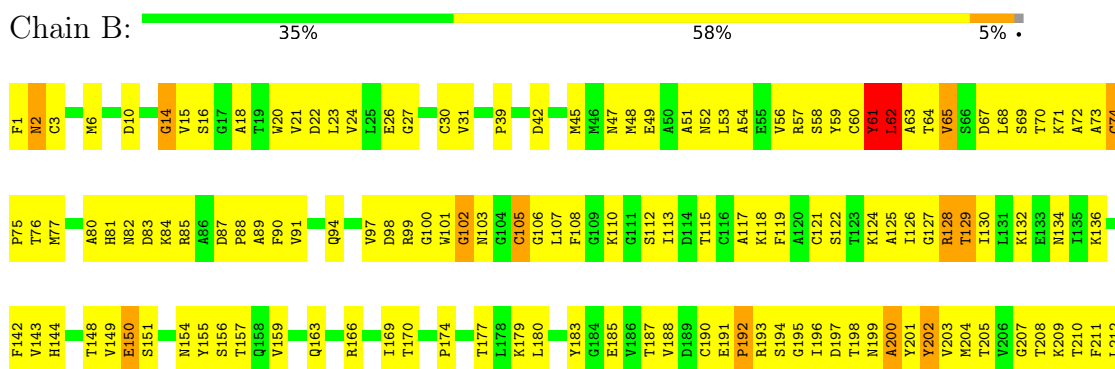
3 Residue-property plots

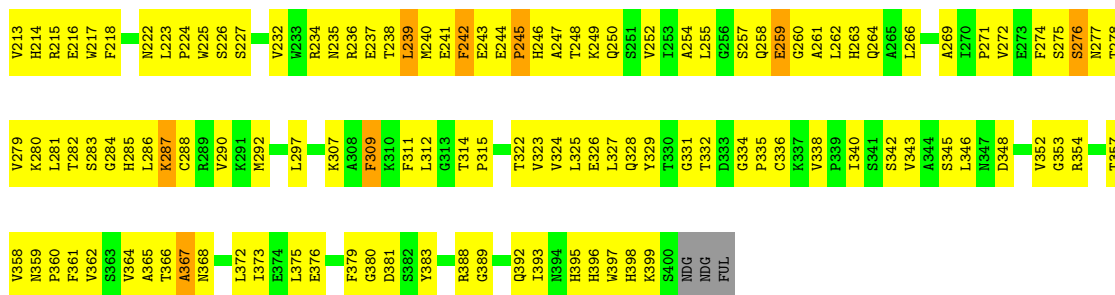
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Polyprotein



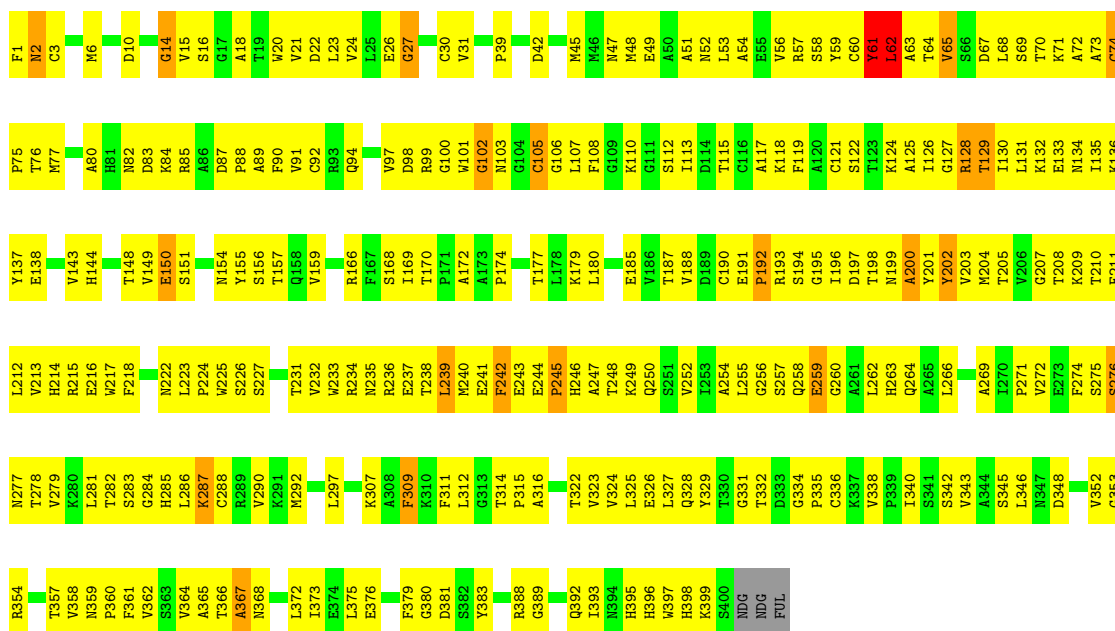
• Molecule 1: Polyprotein





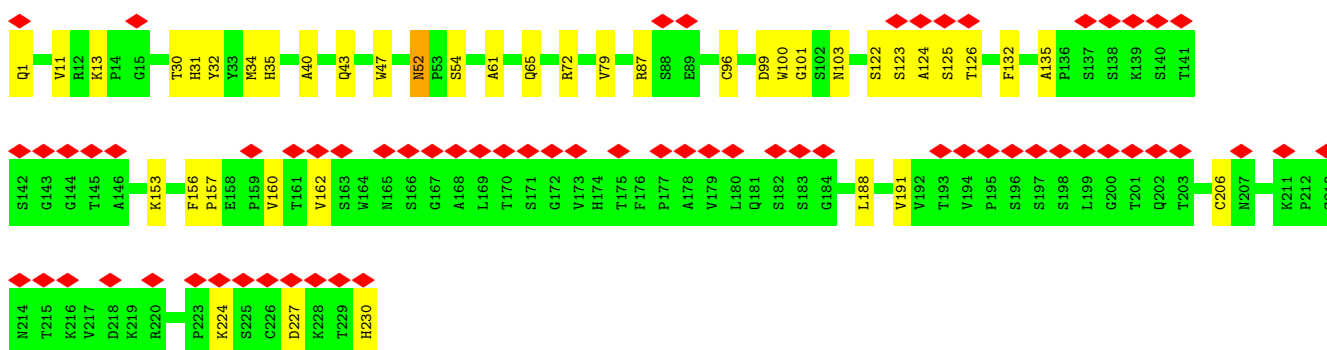
• Molecule 1: Polyprotein

Chain C: 34% 60% 5%



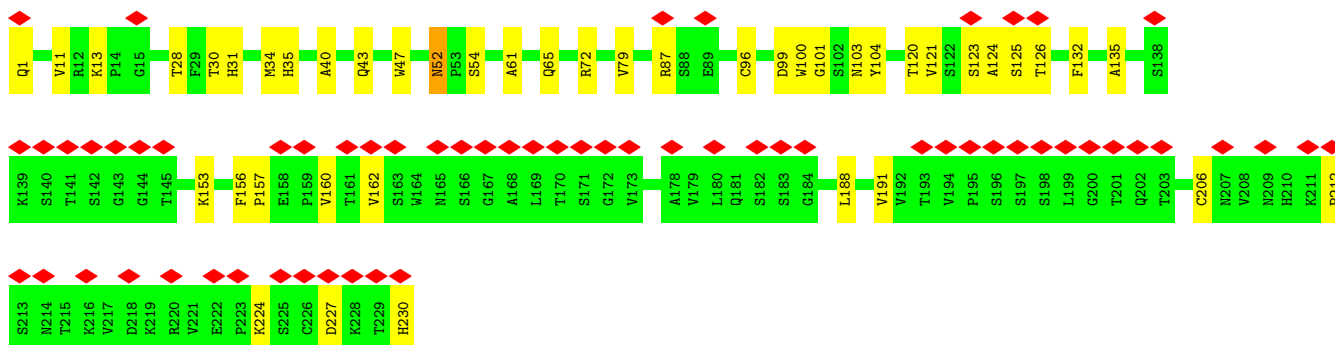
• Molecule 2: CR4354 Fab fragment X1, heavy chain H

Chain H: 29% 82% 17%

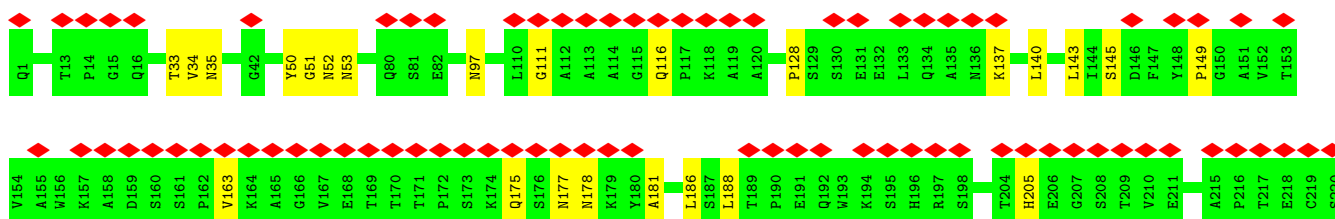


• Molecule 2: CR4354 Fab fragment X1, heavy chain H

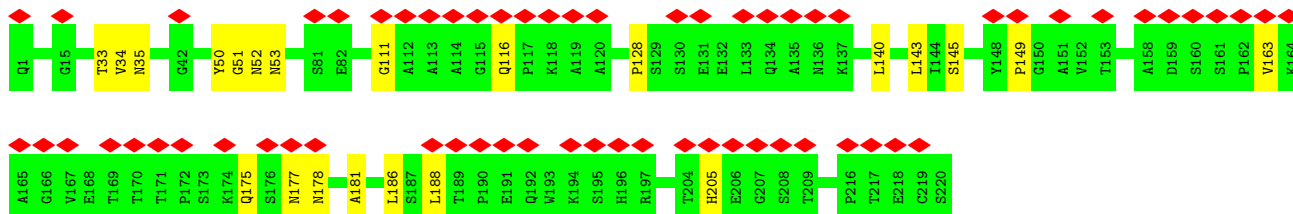
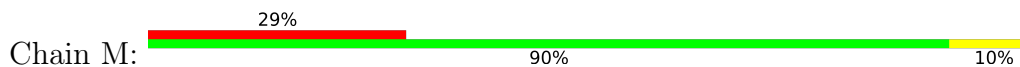
Chain K: 27% 81% 19%



- Molecule 3: CR4354 Fab fragment X1, light chain L



- Molecule 3: CR4354 Fab fragment X1, light chain L



- Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain F: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5006	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	1450	Depositor
Maximum defocus (nm)	3530	Depositor
Magnification	47244	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	4.592	Depositor
Minimum map value	-1.430	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.8	Depositor
Map size (\AA)	814.386, 814.386, 814.386	wwPDB
Map dimensions	299, 299, 299	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.7237, 2.7237, 2.7237	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, NDG, PCA

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	0.65	1/3092 (0.0%)	1.22	6/4193 (0.1%)
1	B	0.39	0/3091	0.74	3/4190 (0.1%)
1	C	0.39	0/3091	0.74	3/4190 (0.1%)
2	H	0.35	0/1959	0.56	0/2661
2	K	0.35	0/1959	0.56	0/2661
3	L	0.32	0/1712	0.54	0/2334
3	M	0.32	0/1712	0.54	0/2334
All	All	0.43	1/16616 (0.0%)	0.78	12/22563 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	GLY	C-N	28.70	2.00	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	GLY	CA-C-N	-46.34	15.26	117.20
1	A	195	GLY	C-N-CA	-41.68	17.49	121.70
1	A	195	GLY	O-C-N	7.06	134.00	122.70
1	C	61	TYR	N-CA-C	-6.72	92.84	111.00
1	B	61	TYR	N-CA-C	-6.72	92.85	111.00
1	A	61	TYR	N-CA-C	-6.72	92.86	111.00
1	C	62	LEU	N-CA-C	6.72	129.14	111.00
1	A	62	LEU	N-CA-C	6.71	129.12	111.00
1	B	62	LEU	N-CA-C	6.70	129.08	111.00
1	A	105	CYS	CA-CB-SG	-6.47	102.36	114.00
1	C	105	CYS	CA-CB-SG	-6.46	102.36	114.00
1	B	105	CYS	CA-CB-SG	-6.46	102.37	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3030	0	2976	419	0
1	B	3030	0	2968	529	0
1	C	3030	0	2966	570	0
2	H	1850	0	1858	99	0
2	K	1850	0	1862	160	0
3	L	1649	0	1620	32	0
3	M	1649	0	1620	18	0
4	D	38	0	32	5	0
4	E	38	0	32	5	0
4	F	38	0	32	5	0
All	All	16202	0	15966	1535	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 48.

