



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 7CN9 / pdb_00007cn9
EMDB ID : EMD-30419
Title : Cryo-EM structure of SARS-CoV-2 Spike ectodomain
Authors : Ho, M.; Chang, Y.; Wang, C.; Wu, Y.; Huang, H.; Chen, T.; Lo, J.M.; Chen, X.; Ma, C.
Deposited on : 2020-07-30
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

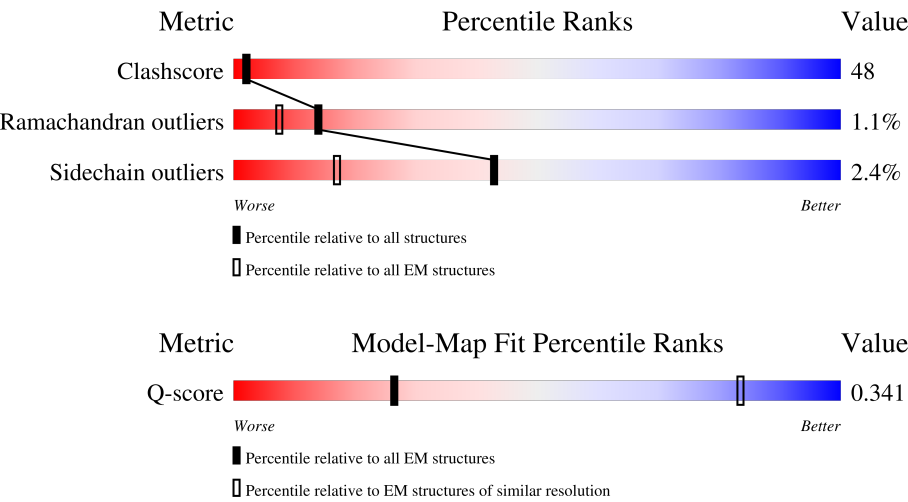
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	1127	44% 36%52%10%
1	B	1127	37% 32%56%10%
1	C	1127	39% 34%55%8%
2	E	2	100% 50%50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	2	50% 100%
2	N	2	50% 50%
2	W	2	50% 50%
2	X	2	50% 100%
2	Z	2	50% 50%
2	d	2	50% 50%
2	f	2	100%
3	k	3	67% 33% 67%
4	V	3	67% 67% 33%
4	p	3	33% 33% 67%
5	h	4	100% 25% 50% 25%
6	Q	4	75% 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24052 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0
			7727	4935	1292	1465	35		
1	B	1010	Total	C	N	O	S	0	0
			7674	4895	1285	1458	36		
1	C	1037	Total	C	N	O	S	0	0
			7889	5040	1316	1498	35		

There are 15 discrepancies between the modelled and reference sequences:

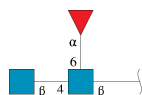
Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



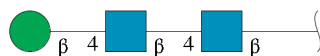
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	k	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	p	3	Total	C	N	O	0	0
			39	22	2	15		
4	V	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

pyranose.



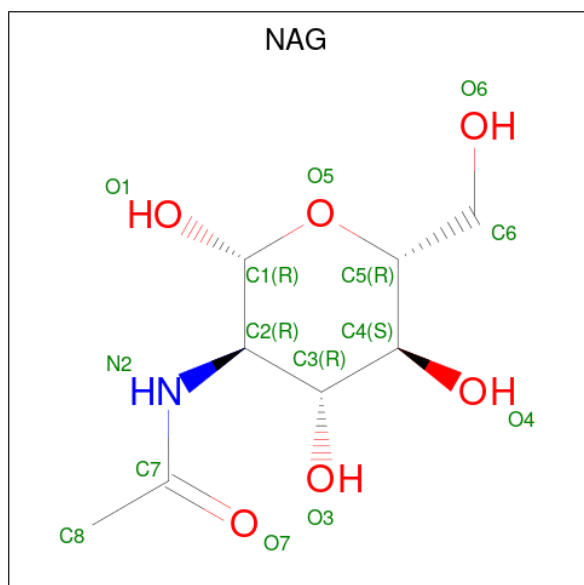
Mol	Chain	Residues	Atoms				AltConf	Trace
5	h	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0

Continued on next page...

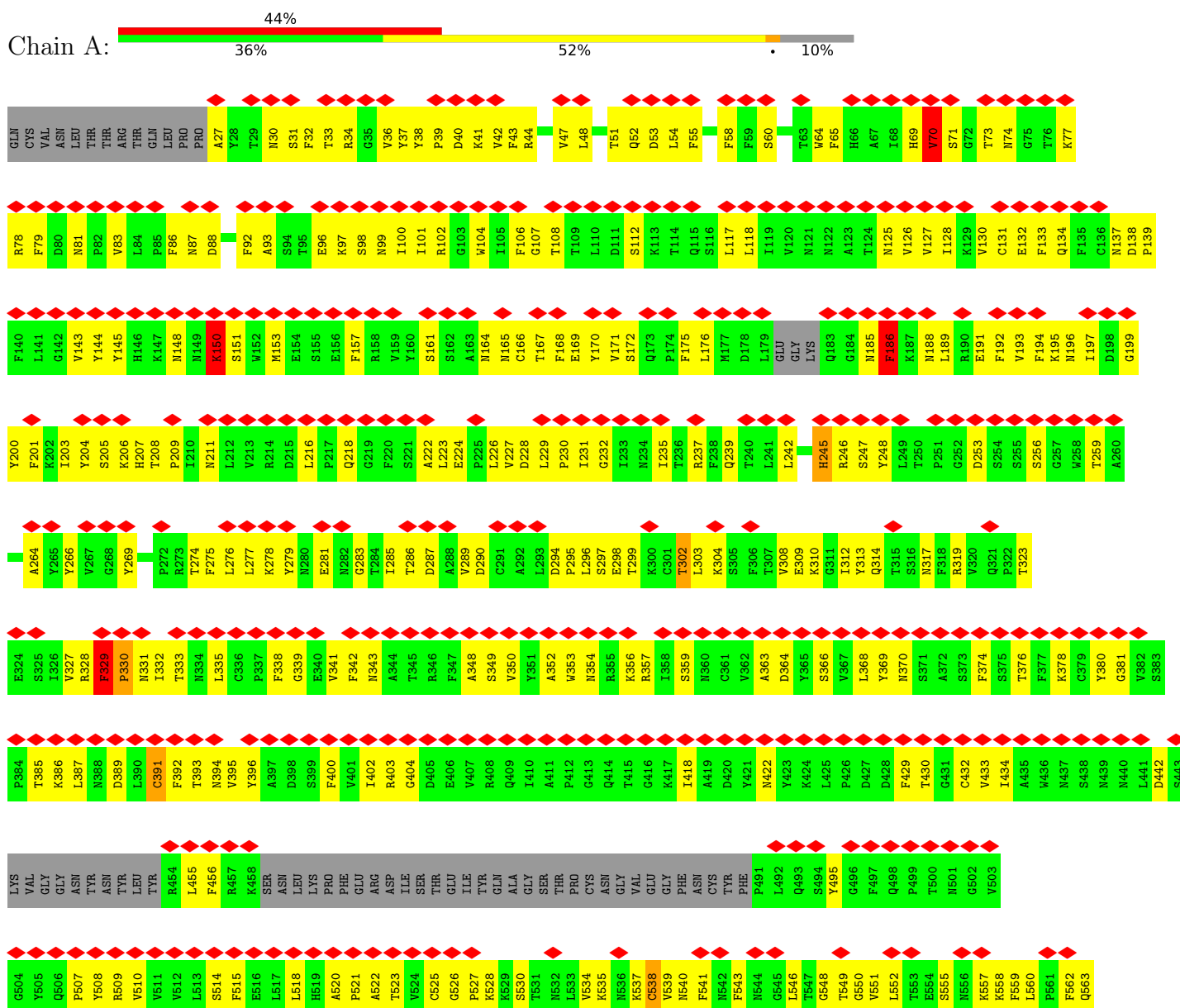
Continued from previous page...

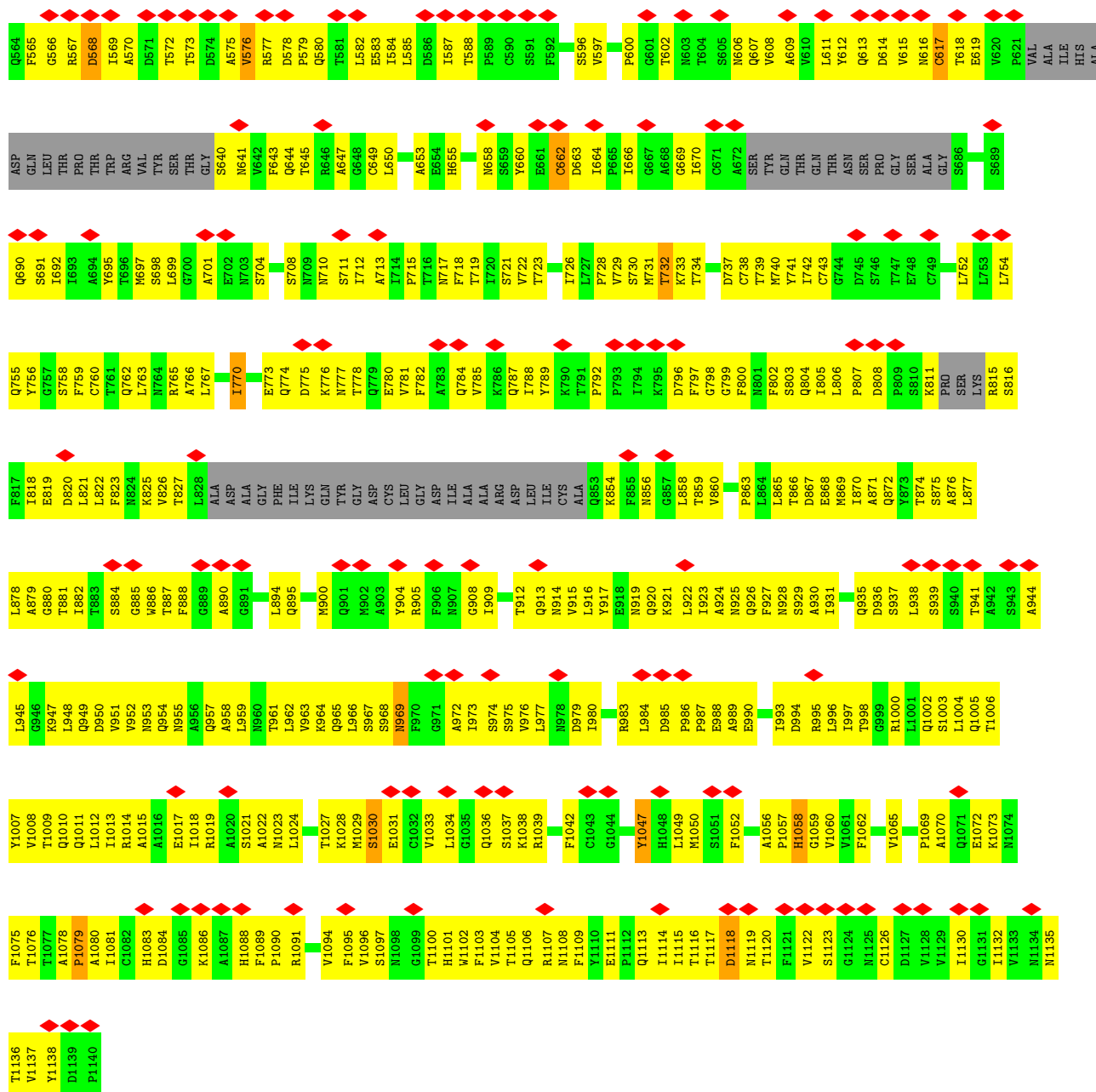
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	C	1	14	8	1	5	0

3 Residue-property plots

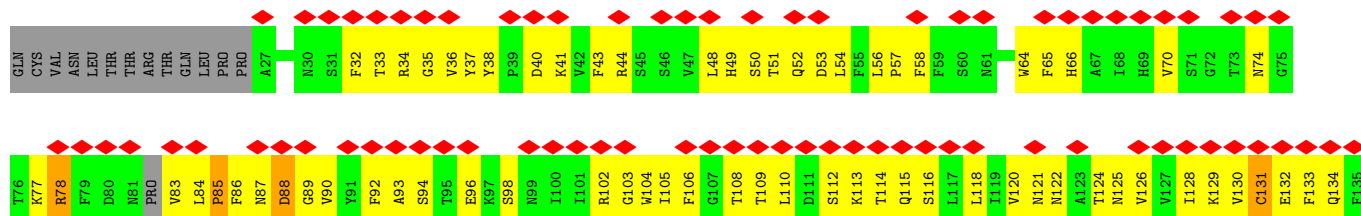
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

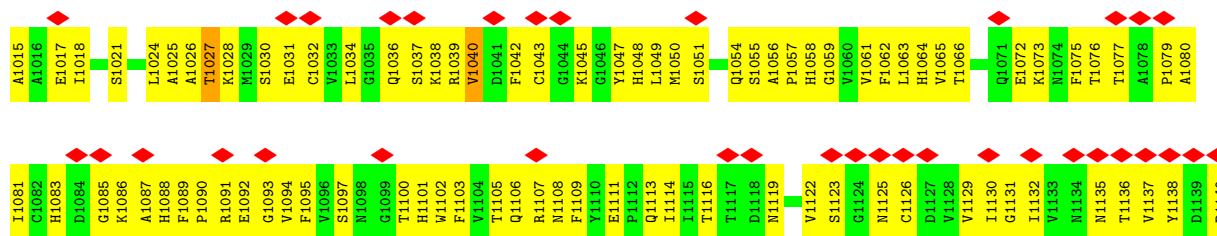




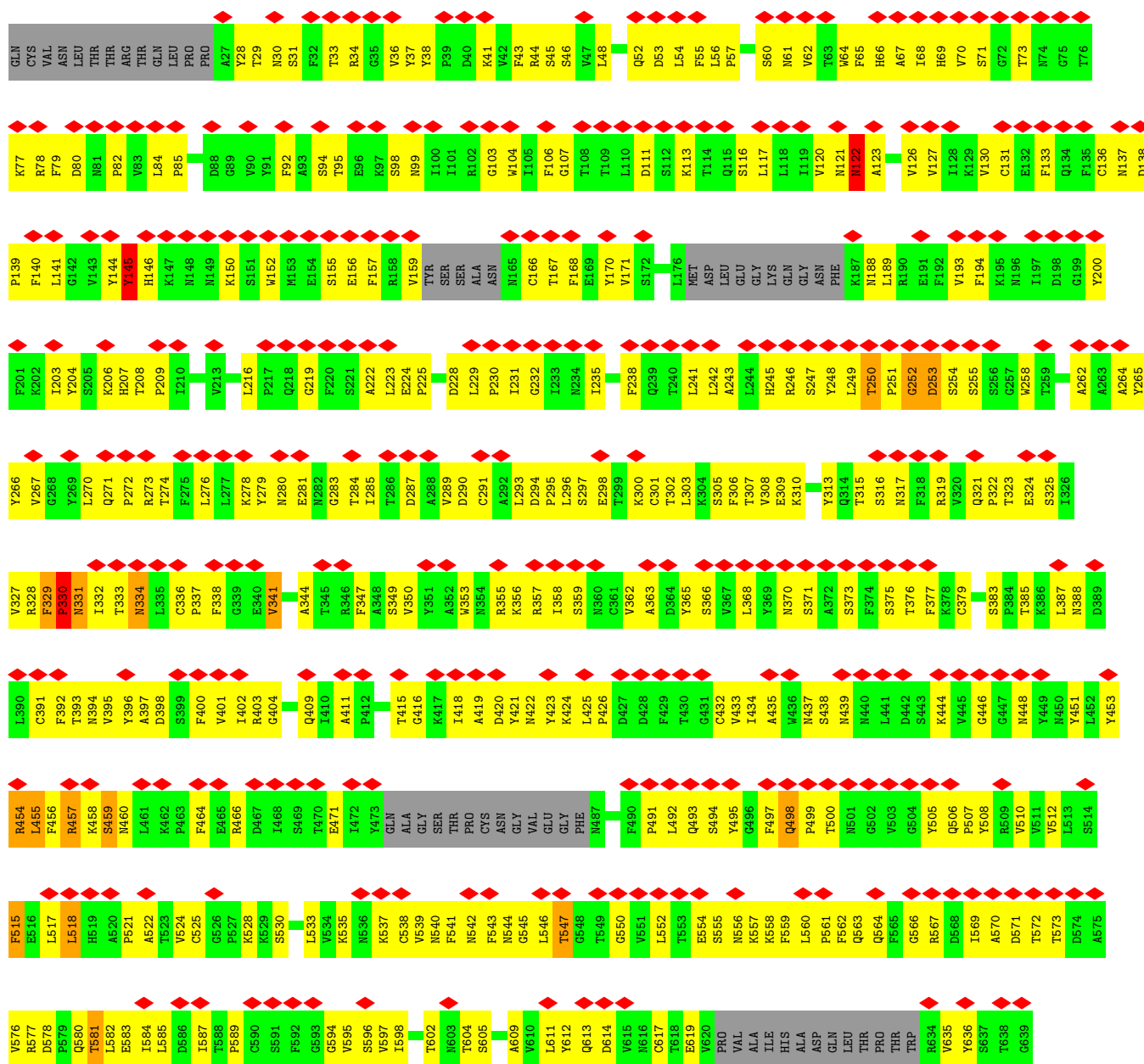
• Molecule 1: Spike glycoprotein

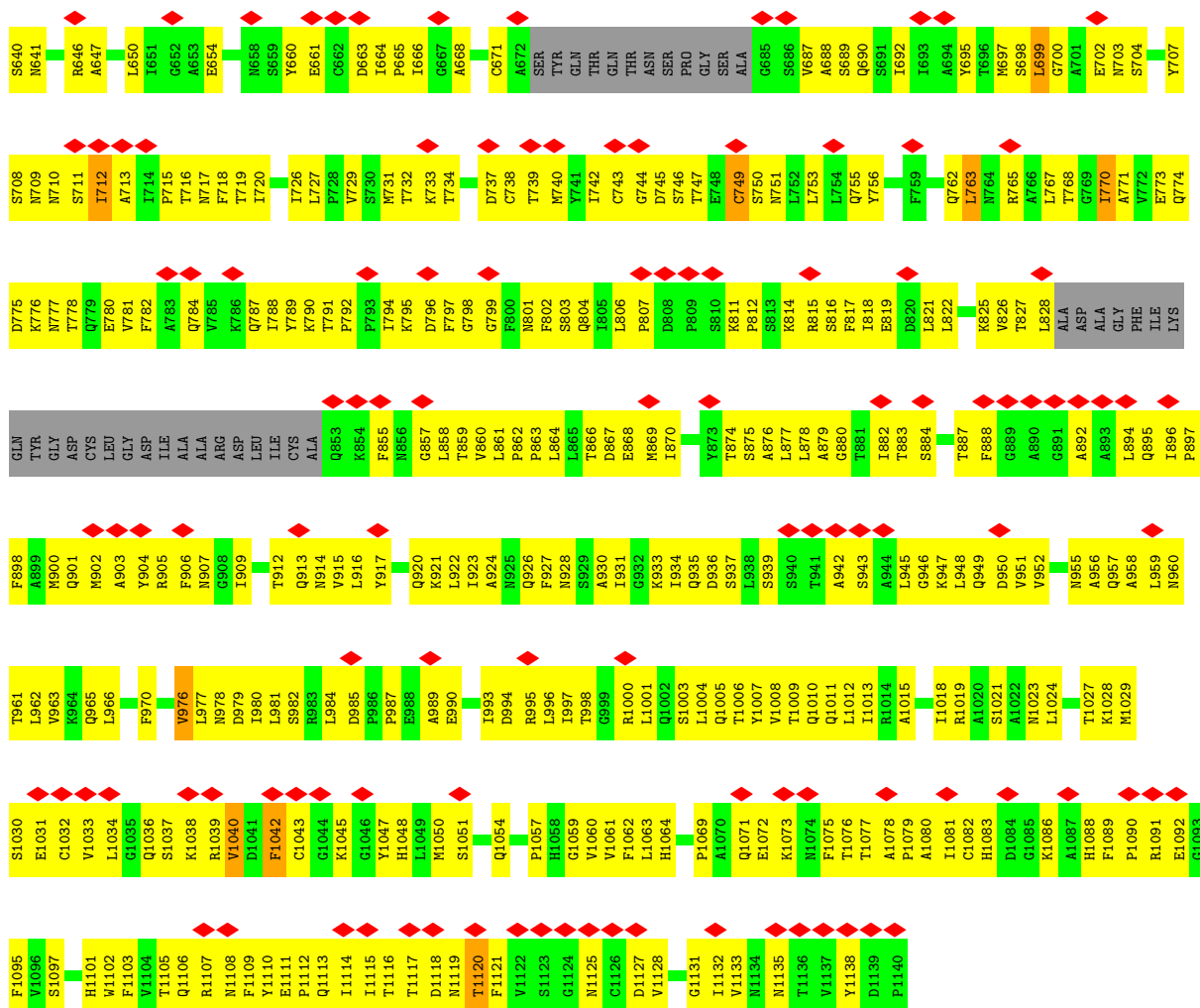






• Molecule 1: Spike glycoprotein





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 100% 50%

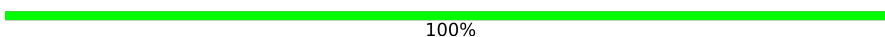


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 50% 50%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

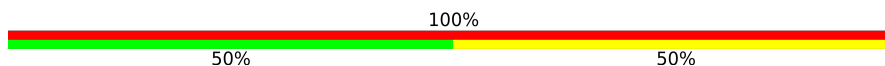


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 100% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



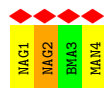
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



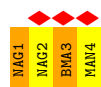
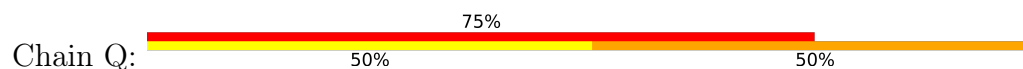
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00738	Depositor
Map size (Å)	354.24, 354.24, 354.24	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	2/7900 (0.0%)	0.74	4/10764 (0.0%)
1	B	0.54	0/7839	0.70	4/10679 (0.0%)
1	C	0.57	2/8069 (0.0%)	0.72	5/11005 (0.0%)
All	All	0.56	4/23808 (0.0%)	0.72	13/32448 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	PRO	N-CA	18.11	1.70	1.47
1	C	330	PRO	N-CA	18.10	1.70	1.47
1	A	329	PHE	C-N	5.09	1.45	1.33
1	C	329	PHE	C-N	5.09	1.45	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PHE	CA-C-N	16.60	140.59	119.84
1	A	329	PHE	C-N-CA	16.60	140.59	119.84
1	C	329	PHE	CA-C-N	15.91	139.73	119.84
1	C	329	PHE	C-N-CA	15.91	139.73	119.84
1	A	330	PRO	CA-N-CD	-9.88	98.17	112.00
1	C	330	PRO	CA-N-CD	-8.74	99.76	112.00
1	B	172	SER	CA-C-N	-6.33	115.80	122.89
1	B	172	SER	C-N-CA	-6.33	115.80	122.89
1	B	124	THR	N-CA-C	-6.31	106.80	114.75
1	A	969	ASN	N-CA-C	-5.53	108.31	114.62
1	B	187	LYS	N-CA-C	5.05	116.82	110.91
1	C	122	ASN	CA-C-N	-5.01	119.00	126.86
1	C	122	ASN	C-N-CA	-5.01	119.00	126.86

