



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:09 PM UTC

PDB ID : 3K6S / pdb_00003k6s
Title : Structure of integrin alphaXbeta2 ectodomain
Authors : Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.
Deposited on : 2009-10-09
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

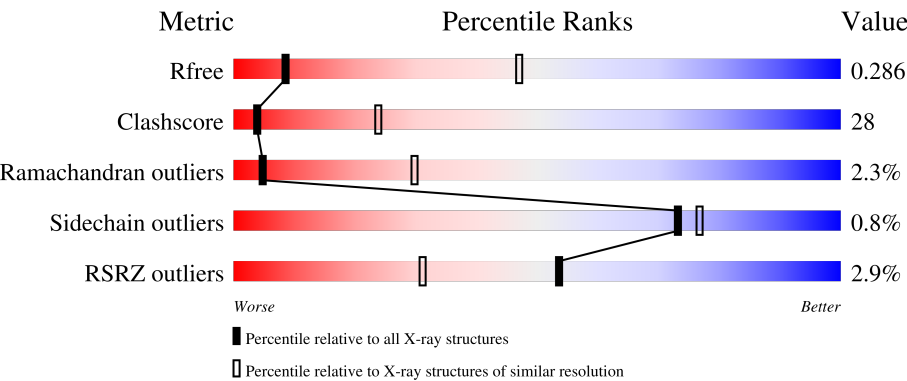
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1095	
1	C	1095	
1	E	1095	
1	G	1095	
2	B	687	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	687	
2	F	687	
2	H	687	
3	I	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	Q	2	
3	R	2	
3	T	2	
4	J	5	
5	P	3	
5	S	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	1	X	-	-	-
4	NAG	J	1	X	-	-	-
4	MAN	J	3	X	-	-	-
5	NAG	P	1	X	-	-	-
5	MAN	P	3	X	-	-	-
5	NAG	S	1	X	-	-	-
5	MAN	S	3	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50187 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1082	Total	C	N	O	S	0	0	0
			8392	5304	1454	1596	38			
1	C	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			
1	E	884	Total	C	N	O	S	0	0	0
			6819	4308	1181	1296	34			
1	G	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	expression tag	UNP P20702
A	1086	CYS	-	expression tag	UNP P20702
A	1087	GLY	-	expression tag	UNP P20702
A	1088	GLY	-	expression tag	UNP P20702
A	1089	LEU	-	expression tag	UNP P20702
A	1090	GLU	-	expression tag	UNP P20702
A	1091	ASN	-	expression tag	UNP P20702
A	1092	LEU	-	expression tag	UNP P20702
A	1093	TYR	-	expression tag	UNP P20702
A	1094	PHE	-	expression tag	UNP P20702
A	1095	GLN	-	expression tag	UNP P20702
C	1085	GLY	-	expression tag	UNP P20702
C	1086	CYS	-	expression tag	UNP P20702
C	1087	GLY	-	expression tag	UNP P20702
C	1088	GLY	-	expression tag	UNP P20702
C	1089	LEU	-	expression tag	UNP P20702
C	1090	GLU	-	expression tag	UNP P20702
C	1091	ASN	-	expression tag	UNP P20702
C	1092	LEU	-	expression tag	UNP P20702
C	1093	TYR	-	expression tag	UNP P20702
C	1094	PHE	-	expression tag	UNP P20702