All (1535) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LYS:HD3	2:K:31:HIS:CA	1.26	1.58
1:B:263:HIS:CB	1:C:258:GLN:HG3	1.23	1.56
2:K:11:VAL:CG2	2:K:157:PRO:HG3	1.13	1.55
1:A:136:LYS:CD	2:H:31:HIS:HA	1.29	1.54
2:H:11:VAL:CG2	2:H:157:PRO:HG3	1.36	1.54
1:B:263:HIS:CB	1:C:258:GLN:CG	1.78	1.53
1:C:136:LYS:CD	2:K:31:HIS:HA	1.40	1.51
1:C:196:ILE:HA	1:C:285:HIS:CD2	1.46	1.50
1:B:101:TRP:CH2	1:C:326:GLU:HB2	1.43	1.50
1:A:136:LYS:HD3	2:H:31:HIS:CA	1.36	1.49
1:B:52:ASN:HD22	1:B:134:ASN:CG	1.19	1.46
1:B:368:ASN:ND2	3:L:97:ASN:HD21	1.09	1.45
1:C:52:ASN:ND2	2:K:100:TRP:HZ3	1.13	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLY:N	1:B:196:ILE:CG1	1.81	1.43
1:B:263:HIS:HB2	1:C:258:GLN:CG	1.33	1.43
2:K:13[A]:LYS:NZ	2:K:126:THR:H	1.12	1.43
1:B:263:HIS:CB	1:C:258:GLN:CD	1.86	1.41
1:C:138:GLU:OE2	2:K:28:THR:CG2	1.68	1.40
2:H:11:VAL:HG21	2:H:157:PRO:CG	1.50	1.40
2:K:11:VAL:HG21	2:K:157:PRO:CG	1.52	1.39
1:C:195:GLY:N	1:C:196:ILE:CG1	1.86	1.38
2:K:11:VAL:CG2	2:K:157:PRO:CG	2.00	1.37
1:A:282:THR:H	1:A:283:SER:N	1.22	1.36
1:B:195:GLY:N	1:B:196:ILE:HG12	1.36	1.36
1:B:255:LEU:HG	1:C:263:HIS:NE2	1.39	1.35
1:A:131:LEU:CD2	1:C:76:THR:HG21	1.55	1.35
1:A:281:LEU:HA	1:A:283:SER:N	1.38	1.35
2:H:13[A]:LYS:NZ	2:H:126:THR:OG1	1.60	1.33
1:A:282:THR:N	1:A:283:SER:N	1.78	1.30
1:B:314:THR:HB	1:C:107:LEU:CD2	1.63	1.28
1:C:138:GLU:CD	2:K:28:THR:CG2	2.02	1.28
1:B:258:GLN:CB	1:C:263:HIS:H	1.35	1.28
2:H:13[A]:LYS:CD	2:H:124:ALA:O	1.81	1.28
1:C:195:GLY:N	1:C:196:ILE:HG13	1.40	1.27
1:C:27:GLY:CA	1:C:282:THR:O	1.82	1.27
2:K:11:VAL:HG21	2:K:157:PRO:CD	1.65	1.27
1:B:195:GLY:C	1:B:196:ILE:HG13	1.53	1.26
1:B:257:SER:O	1:C:259:GLU:HB3	1.27	1.26
1:A:281:LEU:CA	1:A:283:SER:N	1.98	1.26
1:A:136:LYS:HE2	2:H:30:THR:O	1.23	1.25
1:B:194:SER:OG	1:B:196:ILE:HD11	1.11	1.25
1:C:52:ASN:ND2	2:K:100:TRP:CZ3	1.95	1.25
1:B:52:ASN:ND2	1:B:134:ASN:CG	1.88	1.24
2:K:13[A]:LYS:NZ	2:K:126:THR:N	1.84	1.24
2:K:13[A]:LYS:CE	2:K:126:THR:H	1.49	1.24
1:B:108:PHE:H	1:C:316:ALA:CB	1.48	1.24
1:B:260:GLY:N	1:C:260:GLY:N	1.85	1.24
1:A:52:ASN:ND2	2:H:100:TRP:HZ3	1.32	1.24
1:B:263:HIS:HB2	1:C:258:GLN:CD	1.48	1.24
3:L:111:GLY:HA3	3:L:116:GLN:CB	1.66	1.24
1:B:194:SER:CB	1:B:196:ILE:CD1	2.15	1.24
1:B:324:VAL:HB	1:C:108:PHE:CE2	1.73	1.23
1:B:368:ASN:HD22	3:L:97:ASN:ND2	1.35	1.23
1:B:194:SER:OG	1:B:196:ILE:CD1	1.84	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:13[A]:LYS:CE	2:K:125[A]:SER:HA	1.69	1.22
2:K:13[A]:LYS:HE3	2:K:125[A]:SER:CA	1.70	1.21
1:B:149:VAL:CG1	1:C:101:TRP:HB3	1.69	1.21
2:K:13[A]:LYS:HD3	2:K:124:ALA:O	1.37	1.21
1:B:261:ALA:H	1:C:260:GLY:CA	1.51	1.21
1:B:196:ILE:HA	1:B:285:HIS:CD2	1.76	1.20
1:B:196:ILE:HG22	1:B:285:HIS:CG	1.73	1.20
1:B:263:HIS:CG	1:C:258:GLN:CD	2.16	1.19
1:A:136:LYS:CE	2:H:30:THR:O	1.91	1.19
1:A:195:GLY:N	1:A:196:ILE:HG23	1.25	1.19
1:B:108:PHE:HB2	1:C:316:ALA:HB3	1.23	1.19
1:C:133:GLU:HB3	2:K:104:TYR:CE2	1.76	1.19
1:A:281:LEU:HB3	1:A:283:SER:O	1.04	1.19
1:A:52:ASN:ND2	2:H:100:TRP:CZ3	2.10	1.18
1:C:47:ASN:ND2	2:K:28:THR:OG1	1.73	1.18
1:C:138:GLU:CD	2:K:28:THR:HG23	1.60	1.18
1:A:131:LEU:CD2	1:C:76:THR:CG2	2.23	1.17
1:B:194:SER:HB2	1:B:196:ILE:CD1	1.74	1.16
1:B:257:SER:O	1:C:259:GLU:CB	1.91	1.16
1:B:261:ALA:H	1:C:260:GLY:HA3	1.03	1.16
2:K:123[A]:SER:OG	2:K:124:ALA:CA	1.91	1.15
1:A:195:GLY:N	1:A:196:ILE:CG2	2.00	1.15
2:K:11:VAL:CB	2:K:157:PRO:HG3	1.78	1.14
1:A:131:LEU:HD22	1:C:76:THR:HG21	1.14	1.13
2:K:13[A]:LYS:CD	2:K:124:ALA:O	1.95	1.13
2:K:13[B]:LYS:NZ	2:K:125[B]:SER:HA	1.63	1.13
1:B:368:ASN:ND2	3:L:97:ASN:ND2	1.91	1.13
1:C:136:LYS:HD2	2:K:31:HIS:O	1.46	1.12
1:B:52:ASN:HD22	1:B:134:ASN:CB	1.62	1.12
1:A:133:GLU:OE2	1:B:311:PHE:HB2	1.50	1.12
1:C:196:ILE:CA	1:C:285:HIS:HD2	1.61	1.12
1:A:282:THR:H	1:A:283:SER:CA	1.61	1.12
1:B:149:VAL:HG13	1:C:101:TRP:HB3	1.13	1.12
1:C:195:GLY:H	1:C:196:ILE:N	1.48	1.12
1:A:136:LYS:CE	2:H:31:HIS:HA	1.79	1.12
1:B:258:GLN:HG2	1:C:260:GLY:HA2	1.19	1.12
1:C:138:GLU:OE2	2:K:28:THR:HG23	1.47	1.11
1:B:194:SER:C	1:B:196:ILE:HG12	1.70	1.11
1:B:195:GLY:H	1:B:196:ILE:N	1.47	1.11
1:C:194:SER:C	1:C:196:ILE:CG1	2.17	1.11
1:C:138:GLU:OE2	2:K:28:THR:HG22	1.32	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13[A]:LYS:HD3	2:H:124:ALA:O	1.44	1.10
1:A:281:LEU:CB	1:A:283:SER:O	2.00	1.10
1:B:101:TRP:CH2	1:C:326:GLU:CB	2.34	1.10
1:B:101:TRP:CZ2	1:C:326:GLU:HB2	1.87	1.10
1:B:52:ASN:HD22	1:B:134:ASN:ND2	1.49	1.10
1:B:194:SER:HB2	1:B:196:ILE:CG1	1.81	1.09
1:B:62:LEU:HD12	1:B:63:ALA:H	1.17	1.09
1:B:260:GLY:H	1:C:260:GLY:N	1.45	1.08
1:B:108:PHE:H	1:C:316:ALA:HB2	1.10	1.08
1:C:136:LYS:CD	2:K:31:HIS:CA	2.08	1.08
1:C:62:LEU:HD12	1:C:63:ALA:H	1.17	1.08
1:B:196:ILE:HG22	1:B:285:HIS:CD2	1.89	1.08
1:C:168:SER:OG	2:K:54:SER:HB2	1.54	1.08
2:K:13[B]:LYS:HZ3	2:K:125[B]:SER:HA	0.97	1.08
1:B:258:GLN:HG2	1:C:260:GLY:CA	1.83	1.07
2:K:11:VAL:HG23	2:K:157:PRO:HG3	1.17	1.07
3:M:111:GLY:HA3	3:M:116:GLN:HB2	1.36	1.07
1:B:263:HIS:HB3	1:C:258:GLN:CG	1.55	1.07
1:B:263:HIS:CD2	1:C:258:GLN:OE1	2.06	1.07
3:L:111:GLY:CA	3:L:116:GLN:HB2	1.85	1.07
1:B:196:ILE:CG2	1:B:285:HIS:CG	2.38	1.07
2:K:13[A]:LYS:NZ	2:K:126:THR:OG1	1.87	1.07
1:B:57:ARG:HD2	1:B:225:TRP:HB2	1.37	1.07
1:B:314:THR:HB	1:C:107:LEU:HD22	1.30	1.07
1:C:135:ILE:N	2:K:103:ASN:ND2	2.03	1.07
1:B:255:LEU:CG	1:C:263:HIS:NE2	2.16	1.06
2:H:13[A]:LYS:HD2	2:H:124:ALA:O	1.52	1.06
1:A:138:GLU:HB2	2:H:31:HIS:CE1	1.90	1.06
1:C:196:ILE:CA	1:C:285:HIS:CD2	2.36	1.06
2:H:13[B]:LYS:NZ	2:H:125[B]:SER:HA	1.71	1.06
1:C:194:SER:CA	1:C:196:ILE:HG12	1.61	1.06
1:C:137:TYR:C	2:K:31:HIS:NE2	2.10	1.05
1:A:62:LEU:HD12	1:A:63:ALA:H	1.17	1.05
1:A:191:GLU:HB3	1:B:346:LEU:HD22	1.09	1.04
2:H:13[A]:LYS:HE3	2:H:125[A]:SER:HA	1.32	1.04
1:A:57:ARG:HD2	1:A:225:TRP:HB2	1.37	1.04
1:B:101:TRP:CH2	1:C:149:VAL:CG2	2.38	1.04
1:A:51:ALA:CB	2:H:32:TYR:CE2	2.41	1.03
1:A:191:GLU:CB	1:B:346:LEU:HD22	1.89	1.03
1:B:195:GLY:CA	1:B:196:ILE:HG13	1.88	1.03
1:A:136:LYS:CD	2:H:31:HIS:CA	2.10	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ALA:N	1:C:260:GLY:HA3	1.73	1.03
1:B:108:PHE:N	1:C:316:ALA:CB	2.22	1.03
1:B:314:THR:HB	1:C:107:LEU:HD21	1.41	1.03
1:A:282:THR:N	1:A:283:SER:CA	2.16	1.02
1:B:196:ILE:HA	1:B:285:HIS:HD2	1.06	1.02
1:B:258:GLN:CB	1:C:263:HIS:N	2.01	1.02
1:C:27:GLY:HA2	1:C:282:THR:O	1.56	1.02
1:C:195:GLY:H	1:C:196:ILE:CA	1.68	1.02
2:K:13[A]:LYS:NZ	2:K:126:THR:CB	2.22	1.02
1:B:108:PHE:O	1:C:316:ALA:HB1	1.60	1.02
1:C:136:LYS:CE	2:K:31:HIS:HA	1.90	1.02
1:A:334:GLY:HA2	1:A:365:ALA:HA	1.42	1.02
1:B:258:GLN:HG3	1:C:264:GLN:N	1.72	1.01
1:C:57:ARG:HD2	1:C:225:TRP:HB2	1.37	1.01
1:A:194:SER:C	1:A:196:ILE:HG23	1.80	1.01
1:B:196:ILE:CA	1:B:285:HIS:HD2	1.72	1.01
2:K:13[A]:LYS:HE3	2:K:125[A]:SER:HA	1.04	1.01
1:C:136:LYS:HD3	2:K:31:HIS:CB	1.90	1.00
1:C:194:SER:C	1:C:196:ILE:HG12	1.75	1.00
1:B:195:GLY:N	1:B:196:ILE:HG13	1.63	1.00
1:B:260:GLY:HA2	1:C:258:GLN:HG2	1.39	1.00
1:B:101:TRP:CE3	1:C:149:VAL:HA	1.96	1.00
1:B:258:GLN:HB3	1:C:263:HIS:H	0.84	1.00
1:B:334:GLY:HA2	1:B:365:ALA:HA	1.42	0.99
1:C:196:ILE:HG22	1:C:285:HIS:CG	1.86	0.99
2:K:11:VAL:HG21	2:K:157:PRO:HD3	1.41	0.99
2:K:13[A]:LYS:HZ1	2:K:126:THR:CB	1.74	0.99
2:K:13[A]:LYS:CE	2:K:126:THR:N	2.21	0.99
1:B:101:TRP:CE3	1:C:372:LEU:HD12	1.98	0.99
3:L:111:GLY:HA3	3:L:116:GLN:HB2	1.39	0.99
1:B:194:SER:CB	1:B:196:ILE:HG12	1.92	0.99
1:C:27:GLY:HA3	1:C:282:THR:O	1.63	0.98
1:A:281:LEU:C	1:A:283:SER:N	2.17	0.98
1:C:133:GLU:HB3	2:K:104:TYR:HE2	1.16	0.98
1:C:195:GLY:N	1:C:196:ILE:HG12	1.72	0.98
1:A:51:ALA:HB1	2:H:32:TYR:CD2	1.99	0.98
1:B:194:SER:HB2	1:B:196:ILE:HG12	1.45	0.98
1:B:243:GLU:HG2	1:B:245:PRO:HG3	1.45	0.98
1:B:194:SER:HB2	1:B:196:ILE:HD13	1.42	0.97
1:C:136:LYS:CD	2:K:31:HIS:C	2.32	0.97
1:C:135:ILE:N	2:K:103:ASN:HD21	1.26	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:SER:HG	2:K:54:SER:HB2	1.21	0.97
2:K:123[A]:SER:OG	2:K:124:ALA:HA	1.03	0.97
1:C:334:GLY:HA2	1:C:365:ALA:HA	1.42	0.96
1:C:194:SER:C	1:C:196:ILE:HG13	1.83	0.96
1:A:131:LEU:HD21	1:C:76:THR:CG2	1.91	0.96
1:B:263:HIS:CA	1:C:258:GLN:HG3	1.94	0.96
1:B:52:ASN:ND2	1:B:134:ASN:CB	2.25	0.96
1:A:136:LYS:HD3	2:H:31:HIS:CB	1.94	0.96
1:B:69:SER:HB3	1:B:82:ASN:HD21	1.30	0.96
1:A:191:GLU:HB3	1:B:346:LEU:CD2	1.94	0.96
1:B:15:VAL:HG12	1:B:16:SER:H	1.31	0.96
1:A:136:LYS:HG3	1:A:170:THR:HG22	1.48	0.96
1:B:258:GLN:HG3	1:C:264:GLN:H	1.27	0.96
1:C:15:VAL:HG12	1:C:16:SER:H	1.31	0.95
1:A:69:SER:HB3	1:A:82:ASN:HD21	1.31	0.95
1:B:52:ASN:HB2	1:B:134:ASN:ND2	1.80	0.95
2:K:13[A]:LYS:HZ1	2:K:126:THR:H	0.97	0.95
1:C:134:ASN:OD1	2:K:100:TRP:CH2	2.20	0.95
1:C:243:GLU:HG2	1:C:245:PRO:HG3	1.45	0.95
1:B:52:ASN:HB2	1:B:134:ASN:HD22	1.29	0.95
2:K:11:VAL:HG21	2:K:157:PRO:HG3	1.09	0.95
1:B:194:SER:CA	1:B:196:ILE:HG12	1.97	0.95
1:B:263:HIS:HB3	1:C:258:GLN:HG3	1.06	0.95
1:A:307:LYS:HG2	1:A:331:GLY:HA2	1.49	0.94
1:B:101:TRP:HH2	1:C:326:GLU:HB2	1.29	0.94
1:C:136:LYS:HG3	1:C:170:THR:HG22	1.48	0.94
1:A:243:GLU:HG2	1:A:245:PRO:HG3	1.45	0.94
1:C:133:GLU:CB	2:K:104:TYR:HE2	1.79	0.94
1:C:138:GLU:OE1	2:K:28:THR:HG23	1.67	0.94
1:B:136:LYS:HG3	1:B:170:THR:HG22	1.48	0.94
1:B:261:ALA:H	1:C:260:GLY:C	1.67	0.94
1:C:136:LYS:HE2	2:K:30:THR:O	1.68	0.94
1:B:195:GLY:N	1:B:196:ILE:N	2.16	0.93
1:C:69:SER:HB3	1:C:82:ASN:HD21	1.31	0.93
1:A:168:SER:OG	2:H:54:SER:HB2	1.67	0.93
1:C:307:LYS:HG2	1:C:331:GLY:HA2	1.49	0.93
2:K:13[A]:LYS:CD	2:K:125[A]:SER:HA	1.97	0.93
1:B:194:SER:CB	1:B:196:ILE:HD13	1.94	0.93
1:A:15:VAL:HG12	1:A:16:SER:H	1.31	0.93
1:A:200:ALA:O	1:A:215:ARG:HG2	1.69	0.92
1:B:149:VAL:HG13	1:C:101:TRP:CB	2.00	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:HB2	2:K:31:HIS:CE1	2.03	0.92
1:B:258:GLN:CG	1:C:260:GLY:HA2	1.99	0.92
3:L:111:GLY:CA	3:L:116:GLN:CB	2.45	0.92
1:C:52:ASN:CG	2:K:100:TRP:CZ3	2.43	0.92
1:C:51:ALA:O	2:K:101:GLY:O	1.66	0.92
1:B:200:ALA:O	1:B:215:ARG:HG2	1.69	0.92
1:B:108:PHE:HB2	1:C:316:ALA:CB	2.00	0.92
1:B:307:LYS:HG2	1:B:331:GLY:HA2	1.49	0.92
2:K:121:VAL:C	2:K:156:PHE:HZ	1.73	0.91
1:B:196:ILE:CG2	1:B:285:HIS:CD2	2.54	0.91
1:B:195:GLY:H	1:B:196:ILE:HG12	1.23	0.91
1:B:196:ILE:CA	1:B:285:HIS:CD2	2.50	0.91
1:B:75:PRO:O	1:B:76:THR:HG22	1.71	0.91
1:C:14:GLY:HA3	1:C:21:VAL:HG22	1.53	0.91
2:H:13[A]:LYS:HE3	2:H:126:THR:H	1.35	0.90
1:C:200:ALA:O	1:C:215:ARG:HG2	1.69	0.90
1:A:131:LEU:HD21	1:C:76:THR:HG23	1.50	0.90
1:A:195:GLY:H	1:A:196:ILE:HG23	1.29	0.90
1:B:14:GLY:HA3	1:B:21:VAL:HG22	1.53	0.90
1:B:194:SER:CB	1:B:196:ILE:CG1	2.43	0.90
1:B:52:ASN:ND2	1:B:134:ASN:ND2	2.14	0.89
1:C:75:PRO:O	1:C:76:THR:HG22	1.71	0.89
1:A:62:LEU:HD11	1:A:121:CYS:HA	1.54	0.89
1:B:62:LEU:HD11	1:B:121:CYS:HA	1.55	0.89
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.20	0.89
1:A:75:PRO:O	1:A:76:THR:HG22	1.71	0.89
1:B:195:GLY:C	1:B:197:ASP:C	2.30	0.89
1:C:62:LEU:HD11	1:C:121:CYS:HA	1.54	0.88
1:A:14:GLY:HA3	1:A:21:VAL:HG22	1.53	0.88
1:B:194:SER:C	1:B:196:ILE:CG1	2.33	0.88
1:C:168:SER:OG	2:K:54:SER:CB	2.21	0.88
1:C:195:GLY:CA	1:C:196:ILE:HG13	2.03	0.88
2:H:13[A]:LYS:CE	2:H:126:THR:H	1.87	0.88
2:K:11:VAL:HG11	2:K:212:PRO:HB3	1.55	0.88
1:B:108:PHE:CD2	1:C:324:VAL:HB	2.09	0.88
1:B:258:GLN:HB3	1:C:263:HIS:N	1.56	0.87
1:B:52:ASN:ND2	1:B:134:ASN:HB3	1.86	0.87
3:L:111:GLY:HA3	3:L:116:GLN:HB3	1.55	0.87
1:B:73:ALA:HB3	1:B:112:SER:HB3	1.57	0.87
2:K:35:HIS:HD2	2:K:47:TRP:HE1	1.20	0.87
1:A:73:ALA:HB3	1:A:112:SER:HB3	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:NDG:H4	4:F:2:NDG:N2	1.91	0.86
4:E:1:NDG:H4	4:E:2:NDG:N2	1.90	0.86
1:B:261:ALA:N	1:C:260:GLY:CA	2.34	0.86
1:C:52:ASN:CG	2:K:100:TRP:HZ3	1.79	0.86
1:B:108:PHE:CB	1:C:316:ALA:HB3	2.06	0.86
1:A:282:THR:O	1:A:284:GLY:O	1.94	0.86
1:C:73:ALA:HB3	1:C:112:SER:HB3	1.57	0.85
1:C:196:ILE:CG2	1:C:285:HIS:CG	2.56	0.85
2:H:122:SER:O	2:H:124:ALA:O	1.93	0.85
1:A:193:ARG:NH1	1:B:345:SER:OG	2.08	0.85
1:A:194:SER:O	1:A:196:ILE:HG12	1.75	0.85
1:A:51:ALA:HB2	2:H:32:TYR:CE2	2.09	0.85
1:C:48:MET:CE	1:C:282:THR:O	2.24	0.85
2:K:123[A]:SER:HG	2:K:124:ALA:HA	1.39	0.85
1:C:195:GLY:C	1:C:196:ILE:HG13	1.97	0.85
1:A:137:TYR:C	2:H:31:HIS:NE2	2.31	0.85
1:B:263:HIS:HB2	1:C:258:GLN:OE1	1.75	0.85
1:C:135:ILE:H	2:K:103:ASN:ND2	1.75	0.85
1:A:193:ARG:NH1	1:B:345:SER:CB	2.40	0.84
1:C:15:VAL:HB	1:C:18:ALA:HB2	1.59	0.84
4:D:1:NDG:H4	4:D:2:NDG:N2	1.90	0.84
1:A:15:VAL:HB	1:A:18:ALA:HB2	1.59	0.84
1:A:133:GLU:OE2	1:B:311:PHE:CB	2.25	0.84
1:A:233:TRP:HZ2	1:C:85:ARG:CG	1.91	0.84
1:B:260:GLY:CA	1:C:258:GLN:HG2	2.06	0.84
1:C:48:MET:HE3	1:C:282:THR:O	1.76	0.84
1:C:70:THR:HA	1:C:115:THR:HG22	1.59	0.84
1:B:259:GLU:HG3	1:C:257:SER:O	1.78	0.84
2:H:13[A]:LYS:HE3	2:H:126:THR:N	1.91	0.84
2:H:13[B]:LYS:HZ3	2:H:125[B]:SER:HA	1.39	0.84
1:A:62:LEU:HD12	1:A:63:ALA:N	1.93	0.84
1:C:67:ASP:HB2	1:C:90:PHE:HE1	1.43	0.84
2:K:13[A]:LYS:HZ1	2:K:126:THR:N	1.55	0.84
1:B:67:ASP:HB2	1:B:90:PHE:HE1	1.43	0.84
1:C:137:TYR:O	2:K:31:HIS:NE2	2.11	0.84
1:B:15:VAL:HB	1:B:18:ALA:HB2	1.59	0.83
1:C:62:LEU:HD12	1:C:63:ALA:N	1.93	0.83
1:C:136:LYS:HD2	2:K:31:HIS:C	1.98	0.83
1:B:62:LEU:HD12	1:B:63:ALA:N	1.93	0.83
2:H:13[A]:LYS:HE3	2:H:125[A]:SER:CA	2.06	0.83
1:B:101:TRP:CZ3	1:C:372:LEU:HD12	2.14	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLN:HB2	1:C:263:HIS:H	1.43	0.83
1:B:255:LEU:HD21	1:C:263:HIS:CE1	2.14	0.83
1:B:263:HIS:CG	1:C:258:GLN:OE1	2.25	0.83
2:K:13[A]:LYS:HE3	2:K:126:THR:N	1.87	0.83
1:B:101:TRP:CZ2	1:C:326:GLU:CB	2.59	0.82
2:K:13[A]:LYS:HD2	2:K:124:ALA:O	1.79	0.82
1:A:51:ALA:HB1	2:H:32:TYR:CE2	2.09	0.82
1:A:281:LEU:HB3	1:A:283:SER:C	1.99	0.82
1:B:255:LEU:HD11	1:C:266:LEU:HD22	1.59	0.82
1:B:261:ALA:N	1:C:260:GLY:C	2.31	0.82
1:B:314:THR:CB	1:C:107:LEU:HD22	2.07	0.82
1:B:263:HIS:CG	1:C:258:GLN:NE2	2.46	0.82
1:A:67:ASP:HB2	1:A:90:PHE:HE1	1.43	0.82
1:C:135:ILE:H	2:K:103:ASN:HD21	1.23	0.82
3:L:111:GLY:HA3	3:L:116:GLN:N	1.94	0.82
1:A:56:VAL:HG21	1:A:129:THR:HG23	1.61	0.82
1:C:281:LEU:HB3	1:C:283:SER:O	1.80	0.82
1:C:134:ASN:OD1	2:K:100:TRP:HH2	1.59	0.82
1:B:101:TRP:CH2	1:C:149:VAL:HG23	2.14	0.81
1:A:70:THR:HA	1:A:115:THR:HG22	1.60	0.81
1:B:194:SER:CB	1:B:196:ILE:HD11	1.97	0.81
1:B:226:SER:OG	1:B:232:VAL:HG12	1.80	0.81
1:B:388:ARG:HD2	1:B:389:GLY:N	1.94	0.81
1:A:388:ARG:HD2	1:A:389:GLY:N	1.95	0.81
1:B:190:CYS:HB3	1:B:286:LEU:HD11	1.63	0.81
1:B:257:SER:C	1:C:259:GLU:HB3	2.00	0.81
1:B:324:VAL:HB	1:C:108:PHE:CD2	2.15	0.81
3:L:111:GLY:HA2	3:L:116:GLN:HB2	1.60	0.81
1:A:226:SER:OG	1:A:232:VAL:HG12	1.80	0.81
1:B:70:THR:HA	1:B:115:THR:HG22	1.59	0.81
2:K:13[A]:LYS:HZ1	2:K:126:THR:CA	1.94	0.81
1:A:85:ARG:NH1	1:C:231:THR:HG21	1.95	0.80
1:A:169:ILE:HD13	1:A:190:CYS:HB2	1.63	0.80
1:B:56:VAL:HG21	1:B:129:THR:HG23	1.61	0.80
1:B:195:GLY:C	1:B:196:ILE:CG1	2.35	0.80
1:C:56:VAL:HG21	1:C:129:THR:HG23	1.61	0.80
1:C:99:ARG:HB2	1:C:103:ASN:HD21	1.46	0.80
1:B:99:ARG:HB2	1:B:103:ASN:HD21	1.46	0.80
1:C:195:GLY:N	1:C:196:ILE:N	2.27	0.80
1:C:226:SER:OG	1:C:232:VAL:HG12	1.80	0.80
1:A:136:LYS:HD2	2:H:31:HIS:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HD13	1:C:190:CYS:HB2	1.63	0.80
1:C:388:ARG:HD2	1:C:389:GLY:N	1.95	0.80
1:B:155:TYR:O	1:B:159:VAL:HG23	1.82	0.79
1:A:190:CYS:HB3	1:A:286:LEU:HD11	1.63	0.79
1:B:197:ASP:HB3	1:B:201:TYR:CE2	2.18	0.79
2:K:13[A]:LYS:HZ2	2:K:126:THR:N	1.79	0.79
1:A:99:ARG:HB2	1:A:103:ASN:HD21	1.46	0.79
1:B:260:GLY:N	1:C:260:GLY:CA	2.43	0.79
1:B:263:HIS:HB2	1:C:258:GLN:CB	2.11	0.79
1:B:255:LEU:HD11	1:C:266:LEU:CD2	2.13	0.79
1:C:197:ASP:HB3	1:C:201:TYR:CE2	2.18	0.79
1:C:62:LEU:HD21	1:C:121:CYS:HA	1.65	0.79
1:A:136:LYS:HE2	2:H:30:THR:C	2.02	0.78
1:B:169:ILE:HD13	1:B:190:CYS:HB2	1.63	0.78
1:B:195:GLY:CA	1:B:196:ILE:CG1	2.56	0.78
1:C:133:GLU:HB3	2:K:104:TYR:CD2	2.17	0.78
1:A:155:TYR:O	1:A:159:VAL:HG23	1.82	0.78
1:B:108:PHE:CA	1:C:316:ALA:HB1	2.13	0.78
1:C:53:LEU:HD22	1:C:129:THR:O	1.83	0.78
2:K:13[A]:LYS:HE3	2:K:126:THR:H	1.40	0.78
1:B:52:ASN:CB	1:B:134:ASN:ND2	2.46	0.78
1:B:149:VAL:HG22	1:C:101:TRP:CE3	2.18	0.78
1:A:233:TRP:HZ2	1:C:85:ARG:HG2	1.47	0.78
1:B:53:LEU:HD22	1:B:129:THR:O	1.83	0.78
1:C:190:CYS:HB3	1:C:286:LEU:HD11	1.63	0.78
1:A:197:ASP:HB3	1:A:201:TYR:CE2	2.18	0.78
1:B:62:LEU:HD21	1:B:121:CYS:HA	1.65	0.78
3:M:111:GLY:HA3	3:M:116:GLN:CB	2.12	0.78
1:A:282:THR:H	1:A:283:SER:HA	1.49	0.78
1:C:155:TYR:O	1:C:159:VAL:HG23	1.82	0.78
1:C:52:ASN:OD1	2:K:100:TRP:CZ3	2.37	0.78
1:B:101:TRP:CE3	1:C:149:VAL:CA	2.57	0.77
1:B:258:GLN:HG2	1:C:260:GLY:C	2.04	0.77
1:A:53:LEU:HD22	1:A:129:THR:O	1.83	0.77
1:A:168:SER:HG	2:H:54:SER:HB2	1.49	0.77
1:C:138:GLU:N	2:K:31:HIS:NE2	2.32	0.77
1:C:48:MET:CE	1:C:282:THR:C	2.53	0.77
2:K:13[A]:LYS:NZ	2:K:126:THR:CA	2.47	0.77
1:A:48:MET:HE1	1:A:282:THR:O	1.85	0.77
1:C:195:GLY:C	1:C:197:ASP:O	2.05	0.77
1:A:136:LYS:HE2	2:H:31:HIS:HA	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:O	2:H:31:HIS:NE2	2.18	0.77
1:B:258:GLN:CG	1:C:260:GLY:O	2.34	0.76
2:K:13[B]:LYS:NZ	2:K:125[B]:SER:CA	2.46	0.76
1:B:101:TRP:HE3	1:C:149:VAL:HA	1.47	0.76
1:A:62:LEU:HD21	1:A:121:CYS:HA	1.65	0.76
1:B:240:MET:SD	1:C:266:LEU:HD21	2.25	0.76
1:C:196:ILE:HA	1:C:285:HIS:HD2	0.73	0.76
1:B:379:PHE:HA	1:B:399:LYS:HB3	1.68	0.76
1:C:121:CYS:SG	1:C:124:LYS:HG2	2.26	0.76
1:C:379:PHE:HA	1:C:399:LYS:HB3	1.68	0.76
1:B:258:GLN:HG2	1:C:260:GLY:O	1.86	0.76
1:A:136:LYS:CD	2:H:31:HIS:C	2.54	0.75
1:A:121:CYS:SG	1:A:124:LYS:HG2	2.26	0.75
1:B:121:CYS:SG	1:B:124:LYS:HG2	2.26	0.75
2:H:11:VAL:CG2	2:H:157:PRO:CG	2.30	0.75
1:A:379:PHE:HA	1:A:399:LYS:HB3	1.68	0.75
1:C:245:PRO:HG2	1:C:250:GLN:CG	2.17	0.75
1:A:48:MET:CE	1:A:282:THR:O	2.33	0.75
1:A:136:LYS:HE3	2:H:30:THR:O	1.86	0.75
1:B:101:TRP:HE3	1:C:372:LEU:HD12	1.46	0.75
1:C:136:LYS:CE	2:K:30:THR:O	2.34	0.75
2:K:13[A]:LYS:HZ1	2:K:126:THR:HB	1.51	0.75
1:B:245:PRO:HG2	1:B:250:GLN:CG	2.17	0.75
2:H:13[A]:LYS:NZ	2:H:126:THR:H	1.85	0.75
1:C:136:LYS:CD	2:K:31:HIS:O	2.24	0.74
1:B:260:GLY:H	1:C:259:GLU:C	1.90	0.74
1:B:263:HIS:N	1:C:258:GLN:HG3	2.01	0.74
1:A:245:PRO:HG2	1:A:250:GLN:CG	2.17	0.74
1:B:195:GLY:H	1:B:196:ILE:CA	1.99	0.74
1:C:329:TYR:CE2	1:C:331:GLY:HA3	2.23	0.74
1:A:322:THR:HG22	1:A:376:GLU:HB3	1.70	0.74
1:B:108:PHE:CA	1:C:316:ALA:CB	2.65	0.74
1:B:322:THR:HG22	1:B:376:GLU:HB3	1.70	0.74
1:B:329:TYR:CE2	1:B:331:GLY:HA3	2.23	0.74
1:C:322:THR:HG22	1:C:376:GLU:HB3	1.70	0.74
1:A:329:TYR:CE2	1:A:331:GLY:HA3	2.23	0.74
1:C:342:SER:HB3	1:C:353:GLY:HA3	1.70	0.74
1:B:108:PHE:C	1:C:316:ALA:HB1	2.08	0.73
2:H:13[A]:LYS:NZ	2:H:126:THR:CB	2.50	0.73
1:C:282:THR:H	1:C:283:SER:N	1.87	0.73
2:K:11:VAL:HB	2:K:157:PRO:HG3	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:NH1	1:B:345:SER:HB3	2.03	0.73
1:A:282:THR:C	1:A:284:GLY:H	1.91	0.73
1:C:138:GLU:CD	2:K:28:THR:HG21	2.06	0.73
1:B:342:SER:HB3	1:B:353:GLY:HA3	1.70	0.72
1:B:357:THR:O	1:B:360:PRO:HG3	1.90	0.72
1:A:15:VAL:HG12	1:A:16:SER:N	2.04	0.72
1:A:357:THR:O	1:A:360:PRO:HG3	1.90	0.72
1:C:27:GLY:N	1:C:282:THR:O	2.22	0.72
1:C:357:THR:O	1:C:360:PRO:HG3	1.90	0.72
2:K:13[B]:LYS:HZ3	2:K:125[B]:SER:CA	1.89	0.72
1:A:342:SER:HB3	1:A:353:GLY:HA3	1.70	0.72
1:C:136:LYS:HD3	2:K:31:HIS:HA	0.73	0.72
1:A:364:VAL:HG12	1:A:366:THR:H	1.55	0.71
1:A:136:LYS:HD3	2:H:31:HIS:HA	0.71	0.71
1:B:263:HIS:HD2	1:C:258:GLN:OE1	1.73	0.71
2:H:191[A]:VAL:HG21	3:L:143:LEU:CD1	2.20	0.71
2:H:160[B]:VAL:HG23	2:H:188:LEU:HD21	1.71	0.71
2:H:11:VAL:CB	2:H:157:PRO:HG3	2.21	0.71
1:B:108:PHE:N	1:C:316:ALA:HB1	2.04	0.71
3:L:111:GLY:HA3	3:L:116:GLN:CA	2.20	0.71
2:K:160[B]:VAL:HG23	2:K:188:LEU:HD21	1.72	0.71
1:C:195:GLY:H	1:C:196:ILE:CG1	1.77	0.70
1:A:282:THR:N	1:A:283:SER:HA	2.02	0.70
1:B:258:GLN:CG	1:C:260:GLY:CA	2.66	0.70
2:K:191[A]:VAL:HG21	3:M:143:LEU:CD1	2.20	0.70
1:C:208:THR:HB	1:C:209:LYS:HZ3	1.56	0.70
1:C:137:TYR:C	2:K:31:HIS:CE1	2.64	0.70
1:C:364:VAL:HG12	1:C:366:THR:H	1.55	0.70
2:K:13[A]:LYS:HD2	2:K:125[A]:SER:HA	1.71	0.70
1:A:282:THR:C	1:A:284:GLY:N	2.44	0.70
1:B:208:THR:HB	1:B:209:LYS:HZ3	1.56	0.70
1:A:334:GLY:HA2	1:A:365:ALA:CA	2.21	0.70
1:C:138:GLU:HB2	2:K:31:HIS:NE2	2.06	0.70
1:B:364:VAL:HG12	1:B:366:THR:H	1.55	0.70
1:C:62:LEU:CD1	1:C:63:ALA:H	2.02	0.70
1:B:149:VAL:HG11	1:C:101:TRP:HB3	1.72	0.69
1:B:195:GLY:N	1:B:196:ILE:CA	2.54	0.69
2:K:34[B]:MET:HG3	2:K:79:VAL:HG21	1.74	0.69
3:M:111:GLY:CA	3:M:116:GLN:HB2	2.20	0.69
1:C:15:VAL:HG12	1:C:16:SER:N	2.04	0.69
2:K:11:VAL:HG23	2:K:157:PRO:CG	1.95	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:CB	1:C:108:PHE:CE2	2.67	0.69
1:B:15:VAL:HG12	1:B:16:SER:N	2.04	0.69
1:A:244:GLU:N	1:A:245:PRO:HD3	2.07	0.69
2:H:34[B]:MET:HE2	2:H:96[B]:CYS:SG	2.32	0.69
1:C:244:GLU:N	1:C:245:PRO:HD3	2.08	0.69
1:B:51:ALA:O	1:B:52:ASN:ND2	2.25	0.69
1:B:54:ALA:O	1:B:128:ARG:HB3	1.93	0.69
1:B:108:PHE:CB	1:C:316:ALA:CB	2.68	0.69
1:C:23:LEU:HD12	1:C:24:VAL:H	1.58	0.69
1:C:138:GLU:N	2:K:31:HIS:CE1	2.61	0.69
1:B:99:ARG:CB	1:B:103:ASN:HD21	2.06	0.68
1:C:54:ALA:O	1:C:128:ARG:HB3	1.93	0.68
1:B:281:LEU:HB3	1:B:283:SER:O	1.93	0.68
1:A:54:ALA:O	1:A:128:ARG:HB3	1.93	0.68
1:C:99:ARG:CB	1:C:103:ASN:HD21	2.06	0.68
2:H:34[B]:MET:HG3	2:H:79:VAL:HG21	1.75	0.68
1:A:23:LEU:HD12	1:A:24:VAL:H	1.58	0.68
2:H:13[A]:LYS:CE	2:H:125[A]:SER:HA	2.16	0.68
1:B:23:LEU:HD12	1:B:24:VAL:H	1.58	0.68
3:M:128:PRO:HD3	3:M:140[A]:LEU:CD2	2.24	0.68
2:K:120:THR:HG21	2:K:157:PRO:CB	2.24	0.68
1:A:136:LYS:HD2	2:H:31:HIS:C	2.14	0.67
1:C:375:LEU:HD12	1:C:375:LEU:O	1.94	0.67
2:H:160[B]:VAL:CG2	2:H:188:LEU:HD21	2.24	0.67
3:M:35:ASN:HD22	3:M:50:TYR:HA	1.58	0.67
1:A:99:ARG:CB	1:A:103:ASN:HD21	2.06	0.67
1:B:108:PHE:N	1:C:316:ALA:HB2	1.96	0.67
1:B:334:GLY:HA2	1:B:365:ALA:CA	2.21	0.67
2:H:13[A]:LYS:NZ	2:H:126:THR:N	2.42	0.67
1:A:233:TRP:CZ2	1:C:85:ARG:CG	2.75	0.67
1:B:255:LEU:HD21	1:C:263:HIS:HE1	1.58	0.67
1:C:195:GLY:H	1:C:196:ILE:CB	2.06	0.67
1:B:325:LEU:C	1:B:325:LEU:HD12	2.15	0.67
1:C:325:LEU:C	1:C:325:LEU:HD12	2.15	0.67
1:A:193:ARG:HH12	1:B:345:SER:CB	2.02	0.67
1:B:244:GLU:N	1:B:245:PRO:HD3	2.07	0.67
1:B:375:LEU:HD12	1:B:375:LEU:O	1.94	0.67
2:H:13[A]:LYS:CE	2:H:126:THR:N	2.53	0.67
2:K:160[B]:VAL:CG2	2:K:188:LEU:HD21	2.24	0.67
1:B:62:LEU:CD1	1:B:63:ALA:H	2.02	0.67
1:A:51:ALA:CB	2:H:32:TYR:CD2	2.74	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ALA:O	1:B:215:ARG:CG	2.43	0.66
1:B:281:LEU:HA	1:B:283:SER:N	2.10	0.66
1:C:48:MET:SD	1:C:282:THR:C	2.73	0.66
1:C:90:PHE:CE1	1:C:118:LYS:HB2	2.31	0.66
3:L:128:PRO:HD3	3:L:140[A]:LEU:CD2	2.24	0.66
1:A:325:LEU:C	1:A:325:LEU:HD12	2.15	0.66
1:A:375:LEU:HD12	1:A:375:LEU:O	1.94	0.66
1:B:257:SER:C	1:C:259:GLU:CB	2.59	0.66
1:C:136:LYS:HE2	2:K:31:HIS:HA	1.78	0.66
1:A:200:ALA:O	1:A:215:ARG:CG	2.43	0.66
1:A:90:PHE:CE1	1:A:118:LYS:HB2	2.31	0.66
3:M:140[A]:LEU:HD12	3:M:186:LEU:HD23	1.78	0.66
1:A:241:GLU:HG3	1:A:242:PHE:N	2.11	0.66
1:C:195:GLY:N	1:C:196:ILE:CB	2.59	0.66
3:L:175:GLN:HE21	3:L:181:ALA:HB2	1.60	0.66
1:A:274:PHE:HD2	1:A:279:VAL:HG22	1.61	0.66
3:L:35:ASN:HD22	3:L:50:TYR:HA	1.58	0.66
1:A:87:ASP:C	1:A:89:ALA:H	1.99	0.66
1:B:241:GLU:HG3	1:B:242:PHE:N	2.11	0.66
1:B:274:PHE:HD2	1:B:279:VAL:HG22	1.61	0.66
3:L:140[A]:LEU:HD12	3:L:186:LEU:HD23	1.78	0.66
1:A:136:LYS:HE2	2:H:31:HIS:CA	2.25	0.66
1:B:90:PHE:CE1	1:B:118:LYS:HB2	2.31	0.65
1:B:101:TRP:HH2	1:C:326:GLU:CA	2.09	0.65
1:C:334:GLY:HA2	1:C:365:ALA:CA	2.21	0.65
1:C:87:ASP:C	1:C:89:ALA:H	1.99	0.65
1:C:274:PHE:HD2	1:C:279:VAL:HG22	1.61	0.65
1:C:62:LEU:HD11	1:C:121:CYS:CA	2.27	0.65
1:C:241:GLU:HG3	1:C:242:PHE:N	2.11	0.65
2:H:13[B]:LYS:HG2	2:H:124:ALA:O	1.96	0.65
1:C:196:ILE:HG22	1:C:285:HIS:CD2	2.31	0.65
1:A:132:LYS:HG3	1:A:199:ASN:HD22	1.62	0.65
1:C:309:PHE:O	1:C:393:ILE:HD13	1.97	0.65
2:H:13[B]:LYS:HZ2	2:H:125[B]:SER:HA	1.60	0.65
1:B:258:GLN:HB2	1:C:263:HIS:N	2.02	0.64
1:C:133:GLU:CG	2:K:104:TYR:HE2	2.08	0.64
2:K:120:THR:CG2	2:K:157:PRO:CB	2.75	0.64
1:B:309:PHE:O	1:B:393:ILE:HD13	1.97	0.64
1:C:200:ALA:O	1:C:215:ARG:CG	2.43	0.64
1:A:62:LEU:HD11	1:A:121:CYS:CA	2.27	0.64
1:A:168:SER:HB3	2:H:30:THR:OG1	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:PHE:O	1:A:393:ILE:HD13	1.97	0.64
1:C:48:MET:SD	1:C:282:THR:CA	2.85	0.64
1:C:213:VAL:HG12	1:C:269:ALA:HB2	1.80	0.64
2:K:120:THR:HG21	2:K:157:PRO:HB2	1.80	0.64
3:M:175:GLN:HE21	3:M:181:ALA:HB2	1.60	0.64
1:A:136:LYS:HD3	2:H:31:HIS:CG	2.33	0.64
1:A:245:PRO:HG2	1:A:250:GLN:HG3	1.79	0.64
1:B:45:MET:HE1	1:B:48:MET:HG3	1.80	0.64
1:B:69:SER:O	1:B:115:THR:HB	1.98	0.64
1:B:87:ASP:C	1:B:89:ALA:H	1.99	0.64
1:B:69:SER:HB3	1:B:82:ASN:ND2	2.10	0.64
1:C:69:SER:O	1:C:115:THR:HB	1.98	0.64
1:B:255:LEU:CD2	1:C:263:HIS:CE1	2.81	0.64
1:C:52:ASN:ND2	2:K:100:TRP:CH2	2.63	0.64
1:C:364:VAL:HG12	1:C:365:ALA:N	2.13	0.63
1:C:245:PRO:HG2	1:C:250:GLN:HG3	1.79	0.63
2:K:13[B]:LYS:HG2	2:K:124:ALA:O	1.98	0.63
1:B:132:LYS:HG3	1:B:199:ASN:HD22	1.61	0.63
1:B:213:VAL:HG12	1:B:269:ALA:HB2	1.80	0.63
1:B:364:VAL:HG12	1:B:365:ALA:N	2.14	0.63
1:A:97:VAL:HG23	1:A:113:ILE:HD12	1.81	0.63
1:A:364:VAL:HG12	1:A:365:ALA:N	2.14	0.63
1:A:62:LEU:CD1	1:A:63:ALA:H	2.02	0.63
1:B:62:LEU:HD11	1:B:121:CYS:CA	2.27	0.63
1:B:263:HIS:CD2	1:C:258:GLN:CD	2.61	0.63
1:C:202:TYR:CD2	1:C:215:ARG:HA	2.34	0.63
1:C:232:VAL:HG23	1:C:235:ASN:HD21	1.64	0.63
1:A:69:SER:HB3	1:A:82:ASN:ND2	2.10	0.63
1:B:343:VAL:HG13	1:B:348:ASP:HB2	1.81	0.63
1:C:69:SER:HB3	1:C:82:ASN:ND2	2.10	0.63
1:A:69:SER:O	1:A:115:THR:HB	1.98	0.63
1:A:85:ARG:HH12	1:C:231:THR:HG21	1.63	0.63
1:B:97:VAL:HG23	1:B:113:ILE:HD12	1.81	0.63
1:B:132:LYS:HG3	1:B:199:ASN:ND2	2.14	0.63
1:A:52:ASN:HD21	2:H:100:TRP:HZ3	0.85	0.62
1:A:132:LYS:HG3	1:A:199:ASN:ND2	2.14	0.62
1:C:52:ASN:OD1	2:K:100:TRP:CE3	2.51	0.62
1:A:202:TYR:CD2	1:A:215:ARG:HA	2.34	0.62
1:A:232:VAL:HG23	1:A:235:ASN:HD21	1.64	0.62
1:B:243:GLU:HG2	1:B:245:PRO:CG	2.27	0.62
1:C:132:LYS:HG3	1:C:199:ASN:HD22	1.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HB2	1:A:103:ASN:ND2	2.13	0.62
1:B:246:HIS:ND1	1:B:248:THR:HB	2.15	0.62
1:C:99:ARG:HB2	1:C:103:ASN:ND2	2.13	0.62
1:C:281:LEU:HA	1:C:283:SER:N	2.14	0.62
1:B:245:PRO:HG2	1:B:250:GLN:HG3	1.79	0.62
1:C:57:ARG:HG3	1:C:58:SER:N	2.15	0.62
1:C:246:HIS:ND1	1:C:248:THR:HB	2.15	0.62
1:A:213:VAL:HG12	1:A:269:ALA:HB2	1.80	0.62
1:A:246:HIS:ND1	1:A:248:THR:HB	2.15	0.62
1:A:62:LEU:CD1	1:A:121:CYS:HA	2.28	0.62
1:A:208:THR:HB	1:A:209:LYS:NZ	2.15	0.62
1:B:202:TYR:CD2	1:B:215:ARG:HA	2.34	0.62
1:B:255:LEU:CD2	1:C:263:HIS:NE2	2.62	0.62
1:C:89:ALA:O	1:C:118:LYS:HG3	2.00	0.62
1:B:2:ASN:H	1:B:2:ASN:HD22	1.47	0.62
1:C:48:MET:HE1	1:C:282:THR:C	2.19	0.62
1:C:97:VAL:HG23	1:C:113:ILE:HD12	1.81	0.62
1:C:132:LYS:HG3	1:C:199:ASN:ND2	2.14	0.62
1:C:204:MET:HB2	1:C:213:VAL:HG22	1.82	0.62
1:A:166:ARG:HH11	1:A:166:ARG:HB3	1.65	0.62
1:C:91:VAL:HG21	1:C:238:THR:HG21	1.82	0.62
1:C:138:GLU:CA	2:K:31:HIS:NE2	2.63	0.62
1:B:99:ARG:HB2	1:B:103:ASN:ND2	2.13	0.62
1:B:195:GLY:H	1:B:196:ILE:CG1	1.76	0.62
1:B:204:MET:HB2	1:B:213:VAL:HG22	1.82	0.62
1:B:232:VAL:HG23	1:B:235:ASN:HD21	1.64	0.62
1:B:62:LEU:CD1	1:B:121:CYS:HA	2.28	0.61
1:B:263:HIS:HB3	1:C:258:GLN:CD	1.91	0.61
1:C:338:VAL:HG23	1:C:361:PHE:HA	1.82	0.61
2:K:34[B]:MET:HE2	2:K:96[B]:CYS:SG	2.40	0.61
1:A:65:VAL:HG13	1:A:252:VAL:HG12	1.83	0.61
1:B:57:ARG:HG3	1:B:58:SER:N	2.15	0.61
1:C:2:ASN:HD22	1:C:2:ASN:H	1.47	0.61
1:B:195:GLY:CA	1:B:196:ILE:N	2.63	0.61
1:A:51:ALA:HB2	2:H:32:TYR:CZ	2.36	0.61
1:A:57:ARG:HG3	1:A:58:SER:N	2.15	0.61
1:A:338:VAL:HG23	1:A:361:PHE:HA	1.82	0.61
1:A:343:VAL:HG13	1:A:348:ASP:HB2	1.81	0.61
1:B:255:LEU:CD1	1:C:266:LEU:CD2	2.78	0.61
1:B:166:ARG:HH11	1:B:166:ARG:HB3	1.65	0.61
1:C:343:VAL:HG13	1:C:348:ASP:HB2	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:CG2	1:A:283:SER:HA	2.31	0.61
1:B:89:ALA:O	1:B:118:LYS:HG3	2.00	0.61
1:C:65:VAL:HG13	1:C:252:VAL:HG12	1.83	0.61
2:H:227:ASP:OD2	2:H:230:HIS:HD2	1.84	0.61
1:A:243:GLU:HG2	1:A:245:PRO:CG	2.27	0.61
1:C:166:ARG:HH11	1:C:166:ARG:HB3	1.65	0.61
1:C:208:THR:HB	1:C:209:LYS:NZ	2.15	0.61
1:C:62:LEU:CD1	1:C:121:CYS:HA	2.28	0.61
1:C:62:LEU:CD1	1:C:122:SER:N	2.64	0.61
2:K:227:ASP:OD2	2:K:230:HIS:HD2	1.84	0.61
1:A:62:LEU:CD1	1:A:122:SER:N	2.64	0.61
1:A:388:ARG:HA	1:A:392:GLN:HB2	1.83	0.61
1:B:208:THR:HB	1:B:209:LYS:NZ	2.15	0.61
1:A:89:ALA:O	1:A:118:LYS:HG3	2.00	0.60
1:B:338:VAL:HG23	1:B:361:PHE:HA	1.82	0.60
1:A:91:VAL:HG21	1:A:238:THR:HG21	1.82	0.60
1:B:91:VAL:HG21	1:B:238:THR:HG21	1.82	0.60
1:C:62:LEU:HD11	1:C:122:SER:N	2.17	0.60
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.66	0.60
1:A:62:LEU:HD11	1:A:122:SER:N	2.17	0.60
1:A:134:ASN:HA	2:H:103:ASN:N	2.15	0.60
1:B:48:MET:O	1:B:280:LYS:HA	2.02	0.60
1:C:197:ASP:HB3	1:C:201:TYR:HE2	1.65	0.60
1:A:22:ASP:HB3	1:A:287:LYS:NZ	2.17	0.60
1:A:204:MET:HB2	1:A:213:VAL:HG22	1.82	0.60
1:B:388:ARG:HA	1:B:392:GLN:HB2	1.83	0.60
1:C:364:VAL:HG12	1:C:365:ALA:H	1.67	0.60
1:A:168:SER:OG	2:H:54:SER:CB	2.44	0.60
1:A:259:GLU:OE1	1:A:262:LEU:HD12	2.02	0.60
1:C:243:GLU:HG2	1:C:245:PRO:CG	2.26	0.60
1:C:388:ARG:HA	1:C:392:GLN:HB2	1.84	0.60
1:A:62:LEU:HD13	1:A:122:SER:H	1.67	0.59
1:B:62:LEU:CD1	1:B:122:SER:N	2.64	0.59
2:K:120:THR:CG2	2:K:157:PRO:HB3	2.32	0.59
1:A:194:SER:C	1:A:196:ILE:HG12	2.22	0.59
1:B:259:GLU:OE1	1:B:262:LEU:HD12	2.02	0.59
1:B:329:TYR:O	1:B:368:ASN:HA	2.02	0.59
2:K:13[A]:LYS:CD	2:K:125[A]:SER:CA	2.78	0.59
1:B:62:LEU:HD11	1:B:122:SER:N	2.17	0.59
1:B:258:GLN:N	1:C:263:HIS:HB2	2.18	0.59
1:C:97:VAL:CG2	1:C:113:ILE:HD12	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HG2	1:C:128:ARG:HH11	1.66	0.59
1:C:329:TYR:O	1:C:368:ASN:HA	2.02	0.59
1:A:2:ASN:HD22	1:A:2:ASN:H	1.48	0.59
1:B:65:VAL:HG13	1:B:252:VAL:HG12	1.83	0.59
1:A:97:VAL:CG2	1:A:113:ILE:HD12	2.32	0.59
1:B:62:LEU:HD13	1:B:122:SER:H	1.67	0.59
1:B:195:GLY:N	1:B:196:ILE:CB	2.65	0.59
1:B:196:ILE:N	1:B:285:HIS:HD2	2.00	0.59
1:C:138:GLU:CB	2:K:31:HIS:NE2	2.65	0.59
1:B:197:ASP:HB3	1:B:201:TYR:HE2	1.65	0.59
1:C:74:CYS:HB2	1:C:77:MET:HG3	1.84	0.59
1:B:332:THR:HA	1:B:367:ALA:HB2	1.85	0.59
1:B:368:ASN:HD22	3:L:97:ASN:HD21	0.59	0.59
1:C:190:CYS:HB3	1:C:286:LEU:HD21	1.84	0.59
1:A:329:TYR:O	1:A:368:ASN:HA	2.02	0.59
2:H:11:VAL:HG21	2:H:157:PRO:CD	2.29	0.59
1:B:97:VAL:CG2	1:B:113:ILE:HD12	2.32	0.59
1:B:258:GLN:CG	1:C:264:GLN:H	2.09	0.59
1:B:345:SER:O	1:B:348:ASP:OD1	2.21	0.59
1:C:259:GLU:OE1	1:C:262:LEU:HD12	2.02	0.59
2:K:11:VAL:HB	2:K:157:PRO:CG	2.30	0.59
2:K:13[A]:LYS:CE	2:K:125[A]:SER:CA	2.51	0.59
1:A:332:THR:HA	1:A:367:ALA:HB2	1.85	0.58
1:B:22:ASP:HB3	1:B:287:LYS:NZ	2.17	0.58
1:C:22:ASP:HB3	1:C:287:LYS:NZ	2.17	0.58
1:B:74:CYS:HB2	1:B:77:MET:HG3	1.84	0.58
1:C:332:THR:HA	1:C:367:ALA:HB2	1.85	0.58
1:B:23:LEU:HD11	1:B:31:VAL:HG21	1.85	0.58
1:A:364:VAL:HG12	1:A:365:ALA:H	1.67	0.58
1:B:364:VAL:HG12	1:B:365:ALA:H	1.67	0.58
1:C:150:GLU:HG2	1:C:151:SER:N	2.18	0.58
1:C:345:SER:O	1:C:348:ASP:OD1	2.21	0.58
2:K:120:THR:CG2	2:K:157:PRO:HB2	2.33	0.58
1:C:45:MET:HE1	1:C:48:MET:HG3	1.86	0.58
1:A:150:GLU:HG2	1:A:151:SER:N	2.18	0.58
1:A:380:GLY:HA2	1:A:398:HIS:CE1	2.39	0.58
1:B:101:TRP:HH2	1:C:326:GLU:CB	1.94	0.58
1:B:128:ARG:HH11	1:B:128:ARG:HG2	1.66	0.58
1:A:74:CYS:HB2	1:A:77:MET:HG3	1.84	0.58
1:A:143:VAL:HG21	1:A:180:LEU:HD13	1.86	0.58
2:H:122:SER:O	2:H:156:PHE:HE1	1.81	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:CYS:HB3	1:B:286:LEU:HD21	1.85	0.58
1:C:62:LEU:HD13	1:C:122:SER:H	1.67	0.58
1:A:340:ILE:HG21	1:A:373:ILE:HD13	1.86	0.58
1:A:190:CYS:HB3	1:A:286:LEU:HD21	1.85	0.58
1:A:263:HIS:O	1:A:266:LEU:HB2	2.04	0.58
1:B:108:PHE:HD2	1:C:324:VAL:HB	1.63	0.58
1:B:263:HIS:O	1:B:266:LEU:HB2	2.04	0.58
1:B:281:LEU:HD13	1:B:283:SER:O	2.04	0.58
1:A:194:SER:HB2	1:A:196:ILE:CG2	2.33	0.57
1:B:108:PHE:CE2	1:C:324:VAL:HG11	2.39	0.57
1:A:48:MET:SD	1:A:282:THR:HA	2.43	0.57
1:B:150:GLU:HG2	1:B:151:SER:N	2.18	0.57
1:C:380:GLY:HA2	1:C:398:HIS:CE1	2.39	0.57
1:B:48:MET:HB2	1:B:281:LEU:H	1.67	0.57
1:C:57:ARG:HD2	1:C:225:TRP:CB	2.25	0.57
1:C:90:PHE:HD1	1:C:117:ALA:C	2.08	0.57
1:C:143:VAL:HG21	1:C:180:LEU:HD13	1.86	0.57
1:C:194:SER:HB2	1:C:196:ILE:CG2	2.33	0.57
1:A:23:LEU:HD11	1:A:31:VAL:HG21	1.85	0.57
1:B:380:GLY:HA2	1:B:398:HIS:CE1	2.39	0.57
1:C:23:LEU:HD11	1:C:31:VAL:HG21	1.85	0.57
1:C:340:ILE:HG21	1:C:373:ILE:HD13	1.86	0.57
1:A:67:ASP:HB2	1:A:90:PHE:CE1	2.33	0.57
1:B:90:PHE:HD1	1:B:117:ALA:C	2.08	0.57
1:B:246:HIS:CE1	1:B:249:LYS:H	2.23	0.57
1:A:345:SER:O	1:A:348:ASP:OD1	2.21	0.57
1:B:61:TYR:HD2	1:B:257:SER:HB3	1.70	0.57
1:C:191:GLU:O	1:C:193:ARG:N	2.38	0.57
1:A:90:PHE:HD1	1:A:117:ALA:C	2.08	0.57
1:B:15:VAL:CG1	1:B:16:SER:H	2.12	0.57
1:B:61:TYR:CD2	1:B:257:SER:HB3	2.40	0.57
1:B:191:GLU:O	1:B:193:ARG:N	2.38	0.57
1:C:196:ILE:HB	1:C:284:GLY:HA2	1.87	0.57
1:C:263:HIS:O	1:C:266:LEU:HB2	2.04	0.57
1:A:194:SER:CB	1:A:196:ILE:HG23	2.35	0.56
1:A:245:PRO:HG2	1:A:250:GLN:CB	2.35	0.56
1:C:61:TYR:CD2	1:C:257:SER:HB3	2.40	0.56
1:C:61:TYR:HD2	1:C:257:SER:HB3	1.70	0.56
1:A:61:TYR:CD2	1:A:257:SER:HB3	2.40	0.56
1:A:61:TYR:HD2	1:A:257:SER:HB3	1.70	0.56
1:A:191:GLU:O	1:A:193:ARG:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:SER:HB2	1:A:196:ILE:HG23	1.87	0.56
1:A:197:ASP:HB3	1:A:201:TYR:HE2	1.65	0.56
1:B:143:VAL:HG21	1:B:180:LEU:HD13	1.86	0.56
1:B:195:GLY:H	1:B:196:ILE:CB	2.16	0.56
1:B:286:LEU:HG	1:B:288:CYS:SG	2.46	0.56
1:B:340:ILE:HG21	1:B:373:ILE:HD13	1.86	0.56
1:C:62:LEU:CD2	1:C:121:CYS:HA	2.35	0.56
1:A:246:HIS:CE1	1:A:249:LYS:H	2.23	0.56
1:B:263:HIS:H	1:C:258:GLN:HG3	1.70	0.56
1:C:136:LYS:CE	2:K:31:HIS:CA	2.70	0.56
1:A:87:ASP:O	1:A:89:ALA:N	2.39	0.56
1:A:225:TRP:HE1	1:A:234:ARG:HG3	1.70	0.56
1:B:101:TRP:CZ3	1:C:372:LEU:CD1	2.87	0.56
1:C:245:PRO:HG2	1:C:250:GLN:CB	2.35	0.56
1:A:62:LEU:CD2	1:A:121:CYS:HA	2.35	0.56
1:B:190:CYS:CB	1:B:286:LEU:HD21	2.36	0.56
1:B:287:LYS:C	1:B:287:LYS:HD3	2.26	0.56
1:C:87:ASP:O	1:C:89:ALA:N	2.39	0.56
1:C:225:TRP:HE1	1:C:234:ARG:HG3	1.70	0.56
1:A:168:SER:HB2	2:H:31:HIS:HD2	1.71	0.56
1:A:286:LEU:HG	1:A:288:CYS:SG	2.46	0.56
1:C:287:LYS:HD3	1:C:287:LYS:C	2.26	0.56
1:A:136:LYS:HG3	1:A:170:THR:CG2	2.31	0.56
1:B:101:TRP:HZ3	1:C:372:LEU:CG	2.18	0.56
1:B:213:VAL:HG12	1:B:269:ALA:CB	2.36	0.56
3:L:111:GLY:CA	3:L:116:GLN:N	2.65	0.56
1:C:57:ARG:HB3	1:C:218:PHE:CZ	2.41	0.56
1:C:246:HIS:CE1	1:C:249:LYS:H	2.23	0.56
1:B:70:THR:HG22	1:B:115:THR:CG2	2.36	0.55
1:B:258:GLN:CG	1:C:260:GLY:C	2.73	0.55
1:A:191:GLU:CB	1:B:346:LEU:CD2	2.67	0.55
1:A:260:GLY:O	1:A:264:GLN:HG2	2.06	0.55
1:B:57:ARG:HB3	1:B:218:PHE:CZ	2.41	0.55
1:B:245:PRO:HG2	1:B:250:GLN:CB	2.35	0.55
1:C:136:LYS:HE2	2:K:31:HIS:CA	2.36	0.55
1:C:256:GLY:O	1:C:258:GLN:OE1	2.24	0.55
1:A:256:GLY:O	1:A:258:GLN:OE1	2.24	0.55
1:C:15:VAL:CG1	1:C:16:SER:H	2.12	0.55
1:C:154:ASN:OD1	1:C:157:THR:N	2.32	0.55
1:C:286:LEU:HG	1:C:288:CYS:SG	2.46	0.55
1:A:287:LYS:HD3	1:A:287:LYS:C	2.26	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PHE:C	1:B:244:GLU:H	2.08	0.55
1:C:62:LEU:CD1	1:C:122:SER:H	2.19	0.55
1:A:168:SER:HB2	2:H:31:HIS:CD2	2.41	0.55
1:B:225:TRP:HE1	1:B:234:ARG:HG3	1.70	0.55
1:C:213:VAL:HG12	1:C:269:ALA:CB	2.36	0.55
1:C:260:GLY:O	1:C:264:GLN:HG2	2.06	0.55
1:A:190:CYS:CB	1:A:286:LEU:HD21	2.36	0.55
1:B:259:GLU:CG	1:C:257:SER:O	2.53	0.55
1:C:14:GLY:CA	1:C:21:VAL:HG22	2.33	0.55
1:A:70:THR:HG22	1:A:115:THR:CG2	2.36	0.55
1:A:213:VAL:HG12	1:A:269:ALA:CB	2.36	0.55
1:B:45:MET:HE1	1:B:48:MET:CG	2.37	0.55
1:B:240:MET:SD	1:C:266:LEU:CD2	2.93	0.55
2:H:123[B]:SER:OG	2:H:124:ALA:HB1	1.94	0.55
1:A:45:MET:SD	1:A:48:MET:HE2	2.46	0.55
1:B:260:GLY:O	1:B:264:GLN:HG2	2.06	0.55
1:B:263:HIS:CB	1:C:258:GLN:NE2	2.61	0.55
1:B:263:HIS:NE2	1:C:255:LEU:HD21	2.22	0.55
1:B:281:LEU:HB3	1:B:283:SER:C	2.28	0.55
1:C:70:THR:HG22	1:C:115:THR:CG2	2.36	0.55
1:C:242:PHE:C	1:C:244:GLU:N	2.60	0.55
1:B:87:ASP:O	1:B:89:ALA:N	2.39	0.55
1:A:242:PHE:C	1:A:244:GLU:H	2.08	0.55
1:B:67:ASP:HB2	1:B:90:PHE:CE1	2.34	0.55
3:M:34:VAL:H	3:M:52:ASN:ND2	2.05	0.55
1:B:154:ASN:OD1	1:B:157:THR:N	2.32	0.54
1:C:133:GLU:CB	2:K:104:TYR:CE2	2.60	0.54
4:F:1:NDG:C4	4:F:2:NDG:N2	2.69	0.54
1:C:51:ALA:O	1:C:134:ASN:HB3	2.08	0.54
1:C:242:PHE:C	1:C:244:GLU:H	2.08	0.54
2:K:13[A]:LYS:HD2	2:K:124:ALA:C	2.26	0.54
1:C:195:GLY:N	1:C:196:ILE:CA	2.38	0.54
1:A:57:ARG:HB3	1:A:218:PHE:CZ	2.41	0.54
1:B:98:ASP:OD1	1:B:110:LYS:HE2	2.07	0.54
3:L:145[A]:SER:HB2	3:L:175:GLN:HE22	1.73	0.54
3:M:145[A]:SER:HB2	3:M:175:GLN:HE22	1.73	0.54
1:B:62:LEU:CD2	1:B:121:CYS:HA	2.35	0.54
1:B:234:ARG:C	1:B:236:ARG:H	2.10	0.54
2:H:13[A]:LYS:HD2	2:H:124:ALA:C	2.26	0.54
1:A:126:ILE:HG13	1:A:205:THR:HB	1.90	0.54
1:A:193:ARG:CD	1:B:383:TYR:HE1	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:CYS:CB	1:C:286:LEU:HD21	2.36	0.54
1:A:48:MET:HE3	1:A:282:THR:O	2.06	0.54
1:B:51:ALA:O	1:B:134:ASN:HB3	2.08	0.54
1:B:108:PHE:CD2	1:C:324:VAL:CB	2.89	0.54
1:A:15:VAL:CG1	1:A:16:SER:H	2.12	0.54
4:E:1:NDG:C4	4:E:2:NDG:N2	2.69	0.54
1:A:62:LEU:CD1	1:A:122:SER:H	2.19	0.54
1:B:242:PHE:C	1:B:244:GLU:N	2.60	0.54
1:C:68:LEU:HD22	1:C:252:VAL:CG2	2.38	0.54
1:C:134:ASN:CG	2:K:100:TRP:CZ3	2.81	0.54
1:A:51:ALA:O	1:A:134:ASN:HB3	2.08	0.54
1:A:138:GLU:HB2	2:H:31:HIS:NE2	2.20	0.54
1:B:257:SER:O	1:C:259:GLU:HB2	1.99	0.54
1:C:202:TYR:CE2	1:C:215:ARG:HD3	2.43	0.54
1:B:143:VAL:CG2	1:B:180:LEU:HD13	2.38	0.53
3:L:34:VAL:H	3:L:52:ASN:ND2	2.05	0.53
1:A:154:ASN:OD1	1:A:156:SER:HB2	2.08	0.53
1:B:68:LEU:HD22	1:B:252:VAL:CG2	2.38	0.53
1:C:98:ASP:OD1	1:C:110:LYS:HE2	2.07	0.53
1:C:154:ASN:OD1	1:C:156:SER:HB2	2.09	0.53
1:C:234:ARG:C	1:C:236:ARG:H	2.10	0.53
1:A:98:ASP:OD1	1:A:110:LYS:HE2	2.07	0.53
1:A:143:VAL:CG2	1:A:180:LEU:HD13	2.38	0.53
1:A:234:ARG:C	1:A:236:ARG:H	2.10	0.53
1:A:68:LEU:HD22	1:A:252:VAL:CG2	2.38	0.53
1:B:62:LEU:CD1	1:B:122:SER:H	2.19	0.53
1:B:154:ASN:OD1	1:B:156:SER:HB2	2.08	0.53
1:C:67:ASP:HB2	1:C:90:PHE:CE1	2.33	0.53
1:B:126:ILE:HG13	1:B:205:THR:HB	1.90	0.53
1:B:202:TYR:CE2	1:B:215:ARG:HD3	2.43	0.53
1:C:235:ASN:O	1:C:238:THR:HG22	2.09	0.53
1:A:191:GLU:CA	1:B:346:LEU:HD22	2.39	0.53
1:C:143:VAL:CG2	1:C:180:LEU:HD13	2.38	0.53
1:C:342:SER:HB3	1:C:353:GLY:CA	2.39	0.53
1:A:212:LEU:O	1:A:269:ALA:HB1	2.09	0.53
1:B:235:ASN:O	1:B:238:THR:HG22	2.09	0.53
2:H:11:VAL:HG21	2:H:157:PRO:HG3	0.60	0.53
1:A:242:PHE:C	1:A:244:GLU:N	2.60	0.53
1:C:126:ILE:HG13	1:C:205:THR:HB	1.90	0.53
1:B:48:MET:CE	1:B:282:THR:C	2.77	0.52
1:B:59:TYR:HA	1:B:224:PRO:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:HA	1:A:224:PRO:O	2.10	0.52
1:B:149:VAL:HG22	1:C:101:TRP:CD2	2.44	0.52
3:M:128:PRO:HD3	3:M:140[A]:LEU:HD23	1.91	0.52
1:A:202:TYR:CE2	1:A:215:ARG:HD3	2.43	0.52
1:A:57:ARG:HD2	1:A:225:TRP:CB	2.25	0.52
1:C:59:TYR:HA	1:C:224:PRO:O	2.10	0.52
1:C:212:LEU:O	1:C:269:ALA:HB1	2.09	0.52
2:K:11:VAL:HG23	2:K:157:PRO:CB	2.39	0.52
1:B:149:VAL:CG2	1:C:101:TRP:CE3	2.91	0.52
1:A:235:ASN:O	1:A:238:THR:HG22	2.09	0.52
1:C:94:GLN:HA	1:C:113:ILE:O	2.09	0.52
1:A:14:GLY:CA	1:A:21:VAL:HG22	2.33	0.52
1:A:94:GLN:HA	1:A:113:ILE:O	2.09	0.52
1:A:198:THR:HG22	1:A:200:ALA:H	1.75	0.52
1:B:190:CYS:HB3	1:B:286:LEU:CD1	2.39	0.52
1:B:190:CYS:SG	1:B:286:LEU:HD21	2.50	0.52
1:B:212:LEU:O	1:B:269:ALA:HB1	2.09	0.52
1:A:70:THR:HG22	1:A:115:THR:HG22	1.92	0.52
1:C:83:ASP:C	1:C:85:ARG:H	2.13	0.52
1:B:70:THR:HG22	1:B:115:THR:HG22	1.92	0.52
1:B:94:GLN:HA	1:B:113:ILE:O	2.09	0.52
1:C:67:ASP:O	1:C:68:LEU:HD23	2.10	0.52
1:C:198:THR:HG22	1:C:200:ALA:H	1.75	0.52
1:A:67:ASP:O	1:A:68:LEU:HD23	2.10	0.51
1:A:335:PRO:HA	1:A:362:VAL:O	2.10	0.51
1:A:388:ARG:HD2	1:A:389:GLY:H	1.74	0.51
1:B:67:ASP:O	1:B:68:LEU:HD23	2.10	0.51
1:B:388:ARG:HD2	1:B:389:GLY:H	1.74	0.51
1:C:190:CYS:SG	1:C:286:LEU:HD21	2.50	0.51
3:L:128:PRO:HD3	3:L:140[A]:LEU:HD23	1.91	0.51
1:A:48:MET:HE1	1:A:284:GLY:O	2.11	0.51
1:A:138:GLU:N	2:H:31:HIS:CE1	2.79	0.51
1:A:190:CYS:SG	1:A:286:LEU:HD21	2.50	0.51
1:B:75:PRO:HD2	1:B:105:CYS:SG	2.51	0.51
1:B:346:LEU:HD13	1:B:383:TYR:CE1	2.46	0.51
1:B:388:ARG:CA	1:B:392:GLN:HB2	2.40	0.51
1:C:211:PHE:CE1	1:C:271:PRO:HB3	2.46	0.51
1:C:388:ARG:CA	1:C:392:GLN:HB2	2.40	0.51
2:K:120:THR:CB	2:K:157:PRO:HB2	2.40	0.51
1:A:20:TRP:HZ3	1:A:22:ASP:OD2	1.93	0.51
1:A:75:PRO:HD2	1:A:105:CYS:SG	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:HZ3	1:B:22:ASP:OD2	1.93	0.51
1:B:211:PHE:CE1	1:B:271:PRO:HB3	2.46	0.51
1:C:70:THR:HG22	1:C:115:THR:HG22	1.92	0.51
1:C:243:GLU:CG	1:C:245:PRO:HG3	2.31	0.51
1:C:335:PRO:HA	1:C:362:VAL:O	2.10	0.51
1:B:335:PRO:HA	1:B:362:VAL:O	2.11	0.51
1:A:177:THR:OG1	1:A:187:THR:HG23	2.11	0.51
1:A:282:THR:N	1:A:283:SER:C	2.63	0.51
1:B:42:ASP:CG	1:B:144:HIS:HE2	2.14	0.51
1:B:57:ARG:HG3	1:B:58:SER:H	1.76	0.51
1:B:372:LEU:C	1:B:372:LEU:HD23	2.31	0.51
1:C:346:LEU:HD13	1:C:383:TYR:CE1	2.46	0.51
1:A:83:ASP:C	1:A:85:ARG:H	2.14	0.51
1:A:211:PHE:CE1	1:A:271:PRO:HB3	2.46	0.51
1:A:342:SER:HB3	1:A:353:GLY:CA	2.39	0.51
1:A:388:ARG:CA	1:A:392:GLN:HB2	2.40	0.51
1:B:198:THR:HG22	1:B:200:ALA:H	1.75	0.51
1:C:20:TRP:HZ3	1:C:22:ASP:OD2	1.93	0.51
1:C:359:ASN:N	1:C:360:PRO:HD3	2.26	0.51
1:A:137:TYR:C	2:H:31:HIS:CE1	2.84	0.51
1:A:372:LEU:C	1:A:372:LEU:HD23	2.31	0.51
1:B:83:ASP:C	1:B:85:ARG:H	2.13	0.51
1:B:359:ASN:N	1:B:360:PRO:HD3	2.26	0.51
1:A:224:PRO:HD3	1:A:237:GLU:CG	2.41	0.51
1:A:346:LEU:HD13	1:A:383:TYR:CE1	2.46	0.51
1:B:148:THR:OG1	1:B:150:GLU:HB3	2.11	0.51
1:B:149:VAL:CG1	1:C:101:TRP:CB	2.64	0.51
1:C:57:ARG:CG	1:C:58:SER:N	2.74	0.51
1:C:148:THR:OG1	1:C:150:GLU:HB3	2.11	0.51
1:C:325:LEU:CD1	1:C:327:LEU:HD13	2.41	0.51
1:A:325:LEU:CD1	1:A:327:LEU:HD13	2.41	0.51
1:C:134:ASN:CG	2:K:100:TRP:CH2	2.85	0.51
1:A:27:GLY:H	1:A:48:MET:HE3	1.75	0.51
1:A:154:ASN:OD1	1:A:157:THR:N	2.32	0.51
1:B:47:ASN:HD21	1:B:49:GLU:CD	2.15	0.51
1:B:177:THR:OG1	1:B:187:THR:HG23	2.11	0.51
1:C:42:ASP:CG	1:C:144:HIS:HE2	2.14	0.51
1:C:75:PRO:HD2	1:C:105:CYS:SG	2.51	0.51
1:C:224:PRO:HD3	1:C:237:GLU:CG	2.41	0.51
1:C:372:LEU:C	1:C:372:LEU:HD23	2.31	0.51
1:A:72:ALA:HB2	1:A:247:ALA:HB1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:N	2:H:31:HIS:NE2	2.58	0.50
1:B:101:TRP:HH2	1:C:326:GLU:N	2.08	0.50
1:B:224:PRO:HD3	1:B:237:GLU:CG	2.41	0.50
2:K:11:VAL:CB	2:K:157:PRO:CG	2.63	0.50
1:C:39:PRO:HG3	1:C:297:LEU:HD23	1.93	0.50
1:C:177:THR:OG1	1:C:187:THR:HG23	2.11	0.50
1:A:42:ASP:CG	1:A:144:HIS:HE2	2.14	0.50
1:A:148:THR:OG1	1:A:150:GLU:HB3	2.11	0.50
1:B:136:LYS:HG3	1:B:170:THR:CG2	2.31	0.50
1:C:57:ARG:HG3	1:C:58:SER:H	1.76	0.50
3:L:177:ASN:O	3:L:178:ASN:HB2	2.12	0.50
1:B:39:PRO:HG3	1:B:297:LEU:HD23	1.93	0.50
1:C:314:THR:HG22	1:C:315:PRO:O	2.11	0.50
1:A:57:ARG:CG	1:A:58:SER:N	2.74	0.50
1:A:85:ARG:HH12	1:C:231:THR:CG2	2.24	0.50
1:A:119:PHE:CE2	1:A:235:ASN:HB3	2.47	0.50
1:C:47:ASN:HD21	1:C:49:GLU:CD	2.15	0.50
2:K:120:THR:HB	2:K:157:PRO:HB2	1.93	0.50
1:A:242:PHE:O	1:A:242:PHE:CD1	2.65	0.50
1:B:360:PRO:O	1:B:361:PHE:HB3	2.12	0.50
1:C:119:PHE:CE2	1:C:235:ASN:HB3	2.47	0.50
1:A:307:LYS:CG	1:A:331:GLY:HA2	2.34	0.50
1:B:65:VAL:HG12	1:B:65:VAL:O	2.12	0.50
1:B:119:PHE:CE2	1:B:235:ASN:HB3	2.47	0.50
1:C:242:PHE:CD1	1:C:242:PHE:O	2.65	0.50
1:A:359:ASN:N	1:A:360:PRO:HD3	2.26	0.50
1:B:52:ASN:CG	1:B:134:ASN:ND2	2.64	0.50
1:B:342:SER:HB3	1:B:353:GLY:CA	2.39	0.50
1:A:62:LEU:HD11	1:A:121:CYS:C	2.32	0.50
1:B:23:LEU:HG	1:B:24:VAL:N	2.27	0.50
1:B:57:ARG:HD2	1:B:225:TRP:CB	2.25	0.50
1:C:23:LEU:CD1	1:C:24:VAL:H	2.25	0.50
2:K:121:VAL:O	2:K:156:PHE:HZ	1.94	0.50
1:A:244:GLU:N	1:A:245:PRO:CD	2.75	0.49
1:B:62:LEU:HD21	1:B:121:CYS:CA	2.40	0.49
1:B:210:THR:HB	1:B:272:VAL:O	2.12	0.49
1:B:242:PHE:O	1:B:242:PHE:CD1	2.65	0.49
1:C:45:MET:HE1	1:C:48:MET:CG	2.41	0.49
2:H:35:HIS:HE1	2:H:99:ASP:OD1	1.95	0.49
1:A:74:CYS:O	1:A:77:MET:HB2	2.12	0.49
1:B:23:LEU:CD1	1:B:24:VAL:H	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:CG	1:B:58:SER:N	2.74	0.49
1:B:216:GLU:O	1:B:217:TRP:C	2.51	0.49
1:C:72:ALA:HB2	1:C:247:ALA:HB1	1.93	0.49
1:A:39:PRO:HG3	1:A:297:LEU:HD23	1.93	0.49
1:A:168:SER:CB	2:H:31:HIS:HD2	2.24	0.49
1:B:307:LYS:CG	1:B:331:GLY:HA2	2.34	0.49
1:B:325:LEU:CD1	1:B:327:LEU:HD13	2.41	0.49
1:C:210:THR:HB	1:C:272:VAL:O	2.12	0.49
1:A:62:LEU:HD21	1:A:121:CYS:CA	2.39	0.49
1:A:65:VAL:HG12	1:A:65:VAL:O	2.12	0.49
1:B:48:MET:HE3	1:B:282:THR:O	2.12	0.49
1:C:65:VAL:HG12	1:C:65:VAL:O	2.12	0.49
1:C:136:LYS:HD3	2:K:31:HIS:CG	2.46	0.49
2:K:135:ALA:HB3	2:K:224[B]:LYS:HD3	1.94	0.49
1:A:23:LEU:HG	1:A:24:VAL:N	2.27	0.49
1:A:376:GLU:O	1:A:376:GLU:HG3	2.13	0.49
1:B:62:LEU:HD11	1:B:121:CYS:C	2.32	0.49
1:C:360:PRO:O	1:C:361:PHE:HB3	2.12	0.49
1:A:23:LEU:CD1	1:A:24:VAL:H	2.25	0.49
1:B:261:ALA:HB2	1:C:264:GLN:HG2	1.94	0.49
1:B:314:THR:HG22	1:B:315:PRO:O	2.11	0.49
1:C:62:LEU:HD11	1:C:121:CYS:C	2.32	0.49
1:C:241:GLU:CG	1:C:242:PHE:N	2.76	0.49
1:C:307:LYS:CG	1:C:331:GLY:HA2	2.34	0.49
1:C:343:VAL:HG12	1:C:345:SER:H	1.77	0.49
2:K:35:HIS:HE1	2:K:99:ASP:OD1	1.95	0.49
1:A:47:ASN:HD21	1:A:49:GLU:CD	2.15	0.49
1:A:275:SER:O	1:A:277:ASN:N	2.46	0.49
1:B:72:ALA:HB2	1:B:247:ALA:HB1	1.93	0.49
1:B:376:GLU:O	1:B:376:GLU:HG3	2.13	0.49
1:C:74:CYS:O	1:C:77:MET:HB2	2.12	0.49
1:C:190:CYS:HB3	1:C:286:LEU:CD1	2.38	0.49
1:C:195:GLY:C	1:C:196:ILE:CG1	2.77	0.49
1:C:275:SER:O	1:C:277:ASN:N	2.46	0.49
4:D:1:NDG:H4	4:D:2:NDG:HA	1.73	0.49
1:A:65:VAL:CG1	1:A:252:VAL:HG12	2.42	0.49
1:A:250:GLN:O	1:A:252:VAL:HG23	2.13	0.49
1:A:343:VAL:HG12	1:A:345:SER:H	1.77	0.49
1:B:255:LEU:HG	1:C:263:HIS:CD2	2.36	0.49
1:C:65:VAL:CG1	1:C:252:VAL:HG12	2.42	0.49
1:C:136:LYS:HG3	1:C:170:THR:CG2	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:177:ASN:O	3:M:178:ASN:HB2	2.12	0.49
1:A:138:GLU:CB	2:H:31:HIS:CE1	2.80	0.49
1:B:107:LEU:HD22	1:C:314:THR:O	2.12	0.49
1:C:236:ARG:C	1:C:238:THR:H	2.16	0.49
1:A:70:THR:CA	1:A:115:THR:HG22	2.38	0.49
1:B:325:LEU:N	1:C:101:TRP:CZ3	2.69	0.49
1:C:23:LEU:HG	1:C:24:VAL:N	2.27	0.49
1:A:57:ARG:HG3	1:A:58:SER:H	1.76	0.48
1:A:210:THR:HB	1:A:272:VAL:O	2.12	0.48
1:A:360:PRO:O	1:A:361:PHE:HB3	2.12	0.48
1:B:375:LEU:HD12	1:B:375:LEU:C	2.33	0.48
1:C:99:ARG:HD2	1:C:103:ASN:OD1	2.12	0.48
1:C:216:GLU:O	1:C:217:TRP:C	2.51	0.48
1:A:3:CYS:SG	1:A:42:ASP:HB3	2.54	0.48
1:B:65:VAL:CG1	1:B:252:VAL:HG12	2.42	0.48
1:B:74:CYS:O	1:B:77:MET:HB2	2.12	0.48
1:C:244:GLU:H	1:C:245:PRO:HD3	1.76	0.48
2:H:135:ALA:HB3	2:H:224[B]:LYS:HD3	1.94	0.48
4:D:1:NDG:C4	4:D:2:NDG:N2	2.69	0.48
1:A:179:LYS:HA	1:A:185:GLU:HB3	1.96	0.48
1:A:311:PHE:CD2	1:A:393:ILE:HD12	2.48	0.48
1:B:149:VAL:CG2	1:C:101:TRP:CD2	2.96	0.48
1:C:311:PHE:CE2	1:C:395:HIS:HB2	2.48	0.48
1:A:311:PHE:CE2	1:A:395:HIS:HB2	2.48	0.48
1:B:236:ARG:C	1:B:238:THR:H	2.16	0.48
1:B:250:GLN:O	1:B:252:VAL:HG23	2.13	0.48
1:C:196:ILE:CG2	1:C:285:HIS:CD2	2.92	0.48
1:A:31:VAL:O	1:A:42:ASP:HA	2.13	0.48
1:A:57:ARG:CG	1:A:58:SER:H	2.27	0.48
1:A:190:CYS:HB3	1:A:286:LEU:CD1	2.39	0.48
1:A:195:GLY:H	1:A:196:ILE:CG2	1.99	0.48
1:A:244:GLU:H	1:A:245:PRO:HD3	1.76	0.48
1:A:287:LYS:HD3	1:A:288:CYS:N	2.28	0.48
1:A:314:THR:HG22	1:A:315:PRO:O	2.11	0.48
1:B:99:ARG:HD2	1:B:103:ASN:OD1	2.12	0.48
1:B:368:ASN:ND2	3:L:97:ASN:CG	2.65	0.48
1:C:31:VAL:O	1:C:42:ASP:HA	2.13	0.48
1:C:168:SER:HB2	2:K:31:HIS:HD2	1.78	0.48
1:C:179:LYS:HA	1:C:185:GLU:HB3	1.96	0.48
1:C:250:GLN:O	1:C:252:VAL:HG23	2.13	0.48
4:D:1:NDG:O3	4:D:3:FUL:C1	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:NDG:O3	4:F:3:FUL:C1	2.62	0.48
1:A:99:ARG:HD2	1:A:103:ASN:OD1	2.12	0.48
1:A:375:LEU:HD12	1:A:375:LEU:C	2.33	0.48
1:B:3:CYS:SG	1:B:42:ASP:HB3	2.54	0.48
1:B:179:LYS:HA	1:B:185:GLU:HB3	1.96	0.48
1:B:257:SER:O	1:C:259:GLU:CG	2.56	0.48
1:B:275:SER:O	1:B:277:ASN:N	2.46	0.48
1:B:343:VAL:HG12	1:B:345:SER:H	1.77	0.48
1:C:169:ILE:HD13	1:C:190:CYS:CB	2.41	0.48
1:A:216:GLU:O	1:A:217:TRP:C	2.51	0.48
1:A:258:GLN:O	1:A:258:GLN:HG2	2.14	0.48
1:B:31:VAL:O	1:B:42:ASP:HA	2.13	0.48
1:B:241:GLU:CG	1:B:242:PHE:N	2.76	0.48
1:B:258:GLN:HG3	1:C:260:GLY:O	2.13	0.48
1:B:287:LYS:HD3	1:B:288:CYS:N	2.28	0.48
1:B:311:PHE:CD2	1:B:393:ILE:HD12	2.48	0.48
1:C:311:PHE:CD2	1:C:393:ILE:HD12	2.48	0.48
4:E:1:NDG:O3	4:E:3:FUL:C1	2.62	0.48
1:A:236:ARG:C	1:A:238:THR:H	2.16	0.48
1:A:325:LEU:HD12	1:A:325:LEU:O	2.14	0.48
1:A:259:GLU:OE1	1:A:259:GLU:HA	2.14	0.48
1:B:311:PHE:CE2	1:B:395:HIS:HB2	2.48	0.48
1:C:87:ASP:C	1:C:89:ALA:N	2.66	0.48
1:C:244:GLU:N	1:C:245:PRO:CD	2.75	0.48
1:C:258:GLN:HG2	1:C:258:GLN:O	2.13	0.48
1:C:287:LYS:HD3	1:C:288:CYS:N	2.28	0.48
1:C:375:LEU:HD12	1:C:375:LEU:C	2.33	0.48
1:B:358:VAL:CG1	1:B:359:ASN:HD22	2.27	0.48
1:C:90:PHE:HD1	1:C:118:LYS:N	2.11	0.48
1:C:237:GLU:C	1:C:239:LEU:H	2.16	0.48
1:A:237:GLU:C	1:A:239:LEU:H	2.16	0.47
1:A:307:LYS:HG2	1:A:331:GLY:CA	2.33	0.47
1:B:90:PHE:HD1	1:B:118:LYS:N	2.12	0.47
1:B:244:GLU:H	1:B:245:PRO:HD3	1.76	0.47
1:B:259:GLU:OE1	1:B:259:GLU:HA	2.14	0.47
1:C:196:ILE:N	1:C:285:HIS:HB2	2.28	0.47
1:C:325:LEU:HD12	1:C:325:LEU:O	2.14	0.47
1:A:87:ASP:C	1:A:89:ALA:N	2.66	0.47
1:A:241:GLU:CG	1:A:242:PHE:N	2.76	0.47
1:C:69:SER:O	1:C:115:THR:CB	2.63	0.47
1:C:358:VAL:CG1	1:C:359:ASN:HD22	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:123[B]:SER:HB3	2:K:124:ALA:HA	1.30	0.47
4:E:1:NDG:H8C1	4:E:2:NDG:H3	1.96	0.47
1:A:169:ILE:HD13	1:A:190:CYS:CB	2.41	0.47
1:B:57:ARG:CG	1:B:58:SER:H	2.27	0.47
1:B:195:GLY:C	1:B:197:ASP:O	2.53	0.47
1:C:57:ARG:CG	1:C:58:SER:H	2.27	0.47
1:C:376:GLU:HG3	1:C:376:GLU:O	2.13	0.47
1:A:69:SER:O	1:A:115:THR:CB	2.63	0.47
1:A:76:THR:OG1	1:C:131:LEU:HD21	2.14	0.47
1:A:312:LEU:HD21	1:A:328:GLN:HB2	1.96	0.47
1:B:148:THR:O	1:B:149:VAL:C	2.53	0.47
1:C:3:CYS:SG	1:C:42:ASP:HB3	2.54	0.47
1:C:10:ASP:HB2	1:C:31:VAL:HG22	1.96	0.47
1:C:100:GLY:HA3	1:C:108:PHE:CD1	2.50	0.47
1:C:282:THR:N	1:C:283:SER:N	2.59	0.47
1:A:90:PHE:HD1	1:A:118:LYS:N	2.12	0.47
1:B:48:MET:HE1	1:B:282:THR:C	2.33	0.47
1:C:2:ASN:HD22	1:C:2:ASN:N	2.09	0.47
1:C:58:SER:O	1:C:225:TRP:HA	2.15	0.47
1:C:133:GLU:CG	2:K:104:TYR:CE2	2.95	0.47
1:C:138:GLU:OE1	2:K:28:THR:CG2	2.42	0.47
1:C:222:ASN:O	1:C:223:LEU:HG	2.15	0.47
1:B:48:MET:CE	1:B:282:THR:O	2.62	0.47
1:C:133:GLU:HG2	2:K:104:TYR:HE2	1.80	0.47
1:A:222:ASN:O	1:A:223:LEU:HG	2.15	0.47
1:B:237:GLU:C	1:B:239:LEU:H	2.16	0.47
1:B:257:SER:C	1:C:259:GLU:HB2	2.33	0.47
1:C:47:ASN:HD22	2:K:28:THR:CB	2.17	0.47
1:C:127:GLY:HA2	1:C:203:VAL:O	2.15	0.47
1:C:381:ASP:HA	1:C:397:TRP:O	2.15	0.47
2:K:11:VAL:CG2	2:K:157:PRO:HD3	2.30	0.47
4:E:1:NDG:H4	4:E:2:NDG:HA	1.73	0.47
4:F:1:NDG:H8C1	4:F:2:NDG:H3	1.96	0.47
1:B:263:HIS:H	1:C:258:GLN:CB	2.27	0.47
1:C:70:THR:CA	1:C:115:THR:HG22	2.38	0.47
1:C:259:GLU:OE1	1:C:259:GLU:HA	2.14	0.47
1:C:312:LEU:HD21	1:C:328:GLN:HB2	1.97	0.47
2:K:120:THR:HG22	2:K:157:PRO:HB3	1.97	0.47
4:F:1:NDG:H4	4:F:2:NDG:HA	1.73	0.47
1:A:2:ASN:HD22	1:A:2:ASN:N	2.09	0.47
1:B:14:GLY:CA	1:B:21:VAL:HG22	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASP:HA	1:B:397:TRP:O	2.15	0.47
1:A:10:ASP:HB2	1:A:31:VAL:HG22	1.96	0.47
1:A:100:GLY:HA3	1:A:108:PHE:CD1	2.50	0.47
1:A:194:SER:O	1:A:196:ILE:N	2.48	0.47
1:B:127:GLY:HA2	1:B:203:VAL:O	2.15	0.47
1:B:281:LEU:HD22	1:B:283:SER:O	2.15	0.47
1:B:312:LEU:HD21	1:B:328:GLN:HB2	1.96	0.47
1:A:58:SER:O	1:A:225:TRP:HA	2.15	0.46
1:A:358:VAL:CG1	1:A:359:ASN:HD22	2.27	0.46
1:B:101:TRP:HZ3	1:C:372:LEU:HG	1.79	0.46
1:B:314:THR:CG2	1:C:107:LEU:HD22	2.44	0.46
1:C:168:SER:HB2	2:K:31:HIS:CD2	2.50	0.46
1:C:354:ARG:HB3	1:C:376:GLU:OE1	2.15	0.46
1:B:47:ASN:ND2	1:B:49:GLU:HG3	2.31	0.46
1:B:129:THR:HG23	1:B:202:TYR:HE1	1.80	0.46
1:B:222:ASN:O	1:B:223:LEU:HG	2.15	0.46
1:B:311:PHE:CE2	1:B:393:ILE:HD12	2.50	0.46
1:C:62:LEU:HD21	1:C:121:CYS:CA	2.39	0.46
1:A:23:LEU:CG	1:A:24:VAL:N	2.79	0.46
1:B:58:SER:O	1:B:225:TRP:HA	2.15	0.46
1:B:325:LEU:HD12	1:B:325:LEU:O	2.14	0.46
2:H:191[A]:VAL:HG21	3:L:143:LEU:HD13	1.96	0.46
1:A:47:ASN:ND2	1:A:49:GLU:HG3	2.30	0.46
1:A:129:THR:HG23	1:A:202:TYR:HE1	1.80	0.46
1:A:354:ARG:HB3	1:A:376:GLU:OE1	2.15	0.46
1:B:101:TRP:CH2	1:C:326:GLU:N	2.84	0.46
1:C:48:MET:HE1	1:C:282:THR:O	2.14	0.46
1:C:196:ILE:HG23	1:C:285:HIS:HB2	1.42	0.46
1:C:311:PHE:CE2	1:C:393:ILE:HD12	2.50	0.46
1:A:1:PHE:H3	1:A:1:PHE:HD2	1.61	0.46
1:A:381:ASP:HA	1:A:397:TRP:O	2.15	0.46
1:B:307:LYS:HG2	1:B:331:GLY:CA	2.33	0.46
1:B:342:SER:CB	1:B:353:GLY:HA3	2.44	0.46
1:B:354:ARG:HB3	1:B:376:GLU:OE1	2.15	0.46
1:A:282:THR:C	1:A:284:GLY:O	2.53	0.46
1:B:258:GLN:HB2	1:C:262:LEU:N	2.30	0.46
1:A:166:ARG:HB3	1:A:166:ARG:NH1	2.29	0.46
1:B:10:ASP:HB2	1:B:31:VAL:HG22	1.96	0.46
1:B:100:GLY:HA3	1:B:108:PHE:CD1	2.50	0.46
1:C:138:GLU:CB	2:K:31:HIS:CE1	2.90	0.46
2:K:13[A]:LYS:HA	2:K:124:ALA:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:NDG:H8C1	4:D:2:NDG:H3	1.96	0.46
1:B:56:VAL:HG11	1:B:202:TYR:OH	2.16	0.46
1:C:47:ASN:ND2	1:C:49:GLU:HG3	2.31	0.46
1:A:127:GLY:HA2	1:A:203:VAL:O	2.15	0.46
1:A:194:SER:CA	1:A:196:ILE:HG23	2.43	0.46
1:B:204:MET:HB2	1:B:213:VAL:CG2	2.46	0.46
1:C:60:CYS:HB3	1:C:62:LEU:HD22	1.98	0.46
2:K:132:PHE:HE2	2:K:153[B]:LYS:HD3	1.81	0.46
1:A:282:THR:HG22	1:A:283:SER:HA	1.98	0.45
1:B:71:LYS:HG3	1:B:80:ALA:HB1	1.98	0.45
1:B:266:LEU:HD21	1:C:240:MET:SD	2.57	0.45
1:C:51:ALA:HB1	2:K:101:GLY:HA2	1.79	0.45
1:C:56:VAL:HG11	1:C:202:TYR:OH	2.16	0.45
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.13	0.45
1:B:23:LEU:CG	1:B:24:VAL:N	2.79	0.45
1:B:47:ASN:ND2	1:B:49:GLU:CD	2.70	0.45
1:B:69:SER:O	1:B:115:THR:CB	2.63	0.45
1:B:70:THR:CA	1:B:115:THR:HG22	2.38	0.45
1:B:166:ARG:HB3	1:B:166:ARG:NH1	2.29	0.45
1:C:68:LEU:HD22	1:C:252:VAL:HG21	1.98	0.45
1:C:168:SER:CB	2:K:31:HIS:HD2	2.29	0.45
1:C:388:ARG:HD2	1:C:389:GLY:H	1.75	0.45
1:A:47:ASN:ND2	1:A:49:GLU:CD	2.70	0.45
1:A:311:PHE:CE2	1:A:393:ILE:HD12	2.50	0.45
1:C:23:LEU:CG	1:C:24:VAL:N	2.79	0.45
2:K:13[A]:LYS:HZ2	2:K:126:THR:CA	2.24	0.45
1:A:60:CYS:HB3	1:A:62:LEU:HD22	1.98	0.45
1:A:350:THR:HA	1:A:351:PRO:HD3	1.85	0.45
1:B:255:LEU:CD1	1:C:266:LEU:HD22	2.36	0.45
1:C:47:ASN:ND2	1:C:49:GLU:CD	2.70	0.45
1:C:49:GLU:OE1	2:K:28:THR:HB	2.17	0.45
1:A:194:SER:OG	1:A:196:ILE:HD13	2.15	0.45
1:B:128:ARG:HG2	1:B:128:ARG:NH1	2.32	0.45
1:B:169:ILE:HG23	1:B:174:PRO:HA	1.99	0.45
1:B:275:SER:O	1:B:276:SER:C	2.55	0.45
1:A:208:THR:HB	1:A:209:LYS:HZ3	1.80	0.45
1:C:129:THR:HG23	1:C:202:TYR:HE1	1.81	0.45
1:C:196:ILE:CB	1:C:284:GLY:HA2	2.45	0.45
2:H:132:PHE:HE2	2:H:153[B]:LYS:HD3	1.81	0.45
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.32	0.45
1:A:71:LYS:HG3	1:A:80:ALA:HB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:TYR:CD2	1:B:215:ARG:HD3	2.52	0.45
1:C:202:TYR:HD2	1:C:215:ARG:HA	1.80	0.45
1:C:275:SER:O	1:C:276:SER:C	2.55	0.45
1:A:62:LEU:HD23	1:A:119:PHE:CE1	2.52	0.45
1:B:261:ALA:HB2	1:C:264:GLN:CG	2.46	0.45
1:C:71:LYS:HG3	1:C:80:ALA:HB1	1.98	0.45
2:K:13[B]:LYS:HA	2:K:124:ALA:O	2.15	0.45
1:A:26:GLU:HB3	1:A:285:HIS:ND1	2.32	0.45
1:A:56:VAL:HG11	1:A:202:TYR:OH	2.16	0.45
1:B:62:LEU:HD23	1:B:119:PHE:CE1	2.52	0.45
2:K:191[B]:VAL:HG11	3:M:143:LEU:CD1	2.47	0.45
1:A:148:THR:O	1:A:149:VAL:C	2.53	0.44
1:B:169:ILE:HD13	1:B:190:CYS:CB	2.41	0.44
1:B:211:PHE:CZ	1:B:266:LEU:HD11	2.52	0.44
1:B:322:THR:HG22	1:B:376:GLU:CB	2.44	0.44
1:C:26:GLU:HB3	1:C:285:HIS:ND1	2.32	0.44
1:C:166:ARG:HB3	1:C:166:ARG:NH1	2.29	0.44
3:M:33:THR:HB	3:M:51:GLY:HA2	1.99	0.44
1:A:245:PRO:CG	1:A:250:GLN:HA	2.48	0.44
1:C:169:ILE:HG23	1:C:174:PRO:HA	1.99	0.44
1:C:202:TYR:CD2	1:C:215:ARG:HD3	2.52	0.44
1:C:211:PHE:CZ	1:C:266:LEU:HD11	2.52	0.44
1:C:334:GLY:HA2	1:C:365:ALA:CB	2.48	0.44
1:C:342:SER:CB	1:C:353:GLY:HA3	2.44	0.44
2:K:11:VAL:CG1	2:K:212:PRO:HB3	2.36	0.44
1:A:6:MET:SD	1:A:30:CYS:HB2	2.58	0.44
1:A:258:GLN:CD	1:A:258:GLN:H	2.20	0.44
1:A:367:ALA:O	1:A:368:ASN:OD1	2.35	0.44
1:C:62:LEU:HD23	1:C:119:PHE:CE1	2.52	0.44
1:C:258:GLN:CD	1:C:258:GLN:H	2.20	0.44
3:L:33:THR:HB	3:L:51:GLY:HA2	1.99	0.44
1:A:101:TRP:O	1:A:102:GLY:C	2.56	0.44
1:B:323:VAL:HG22	1:B:375:LEU:HD12	2.00	0.44
1:C:6:MET:SD	1:C:30:CYS:HB2	2.58	0.44
1:C:204:MET:HB2	1:C:213:VAL:CG2	2.46	0.44
1:C:245:PRO:CG	1:C:250:GLN:HA	2.48	0.44
3:L:34:VAL:H	3:L:52:ASN:HD22	1.66	0.44
1:A:195:GLY:C	1:A:197:ASP:N	2.40	0.44
1:A:211:PHE:CZ	1:A:266:LEU:HD11	2.52	0.44
1:B:26:GLU:HB3	1:B:285:HIS:ND1	2.32	0.44
1:B:68:LEU:HD22	1:B:252:VAL:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TRP:HZ3	1:C:372:LEU:HD12	1.78	0.44
1:C:195:GLY:H	1:C:196:ILE:HG12	1.55	0.44
1:A:68:LEU:HD22	1:A:252:VAL:HG21	1.98	0.44
1:A:204:MET:HB2	1:A:213:VAL:CG2	2.46	0.44
1:A:237:GLU:HA	1:A:237:GLU:OE1	2.18	0.44
1:B:196:ILE:CB	1:B:285:HIS:CD2	2.99	0.44
1:B:237:GLU:OE1	1:B:237:GLU:HA	2.18	0.44
1:B:244:GLU:N	1:B:245:PRO:CD	2.75	0.44
1:B:245:PRO:CG	1:B:250:GLN:HA	2.48	0.44
1:B:255:LEU:CD1	1:C:263:HIS:NE2	2.78	0.44
1:B:258:GLN:CD	1:B:258:GLN:H	2.20	0.44
1:C:126:ILE:HD12	1:C:128:ARG:HH21	1.83	0.44
1:C:307:LYS:HG2	1:C:331:GLY:CA	2.33	0.44
1:B:60:CYS:HB3	1:B:62:LEU:HD22	1.98	0.44
1:B:87:ASP:C	1:B:89:ALA:N	2.66	0.44
1:B:101:TRP:O	1:B:102:GLY:C	2.56	0.44
1:B:202:TYR:HD2	1:B:215:ARG:HA	1.80	0.44
1:B:367:ALA:O	1:B:368:ASN:OD1	2.35	0.44
1:C:325:LEU:C	1:C:325:LEU:CD1	2.86	0.44
2:H:191[B]:VAL:HG11	3:L:143:LEU:CD1	2.47	0.44
2:K:52:ASN:C	2:K:52:ASN:HD22	2.21	0.44
1:A:138:GLU:CB	2:H:31:HIS:NE2	2.79	0.44
1:A:138:GLU:CA	2:H:31:HIS:NE2	2.81	0.44
1:A:202:TYR:CD2	1:A:215:ARG:HD3	2.52	0.44
1:A:334:GLY:HA2	1:A:365:ALA:CB	2.48	0.44
1:C:101:TRP:O	1:C:102:GLY:C	2.56	0.44
1:A:136:LYS:HD3	2:H:31:HIS:CD2	2.53	0.44
1:A:364:VAL:CG1	1:A:365:ALA:N	2.81	0.44
1:B:258:GLN:CB	1:C:260:GLY:CA	2.93	0.44
1:B:334:GLY:HA2	1:B:365:ALA:CB	2.48	0.44
1:B:364:VAL:CG1	1:B:365:ALA:N	2.81	0.44
1:A:169:ILE:HG23	1:A:174:PRO:HA	1.99	0.43
1:B:126:ILE:HD12	1:B:128:ARG:HH21	1.83	0.43
1:B:263:HIS:HB3	1:C:258:GLN:NE2	2.30	0.43
1:C:172:ALA:HB2	2:K:103:ASN:O	2.18	0.43
1:C:198:THR:HG22	1:C:199:ASN:OD1	2.18	0.43
2:H:34[B]:MET:CE	2:H:96[B]:CYS:SG	3.05	0.43
2:K:34[B]:MET:CE	2:K:96[B]:CYS:SG	3.05	0.43
1:A:198:THR:HG22	1:A:199:ASN:OD1	2.18	0.43
1:B:198:THR:HG22	1:B:199:ASN:OD1	2.18	0.43
1:C:367:ALA:O	1:C:368:ASN:OD1	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:HB1	2:H:101:GLY:HA2	1.61	0.43
1:C:128:ARG:HG2	1:C:128:ARG:NH1	2.32	0.43
2:H:52:ASN:C	2:H:52:ASN:HD22	2.21	0.43
1:A:14:GLY:HA3	1:A:21:VAL:CG2	2.38	0.43
1:A:322:THR:HG22	1:A:376:GLU:CB	2.44	0.43
1:B:6:MET:SD	1:B:30:CYS:HB2	2.58	0.43
1:B:243:GLU:OE2	1:B:245:PRO:HB3	2.19	0.43
1:A:342:SER:CB	1:A:353:GLY:HA3	2.44	0.43
1:B:196:ILE:CB	1:B:284:GLY:HA2	2.49	0.43
1:C:68:LEU:HD21	1:C:252:VAL:HB	2.01	0.43
1:C:345:SER:O	1:C:346:LEU:C	2.57	0.43
1:A:323:VAL:HG22	1:A:375:LEU:HD12	2.00	0.43
1:B:101:TRP:HZ3	1:C:372:LEU:CD1	2.31	0.43
1:B:243:GLU:CG	1:B:245:PRO:HG3	2.31	0.43
1:C:148:THR:O	1:C:149:VAL:C	2.53	0.43
2:K:35:HIS:CD2	2:K:47:TRP:HE1	2.13	0.43
3:M:34:VAL:H	3:M:52:ASN:HD22	1.66	0.43
1:A:85:ARG:HH21	1:C:233:TRP:HE1	1.65	0.43
1:B:68:LEU:HD21	1:B:252:VAL:HB	2.01	0.43
1:B:263:HIS:CB	1:C:258:GLN:OE1	2.34	0.43
1:A:22:ASP:HB3	1:A:287:LYS:HZ1	1.84	0.43
1:A:275:SER:O	1:A:276:SER:C	2.55	0.43
1:B:101:TRP:HH2	1:C:325:LEU:C	2.21	0.43
3:M:149:PRO:O	3:M:205:HIS:HE1	2.02	0.43
1:A:202:TYR:HD2	1:A:215:ARG:HA	1.80	0.43
1:B:174:PRO:HB3	1:B:192:PRO:HD3	2.01	0.43
1:C:90:PHE:CD1	1:C:118:LYS:N	2.87	0.43
1:C:234:ARG:C	1:C:236:ARG:N	2.72	0.43
1:C:243:GLU:OE2	1:C:245:PRO:HB3	2.19	0.43
1:C:290:VAL:O	1:C:292:MET:HE2	2.19	0.43
1:B:325:LEU:C	1:B:325:LEU:CD1	2.86	0.43
1:C:198:THR:C	1:C:200:ALA:N	2.72	0.43
2:K:121:VAL:C	2:K:156:PHE:CZ	2.61	0.43
2:K:191[A]:VAL:HG21	3:M:143:LEU:HD13	1.96	0.43
1:A:48:MET:SD	1:A:282:THR:CA	3.07	0.42
1:A:90:PHE:CD1	1:A:118:LYS:N	2.87	0.42
1:A:366:THR:O	1:A:367:ALA:O	2.36	0.42
1:B:90:PHE:CD1	1:B:118:LYS:N	2.87	0.42
1:B:101:TRP:CH2	1:C:325:LEU:C	2.93	0.42
1:C:80:ALA:N	1:C:112:SER:OG	2.52	0.42
1:C:85:ARG:HG2	1:C:85:ARG:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:CYS:SG	1:C:106:GLY:N	2.92	0.42
1:A:15:VAL:HB	1:A:18:ALA:CB	2.40	0.42
1:A:68:LEU:HD21	1:A:252:VAL:HB	2.01	0.42
1:A:345:SER:O	1:A:346:LEU:C	2.57	0.42
1:B:22:ASP:HB3	1:B:287:LYS:HZ1	1.83	0.42
1:B:198:THR:C	1:B:200:ALA:N	2.72	0.42
1:B:263:HIS:H	1:C:258:GLN:CG	2.31	0.42
1:B:366:THR:O	1:B:367:ALA:O	2.36	0.42
1:C:15:VAL:HB	1:C:18:ALA:CB	2.40	0.42
1:C:190:CYS:HA	1:C:288:CYS:HA	2.00	0.42
1:C:237:GLU:OE1	1:C:237:GLU:HA	2.18	0.42
1:A:174:PRO:HB3	1:A:192:PRO:HD3	2.01	0.42
1:A:290:VAL:O	1:A:292:MET:HE2	2.19	0.42
1:C:59:TYR:O	1:C:125:ALA:N	2.51	0.42
2:K:13[A]:LYS:CD	2:K:124:ALA:C	2.79	0.42
1:A:52:ASN:ND2	2:H:100:TRP:CE3	2.77	0.42
1:A:131:LEU:HD23	1:C:76:THR:OG1	2.19	0.42
1:B:59:TYR:CD1	1:B:223:LEU:HB2	2.54	0.42
1:B:85:ARG:O	1:B:85:ARG:HG2	2.19	0.42
1:B:258:GLN:HA	1:C:259:GLU:HB3	1.34	0.42
1:C:59:TYR:CD1	1:C:223:LEU:HB2	2.54	0.42
1:C:134:ASN:OD1	2:K:100:TRP:CZ3	2.71	0.42
3:L:111:GLY:C	3:L:116:GLN:N	2.73	0.42
1:A:105:CYS:SG	1:A:106:GLY:N	2.92	0.42
1:C:364:VAL:CG1	1:C:365:ALA:N	2.81	0.42
1:C:366:THR:O	1:C:367:ALA:O	2.36	0.42
1:A:80:ALA:N	1:A:112:SER:OG	2.52	0.42
1:A:198:THR:C	1:A:200:ALA:N	2.72	0.42
1:B:59:TYR:O	1:B:125:ALA:N	2.51	0.42
1:B:65:VAL:HG11	1:B:254:ALA:HA	2.02	0.42
1:B:190:CYS:HA	1:B:288:CYS:HA	2.00	0.42
1:B:246:HIS:CE1	1:B:249:LYS:N	2.87	0.42
1:C:323:VAL:HG22	1:C:375:LEU:HD12	2.00	0.42
1:A:190:CYS:HA	1:A:288:CYS:HA	2.00	0.42
1:A:246:HIS:CE1	1:A:249:LYS:N	2.87	0.42
1:B:1:PHE:H3	1:B:1:PHE:HD2	1.62	0.42
1:B:75:PRO:O	1:B:76:THR:CG2	2.55	0.42
1:B:196:ILE:HB	1:B:284:GLY:HA2	2.00	0.42
1:B:232:VAL:HG23	1:B:235:ASN:ND2	2.34	0.42
1:B:234:ARG:C	1:B:236:ARG:N	2.72	0.42
1:A:59:TYR:CD1	1:A:223:LEU:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:HG2	1:A:85:ARG:O	2.19	0.42
1:A:243:GLU:OE2	1:A:245:PRO:HB3	2.19	0.42
1:A:325:LEU:HD13	1:A:327:LEU:HD13	2.02	0.42
1:A:364:VAL:CG1	1:A:365:ALA:H	2.33	0.42
1:B:108:PHE:CE2	1:C:324:VAL:CG1	3.01	0.42
1:A:282:THR:HG23	1:A:283:SER:HA	2.02	0.42
1:B:80:ALA:N	1:B:112:SER:OG	2.53	0.42
1:B:99:ARG:CD	1:B:103:ASN:OD1	2.68	0.42
1:B:245:PRO:HG2	1:B:250:GLN:HA	2.02	0.42
1:C:126:ILE:O	1:C:205:THR:HB	2.20	0.42
1:C:246:HIS:CE1	1:C:249:LYS:N	2.87	0.42
1:A:99:ARG:CD	1:A:103:ASN:OD1	2.68	0.42
1:A:130:ILE:HG13	1:A:203:VAL:CG2	2.50	0.42
1:A:274:PHE:CD2	1:A:279:VAL:HG22	2.49	0.42
1:B:105:CYS:SG	1:B:106:GLY:N	2.92	0.42
1:C:136:LYS:CE	2:K:31:HIS:C	2.86	0.42
1:C:325:LEU:HD13	1:C:327:LEU:HD13	2.02	0.42
2:K:61:ALA:O	2:K:65[B]:GLN:HG3	2.20	0.42
1:A:27:GLY:N	1:A:48:MET:HE3	2.35	0.41
1:B:261:ALA:CB	1:C:260:GLY:HA3	2.49	0.41
1:B:290:VAL:O	1:B:292:MET:HE2	2.19	0.41
2:H:153[B]:LYS:HZ1	3:L:137:LYS:HD3	1.84	0.41
3:L:149:PRO:O	3:L:205:HIS:HE1	2.02	0.41
1:A:84:LYS:HD2	1:A:90:PHE:CD2	2.55	0.41
1:B:196:ILE:HG23	1:B:285:HIS:HB2	1.38	0.41
1:B:345:SER:O	1:B:346:LEU:C	2.57	0.41
1:C:84:LYS:HD2	1:C:90:PHE:CD2	2.55	0.41
1:A:75:PRO:O	1:A:76:THR:CG2	2.55	0.41
1:A:126:ILE:HD12	1:A:128:ARG:HH21	1.83	0.41
1:A:194:SER:CB	1:A:196:ILE:CG2	2.96	0.41
1:A:214:HIS:O	1:A:215:ARG:C	2.59	0.41
1:A:258:GLN:C	1:A:260:GLY:H	2.23	0.41
1:C:75:PRO:O	1:C:76:THR:CG2	2.55	0.41
1:C:99:ARG:CD	1:C:103:ASN:OD1	2.68	0.41
2:H:61:ALA:O	2:H:65[B]:GLN:HG3	2.20	0.41
1:B:126:ILE:O	1:B:205:THR:HB	2.20	0.41
1:B:329:TYR:CD2	1:B:331:GLY:HA3	2.56	0.41
1:C:92:CYS:HA	1:C:115:THR:O	2.21	0.41
1:C:130:ILE:HG13	1:C:203:VAL:CG2	2.50	0.41
1:C:174:PRO:HB3	1:C:192:PRO:HD3	2.01	0.41
1:C:198:THR:O	1:C:201:TYR:CD2	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:C	1:A:200:ALA:H	2.24	0.41
1:A:245:PRO:HG2	1:A:250:GLN:HA	2.02	0.41
1:A:252:VAL:HG12	1:A:252:VAL:O	2.21	0.41
1:B:84:LYS:HD2	1:B:90:PHE:CD2	2.55	0.41
1:B:130:ILE:HG13	1:B:203:VAL:CG2	2.50	0.41
1:C:67:ASP:CB	1:C:90:PHE:HE1	2.24	0.41
1:A:92:CYS:HA	1:A:115:THR:O	2.21	0.41
1:B:6:MET:CE	1:B:30:CYS:HB2	2.51	0.41
1:B:101:TRP:CE3	1:C:372:LEU:CD1	2.86	0.41
1:B:198:THR:O	1:B:201:TYR:CD2	2.74	0.41
2:H:40:ALA:HB3	2:H:43[B]:GLN:OE1	2.21	0.41
2:K:13[A]:LYS:HD2	2:K:125[A]:SER:CA	2.47	0.41
1:A:329:TYR:CD2	1:A:331:GLY:HA3	2.56	0.41
1:C:336:CYS:O	1:C:361:PHE:HB2	2.21	0.41
1:C:364:VAL:CG1	1:C:365:ALA:H	2.33	0.41
2:K:188:LEU:HD12	2:K:188:LEU:C	2.41	0.41
1:A:194:SER:HB3	1:A:285:HIS:O	2.21	0.41
1:A:325:LEU:C	1:A:325:LEU:CD1	2.86	0.41
1:A:346:LEU:HD13	1:A:383:TYR:CZ	2.56	0.41
1:B:194:SER:HB3	1:B:285:HIS:O	2.21	0.41
1:B:358:VAL:HG12	1:B:359:ASN:HD22	1.86	0.41
1:C:65:VAL:HG11	1:C:254:ALA:HA	2.02	0.41
2:K:40:ALA:HB3	2:K:43[B]:GLN:OE1	2.21	0.41
1:A:6:MET:CE	1:A:30:CYS:HB2	2.51	0.41
1:A:65:VAL:HG11	1:A:254:ALA:HA	2.02	0.41
1:A:81:HIS:CE1	1:A:85:ARG:HD3	2.56	0.41
1:A:149:VAL:HG23	1:A:326:GLU:CD	2.42	0.41
1:A:168:SER:CB	2:H:31:HIS:CD2	3.02	0.41
1:A:198:THR:O	1:A:201:TYR:CD2	2.74	0.41
1:A:358:VAL:HG12	1:A:359:ASN:HD22	1.86	0.41
1:B:15:VAL:HB	1:B:18:ALA:CB	2.40	0.41
1:B:48:MET:HB2	1:B:281:LEU:N	2.34	0.41
1:B:57:ARG:CD	1:B:58:SER:H	2.34	0.41
1:B:91:VAL:N	1:B:117:ALA:O	2.46	0.41
1:B:142:PHE:CG	1:B:143:VAL:N	2.89	0.41
1:B:396:HIS:CG	1:B:397:TRP:N	2.89	0.41
1:C:1:PHE:H3	1:C:1:PHE:HD2	1.63	0.41
1:C:191:GLU:C	1:C:193:ARG:N	2.74	0.41
1:C:214:HIS:O	1:C:215:ARG:C	2.59	0.41
1:A:90:PHE:HA	1:A:117:ALA:O	2.22	0.41
1:A:126:ILE:O	1:A:205:THR:HB	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HG2	1:A:183:TYR:HE2	1.85	0.41
1:A:194:SER:C	1:A:196:ILE:CG2	2.67	0.41
1:A:234:ARG:C	1:A:236:ARG:N	2.72	0.41
1:C:6:MET:CE	1:C:30:CYS:HB2	2.51	0.41
1:C:242:PHE:HA	1:C:250:GLN:HE21	1.87	0.41
2:H:11:VAL:CG2	2:H:157:PRO:CB	2.99	0.41
1:A:51:ALA:CA	2:H:32:TYR:CE2	3.04	0.40
1:A:138:GLU:HB2	2:H:31:HIS:HE1	1.73	0.40
1:B:191:GLU:C	1:B:193:ARG:N	2.74	0.40
1:C:117:ALA:HB2	1:C:252:VAL:HG11	2.03	0.40
1:A:193:ARG:CD	1:B:383:TYR:CE1	3.04	0.40
1:B:163:GLN:HG2	1:B:183:TYR:HE2	1.85	0.40
1:B:242:PHE:HA	1:B:250:GLN:HE21	1.87	0.40
1:B:336:CYS:O	1:B:361:PHE:HB2	2.21	0.40
1:C:149:VAL:HG23	1:C:326:GLU:CD	2.42	0.40
1:C:198:THR:C	1:C:200:ALA:H	2.24	0.40
2:H:123[B]:SER:HB3	2:H:124:ALA:HA	1.06	0.40
2:K:162:VAL:HG13	2:K:206[B]:CYS:SG	2.62	0.40
1:A:142:PHE:CG	1:A:143:VAL:N	2.89	0.40
1:B:346:LEU:HD13	1:B:383:TYR:CZ	2.56	0.40
3:L:188[B]:LEU:HD23	3:L:188[B]:LEU:H	1.86	0.40
1:A:3:CYS:HB3	1:A:9:ARG:CD	2.52	0.40
1:A:191:GLU:C	1:A:193:ARG:H	2.25	0.40
1:A:232:VAL:HG23	1:A:235:ASN:ND2	2.34	0.40
1:A:380:GLY:HA2	1:A:398:HIS:ND1	2.37	0.40
1:B:81:HIS:CE1	1:B:85:ARG:HD3	2.56	0.40
1:B:195:GLY:HA3	1:B:196:ILE:N	2.29	0.40
1:C:57:ARG:CD	1:C:58:SER:H	2.34	0.40
1:C:100:GLY:O	1:C:105:CYS:N	2.53	0.40
1:C:396:HIS:CG	1:C:397:TRP:N	2.89	0.40
2:H:162:VAL:HG13	2:H:206[B]:CYS:SG	2.62	0.40
1:A:57:ARG:CD	1:A:58:SER:H	2.34	0.40
1:A:183:TYR:O	1:A:295:LEU:HD12	2.22	0.40
1:B:2:ASN:HD22	1:B:2:ASN:N	2.09	0.40
1:B:90:PHE:HA	1:B:117:ALA:O	2.22	0.40
1:B:149:VAL:HG23	1:B:326:GLU:CD	2.42	0.40
1:B:214:HIS:O	1:B:215:ARG:C	2.59	0.40
1:B:325:LEU:HD13	1:B:327:LEU:HD13	2.02	0.40
1:C:245:PRO:HG2	1:C:250:GLN:HA	2.02	0.40
1:C:380:GLY:HA2	1:C:398:HIS:ND1	2.37	0.40
2:K:123[A]:SER:OG	2:K:124:ALA:CB	2.65	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	392/403 (97%)	328 (84%)	46 (12%)	18 (5%)	2	21
1	B	390/403 (97%)	327 (84%)	45 (12%)	18 (5%)	2	21
1	C	390/403 (97%)	327 (84%)	45 (12%)	18 (5%)	2	21
2	H	249/230 (108%)	246 (99%)	3 (1%)	0	100	100
2	K	249/230 (108%)	246 (99%)	3 (1%)	0	100	100
3	L	225/220 (102%)	217 (96%)	8 (4%)	0	100	100
3	M	225/220 (102%)	217 (96%)	8 (4%)	0	100	100
All	All	2120/2109 (100%)	1908 (90%)	158 (8%)	54 (2%)	8	32