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	7727	0	7433	716	0
1	B	7674	0	7325	798	0
1	C	7889	0	7542	780	0
2	E	28	0	25	1	0
2	H	28	0	25	0	0
2	N	28	0	25	0	0
2	W	28	0	25	1	0
2	X	28	0	25	6	0
2	Z	28	0	25	0	0
2	d	28	0	25	2	0
2	f	28	0	25	0	0
3	k	38	0	34	0	0
4	V	39	0	34	5	0
4	p	39	0	34	4	0
5	h	50	0	43	4	0
6	Q	50	0	43	3	0
7	A	98	0	91	6	0
7	B	126	0	117	10	0
7	C	98	0	91	7	0
All	All	24052	0	22987	2244	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 (2244) 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:330:PRO:N	1:C:330:PRO:CA	1.70	1.45
1:C:328:ARG:NH1	1:C:533:LEU:HD13	1.39	1.37
1:A:330:PRO:N	1:A:330:PRO:CA	1.70	1.36
1:A:538:CYS:SG	1:A:550:GLY:HA2	1.67	1.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:TYR:CE2	1:C:458:LYS:HA	1.62	1.33
1:C:329:PHE:CE1	1:C:528:LYS:CB	2.11	1.32
1:B:86:PHE:CE2	1:B:89:GLY:HA2	1.66	1.31
1:C:421:TYR:CZ	1:C:458:LYS:HA	1.65	1.31
1:C:421:TYR:HE2	1:C:458:LYS:CA	1.40	1.30
1:B:86:PHE:CZ	1:B:89:GLY:N	1.99	1.30
1:C:421:TYR:CE2	1:C:458:LYS:CA	2.15	1.29
1:A:329:PHE:CB	1:A:330:PRO:HD3	1.59	1.28
1:B:86:PHE:CE2	1:B:89:GLY:CA	2.17	1.26
1:A:145:TYR:CD1	1:A:150:LYS:HD3	1.71	1.25
1:B:86:PHE:CZ	1:B:89:GLY:CA	2.20	1.23
1:B:86:PHE:CZ	1:B:89:GLY:HA2	1.71	1.22
1:C:455:LEU:O	1:C:456:PHE:CD1	1.93	1.22
1:C:421:TYR:OH	1:C:458:LYS:HA	1.36	1.19
1:B:310:LYS:HG2	1:B:600:PRO:O	1.38	1.17
1:A:148:ASN:ND2	1:A:150:LYS:H	1.43	1.16
1:A:538:CYS:SG	1:A:550:GLY:CA	2.33	1.15
1:C:421:TYR:CE2	1:C:459:SER:N	2.14	1.14
1:C:498:GLN:H	1:C:499:PRO:HD2	1.02	1.14
1:B:86:PHE:CD2	1:B:90:VAL:HG13	1.83	1.13
1:B:337:PRO:CG	1:B:358:ILE:HG21	1.78	1.13
1:C:422:ASN:OD1	1:C:455:LEU:HB2	1.50	1.11
1:B:86:PHE:HD2	1:B:90:VAL:HG13	1.05	1.11
1:A:145:TYR:H	1:A:150:LYS:HD2	1.11	1.08
1:B:84:LEU:HB2	1:B:269:TYR:OH	1.51	1.08
1:B:337:PRO:HG3	1:B:358:ILE:HD13	1.10	1.08
1:B:275:PHE:CE1	1:B:290:ASP:CG	2.32	1.08
1:A:329:PHE:HB3	1:A:330:PRO:CD	1.84	1.07
1:C:515:PHE:O	1:C:515:PHE:HD1	1.36	1.07
7:C:1205:NAG:H83	7:C:1205:NAG:H3	1.39	1.05
1:B:881:THR:HA	1:B:888:PHE:HE2	1.23	1.03
1:B:105:ILE:O	1:B:238:PHE:HA	1.58	1.03
1:A:1086:LYS:HE2	1:A:1088:HIS:CE1	1.93	1.02
1:A:329:PHE:CB	1:A:330:PRO:CD	2.38	1.02
1:B:275:PHE:CD1	1:B:290:ASP:HA	1.95	1.02
1:B:875:SER:HA	1:B:878:LEU:HD21	1.37	1.02
1:B:275:PHE:CG	1:B:290:ASP:HA	1.94	1.02
1:A:966:LEU:HG	1:A:1000:ARG:HH12	1.20	1.02
1:A:1028:LYS:HD3	1:A:1042:PHE:CE2	1.95	1.02
1:C:455:LEU:O	1:C:456:PHE:HD1	1.29	1.02
1:A:145:TYR:N	1:A:150:LYS:HD2	1.74	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HH12	1:C:533:LEU:CD1	1.72	1.02
1:C:517:LEU:O	1:C:518:LEU:HB2	1.60	1.01
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.43	1.00
1:C:421:TYR:HE2	1:C:458:LYS:C	1.68	1.00
1:B:521:PRO:HA	1:B:564:GLN:HG3	1.45	0.99
1:C:250:THR:H	1:C:251:PRO:HD2	1.23	0.98
1:B:310:LYS:CG	1:B:600:PRO:O	2.12	0.98
1:B:337:PRO:CG	1:B:358:ILE:HD13	1.95	0.97
1:C:739:THR:O	1:C:743:CYS:HB2	1.64	0.96
1:A:148:ASN:ND2	1:A:150:LYS:N	2.14	0.96
1:B:337:PRO:HG3	1:B:358:ILE:CD1	1.97	0.95
1:B:112:SER:HA	1:B:132:GLU:HG2	1.47	0.94
1:C:392:PHE:CE2	1:C:515:PHE:CZ	2.54	0.94
1:B:811:LYS:HB2	1:B:811:LYS:HZ3	1.30	0.94
1:B:273:ARG:HB3	1:B:275:PHE:HE1	1.31	0.94
1:B:576:VAL:HB	1:B:585:LEU:HB2	1.48	0.93
1:C:498:GLN:H	1:C:499:PRO:CD	1.79	0.93
1:B:1010:GLN:HA	1:B:1013:ILE:HD12	1.48	0.93
1:A:966:LEU:HG	1:A:1000:ARG:NH1	1.82	0.93
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.50	0.93
1:A:329:PHE:O	1:A:579:PRO:HG2	1.68	0.92
1:A:145:TYR:CD1	1:A:150:LYS:CD	2.53	0.91
1:B:613:GLN:NE2	1:B:614:ASP:OD1	2.03	0.91
1:C:498:GLN:N	1:C:499:PRO:HD2	1.86	0.91
1:C:328:ARG:HH12	1:C:533:LEU:HD13	0.98	0.91
1:A:538:CYS:SG	1:A:550:GLY:C	2.54	0.91
1:C:328:ARG:NH1	1:C:533:LEU:CD1	2.28	0.91
1:C:444:LYS:HE3	1:C:500:THR:HA	1.53	0.90
1:A:546:LEU:HD11	1:A:565:PHE:HB3	1.52	0.90
1:A:329:PHE:HB3	1:A:330:PRO:HD3	0.90	0.90
1:A:145:TYR:CE1	1:A:150:LYS:HD3	2.07	0.90
1:A:788:ILE:HD11	1:C:699:LEU:HB2	1.53	0.90
1:A:989:ALA:O	1:A:993:ILE:HG23	1.72	0.90
1:B:522:ALA:H	1:B:564:GLN:HE21	1.18	0.90
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.55	0.89
1:C:356:LYS:NZ	1:C:357:ARG:O	2.06	0.88
1:C:1106:GLN:NE2	1:C:1109:PHE:O	2.06	0.88
1:B:729:VAL:HG12	1:B:1059:GLY:HA2	1.56	0.88
1:C:903:ALA:HB1	1:C:913:GLN:HB3	1.55	0.88
1:C:921:LYS:O	1:C:924:ALA:HB3	1.74	0.88
1:B:881:THR:HA	1:B:888:PHE:CE2	2.09	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ARG:HA	1:A:584:ILE:HD12	1.56	0.87
1:B:85:PRO:HB3	1:B:237:ARG:HH12	1.37	0.87
1:B:404:GLY:N	1:B:506:GLN:O	2.06	0.87
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.07	0.87
1:B:900:MET:SD	1:B:917:TYR:OH	2.33	0.87
1:C:740:MET:O	1:C:744:GLY:N	2.07	0.87
1:C:69:HIS:HB2	1:C:77:LYS:HG3	1.56	0.87
1:B:86:PHE:CE2	1:B:89:GLY:C	2.53	0.87
1:C:453:TYR:CD2	1:C:454:ARG:HG3	2.10	0.87
1:C:515:PHE:O	1:C:515:PHE:CD1	2.27	0.87
1:B:1085:GLY:O	1:B:1126:CYS:N	2.07	0.86
1:C:731:MET:SD	1:C:1011:GLN:NE2	2.48	0.86
1:C:122:ASN:OD1	1:C:127:VAL:HG21	1.75	0.86
1:C:329:PHE:CD1	1:C:528:LYS:CB	2.59	0.86
1:C:421:TYR:CE2	1:C:458:LYS:C	2.48	0.86
1:C:451:TYR:HB2	1:C:495:TYR:O	1.76	0.86
1:B:365:TYR:O	1:B:369:TYR:CB	2.23	0.85
1:A:1104:VAL:HG13	1:A:1115:ILE:HG13	1.56	0.85
1:C:438:SER:N	1:C:507:PRO:O	2.09	0.85
1:B:875:SER:HA	1:B:878:LEU:CD2	2.05	0.85
1:C:726:ILE:HG22	1:C:1061:VAL:HG12	1.58	0.85
1:A:963:VAL:O	1:A:966:LEU:HD13	1.76	0.85
1:B:874:THR:O	1:B:878:LEU:HD23	1.76	0.85
1:C:329:PHE:HE1	1:C:528:LYS:CB	1.89	0.85
1:B:151:SER:HB3	1:B:153:MET:HG3	1.59	0.84
1:C:353:TRP:O	1:C:466:ARG:NH2	2.09	0.84
1:B:449:TYR:N	1:B:495:TYR:O	2.10	0.84
1:A:139:PRO:HB2	1:A:157:PHE:HB2	1.60	0.84
1:B:526:GLY:O	1:B:528:LYS:NZ	2.10	0.84
1:C:457:ARG:HG2	1:C:471:GLU:HG2	1.59	0.84
1:A:206:LYS:NZ	1:A:208:THR:OG1	2.11	0.84
1:B:874:THR:C	1:B:878:LEU:HD23	2.03	0.83
1:A:70:VAL:HG13	1:A:79:PHE:CB	2.08	0.83
1:C:455:LEU:HD22	1:C:492:LEU:CB	2.08	0.83
1:A:53:ASP:OD1	1:A:54:LEU:N	2.11	0.83
1:C:73:THR:HB	1:C:78:ARG:HA	1.60	0.83
1:C:666:ILE:HG22	1:C:671:CYS:HA	1.59	0.83
1:B:875:SER:O	1:B:878:LEU:HG	1.79	0.82
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.61	0.82
1:C:145:TYR:H	1:C:145:TYR:HD1	1.26	0.82
1:A:660:TYR:HB2	1:A:695:TYR:CZ	2.14	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:GLN:NE2	1:B:647:ALA:O	2.11	0.82
1:B:86:PHE:HE2	1:B:89:GLY:HA2	1.38	0.82
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.61	0.82
1:A:1106:GLN:NE2	1:A:1109:PHE:O	2.12	0.82
1:B:819:GLU:HA	1:B:822:LEU:HD12	1.61	0.82
1:A:1106:GLN:OE1	1:A:1108:ASN:N	2.11	0.82
1:B:811:LYS:HB2	1:B:811:LYS:NZ	1.86	0.82
1:B:439:ASN:OD1	1:B:449:TYR:N	2.12	0.82
1:C:206:LYS:NZ	1:C:207:HIS:O	2.12	0.82
1:B:740:MET:O	1:B:744:GLY:N	2.13	0.81
1:C:457:ARG:O	1:C:457:ARG:HD3	1.79	0.81
1:A:354:ASN:HB3	1:A:356:LYS:HE3	1.62	0.81
1:A:429:PHE:HB2	1:A:515:PHE:H	1.45	0.81
1:B:84:LEU:CB	1:B:269:TYR:OH	2.27	0.81
1:C:421:TYR:CE2	1:C:458:LYS:N	2.48	0.81
1:C:997:ILE:O	1:C:1001:LEU:HB2	1.80	0.81
1:B:337:PRO:HG3	1:B:358:ILE:HG21	1.59	0.81
1:C:578:ASP:OD1	1:C:583:GLU:N	2.11	0.81
1:A:145:TYR:H	1:A:150:LYS:CD	1.91	0.81
1:B:499:PRO:O	1:B:503:VAL:N	2.14	0.81
1:A:905:ARG:O	1:A:1036:GLN:NE2	2.14	0.80
1:B:417:LYS:O	1:B:421:TYR:HB2	1.81	0.80
1:B:728:PRO:HB3	1:B:951:VAL:HG21	1.63	0.80
1:C:122:ASN:O	1:C:123:ALA:HB3	1.79	0.80
1:A:107:GLY:O	1:A:237:ARG:N	2.14	0.80
1:B:825:LYS:HE3	1:B:945:LEU:HD11	1.63	0.80
1:C:990:GLU:HA	1:C:993:ILE:HD12	1.64	0.80
1:A:613:GLN:NE2	1:A:614:ASP:OD1	2.15	0.80
1:B:815:ARG:NH2	1:B:819:GLU:OE2	2.14	0.80
1:B:275:PHE:CZ	1:B:290:ASP:HB2	2.17	0.80
1:C:422:ASN:OD1	1:C:455:LEU:N	2.15	0.80
1:B:273:ARG:CB	1:B:275:PHE:HE1	1.95	0.79
1:C:855:PHE:H	1:C:858:LEU:HD11	1.45	0.79
1:A:108:THR:O	1:A:237:ARG:NH1	2.14	0.79
1:A:330:PRO:HD2	1:A:527:PRO:HA	1.64	0.79
1:C:421:TYR:OH	1:C:458:LYS:CA	2.25	0.79
1:A:966:LEU:H	1:A:966:LEU:HD12	1.48	0.79
1:A:973:ILE:HD11	1:A:984:LEU:HD11	1.65	0.79
1:A:70:VAL:HG13	1:A:79:PHE:HB3	1.63	0.79
1:C:567:ARG:HG3	1:C:571:ASP:HA	1.65	0.79
1:B:275:PHE:CE1	1:B:290:ASP:CB	2.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:827:THR:OG1	1:C:949:GLN:NE2	2.15	0.78
1:C:1003:SER:O	1:C:1006:THR:OG1	2.00	0.78
1:A:767:LEU:O	1:A:770:ILE:HG23	1.82	0.78
1:B:118:LEU:HD11	1:B:129:LYS:HD2	1.66	0.78
1:B:1027:THR:HG23	1:B:1031:GLU:CD	2.08	0.78
1:B:85:PRO:HB3	1:B:237:ARG:NH1	1.97	0.78
1:C:614:ASP:H	1:C:647:ALA:C	1.91	0.78
1:C:421:TYR:HE2	1:C:458:LYS:N	1.81	0.78
1:B:355:ARG:HD3	1:B:466:ARG:HH12	1.47	0.78
1:A:148:ASN:HD22	1:A:150:LYS:H	1.32	0.78
1:B:86:PHE:HD2	1:B:90:VAL:CG1	1.90	0.78
1:C:53:ASP:HB3	1:C:55:PHE:HE1	1.49	0.78
1:B:274:THR:C	1:B:275:PHE:HD1	1.92	0.77
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.20	0.77
1:B:308:VAL:N	1:B:602:THR:OG1	2.17	0.77
1:C:454:ARG:HB2	1:C:493:GLN:CB	2.14	0.77
1:A:132:GLU:H	1:A:166:CYS:HA	1.46	0.77
1:B:1003:SER:O	1:B:1006:THR:OG1	2.02	0.77
1:C:883:THR:O	1:C:896:ILE:N	2.16	0.77
1:C:804:GLN:HG3	4:p:1:NAG:H62	1.67	0.77
1:B:905:ARG:HB3	1:B:1036:GLN:HE22	1.49	0.77
1:C:422:ASN:OD1	1:C:455:LEU:CB	2.33	0.77
1:B:563:GLN:O	1:B:577:ARG:NH1	2.17	0.77
1:C:421:TYR:HE2	1:C:459:SER:N	1.66	0.76
1:A:299:THR:O	1:A:303:LEU:HG	1.84	0.76
1:B:337:PRO:HG2	1:B:358:ILE:HG21	1.65	0.76
1:C:521:PRO:HB3	1:C:564:GLN:HG3	1.66	0.76
1:B:87:ASN:O	1:B:88:ASP:HB2	1.84	0.76
7:B:1209:NAG:O7	7:B:1209:NAG:H3	1.83	0.76
1:A:387:LEU:HG	1:A:392:PHE:HE1	1.49	0.76
1:C:150:LYS:HD2	1:C:150:LYS:H	1.49	0.76
1:A:299:THR:OG1	1:A:303:LEU:CD1	2.34	0.76
1:C:138:ASP:OD2	1:C:157:PHE:HB2	1.86	0.76
1:C:250:THR:H	1:C:251:PRO:CD	1.99	0.76
1:B:131:CYS:SG	1:B:169:GLU:OE1	2.43	0.76
1:C:557:LYS:NZ	1:C:558:LYS:O	2.19	0.76
1:C:122:ASN:OD1	1:C:127:VAL:CG2	2.34	0.76
1:C:188:ASN:ND2	1:C:208:THR:O	2.17	0.76
1:B:329:PHE:O	1:B:580:GLN:NE2	2.17	0.76
1:C:920:GLN:O	1:C:923:ILE:HB	1.86	0.76
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:ILE:HD12	1:B:715:PRO:HD2	1.68	0.75
1:C:328:ARG:HH11	1:C:533:LEU:HD13	1.46	0.75
1:C:1114:ILE:O	1:C:1119:ASN:ND2	2.19	0.75
1:B:826:VAL:HG12	1:B:828:LEU:H	1.51	0.75
1:C:874:THR:HG22	1:C:878:LEU:HD11	1.66	0.75
1:B:201:PHE:HB3	1:B:229:LEU:O	1.86	0.75
1:B:542:ASN:HA	1:B:547:THR:HG22	1.69	0.75
1:B:789:TYR:CD2	1:B:876:ALA:HB1	2.22	0.75
1:C:455:LEU:CD1	1:C:491:PRO:HB2	2.17	0.75
1:C:471:GLU:H	1:C:491:PRO:HD3	1.51	0.75
1:B:874:THR:O	1:B:878:LEU:CD2	2.35	0.75
1:A:148:ASN:HD21	1:A:150:LYS:HA	1.51	0.75
1:B:273:ARG:CB	1:B:275:PHE:CE1	2.70	0.75
1:B:275:PHE:HB3	1:B:289:VAL:O	1.86	0.75
1:A:396:TYR:N	1:A:514:SER:O	2.20	0.74
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.68	0.74
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.69	0.74
1:B:1091:ARG:HG3	1:B:1092:GLU:H	1.52	0.74
1:C:887:THR:HG21	1:C:894:LEU:HB2	1.68	0.74
1:B:357:ARG:NH2	1:B:359:SER:OG	2.19	0.74
1:C:790:LYS:NZ	1:C:791:THR:O	2.19	0.74
1:B:316:SER:O	1:B:595:VAL:N	2.15	0.74
1:A:422:ASN:HD21	1:A:456:PHE:HB2	1.52	0.74
1:B:404:GLY:HA3	1:B:508:TYR:CD1	2.22	0.74
1:A:1109:PHE:CD2	1:A:1111:GLU:HG3	2.23	0.74
1:B:1116:THR:HG21	1:B:1140:PRO:HD3	1.70	0.74
1:B:747:THR:OG1	1:B:748:GLU:OE1	2.05	0.74
1:B:970:PHE:O	1:B:995:ARG:NH2	2.16	0.74
1:C:1006:THR:HB	1:C:1010:GLN:HE22	1.53	0.74
1:C:1120:THR:CG2	1:C:1121:PHE:N	2.50	0.73
1:B:113:LYS:HD3	1:B:114:THR:HG23	1.70	0.73
1:B:273:ARG:HB3	1:B:275:PHE:CE1	2.21	0.73
1:A:602:THR:O	1:A:606:ASN:ND2	2.15	0.73
1:A:609:ALA:HB2	1:A:692:ILE:HG13	1.69	0.73
1:B:789:TYR:HD2	1:B:876:ALA:HB1	1.53	0.73
1:C:1029:MET:O	1:C:1033:VAL:HB	1.86	0.73
1:A:200:TYR:HD1	1:A:230:PRO:HA	1.53	0.73
1:C:246:ARG:HD2	1:C:249:LEU:HD13	1.68	0.73
1:C:920:GLN:OE1	1:C:920:GLN:N	2.22	0.73
1:B:726:ILE:HB	1:B:948:LEU:HD11	1.70	0.73
1:C:34:ARG:NH2	1:C:219:GLY:O	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:CE1	1:B:89:GLY:N	2.50	0.73
1:A:704:SER:OG	1:B:790:LYS:N	2.16	0.73
1:A:880:GLY:O	1:A:884:SER:N	2.21	0.73
1:B:323:THR:H	1:B:539:VAL:HG12	1.54	0.72
7:C:1205:NAG:H3	7:C:1205:NAG:C8	2.17	0.72
1:A:730:SER:OG	1:A:731:MET:N	2.21	0.72
1:B:1027:THR:HG22	1:B:1028:LYS:N	2.02	0.72
1:A:393:THR:OG1	1:A:520:ALA:O	2.07	0.72
1:C:140:PHE:HE1	1:C:245:HIS:CD2	2.08	0.72
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.69	0.72
1:B:521:PRO:HD3	1:C:41:LYS:HG2	1.70	0.72
1:A:1073:LYS:HB2	1:A:1075:PHE:CE2	2.24	0.72
1:C:455:LEU:CD2	1:C:492:LEU:CB	2.67	0.72
1:B:1040:VAL:N	1:C:1031:GLU:OE1	2.22	0.72
1:C:319:ARG:NH2	1:C:321:GLN:OE1	2.21	0.72
1:B:578:ASP:OD1	1:B:583:GLU:N	2.19	0.72
1:A:770:ILE:HD12	1:A:1015:ALA:HB2	1.72	0.72
1:B:881:THR:HB	1:B:888:PHE:HZ	1.53	0.72
1:C:454:ARG:O	1:C:493:GLN:N	2.19	0.72
1:B:767:LEU:O	1:B:770:ILE:HG22	1.89	0.71
1:B:294:ASP:O	1:B:297:SER:N	2.22	0.71
1:A:36:VAL:HG13	1:A:222:ALA:HA	1.72	0.71
1:C:444:LYS:CE	1:C:500:THR:HA	2.20	0.71
1:B:640:SER:N	1:B:654:GLU:OE2	2.23	0.71
1:C:875:SER:HA	1:C:878:LEU:HD12	1.71	0.71
1:A:726:ILE:HD12	1:A:948:LEU:HG	1.71	0.71
1:B:54:LEU:HB3	1:B:270:LEU:HB2	1.72	0.71
1:C:867:ASP:HA	1:C:870:ILE:HD12	1.73	0.71
1:A:308:VAL:N	1:A:602:THR:OG1	2.24	0.71
1:A:1091:ARG:NH2	1:A:1117:THR:O	2.20	0.71
1:B:998:THR:OG1	1:B:1002:GLN:OE1	2.08	0.71
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.22	0.71
1:C:818:ILE:HA	1:C:821:LEU:HD12	1.72	0.71
1:B:790:LYS:NZ	1:B:791:THR:O	2.22	0.71
1:A:107:GLY:N	1:A:237:ARG:O	2.23	0.71
1:A:731:MET:SD	1:A:1011:GLN:NE2	2.59	0.71
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.71
1:C:453:TYR:CE2	1:C:454:ARG:HG3	2.26	0.70
1:A:391:CYS:HB3	1:A:525:CYS:HA	1.73	0.70
1:C:767:LEU:HD12	1:C:770:ILE:HG12	1.71	0.70
1:C:958:ALA:O	1:C:961:THR:OG1	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:GLN:HA	1:C:700:GLY:HA3	1.73	0.70
1:B:616:ASN:HB2	7:B:1203:NAG:N2	2.06	0.70
1:B:660:TYR:HB2	1:B:695:TYR:CZ	2.26	0.70
1:B:787:GLN:OE1	1:B:789:TYR:OH	2.08	0.70
1:C:33:THR:OG1	1:C:34:ARG:NH1	2.24	0.70
1:B:51:THR:HG22	1:B:275:PHE:O	1.91	0.70
1:C:251:PRO:O	1:C:252:GLY:O	2.09	0.70
6:Q:1:NAG:H83	6:Q:1:NAG:H3	1.72	0.70
1:A:70:VAL:CG1	1:A:79:PHE:CB	2.69	0.70
1:A:1109:PHE:CE2	1:A:1111:GLU:HG3	2.27	0.70
1:B:102:ARG:CB	1:B:139:PRO:HG3	2.21	0.70
1:B:275:PHE:CD1	1:B:290:ASP:CA	2.75	0.70
1:B:774:GLN:HA	1:B:777:ASN:ND2	2.07	0.70
1:B:874:THR:O	1:B:878:LEU:CG	2.39	0.70
1:C:826:VAL:HG21	1:C:1057:PRO:HG3	1.74	0.70
1:A:133:PHE:CD1	1:A:161:SER:HA	2.26	0.70
1:B:428:ASP:O	1:B:430:THR:OG1	2.10	0.70
1:B:748:GLU:OE1	1:B:748:GLU:N	2.24	0.70
1:C:878:LEU:O	1:C:882:ILE:HG13	1.92	0.70
1:A:166:CYS:SG	1:A:167:THR:N	2.64	0.70
1:C:912:THR:HG22	1:C:914:ASN:H	1.57	0.70
1:A:125:ASN:HD22	7:A:1206:NAG:H5	1.56	0.70
1:A:1003:SER:O	1:A:1006:THR:OG1	2.10	0.70
2:X:1:NAG:O7	2:X:1:NAG:O3	2.08	0.70
1:A:578:ASP:HB3	1:A:583:GLU:O	1.92	0.70
1:A:787:GLN:NE2	1:A:789:TYR:OH	2.25	0.70
1:A:1106:GLN:HE22	1:A:1109:PHE:H	1.39	0.70
1:A:189:LEU:HB3	1:A:208:THR:HB	1.74	0.70
1:A:1000:ARG:O	1:A:1004:LEU:HD23	1.92	0.70
1:B:565:PHE:HA	1:B:575:ALA:HB3	1.74	0.69
1:B:881:THR:HB	1:B:888:PHE:CZ	2.27	0.69
1:B:983:ARG:HD3	1:B:984:LEU:HG	1.73	0.69
1:A:1086:LYS:CE	1:A:1088:HIS:CE1	2.73	0.69
1:B:221:SER:OG	1:B:222:ALA:N	2.24	0.69
1:A:330:PRO:HG2	1:A:526:GLY:O	1.92	0.69
1:A:442:ASP:HB3	1:A:507:PRO:HG3	1.74	0.69
1:B:337:PRO:CD	1:B:358:ILE:HG21	2.22	0.69
1:A:995:ARG:O	1:A:998:THR:OG1	2.09	0.69
1:B:1051:SER:OG	1:B:1063:LEU:O	2.08	0.69
1:C:377:PHE:HA	1:C:434:ILE:HD12	1.74	0.69
1:A:133:PHE:HD1	1:A:161:SER:HA	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:LEU:H	1:A:966:LEU:CD1	2.04	0.69
1:B:619:GLU:C	1:B:621:PRO:CD	2.66	0.69
1:A:314:GLN:HA	1:A:596:SER:HB2	1.73	0.69
1:B:296:LEU:HB2	1:B:608:VAL:HG21	1.74	0.69
1:B:342:PHE:CE2	1:B:371:SER:HB2	2.27	0.69
1:C:715:PRO:O	1:C:1110:TYR:N	2.25	0.69
1:A:144:TYR:CG	1:A:245:HIS:HB2	2.28	0.69
1:C:107:GLY:HA2	1:C:235:ILE:HD12	1.74	0.69
1:A:70:VAL:CG1	1:A:79:PHE:HB2	2.23	0.69
1:A:329:PHE:HB2	1:A:330:PRO:CD	2.23	0.69
1:A:826:VAL:HG11	1:A:1057:PRO:HG3	1.75	0.69
1:A:925:ASN:HA	1:A:928:ASN:HD22	1.57	0.69
1:B:86:PHE:HZ	1:B:89:GLY:HA2	1.50	0.69
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.73	0.69
1:B:762:GLN:HA	1:B:765:ARG:HE	1.58	0.69
1:C:936:ASP:OD1	1:C:937:SER:N	2.25	0.69
1:C:1127:ASP:OD1	1:C:1128:VAL:N	2.25	0.69
1:B:737:ASP:HA	1:B:764:ASN:HD21	1.58	0.69
1:C:394:ASN:O	1:C:515:PHE:HB2	1.92	0.69
1:C:1083:HIS:HB3	1:C:1088:HIS:NE2	2.08	0.69
1:C:1105:THR:HG21	1:C:1111:GLU:H	1.58	0.69
1:A:708:SER:OG	1:A:711:SER:O	2.11	0.69
1:C:453:TYR:O	1:C:454:ARG:C	2.35	0.69
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.57	0.69
1:A:37:TYR:HB2	1:A:204:TYR:CE2	2.28	0.68
1:A:327:VAL:HG22	1:A:329:PHE:CE1	2.28	0.68
1:B:538:CYS:HA	1:B:550:GLY:O	1.93	0.68
1:B:1114:ILE:O	1:B:1119:ASN:ND2	2.26	0.68
1:A:534:VAL:HG21	1:A:539:VAL:HG21	1.74	0.68
1:A:770:ILE:O	1:A:774:GLN:NE2	2.24	0.68
1:C:826:VAL:HG12	1:C:828:LEU:H	1.58	0.68
1:A:966:LEU:CG	1:A:1000:ARG:HH12	2.02	0.68
1:B:139:PRO:HD3	1:B:242:LEU:C	2.19	0.68
1:A:393:THR:HA	1:A:522:ALA:HA	1.76	0.68
1:A:924:ALA:O	1:A:928:ASN:ND2	2.27	0.68
1:B:305:SER:HG	1:B:307:THR:HG1	1.41	0.68
1:B:383:SER:OG	1:B:385:THR:OG1	2.12	0.68
1:A:200:TYR:CD1	1:A:230:PRO:HA	2.29	0.68
1:B:271:GLN:HG3	1:B:273:ARG:HG2	1.76	0.68
1:B:330:PRO:HA	1:B:580:GLN:HG2	1.75	0.68
1:B:950:ASP:OD1	1:B:951:VAL:N	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:THR:HA	1:C:1012:LEU:HD12	1.76	0.68
1:A:329:PHE:O	1:A:579:PRO:CG	2.42	0.67
1:B:787:GLN:HB2	1:B:789:TYR:CE1	2.29	0.67
1:A:137:ASN:OD1	1:A:138:ASP:N	2.28	0.67
1:A:762:GLN:HA	1:A:765:ARG:HH11	1.59	0.67
1:B:730:SER:OG	1:B:1058:HIS:O	2.11	0.67
1:C:563:GLN:H	1:C:577:ARG:NH2	1.92	0.67
1:A:41:LYS:HD3	1:C:521:PRO:HD2	1.75	0.67
1:B:274:THR:O	1:B:275:PHE:HD1	1.77	0.67
1:B:330:PRO:HG3	1:B:579:PRO:HB2	1.77	0.67
1:C:146:HIS:HA	1:C:150:LYS:HE3	1.76	0.67
1:C:963:VAL:HA	1:C:966:LEU:HD23	1.76	0.67
1:A:558:LYS:NZ	5:h:2:NAG:O5	2.28	0.67
1:B:866:THR:HG23	1:B:869:MET:H	1.58	0.67
1:B:867:ASP:OD1	1:B:867:ASP:N	2.25	0.67
1:C:1037:SER:OG	1:C:1039:ARG:N	2.22	0.67
1:A:330:PRO:HD2	1:A:527:PRO:C	2.19	0.67
1:A:770:ILE:HG13	1:A:774:GLN:NE2	2.10	0.67
1:C:152:TRP:CD2	1:C:155:SER:HB2	2.29	0.67
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.28	0.67
1:B:518:LEU:HB3	1:B:565:PHE:HZ	1.60	0.67
1:A:299:THR:OG1	1:A:303:LEU:HD11	1.95	0.67
1:A:756:TYR:HB3	1:A:759:PHE:CE1	2.30	0.67
1:B:623:ALA:HA	1:B:626:ALA:HB3	1.76	0.67
1:A:104:TRP:HB3	1:A:106:PHE:HE1	1.60	0.66
1:A:974:SER:OG	1:A:983:ARG:NH2	2.28	0.66
1:C:444:LYS:HE3	1:C:500:THR:CA	2.23	0.66
1:A:422:ASN:ND2	1:A:455:LEU:O	2.26	0.66
1:A:712:ILE:HG21	1:B:896:ILE:HD13	1.76	0.66
1:B:54:LEU:HD22	1:B:88:ASP:HB3	1.75	0.66
1:B:106:PHE:HA	1:B:237:ARG:O	1.95	0.66
1:B:138:ASP:OD1	1:B:242:LEU:HG	1.95	0.66
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.75	0.66
1:A:298:GLU:O	1:A:302:THR:HG22	1.95	0.66
1:C:122:ASN:O	1:C:123:ALA:CB	2.43	0.66
1:C:957:GLN:O	1:C:961:THR:HG23	1.96	0.66
1:C:1120:THR:HG23	1:C:1121:PHE:H	1.60	0.66
1:B:882:ILE:HB	1:B:898:PHE:HE1	1.60	0.66
1:C:517:LEU:O	1:C:518:LEU:CB	2.42	0.66
4:V:1:NAG:C3	4:V:1:NAG:H83	2.26	0.66
1:A:27:ALA:O	1:A:64:TRP:N	2.24	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:CE1	1:C:245:HIS:CD2	2.82	0.66
1:C:563:GLN:O	1:C:577:ARG:NE	2.28	0.66
1:A:660:TYR:C	1:A:698:SER:HB3	2.20	0.66
1:B:646:ARG:HG3	1:B:668:ALA:HB1	1.77	0.66
1:C:708:SER:N	1:C:711:SER:OG	2.27	0.66
1:B:133:PHE:CD2	1:B:160:TYR:HA	2.30	0.66
1:A:1028:LYS:CD	1:A:1042:PHE:CE2	2.77	0.66
1:B:875:SER:CA	1:B:878:LEU:HD21	2.20	0.66
7:C:1205:NAG:C1	7:C:1205:NAG:H82	2.26	0.66
1:A:1009:THR:OG1	1:A:1010:GLN:NE2	2.29	0.66
1:C:334:ASN:O	1:C:362:VAL:N	2.29	0.66
1:C:729:VAL:HG13	1:C:1059:GLY:HA2	1.78	0.66
1:C:879:ALA:HA	1:C:882:ILE:HD12	1.78	0.66
1:C:961:THR:O	1:C:965:GLN:NE2	2.28	0.66
1:C:578:ASP:OD2	1:C:581:THR:OG1	2.13	0.65
1:A:966:LEU:HD12	1:A:966:LEU:N	2.10	0.65
1:B:138:ASP:OD1	1:B:242:LEU:CD1	2.45	0.65
1:C:392:PHE:CZ	1:C:515:PHE:CZ	2.83	0.65
1:C:542:ASN:OD1	1:C:545:GLY:N	2.29	0.65
7:C:1202:NAG:H3	7:C:1202:NAG:H83	1.78	0.65
1:A:54:LEU:HB2	1:A:195:LYS:HZ1	1.61	0.65
1:B:557:LYS:NZ	1:B:558:LYS:O	2.30	0.65
1:A:126:VAL:O	1:A:172:SER:OG	2.11	0.65
1:A:348:ALA:HB3	1:A:353:TRP:HE3	1.59	0.65
4:p:2:NAG:O7	4:p:2:NAG:H3	1.95	0.65
1:A:286:THR:OG1	1:A:287:ASP:OD1	2.15	0.65
1:B:57:PRO:HG3	1:B:271:GLN:HB3	1.77	0.65
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.78	0.65
1:B:499:PRO:HB2	1:B:506:GLN:HE22	1.61	0.65
1:B:871:ALA:O	1:B:874:THR:OG1	2.14	0.65
1:C:315:THR:HG23	1:C:596:SER:HA	1.78	0.65
1:C:337:PRO:O	1:C:341:VAL:HG23	1.97	0.65
1:C:1091:ARG:HE	1:C:1119:ASN:C	2.04	0.65
4:V:1:NAG:H83	4:V:1:NAG:H3	1.77	0.65
1:A:1080:ALA:HA	1:A:1095:PHE:CE2	2.32	0.65
1:C:295:PRO:HB3	1:C:597:VAL:HG22	1.78	0.65
1:B:874:THR:O	1:B:878:LEU:HG	1.97	0.65
1:C:1004:LEU:O	1:C:1008:VAL:HG23	1.97	0.65
1:B:126:VAL:HG21	1:B:174:PRO:HB2	1.79	0.64
1:B:775:ASP:O	1:B:778:THR:OG1	2.13	0.64
1:B:1002:GLN:O	1:B:1006:THR:HG23	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:H	1:A:949:GLN:HE22	1.45	0.64
1:B:355:ARG:O	1:B:356:LYS:NZ	2.29	0.64
1:B:1030:SER:HA	1:B:1034:LEU:HD13	1.79	0.64
1:B:881:THR:CA	1:B:888:PHE:CE2	2.80	0.64
1:C:29:THR:HG21	1:C:216:LEU:HD13	1.79	0.64
1:C:1028:LYS:O	1:C:1032:CYS:HB2	1.97	0.64
1:A:825:LYS:NZ	1:A:938:LEU:O	2.23	0.64
1:B:109:THR:OG1	1:B:114:THR:OG1	2.11	0.64
1:C:375:SER:OG	1:C:435:ALA:O	2.14	0.64
1:C:403:ARG:NH2	1:C:505:TYR:CE1	2.65	0.64
1:C:455:LEU:HD12	1:C:491:PRO:HB2	1.78	0.64
1:A:1006:THR:O	1:A:1010:GLN:NE2	2.30	0.64
1:B:51:THR:O	1:B:274:THR:OG1	2.14	0.64
1:B:273:ARG:HB2	1:B:275:PHE:CE1	2.31	0.64
1:B:404:GLY:HA3	1:B:508:TYR:CG	2.33	0.64
1:C:774:GLN:HA	1:C:777:ASN:ND2	2.12	0.64
2:d:1:NAG:O3	2:d:2:NAG:O5	2.15	0.64
1:A:1030:SER:OG	1:A:1031:GLU:N	2.30	0.64
1:B:90:VAL:HG23	1:B:194:PHE:HB2	1.80	0.64
1:C:609:ALA:HB2	1:C:692:ILE:HD12	1.78	0.64
1:B:50:SER:OG	1:B:51:THR:N	2.31	0.64
1:A:980:ILE:HD12	1:A:993:ILE:HG22	1.79	0.64
7:B:1209:NAG:O7	7:B:1209:NAG:C3	2.46	0.64
1:C:782:PHE:O	1:C:784:GLN:N	2.29	0.64
1:C:1037:SER:OG	1:C:1038:LYS:N	2.29	0.64
1:A:912:THR:O	1:A:915:VAL:HG12	1.96	0.64
1:B:305:SER:OG	1:B:307:THR:OG1	2.13	0.64
1:B:309:GLU:N	1:B:309:GLU:OE1	2.31	0.64
1:C:550:GLY:HA2	1:C:589:PRO:HA	1.79	0.64
1:A:895:GLN:OE1	1:C:713:ALA:HB2	1.97	0.64
1:B:521:PRO:CA	1:B:564:GLN:HG3	2.22	0.64
1:A:773:GLU:O	1:A:777:ASN:ND2	2.30	0.63
1:A:1083:HIS:HD2	1:A:1136:THR:HA	1.63	0.63
1:B:284:THR:HG22	1:B:285:ILE:H	1.64	0.63
1:B:423:TYR:OH	1:B:466:ARG:NH1	2.31	0.63
1:B:954:GLN:NE2	1:B:1014:ARG:HH21	1.96	0.63
1:A:188:ASN:HB3	1:A:207:HIS:HE1	1.63	0.63
1:A:359:SER:HB3	1:A:523:THR:OG1	1.98	0.63
1:C:1091:ARG:NE	1:C:1119:ASN:O	2.28	0.63
7:A:1205:NAG:H3	7:A:1205:NAG:H83	1.81	0.63
1:B:34:ARG:HH21	1:B:218:GLN:C	2.07	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:N	1:B:84:LEU:HD12	2.12	0.63
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.80	0.63
1:B:290:ASP:OD1	1:B:291:CYS:N	2.31	0.63
1:C:316:SER:OG	1:C:317:ASN:N	2.29	0.63
1:C:775:ASP:O	1:C:778:THR:OG1	2.16	0.63
1:A:543:PHE:CE2	1:A:576:VAL:HB	2.33	0.63
1:A:881:THR:HA	1:A:885:GLY:HA2	1.80	0.63
1:C:395:VAL:HA	1:C:515:PHE:HB3	1.81	0.63
1:C:710:ASN:N	1:C:710:ASN:OD1	2.30	0.63
1:C:1062:PHE:HB3	1:C:1064:HIS:CE1	2.34	0.63
1:A:38:TYR:OH	1:A:285:ILE:N	2.30	0.63
1:A:310:LYS:HG2	1:A:664:ILE:HD11	1.81	0.63
1:B:336:CYS:N	1:B:361:CYS:SG	2.72	0.63
1:C:559:PHE:HE2	1:C:563:GLN:HB2	1.63	0.63
1:C:1116:THR:H	1:C:1119:ASN:HD21	1.46	0.63
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.81	0.63
1:C:457:ARG:HH11	1:C:457:ARG:C	2.07	0.63
1:A:70:VAL:HG11	1:A:79:PHE:HB2	1.81	0.62
1:C:822:LEU:HD21	1:C:1057:PRO:HD3	1.81	0.62
1:A:645:THR:HG23	1:A:647:ALA:H	1.63	0.62
1:B:949:GLN:HG3	1:B:953:ASN:HD21	1.62	0.62
1:A:37:TYR:HB2	1:A:204:TYR:CD2	2.34	0.62
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.35	0.62
1:A:369:TYR:OH	1:A:376:THR:O	2.14	0.62
1:A:541:PHE:O	1:A:548:GLY:N	2.30	0.62
1:A:1006:THR:O	1:A:1009:THR:OG1	2.17	0.62
1:B:641:ASN:H	1:B:654:GLU:HG2	1.63	0.62
1:B:1088:HIS:HA	1:B:1122:VAL:HA	1.81	0.62
1:C:456:PHE:O	1:C:471:GLU:HG3	2.00	0.62
1:C:702:GLU:OE2	1:C:704:SER:N	2.32	0.62
1:A:246:ARG:N	1:A:246:ARG:HD2	2.15	0.62
1:A:366:SER:HB3	1:A:387:LEU:HD22	1.82	0.62
1:B:84:LEU:HB3	1:B:85:PRO:HD2	1.79	0.62
1:B:392:PHE:N	1:B:524:VAL:O	2.22	0.62
1:A:1023:ASN:O	1:A:1027:THR:HG23	1.99	0.62
1:B:439:ASN:ND2	1:B:495:TYR:O	2.29	0.62
1:B:931:ILE:O	1:B:934:ILE:HG22	1.99	0.62
1:C:708:SER:OG	1:C:711:SER:N	2.32	0.62
1:A:204:TYR:HB3	1:A:223:LEU:HB2	1.81	0.62
1:B:1037:SER:OG	1:B:1038:LYS:N	2.31	0.62
1:B:1136:THR:HG23	1:B:1138:TYR:HE1	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LYS:HD2	1:C:500:THR:O	1.98	0.62
1:C:458:LYS:HG2	1:C:458:LYS:O	2.00	0.62
1:C:807:PRO:HB3	1:C:815:ARG:CG	2.30	0.62
1:C:1120:THR:CG2	1:C:1121:PHE:H	2.11	0.62
1:A:102:ARG:HB2	1:A:242:LEU:HD22	1.81	0.62
1:A:245:HIS:C	1:A:246:ARG:HD2	2.24	0.62
1:A:330:PRO:HD2	1:A:527:PRO:CA	2.29	0.62
1:A:1106:GLN:HE22	1:A:1109:PHE:N	1.97	0.62
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.33	0.62
1:A:964:LYS:O	1:A:967:SER:OG	2.10	0.62
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.33	0.62
1:B:619:GLU:C	1:B:621:PRO:HD2	2.25	0.62
1:C:455:LEU:HA	1:C:492:LEU:HA	1.80	0.62
1:A:148:ASN:HD22	1:A:150:LYS:N	1.90	0.61
1:A:968:SER:OG	1:A:969:ASN:N	2.31	0.61
1:B:560:LEU:HB2	1:B:563:GLN:HE21	1.64	0.61
1:A:357:ARG:NE	1:A:394:ASN:OD1	2.34	0.61
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.35	0.61
1:A:1106:GLN:OE1	1:A:1107:ARG:N	2.33	0.61
1:B:924:ALA:O	1:B:928:ASN:ND2	2.33	0.61
1:B:925:ASN:HA	1:B:928:ASN:HD22	1.64	0.61
1:C:37:TYR:CB	1:C:223:LEU:HB2	2.29	0.61
1:A:712:ILE:CG2	1:B:897:PRO:HD3	2.31	0.61
1:B:89:GLY:C	1:B:270:LEU:HG	2.25	0.61
1:B:429:PHE:CZ	1:C:984:LEU:HD11	2.34	0.61
1:B:743:CYS:O	1:B:746:SER:OG	2.14	0.61
1:A:148:ASN:HD21	1:A:150:LYS:CA	2.12	0.61
1:A:339:GLY:O	1:A:343:ASN:N	2.28	0.61
1:C:717:ASN:OD1	2:X:1:NAG:N2	2.32	0.61
1:B:52:GLN:HB3	1:B:274:THR:HB	1.81	0.61
1:B:811:LYS:CB	1:B:812:PRO:HD3	2.30	0.61
1:B:825:LYS:NZ	1:B:938:LEU:O	2.23	0.61
1:C:455:LEU:HD13	1:C:492:LEU:CA	2.31	0.61
1:C:1120:THR:HG22	1:C:1121:PHE:N	2.13	0.61
1:A:71:SER:HB3	1:A:259:THR:HA	1.83	0.61
1:A:148:ASN:ND2	1:A:150:LYS:CA	2.64	0.61
1:A:660:TYR:O	1:A:698:SER:N	2.33	0.61
1:A:866:THR:OG1	1:A:868:GLU:OE1	2.14	0.61
1:B:274:THR:C	1:B:275:PHE:CD1	2.78	0.61
1:B:1106:GLN:H	1:B:1106:GLN:CD	2.09	0.61
1:C:297:SER:OG	1:C:298:GLU:OE2	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:PHE:O	1:C:806:LEU:N	2.26	0.61
1:C:1116:THR:HA	1:C:1138:TYR:HB2	1.82	0.61
1:A:127:VAL:HG12	1:A:171:VAL:HA	1.82	0.61
1:A:204:TYR:HB3	1:A:223:LEU:CB	2.30	0.61
1:A:728:PRO:HB3	1:A:951:VAL:HG11	1.82	0.61
1:C:365:TYR:HD1	1:C:388:ASN:HA	1.65	0.61
1:C:411:ALA:H	1:C:425:LEU:HD21	1.64	0.61
1:A:175:PHE:HD1	1:A:176:LEU:HD12	1.64	0.61
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.81	0.61
1:A:776:LYS:O	1:A:780:GLU:HG3	2.00	0.61
1:B:433:VAL:HG23	1:B:511:VAL:HG13	1.82	0.61
1:C:336:CYS:HB3	1:C:338:PHE:CD2	2.35	0.61
1:C:424:LYS:HA	1:C:460:ASN:HD21	1.64	0.61
1:C:970:PHE:O	1:C:995:ARG:NH2	2.34	0.61
1:A:328:ARG:HB2	1:A:543:PHE:CE1	2.36	0.61
1:A:618:THR:OG1	1:A:619:GLU:OE1	2.18	0.61
1:A:641:ASN:ND2	1:A:653:ALA:O	2.34	0.61
1:A:1089:PHE:O	1:A:1120:THR:OG1	2.15	0.61
1:C:495:TYR:CZ	1:C:497:PHE:O	2.53	0.61
1:A:770:ILE:HA	1:A:773:GLU:CD	2.26	0.61
1:B:874:THR:C	1:B:878:LEU:CD2	2.72	0.61
1:C:426:PRO:HG3	1:C:464:PHE:CE2	2.36	0.61
1:C:717:ASN:CG	2:X:1:NAG:HN2	2.09	0.61
1:A:541:PHE:N	1:A:548:GLY:O	2.24	0.60
1:B:1091:ARG:HG3	1:B:1092:GLU:N	2.16	0.60
1:C:43:PHE:CE2	1:C:45:SER:HB3	2.36	0.60
1:C:383:SER:HG	1:C:385:THR:HG1	1.37	0.60
1:C:402:ILE:O	1:C:507:PRO:HB2	2.01	0.60
1:A:338:PHE:O	1:A:342:PHE:N	2.33	0.60
7:A:1207:NAG:H3	7:A:1207:NAG:H83	1.81	0.60
1:B:134:GLN:H	1:B:161:SER:HG	1.47	0.60
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.36	0.60
1:B:1093:GLY:H	1:B:1107:ARG:NH2	2.00	0.60
1:C:1062:PHE:O	1:C:1063:LEU:HD23	2.02	0.60
1:C:1105:THR:OG1	1:C:1111:GLU:O	2.17	0.60
1:B:895:GLN:OE1	1:B:895:GLN:N	2.34	0.60
1:A:562:PHE:HB3	1:B:224:GLU:HB2	1.84	0.60
1:C:98:SER:OG	1:C:99:ASN:OD1	2.16	0.60
1:A:39:PRO:HG3	1:A:44:ARG:HH12	1.65	0.60
1:A:969:ASN:O	1:A:972:ALA:N	2.32	0.60
1:B:37:TYR:HD2	1:B:204:TYR:CE2	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:VAL:HA	1:B:511:VAL:HG22	1.83	0.60
1:B:691:SER:OG	1:B:692:ILE:N	2.34	0.60
1:B:710:ASN:O	1:B:1077:THR:N	2.26	0.60
1:B:752:LEU:O	1:B:755:GLN:HB3	2.01	0.60
2:d:1:NAG:O3	2:d:1:NAG:O7	2.19	0.60
1:A:756:TYR:HB3	1:A:759:PHE:CD1	2.37	0.60
1:A:962:LEU:HD12	1:A:1007:TYR:CE1	2.36	0.60
1:B:826:VAL:HG21	1:B:1057:PRO:HG2	1.83	0.60
1:B:1043:CYS:HB2	1:B:1048:HIS:CE1	2.36	0.60
1:A:741:TYR:CZ	1:A:1004:LEU:HD21	2.37	0.60
1:A:820:ASP:O	1:A:823:PHE:N	2.34	0.60
1:B:659:SER:HB2	1:B:698:SER:HB2	1.83	0.60
1:B:867:ASP:HA	1:B:870:ILE:HD12	1.84	0.60
1:B:954:GLN:HE21	1:B:1014:ARG:HH21	1.48	0.60
1:C:139:PRO:HG2	1:C:242:LEU:HA	1.84	0.60
1:C:455:LEU:C	1:C:456:PHE:CD1	2.78	0.60
1:C:560:LEU:HB3	1:C:562:PHE:CE2	2.36	0.60
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.35	0.60
1:C:901:GLN:NE2	1:C:905:ARG:HE	2.00	0.60
1:C:976:VAL:HG13	1:C:979:ASP:HB2	1.84	0.60
1:A:1028:LYS:HD3	1:A:1042:PHE:CD2	2.36	0.60
1:B:376:THR:HG23	1:B:378:LYS:HG2	1.84	0.60
1:B:812:PRO:HB2	1:B:815:ARG:HD2	1.84	0.60
1:A:1031:GLU:OE1	1:C:1039:ARG:HA	2.01	0.60
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.84	0.60
1:B:1083:HIS:HD2	1:B:1137:VAL:HG22	1.67	0.60
1:C:294:ASP:OD2	1:C:296:LEU:N	2.27	0.60
1:A:203:ILE:HG12	1:A:227:VAL:HG22	1.84	0.60
1:B:86:PHE:HZ	1:B:89:GLY:CA	2.06	0.60
1:B:139:PRO:CD	1:B:242:LEU:C	2.75	0.60
1:B:518:LEU:HB3	1:B:565:PHE:CZ	2.37	0.60
1:B:1129:VAL:HG21	1:C:917:TYR:HB3	1.82	0.60
1:B:133:PHE:CE2	1:B:159:VAL:O	2.55	0.59
1:C:315:THR:OG1	1:C:316:SER:N	2.34	0.59
1:A:294:ASP:OD1	1:A:297:SER:OG	2.16	0.59
1:B:1076:THR:O	1:B:1097:SER:N	2.32	0.59
1:B:1105:THR:HG21	1:B:1111:GLU:H	1.66	0.59
1:C:884:SER:OG	1:C:894:LEU:N	2.35	0.59
1:C:887:THR:OG1	1:C:894:LEU:N	2.27	0.59
1:A:168:PHE:CE2	1:A:170:TYR:HB2	2.37	0.59
1:A:319:ARG:HH11	1:B:740:MET:HB2	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:O	1:C:223:LEU:HG	2.02	0.59
1:C:228:ASP:OD1	1:C:229:LEU:N	2.35	0.59
1:C:817:PHE:HD1	1:C:821:LEU:HD11	1.67	0.59
2:E:2:NAG:H3	2:E:2:NAG:H83	1.84	0.59
1:A:102:ARG:HG2	1:A:242:LEU:HD13	1.83	0.59
1:A:550:GLY:HA3	1:A:588:THR:O	2.02	0.59
1:C:251:PRO:O	1:C:252:GLY:C	2.45	0.59
1:C:1109:PHE:CE2	1:C:1111:GLU:HB2	2.38	0.59
1:B:619:GLU:C	1:B:621:PRO:HD3	2.28	0.59
1:B:1080:ALA:HB3	1:B:1132:ILE:HG12	1.85	0.59
1:A:538:CYS:SG	1:A:551:VAL:N	2.76	0.59
1:A:958:ALA:O	1:A:961:THR:OG1	2.21	0.59
1:A:1080:ALA:HA	1:A:1095:PHE:HE2	1.66	0.59
1:C:665:PRO:HA	1:C:671:CYS:HB2	1.85	0.59
1:C:717:ASN:HB3	1:C:1071:GLN:HG3	1.83	0.59
1:A:782:PHE:O	1:A:784:GLN:N	2.32	0.59
1:B:130:VAL:HG13	1:B:167:THR:HB	1.85	0.59
1:B:374:PHE:CE2	1:B:434:ILE:HA	2.37	0.59
1:B:1089:PHE:CZ	1:C:914:ASN:HA	2.38	0.59
1:C:146:HIS:HE1	1:C:248:TYR:CG	2.21	0.59
1:A:304:LYS:N	1:A:304:LYS:HD2	2.18	0.59
1:A:969:ASN:C	1:A:972:ALA:H	2.11	0.59
1:A:1056:ALA:HB3	1:A:1059:GLY:C	2.27	0.59
1:B:105:ILE:O	1:B:238:PHE:CA	2.43	0.59
1:B:1087:ALA:O	1:B:1123:SER:N	2.33	0.59
1:C:920:GLN:O	1:C:924:ALA:N	2.24	0.59
1:C:1018:ILE:O	1:C:1021:SER:OG	2.20	0.59
1:C:1111:GLU:HG3	1:C:1113:GLN:HE22	1.68	0.59
1:A:732:THR:O	1:A:734:THR:N	2.36	0.59
1:A:878:LEU:O	1:A:882:ILE:HG12	2.02	0.59
1:B:583:GLU:OE2	1:B:584:ILE:N	2.34	0.59
1:B:875:SER:C	1:B:878:LEU:HG	2.28	0.59
1:C:152:TRP:CE3	1:C:155:SER:HB2	2.37	0.59
1:C:276:LEU:HD11	1:C:291:CYS:HB2	1.85	0.59
1:C:379:CYS:HA	1:C:432:CYS:CB	2.33	0.59
7:C:1206:NAG:H83	7:C:1206:NAG:H3	1.85	0.59
1:A:1024:LEU:O	1:A:1028:LYS:HG2	2.03	0.58
1:C:188:ASN:ND2	1:C:189:LEU:H	2.01	0.58
1:C:332:ILE:O	1:C:332:ILE:HG23	2.01	0.58
1:C:455:LEU:HD13	1:C:492:LEU:N	2.18	0.58
1:C:821:LEU:O	1:C:825:LYS:HG2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:955:ASN:O	1:C:959:LEU:HG	2.02	0.58
1:A:31:SER:OG	1:A:60:SER:N	2.29	0.58
1:A:299:THR:O	1:A:303:LEU:HB2	2.03	0.58
1:B:381:GLY:HA2	1:B:429:PHE:CZ	2.38	0.58
1:B:396:TYR:H	1:B:514:SER:CB	2.17	0.58
1:C:799:GLY:O	1:C:928:ASN:ND2	2.26	0.58
1:A:47:VAL:HG21	1:C:567:ARG:HH12	1.68	0.58
1:A:168:PHE:HE2	1:A:170:TYR:HB2	1.67	0.58
1:A:582:LEU:HG	1:A:582:LEU:O	2.03	0.58
1:B:298:GLU:OE1	1:B:298:GLU:N	2.35	0.58
1:B:731:MET:HG3	1:B:955:ASN:HD22	1.69	0.58
1:C:28:TYR:HD2	7:C:1206:NAG:H5	1.68	0.58
1:C:250:THR:N	1:C:251:PRO:HD2	2.06	0.58
1:B:975:SER:O	1:B:1000:ARG:NH2	2.36	0.58
1:C:594:GLY:H	1:C:613:GLN:HE22	1.49	0.58
1:C:901:GLN:O	1:C:905:ARG:HG3	2.03	0.58
1:A:562:PHE:O	1:B:41:LYS:HA	2.02	0.58
1:A:980:ILE:O	1:A:984:LEU:N	2.36	0.58
1:A:1097:SER:OG	1:A:1101:HIS:O	2.13	0.58
1:B:128:ILE:HD13	1:B:170:TYR:CD1	2.39	0.58
1:B:914:ASN:OD1	1:B:915:VAL:N	2.33	0.58
1:C:307:THR:OG1	1:C:309:GLU:OE2	2.13	0.58
1:C:1030:SER:OG	1:C:1031:GLU:N	2.35	0.58
1:A:143:VAL:HG22	1:A:150:LYS:HG2	1.86	0.58
1:A:915:VAL:HG13	1:A:916:LEU:H	1.67	0.58
1:B:937:SER:O	1:B:941:THR:N	2.37	0.58
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.19	0.58
1:C:901:GLN:HE22	1:C:905:ARG:HE	1.52	0.58
1:A:100:ILE:HG23	1:A:101:ILE:HG12	1.86	0.58
1:A:393:THR:OG1	1:A:394:ASN:ND2	2.37	0.58
1:B:216:LEU:O	1:B:218:GLN:N	2.36	0.58
1:B:275:PHE:CE1	1:B:290:ASP:HB2	2.35	0.58
1:B:775:ASP:OD1	1:B:776:LYS:N	2.36	0.58
1:C:204:TYR:HA	1:C:224:GLU:O	2.03	0.58
1:C:319:ARG:HH21	1:C:322:PRO:HD2	1.69	0.58
1:C:333:THR:O	1:C:333:THR:HG22	2.02	0.58
1:C:365:TYR:CD1	1:C:388:ASN:HA	2.39	0.58
1:C:455:LEU:HD13	1:C:492:LEU:HA	1.86	0.58
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.39	0.58
1:A:805:ILE:HG13	1:A:806:LEU:N	2.19	0.58
1:B:620:VAL:N	1:B:621:PRO:CD	2.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ASP:HB3	1:C:55:PHE:CE1	2.35	0.58
1:C:104:TRP:CD1	1:C:194:PHE:HE2	2.21	0.58
1:C:250:THR:OG1	1:C:251:PRO:HD3	2.04	0.58
1:C:422:ASN:CG	1:C:455:LEU:HB2	2.27	0.58
1:C:762:GLN:HA	1:C:765:ARG:HH11	1.69	0.58
1:A:669:GLY:H	1:B:864:LEU:HD12	1.69	0.58
1:B:328:ARG:NH1	1:B:580:GLN:OE1	2.37	0.58
1:B:566:GLY:H	1:B:575:ALA:HB3	1.68	0.58
1:B:623:ALA:O	1:B:627:ASP:N	2.36	0.58
1:B:965:GLN:O	1:B:968:SER:N	2.32	0.58
1:A:949:GLN:O	1:A:953:ASN:ND2	2.37	0.58
7:A:1207:NAG:H62	1:C:558:LYS:NZ	2.19	0.58
1:B:782:PHE:O	1:B:784:GLN:N	2.34	0.58
1:B:922:LEU:O	1:B:926:GLN:HG3	2.03	0.58
1:B:1094:VAL:HG22	1:B:1107:ARG:HG2	1.85	0.58
1:C:453:TYR:CD1	1:C:495:TYR:HB2	2.39	0.58
1:C:719:THR:OG1	1:C:720:ILE:N	2.37	0.58
1:B:275:PHE:CG	1:B:290:ASP:CA	2.81	0.57
1:B:433:VAL:HG13	1:B:508:TYR:HD2	1.68	0.57
1:B:122:ASN:N	1:B:125:ASN:O	2.27	0.57
1:B:663:ASP:HB3	1:B:672:ALA:HB3	1.85	0.57
1:C:329:PHE:CB	1:C:330:PRO:HD2	2.30	0.57
1:C:660:TYR:HB2	1:C:695:TYR:OH	2.04	0.57
1:A:354:ASN:O	1:A:356:LYS:HG2	2.04	0.57
1:A:607:GLN:OE1	1:A:691:SER:HA	2.03	0.57
7:B:1204:NAG:H83	7:B:1204:NAG:H3	1.85	0.57
1:C:1117:THR:N	1:C:1138:TYR:O	2.37	0.57
1:A:247:SER:OG	1:A:248:TYR:N	2.37	0.57
1:A:878:LEU:HA	1:A:881:THR:HG22	1.87	0.57
1:A:905:ARG:HA	1:A:1036:GLN:OE1	2.04	0.57
1:B:1086:LYS:HB3	1:B:1088:HIS:HE2	1.67	0.57
1:C:583:GLU:OE2	1:C:584:ILE:N	2.33	0.57
1:A:909:ILE:HD12	1:A:1047:TYR:HD2	1.70	0.57
1:A:926:GLN:O	1:A:929:SER:OG	2.18	0.57
1:B:1089:PHE:HD1	1:B:1090:PRO:HD2	1.69	0.57
1:B:86:PHE:CE2	1:B:89:GLY:N	2.50	0.57
1:C:421:TYR:HA	1:C:460:ASN:HB3	1.86	0.57
1:C:444:LYS:CD	1:C:500:THR:HA	2.34	0.57
1:C:740:MET:HG2	1:C:745:ASP:N	2.19	0.57
1:C:1005:GLN:O	1:C:1009:THR:HG23	2.04	0.57
1:A:309:GLU:O	1:A:313:TYR:OH	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:ASN:O	1:A:618:THR:N	2.37	0.57
1:A:908:GLY:C	1:A:1038:LYS:HZ3	2.13	0.57
1:A:1028:LYS:HD3	1:A:1042:PHE:HE2	1.66	0.57
1:B:611:LEU:HD12	1:B:612:TYR:H	1.68	0.57
1:B:712:ILE:HG13	1:B:1077:THR:HG21	1.85	0.57
1:B:973:ILE:HD13	1:B:983:ARG:HG3	1.85	0.57
1:C:356:LYS:NZ	1:C:358:ILE:HG12	2.19	0.57
1:C:356:LYS:HZ2	1:C:358:ILE:HG12	1.70	0.57
1:C:802:PHE:HB2	1:C:806:LEU:HB2	1.85	0.57
1:A:201:PHE:HZ	1:A:235:ILE:HG21	1.69	0.57
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.87	0.57
1:A:770:ILE:O	1:A:773:GLU:HG2	2.04	0.57
1:A:919:ASN:OD1	1:A:922:LEU:HB2	2.05	0.57
1:B:77:LYS:O	1:B:78:ARG:HB3	2.02	0.57
1:B:768:THR:O	1:B:772:VAL:HG23	2.05	0.57
1:B:949:GLN:O	1:B:953:ASN:ND2	2.38	0.57
1:C:30:ASN:HA	1:C:61:ASN:HA	1.86	0.57
1:C:357:ARG:HB2	1:C:396:TYR:CE2	2.39	0.57
1:C:392:PHE:CD2	1:C:517:LEU:HD13	2.39	0.57
1:C:446:GLY:O	1:C:448:ASN:ND2	2.37	0.57
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.70	0.57
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.38	0.57
1:B:424:LYS:O	1:B:463:PRO:HG3	2.05	0.57
1:B:624:ILE:O	1:B:628:GLN:N	2.37	0.57
1:C:928:ASN:O	1:C:931:ILE:HB	2.04	0.57
1:C:1111:GLU:HG3	1:C:1113:GLN:NE2	2.19	0.57
1:B:316:SER:OG	1:B:317:ASN:N	2.38	0.57
1:C:739:THR:O	1:C:743:CYS:CB	2.45	0.57
1:A:144:TYR:O	1:A:246:ARG:HD3	2.05	0.56
1:A:185:ASN:CG	1:A:211:ASN:OD1	2.48	0.56
1:C:294:ASP:O	1:C:297:SER:N	2.38	0.56
1:C:543:PHE:HB2	1:C:546:LEU:HB2	1.87	0.56
1:C:559:PHE:CE2	1:C:563:GLN:HB2	2.40	0.56
1:A:872:GLN:O	1:A:875:SER:OG	2.22	0.56
1:A:959:LEU:O	1:A:963:VAL:HG23	2.04	0.56
1:B:315:THR:HG23	1:B:595:VAL:HG23	1.87	0.56
1:B:577:ARG:HA	1:B:583:GLU:O	2.05	0.56
1:B:640:SER:HB2	1:B:654:GLU:HG2	1.87	0.56
1:B:969:ASN:OD1	1:B:972:ALA:N	2.38	0.56
1:B:1034:LEU:H	1:B:1034:LEU:HD12	1.70	0.56
1:B:1097:SER:HB2	1:B:1102:TRP:CE2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:HA	1:C:522:ALA:HA	1.87	0.56
1:C:395:VAL:HG12	1:C:515:PHE:HD2	1.71	0.56
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	1.87	0.56
1:A:820:ASP:HA	1:A:823:PHE:HB3	1.87	0.56
1:B:109:THR:HG21	1:B:113:LYS:HD2	1.87	0.56
1:B:322:PRO:CB	1:B:539:VAL:HA	2.35	0.56
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.70	0.56
1:C:103:GLY:HA3	1:C:120:VAL:HG22	1.87	0.56
1:C:280:ASN:H	1:C:284:THR:H	1.50	0.56
1:C:323:THR:O	1:C:539:VAL:HG22	2.05	0.56
1:C:882:ILE:HA	1:C:898:PHE:CE1	2.39	0.56
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.35	0.56
1:B:610:VAL:HG22	1:B:611:LEU:H	1.70	0.56
1:B:870:ILE:HA	1:B:873:TYR:HD2	1.69	0.56
1:B:1006:THR:O	1:B:1009:THR:OG1	2.21	0.56
1:C:453:TYR:CE1	1:C:495:TYR:HB2	2.40	0.56
1:C:636:TYR:O	1:C:640:SER:OG	2.18	0.56
1:A:1009:THR:O	1:A:1013:ILE:HG12	2.05	0.56
1:B:84:LEU:HB2	1:B:269:TYR:HH	1.67	0.56
1:B:560:LEU:O	1:B:562:PHE:N	2.39	0.56
1:C:740:MET:SD	1:C:744:GLY:HA2	2.46	0.56
1:A:70:VAL:HG21	1:A:77:LYS:O	2.05	0.56
1:A:1031:GLU:OE2	1:C:1040:VAL:N	2.38	0.56
1:A:1126:CYS:HB2	1:A:1132:ILE:HG21	1.88	0.56
1:B:758:SER:O	1:B:761:THR:OG1	2.11	0.56
1:C:1089:PHE:O	1:C:1120:THR:HG23	2.05	0.56
1:A:299:THR:O	1:A:303:LEU:CG	2.53	0.56
1:A:613:GLN:NE2	1:A:647:ALA:O	2.38	0.56
1:A:759:PHE:HA	1:A:762:GLN:NE2	2.21	0.56
1:C:188:ASN:HD21	1:C:209:PRO:HA	1.71	0.56
1:C:933:LYS:O	1:C:937:SER:OG	2.19	0.56
1:B:866:THR:OG1	1:B:868:GLU:OE1	2.21	0.56
1:B:1054:GLN:HG3	1:B:1055:SER:H	1.69	0.56
1:C:308:VAL:N	1:C:602:THR:OG1	2.27	0.56
1:C:515:PHE:CD1	1:C:515:PHE:C	2.83	0.56
1:A:256:SER:HB3	1:A:259:THR:O	2.06	0.56
1:A:660:TYR:HB2	1:A:695:TYR:OH	2.05	0.56
1:A:948:LEU:O	1:A:951:VAL:HG22	2.06	0.56
1:A:1012:LEU:O	1:A:1015:ALA:HB3	2.06	0.56
1:B:355:ARG:HB2	1:B:400:PHE:HB3	1.87	0.56
1:B:429:PHE:CE2	1:C:984:LEU:HD11	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:GLN:HA	1:B:765:ARG:NE	2.21	0.56
1:C:271:GLN:O	1:C:273:ARG:N	2.39	0.56
1:A:112:SER:HB2	1:A:134:GLN:HE21	1.71	0.56
1:A:1094:VAL:HG12	1:B:900:MET:HE2	1.87	0.56
1:B:434:ILE:HB	1:B:436:TRP:CZ3	2.41	0.56
1:B:762:GLN:HG2	1:B:765:ARG:HH21	1.71	0.56
1:B:973:ILE:HG22	1:B:980:ILE:HD12	1.87	0.56
1:C:411:ALA:N	1:C:425:LEU:HD21	2.21	0.56
1:C:687:VAL:HG12	1:C:688:ALA:H	1.71	0.56
1:C:738:CYS:SG	1:C:739:THR:N	2.79	0.56
1:A:52:GLN:HA	1:A:274:THR:HA	1.88	0.55
1:A:740:MET:HE3	1:C:317:ASN:HD22	1.69	0.55
1:C:796:ASP:N	1:C:796:ASP:OD1	2.39	0.55
1:C:1091:ARG:NH2	1:C:1118:ASP:O	2.38	0.55
5:h:1:NAG:O3	5:h:2:NAG:N2	2.39	0.55
1:A:192:PHE:HD1	1:A:205:SER:HA	1.71	0.55
1:B:53:ASP:OD1	1:B:54:LEU:N	2.30	0.55
1:B:927:PHE:O	1:B:931:ILE:HG12	2.07	0.55
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	2.21	0.55
1:C:309:GLU:O	1:C:313:TYR:OH	2.18	0.55
1:C:349:SER:HA	1:C:451:TYR:HE1	1.72	0.55
1:C:34:ARG:O	1:C:56:LEU:HD23	2.06	0.55
1:B:364:ASP:OD1	1:B:366:SER:OG	2.19	0.55
1:A:543:PHE:HE2	1:A:576:VAL:HB	1.71	0.55
1:B:236:THR:HG23	1:B:237:ARG:HD2	1.88	0.55
1:B:997:ILE:O	1:B:1001:LEU:HB2	2.07	0.55
1:C:422:ASN:HD21	1:C:455:LEU:H	1.52	0.55
1:C:960:ASN:HA	1:C:963:VAL:HG12	1.89	0.55
1:A:64:TRP:CD1	1:A:65:PHE:H	2.24	0.55
1:B:103:GLY:O	1:B:240:THR:HA	2.07	0.55
1:B:616:ASN:O	1:B:618:THR:N	2.37	0.55
1:B:1025:ALA:O	1:B:1028:LYS:N	2.40	0.55
1:B:1109:PHE:CE2	1:B:1111:GLU:HB2	2.41	0.55
1:C:57:PRO:HG3	1:C:273:ARG:HE	1.71	0.55
1:A:966:LEU:O	1:A:975:SER:OG	2.23	0.55
1:B:396:TYR:H	1:B:514:SER:HB2	1.71	0.55
1:C:905:ARG:HG2	1:C:1036:GLN:OE1	2.07	0.55
1:A:1004:LEU:O	1:A:1008:VAL:HG13	2.07	0.55
1:B:40:ASP:CG	1:B:41:LYS:H	2.14	0.55
1:B:305:SER:C	1:B:307:THR:H	2.15	0.55
1:B:314:GLN:OE1	1:B:314:GLN:N	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LEU:HD12	1:B:612:TYR:N	2.22	0.55
1:A:70:VAL:CG1	1:A:79:PHE:HB3	2.32	0.55
1:A:1050:MET:SD	1:A:1052:PHE:HE1	2.30	0.55
1:A:1088:HIS:CD2	1:A:1137:VAL:HG11	2.41	0.55
1:C:422:ASN:ND2	1:C:455:LEU:H	2.05	0.55
1:C:1024:LEU:HG	1:C:1028:LYS:HE2	1.89	0.55
1:A:948:LEU:O	1:A:952:VAL:HG22	2.06	0.55
1:A:954:GLN:O	1:A:957:GLN:HG2	2.07	0.55
1:A:1037:SER:OG	1:A:1038:LYS:N	2.40	0.55
1:B:955:ASN:O	1:B:959:LEU:HG	2.07	0.55
1:C:737:ASP:O	1:C:738:CYS:C	2.50	0.55
1:A:596:SER:OG	1:A:597:VAL:N	2.40	0.54
1:B:880:GLY:O	1:B:884:SER:N	2.40	0.54
1:B:1129:VAL:HG22	1:C:917:TYR:O	2.06	0.54
1:C:145:TYR:CD1	1:C:145:TYR:N	2.73	0.54
1:C:498:GLN:N	1:C:499:PRO:CD	2.53	0.54
1:C:930:ALA:O	1:C:933:LYS:HB3	2.07	0.54
1:A:52:GLN:HB3	1:A:274:THR:HB	1.89	0.54
1:A:433:VAL:HG23	1:A:510:VAL:HG11	1.87	0.54
1:A:27:ALA:N	1:A:64:TRP:O	2.40	0.54
1:A:558:LYS:HZ2	5:h:1:NAG:H62	1.71	0.54
1:A:566:GLY:H	1:A:575:ALA:HB3	1.71	0.54
1:A:915:VAL:HG13	1:A:916:LEU:N	2.23	0.54
1:A:1083:HIS:HB2	1:A:1137:VAL:HG13	1.89	0.54
1:A:569:ILE:HD12	1:A:570:ALA:H	1.72	0.54
1:A:752:LEU:O	1:A:755:GLN:HB3	2.07	0.54
1:A:937:SER:O	1:A:941:THR:OG1	2.25	0.54
1:B:436:TRP:NE1	1:B:508:TYR:HA	2.22	0.54
1:B:737:ASP:N	1:B:737:ASP:OD1	2.40	0.54
1:B:875:SER:HA	1:B:878:LEU:CG	2.37	0.54
1:A:281:GLU:O	1:C:557:LYS:HE2	2.08	0.54
1:A:759:PHE:O	1:A:762:GLN:HG2	2.08	0.54
1:A:799:GLY:O	1:A:924:ALA:HB1	2.08	0.54
1:B:619:GLU:O	1:B:621:PRO:HD2	2.07	0.54
1:C:611:LEU:HG	1:C:612:TYR:N	2.22	0.54
1:C:956:ALA:HA	1:C:959:LEU:HD12	1.90	0.54
1:C:1116:THR:H	1:C:1119:ASN:ND2	2.05	0.54
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.88	0.54
1:A:871:ALA:O	1:A:874:THR:OG1	2.23	0.54
1:B:231:ILE:HG12	1:B:233:ILE:HB	1.90	0.54
1:B:336:CYS:HB2	1:B:337:PRO:HD2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.54
1:C:740:MET:HG2	1:C:745:ASP:H	1.72	0.54
1:A:44:ARG:HD2	1:A:279:TYR:CE1	2.43	0.54
1:A:186:PHE:CD1	1:A:186:PHE:C	2.86	0.54
1:A:287:ASP:OD1	1:A:287:ASP:N	2.38	0.54
1:A:758:SER:OG	1:C:965:GLN:NE2	2.40	0.54
1:C:874:THR:O	1:C:878:LEU:HG	2.08	0.54
7:C:1205:NAG:C8	7:C:1205:NAG:C1	2.86	0.54
1:A:350:VAL:HG22	1:A:400:PHE:CE2	2.43	0.54
1:A:765:ARG:HH21	1:C:957:GLN:HG2	1.71	0.54
1:B:77:LYS:HG3	1:B:78:ARG:N	2.23	0.54
1:C:278:LYS:HG2	1:C:279:TYR:H	1.73	0.54
1:C:298:GLU:OE2	1:C:298:GLU:N	2.41	0.54
1:C:742:ILE:HG12	1:C:997:ILE:HG13	1.89	0.54
1:C:1019:ARG:O	1:C:1023:ASN:ND2	2.41	0.54
1:A:607:GLN:HB3	1:A:692:ILE:HG12	1.90	0.54
1:A:699:LEU:HD12	1:B:788:ILE:HG21	1.89	0.54
1:A:738:CYS:O	1:A:742:ILE:HG22	2.08	0.54
1:C:64:TRP:HE1	1:C:66:HIS:CD2	2.26	0.54
1:A:96:GLU:OE1	1:A:100:ILE:HB	2.08	0.54
1:A:577:ARG:HH21	1:A:584:ILE:H	1.55	0.54
1:A:1037:SER:C	1:A:1038:LYS:HD2	2.32	0.54
1:A:1083:HIS:CG	1:A:1137:VAL:HG22	2.43	0.54
1:B:151:SER:C	1:B:153:MET:H	2.16	0.54
1:B:901:GLN:HE21	1:B:905:ARG:NH2	2.06	0.54
1:C:140:PHE:H	1:C:243:ALA:HB3	1.73	0.54
1:C:1102:TRP:HD1	1:C:1135:ASN:HD22	1.56	0.54
1:A:308:VAL:O	1:A:602:THR:OG1	2.26	0.53
1:A:1015:ALA:O	1:A:1019:ARG:HG3	2.08	0.53
1:B:772:VAL:HA	1:B:775:ASP:OD2	2.07	0.53
1:B:1072:GLU:H	1:B:1072:GLU:CD	2.12	0.53
1:C:635:VAL:HG12	1:C:636:TYR:H	1.73	0.53
1:A:193:VAL:HG22	1:A:194:PHE:H	1.73	0.53
1:A:1086:LYS:NZ	1:A:1122:VAL:HG11	2.23	0.53
1:B:311:GLY:O	1:B:664:ILE:HD13	2.08	0.53
1:B:554:GLU:N	1:B:554:GLU:OE1	2.39	0.53
1:B:732:THR:O	1:B:734:THR:N	2.40	0.53
1:B:1100:THR:OG1	1:B:1101:HIS:N	2.41	0.53
1:C:38:TYR:OH	1:C:285:ILE:N	2.28	0.53
1:C:742:ILE:HG23	1:C:743:CYS:SG	2.49	0.53
1:A:328:ARG:HB3	1:A:328:ARG:NH1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HG13	1:A:495:TYR:OH	2.08	0.53
1:A:805:ILE:HG13	1:A:806:LEU:H	1.72	0.53
1:B:294:ASP:OD1	1:B:296:LEU:N	2.36	0.53
1:B:737:ASP:OD2	1:B:740:MET:HB3	2.08	0.53
1:B:825:LYS:HB3	1:B:945:LEU:HD11	1.90	0.53
1:B:875:SER:CA	1:B:878:LEU:CD2	2.81	0.53
1:C:144:TYR:O	1:C:146:HIS:N	2.38	0.53
1:C:594:GLY:N	1:C:613:GLN:HE22	2.07	0.53
1:C:811:LYS:HD3	1:C:815:ARG:NH2	2.22	0.53
1:A:299:THR:O	1:A:303:LEU:CB	2.56	0.53
1:A:349:SER:H	1:A:352:ALA:HB3	1.74	0.53
1:A:985:ASP:HB3	1:A:987:PRO:HD2	1.91	0.53
1:B:586:ASP:OD1	1:B:587:ILE:N	2.41	0.53
1:B:747:THR:OG1	1:B:748:GLU:N	2.42	0.53
1:B:808:ASP:O	1:B:810:SER:N	2.40	0.53
1:B:896:ILE:HG21	1:B:901:GLN:OE1	2.09	0.53
1:C:392:PHE:CE2	1:C:515:PHE:CE2	2.96	0.53
1:C:611:LEU:HD13	1:C:650:LEU:HD12	1.90	0.53
1:C:1050:MET:SD	1:C:1051:SER:N	2.80	0.53
1:A:333:THR:HG22	1:A:527:PRO:HG2	1.91	0.53
1:A:402:ILE:HG22	1:A:403:ARG:H	1.74	0.53
1:B:57:PRO:HG3	1:B:271:GLN:CB	2.38	0.53
1:B:811:LYS:HB2	1:B:812:PRO:HD3	1.90	0.53
1:C:355:ARG:HA	1:C:397:ALA:O	2.08	0.53
1:A:796:ASP:OD1	1:C:709:ASN:HB3	2.09	0.53
1:B:121:ASN:HA	1:B:126:VAL:HG22	1.89	0.53
1:B:1027:THR:HG23	1:B:1031:GLU:OE2	2.07	0.53
1:C:365:TYR:CG	1:C:387:LEU:HG	2.44	0.53
1:C:747:THR:O	1:C:751:ASN:HB2	2.09	0.53
1:A:715:PRO:HB2	1:A:1069:PRO:HB2	1.91	0.53
1:B:275:PHE:CD1	1:B:290:ASP:CB	2.91	0.53
1:B:522:ALA:N	1:B:564:GLN:HE21	1.98	0.53
1:B:710:ASN:OD1	1:B:710:ASN:N	2.41	0.53
1:B:1136:THR:HG23	1:B:1138:TYR:CE1	2.43	0.53
1:C:689:SER:O	1:C:690:GLN:HG3	2.08	0.53
1:C:708:SER:C	1:C:710:ASN:H	2.17	0.53
1:C:777:ASN:O	1:C:780:GLU:HG2	2.09	0.53
1:B:342:PHE:CZ	1:B:371:SER:HB2	2.44	0.53
1:C:931:ILE:O	1:C:934:ILE:HG22	2.09	0.53
1:C:996:LEU:HD21	1:C:1000:ARG:CZ	2.38	0.53
1:C:1103:PHE:CD2	1:C:1112:PRO:HB3	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TYR:O	1:A:514:SER:N	2.42	0.53
1:A:1037:SER:OG	1:A:1039:ARG:HG2	2.08	0.53
1:B:112:SER:HA	1:B:132:GLU:CG	2.29	0.53
1:B:382:VAL:HG12	1:B:384:PRO:HD3	1.91	0.53
1:B:1105:THR:HG22	1:B:1106:GLN:O	2.09	0.53
1:C:68:ILE:HG13	1:C:80:ASP:OD2	2.07	0.53
1:C:860:VAL:C	1:C:861:LEU:HD22	2.34	0.53
1:A:559:PHE:HB3	1:A:563:GLN:HB2	1.91	0.53
1:A:698:SER:O	1:A:698:SER:OG	2.27	0.53
1:A:770:ILE:O	1:A:774:GLN:HG2	2.09	0.53
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.91	0.53
1:C:753:LEU:O	1:C:756:TYR:N	2.43	0.53
1:A:577:ARG:HH21	1:A:584:ILE:N	2.07	0.52
1:A:699:LEU:HG	1:B:788:ILE:HG13	1.91	0.52
1:A:759:PHE:O	1:A:763:LEU:HD23	2.09	0.52
1:B:179:LEU:HD22	1:B:190:ARG:CZ	2.39	0.52
1:B:275:PHE:CD1	1:B:290:ASP:CG	2.84	0.52
1:B:280:ASN:O	1:B:283:GLY:N	2.34	0.52
1:B:613:GLN:HE21	1:B:614:ASP:CG	2.14	0.52
1:B:969:ASN:HB2	1:B:974:SER:O	2.09	0.52
1:C:328:ARG:NH1	1:C:533:LEU:HD22	2.25	0.52
1:C:578:ASP:CG	1:C:583:GLU:H	2.13	0.52
1:A:195:LYS:O	1:A:201:PHE:HA	2.10	0.52
1:A:1081:ILE:HG21	1:A:1135:ASN:HB3	1.92	0.52
1:B:52:GLN:HA	1:B:274:THR:HA	1.92	0.52
1:B:133:PHE:HB2	1:B:161:SER:N	2.25	0.52
1:B:906:PHE:HB3	1:B:911:VAL:HG23	1.91	0.52
1:B:909:ILE:HG21	1:B:1047:TYR:HB3	1.91	0.52
1:B:1089:PHE:CD1	1:B:1090:PRO:HD2	2.45	0.52
1:C:421:TYR:CD2	1:C:459:SER:N	2.51	0.52
1:C:980:ILE:HG13	1:C:989:ALA:HB1	1.91	0.52
1:A:193:VAL:HG12	1:A:204:TYR:HB2	1.91	0.52
1:C:1012:LEU:O	1:C:1015:ALA:HB3	2.09	0.52
1:A:616:ASN:O	1:A:618:THR:HG23	2.10	0.52
1:A:919:ASN:HB3	1:A:923:ILE:HD11	1.92	0.52
1:A:1069:PRO:HD2	1:B:890:ALA:O	2.08	0.52
1:C:121:ASN:HA	1:C:126:VAL:HA	1.90	0.52
1:C:137:ASN:CG	1:C:241:LEU:HD21	2.35	0.52
1:A:381:GLY:HA3	1:A:430:THR:OG1	2.10	0.52
1:C:94:SER:OG	1:C:95:THR:N	2.42	0.52
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:VAL:O	1:C:434:ILE:HD13	2.09	0.52
1:C:985:ASP:HB2	1:C:987:PRO:HD2	1.92	0.52
1:A:65:PHE:HB2	1:A:264:ALA:HA	1.92	0.52
1:A:576:VAL:HG22	1:A:585:LEU:O	2.09	0.52
1:A:886:TRP:HB2	1:A:1034:LEU:O	2.09	0.52
1:B:48:LEU:HB3	1:B:276:LEU:HD11	1.92	0.52
1:B:1107:ARG:HD2	1:C:904:TYR:CE2	2.45	0.52
1:C:38:TYR:CE2	1:C:285:ILE:HG13	2.45	0.52
1:C:359:SER:HA	1:C:524:VAL:HG22	1.92	0.52
1:A:33:THR:HA	1:A:58:PHE:CE2	2.44	0.52
1:A:653:ALA:HA	1:A:692:ILE:O	2.10	0.52
1:B:1015:ALA:HA	1:B:1018:ILE:HG22	1.92	0.52
1:B:1129:VAL:HG11	1:C:917:TYR:CD2	2.45	0.52
1:C:146:HIS:HE1	1:C:248:TYR:CD2	2.27	0.52
1:C:193:VAL:HG12	1:C:204:TYR:O	2.09	0.52
1:C:594:GLY:H	1:C:613:GLN:NE2	2.07	0.52
1:C:641:ASN:HB3	1:C:654:GLU:OE1	2.09	0.52
1:C:803:SER:OG	4:p:1:NAG:H5	2.09	0.52
1:C:816:SER:OG	1:C:819:GLU:OE2	2.21	0.52
1:A:614:ASP:N	1:A:647:ALA:O	2.24	0.52
1:A:777:ASN:O	1:A:781:VAL:HG23	2.10	0.52
1:A:969:ASN:HB2	1:B:755:GLN:OE1	2.10	0.52
1:B:33:THR:HA	1:B:58:PHE:CE2	2.45	0.52
1:B:402:ILE:HD13	1:B:410:ILE:HG21	1.90	0.52
1:B:596:SER:OG	1:B:597:VAL:N	2.32	0.52
1:B:882:ILE:HB	1:B:898:PHE:CE1	2.44	0.52
1:C:254:SER:OG	1:C:255:SER:N	2.43	0.52
1:A:43:PHE:HD2	1:C:566:GLY:HA3	1.74	0.51
1:A:650:LEU:HD13	1:A:653:ALA:HB3	1.92	0.51
1:A:1107:ARG:HG2	1:B:886:TRP:HZ2	1.75	0.51
1:B:1086:LYS:HG2	1:B:1088:HIS:CD2	2.45	0.51
1:C:437:ASN:ND2	1:C:506:GLN:O	2.36	0.51
1:A:132:GLU:N	1:A:166:CYS:HA	2.22	0.51
1:A:976:VAL:HG12	1:A:979:ASP:H	1.76	0.51
1:B:1083:HIS:CD2	1:B:1137:VAL:H	2.28	0.51
1:C:578:ASP:OD1	1:C:582:LEU:N	2.43	0.51
1:C:717:ASN:CG	2:X:1:NAG:N2	2.67	0.51
1:B:138:ASP:OD1	1:B:242:LEU:CG	2.58	0.51
1:B:147:LYS:O	1:B:147:LYS:HG2	2.10	0.51
1:B:567:ARG:HG2	1:B:573:THR:HA	1.92	0.51
1:A:278:LYS:HE3	1:A:287:ASP:OD1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TRP:HB3	1:B:106:PHE:HE1	1.76	0.51
1:B:105:ILE:CB	1:B:239:GLN:O	2.59	0.51
1:B:382:VAL:HG13	1:B:387:LEU:HD12	1.91	0.51
1:B:394:ASN:HD21	1:B:515:PHE:C	2.19	0.51
1:B:1028:LYS:HG2	1:B:1042:PHE:CE2	2.45	0.51
1:C:375:SER:OG	1:C:376:THR:N	2.44	0.51