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	expression tag	UNP P20702
E	1085	GLY	-	expression tag	UNP P20702
E	1086	CYS	-	expression tag	UNP P20702
E	1087	GLY	-	expression tag	UNP P20702
E	1088	GLY	-	expression tag	UNP P20702
E	1089	LEU	-	expression tag	UNP P20702
E	1090	GLU	-	expression tag	UNP P20702
E	1091	ASN	-	expression tag	UNP P20702
E	1092	LEU	-	expression tag	UNP P20702
E	1093	TYR	-	expression tag	UNP P20702
E	1094	PHE	-	expression tag	UNP P20702
E	1095	GLN	-	expression tag	UNP P20702
G	1085	GLY	-	expression tag	UNP P20702
G	1086	CYS	-	expression tag	UNP P20702
G	1087	GLY	-	expression tag	UNP P20702
G	1088	GLY	-	expression tag	UNP P20702
G	1089	LEU	-	expression tag	UNP P20702
G	1090	GLU	-	expression tag	UNP P20702
G	1091	ASN	-	expression tag	UNP P20702
G	1092	LEU	-	expression tag	UNP P20702
G	1093	TYR	-	expression tag	UNP P20702
G	1094	PHE	-	expression tag	UNP P20702
G	1095	GLN	-	expression tag	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	D	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	F	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	H	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	expression tag	UNP P05107
B	679	GLY	-	expression tag	UNP P05107
B	680	CYS	-	expression tag	UNP P05107

Continued on next page...

Continued from previous page...

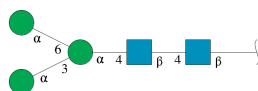
Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	expression tag	UNP P05107
B	682	GLU	-	expression tag	UNP P05107
B	684	LEU	-	expression tag	UNP P05107
B	685	TYR	-	expression tag	UNP P05107
B	686	PHE	-	expression tag	UNP P05107
B	687	GLN	-	expression tag	UNP P05107
D	678	ASP	-	expression tag	UNP P05107
D	679	GLY	-	expression tag	UNP P05107
D	680	CYS	-	expression tag	UNP P05107
D	681	GLY	-	expression tag	UNP P05107
D	682	GLU	-	expression tag	UNP P05107
D	684	LEU	-	expression tag	UNP P05107
D	685	TYR	-	expression tag	UNP P05107
D	686	PHE	-	expression tag	UNP P05107
D	687	GLN	-	expression tag	UNP P05107
F	678	ASP	-	expression tag	UNP P05107
F	679	GLY	-	expression tag	UNP P05107
F	680	CYS	-	expression tag	UNP P05107
F	681	GLY	-	expression tag	UNP P05107
F	682	GLU	-	expression tag	UNP P05107
F	684	LEU	-	expression tag	UNP P05107
F	685	TYR	-	expression tag	UNP P05107
F	686	PHE	-	expression tag	UNP P05107
F	687	GLN	-	expression tag	UNP P05107
H	678	ASP	-	expression tag	UNP P05107
H	679	GLY	-	expression tag	UNP P05107
H	680	CYS	-	expression tag	UNP P05107
H	681	GLY	-	expression tag	UNP P05107
H	682	GLU	-	expression tag	UNP P05107
H	684	LEU	-	expression tag	UNP P05107
H	685	TYR	-	expression tag	UNP P05107
H	686	PHE	-	expression tag	UNP P05107
H	687	GLN	-	expression tag	UNP P05107

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



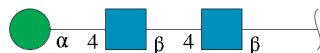
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



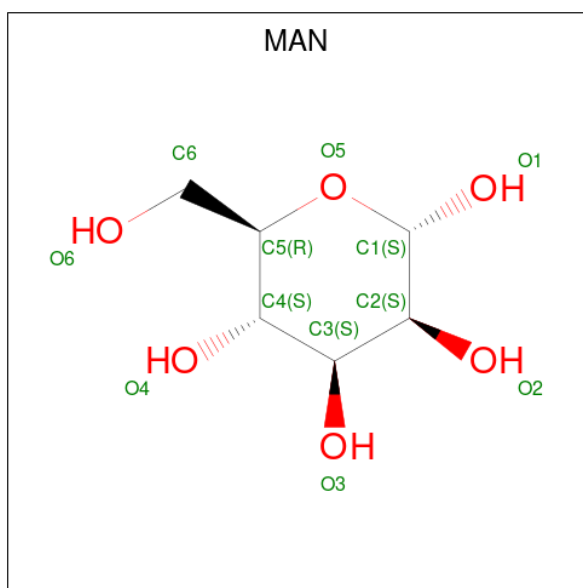
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