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ILE
1	A	227	SER
1	A	276	SER
1	A	367	ALA
1	B	227	SER
1	B	276	SER
1	B	367	ALA
1	C	227	SER
1	C	276	SER
1	C	367	ALA
1	A	14	GLY
1	A	27	GLY
1	A	64	THR
1	A	150	GLU
1	A	192	PRO
1	A	242	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	14	GLY
1	B	27	GLY
1	B	64	THR
1	B	150	GLU
1	B	192	PRO
1	B	242	PHE
1	C	14	GLY
1	C	27	GLY
1	C	64	THR
1	C	150	GLU
1	C	192	PRO
1	C	242	PHE
1	A	239	LEU
1	B	239	LEU
1	C	239	LEU
1	A	88	PRO
1	B	88	PRO
1	C	88	PRO
1	A	259	GLU
1	B	259	GLU
1	C	259	GLU
1	A	207	GLY
1	A	352	VAL
1	B	200	ALA
1	B	207	GLY
1	B	352	VAL
1	C	200	ALA
1	C	207	GLY
1	C	352	VAL
1	B	102	GLY
1	A	102	GLY
1	C	102	GLY
1	A	65	VAL
1	B	65	VAL
1	C	65	VAL
1	A	245	PRO
1	B	245	PRO
1	C	245	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	320 (97%)	11 (3%)	38	61
1	B	331/331 (100%)	320 (97%)	11 (3%)	38	61
1	C	331/331 (100%)	320 (97%)	11 (3%)	38	61
2	H	219/195 (112%)	215 (98%)	4 (2%)	59	77
2	K	219/195 (112%)	215 (98%)	4 (2%)	59	77
3	L	190/181 (105%)	188 (99%)	2 (1%)	73	84
3	M	190/181 (105%)	188 (99%)	2 (1%)	73	84
All	All	1811/1745 (104%)	1766 (98%)	45 (2%)	50	68