1:C:924:ALA:C	1:C:928:ASN:HD22	2.19	0.51
1:C:1054:GLN:HB2	1:C:1061:VAL:HG23	1.93	0.51
1:B:435:ALA:HA	1:B:508:TYR:CE1	2.44	0.51
1:B:660:TYR:HB2	1:B:695:TYR:CE1	2.45	0.51
1:B:967:SER:O	1:B:975:SER:OG	2.23	0.51
1:C:535:LYS:HG3	1:C:552:LEU:HB2	1.93	0.51
1:C:762:GLN:O	1:C:765:ARG:HG2	2.11	0.51
1:C:904:TYR:O	1:C:907:ASN:HB3	2.10	0.51
2:X:1:NAG:HO3	2:X:1:NAG:C7	2.19	0.51
1:A:348:ALA:HB3	1:A:353:TRP:CE3	2.44	0.51
1:A:535:LYS:O	1:A:537:LYS:HG2	2.10	0.51
1:C:53:ASP:OD2	1:C:54:LEU:HD12	2.09	0.51
1:C:222:ALA:O	1:C:223:LEU:HD23	2.10	0.51
1:C:305:SER:OG	1:C:307:THR:O	2.26	0.51
1:C:619:GLU:OE1	1:C:619:GLU:N	2.44	0.51
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.26	0.51
1:A:370:ASN:OD1	1:A:370:ASN:N	2.40	0.51
1:B:52:GLN:HB3	1:B:274:THR:CB	2.40	0.51
1:B:314:GLN:H	1:B:314:GLN:CD	2.17	0.51
1:B:746:SER:HB2	1:B:749:CYS:HB3	1.92	0.51
1:C:34:ARG:HH22	1:C:219:GLY:C	2.14	0.51
1:C:661:GLU:O	1:C:695:TYR:OH	2.14	0.51
1:A:168:PHE:CG	1:A:169:GLU:N	2.78	0.51
1:C:138:ASP:HB2	1:C:140:PHE:CD2	2.45	0.51
1:C:1106:GLN:HE22	1:C:1109:PHE:C	2.17	0.51
1:B:641:ASN:N	1:B:654:GLU:HG2	2.25	0.51
1:B:1027:THR:CG2	1:B:1028:LYS:N	2.72	0.51
1:C:104:TRP:HB3	1:C:106:PHE:CZ	2.46	0.51
1:C:438:SER:HB2	1:C:507:PRO:HG2	1.93	0.51
1:C:859:THR:OG1	1:C:860:VAL:N	2.42	0.51
1:C:1029:MET:HG2	1:C:1033:VAL:HG21	1.93	0.51
1:A:645:THR:HG23	1:A:647:ALA:N	2.25	0.51
1:A:1027:THR:C	1:A:1030:SER:HG	2.13	0.51
1:B:164:ASN:OD1	1:B:165:ASN:N	2.44	0.51
1:B:553:THR:O	1:B:586:ASP:N	2.37	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LYS:NZ	1:B:559:PHE:HA	2.26	0.51
1:B:1005:GLN:O	1:B:1009:THR:HG23	2.11	0.51
1:C:33:THR:OG1	1:C:219:GLY:O	2.21	0.51
1:C:144:TYR:C	1:C:146:HIS:H	2.18	0.51
1:C:276:LEU:HD22	1:C:301:CYS:HA	1.93	0.51
1:C:435:ALA:HB2	1:C:510:VAL:HG13	1.92	0.51
1:C:453:TYR:CE2	1:C:454:ARG:CG	2.92	0.51
1:C:807:PRO:HB3	1:C:815:ARG:HG3	1.92	0.51
1:C:818:ILE:HD11	1:C:935:GLN:HB2	1.93	0.51
1:C:866:THR:HG23	1:C:868:GLU:H	1.76	0.51
1:B:112:SER:OG	1:B:132:GLU:OE1	2.19	0.50
1:B:551:VAL:HG22	1:B:552:LEU:H	1.76	0.50
1:C:995:ARG:O	1:C:998:THR:HG22	2.11	0.50
1:C:996:LEU:HG	1:C:1000:ARG:HD2	1.92	0.50
1:C:1082:CYS:HA	1:C:1086:LYS:O	2.11	0.50
1:A:711:SER:HG	1:A:1076:THR:HA	1.75	0.50
1:A:858:LEU:HD12	1:A:859:THR:H	1.76	0.50
1:B:929:SER:O	1:B:933:LYS:HG2	2.11	0.50
1:A:43:PHE:HB2	1:C:563:GLN:HG2	1.93	0.50
1:B:699:LEU:HB3	1:C:788:ILE:HD11	1.91	0.50
1:C:1062:PHE:C	1:C:1063:LEU:HD23	2.37	0.50
1:A:729:VAL:HG11	1:A:1060:VAL:HG13	1.93	0.50
7:A:1207:NAG:H62	1:C:558:LYS:HZ2	1.75	0.50
1:B:619:GLU:OE1	1:B:619:GLU:N	2.45	0.50
1:C:315:THR:OG1	1:C:595:VAL:O	2.16	0.50
1:B:54:LEU:HD13	1:B:88:ASP:C	2.37	0.50
1:B:383:SER:C	1:B:387:LEU:HG	2.36	0.50
1:B:1076:THR:OG1	1:B:1097:SER:HB3	2.11	0.50
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.47	0.50
1:C:303:LEU:HD11	1:C:313:TYR:CD1	2.46	0.50
1:C:308:VAL:HG22	1:C:602:THR:OG1	2.11	0.50
1:C:398:ASP:O	1:C:512:VAL:HG22	2.12	0.50
1:C:444:LYS:HE3	1:C:500:THR:CB	2.41	0.50
1:A:820:ASP:OD1	1:A:821:LEU:N	2.45	0.50
1:B:711:SER:HA	1:B:1077:THR:HG23	1.94	0.50
1:B:922:LEU:H	1:B:922:LEU:HD12	1.76	0.50
1:C:774:GLN:O	1:C:777:ASN:HB2	2.11	0.50
1:C:866:THR:H	1:C:869:MET:CE	2.24	0.50
1:A:108:THR:HA	1:A:237:ARG:HB3	1.93	0.50
1:A:816:SER:N	1:A:819:GLU:OE1	2.45	0.50
1:A:985:ASP:O	1:A:989:ALA:N	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:GLU:CD	1:C:1039:ARG:HA	2.37	0.50
1:B:204:TYR:HB3	1:B:223:LEU:CB	2.41	0.50
1:B:1045:LYS:C	1:B:1066:THR:HG21	2.37	0.50
1:C:92:PHE:HA	1:C:266:TYR:O	2.12	0.50
1:C:403:ARG:HH11	1:C:404:GLY:H	1.58	0.50
1:A:644:GLN:OE1	1:A:649:CYS:N	2.45	0.50
1:B:182:LYS:C	1:B:184:GLY:H	2.19	0.50
1:C:73:THR:HG22	1:C:77:LYS:O	2.12	0.50
1:C:203:ILE:O	1:C:225:PRO:HA	2.11	0.50
1:C:368:LEU:HD12	1:C:368:LEU:H	1.76	0.50
1:C:409:GLN:HB3	1:C:415:THR:O	2.12	0.50
1:C:567:ARG:CG	1:C:571:ASP:HA	2.40	0.50
1:C:733:LYS:NZ	1:C:862:PRO:O	2.33	0.50
1:C:960:ASN:HD22	1:C:963:VAL:CG1	2.25	0.50
1:A:607:GLN:CD	1:A:691:SER:HA	2.37	0.50
1:A:856:ASN:OD1	1:A:856:ASN:N	2.44	0.50
1:B:544:ASN:ND2	1:B:579:PRO:HB3	2.26	0.50
1:A:96:GLU:CD	1:A:97:LYS:H	2.20	0.49
1:A:328:ARG:HG2	1:A:530:SER:OG	2.12	0.49
1:A:774:GLN:HA	1:A:777:ASN:HD22	1.77	0.49
1:A:890:ALA:HB2	1:C:1047:TYR:CE1	2.47	0.49
1:A:909:ILE:HB	1:A:1047:TYR:HB3	1.93	0.49
1:B:742:ILE:HG21	1:B:997:ILE:HD13	1.94	0.49
1:B:816:SER:OG	1:B:819:GLU:N	2.39	0.49
1:B:859:THR:OG1	1:B:860:VAL:N	2.45	0.49
1:C:278:LYS:HD2	1:C:306:PHE:CE2	2.46	0.49
1:C:471:GLU:HB2	1:C:491:PRO:HB3	1.93	0.49
1:C:564:GLN:HG2	1:C:577:ARG:HD2	1.94	0.49
1:C:867:ASP:N	1:C:867:ASP:OD1	2.45	0.49
1:A:295:PRO:O	1:A:298:GLU:HB2	2.12	0.49
1:A:737:ASP:OD1	1:A:740:MET:HB3	2.12	0.49
1:B:426:PRO:HD3	1:B:463:PRO:HG2	1.93	0.49
1:B:641:ASN:H	1:B:654:GLU:CG	2.25	0.49
1:B:1056:ALA:HB3	1:B:1059:GLY:C	2.36	0.49
1:B:1094:VAL:HG13	1:B:1107:ARG:HE	1.76	0.49
1:C:660:TYR:HB2	1:C:695:TYR:CE2	2.46	0.49
1:A:42:VAL:HG11	1:A:44:ARG:NH2	2.28	0.49
1:A:43:PHE:HZ	1:C:557:LYS:HE3	1.77	0.49
1:A:78:ARG:HB2	1:A:81:ASN:HD21	1.76	0.49
1:A:200:TYR:HB3	1:A:228:ASP:OD1	2.11	0.49
1:A:568:ASP:OD1	1:A:568:ASP:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:PRO:HB3	1:A:815:ARG:N	2.27	0.49
1:A:920:GLN:HG3	1:A:921:LYS:HD2	1.94	0.49
1:A:964:LYS:HZ3	1:C:570:ALA:H	1.60	0.49
1:B:34:ARG:C	1:B:56:LEU:HD23	2.37	0.49
1:B:722:VAL:HA	1:B:1064:HIS:O	2.11	0.49
1:B:1032:CYS:HB2	1:B:1048:HIS:HE1	1.77	0.49
1:C:577:ARG:HB3	1:C:584:ILE:HG13	1.95	0.49
1:A:51:THR:O	1:A:274:THR:OG1	2.21	0.49
1:A:1089:PHE:HB3	1:A:1090:PRO:HD2	1.94	0.49
1:B:658:ASN:HB2	1:B:660:TYR:CE1	2.48	0.49
1:B:1049:LEU:HB2	1:B:1065:VAL:HG23	1.93	0.49
1:C:280:ASN:CG	1:C:281:GLU:H	2.20	0.49
1:C:726:ILE:HD11	1:C:947:LYS:HB2	1.94	0.49
1:A:323:THR:O	1:A:539:VAL:HG12	2.13	0.49
1:A:640:SER:OG	1:A:641:ASN:N	2.43	0.49
1:A:866:THR:HG1	1:A:868:GLU:CD	2.17	0.49
1:B:430:THR:HA	1:B:513:LEU:HB2	1.94	0.49
1:C:409:GLN:OE1	1:C:409:GLN:N	2.45	0.49
1:C:422:ASN:CG	1:C:455:LEU:H	2.21	0.49
1:C:707:TYR:CG	1:C:708:SER:N	2.80	0.49
1:C:753:LEU:O	1:C:755:GLN:N	2.46	0.49
1:A:578:ASP:N	1:A:579:PRO:HD3	2.28	0.49
1:A:900:MET:HE1	1:C:1077:THR:HB	1.95	0.49
1:B:303:LEU:HD11	1:B:313:TYR:CG	2.47	0.49
1:B:355:ARG:HH11	1:B:466:ARG:NH1	2.10	0.49
1:B:906:PHE:CE1	1:B:1049:LEU:HD11	2.47	0.49
1:C:416:GLY:O	1:C:420:ASP:N	2.45	0.49
1:C:614:ASP:N	1:C:647:ALA:O	2.34	0.49
1:C:866:THR:HG22	1:C:869:MET:SD	2.53	0.49
1:A:732:THR:O	1:A:734:THR:HG23	2.12	0.49
1:A:733:LYS:HZ1	1:A:863:PRO:HA	1.77	0.49
1:A:765:ARG:NH2	1:C:957:GLN:HG2	2.28	0.49
1:A:1019:ARG:HB3	1:A:1019:ARG:CZ	2.42	0.49
1:A:1028:LYS:NZ	1:A:1042:PHE:CD2	2.75	0.49
1:B:604:THR:O	1:B:606:ASN:N	2.46	0.49
1:B:655:HIS:CG	1:B:656:VAL:N	2.81	0.49
1:B:726:ILE:HD12	1:B:948:LEU:HG	1.94	0.49
1:B:1103:PHE:HZ	7:B:1206:NAG:HO6	1.59	0.49
1:C:216:LEU:H	1:C:216:LEU:HD12	1.78	0.49
1:C:1078:ALA:HB2	1:C:1102:TRP:CH2	2.48	0.49
1:A:332:ILE:HD12	4:V:1:NAG:C8	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:TYR:CE1	1:A:1004:LEU:HD21	2.48	0.49
1:A:989:ALA:O	1:A:993:ILE:HG12	2.12	0.49
1:B:53:ASP:O	1:B:272:PRO:HA	2.13	0.49
1:B:86:PHE:HE2	1:B:89:GLY:C	2.16	0.49
1:B:439:ASN:ND2	1:B:496:GLY:O	2.45	0.49
1:B:643:PHE:CG	1:B:655:HIS:HB2	2.47	0.49
1:B:1040:VAL:HG22	1:C:1031:GLU:OE2	2.12	0.49
1:C:817:PHE:CD1	1:C:821:LEU:HD11	2.46	0.49
1:A:278:LYS:HD2	1:A:278:LYS:C	2.38	0.49
1:A:341:VAL:HG12	1:A:342:PHE:CD1	2.47	0.49
1:A:662:CYS:HB3	1:A:697:MET:HB3	1.95	0.49
1:A:947:LYS:O	1:A:950:ASP:HB3	2.13	0.49
1:B:83:VAL:HG11	1:B:239:GLN:OE1	2.13	0.49
1:B:116:SER:O	1:B:130:VAL:HA	2.13	0.49
1:C:44:ARG:NH2	1:C:279:TYR:OH	2.43	0.49
1:C:370:ASN:OD1	1:C:371:SER:N	2.46	0.49
1:C:866:THR:H	1:C:869:MET:HE2	1.77	0.49
1:C:912:THR:O	1:C:915:VAL:HG12	2.13	0.49
1:C:1102:TRP:NE1	1:C:1133:VAL:HG21	2.27	0.49
1:A:540:ASN:HA	1:A:549:THR:HG22	1.95	0.49
1:A:739:THR:O	1:A:743:CYS:N	2.36	0.49
1:A:777:ASN:O	1:A:778:THR:C	2.56	0.49
1:B:83:VAL:HG23	1:B:83:VAL:O	2.11	0.49
1:B:129:LYS:HG2	1:B:169:GLU:HG3	1.95	0.49
1:B:377:PHE:CZ	1:B:382:VAL:HG11	2.48	0.49
1:B:748:GLU:N	1:B:748:GLU:CD	2.71	0.49
1:B:897:PRO:HG2	1:B:900:MET:HB2	1.95	0.49
1:B:987:PRO:O	1:B:990:GLU:HB2	2.13	0.49
1:C:353:TRP:HB3	1:C:423:TYR:HE1	1.78	0.49
1:C:914:ASN:OD1	1:C:915:VAL:N	2.46	0.49
1:A:33:THR:OG1	1:A:33:THR:O	2.29	0.48
1:B:371:SER:O	1:B:373:SER:N	2.45	0.48
1:C:37:TYR:CZ	1:C:55:PHE:CE2	3.01	0.48
1:C:537:LYS:O	1:C:539:VAL:HG23	2.13	0.48
1:C:1005:GLN:OE1	1:C:1006:THR:N	2.45	0.48
1:B:604:THR:OG1	7:B:1202:NAG:H82	2.13	0.48
1:B:693:ILE:HG13	1:B:694:ALA:H	1.78	0.48
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.48	0.48
1:B:954:GLN:HE21	1:B:1014:ARG:NH2	2.09	0.48
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.29	0.48
1:B:1116:THR:HA	1:B:1138:TYR:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:SER:HG	1:C:1031:GLU:H	1.62	0.48
1:B:808:ASP:OD1	1:B:808:ASP:N	2.46	0.48
1:C:315:THR:OG1	1:C:595:VAL:HG13	2.12	0.48
1:C:366:SER:N	1:C:388:ASN:OD1	2.46	0.48
1:C:437:ASN:HA	1:C:508:TYR:HA	1.95	0.48
1:C:546:LEU:HD22	1:C:573:THR:HG21	1.95	0.48
1:C:687:VAL:HG12	1:C:688:ALA:N	2.29	0.48
1:C:787:GLN:O	1:C:788:ILE:HD13	2.14	0.48
1:A:1010:GLN:HB3	1:A:1014:ARG:NH2	2.28	0.48
1:B:317:ASN:CG	1:B:594:GLY:HA2	2.37	0.48
1:B:972:ALA:HA	1:B:992:GLN:HE21	1.78	0.48
1:C:328:ARG:HH21	1:C:580:GLN:HB2	1.78	0.48
1:C:1047:TYR:OH	1:C:1108:ASN:ND2	2.45	0.48
1:A:859:THR:OG1	1:A:860:VAL:N	2.47	0.48
1:A:1103:PHE:HB3	1:A:1113:GLN:H	1.79	0.48
1:A:1104:VAL:O	1:A:1105:THR:OG1	2.31	0.48
1:B:37:TYR:HB3	1:B:223:LEU:HD12	1.94	0.48
1:B:38:TYR:OH	1:B:285:ILE:HG13	2.13	0.48
1:B:136:CYS:HB3	1:B:241:LEU:HD23	1.95	0.48
1:C:310:LYS:HG3	1:C:664:ILE:HD11	1.95	0.48
1:C:578:ASP:N	1:C:583:GLU:O	2.40	0.48
1:C:947:LYS:HA	1:C:950:ASP:HB2	1.95	0.48
1:A:37:TYR:HB2	1:A:204:TYR:CZ	2.49	0.48
1:A:73:THR:OG1	1:A:74:ASN:N	2.45	0.48
1:A:797:PHE:O	1:A:799:GLY:N	2.47	0.48
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.14	0.48
1:B:383:SER:HG	1:B:385:THR:HG1	1.42	0.48
1:B:776:LYS:HG2	1:B:780:GLU:OE1	2.14	0.48
1:B:903:ALA:HB1	1:B:913:GLN:HB3	1.95	0.48
1:C:392:PHE:CZ	1:C:515:PHE:CE2	3.02	0.48
1:A:201:PHE:O	1:A:228:ASP:HA	2.14	0.48
1:A:613:GLN:O	1:A:615:VAL:HG23	2.14	0.48
1:A:818:ILE:HG22	1:A:822:LEU:HD23	1.96	0.48
1:A:867:ASP:O	1:A:870:ILE:HG12	2.14	0.48
1:B:133:PHE:HB2	1:B:161:SER:OG	2.14	0.48
1:B:381:GLY:HA3	1:B:430:THR:O	2.14	0.48
1:B:731:MET:HG3	1:B:955:ASN:ND2	2.28	0.48
1:B:1012:LEU:O	1:B:1015:ALA:HB3	2.14	0.48
1:C:287:ASP:OD2	1:C:300:LYS:NZ	2.47	0.48
1:C:453:TYR:HE1	1:C:494:SER:O	1.96	0.48
1:C:617:CYS:HB2	1:C:619:GLU:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:MET:HG2	1:C:774:GLN:HE22	1.77	0.48
1:C:1078:ALA:O	1:C:1095:PHE:HB2	2.12	0.48
1:A:865:LEU:HB3	1:A:870:ILE:HG22	1.95	0.48
1:A:1029:MET:HE2	1:A:1029:MET:HB3	1.75	0.48
1:B:86:PHE:HE2	1:B:90:VAL:N	2.12	0.48
1:B:275:PHE:HE1	1:B:290:ASP:CG	2.09	0.48
1:B:322:PRO:HB2	1:B:539:VAL:HA	1.95	0.48
1:B:700:GLY:HA3	1:C:787:GLN:HA	1.96	0.48
1:B:856:ASN:C	1:B:858:LEU:H	2.21	0.48
1:B:1094:VAL:HG13	1:B:1107:ARG:NE	2.29	0.48
1:C:400:PHE:CE2	1:C:510:VAL:HB	2.49	0.48
1:C:538:CYS:HA	1:C:550:GLY:C	2.39	0.48
1:C:663:ASP:N	1:C:663:ASP:OD1	2.44	0.48
1:C:1082:CYS:HB2	1:C:1132:ILE:HD13	1.95	0.48
1:A:131:CYS:O	1:A:133:PHE:N	2.46	0.48
1:A:1114:ILE:O	1:A:1119:ASN:ND2	2.46	0.48
1:B:980:ILE:HD11	1:B:992:GLN:HG2	1.95	0.48
1:B:1001:LEU:O	1:B:1004:LEU:HG	2.14	0.48
1:C:801:ASN:OD1	1:C:803:SER:OG	2.11	0.48
1:C:961:THR:O	1:C:965:GLN:HG2	2.14	0.48
1:A:617:CYS:H	1:A:644:GLN:HE22	1.62	0.48
1:A:763:LEU:HA	1:A:763:LEU:HD13	1.54	0.48
1:A:805:ILE:O	1:A:816:SER:OG	2.25	0.48
1:A:885:GLY:O	1:A:888:PHE:N	2.41	0.48
1:A:1047:TYR:N	1:A:1047:TYR:CD1	2.82	0.48
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.95	0.48
1:B:36:VAL:O	1:B:222:ALA:HA	2.13	0.48
1:B:84:LEU:HB3	1:B:85:PRO:CD	2.44	0.48
1:B:108:THR:HA	1:B:237:ARG:HG2	1.95	0.48
1:B:238:PHE:O	1:B:238:PHE:CG	2.67	0.48
1:B:949:GLN:HG3	1:B:953:ASN:ND2	2.29	0.48
1:B:950:ASP:OD1	1:B:951:VAL:HG23	2.14	0.48
1:A:30:ASN:HB3	1:A:32:PHE:HE1	1.79	0.47
1:B:48:LEU:HD21	1:B:306:PHE:HD1	1.79	0.47
1:C:189:LEU:HG	1:C:208:THR:OG1	2.14	0.47
1:C:365:TYR:HB2	1:C:388:ASN:ND2	2.28	0.47
1:A:93:ALA:CB	1:A:191:GLU:HG3	2.44	0.47
1:A:117:LEU:C	1:A:118:LEU:HD12	2.39	0.47
1:A:442:ASP:HB2	1:A:509:ARG:NH1	2.29	0.47
1:A:560:LEU:HD12	1:A:562:PHE:HE1	1.79	0.47
1:A:1123:SER:CB	1:B:914:ASN:HD22	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HB2	1:B:279:TYR:CD2	2.49	0.47
1:B:193:VAL:HG22	1:B:194:PHE:N	2.29	0.47
1:B:316:SER:C	1:B:595:VAL:HG22	2.39	0.47
1:B:560:LEU:HB3	1:B:562:PHE:CE2	2.48	0.47
1:C:52:GLN:HA	1:C:274:THR:HA	1.95	0.47
1:C:66:HIS:CE1	1:C:264:ALA:HB2	2.48	0.47
1:C:325:SER:HA	1:C:539:VAL:HG13	1.95	0.47
1:C:432:CYS:SG	1:C:434:ILE:HD11	2.54	0.47
1:C:660:TYR:C	1:C:698:SER:HG	2.21	0.47
1:C:811:LYS:HE3	1:C:814:LYS:O	2.14	0.47
6:Q:3:BMA:O6	6:Q:3:BMA:O4	2.25	0.47
1:A:139:PRO:HB2	1:A:157:PHE:CB	2.39	0.47
1:B:210:ILE:HG23	1:B:212:LEU:HD23	1.95	0.47
1:B:547:THR:OG1	1:C:978:ASN:ND2	2.48	0.47
1:B:777:ASN:O	1:B:780:GLU:HG2	2.14	0.47
1:B:1079:PRO:HB2	1:C:917:TYR:CE2	2.49	0.47
1:C:278:LYS:HG2	1:C:279:TYR:N	2.29	0.47
1:C:884:SER:HA	1:C:895:GLN:HA	1.96	0.47
1:A:246:ARG:N	1:A:246:ARG:CD	2.77	0.47
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.97	0.47
1:A:732:THR:HG23	1:A:734:THR:HG22	1.94	0.47
1:A:966:LEU:HA	1:A:1000:ARG:NH2	2.29	0.47
1:A:1018:ILE:HA	1:A:1021:SER:OG	2.15	0.47
1:B:718:PHE:C	1:B:718:PHE:CD1	2.93	0.47
1:B:1088:HIS:ND1	1:B:1137:VAL:HG11	2.29	0.47
1:C:392:PHE:CE2	1:C:515:PHE:CE1	3.01	0.47
1:C:703:ASN:OD1	1:C:703:ASN:N	2.45	0.47
1:C:792:PRO:HB2	1:C:794:ILE:HG22	1.95	0.47
1:C:802:PHE:CB	1:C:806:LEU:HB2	2.45	0.47
1:A:126:VAL:HG13	1:A:172:SER:OG	2.13	0.47
1:A:245:HIS:C	1:A:245:HIS:ND1	2.73	0.47
1:A:1028:LYS:NZ	1:A:1042:PHE:CG	2.75	0.47
1:B:202:LYS:HD2	1:B:204:TYR:HE1	1.78	0.47
1:B:275:PHE:CE1	1:B:290:ASP:OD2	2.65	0.47
1:B:760:CYS:HA	1:B:763:LEU:CD1	2.44	0.47
1:B:860:VAL:O	1:B:860:VAL:HG13	2.15	0.47
1:B:1027:THR:O	1:B:1028:LYS:C	2.57	0.47
1:B:1050:MET:HB2	1:B:1050:MET:HE3	1.73	0.47
1:C:62:VAL:HG21	1:C:266:TYR:HB3	1.97	0.47
1:C:541:PHE:O	1:C:547:THR:HA	2.15	0.47
6:Q:1:NAG:H3	6:Q:1:NAG:C8	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:NZ	1:A:98:SER:OG	2.47	0.47
1:A:733:LYS:NZ	1:A:775:ASP:OD1	2.47	0.47
1:A:868:GLU:OE1	1:A:868:GLU:N	2.42	0.47
1:A:964:LYS:O	1:A:965:GLN:C	2.57	0.47
1:B:96:GLU:O	1:B:98:SER:N	2.44	0.47
1:B:275:PHE:CE2	1:B:290:ASP:HB2	2.49	0.47
1:B:312:ILE:HG13	1:B:596:SER:OG	2.15	0.47
1:B:507:PRO:O	1:B:508:TYR:HD1	1.98	0.47
1:B:534:VAL:C	1:B:535:LYS:HG3	2.40	0.47
1:B:604:THR:C	1:B:606:ASN:H	2.22	0.47
1:C:401:VAL:HG13	1:C:508:TYR:O	2.13	0.47
1:C:419:ALA:O	1:C:460:ASN:OD1	2.32	0.47
1:C:457:ARG:C	1:C:457:ARG:NH1	2.73	0.47
1:C:1034:LEU:HD12	1:C:1034:LEU:H	1.80	0.47
1:A:145:TYR:CA	1:A:150:LYS:HD2	2.43	0.47
1:A:717:ASN:O	1:A:1070:ALA:N	2.41	0.47
1:A:977:LEU:H	1:A:977:LEU:HD12	1.80	0.47
1:B:202:LYS:O	1:B:203:ILE:HD13	2.15	0.47
1:B:328:ARG:HH21	1:B:578:ASP:HB2	1.80	0.47
1:B:382:VAL:HA	1:B:387:LEU:HD11	1.95	0.47
1:B:521:PRO:HA	1:B:564:GLN:CG	2.30	0.47
1:B:740:MET:CE	1:B:857:GLY:H	2.28	0.47
1:B:884:SER:HA	1:B:896:ILE:N	2.29	0.47
1:B:925:ASN:HA	1:B:928:ASN:ND2	2.29	0.47
1:B:1024:LEU:O	1:B:1028:LYS:HG3	2.14	0.47
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.46	0.47
1:C:38:TYR:OH	1:C:284:THR:HA	2.15	0.47
1:C:167:THR:HB	1:C:168:PHE:CE2	2.49	0.47
1:C:332:ILE:HA	1:C:362:VAL:CG2	2.44	0.47
1:C:393:THR:OG1	1:C:394:ASN:N	2.47	0.47
1:C:418:ILE:O	1:C:423:TYR:N	2.46	0.47
1:C:665:PRO:HA	1:C:671:CYS:CB	2.44	0.47
1:C:731:MET:H	1:C:774:GLN:CD	2.20	0.47
1:C:743:CYS:SG	1:C:750:SER:OG	2.60	0.47
1:C:771:ALA:O	1:C:774:GLN:N	2.48	0.47
1:C:818:ILE:HD13	1:C:821:LEU:HD12	1.97	0.47
1:C:990:GLU:CA	1:C:993:ILE:HD12	2.41	0.47
1:C:1073:LYS:HB3	1:C:1075:PHE:CE2	2.49	0.47
1:A:200:TYR:HA	1:A:229:LEU:O	2.14	0.47
1:A:329:PHE:HB2	1:A:528:LYS:HA	1.96	0.47
1:A:619:GLU:OE1	1:A:619:GLU:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:SER:C	1:A:805:ILE:H	2.22	0.47
1:A:904:TYR:HD2	1:C:1107:ARG:CZ	2.27	0.47
1:B:193:VAL:HG22	1:B:194:PHE:H	1.78	0.47
1:B:316:SER:O	1:B:595:VAL:HG22	2.14	0.47
1:B:369:TYR:O	1:B:377:PHE:HB2	2.15	0.47
1:B:425:LEU:HD12	1:B:426:PRO:HD2	1.95	0.47
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.96	0.47
1:B:560:LEU:O	1:B:563:GLN:HG3	2.14	0.47
1:B:576:VAL:O	1:B:585:LEU:N	2.47	0.47
1:B:656:VAL:HG22	1:B:658:ASN:H	1.80	0.47
1:C:718:PHE:CB	1:C:1069:PRO:HA	2.44	0.47
1:A:224:GLU:OE1	1:A:224:GLU:N	2.41	0.47
1:A:330:PRO:HD2	1:A:528:LYS:N	2.30	0.47
1:A:713:ALA:O	1:B:894:LEU:HD13	2.15	0.47
1:A:1116:THR:H	1:A:1119:ASN:ND2	2.13	0.47
1:B:356:LYS:O	1:B:398:ASP:HA	2.15	0.47
1:B:422:ASN:ND2	1:B:454:ARG:O	2.48	0.47
1:B:726:ILE:HG13	1:B:947:LYS:HB2	1.97	0.47
1:B:1049:LEU:HB2	1:B:1065:VAL:O	2.14	0.47
1:C:43:PHE:HE1	1:C:283:GLY:HA3	1.78	0.47
1:A:402:ILE:HG22	1:A:403:ARG:N	2.29	0.47
1:A:742:ILE:HD11	1:A:997:ILE:HG22	1.96	0.47
1:A:1005:GLN:O	1:A:1008:VAL:HG22	2.15	0.47
1:B:614:ASP:H	1:B:648:GLY:HA3	1.80	0.47
1:C:332:ILE:HA	1:C:362:VAL:HG22	1.97	0.47
1:C:727:LEU:HA	1:C:727:LEU:HD23	1.68	0.47
1:C:935:GLN:O	1:C:939:SER:N	2.33	0.47
1:A:341:VAL:HG12	1:A:342:PHE:HD1	1.80	0.46
1:A:987:PRO:HB2	1:A:988:GLU:OE1	2.14	0.46
1:A:1089:PHE:HE2	1:A:1123:SER:O	1.98	0.46
1:B:92:PHE:CZ	1:B:265:TYR:HB2	2.50	0.46
1:B:110:LEU:HA	1:B:116:SER:OG	2.16	0.46
1:B:1097:SER:HB2	1:B:1102:TRP:CE3	2.50	0.46
1:C:530:SER:CB	1:C:580:GLN:HE22	2.28	0.46
1:C:560:LEU:HB3	1:C:562:PHE:CZ	2.50	0.46
1:C:770:ILE:HG13	1:C:771:ALA:N	2.26	0.46
1:A:378:LYS:O	1:A:434:ILE:HD11	2.16	0.46
1:A:752:LEU:HD11	1:A:990:GLU:OE2	2.15	0.46
1:A:858:LEU:HD12	1:A:859:THR:N	2.31	0.46
1:B:294:ASP:O	1:B:296:LEU:N	2.48	0.46
1:B:312:ILE:HG21	1:B:665:PRO:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:NH2	1:B:578:ASP:OD2	2.49	0.46
1:B:359:SER:HA	1:B:395:VAL:HB	1.98	0.46
1:B:641:ASN:O	1:B:654:GLU:HG3	2.16	0.46
1:B:1045:LYS:HA	1:B:1045:LYS:HD3	1.71	0.46
1:C:111:ASP:OD1	1:C:111:ASP:N	2.46	0.46
1:B:126:VAL:HB	1:B:174:PRO:HD2	1.97	0.46
1:B:174:PRO:HB3	1:B:178:ASP:OD2	2.16	0.46
1:B:650:LEU:HA	1:B:650:LEU:HD13	1.69	0.46
1:C:646:ARG:HB3	1:C:668:ALA:HB1	1.96	0.46
1:C:915:VAL:HG13	1:C:916:LEU:N	2.30	0.46
1:A:580:GLN:OE1	1:A:580:GLN:HA	2.15	0.46
1:A:701:ALA:O	1:B:787:GLN:HB3	2.14	0.46
1:B:1009:THR:O	1:B:1012:LEU:HB2	2.14	0.46
1:C:816:SER:N	1:C:819:GLU:OE1	2.45	0.46
1:C:1079:PRO:HD2	1:C:1131:GLY:O	2.16	0.46
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.51	0.46
1:A:296:LEU:HD13	1:A:608:VAL:HG22	1.96	0.46
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.96	0.46
1:A:328:ARG:NH2	1:A:580:GLN:HB2	2.31	0.46
1:A:528:LYS:O	1:A:530:SER:N	2.48	0.46
1:A:983:ARG:C	1:A:984:LEU:HD12	2.41	0.46
1:B:276:LEU:HD23	1:B:300:LYS:HG2	1.98	0.46
1:B:560:LEU:C	1:B:562:PHE:H	2.23	0.46
1:B:808:ASP:HB2	1:B:809:PRO:HD2	1.97	0.46
1:B:1081:ILE:N	1:B:1095:PHE:HE2	2.14	0.46
1:A:330:PRO:CD	1:A:527:PRO:HA	2.39	0.46
1:A:938:LEU:HD23	1:A:944:ALA:HB1	1.97	0.46
1:A:1029:MET:O	1:A:1033:VAL:HB	2.15	0.46
1:B:707:TYR:CG	1:B:708:SER:N	2.82	0.46
1:B:1025:ALA:O	1:B:1026:ALA:C	2.59	0.46
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.16	0.46
1:C:138:ASP:OD1	1:C:138:ASP:N	2.46	0.46
1:C:541:PHE:CD1	1:C:543:PHE:HD2	2.34	0.46
1:C:611:LEU:HD22	1:C:666:ILE:HD11	1.97	0.46
1:A:1049:LEU:HB2	1:A:1065:VAL:CG2	2.45	0.46
1:B:322:PRO:HB3	1:B:539:VAL:HA	1.98	0.46
1:B:402:ILE:HD12	1:B:410:ILE:HD13	1.96	0.46
1:B:421:TYR:HB3	1:B:422:ASN:ND2	2.30	0.46
1:B:434:ILE:HG22	1:B:435:ALA:N	2.30	0.46
1:B:902:MET:SD	1:B:905:ARG:HD2	2.56	0.46
1:C:67:ALA:HB1	1:C:69:HIS:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2:NAG:O7	2:X:2:NAG:O3	2.29	0.46
1:A:40:ASP:OD1	1:A:41:LYS:N	2.47	0.46
1:A:64:TRP:CD1	1:A:266:TYR:CE1	3.03	0.46
1:A:666:ILE:HD12	1:A:670:ILE:HG22	1.98	0.46
1:A:712:ILE:HG21	1:B:897:PRO:HD3	1.97	0.46
1:A:869:MET:HB3	1:A:869:MET:HE2	1.76	0.46
1:A:936:ASP:HA	1:A:939:SER:OG	2.16	0.46
1:B:290:ASP:HB3	1:B:293:LEU:HG	1.98	0.46
1:B:499:PRO:HB2	1:B:506:GLN:NE2	2.28	0.46
1:B:598:ILE:HG23	1:B:609:ALA:HB3	1.97	0.46
1:B:738:CYS:HB2	1:B:753:LEU:HD11	1.98	0.46
1:B:778:THR:O	1:B:781:VAL:HB	2.15	0.46
1:C:350:VAL:HG21	1:C:402:ILE:HG13	1.97	0.46
1:C:573:THR:O	1:C:587:ILE:HD12	2.16	0.46
1:A:710:ASN:OD1	1:A:710:ASN:N	2.49	0.46
1:A:961:THR:O	1:A:965:GLN:NE2	2.28	0.46
1:A:993:ILE:O	1:A:997:ILE:HG12	2.16	0.46
1:B:94:SER:OG	1:B:265:TYR:HA	2.16	0.46
1:B:191:GLU:OE1	1:B:191:GLU:N	2.49	0.46
1:C:743:CYS:SG	1:C:750:SER:N	2.89	0.46
1:C:1029:MET:O	1:C:1033:VAL:CB	2.60	0.46
1:C:1091:ARG:HG3	1:C:1092:GLU:H	1.80	0.46
1:A:380:TYR:CD1	1:A:432:CYS:HA	2.51	0.46
1:A:808:ASP:HB3	1:A:811:LYS:HE2	1.98	0.46
1:A:1079:PRO:HG3	1:A:1130:ILE:O	2.16	0.46
1:B:430:THR:C	1:B:513:LEU:HD12	2.41	0.46
1:B:739:THR:OG1	1:B:740:MET:N	2.48	0.46
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.51	0.46
1:C:699:LEU:H	1:C:699:LEU:HD12	1.79	0.46
1:C:867:ASP:OD1	1:C:868:GLU:N	2.47	0.46
1:C:1039:ARG:CZ	1:C:1042:PHE:CE1	2.99	0.46
1:A:1028:LYS:CE	1:A:1042:PHE:CE2	2.99	0.45
1:A:1083:HIS:ND1	1:A:1084:ASP:OD1	2.50	0.45
1:B:326:ILE:HD11	1:B:541:PHE:HB3	1.98	0.45
1:A:422:ASN:ND2	1:A:456:PHE:HB2	2.28	0.45
1:A:785:VAL:HG11	1:A:789:TYR:CE1	2.51	0.45
1:A:1116:THR:H	1:A:1119:ASN:CG	2.23	0.45
1:B:977:LEU:N	1:B:977:LEU:HD23	2.31	0.45
1:C:122:ASN:CG	1:C:127:VAL:HG23	2.41	0.45
1:C:906:PHE:HD2	1:C:916:LEU:HB2	1.81	0.45
1:C:948:LEU:O	1:C:952:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:THR:OG1	1:C:1010:GLN:N	2.49	0.45
4:V:1:NAG:C3	4:V:1:NAG:C8	2.92	0.45
1:A:100:ILE:HG23	1:A:101:ILE:N	2.31	0.45
1:A:196:ASN:OD1	1:A:196:ASN:N	2.50	0.45
1:A:429:PHE:CD2	1:A:515:PHE:HB2	2.51	0.45
1:A:1105:THR:OG1	1:A:1111:GLU:O	2.33	0.45
1:B:603:ASN:OD1	1:B:603:ASN:N	2.48	0.45
1:B:738:CYS:SG	1:B:739:THR:N	2.90	0.45
1:B:1083:HIS:HB3	1:B:1088:HIS:CE1	2.51	0.45
1:B:1130:ILE:H	1:B:1130:ILE:HD12	1.80	0.45
1:C:555:SER:O	1:C:555:SER:OG	2.33	0.45
1:C:732:THR:O	1:C:734:THR:N	2.49	0.45
1:C:770:ILE:HA	1:C:773:GLU:OE1	2.16	0.45
1:A:189:LEU:HG	1:A:191:GLU:OE2	2.16	0.45
1:A:294:ASP:O	1:A:296:LEU:N	2.49	0.45
1:A:327:VAL:CG2	1:A:329:PHE:CZ	2.99	0.45
1:A:866:THR:O	1:A:870:ILE:HG23	2.16	0.45
1:A:869:MET:O	1:A:872:GLN:N	2.49	0.45
1:B:84:LEU:N	1:B:84:LEU:CD1	2.79	0.45
1:B:128:ILE:O	1:B:169:GLU:HA	2.17	0.45
1:B:779:GLN:CD	1:B:783:ALA:HB2	2.42	0.45
1:C:355:ARG:NH1	1:C:355:ARG:O	2.49	0.45
1:C:942:ALA:O	1:C:943:SER:OG	2.28	0.45
1:C:1116:THR:OG1	1:C:1117:THR:N	2.48	0.45
1:A:567:ARG:HB2	1:A:572:THR:C	2.41	0.45
1:A:1049:LEU:HB2	1:A:1065:VAL:HG23	1.98	0.45
1:B:85:PRO:CB	1:B:237:ARG:NH1	2.74	0.45
1:B:898:PHE:O	1:B:901:GLN:HB3	2.16	0.45
1:B:919:ASN:O	1:B:920:GLN:C	2.58	0.45
1:B:955:ASN:OD1	1:B:959:LEU:HD11	2.16	0.45
1:B:1093:GLY:O	1:B:1107:ARG:NH2	2.50	0.45
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.40	0.45
1:C:777:ASN:HA	1:C:780:GLU:OE1	2.16	0.45
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.17	0.45
1:A:148:ASN:ND2	1:A:150:LYS:HA	2.24	0.45
1:A:391:CYS:HB3	1:A:525:CYS:CA	2.45	0.45
1:A:718:PHE:HA	1:A:1069:PRO:HA	1.99	0.45
1:A:788:ILE:CD1	1:C:699:LEU:HB2	2.37	0.45
1:B:37:TYR:HB2	1:B:223:LEU:HB2	1.99	0.45
1:B:355:ARG:HD3	1:B:466:ARG:NH1	2.22	0.45
1:B:431:GLY:H	1:B:513:LEU:HB2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:THR:HB	1:B:586:ASP:HB3	1.99	0.45
1:B:597:VAL:CG1	1:B:599:THR:HG23	2.46	0.45
1:C:811:LYS:HD3	1:C:815:ARG:HH22	1.81	0.45
1:C:902:MET:SD	1:C:905:ARG:HD2	2.57	0.45
1:C:1010:GLN:HA	1:C:1013:ILE:HG12	1.97	0.45
1:A:199:GLY:O	1:A:231:ILE:HG12	2.17	0.45
1:A:328:ARG:HB2	1:A:543:PHE:HE1	1.79	0.45
1:A:333:THR:HG22	1:A:527:PRO:HB2	1.99	0.45
1:A:541:PHE:HZ	1:A:576:VAL:HG11	1.80	0.45
1:A:663:ASP:OD1	1:A:663:ASP:N	2.32	0.45
1:A:913:GLN:OE1	1:C:1090:PRO:HG2	2.17	0.45
1:B:507:PRO:C	1:B:508:TYR:HD1	2.24	0.45
1:B:767:LEU:HD12	1:B:767:LEU:HA	1.69	0.45
1:C:319:ARG:NH2	1:C:322:PRO:HD2	2.32	0.45
1:C:453:TYR:CE2	1:C:454:ARG:CD	2.99	0.45
1:A:276:LEU:C	1:A:277:LEU:HD22	2.42	0.45
1:A:369:TYR:CE1	1:A:374:PHE:HD2	2.35	0.45
1:A:434:ILE:O	1:A:510:VAL:HG13	2.17	0.45
1:A:558:LYS:HD2	5:h:1:NAG:H62	1.97	0.45
1:A:731:MET:HE3	1:A:955:ASN:HB2	1.99	0.45
1:A:789:TYR:HB2	1:A:876:ALA:HB1	1.98	0.45
1:A:1050:MET:O	1:A:1065:VAL:HG22	2.17	0.45
1:A:1107:ARG:NE	1:A:1107:ARG:HA	2.32	0.45
1:B:33:THR:HA	1:B:58:PHE:CZ	2.51	0.45
1:C:55:PHE:HB2	1:C:273:ARG:HB2	1.99	0.45
1:C:253:ASP:OD1	1:C:253:ASP:N	2.48	0.45
1:C:421:TYR:HH	1:C:458:LYS:HA	1.69	0.45
1:C:451:TYR:HB3	1:C:495:TYR:HB3	1.99	0.45
1:C:789:TYR:HB2	1:C:876:ALA:HB1	1.99	0.45
1:C:977:LEU:HD23	1:C:977:LEU:H	1.82	0.45
1:C:1106:GLN:HE22	1:C:1109:PHE:CA	2.30	0.45
1:A:800:PHE:HB3	1:A:802:PHE:CE1	2.52	0.45
1:A:854:LYS:HD2	1:A:854:LYS:C	2.42	0.45
1:B:201:PHE:CB	1:B:229:LEU:O	2.62	0.45
1:B:382:VAL:HG12	1:B:384:PRO:CD	2.46	0.45
1:B:787:GLN:HB2	1:B:789:TYR:CZ	2.52	0.45
1:B:934:ILE:HD12	1:B:934:ILE:HA	1.71	0.45
1:B:1080:ALA:C	1:B:1095:PHE:HE2	2.24	0.45
1:B:1081:ILE:HG22	1:B:1088:HIS:O	2.17	0.45
1:C:200:TYR:CE1	1:C:230:PRO:HA	2.52	0.45
1:C:401:VAL:HB	1:C:451:TYR:OH	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:ASN:OD1	1:C:540:ASN:N	2.45	0.45
1:C:613:GLN:HG2	1:C:613:GLN:O	2.17	0.45
1:C:994:ASP:HA	1:C:997:ILE:HG22	1.97	0.45
1:A:763:LEU:HD12	1:A:1008:VAL:HG11	1.99	0.45
1:A:787:GLN:HG2	1:A:789:TYR:CE1	2.52	0.45
1:A:1030:SER:HA	1:A:1034:LEU:HD13	1.99	0.45
1:B:206:LYS:HG2	1:B:208:THR:OG1	2.17	0.45
1:B:712:ILE:H	1:B:1077:THR:HG21	1.82	0.45
1:B:1051:SER:HG	1:B:1064:HIS:HD1	1.61	0.45
1:C:140:PHE:HZ	1:C:156:GLU:H	1.61	0.45
1:C:141:LEU:HD23	1:C:141:LEU:H	1.82	0.45
1:C:1115:ILE:HA	1:C:1119:ASN:ND2	2.32	0.45
1:A:71:SER:CB	1:A:259:THR:HA	2.45	0.44
1:A:387:LEU:HG	1:A:392:PHE:CE1	2.39	0.44
1:A:389:ASP:O	1:A:526:GLY:HA3	2.18	0.44
1:A:752:LEU:HD21	1:A:990:GLU:OE1	2.17	0.44
1:A:969:ASN:HB3	1:A:972:ALA:O	2.16	0.44
1:A:1015:ALA:O	1:A:1018:ILE:HG22	2.17	0.44
1:B:961:THR:O	1:B:965:GLN:HG2	2.17	0.44
1:C:64:TRP:CD1	1:C:65:PHE:N	2.85	0.44
1:C:207:HIS:CE1	1:C:209:PRO:HB3	2.52	0.44
1:C:767:LEU:HA	1:C:770:ILE:HG23	1.98	0.44
1:A:83:VAL:HG11	1:A:237:ARG:HG3	1.99	0.44
1:A:197:ILE:O	1:A:197:ILE:HG13	2.17	0.44
1:A:368:LEU:HD23	1:A:368:LEU:H	1.82	0.44
1:A:1072:GLU:CD	1:A:1072:GLU:H	2.25	0.44
1:A:1084:ASP:HB2	1:A:1086:LYS:HG3	1.98	0.44
1:A:1107:ARG:HA	1:A:1107:ARG:HE	1.82	0.44
1:B:93:ALA:HB2	1:B:191:GLU:HA	1.98	0.44
1:B:584:ILE:C	1:B:585:LEU:HD22	2.41	0.44
1:B:712:ILE:HG12	1:C:897:PRO:HD3	1.99	0.44
1:B:1049:LEU:HA	1:B:1049:LEU:HD23	1.76	0.44
1:C:48:LEU:HD23	1:C:278:LYS:HG3	1.99	0.44
1:C:325:SER:OG	1:C:540:ASN:OD1	2.30	0.44
1:C:750:SER:HA	1:C:753:LEU:HB3	2.00	0.44
1:C:900:MET:HE2	1:C:900:MET:HB3	1.67	0.44
1:C:1045:LYS:HA	1:C:1045:LYS:HD2	1.78	0.44
1:C:1050:MET:HE2	1:C:1050:MET:HB2	1.79	0.44
1:C:1089:PHE:H	1:C:1120:THR:CG2	2.30	0.44
1:A:55:PHE:HB3	1:A:275:PHE:CZ	2.53	0.44
1:A:434:ILE:C	1:A:510:VAL:HG22	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.52	0.44
1:B:1048:HIS:CD2	1:B:1048:HIS:C	2.95	0.44
1:C:861:LEU:HA	1:C:861:LEU:HD13	1.86	0.44
1:C:1024:LEU:O	1:C:1027:THR:OG1	2.29	0.44
4:V:1:NAG:H83	4:V:1:NAG:O3	2.17	0.44
1:A:87:ASN:HD22	1:A:269:TYR:CB	2.30	0.44
1:A:93:ALA:HB1	1:A:191:GLU:HG3	1.99	0.44
1:A:692:ILE:HD13	1:A:692:ILE:HA	1.74	0.44
1:A:726:ILE:HB	1:A:948:LEU:HD11	2.00	0.44
1:A:785:VAL:HG11	1:A:789:TYR:HE1	1.83	0.44
1:A:990:GLU:O	1:A:994:ASP:HB2	2.17	0.44
1:A:1039:ARG:NH2	1:B:1031:GLU:CD	2.75	0.44
1:B:290:ASP:CG	1:B:292:ALA:H	2.25	0.44
1:B:383:SER:H	1:B:387:LEU:HD11	1.82	0.44
1:B:388:ASN:HD21	1:B:528:LYS:NZ	2.16	0.44
1:B:615:VAL:O	1:B:644:GLN:NE2	2.34	0.44
1:B:709:ASN:OD1	7:B:1205:NAG:N2	2.50	0.44
1:B:805:ILE:HG13	1:B:818:ILE:HD11	1.99	0.44
1:B:886:TRP:CH2	1:B:904:TYR:CD1	3.06	0.44
1:C:69:HIS:CB	1:C:77:LYS:HG3	2.39	0.44
1:C:136:CYS:SG	1:C:159:VAL:HG23	2.57	0.44
1:C:762:GLN:HA	1:C:765:ARG:NH1	2.33	0.44
1:C:822:LEU:O	1:C:825:LYS:N	2.50	0.44
1:C:1024:LEU:O	1:C:1028:LYS:HG3	2.18	0.44
1:C:1061:VAL:C	1:C:1062:PHE:HD1	2.25	0.44
1:C:1094:VAL:HG12	1:C:1095:PHE:O	2.17	0.44
1:A:763:LEU:CD1	1:A:1008:VAL:HG11	2.47	0.44
1:A:1079:PRO:HA	1:B:900:MET:SD	2.58	0.44
1:B:284:THR:HG22	1:B:285:ILE:N	2.29	0.44
1:A:144:TYR:CB	1:A:245:HIS:HB2	2.47	0.44
1:A:429:PHE:HB2	1:A:515:PHE:N	2.24	0.44
1:A:552:LEU:HD23	1:A:587:ILE:HG22	2.00	0.44
1:A:1089:PHE:CE2	1:A:1123:SER:O	2.71	0.44
1:B:442:ASP:OD1	1:B:442:ASP:N	2.49	0.44
1:B:858:LEU:HD12	1:B:859:THR:N	2.33	0.44
1:B:869:MET:HA	1:B:872:GLN:OE1	2.17	0.44
1:B:978:ASN:O	1:B:981:LEU:HG	2.17	0.44
1:C:46:SER:H	1:C:279:TYR:HB2	1.81	0.44
1:C:113:LYS:HE2	1:C:113:LYS:HB3	1.84	0.44
1:C:166:CYS:SG	1:C:167:THR:N	2.90	0.44
1:C:563:GLN:H	1:C:577:ARG:HH21	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:VAL:HG12	1:C:782:PHE:CG	2.53	0.44
1:C:874:THR:O	1:C:877:LEU:N	2.50	0.44
1:C:945:LEU:O	1:C:946:GLY:C	2.61	0.44
1:C:1080:ALA:O	1:C:1081:ILE:HD13	2.17	0.44
1:A:164:ASN:O	1:A:165:ASN:HB2	2.17	0.44
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.99	0.44
1:A:289:VAL:HG22	1:A:290:ASP:O	2.17	0.44
1:A:404:GLY:H	1:A:508:TYR:HB2	1.83	0.44
1:A:818:ILE:O	1:A:822:LEU:HG	2.18	0.44
1:B:325:SER:HB2	1:B:540:ASN:ND2	2.33	0.44
1:B:434:ILE:HG22	1:B:435:ALA:H	1.83	0.44
1:B:559:PHE:CD1	1:B:563:GLN:OE1	2.71	0.44
1:B:1008:VAL:O	1:B:1012:LEU:HD23	2.17	0.44
1:B:1021:SER:O	1:B:1024:LEU:HB3	2.18	0.44
1:B:1047:TYR:CE2	1:B:1108:ASN:ND2	2.86	0.44
1:C:419:ALA:HA	1:C:423:TYR:O	2.17	0.44
1:C:497:PHE:CB	1:C:499:PRO:HD2	2.48	0.44
1:C:555:SER:HB3	1:C:584:ILE:O	2.18	0.44
1:C:767:LEU:O	1:C:770:ILE:N	2.51	0.44
1:C:1006:THR:O	1:C:1009:THR:N	2.51	0.44
1:A:34:ARG:HA	1:A:34:ARG:HD2	1.79	0.44
1:B:337:PRO:CD	1:B:358:ILE:CG2	2.94	0.44
1:B:884:SER:OG	1:B:894:LEU:O	2.30	0.44
1:C:924:ALA:O	1:C:928:ASN:ND2	2.38	0.44
1:A:186:PHE:CD1	1:A:186:PHE:O	2.71	0.44
1:A:752:LEU:HD13	1:A:752:LEU:HA	1.80	0.44
1:A:762:GLN:HA	1:A:765:ARG:NH1	2.31	0.44
1:B:377:PHE:CE2	1:B:382:VAL:HG11	2.53	0.44
1:B:731:MET:SD	1:B:1011:GLN:NE2	2.76	0.44
1:B:780:GLU:O	1:B:784:GLN:NE2	2.51	0.44
1:B:791:THR:HG21	1:B:806:LEU:HD12	1.99	0.44
1:B:819:GLU:O	1:B:822:LEU:HB2	2.17	0.44
1:B:909:ILE:CG2	1:B:1047:TYR:HB3	2.48	0.44
1:B:1037:SER:O	1:B:1038:LYS:HD3	2.18	0.44
1:C:64:TRP:HA	1:C:266:TYR:CE1	2.52	0.44
1:C:305:SER:OG	1:C:305:SER:O	2.35	0.44
1:C:437:ASN:OD1	1:C:438:SER:N	2.51	0.44
1:C:1081:ILE:C	1:C:1132:ILE:HD11	2.43	0.44
1:C:1089:PHE:O	1:C:1120:THR:CG2	2.65	0.44
1:A:712:ILE:HA	1:B:895:GLN:CD	2.42	0.43
1:B:194:PHE:HD1	1:B:203:ILE:HD12	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TYR:N	1:B:514:SER:OG	2.51	0.43
1:B:555:SER:OG	1:B:584:ILE:HG13	2.17	0.43
1:B:1087:ALA:HB2	1:B:1126:CYS:HA	1.99	0.43
1:C:400:PHE:CZ	1:C:510:VAL:HB	2.53	0.43
1:C:613:GLN:H	1:C:613:GLN:CD	2.25	0.43
1:C:737:ASP:OD1	1:C:857:GLY:HA2	2.18	0.43
1:C:926:GLN:O	1:C:927:PHE:C	2.61	0.43
1:A:43:PHE:CG	1:A:44:ARG:N	2.86	0.43
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.78	0.43
1:A:729:VAL:HG22	1:A:1058:HIS:O	2.19	0.43
1:A:914:ASN:HA	1:A:917:TYR:HB2	2.00	0.43
1:A:947:LYS:O	1:A:951:VAL:HG13	2.18	0.43
1:A:1076:THR:HG23	1:A:1097:SER:HB3	1.99	0.43
1:B:144:TYR:C	1:B:146:HIS:N	2.75	0.43
1:B:738:CYS:HB3	1:B:760:CYS:HB2	1.44	0.43
1:B:804:GLN:OE1	1:B:804:GLN:N	2.51	0.43
1:B:936:ASP:HA	1:B:939:SER:OG	2.17	0.43
1:B:995:ARG:HA	1:B:998:THR:HG22	1.99	0.43
1:C:82:PRO:HD2	1:C:265:TYR:OH	2.18	0.43
1:C:743:CYS:O	1:C:746:SER:N	2.52	0.43
1:A:577:ARG:NH2	1:A:584:ILE:HB	2.32	0.43
1:B:1083:HIS:CG	1:B:1136:THR:HA	2.53	0.43
7:B:1203:NAG:O7	7:B:1203:NAG:O3	2.32	0.43
1:C:331:ASN:HD22	1:C:331:ASN:HA	1.67	0.43
1:C:353:TRP:HB3	1:C:423:TYR:CE1	2.53	0.43
1:C:880:GLY:C	1:C:888:PHE:HE2	2.26	0.43
1:C:961:THR:C	1:C:965:GLN:HE21	2.24	0.43
1:C:979:ASP:O	1:C:982:SER:OG	2.31	0.43
1:C:1039:ARG:HD3	1:C:1042:PHE:CE2	2.53	0.43
1:A:96:GLU:CD	1:A:100:ILE:HB	2.44	0.43
1:A:329:PHE:O	1:A:579:PRO:CB	2.67	0.43
1:A:752:LEU:HD21	1:A:990:GLU:CD	2.44	0.43
1:A:969:ASN:HB3	1:A:972:ALA:N	2.33	0.43
1:A:979:ASP:OD1	1:A:983:ARG:NE	2.45	0.43
1:A:1106:GLN:CD	1:A:1106:GLN:C	2.87	0.43
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.99	0.43
1:B:120:VAL:C	1:B:126:VAL:HG13	2.43	0.43
1:B:121:ASN:HB3	1:B:175:PHE:HD2	1.82	0.43
1:B:128:ILE:HD13	1:B:170:TYR:HD1	1.82	0.43
1:B:699:LEU:CB	1:C:788:ILE:HD11	2.49	0.43
1:B:1106:GLN:HE22	1:B:1113:GLN:NE2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:SER:C	1:C:117:LEU:HD23	2.43	0.43
1:C:327:VAL:O	1:C:530:SER:HA	2.19	0.43
1:C:1051:SER:OG	1:C:1064:HIS:HA	2.18	0.43
1:A:188:ASN:HB3	1:A:207:HIS:CE1	2.48	0.43
1:B:327:VAL:H	1:B:531:THR:HG1	1.62	0.43
1:B:868:GLU:H	1:B:868:GLU:CD	2.26	0.43
1:B:1063:LEU:C	1:B:1064:HIS:ND1	2.76	0.43
1:C:53:ASP:C	1:C:55:PHE:HD1	2.26	0.43
1:C:130:VAL:HG11	1:C:168:PHE:HB2	2.00	0.43
1:C:188:ASN:ND2	1:C:209:PRO:HA	2.33	0.43
1:C:224:GLU:N	1:C:224:GLU:OE1	2.52	0.43
1:C:356:LYS:O	1:C:396:TYR:HA	2.18	0.43
1:C:521:PRO:HA	1:C:564:GLN:OE1	2.19	0.43
1:C:584:ILE:C	1:C:585:LEU:HD12	2.43	0.43
1:C:604:THR:OG1	1:C:605:SER:N	2.51	0.43
1:C:819:GLU:O	1:C:822:LEU:HB3	2.18	0.43
1:C:1078:ALA:HB3	1:C:1095:PHE:HB3	2.00	0.43
1:A:733:LYS:NZ	1:A:863:PRO:HA	2.33	0.43
1:B:703:ASN:O	1:C:789:TYR:HA	2.19	0.43
1:B:914:ASN:OD1	1:B:915:VAL:HG13	2.19	0.43
1:C:1054:GLN:O	1:C:1060:VAL:HG23	2.18	0.43
1:C:1091:ARG:HH21	1:C:1120:THR:N	2.16	0.43
1:A:560:LEU:H	1:A:563:GLN:HB2	1.84	0.43
1:A:743:CYS:HA	1:A:977:LEU:HD22	1.99	0.43
1:A:894:LEU:HB3	1:C:713:ALA:HB3	2.01	0.43
1:A:954:GLN:HA	1:A:957:GLN:CD	2.44	0.43
1:B:327:VAL:HB	1:B:531:THR:HG23	2.00	0.43
1:B:537:LYS:O	1:B:539:VAL:N	2.52	0.43
1:B:698:SER:C	1:B:700:GLY:H	2.26	0.43
1:B:815:ARG:HB3	1:B:819:GLU:OE1	2.19	0.43
1:B:915:VAL:O	1:B:918:GLU:HB2	2.18	0.43
1:C:424:LYS:HA	1:C:460:ASN:ND2	2.31	0.43
1:C:795:LYS:HE2	1:C:795:LYS:HB3	1.71	0.43
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.54	0.43
1:C:1080:ALA:O	1:C:1132:ILE:HG13	2.18	0.43
1:A:231:ILE:HG13	1:A:232:GLY:N	2.33	0.43
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.77	0.43
1:A:1116:THR:C	1:A:1118:ASP:N	2.76	0.43
1:B:86:PHE:HB3	1:B:236:THR:OG1	2.19	0.43
1:B:275:PHE:CE1	1:B:290:ASP:OD1	2.71	0.43
1:B:434:ILE:HB	1:B:436:TRP:HZ3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LYS:HZ2	1:B:559:PHE:HA	1.83	0.43
1:B:733:LYS:HE3	1:B:733:LYS:HB2	1.75	0.43
1:C:122:ASN:HD22	1:C:122:ASN:HA	1.54	0.43
1:C:439:ASN:HA	1:C:506:GLN:HG2	2.01	0.43
1:C:731:MET:HE3	1:C:955:ASN:ND2	2.34	0.43
1:A:338:PHE:HA	1:A:341:VAL:HB	2.00	0.43
1:A:787:GLN:HG3	1:C:703:ASN:OD1	2.19	0.43
1:B:77:LYS:HG3	1:B:78:ARG:H	1.83	0.43
1:B:740:MET:O	1:B:741:TYR:C	2.62	0.43
1:C:53:ASP:CG	1:C:54:LEU:H	2.27	0.43
1:C:73:THR:H	1:C:258:TRP:HZ3	1.67	0.43
1:C:85:PRO:O	1:C:238:PHE:HE1	2.02	0.43
1:C:141:LEU:O	1:C:141:LEU:HG	2.19	0.43
1:C:170:TYR:CG	1:C:171:VAL:N	2.86	0.43
1:C:289:VAL:HG12	1:C:290:ASP:N	2.34	0.43
1:C:597:VAL:O	1:C:598:ILE:HD13	2.19	0.43
1:C:1006:THR:O	1:C:1007:TYR:C	2.61	0.43
1:C:1006:THR:O	1:C:1009:THR:OG1	2.25	0.43
1:A:188:ASN:CB	1:A:207:HIS:HE1	2.31	0.43
1:A:712:ILE:CG2	1:B:896:ILE:HD13	2.48	0.43
1:B:620:VAL:N	1:B:621:PRO:HD3	2.32	0.43
1:B:762:GLN:HA	1:B:765:ARG:HH21	1.83	0.43
1:B:949:GLN:O	1:B:952:VAL:HG12	2.18	0.43
1:B:1043:CYS:O	1:B:1048:HIS:CE1	2.72	0.43
1:C:576:VAL:HG22	1:C:577:ARG:O	2.19	0.43
1:C:716:THR:HG22	1:C:1071:GLN:O	2.19	0.43
1:C:1073:LYS:HB3	1:C:1075:PHE:HE2	1.83	0.43
1:A:538:CYS:N	1:A:551:VAL:HG12	2.34	0.42
1:A:1039:ARG:NH2	1:B:1031:GLU:OE2	2.46	0.42
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.99	0.42
1:B:1103:PHE:HB3	1:B:1113:GLN:H	1.83	0.42
1:C:763:LEU:H	1:C:763:LEU:HG	1.59	0.42
1:C:1076:THR:OG1	1:C:1097:SER:HB3	2.19	0.42
1:A:540:ASN:OD1	1:A:540:ASN:N	2.52	0.42
1:A:819:GLU:O	1:A:823:PHE:HB2	2.19	0.42
1:A:1078:ALA:HB1	1:A:1079:PRO:HD2	2.01	0.42
1:B:44:ARG:NH2	1:B:49:HIS:CE1	2.87	0.42
1:B:275:PHE:CD1	1:B:275:PHE:N	2.87	0.42
1:B:665:PRO:HB3	1:C:864:LEU:HD11	2.01	0.42
1:B:881:THR:HA	1:B:885:GLY:O	2.18	0.42
1:B:948:LEU:HA	1:B:951:VAL:HG23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.84	0.42
1:C:344:ALA:O	1:C:347:PHE:CE1	2.71	0.42
1:A:792:PRO:HG3	1:C:707:TYR:HB3	2.02	0.42
1:A:885:GLY:O	1:A:888:PHE:HD2	2.02	0.42
1:A:1039:ARG:HH21	1:B:1031:GLU:CD	2.28	0.42
1:B:106:PHE:HB3	1:B:235:ILE:HD12	2.02	0.42
1:B:275:PHE:CB	1:B:290:ASP:HA	2.47	0.42
1:B:903:ALA:O	1:B:913:GLN:HG2	2.18	0.42
1:B:1081:ILE:HD11	1:B:1135:ASN:HB3	2.00	0.42
1:C:577:ARG:HA	1:C:584:ILE:HG13	2.01	0.42
1:C:718:PHE:HD2	1:C:719:THR:O	2.02	0.42
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.68	0.42
1:A:354:ASN:ND2	1:A:356:LYS:HD3	2.34	0.42
1:A:389:ASP:OD1	1:A:527:PRO:HD2	2.19	0.42
1:A:658:ASN:OD1	1:A:658:ASN:N	2.52	0.42
1:B:560:LEU:HB3	1:B:562:PHE:CZ	2.53	0.42
1:B:704:SER:HB2	1:C:790:LYS:H	1.84	0.42
1:B:912:THR:HG22	1:B:914:ASN:H	1.84	0.42
1:B:1045:LYS:HD3	1:B:1045:LYS:N	2.30	0.42
1:B:1049:LEU:CB	1:B:1065:VAL:HG23	2.50	0.42
1:C:31:SER:N	1:C:60:SER:O	2.50	0.42
1:C:139:PRO:HD2	1:C:242:LEU:C	2.44	0.42
1:C:611:LEU:HD22	1:C:666:ILE:CD1	2.49	0.42
1:C:892:ALA:O	1:C:894:LEU:HG	2.20	0.42
1:C:1062:PHE:CD2	1:C:1064:HIS:HE1	2.37	0.42
1:C:1127:ASP:CG	1:C:1128:VAL:N	2.77	0.42
1:A:30:ASN:HB3	1:A:32:PHE:CE1	2.54	0.42
1:A:43:PHE:HE1	1:A:283:GLY:HA3	1.84	0.42
1:A:83:VAL:HG22	1:A:239:GLN:CB	2.49	0.42
1:A:613:GLN:HE21	1:A:614:ASP:CG	2.28	0.42
1:A:886:TRP:CZ2	1:A:904:TYR:CZ	3.07	0.42
1:A:994:ASP:HA	1:A:997:ILE:HD11	2.00	0.42
1:B:314:GLN:HE21	1:C:768:THR:HG21	1.83	0.42
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.00	0.42
1:B:649:CYS:C	1:B:650:LEU:HD22	2.43	0.42
1:B:865:LEU:HA	1:B:865:LEU:HD13	1.72	0.42
1:B:1009:THR:OG1	1:B:1010:GLN:N	2.52	0.42
1:C:455:LEU:HD21	1:C:492:LEU:CB	2.46	0.42
1:A:552:LEU:CD2	1:A:587:ILE:HG22	2.48	0.42
1:A:701:ALA:H	1:B:787:GLN:HA	1.84	0.42
1:A:732:THR:HG23	1:A:734:THR:CG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:CE	1:C:317:ASN:HD22	2.31	0.42
1:A:803:SER:O	1:A:805:ILE:N	2.53	0.42
1:A:1083:HIS:CD2	1:A:1136:THR:HA	2.51	0.42
1:C:70:VAL:HG22	1:C:71:SER:H	1.85	0.42
1:C:582:LEU:HA	1:C:582:LEU:HD13	1.79	0.42
1:C:614:ASP:N	1:C:647:ALA:C	2.70	0.42
1:C:712:ILE:HB	1:C:1077:THR:CG2	2.50	0.42
1:C:874:THR:O	1:C:875:SER:C	2.62	0.42
1:B:38:TYR:OH	1:B:283:GLY:O	2.28	0.42
1:B:70:VAL:O	1:B:70:VAL:HG13	2.19	0.42
1:B:86:PHE:CE2	1:B:90:VAL:N	2.84	0.42
1:B:338:PHE:HA	1:B:341:VAL:CG2	2.50	0.42
1:B:997:ILE:O	1:B:1001:LEU:CB	2.68	0.42
1:C:130:VAL:HG13	1:C:167:THR:OG1	2.19	0.42
1:C:539:VAL:H	1:C:550:GLY:H	1.66	0.42
1:C:708:SER:C	1:C:710:ASN:N	2.77	0.42
1:C:866:THR:O	1:C:870:ILE:HG13	2.20	0.42
2:W:2:NAG:O7	2:W:2:NAG:O3	2.27	0.42
1:A:108:THR:CA	1:A:237:ARG:HB3	2.49	0.42
1:A:385:THR:HG23	1:A:386:LYS:N	2.34	0.42
1:A:877:LEU:HA	1:A:877:LEU:HD12	1.75	0.42
1:A:1060:VAL:HG23	1:A:1062:PHE:HE1	1.84	0.42
1:B:66:HIS:O	1:B:264:ALA:HB2	2.20	0.42
1:B:1076:THR:OG1	1:B:1097:SER:O	2.29	0.42
1:C:815:ARG:HA	1:C:815:ARG:NE	2.33	0.42
1:A:231:ILE:HG13	1:A:232:GLY:H	1.84	0.42
1:A:328:ARG:O	1:A:329:PHE:CG	2.73	0.42
1:A:386:LYS:HD3	1:A:386:LYS:HA	1.83	0.42
1:A:577:ARG:NH2	1:A:584:ILE:H	2.18	0.42
1:A:916:LEU:HD12	1:A:923:ILE:CD1	2.49	0.42
1:A:966:LEU:CD1	1:A:966:LEU:N	2.73	0.42
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.67	0.42
1:B:34:ARG:HA	1:B:34:ARG:HD3	1.84	0.42
1:B:88:ASP:O	1:B:270:LEU:HB2	2.20	0.42
1:B:132:GLU:OE2	1:B:165:ASN:HB3	2.20	0.42
1:B:370:ASN:HA	1:B:377:PHE:HB2	2.02	0.42
1:B:654:GLU:H	1:B:693:ILE:HD12	1.85	0.42
1:B:726:ILE:C	1:B:948:LEU:HD21	2.45	0.42
1:B:787:GLN:HB2	1:B:789:TYR:HE1	1.84	0.42
1:B:1027:THR:O	1:B:1030:SER:N	2.53	0.42
1:B:1091:ARG:HG2	1:B:1119:ASN:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD11	1:C:265:TYR:OH	2.20	0.42
1:C:280:ASN:ND2	1:C:281:GLU:H	2.17	0.42
1:A:99:ASN:HA	1:A:102:ARG:NH1	2.34	0.42
1:A:299:THR:HG23	1:A:308:VAL:HG11	2.01	0.42
1:A:541:PHE:CZ	1:A:548:GLY:HA3	2.55	0.42
1:A:650:LEU:HA	1:A:650:LEU:HD23	1.86	0.42
1:A:919:ASN:O	1:A:920:GLN:C	2.62	0.42
1:A:990:GLU:HA	1:A:993:ILE:HG12	2.02	0.42
1:A:1019:ARG:O	1:A:1022:ALA:HB3	2.20	0.42
1:A:1031:GLU:OE2	1:C:1040:VAL:HG22	2.20	0.42
1:A:1075:PHE:HB3	1:A:1096:VAL:HG23	2.01	0.42
1:B:693:ILE:HD12	1:B:693:ILE:HA	1.88	0.42
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	2.00	0.42
1:B:985:ASP:N	1:B:985:ASP:OD1	2.52	0.42
1:C:927:PHE:O	1:C:931:ILE:HG12	2.20	0.42
1:C:945:LEU:O	1:C:948:LEU:HB2	2.20	0.42
1:A:867:ASP:N	1:A:867:ASP:OD1	2.51	0.41
1:A:927:PHE:O	1:A:931:ILE:HG12	2.20	0.41
1:A:1100:THR:HG1	1:A:1101:HIS:CE1	2.33	0.41
1:B:1017:GLU:OE1	1:C:1019:ARG:NH1	2.53	0.41
1:C:70:VAL:O	1:C:77:LYS:HB3	2.20	0.41
1:C:79:PHE:CG	1:C:262:ALA:HB2	2.55	0.41
1:C:451:TYR:CB	1:C:495:TYR:HB3	2.50	0.41
1:C:746:SER:O	1:C:749:CYS:HB3	2.20	0.41
1:C:960:ASN:HD22	1:C:963:VAL:HG13	1.85	0.41
1:C:1117:THR:HG23	1:C:1138:TYR:O	2.20	0.41
1:A:117:LEU:HD11	1:A:130:VAL:HG22	2.01	0.41
1:A:216:LEU:HG	1:A:266:TYR:CE1	2.55	0.41
1:A:711:SER:OG	1:A:1076:THR:HA	2.19	0.41
1:A:738:CYS:HB2	1:A:760:CYS:HB3	1.95	0.41
1:A:754:LEU:HD23	1:A:754:LEU:HA	1.79	0.41
1:A:1030:SER:HG	1:A:1031:GLU:H	1.64	0.41
1:A:1076:THR:CG2	1:A:1097:SER:HB3	2.51	0.41
1:B:303:LEU:HA	1:B:303:LEU:HD23	1.80	0.41
1:B:906:PHE:HD2	1:B:916:LEU:HB2	1.82	0.41
1:B:977:LEU:HD22	1:B:1000:ARG:HH12	1.84	0.41
1:C:207:HIS:CD2	1:C:208:THR:N	2.88	0.41
1:C:231:ILE:HG23	1:C:232:GLY:N	2.35	0.41
1:C:336:CYS:SG	1:C:337:PRO:HD2	2.60	0.41
1:C:577:ARG:HA	1:C:584:ILE:HA	2.02	0.41
1:C:814:LYS:HB2	1:C:814:LYS:HE2	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:HB2	1:A:165:ASN:O	2.21	0.41
1:A:335:LEU:HB3	1:A:364:ASP:O	2.21	0.41
1:A:643:PHE:CE1	1:A:655:HIS:CD2	3.08	0.41
1:B:126:VAL:HG23	1:B:175:PHE:H	1.84	0.41
1:B:130:VAL:HG13	1:B:130:VAL:O	2.19	0.41
1:B:294:ASP:C	1:B:296:LEU:N	2.78	0.41
1:B:438:SER:H	1:B:507:PRO:HG3	1.84	0.41
1:B:496:GLY:C	1:B:498:GLN:H	2.29	0.41
1:B:759:PHE:CE2	1:B:763:LEU:HD11	2.55	0.41
1:B:1087:ALA:HB3	1:B:1123:SER:O	2.20	0.41
1:B:1094:VAL:HG13	1:B:1107:ARG:CD	2.51	0.41
1:C:131:CYS:O	1:C:133:PHE:N	2.53	0.41
1:C:136:CYS:C	1:C:138:ASP:H	2.29	0.41
1:C:416:GLY:O	1:C:419:ALA:N	2.54	0.41
1:C:521:PRO:HB3	1:C:564:GLN:CG	2.43	0.41
1:C:905:ARG:HA	1:C:1036:GLN:OE1	2.19	0.41
1:C:915:VAL:HG13	1:C:916:LEU:H	1.85	0.41
1:C:1039:ARG:O	1:C:1042:PHE:HB2	2.20	0.41
1:C:1062:PHE:HD2	1:C:1064:HIS:CE1	2.38	0.41
1:C:1103:PHE:HB3	1:C:1113:GLN:H	1.85	0.41
1:A:137:ASN:C	1:A:139:PRO:HD3	2.46	0.41
1:A:145:TYR:H	1:A:150:LYS:CG	2.32	0.41
1:A:894:LEU:HD22	1:C:713:ALA:HB1	2.02	0.41
1:B:34:ARG:HH11	1:B:34:ARG:HG3	1.85	0.41
1:B:622:VAL:O	1:B:622:VAL:HG13	2.20	0.41
1:B:707:TYR:CD2	1:B:707:TYR:C	2.96	0.41
1:B:753:LEU:O	1:B:753:LEU:HD23	2.20	0.41
1:B:973:ILE:HG22	1:B:980:ILE:CD1	2.51	0.41
1:C:122:ASN:OD1	1:C:127:VAL:HG23	2.18	0.41
1:C:323:THR:OG1	1:C:324:GLU:N	2.52	0.41
1:C:371:SER:C	1:C:373:SER:H	2.29	0.41
1:C:383:SER:OG	1:C:385:THR:OG1	2.13	0.41
1:C:569:ILE:O	1:C:572:THR:HG23	2.19	0.41
1:C:646:ARG:HA	1:C:646:ARG:HD2	1.83	0.41
1:C:740:MET:C	1:C:743:CYS:H	2.29	0.41
1:A:429:PHE:CB	1:A:515:PHE:H	2.25	0.41
1:A:879:ALA:HA	1:A:882:ILE:HD11	2.03	0.41
1:A:1102:TRP:HD1	1:A:1135:ASN:HD22	1.67	0.41
1:A:1107:ARG:NH1	1:B:904:TYR:CD2	2.89	0.41
1:B:312:ILE:C	1:B:313:TYR:CD1	2.99	0.41
1:B:378:LYS:HA	1:B:378:LYS:HD3	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1073:LYS:HE2	1:B:1073:LYS:HB3	1.89	0.41
1:C:241:LEU:HD12	1:C:242:LEU:H	1.84	0.41
1:C:554:GLU:OE2	1:C:556:ASN:HB3	2.21	0.41
1:C:1028:LYS:O	1:C:1032:CYS:CB	2.66	0.41
1:A:557:LYS:HD3	1:B:43:PHE:CE1	2.55	0.41
1:A:719:THR:O	1:A:721:SER:OG	2.31	0.41
1:A:1062:PHE:CD1	1:A:1062:PHE:N	2.88	0.41
1:A:1086:LYS:HE2	1:A:1088:HIS:HE1	1.69	0.41
7:A:1201:NAG:O7	7:A:1201:NAG:O3	2.33	0.41
1:B:144:TYR:C	1:B:146:HIS:H	2.29	0.41
1:B:308:VAL:HG13	1:B:308:VAL:O	2.20	0.41
1:B:610:VAL:HG22	1:B:611:LEU:N	2.36	0.41
1:B:726:ILE:HG22	1:B:1061:VAL:HG13	2.03	0.41
1:B:816:SER:O	1:B:819:GLU:HB3	2.20	0.41
1:B:1007:TYR:CZ	1:B:1011:GLN:HB2	2.55	0.41
1:C:107:GLY:CA	1:C:235:ILE:HG23	2.51	0.41
1:C:338:PHE:HE2	1:C:363:ALA:HA	1.85	0.41
1:C:1043:CYS:HB2	1:C:1048:HIS:CD2	2.55	0.41
1:A:133:PHE:CE1	1:A:161:SER:HA	2.56	0.41
1:A:286:THR:OG1	1:A:287:ASP:N	2.54	0.41
1:A:312:ILE:HG13	1:A:597:VAL:O	2.21	0.41
1:A:328:ARG:HB3	1:A:328:ARG:CZ	2.51	0.41
1:A:1056:ALA:HB3	1:A:1059:GLY:O	2.20	0.41
1:B:89:GLY:HA3	1:B:270:LEU:HD12	2.01	0.41
1:B:174:PRO:O	1:B:178:ASP:N	2.26	0.41
1:B:616:ASN:HB2	7:B:1203:NAG:C2	2.50	0.41
1:B:698:SER:O	1:B:700:GLY:N	2.54	0.41
1:B:727:LEU:HA	1:B:727:LEU:HD23	1.80	0.41
1:B:806:LEU:HD13	1:B:806:LEU:HA	1.85	0.41
1:B:816:SER:O	1:B:819:GLU:N	2.53	0.41
1:B:1079:PRO:HD2	1:B:1131:GLY:O	2.20	0.41
1:C:62:VAL:HG23	1:C:267:VAL:C	2.45	0.41
1:C:377:PHE:CD1	1:C:434:ILE:HD12	2.55	0.41
1:C:561:PRO:HD2	1:C:562:PHE:CD2	2.56	0.41
1:C:776:LYS:HD2	1:C:780:GLU:OE1	2.21	0.41
1:C:934:ILE:HA	1:C:934:ILE:HD12	1.84	0.41
1:A:33:THR:HG21	1:A:218:GLN:HA	2.03	0.41
1:A:1086:LYS:HE2	1:A:1088:HIS:NE2	2.30	0.41
1:B:102:ARG:O	1:B:120:VAL:HG22	2.21	0.41
1:B:115:GLN:CB	1:B:130:VAL:HG22	2.51	0.41
1:B:628:GLN:O	1:B:629:LEU:HD12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LEU:HD13	1:C:561:PRO:HD3	2.01	0.41
1:C:697:MET:HE3	1:C:697:MET:HB2	1.89	0.41
1:C:797:PHE:O	1:C:799:GLY:N	2.53	0.41
1:C:905:ARG:O	1:C:909:ILE:HG12	2.20	0.41
1:A:54:LEU:HB2	1:A:195:LYS:NZ	2.32	0.41
1:A:327:VAL:CG2	1:A:329:PHE:CE1	3.02	0.41
1:A:509:ARG:H	1:A:509:ARG:HG2	1.73	0.41
1:A:778:THR:O	1:A:781:VAL:HB	2.20	0.41
1:A:808:ASP:O	1:A:811:LYS:N	2.46	0.41
1:A:909:ILE:HA	1:A:1038:LYS:NZ	2.35	0.41
1:A:980:ILE:HB	1:A:984:LEU:HD13	2.03	0.41
1:A:1116:THR:HA	1:A:1138:TYR:O	2.21	0.41
1:B:276:LEU:HD22	1:B:301:CYS:HA	2.03	0.41
1:B:736:VAL:HG12	1:B:737:ASP:H	1.86	0.41
1:B:861:LEU:HD23	1:B:862:PRO:O	2.21	0.41
1:B:1018:ILE:HD12	1:B:1018:ILE:HA	1.85	0.41
1:B:1062:PHE:O	1:B:1063:LEU:HD23	2.20	0.41
1:B:1100:THR:HG21	7:B:1206:NAG:HN2	1.85	0.41
1:C:62:VAL:HG23	1:C:267:VAL:O	2.21	0.41
1:C:307:THR:HB	1:C:602:THR:HB	2.03	0.41
1:C:359:SER:HA	1:C:524:VAL:CG2	2.51	0.41
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.86	0.41
1:C:453:TYR:CE2	1:C:454:ARG:HD2	2.56	0.41
1:C:803:SER:OG	4:p:1:NAG:C5	2.69	0.41
1:C:887:THR:HB	1:C:894:LEU:HG	2.03	0.41
1:C:922:LEU:O	1:C:923:ILE:C	2.64	0.41
1:C:923:ILE:O	1:C:924:ALA:C	2.64	0.41
1:C:978:ASN:HA	1:C:981:LEU:HG	2.03	0.41
1:C:1047:TYR:N	1:C:1047:TYR:CD1	2.86	0.41
1:C:1062:PHE:CD2	1:C:1064:HIS:CE1	3.09	0.41
1:A:86:PHE:H	1:A:86:PHE:HD1	1.69	0.41
1:A:185:ASN:ND2	1:A:209:PRO:HB2	2.36	0.41
1:A:196:ASN:HB3	1:A:201:PHE:HE1	1.85	0.41
1:A:304:LYS:N	1:A:304:LYS:CD	2.83	0.41
1:A:433:VAL:O	1:A:433:VAL:HG13	2.21	0.41
1:A:607:GLN:NE2	1:A:690:GLN:O	2.54	0.41
1:B:203:ILE:O	1:B:225:PRO:HA	2.21	0.41
1:B:611:LEU:HD13	1:B:650:LEU:CD2	2.51	0.41
1:B:880:GLY:HA2	1:B:883:THR:HG22	2.03	0.41
1:B:1075:PHE:O	1:B:1077:THR:HG23	2.21	0.41
1:C:55:PHE:HA	1:C:270:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:LEU:O	1:C:962:LEU:HB3	2.21	0.41
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.86	0.40
1:A:92:PHE:HE2	1:A:104:TRP:HZ2	1.69	0.40
1:A:395:VAL:HG22	1:A:515:PHE:CE1	2.56	0.40
1:A:567:ARG:HE	1:A:573:THR:HG22	1.86	0.40
1:A:804:GLN:O	1:A:818:ILE:HG12	2.21	0.40
1:A:886:TRP:N	1:A:886:TRP:CE3	2.89	0.40
1:A:886:TRP:CZ3	1:A:887:THR:HG23	2.56	0.40
1:B:190:ARG:HD2	1:B:192:PHE:HZ	1.86	0.40
1:B:906:PHE:CE2	1:B:916:LEU:HD13	2.56	0.40
1:C:302:THR:O	1:C:303:LEU:HD23	2.22	0.40
1:C:708:SER:OG	1:C:710:ASN:OD1	2.18	0.40
1:C:948:LEU:O	1:C:951:VAL:HG22	2.21	0.40
1:A:54:LEU:HD23	1:A:88:ASP:C	2.46	0.40
1:A:193:VAL:HG22	1:A:194:PHE:N	2.34	0.40
1:B:43:PHE:CD1	1:B:43:PHE:C	2.99	0.40
1:B:65:PHE:HD2	1:B:263:ALA:O	2.04	0.40
1:B:731:MET:CE	1:B:1011:GLN:HE22	2.35	0.40
1:B:733:LYS:HZ3	1:B:864:LEU:H	1.69	0.40
1:B:826:VAL:HG12	1:B:828:LEU:N	2.29	0.40
1:B:1027:THR:O	1:B:1030:SER:OG	2.17	0.40
1:C:246:ARG:HD2	1:C:249:LEU:CD1	2.44	0.40
1:C:1040:VAL:C	1:C:1042:PHE:H	2.29	0.40
1:C:1125:ASN:OD1	1:C:1125:ASN:N	2.54	0.40
1:A:247:SER:N	1:A:253:ASP:HB2	2.36	0.40
1:A:518:LEU:HD22	1:A:521:PRO:HA	2.02	0.40
1:A:555:SER:OG	1:A:584:ILE:HG23	2.20	0.40
1:A:712:ILE:HG22	1:B:896:ILE:HA	2.02	0.40
1:A:767:LEU:HD12	1:A:767:LEU:HA	1.84	0.40
1:A:885:GLY:O	1:A:887:THR:N	2.54	0.40
1:A:886:TRP:N	1:A:886:TRP:HE3	2.20	0.40
1:A:935:GLN:NE2	1:A:939:SER:OG	2.54	0.40
1:A:1004:LEU:HD13	1:A:1004:LEU:HA	1.94	0.40
1:A:1014:ARG:HA	1:A:1017:GLU:OE2	2.22	0.40
1:A:1116:THR:O	1:A:1120:THR:HG22	2.21	0.40
1:B:64:TRP:HB2	1:B:266:TYR:CZ	2.56	0.40
1:B:1039:ARG:H	1:B:1039:ARG:HG2	1.67	0.40
1:B:1091:ARG:HG2	1:B:1119:ASN:C	2.46	0.40
1:C:38:TYR:CD1	1:C:285:ILE:HD12	2.57	0.40
1:C:900:MET:HG2	1:C:917:TYR:OH	2.21	0.40
1:A:40:ASP:C	1:A:42:VAL:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:CE1	1:A:253:ASP:OD2	2.75	0.40
1:A:299:THR:OG1	1:A:303:LEU:HD12	2.21	0.40
1:A:766:ALA:O	1:A:770:ILE:HG22	2.22	0.40
1:A:938:LEU:HD22	1:A:945:LEU:HD21	2.02	0.40
1:A:1091:ARG:NH2	1:A:1120:THR:O	2.55	0.40
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.90	0.40
1:B:271:GLN:O	1:B:273:ARG:N	2.54	0.40
1:B:726:ILE:HG13	1:B:726:ILE:O	2.21	0.40
1:B:908:GLY:C	1:B:909:ILE:HD13	2.47	0.40
1:B:1065:VAL:HG23	1:B:1065:VAL:O	2.21	0.40
1:B:1114:ILE:HA	1:B:1114:ILE:HD12	1.79	0.40
1:C:1061:VAL:O	1:C:1062:PHE:HD1	2.04	0.40
1:C:1118:ASP:O	1:C:1120:THR:N	2.55	0.40
1:A:77:LYS:O	1:A:77:LYS:HG3	2.22	0.40
1:A:363:ALA:HB1	1:A:392:PHE:CD2	2.56	0.40
1:A:611:LEU:HD12	1:A:612:TYR:N	2.36	0.40
1:A:669:GLY:C	1:A:670:ILE:HD12	2.47	0.40
1:B:92:PHE:CD2	1:B:240:THR:HG21	2.56	0.40
1:B:130:VAL:O	1:B:130:VAL:HG22	2.21	0.40
1:B:380:TYR:OH	1:B:411:ALA:HB1	2.21	0.40
1:B:697:MET:HE2	1:B:697:MET:HB3	1.98	0.40
1:B:727:LEU:HD12	1:B:1062:PHE:HE2	1.86	0.40
1:B:825:LYS:HB3	1:B:945:LEU:CD1	2.51	0.40
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.80	0.40
1:B:1081:ILE:CG2	1:B:1088:HIS:HB2	2.52	0.40
1:C:863:PRO:O	1:C:864:LEU:C	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	995/1127 (88%)	780 (78%)	205 (21%)	10 (1%)	12	47
1	B	988/1127 (88%)	770 (78%)	206 (21%)	12 (1%)	10	43
1	C	1023/1127 (91%)	780 (76%)	231 (23%)	12 (1%)	10	43
All	All	3006/3381 (89%)	2330 (78%)	642 (21%)	34 (1%)	14	45