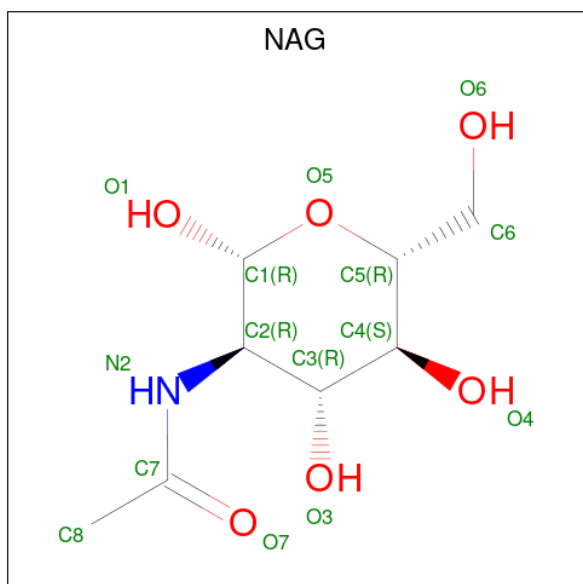
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	Ca	0	0
			3	3		
8	B	1	Total	Ca	0	0
			1	1		
8	C	3	Total	Ca	0	0
			3	3		
8	D	1	Total	Ca	0	0
			1	1		
8	E	3	Total	Ca	0	0
			3	3		
8	F	1	Total	Ca	0	0
			1	1		
8	G	3	Total	Ca	0	0
			3	3		
8	H	1	Total	Ca	0	0
			1	1		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Mg 1	0	0

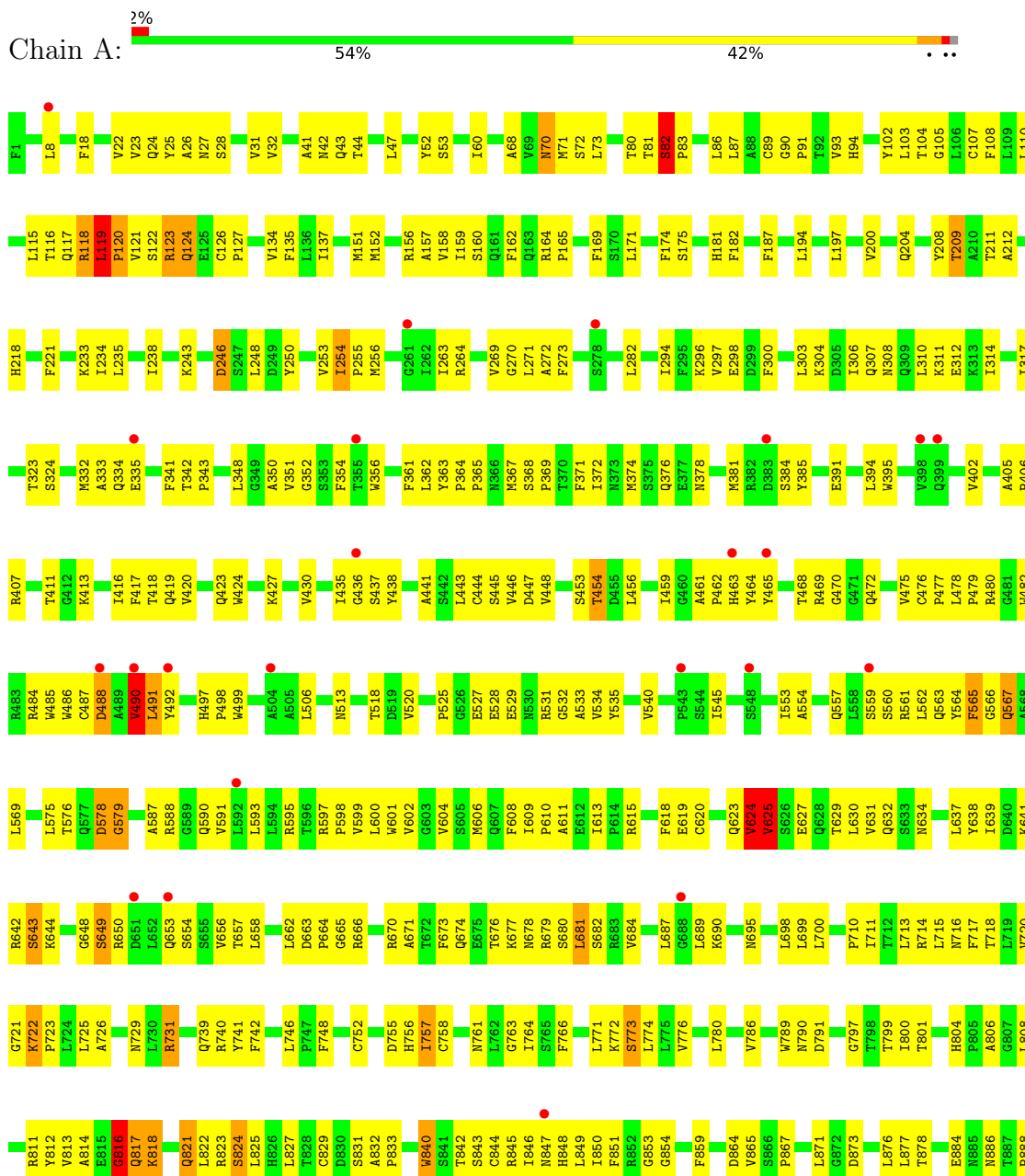
- Molecule 10 is water.