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	61	TYR
1	A	62	LEU
1	A	74	CYS
1	A	128	ARG
1	A	129	THR
1	A	188	VAL
1	A	202	TYR
1	A	278	THR
1	A	287	LYS
1	A	309	PHE
1	B	2	ASN
1	B	61	TYR
1	B	62	LEU
1	B	74	CYS
1	B	128	ARG
1	B	129	THR
1	B	188	VAL
1	B	202	TYR
1	B	278	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	287	LYS
1	B	309	PHE
1	C	2	ASN
1	C	61	TYR
1	C	62	LEU
1	C	74	CYS
1	C	128	ARG
1	C	129	THR
1	C	188	VAL
1	C	202	TYR
1	C	278	THR
1	C	287	LYS
1	C	309	PHE
2	H	52	ASN
2	H	72	ARG
2	H	87[A]	ARG
2	H	87[B]	ARG
3	L	53	ASN
3	L	163	VAL
2	K	52	ASN
2	K	72	ARG
2	K	87[A]	ARG
2	K	87[B]	ARG
3	M	53	ASN
3	M	163	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	8	ASN
1	A	47	ASN
1	A	152	HIS
1	A	328	GLN
1	A	359	ASN
1	A	392	GLN
1	B	2	ASN
1	B	8	ASN
1	B	47	ASN
1	B	52	ASN
1	B	134	ASN
1	B	152	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	258	GLN
1	B	263	HIS
1	B	285	HIS
1	B	359	ASN
1	B	368	ASN
1	B	392	GLN
1	C	2	ASN
1	C	8	ASN
1	C	47	ASN
1	C	152	HIS
1	C	263	HIS
1	C	328	GLN
1	C	359	ASN
1	C	392	GLN
2	H	35	HIS
2	H	52	ASN
2	H	230	HIS
3	L	1	GLN
3	L	32	ASN
3	L	35	ASN
3	L	52	ASN
3	L	53	ASN
3	L	116	GLN
3	L	175	GLN
3	L	205	HIS
2	K	35	HIS
2	K	52	ASN
2	K	230	HIS
3	M	1	GLN
3	M	32	ASN
3	M	35	ASN
3	M	52	ASN
3	M	53	ASN
3	M	116	GLN
3	M	175	GLN
3	M	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PCA	H	1	2	7,8,9	1.62	1 (14%)	9,10,12	1.73	3 (33%)
2	PCA	K	1	2	7,8,9	1.63	1 (14%)	9,10,12	1.73	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	K	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	PCA	CD-N	4.17	1.45	1.34
2	H	1	PCA	CD-N	4.15	1.45	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	PCA	CA-N-CD	-2.63	104.57	113.58
2	H	1	PCA	CA-N-CD	-2.63	104.58	113.58
2	K	1	PCA	CB-CA-N	2.38	110.14	103.30
2	H	1	PCA	CB-CA-N	2.37	110.11	103.30
2	H	1	PCA	CG-CD-N	2.19	114.06	108.39
2	K	1	PCA	CG-CD-N	2.18	114.05	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NDG	D	1	4	14,14,15	0.61	0	17,19,21	1.06	2 (11%)
4	NDG	D	2	4	14,14,15	0.64	0	17,19,21	0.94	1 (5%)
4	FUL	D	3	4	10,10,11	0.65	0	14,14,16	0.52	0
4	NDG	E	1	4	14,14,15	0.61	0	17,19,21	1.06	3 (17%)
4	NDG	E	2	4	14,14,15	0.64	0	17,19,21	0.94	1 (5%)
4	FUL	E	3	4	10,10,11	0.65	0	14,14,16	0.53	0
4	NDG	F	1	4	14,14,15	0.60	0	17,19,21	1.06	2 (11%)
4	NDG	F	2	4	14,14,15	0.65	0	17,19,21	0.95	1 (5%)
4	FUL	F	3	4	10,10,11	0.66	0	14,14,16	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	D	1	4	-	4/6/23/26	0/1/1/1
4	NDG	D	2	4	-	3/6/23/26	0/1/1/1
4	FUL	D	3	4	-	-	0/1/1/1
4	NDG	E	1	4	-	4/6/23/26	0/1/1/1
4	NDG	E	2	4	-	3/6/23/26	0/1/1/1
4	FUL	E	3	4	-	-	0/1/1/1
4	NDG	F	1	4	-	4/6/23/26	0/1/1/1
4	NDG	F	2	4	-	3/6/23/26	0/1/1/1
4	FUL	F	3	4	-	-	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NDG	C6-C5-C4	2.36	118.53	113.00
4	D	1	NDG	C6-C5-C4	2.35	118.52	113.00
4	E	1	NDG	C6-C5-C4	2.33	118.47	113.00
4	F	2	NDG	C2-N2-C7	-2.29	119.65	122.90
4	E	2	NDG	C2-N2-C7	-2.27	119.66	122.90
4	D	2	NDG	C2-N2-C7	-2.27	119.67	122.90
4	F	1	NDG	C2-N2-C7	-2.23	119.72	122.90
4	D	1	NDG	C2-N2-C7	-2.21	119.76	122.90
4	E	1	NDG	C2-N2-C7	-2.19	119.79	122.90
4	E	1	NDG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