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PHE
1	B	538	CYS
1	C	145	TYR
1	C	330	PRO
1	C	498	GLN
1	C	518	LEU
1	A	70	VAL
1	A	150	LYS
1	B	88	ASP
1	B	622	VAL
1	C	250	THR
1	C	252	GLY
1	C	454	ARG
1	A	617	CYS
1	B	78	ARG
1	B	85	PRO
1	A	69	HIS
1	A	151	SER
1	B	153	MET
1	B	295	PRO
1	A	186	PHE
1	A	1030	SER
1	B	74	ASN
1	B	605	SER
1	B	783	ALA
1	B	823	PHE
1	C	749	CYS
1	C	812	PRO
1	C	247	SER
1	A	798	GLY
1	A	1079	PRO
1	C	798	GLY
1	B	491	PRO
1	C	272	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	838/976 (86%)	819 (98%)	19 (2%)	44	64
1	B	827/976 (85%)	809 (98%)	18 (2%)	45	64
1	C	850/976 (87%)	827 (97%)	23 (3%)	39	60
All	All	2515/2928 (86%)	2455 (98%)	60 (2%)	43	63

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	150	LYS
1	A	153	MET
1	A	186	PHE
1	A	245	HIS
1	A	302	THR
1	A	317	ASN
1	A	331	ASN
1	A	391	CYS
1	A	538	CYS
1	A	568	ASP
1	A	576	VAL
1	A	662	CYS
1	A	723	THR
1	A	732	THR
1	A	770	ILE
1	A	1047	TYR
1	A	1058	HIS
1	A	1118	ASP
1	B	32	PHE
1	B	131	CYS
1	B	138	ASP
1	B	144	TYR
1	B	312	ILE
1	B	315	THR
1	B	336	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	497	PHE
1	B	508	TYR
1	B	622	VAL
1	B	763	LEU
1	B	785	VAL
1	B	811	LYS
1	B	813	SER
1	B	814	LYS
1	B	883	THR
1	B	1027	THR
1	B	1040	VAL
1	C	122	ASN
1	C	145	TYR
1	C	253	ASP
1	C	293	LEU
1	C	331	ASN
1	C	334	ASN
1	C	341	VAL
1	C	455	LEU
1	C	457	ARG
1	C	459	SER
1	C	515	PHE
1	C	544	ASN
1	C	547	THR
1	C	581	THR
1	C	699	LEU
1	C	712	ILE
1	C	763	LEU
1	C	770	ILE
1	C	976	VAL
1	C	1040	VAL
1	C	1042	PHE
1	C	1101	HIS
1	C	1120	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	87	ASN
1	A	99	ASN
1	A	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	134	GLN
1	A	146	HIS
1	A	148	ASN
1	A	207	HIS
1	A	317	ASN
1	A	613	GLN
1	A	644	GLN
1	A	655	HIS
1	A	755	GLN
1	A	777	ASN
1	A	784	GLN
1	A	787	GLN
1	A	901	GLN
1	A	920	GLN
1	A	928	ASN
1	A	935	GLN
1	A	955	ASN
1	A	969	ASN
1	A	1010	GLN
1	A	1023	ASN
1	A	1048	HIS
1	A	1054	GLN
1	A	1088	HIS
1	A	1108	ASN
1	B	49	HIS
1	B	87	ASN
1	B	121	ASN
1	B	185	ASN
1	B	343	ASN
1	B	388	ASN
1	B	542	ASN
1	B	564	GLN
1	B	607	GLN
1	B	655	HIS
1	B	764	ASN
1	B	784	GLN
1	B	953	ASN
1	B	954	GLN
1	B	992	GLN
1	B	1048	HIS
1	B	1058	HIS
1	B	1071	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1083	HIS
1	B	1101	HIS
1	B	1113	GLN
1	C	49	HIS
1	C	66	HIS
1	C	87	ASN
1	C	146	HIS
1	C	188	ASN
1	C	207	HIS
1	C	245	HIS
1	C	280	ASN
1	C	460	ASN
1	C	506	GLN
1	C	580	GLN
1	C	804	GLN
1	C	965	GLN
1	C	978	ASN
1	C	992	GLN
1	C	1048	HIS
1	C	1108	ASN
1	C	1135	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