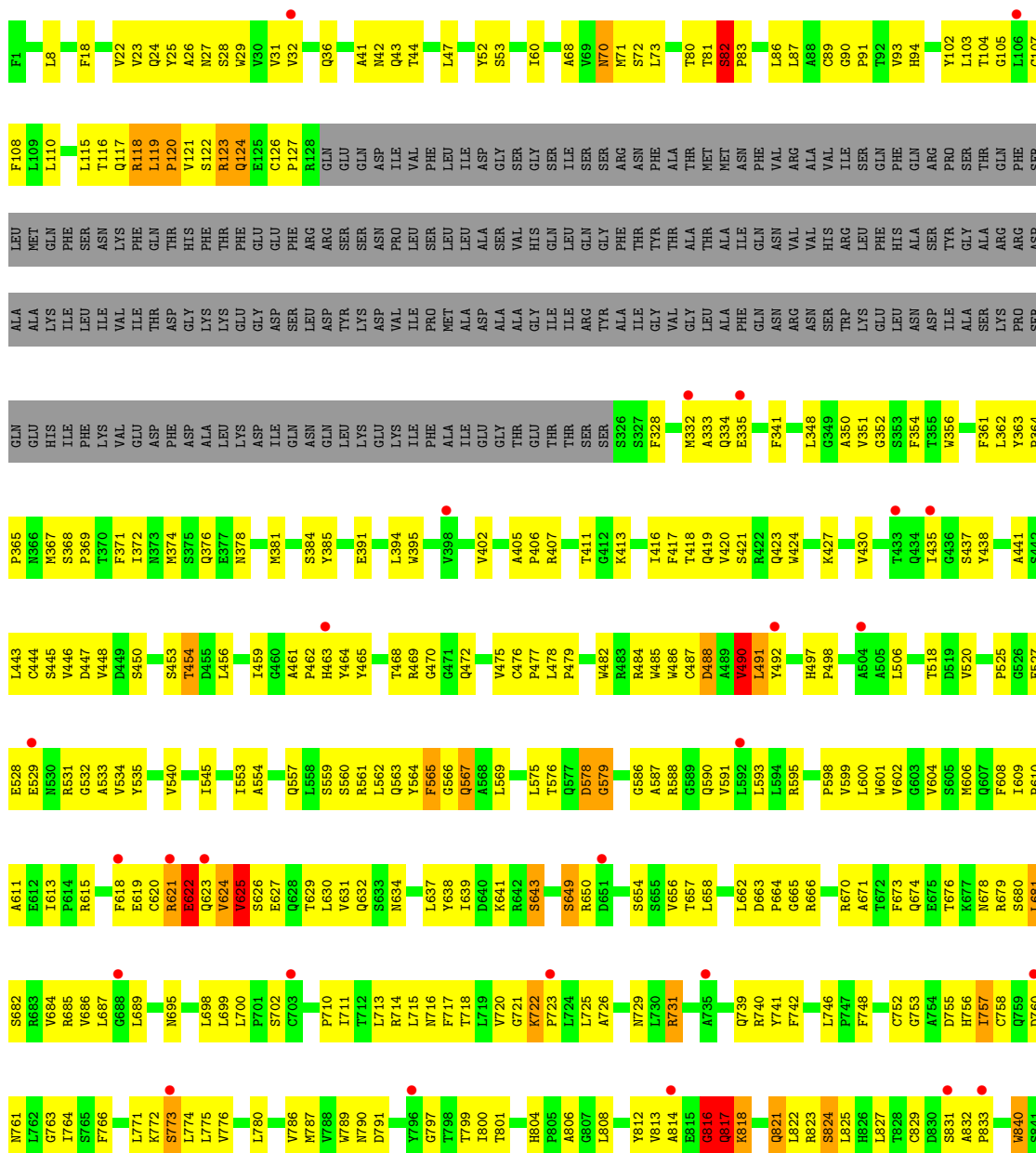
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total 3	O 3	0	0