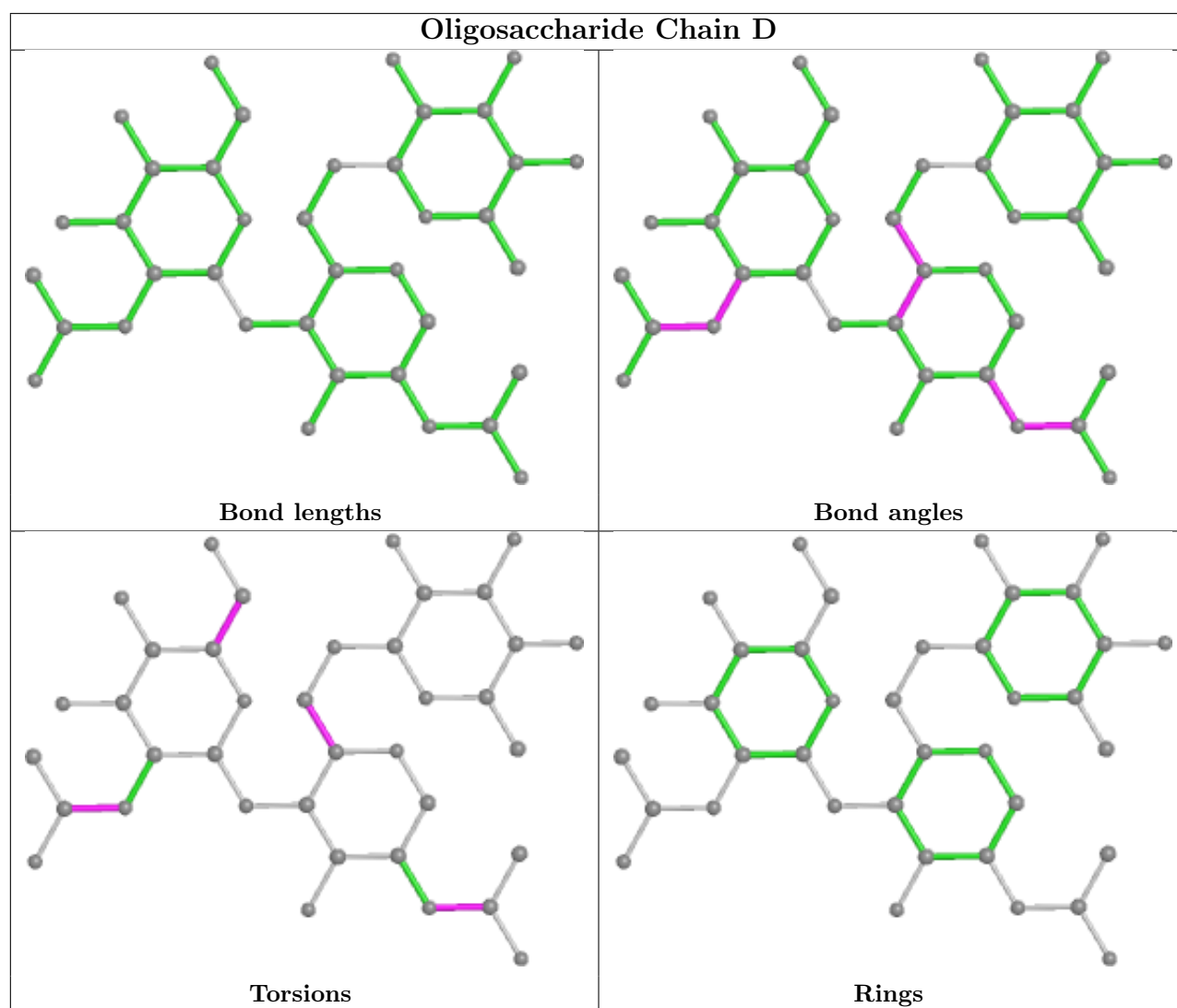
Mol	Chain	Res	Type	Atoms
4	D	1	NDG	C8-C7-N2-C2
4	D	1	NDG	O7-C7-N2-C2
4	D	2	NDG	C8-C7-N2-C2
4	D	2	NDG	O7-C7-N2-C2
4	E	1	NDG	C8-C7-N2-C2
4	E	1	NDG	O7-C7-N2-C2
4	E	2	NDG	C8-C7-N2-C2
4	E	2	NDG	O7-C7-N2-C2
4	F	1	NDG	C8-C7-N2-C2
4	F	1	NDG	O7-C7-N2-C2
4	F	2	NDG	C8-C7-N2-C2
4	F	2	NDG	O7-C7-N2-C2
4	D	1	NDG	C4-C5-C6-O6
4	E	1	NDG	C4-C5-C6-O6
4	F	1	NDG	C4-C5-C6-O6
4	D	1	NDG	O5-C5-C6-O6
4	E	1	NDG	O5-C5-C6-O6
4	F	1	NDG	O5-C5-C6-O6
4	D	2	NDG	O5-C5-C6-O6
4	E	2	NDG	O5-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6