33 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
2	NAG	E	1	2,1	14,14,15	0.41	0	17,19,21	0.51	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	1.32	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.47	0	17,19,21	0.55	0
2	NAG	H	2	2	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	N	1	2,1	14,14,15	0.65	1 (7%)	17,19,21	1.11	1 (5%)
2	NAG	N	2	2	14,14,15	0.43	0	17,19,21	0.38	0
6	NAG	Q	1	6,1	14,14,15	1.67	1 (7%)	17,19,21	1.61	3 (17%)
6	NAG	Q	2	6	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
6	BMA	Q	3	6	11,11,12	0.82	0	15,15,17	0.90	1 (6%)
6	MAN	Q	4	6	11,11,12	0.94	0	15,15,17	1.61	2 (13%)
4	NAG	V	1	1,4	14,14,15	0.26	0	17,19,21	0.61	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.63	0
4	BMA	V	3	4	11,11,12	0.24	0	15,15,17	0.74	0
2	NAG	W	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.75	0
2	NAG	W	2	2	14,14,15	0.87	1 (7%)	17,19,21	0.74	0
2	NAG	X	1	2,1	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	X	2	2	14,14,15	0.31	0	17,19,21	0.56	0
2	NAG	Z	1	2,1	14,14,15	0.58	1 (7%)	17,19,21	0.47	0
2	NAG	Z	2	2	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	d	1	2,1	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	d	2	2	14,14,15	0.15	0	17,19,21	0.87	1 (5%)
2	NAG	f	1	2,1	14,14,15	0.70	0	17,19,21	0.50	0
2	NAG	f	2	2	14,14,15	0.33	0	17,19,21	0.52	0
5	NAG	h	1	5,1	14,14,15	0.36	0	17,19,21	0.74	0
5	NAG	h	2	5	14,14,15	0.26	0	17,19,21	0.85	1 (5%)
5	BMA	h	3	5	11,11,12	0.72	0	15,15,17	0.81	0
5	MAN	h	4	5	11,11,12	0.78	1 (9%)	15,15,17	1.28	2 (13%)
3	NAG	k	1	3,1	14,14,15	0.31	0	17,19,21	0.56	0
3	NAG	k	2	3	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
3	FUC	k	3	3	10,10,11	0.87	0	14,14,16	1.74	2 (14%)
4	NAG	p	1	1,4	14,14,15	0.36	0	17,19,21	0.75	0
4	NAG	p	2	4	14,14,15	0.33	0	17,19,21	0.62	0
4	BMA	p	3	4	11,11,12	0.26	0	15,15,17	0.58	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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
2	NAG	W	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	X	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	4/6/23/26	0/1/1/1
5	NAG	h	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	1/6/23/26	0/1/1/1
5	BMA	h	3	5	-	0/2/19/22	0/1/1/1
5	MAN	h	4	5	-	1/2/19/22	0/1/1/1
3	NAG	k	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	k	2	3	-	4/6/23/26	0/1/1/1
3	FUC	k	3	3	-	-	0/1/1/1
4	NAG	p	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	p	2	4	-	5/6/23/26	0/1/1/1
4	BMA	p	3	4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	1	NAG	O5-C1	-6.16	1.33	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	1	NAG	O5-C1	-2.60	1.39	1.43
2	W	2	NAG	C1-C2	2.35	1.55	1.52
5	h	4	MAN	C1-C2	2.21	1.57	1.52
2	Z	1	NAG	O5-C1	-2.07	1.40	1.43
2	N	1	NAG	C1-C2	2.05	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	4	MAN	C1-O5-C5	4.73	118.53	112.19
6	Q	1	NAG	C2-N2-C7	4.57	129.03	122.90
2	E	2	NAG	C2-N2-C7	4.46	128.87	122.90
3	k	3	FUC	O5-C5-C4	3.85	116.48	109.55
3	k	3	FUC	C1-O5-C5	3.77	121.87	112.97
3	k	2	NAG	C1-O5-C5	3.15	116.41	112.19
2	N	1	NAG	C1-O5-C5	3.08	116.31	112.19
2	d	2	NAG	C1-O5-C5	2.80	115.93	112.19
5	h	4	MAN	C1-O5-C5	2.79	115.93	112.19
5	h	4	MAN	O2-C2-C3	-2.57	104.83	110.15
6	Q	1	NAG	C1-O5-C5	-2.45	108.90	112.19
6	Q	2	NAG	C1-O5-C5	2.37	115.36	112.19
5	h	2	NAG	C1-O5-C5	2.35	115.34	112.19
6	Q	4	MAN	C1-C2-C3	-2.33	106.25	109.64
6	Q	1	NAG	O4-C4-C5	-2.21	103.88	109.32
6	Q	3	BMA	C3-C4-C5	-2.15	106.33	110.23
2	E	2	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	1	NAG	C3-C2-N2-C7
2	X	1	NAG	O7-C7-N2-C2
4	p	1	NAG	C1-C2-N2-C7
4	p	2	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
2	X	1	NAG	C8-C7-N2-C2
4	p	1	NAG	C8-C7-N2-C2
4	p	1	NAG	O7-C7-N2-C2
2	d	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
4	p	3	BMA	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
4	p	3	BMA	C4-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	X	2	NAG	C8-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
3	k	1	NAG	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O7-C7-N2-C2
2	N	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
5	h	4	MAN	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	X	2	NAG	C3-C2-N2-C7
3	k	2	NAG	C4-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	C1-C2-N2-C7
4	p	2	NAG	C4-C5-C6-O6
4	p	2	NAG	C8-C7-N2-C2
4	p	2	NAG	O5-C5-C6-O6
2	W	1	NAG	C3-C2-N2-C7
2	W	2	NAG	C3-C2-N2-C7
2	d	1	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7
6	Q	1	NAG	C3-C2-N2-C7
6	Q	2	NAG	C3-C2-N2-C7
4	p	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C1-C2-N2-C7
2	W	1	NAG	C1-C2-N2-C7
2	W	2	NAG	C1-C2-N2-C7
3	k	2	NAG	C1-C2-N2-C7
6	Q	1	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
3	k	1	NAG	C3-C2-N2-C7