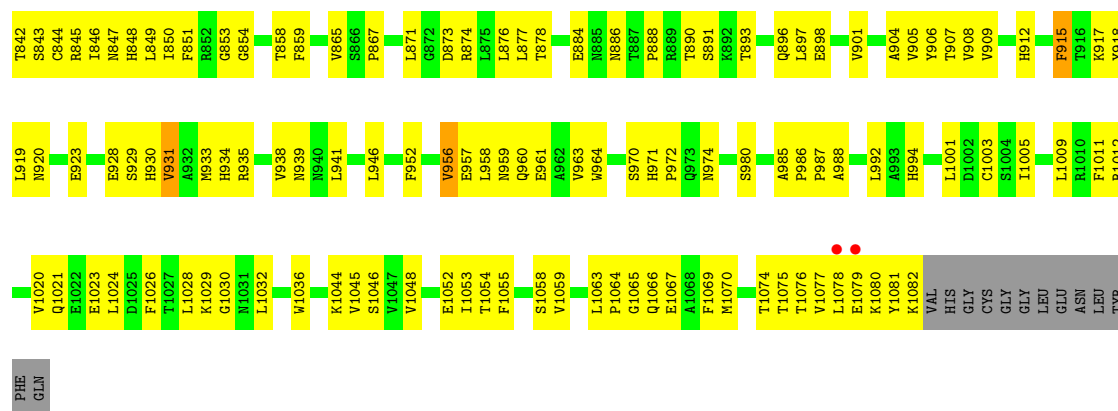
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