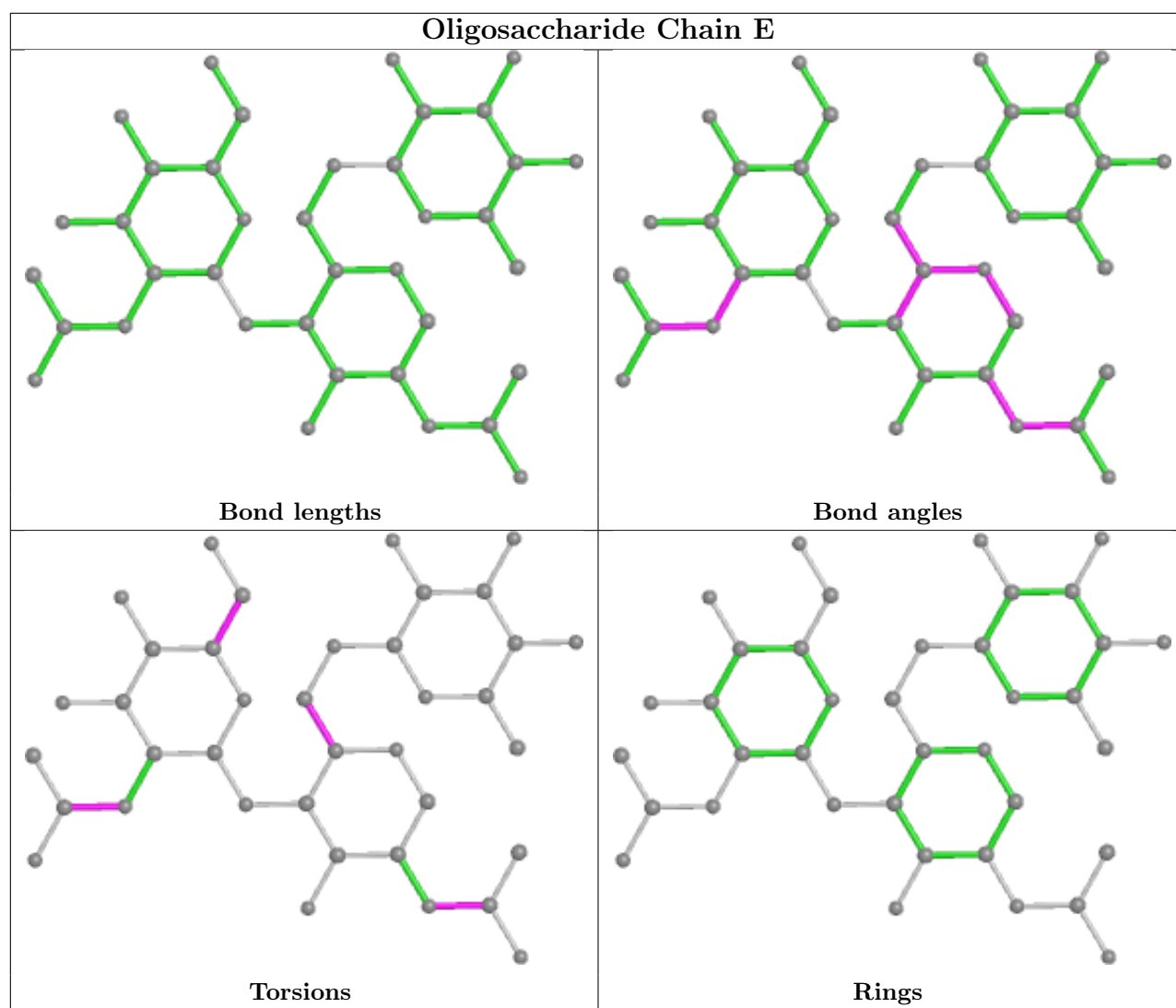
There are no ring outliers.