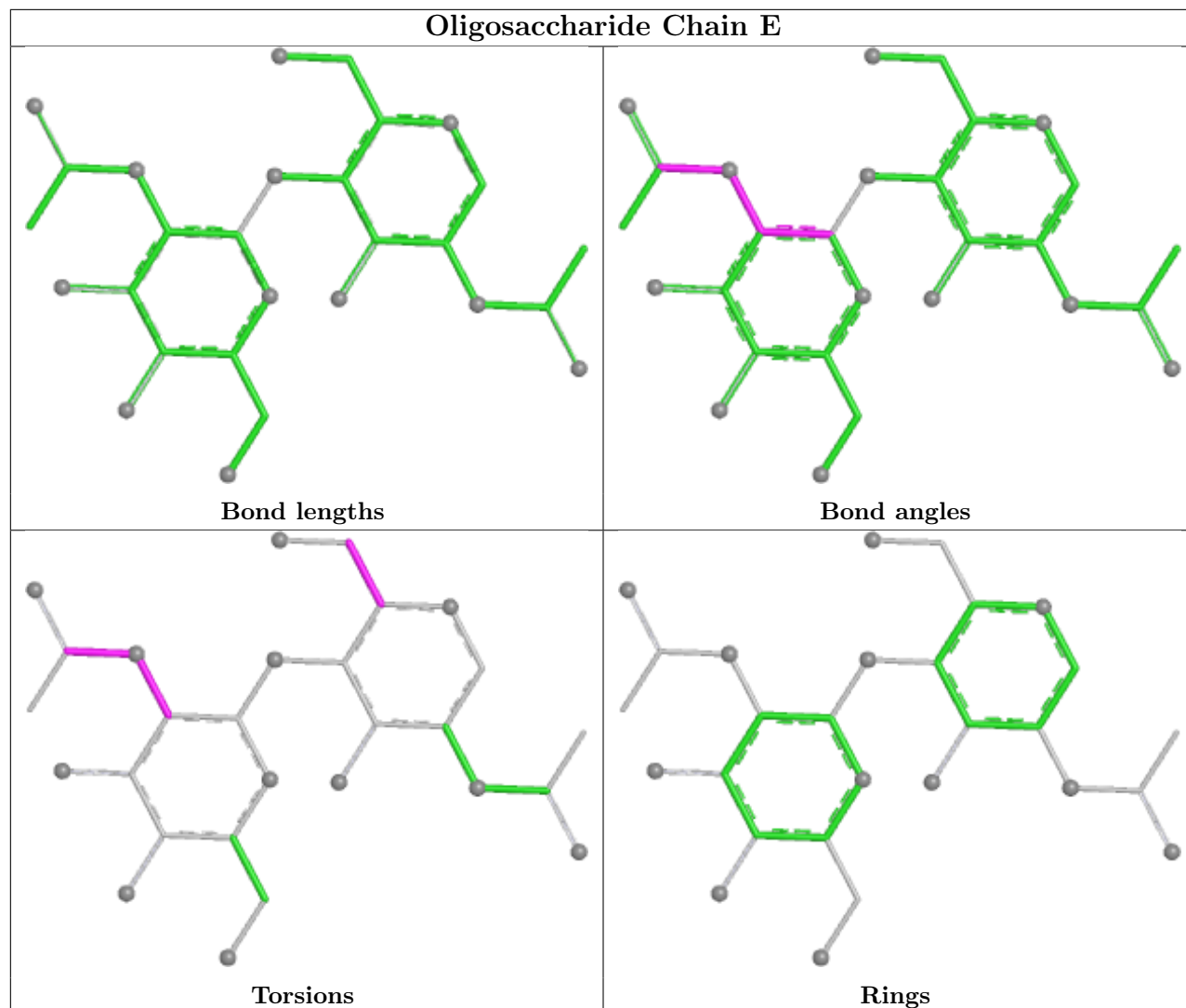
There are no ring outliers.