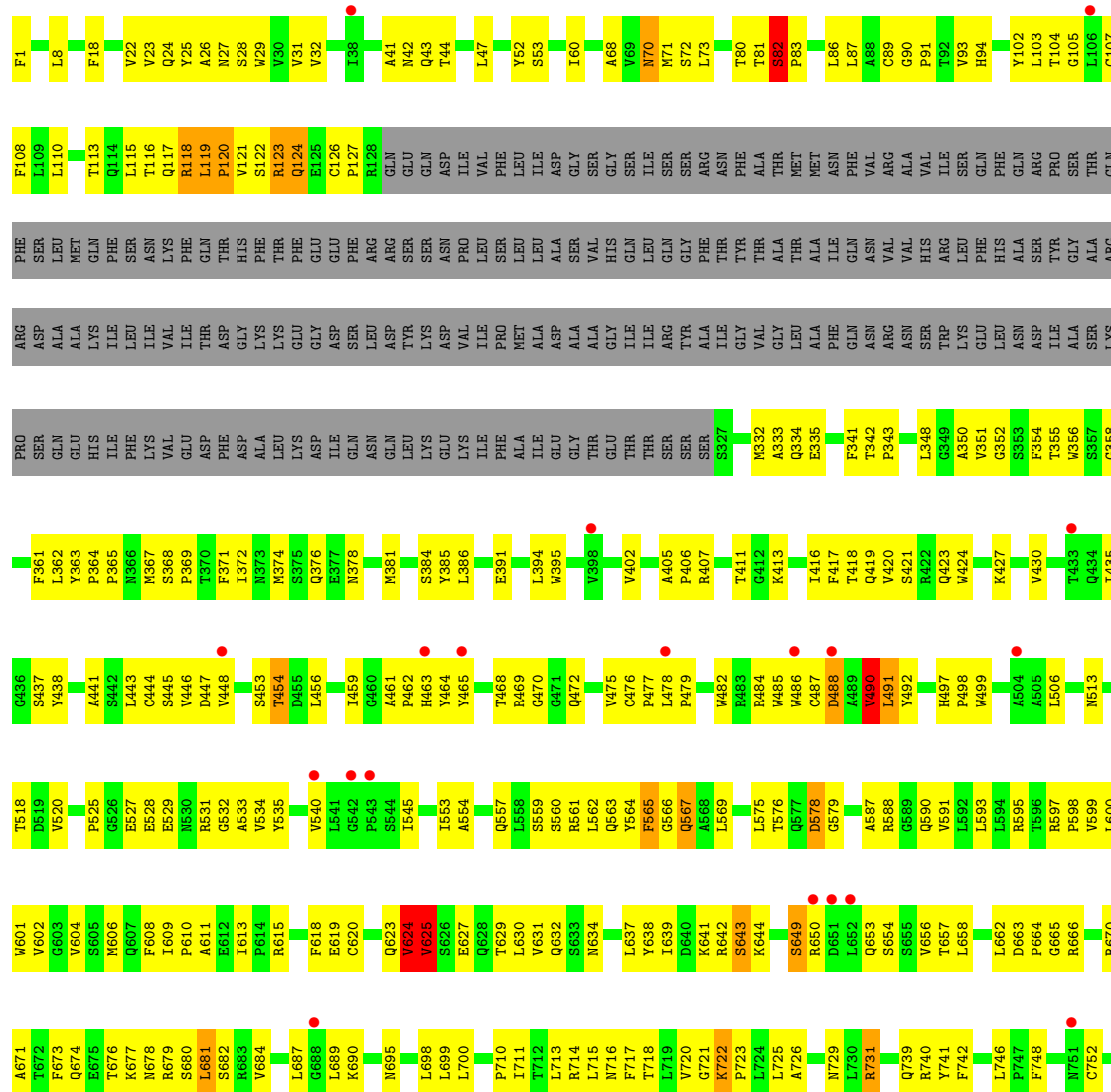
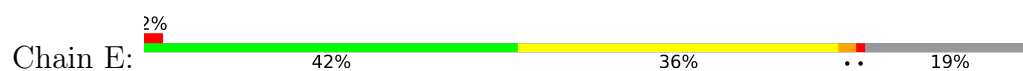
• Molecule 1: Integrin alpha-X