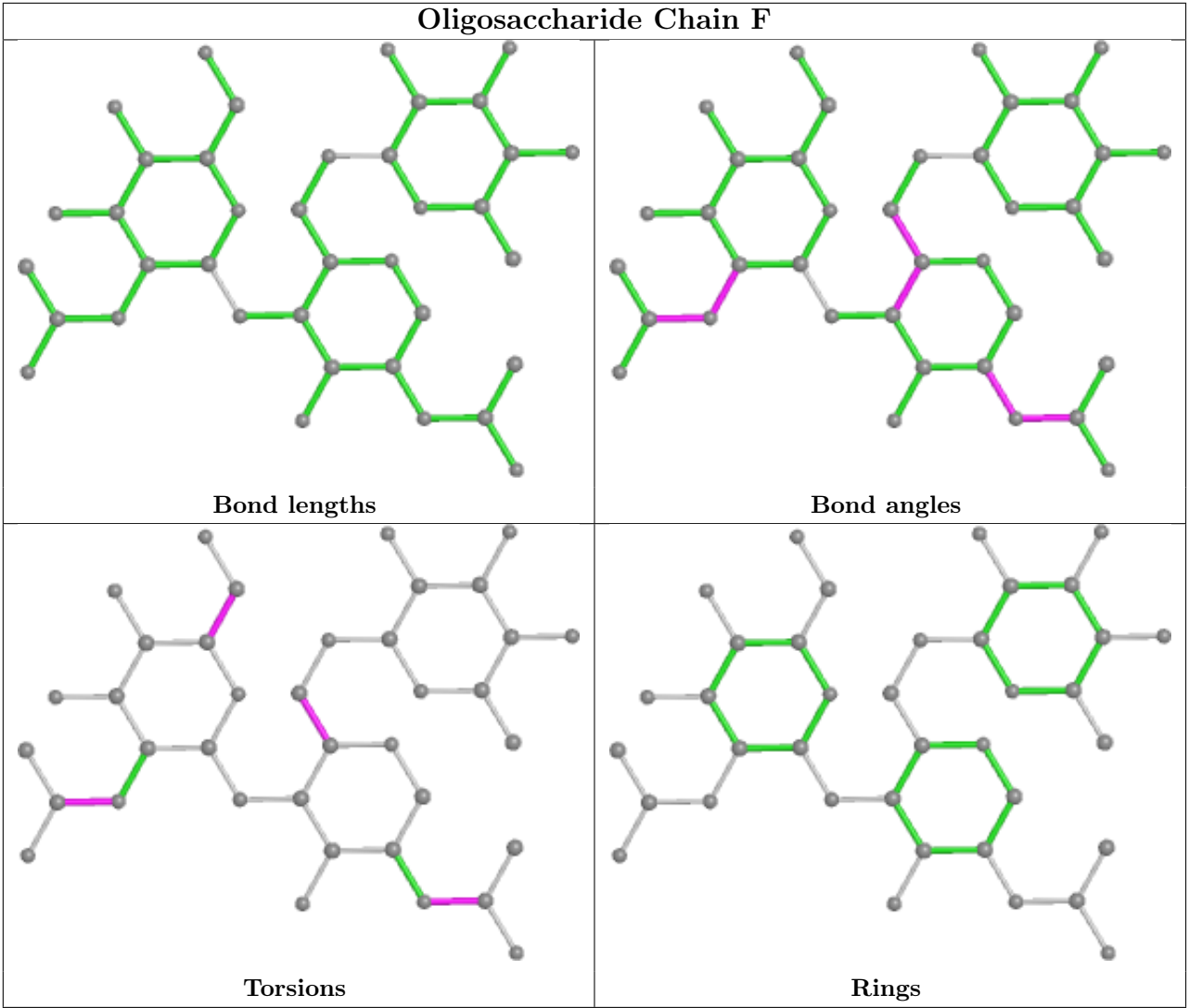
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NDG	4	0
4	F	2	NDG	4	0
4	F	1	NDG	5	0
4	E	3	FUL	1	0
4	D	2	NDG	4	0
4	D	3	FUL	1	0
4	F	3	FUL	1	0
4	D	1	NDG	5	0
4	E	1	NDG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	C	4
1	B	4
2	K	1
2	H	1
3	L	1
3	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	51:ALA	C	52:ASN	N	6.66
1	C	51:ALA	C	52:ASN	N	5.87
1	A	132:LYS	C	133:GLU	N	5.75
1	C	132:LYS	C	133:GLU	N	4.95
1	K	123:SER	C	124:ALA	N	4.88
1	B	132:LYS	C	133:GLU	N	4.78
1	B	51:ALA	C	52:ASN	N	4.72
1	B	282:THR	C	283:SER	N	4.62
1	H	123:SER	C	124:ALA	N	4.60
1	C	282:THR	C	283:SER	N	4.28
1	A	282:THR	C	283:SER	N	3.92
1	C	195:GLY	C	196:ILE	N	3.83
1	L	115:GLY	C	116:GLN	N	3.64
1	B	195:GLY	C	196:ILE	N	3.39
1	M	115:GLY	C	116:GLN	N	3.24
1	A	195:GLY	C	196:ILE	N	2.00

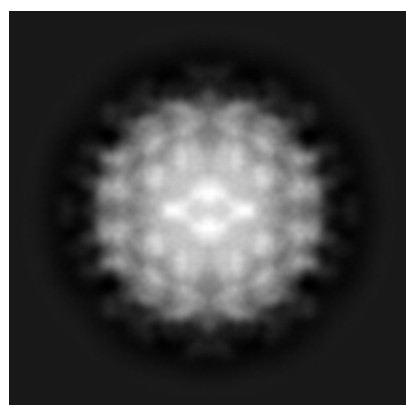
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5190. These allow visual inspection of the internal detail of the map and identification of artifacts.

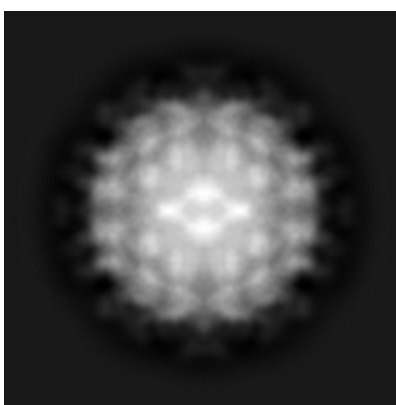
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

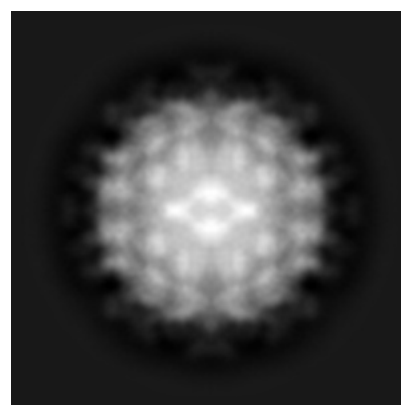
6.1.1 Primary map



X



Y

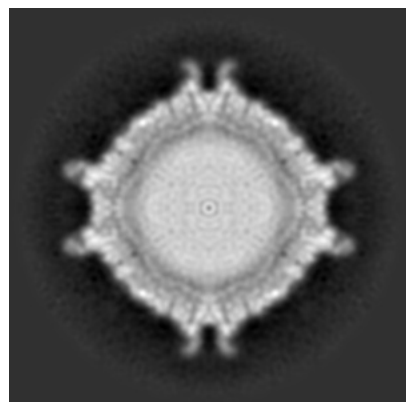


Z

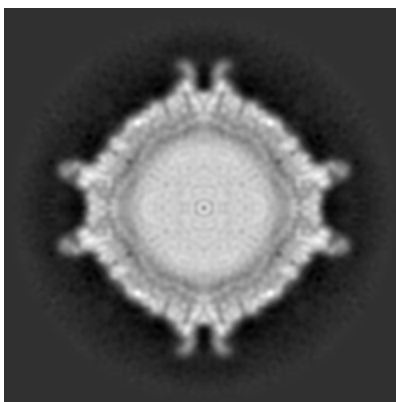
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

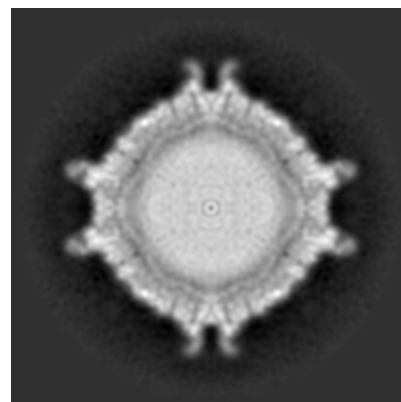
6.2.1 Primary map



X Index: 149



Y Index: 149

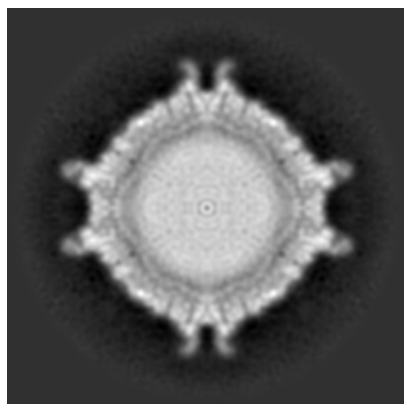


Z Index: 149

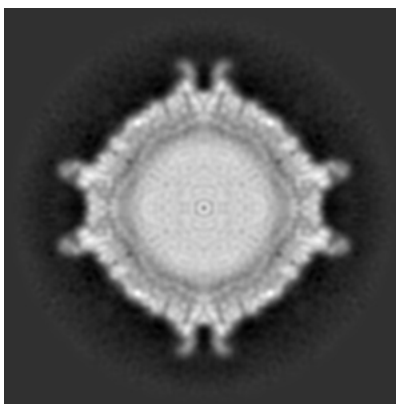
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

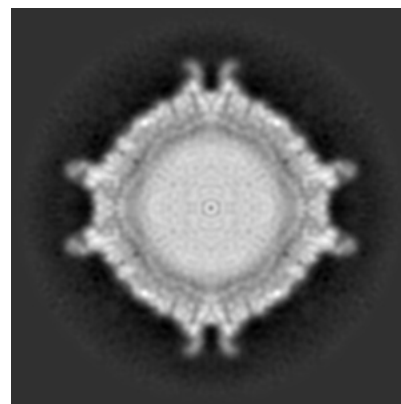
6.3.1 Primary map



X Index: 149



Y Index: 149

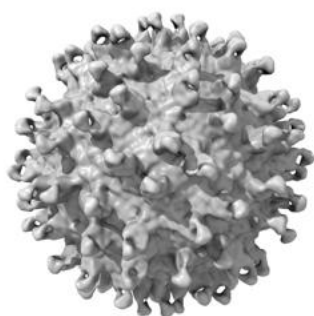


Z Index: 149

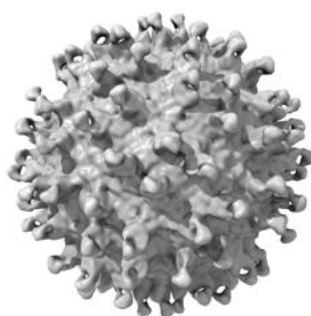
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