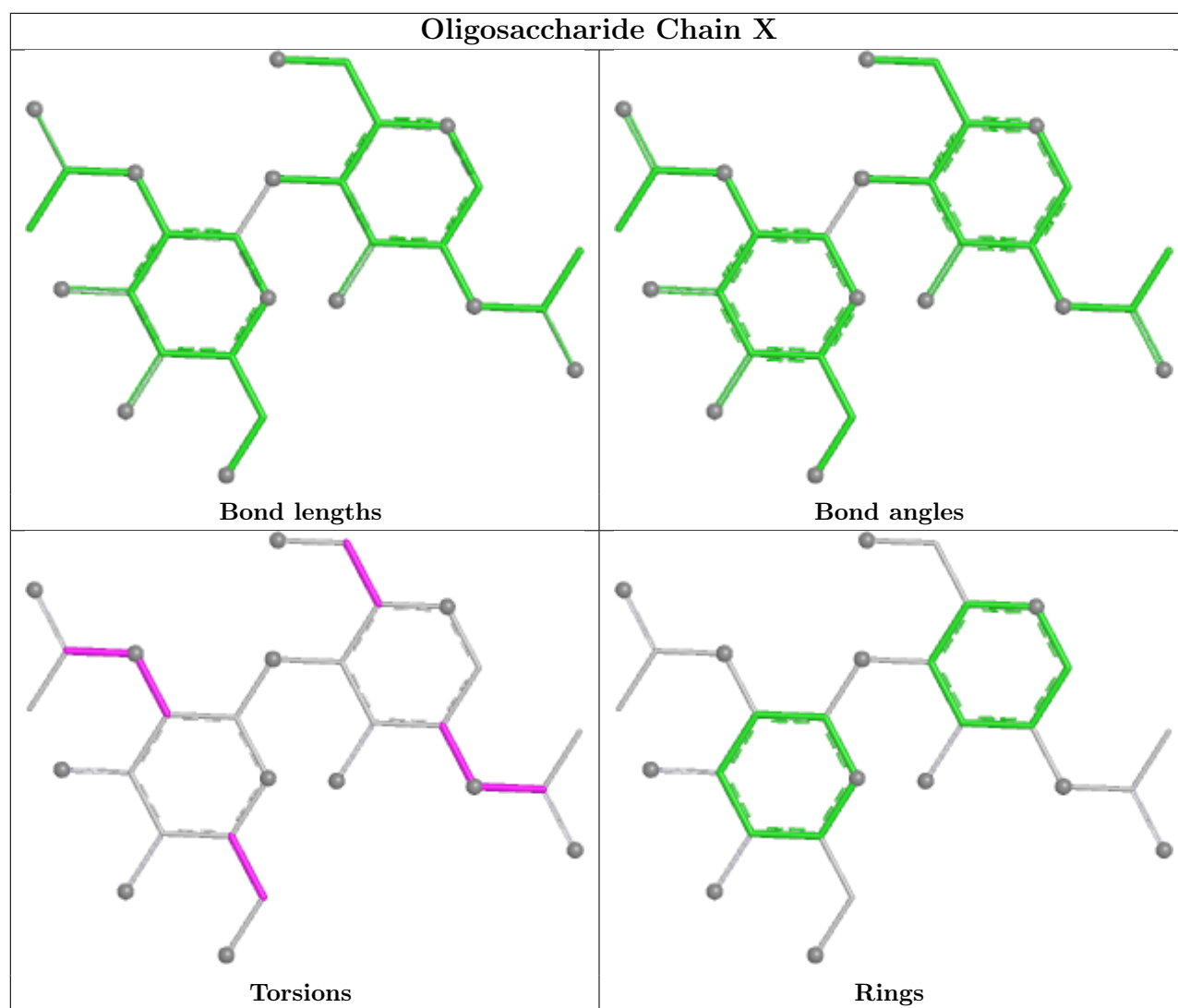
13 monomers are involved in 26 short contacts:

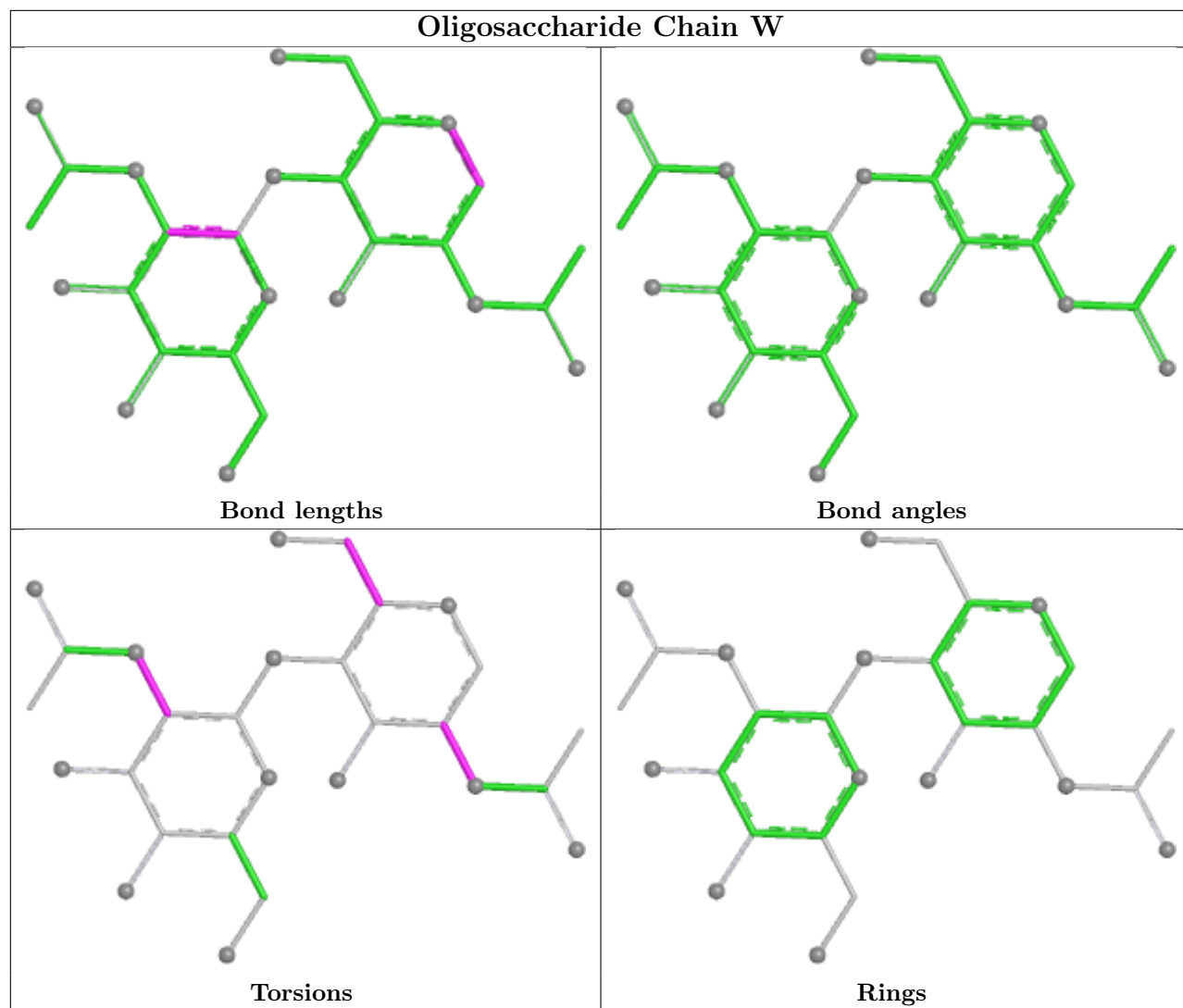
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
4	p	1	NAG	3	0
6	Q	1	NAG	2	0
2	d	2	NAG	1	0
5	h	1	NAG	3	0
2	X	2	NAG	1	0
4	p	2	NAG	1	0
4	V	1	NAG	5	0
5	h	2	NAG	2	0
2	d	1	NAG	2	0
2	X	1	NAG	5	0
2	W	2	NAG	1	0
6	Q	3	BMA	1	0

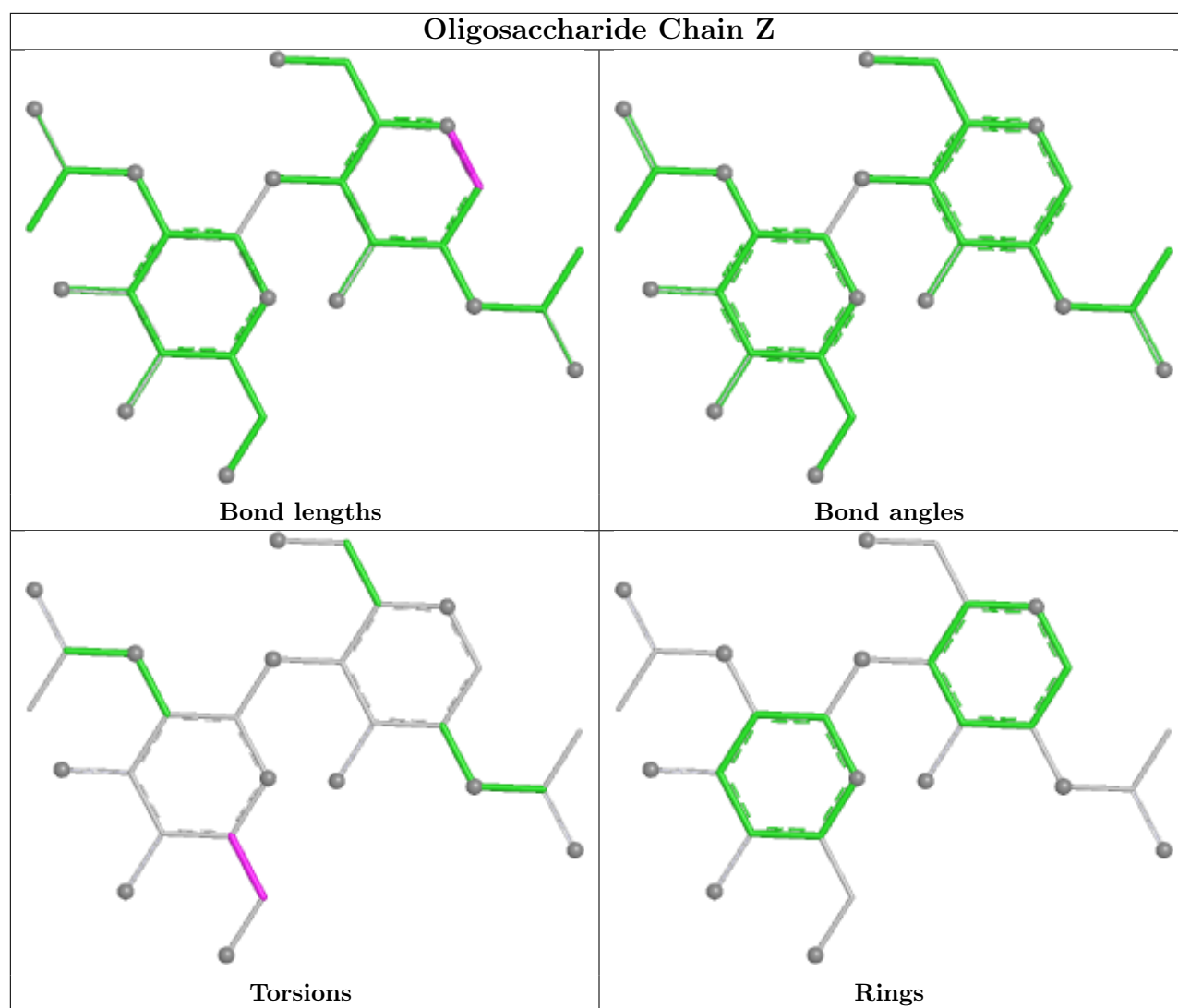
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

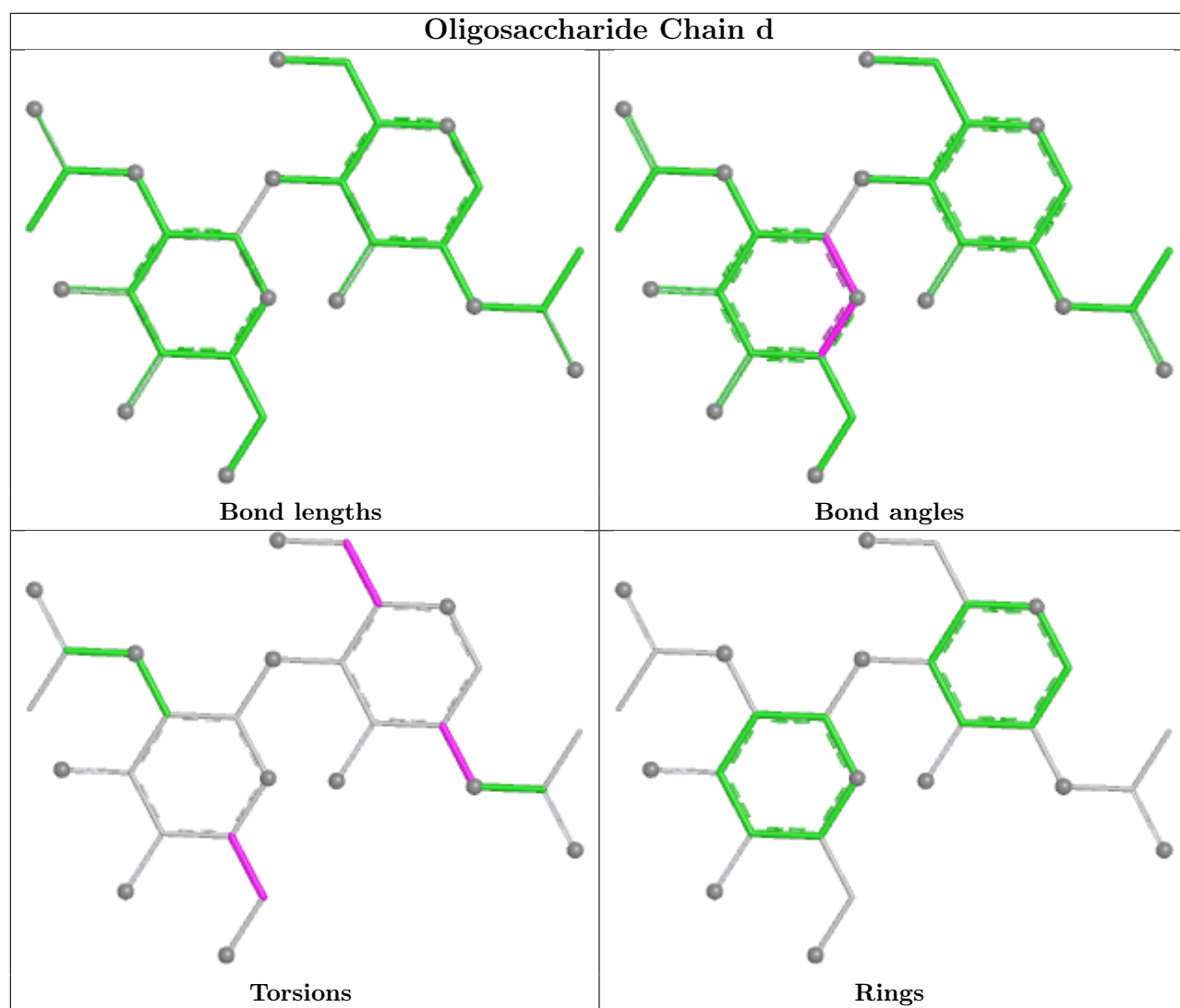
bond angles, torsion angles, and ring geometry for oligosaccharide.

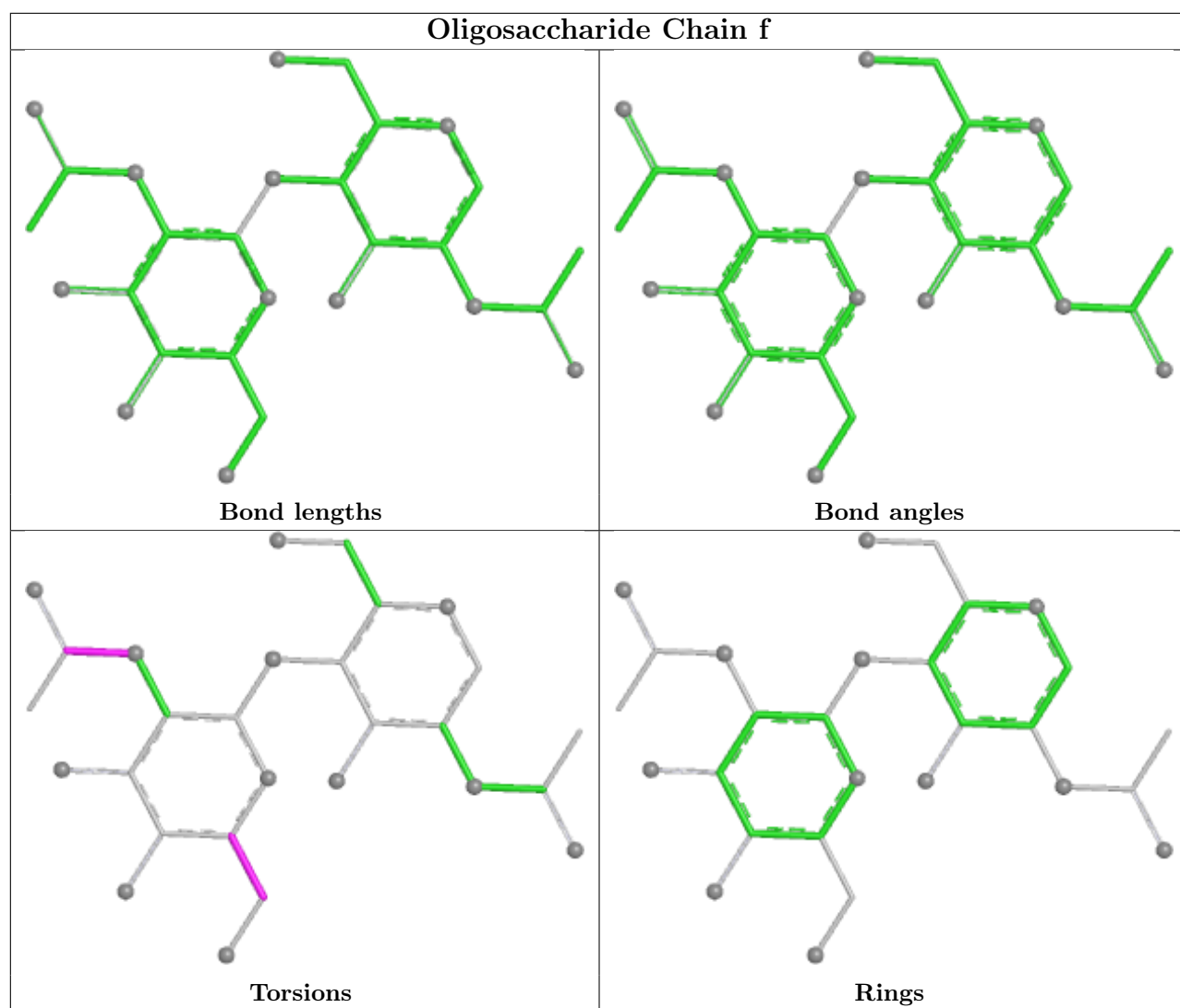


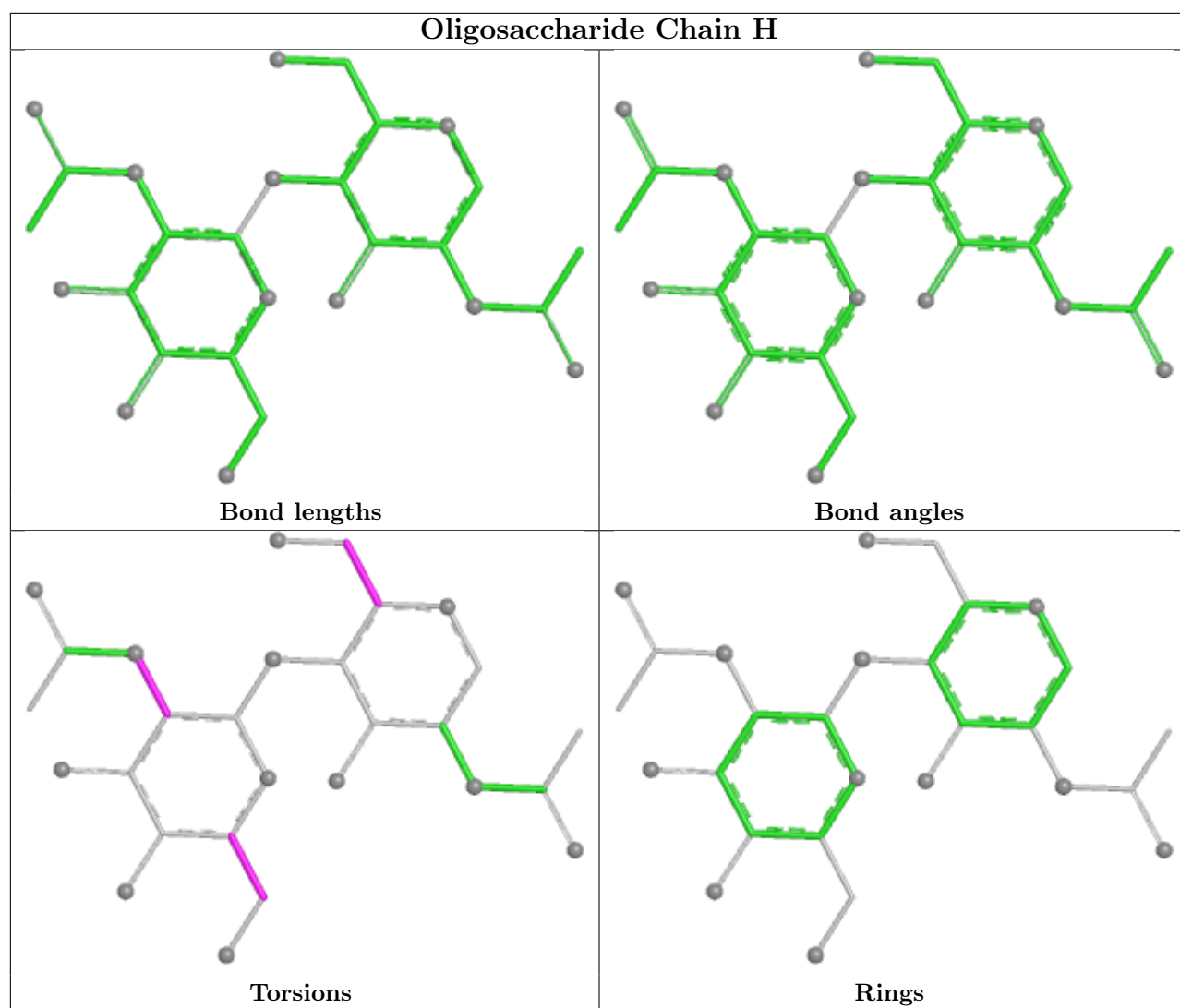


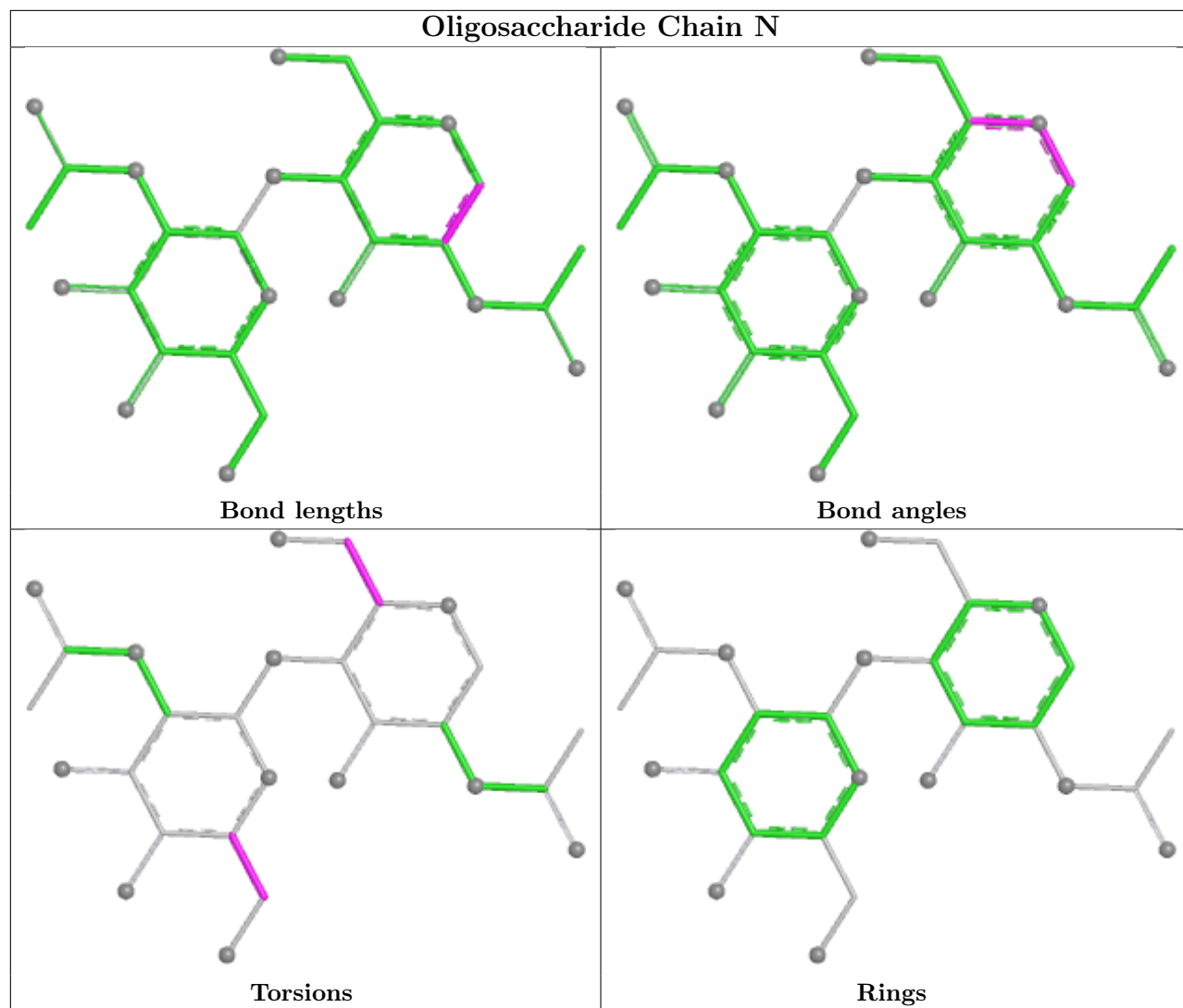


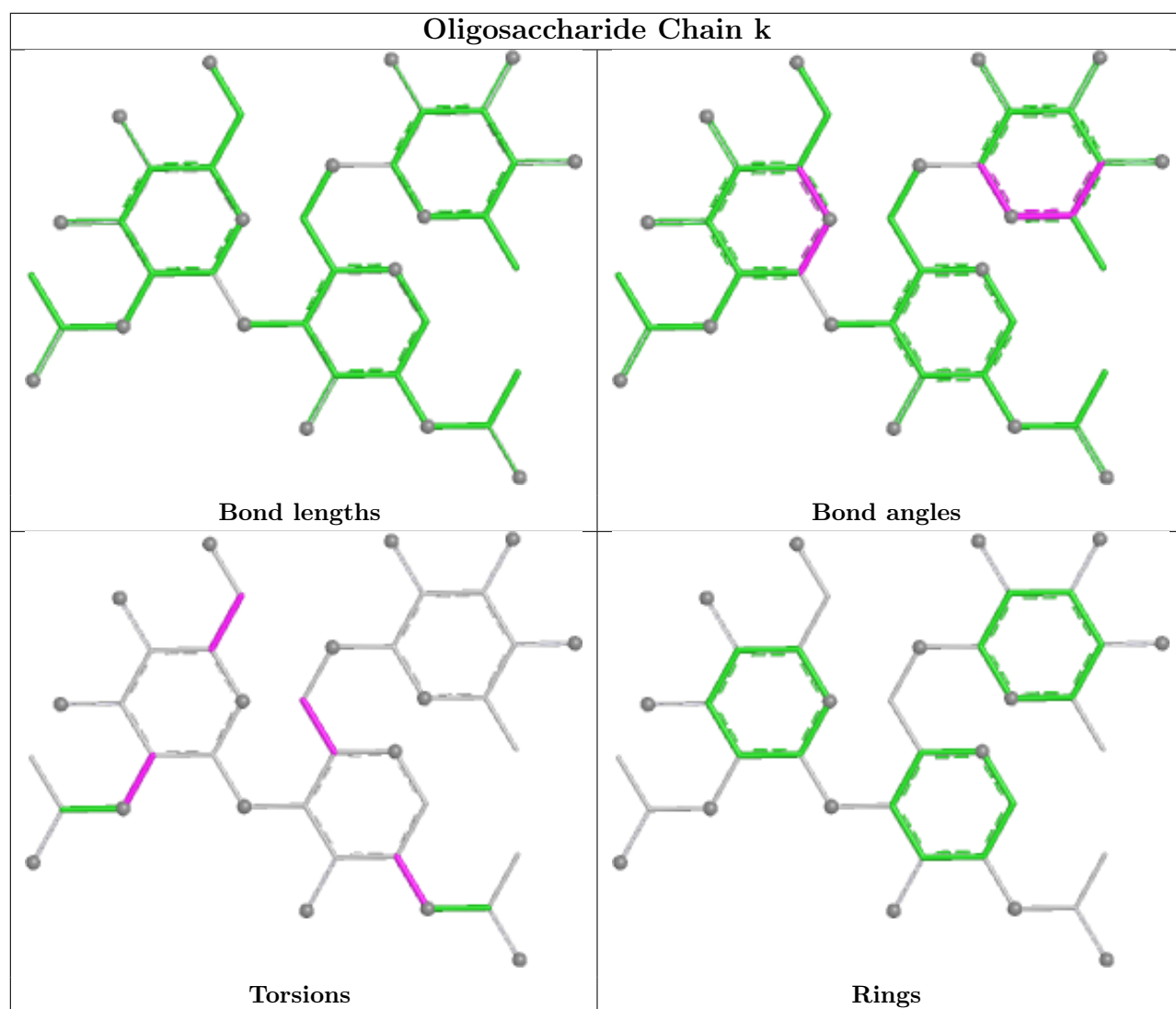


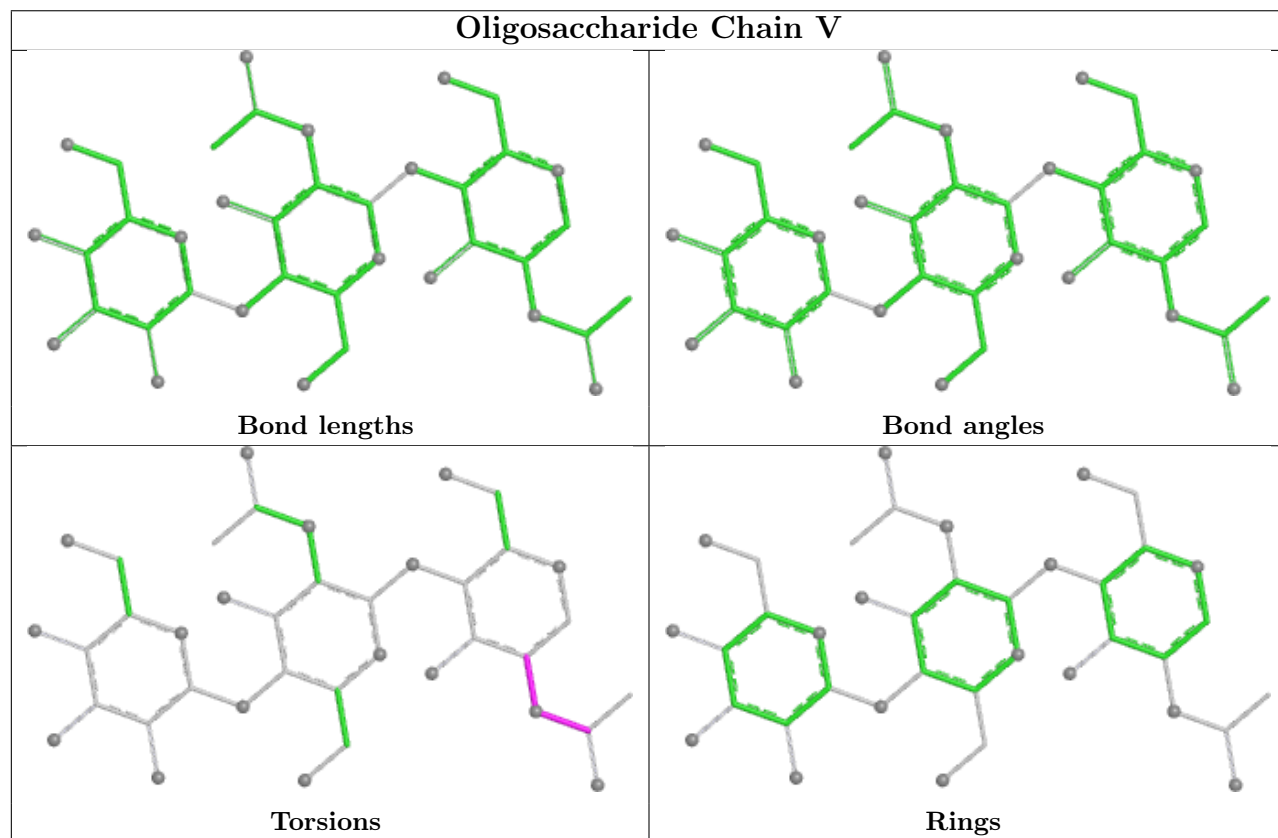
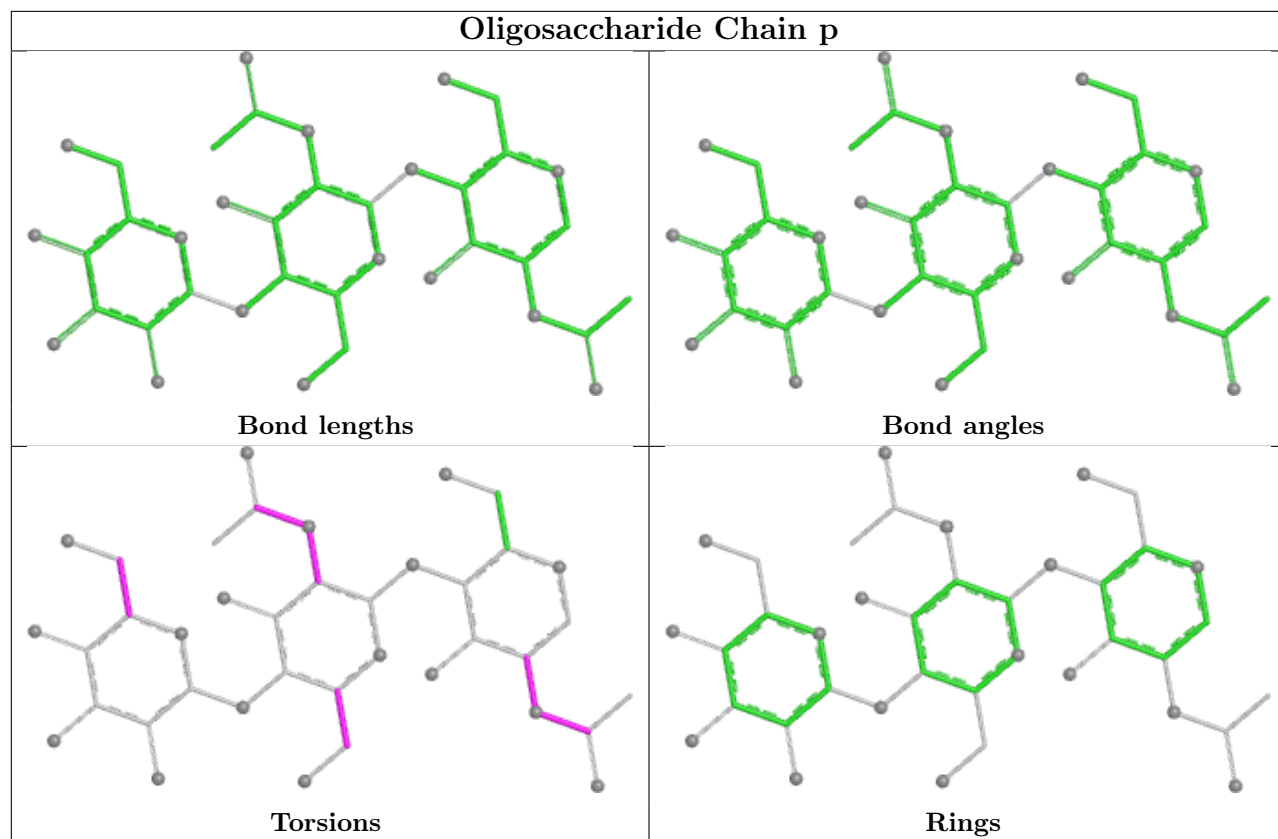