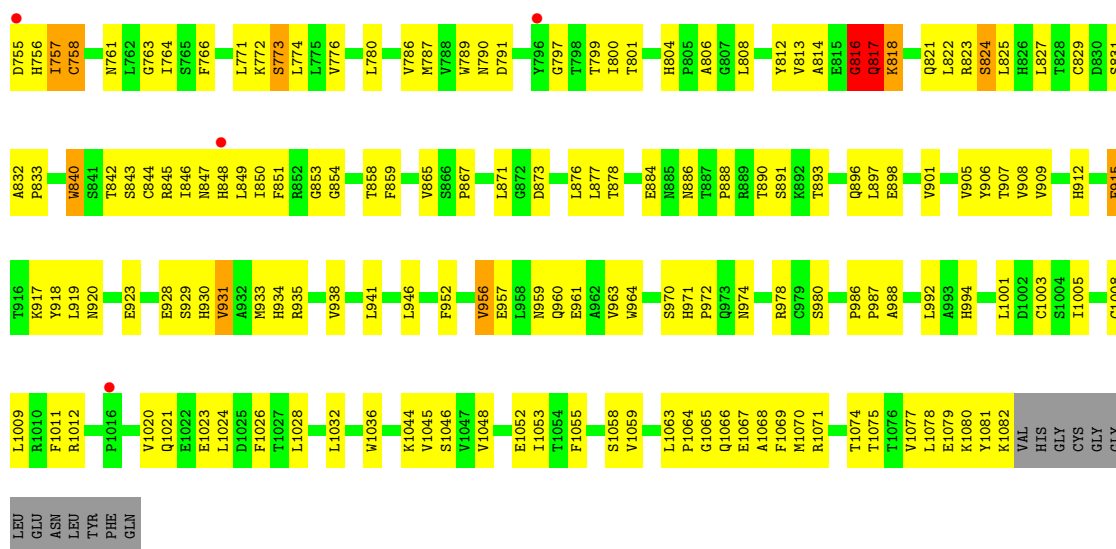




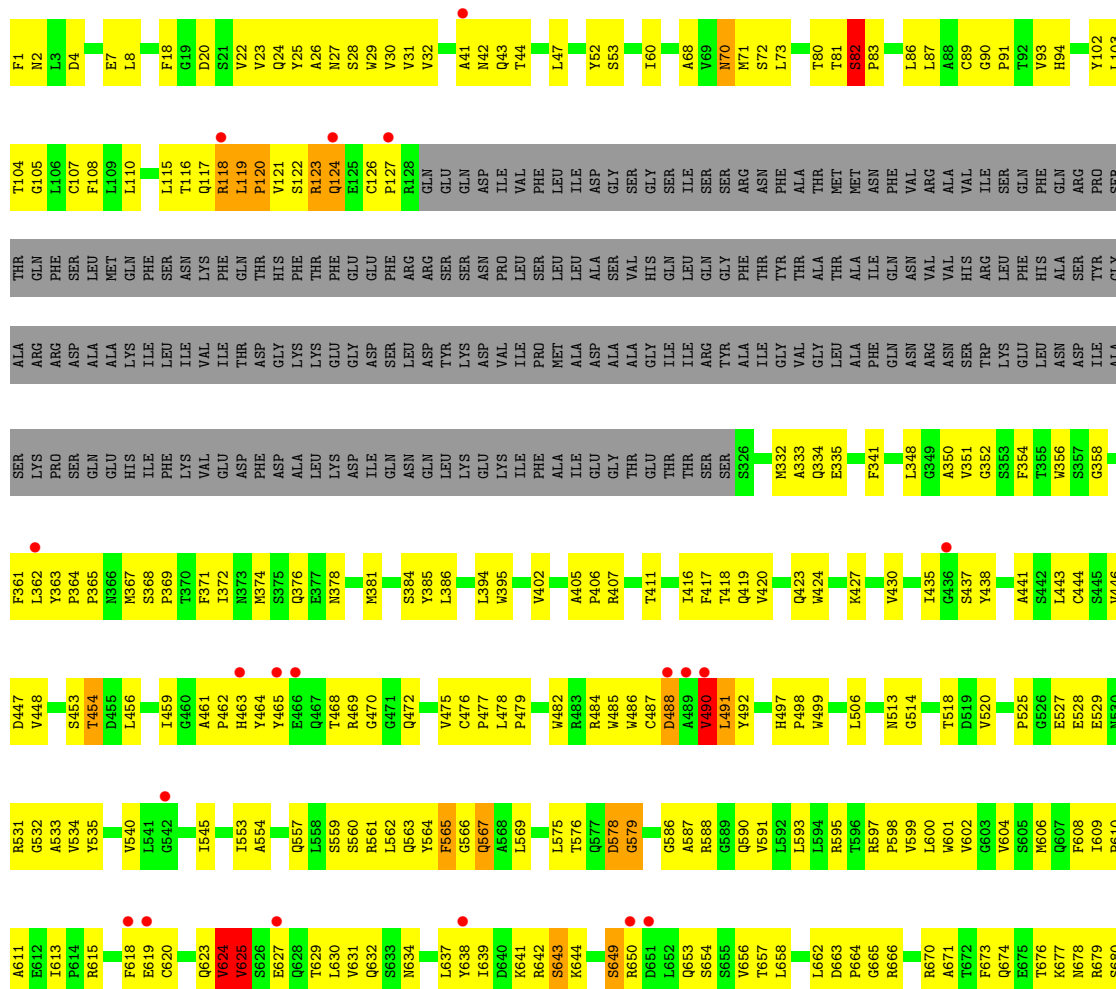
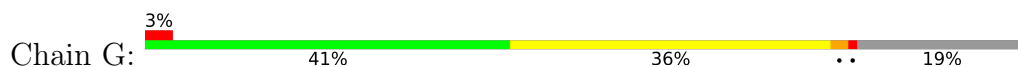