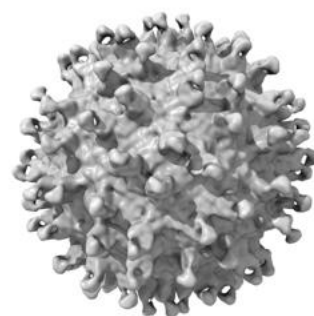
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

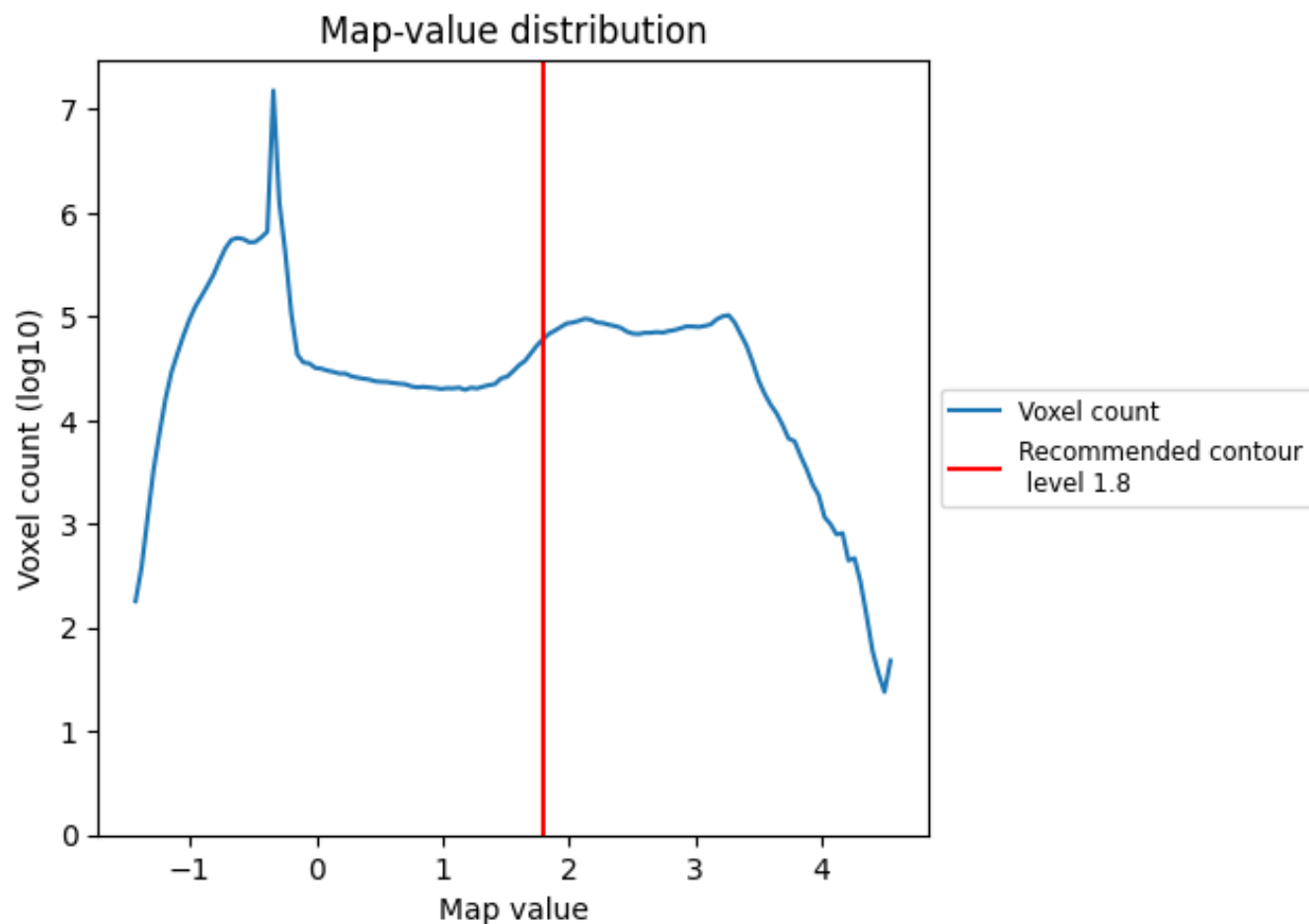
6.5 Mask visualisation

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

7 Map analysis [i](#)

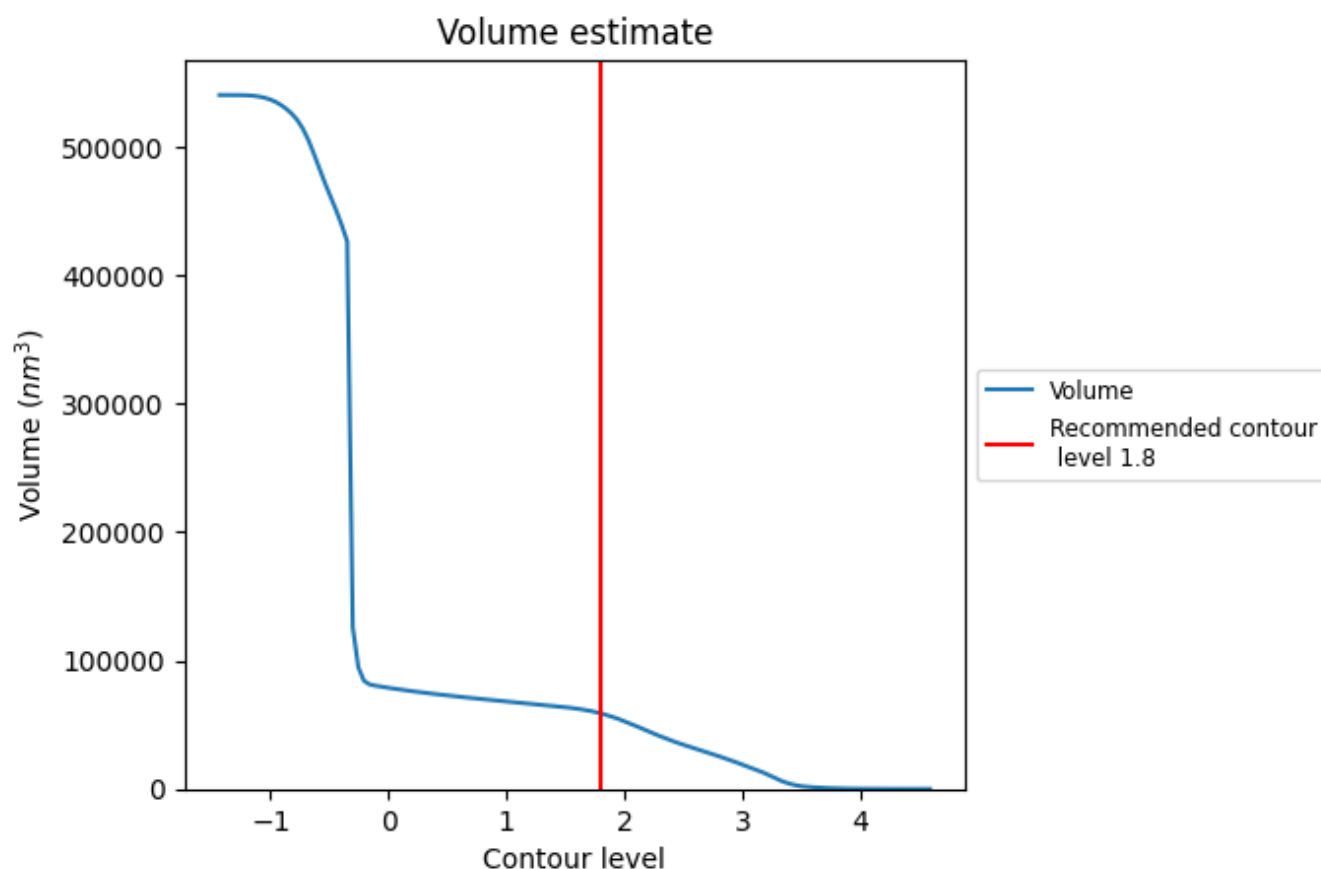
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

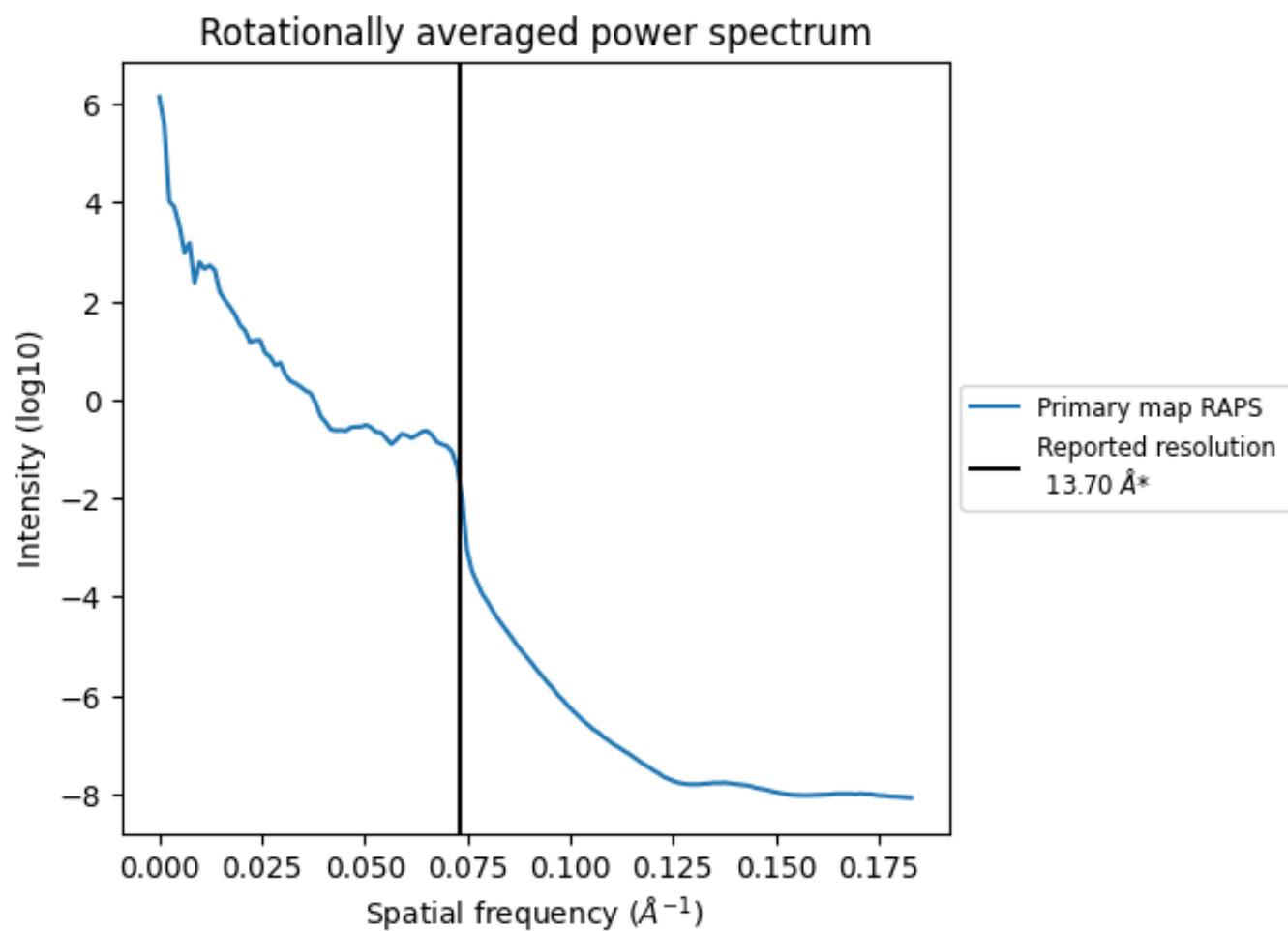
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58861 nm^3 ; this corresponds to an approximate mass of 53171 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.073 Å⁻¹

8 Fourier-Shell correlation

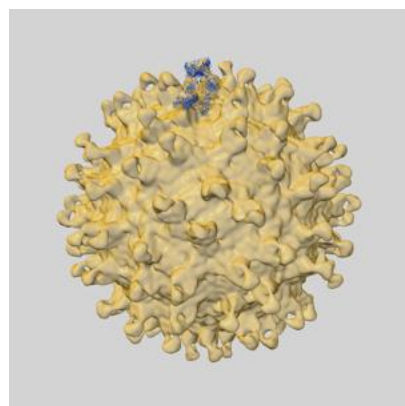
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

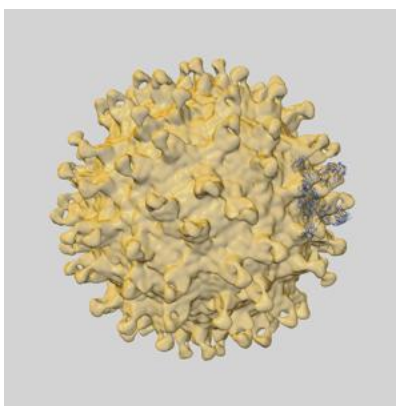
This section contains information regarding the fit between EMDB map EMD-5190 and PDB model 3IYW. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

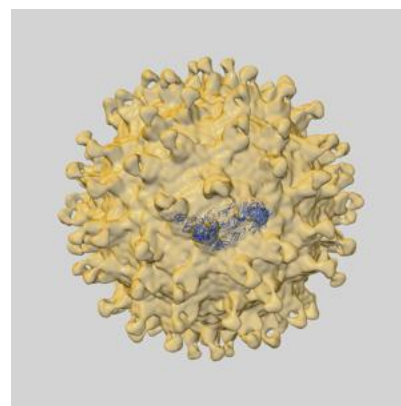
9.1.1 Map-model overlay [i](#)



X

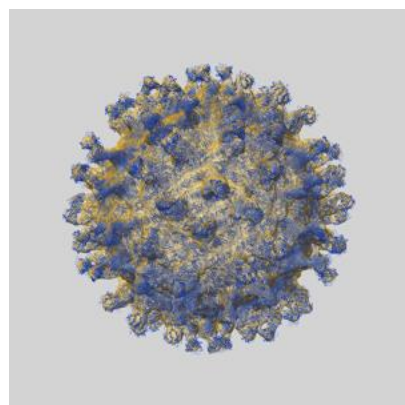


Y

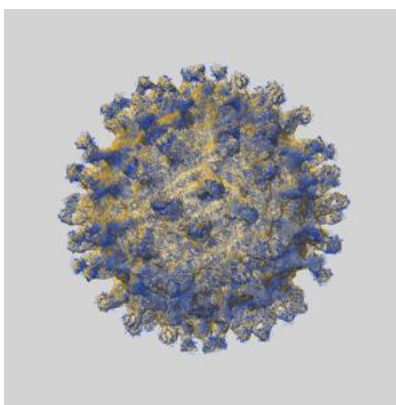


Z

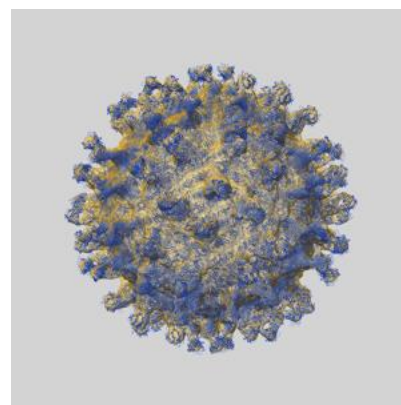
9.1.2 Map-model assembly overlay [i](#)



X



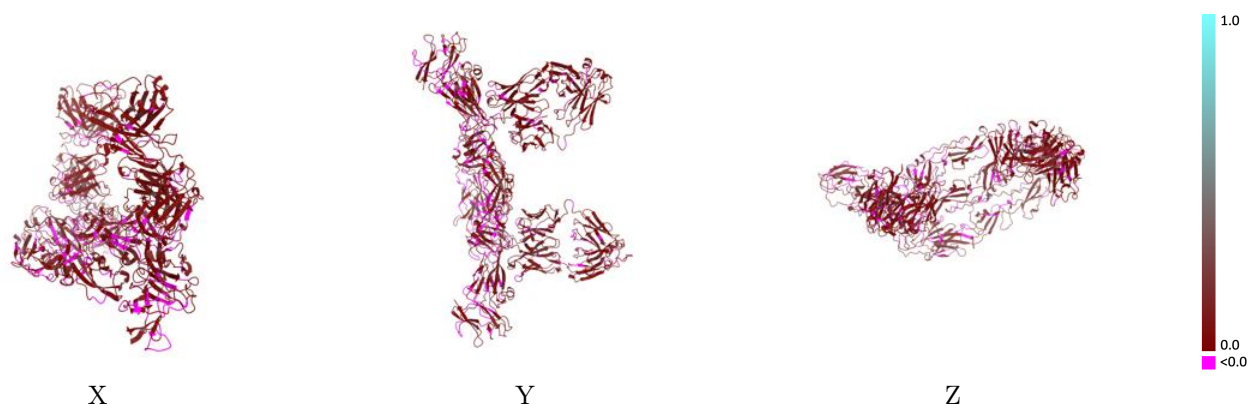
Y



Z

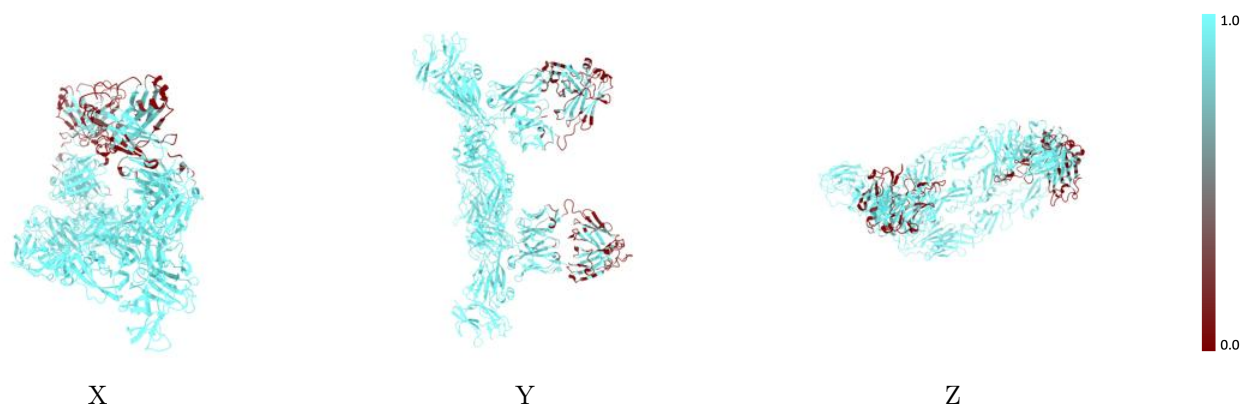
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



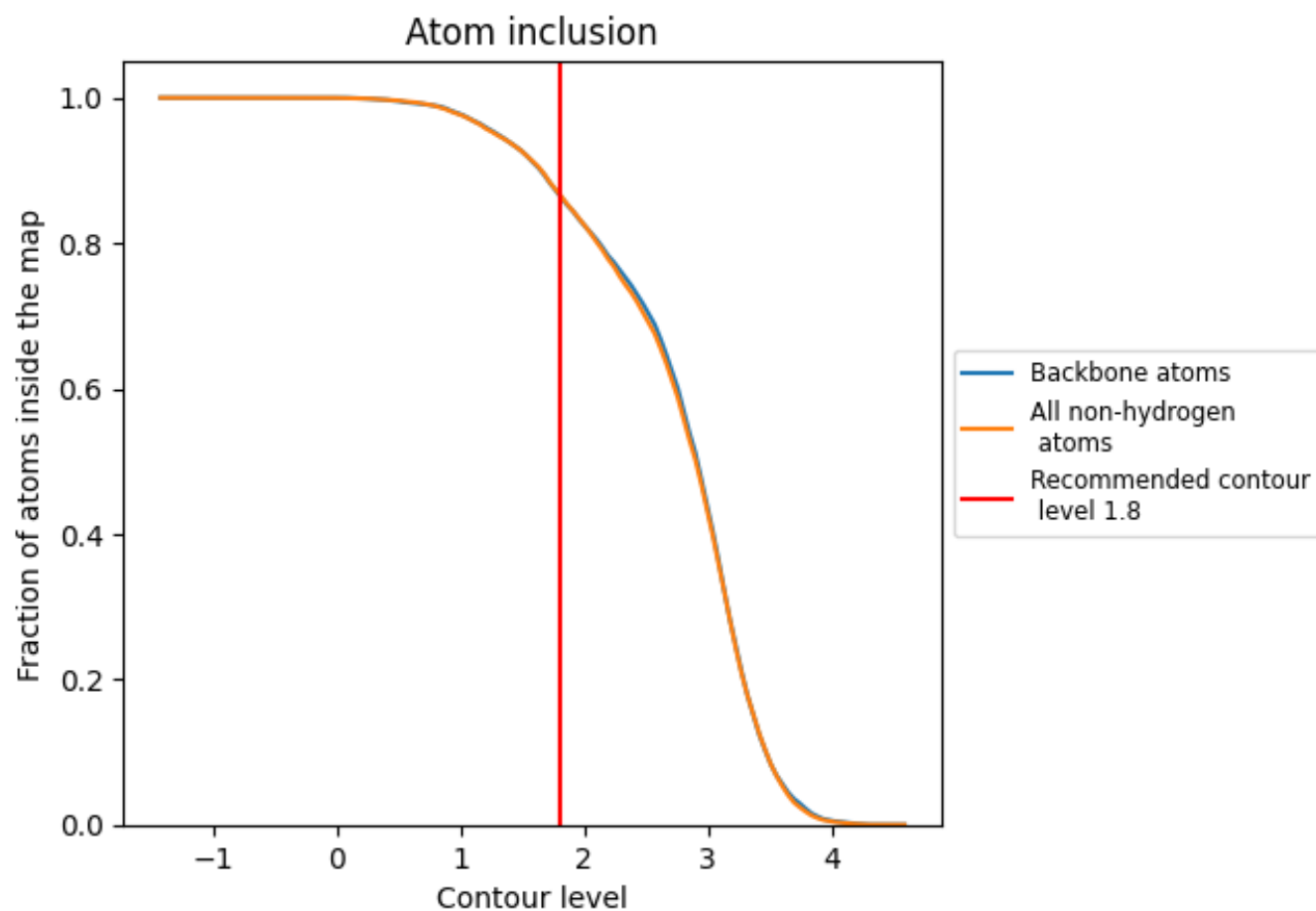
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8671	<div></div> 0.0710
A	<div></div> 0.9993	<div></div> 0.0610
B	<div></div> 0.9997	<div></div> 0.0700
C	<div></div> 1.0000	<div></div> 0.0660
D	<div></div> 0.7632	<div></div> 0.0010
E	<div></div> 0.7368	<div></div> 0.0570
F	<div></div> 0.5789	<div></div> 0.0480
H	<div></div> 0.7157	<div></div> 0.0840
K	<div></div> 0.7227	<div></div> 0.0730
L	<div></div> 0.6283	<div></div> 0.0720
M	<div></div> 0.6887	<div></div> 0.0810

1.0

0.0

<0.0