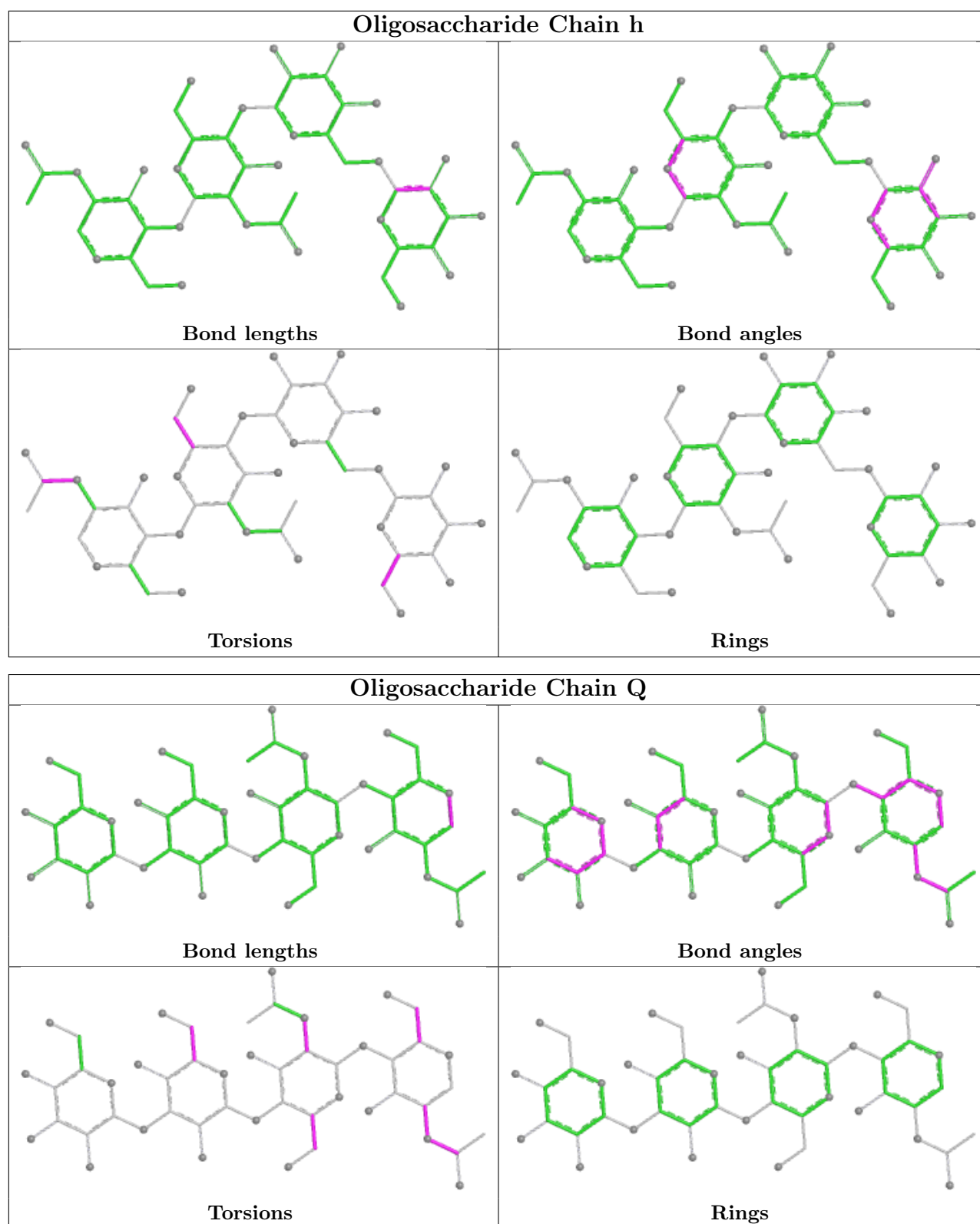












5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	1206	1	14,14,15	0.52	0	17,19,21	1.24	2 (11%)
7	NAG	B	1207	1	14,14,15	0.30	0	17,19,21	0.40	0
7	NAG	B	1206	1	14,14,15	0.20	0	17,19,21	0.71	1 (5%)
7	NAG	B	1201	1	14,14,15	0.28	0	17,19,21	0.64	0
7	NAG	B	1209	1	14,14,15	0.28	0	17,19,21	0.64	0
7	NAG	C	1204	-	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
7	NAG	A	1207	1	14,14,15	0.99	1 (7%)	17,19,21	1.47	2 (11%)
7	NAG	C	1201	1	14,14,15	0.22	0	17,19,21	0.57	0
7	NAG	C	1203	1	14,14,15	0.40	0	17,19,21	0.48	0
7	NAG	C	1205	1	14,14,15	0.29	0	17,19,21	0.52	0
7	NAG	B	1204	1	14,14,15	0.47	0	17,19,21	1.30	1 (5%)
7	NAG	A	1204	1	14,14,15	0.24	0	17,19,21	0.67	0
7	NAG	A	1206	1	14,14,15	0.26	0	17,19,21	0.48	0
7	NAG	B	1208	1	14,14,15	0.77	1 (7%)	17,19,21	0.54	0
7	NAG	B	1202	1	14,14,15	0.40	0	17,19,21	0.61	0
7	NAG	B	1203	1	14,14,15	0.63	1 (7%)	17,19,21	0.55	0
7	NAG	B	1205	1	14,14,15	1.60	2 (14%)	17,19,21	0.97	1 (5%)
7	NAG	A	1202	1	14,14,15	0.20	0	17,19,21	0.57	0
7	NAG	C	1202	1	14,14,15	0.66	1 (7%)	17,19,21	1.33	2 (11%)
7	NAG	C	1207	1	14,14,15	0.26	0	17,19,21	0.67	0
7	NAG	A	1201	1	14,14,15	0.62	0	17,19,21	0.81	0
7	NAG	A	1203	1	14,14,15	0.29	0	17,19,21	0.56	0
7	NAG	A	1205	1	14,14,15	0.43	0	17,19,21	1.50	2 (11%)

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
7	NAG	C	1206	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1207	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1201	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1209	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1204	-	-	2/6/23/26	0/1/1/1
7	NAG	A	1207	1	-	5/6/23/26	0/1/1/1
7	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1203	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1205	1	-	5/6/23/26	0/1/1/1
7	NAG	B	1204	1	-	6/6/23/26	0/1/1/1
7	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1206	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1203	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1205	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1202	1	-	6/6/23/26	0/1/1/1
7	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1205	1	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1205	NAG	O5-C1	-5.53	1.34	1.43
7	A	1207	NAG	C1-C2	3.31	1.56	1.52
7	B	1208	NAG	O5-C1	-2.44	1.39	1.43
7	C	1202	NAG	O5-C1	-2.23	1.40	1.43
7	B	1203	NAG	C1-C2	2.20	1.55	1.52
7	B	1205	NAG	C1-C2	-2.04	1.49	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1205	NAG	C2-N2-C7	4.71	129.22	122.90
7	B	1204	NAG	C2-N2-C7	4.53	128.97	122.90
7	C	1202	NAG	C2-N2-C7	4.37	128.75	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1207	NAG	C2-N2-C7	4.09	128.38	122.90
7	C	1206	NAG	C2-N2-C7	3.73	127.90	122.90
7	A	1207	NAG	C1-O5-C5	3.35	116.67	112.19
7	A	1205	NAG	C1-C2-N2	2.95	115.08	110.43
7	B	1205	NAG	C3-C4-C5	2.80	115.30	110.23
7	C	1204	NAG	C1-O5-C5	2.38	115.38	112.19
7	B	1206	NAG	C1-O5-C5	2.30	115.27	112.19
7	C	1206	NAG	C1-C2-N2	2.30	114.05	110.43
7	C	1202	NAG	C1-C2-N2	2.27	114.01	110.43

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1209	NAG	C3-C2-N2-C7
7	B	1208	NAG	O5-C5-C6-O6
7	A	1202	NAG	C4-C5-C6-O6
7	B	1204	NAG	O5-C5-C6-O6
7	B	1206	NAG	C4-C5-C6-O6
7	B	1206	NAG	O5-C5-C6-O6
7	B	1208	NAG	C4-C5-C6-O6
7	B	1202	NAG	O5-C5-C6-O6
7	B	1203	NAG	O5-C5-C6-O6
7	A	1202	NAG	O5-C5-C6-O6
7	C	1203	NAG	O5-C5-C6-O6
7	C	1203	NAG	C4-C5-C6-O6
7	B	1203	NAG	C4-C5-C6-O6
7	B	1207	NAG	O5-C5-C6-O6
7	A	1205	NAG	C8-C7-N2-C2
7	A	1205	NAG	O7-C7-N2-C2
7	A	1207	NAG	C8-C7-N2-C2
7	A	1207	NAG	O7-C7-N2-C2
7	B	1204	NAG	C8-C7-N2-C2
7	B	1204	NAG	O7-C7-N2-C2
7	C	1202	NAG	C8-C7-N2-C2
7	C	1202	NAG	O7-C7-N2-C2
7	C	1203	NAG	C8-C7-N2-C2
7	C	1203	NAG	O7-C7-N2-C2
7	C	1205	NAG	C8-C7-N2-C2
7	C	1205	NAG	O7-C7-N2-C2
7	C	1206	NAG	C8-C7-N2-C2
7	C	1206	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	1205	NAG	O5-C5-C6-O6
7	B	1205	NAG	C4-C5-C6-O6
7	B	1204	NAG	C4-C5-C6-O6
7	A	1204	NAG	O5-C5-C6-O6
7	A	1201	NAG	O5-C5-C6-O6
7	C	1205	NAG	O5-C5-C6-O6
7	B	1201	NAG	O5-C5-C6-O6
7	C	1202	NAG	C4-C5-C6-O6
7	C	1201	NAG	C4-C5-C6-O6
7	C	1202	NAG	O5-C5-C6-O6
7	C	1205	NAG	C1-C2-N2-C7
7	A	1207	NAG	C4-C5-C6-O6
7	A	1201	NAG	C3-C2-N2-C7
7	A	1205	NAG	C3-C2-N2-C7
7	B	1201	NAG	C3-C2-N2-C7
7	B	1205	NAG	C3-C2-N2-C7
7	C	1202	NAG	C3-C2-N2-C7
7	C	1204	NAG	C3-C2-N2-C7
7	C	1205	NAG	C3-C2-N2-C7
7	A	1204	NAG	C4-C5-C6-O6
7	C	1201	NAG	O5-C5-C6-O6
7	B	1202	NAG	C4-C5-C6-O6
7	A	1207	NAG	C1-C2-N2-C7
7	B	1201	NAG	C1-C2-N2-C7
7	B	1204	NAG	C1-C2-N2-C7
7	C	1202	NAG	C1-C2-N2-C7
7	C	1204	NAG	C1-C2-N2-C7
7	C	1206	NAG	C1-C2-N2-C7
7	A	1207	NAG	C3-C2-N2-C7
7	B	1203	NAG	C3-C2-N2-C7
7	B	1204	NAG	C3-C2-N2-C7
7	C	1206	NAG	C3-C2-N2-C7
7	B	1207	NAG	C4-C5-C6-O6
7	B	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1206	NAG	2	0
7	B	1206	NAG	2	0
7	B	1209	NAG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1207	NAG	3	0
7	C	1205	NAG	4	0
7	B	1204	NAG	1	0
7	A	1206	NAG	1	0
7	B	1202	NAG	1	0
7	B	1203	NAG	3	0
7	B	1205	NAG	1	0
7	C	1202	NAG	1	0
7	A	1201	NAG	1	0
7	A	1205	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

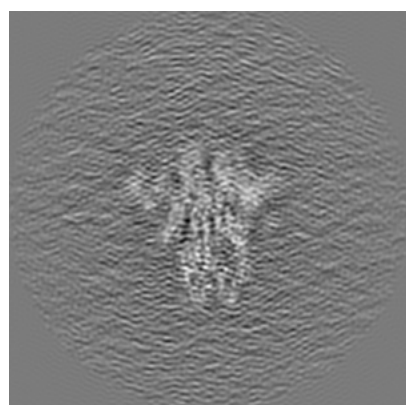
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30419. These allow visual inspection of the internal detail of the map and identification of artifacts.

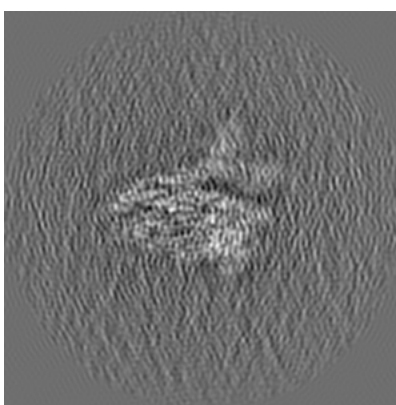
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

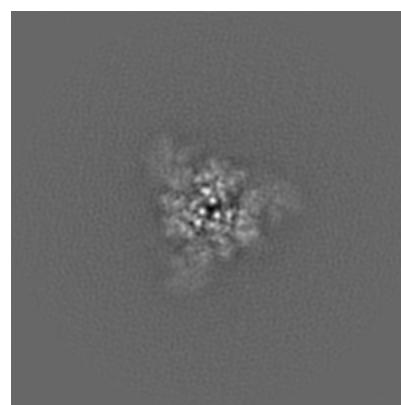
6.1.1 Primary map



X



Y

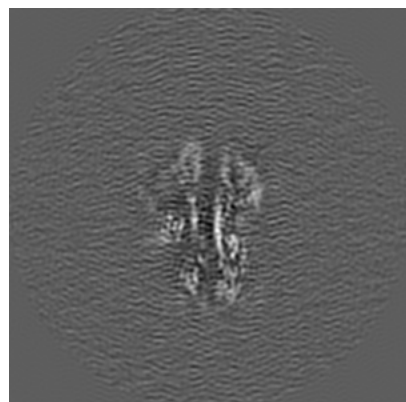


Z

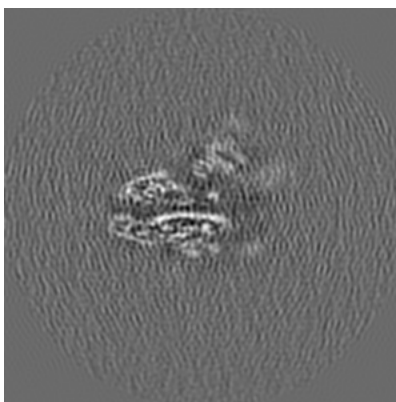
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

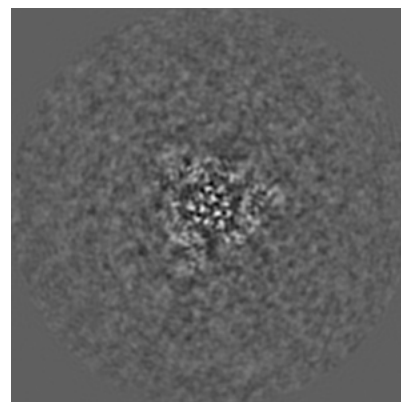
6.2.1 Primary map



X Index: 216



Y Index: 216

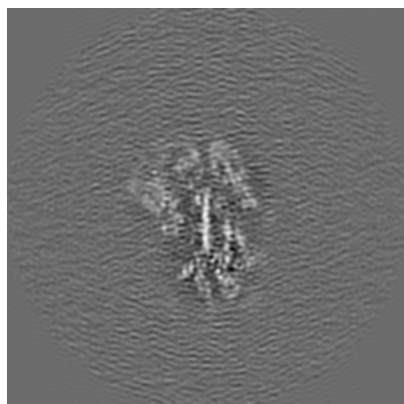


Z Index: 216

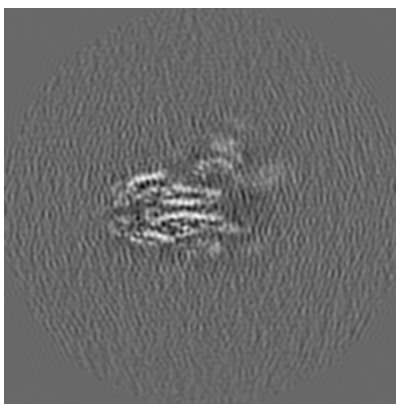
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

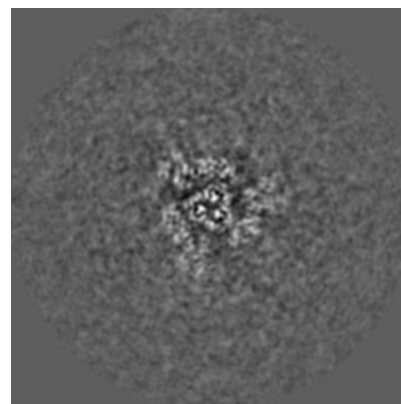
6.3.1 Primary map



X Index: 207



Y Index: 213

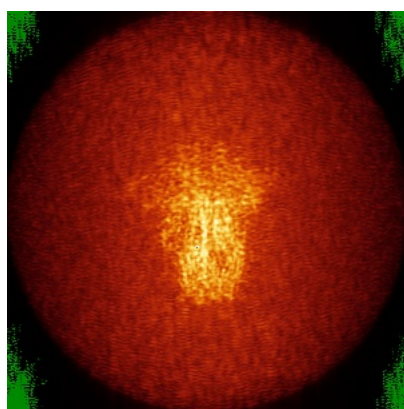


Z Index: 224

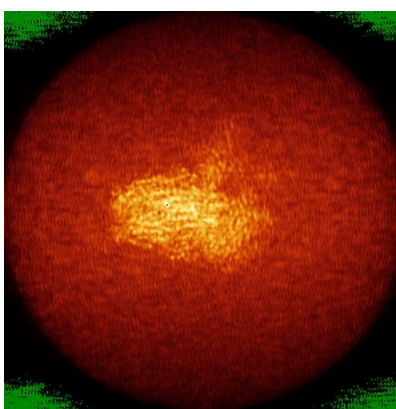
The images above show the largest variance slices of the map in three orthogonal directions.

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

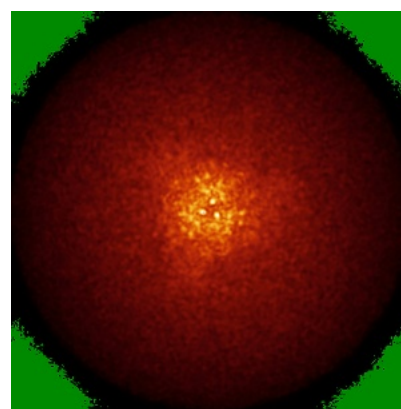
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

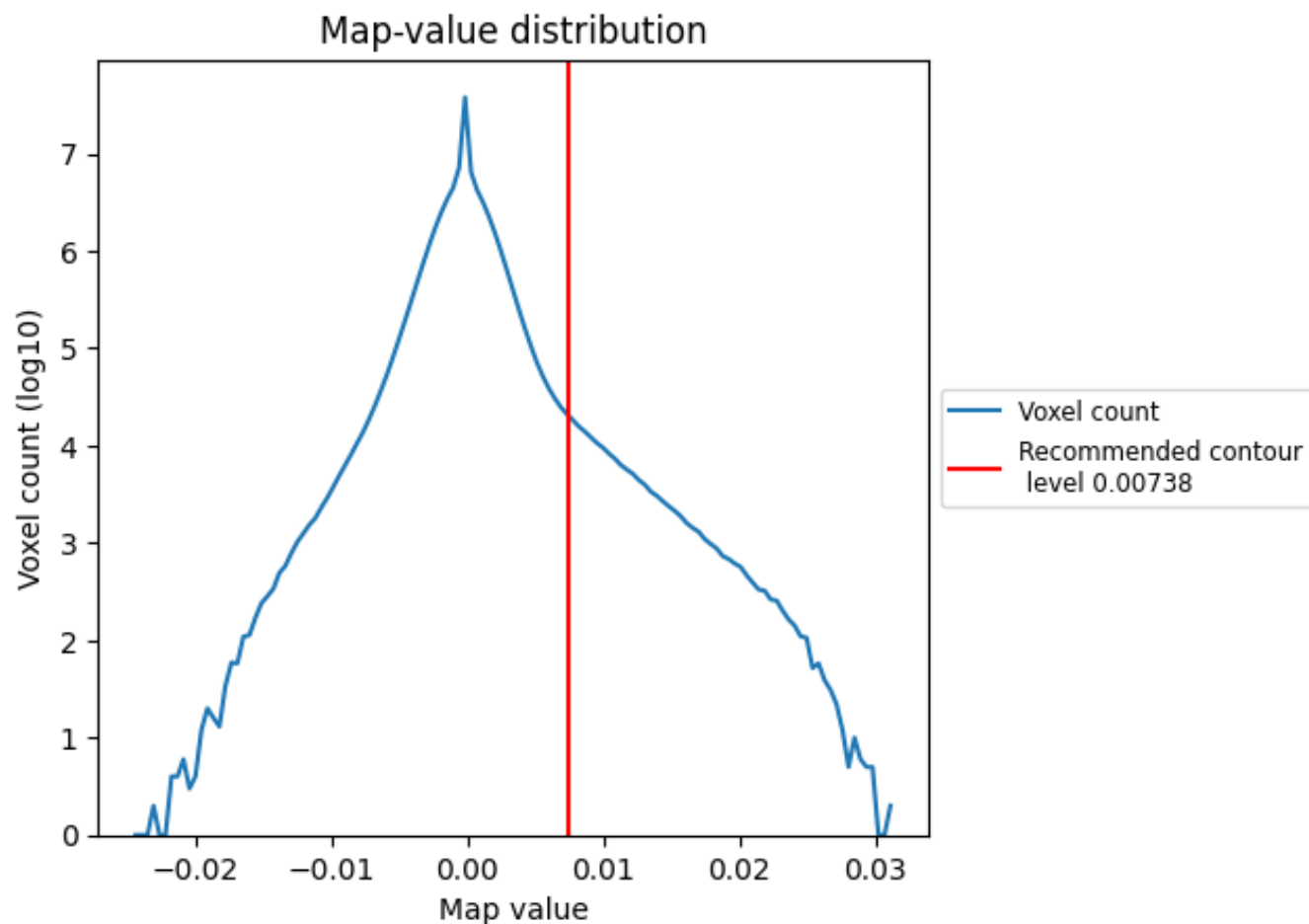
6.6 Mask visualisation

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

7 Map analysis [i](#)

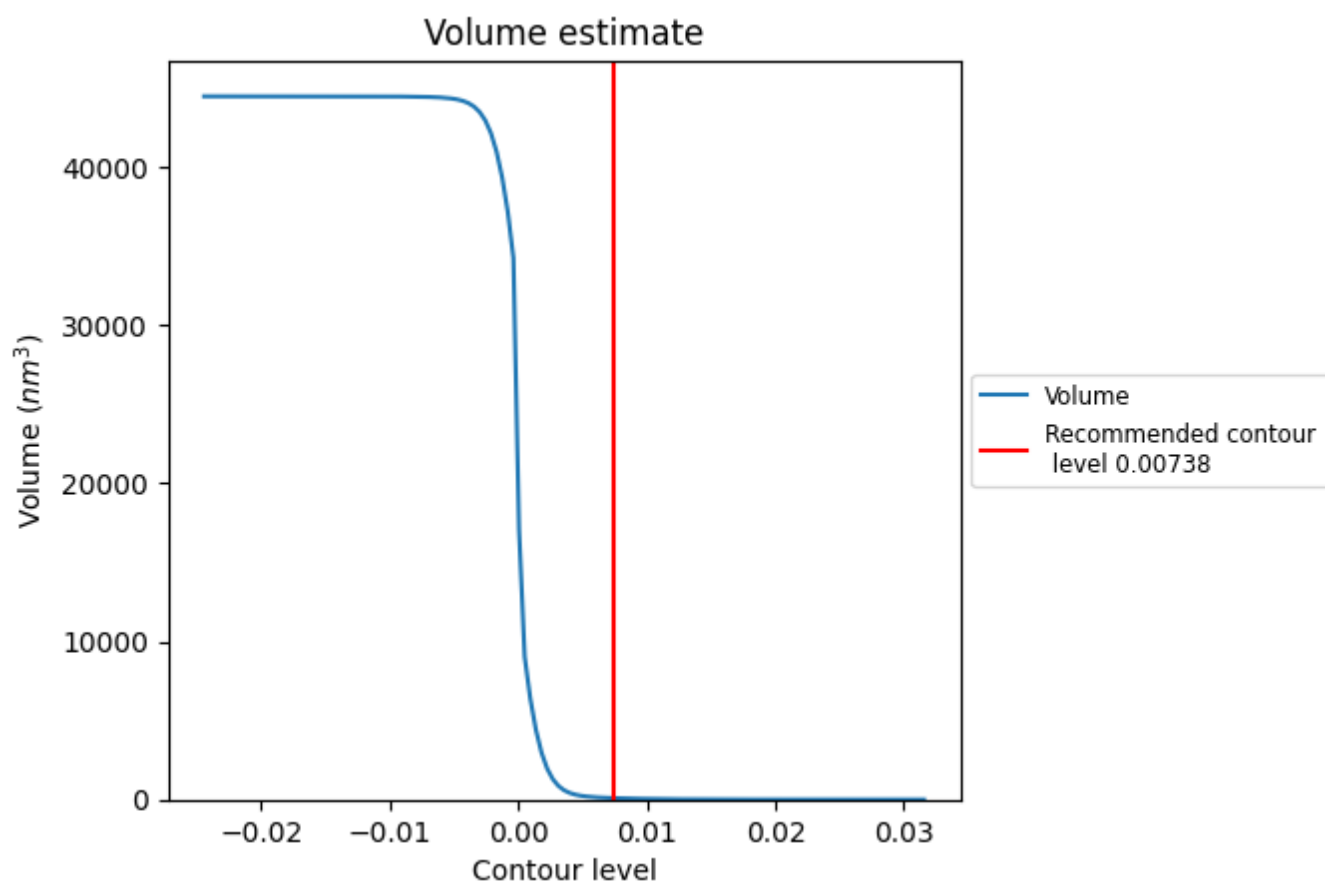
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

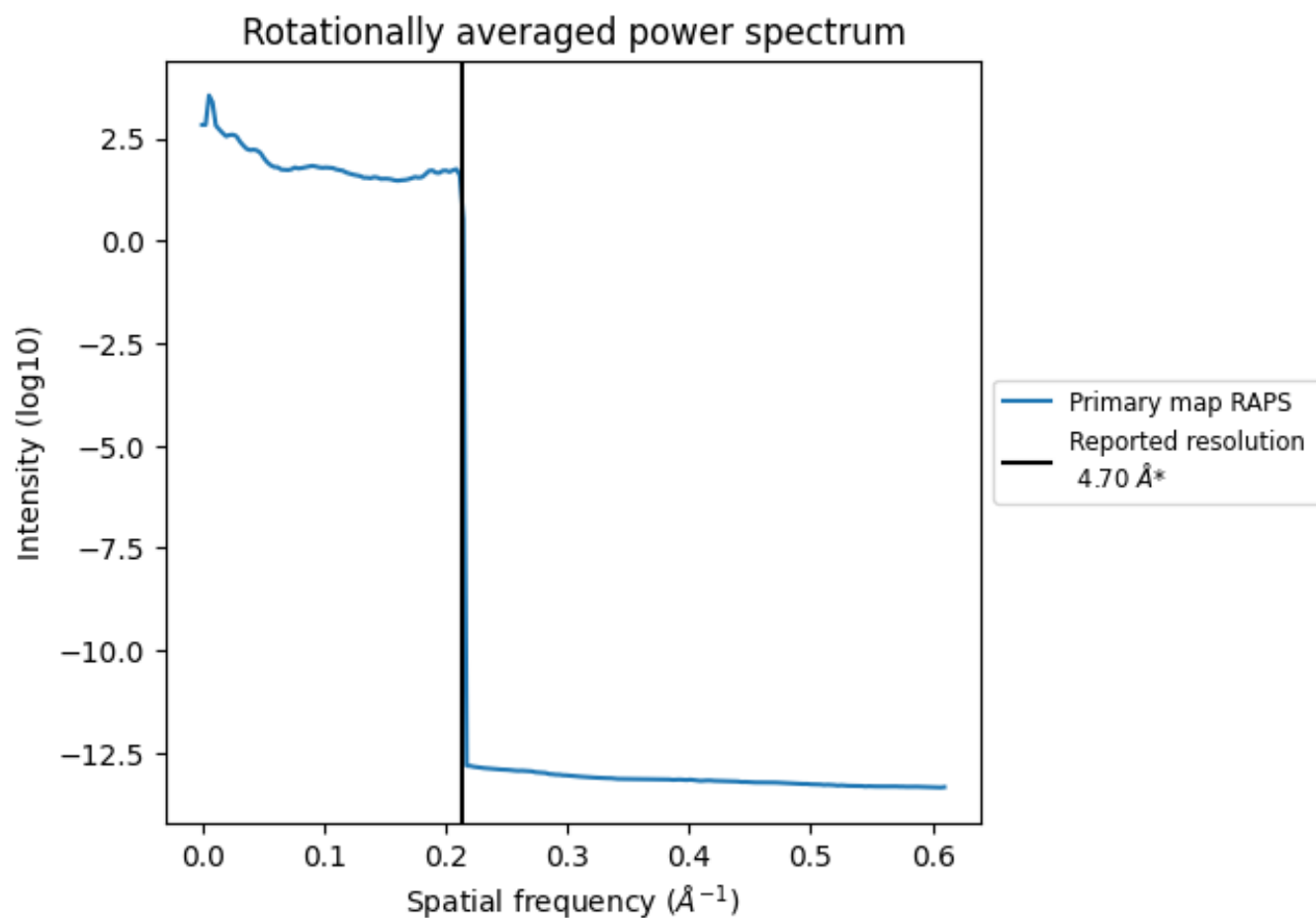
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 84 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 0.213 Å⁻¹

8 Fourier-Shell correlation

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

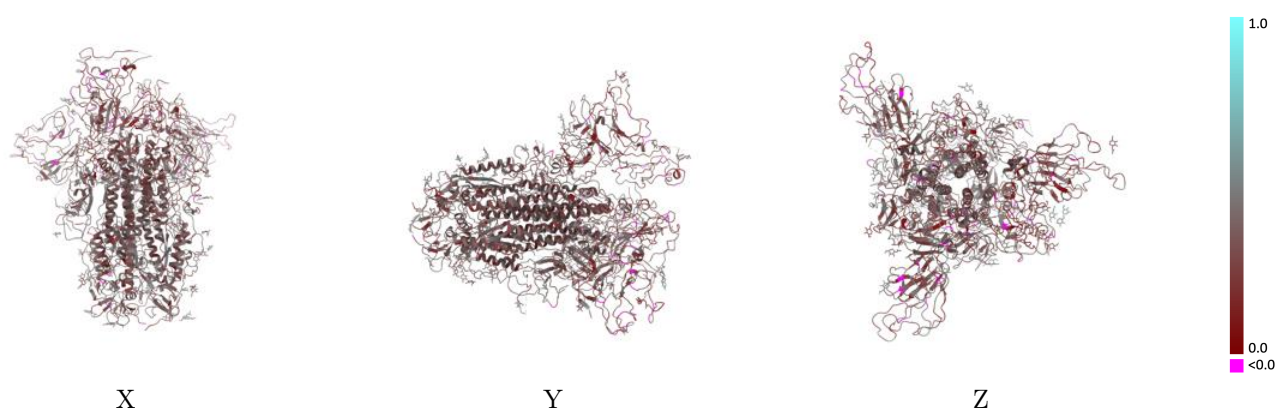
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30419 and PDB model 7CN9. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

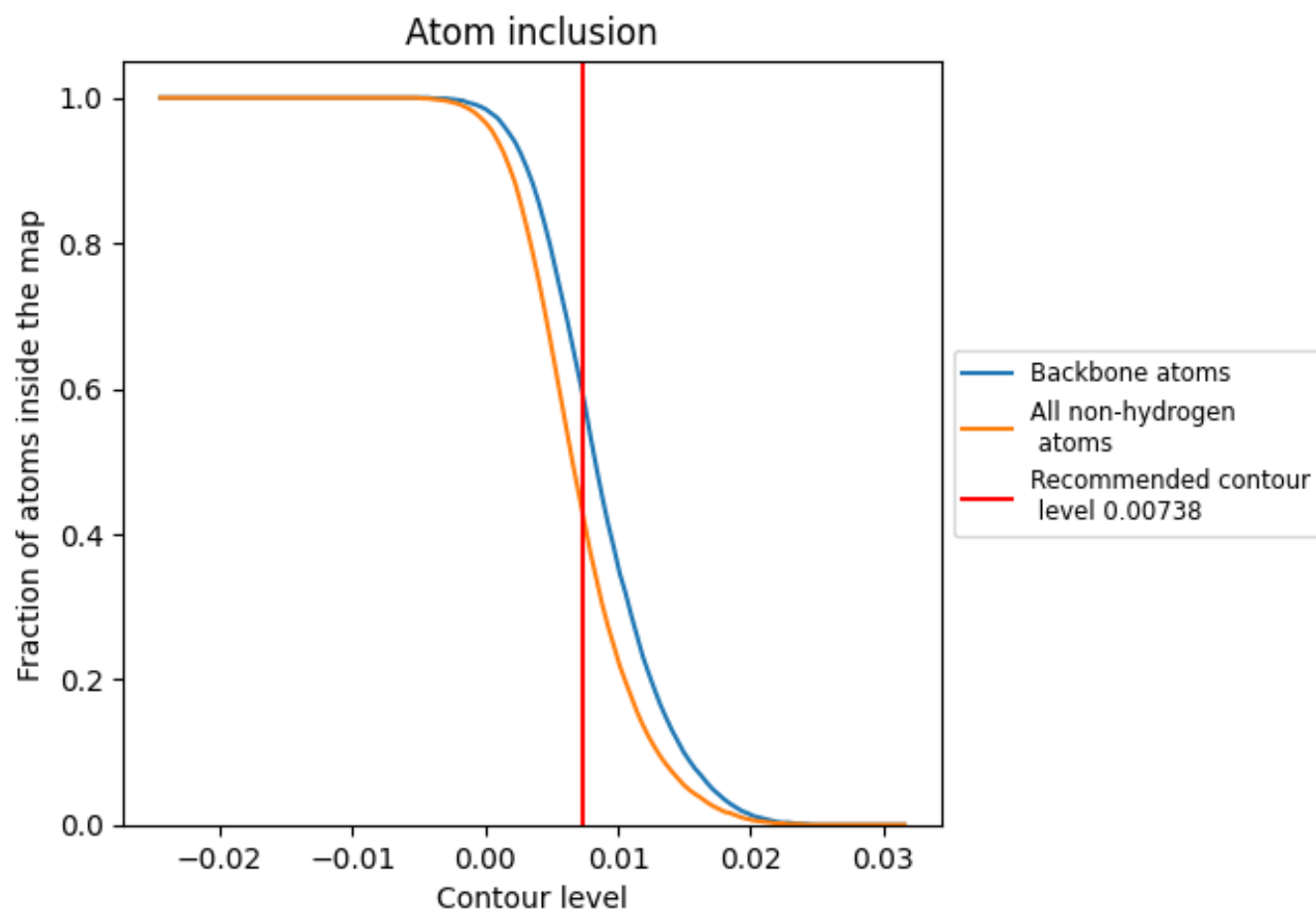


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00738) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4250	 0.3410
A	 0.3970	 0.3420
B	 0.4410	 0.3360
C	 0.4450	 0.3410
E	 0.1070	 0.4070
H	 0.3570	 0.3700
N	 0.0710	 0.4400
Q	 0.2200	 0.3940
V	 0.2310	 0.2700
W	 0.4640	 0.4550
X	 0.2860	 0.4050
Z	 0.0000	 0.4640
d	 0.3210	 0.4190
f	 0.5360	 0.4710
h	 0.0800	 0.4670
k	 0.3950	 0.4780
p	 0.4100	 0.3900