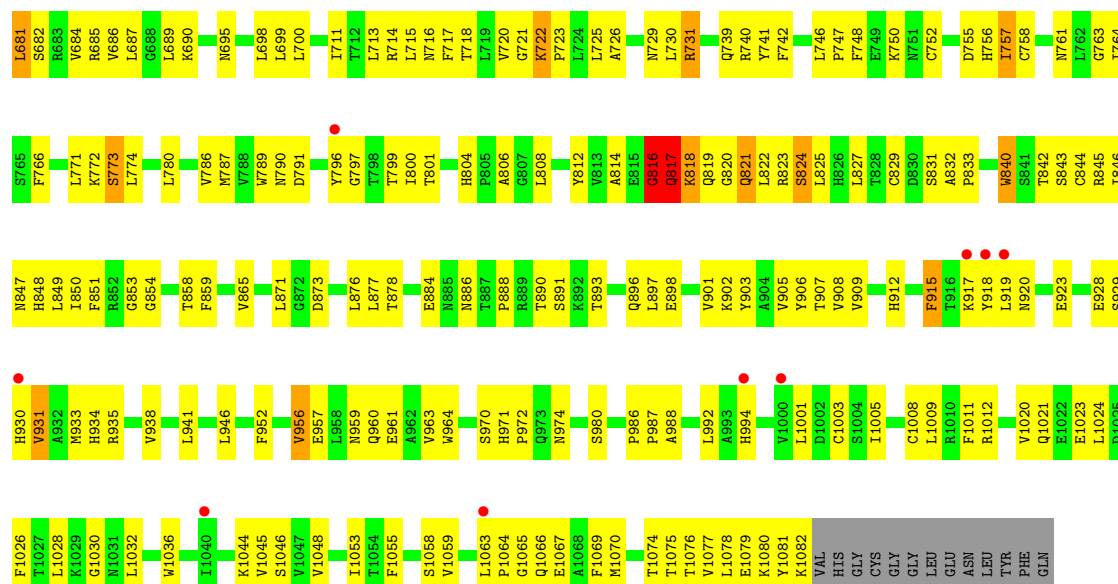
• Molecule 1: Integrin alpha-X



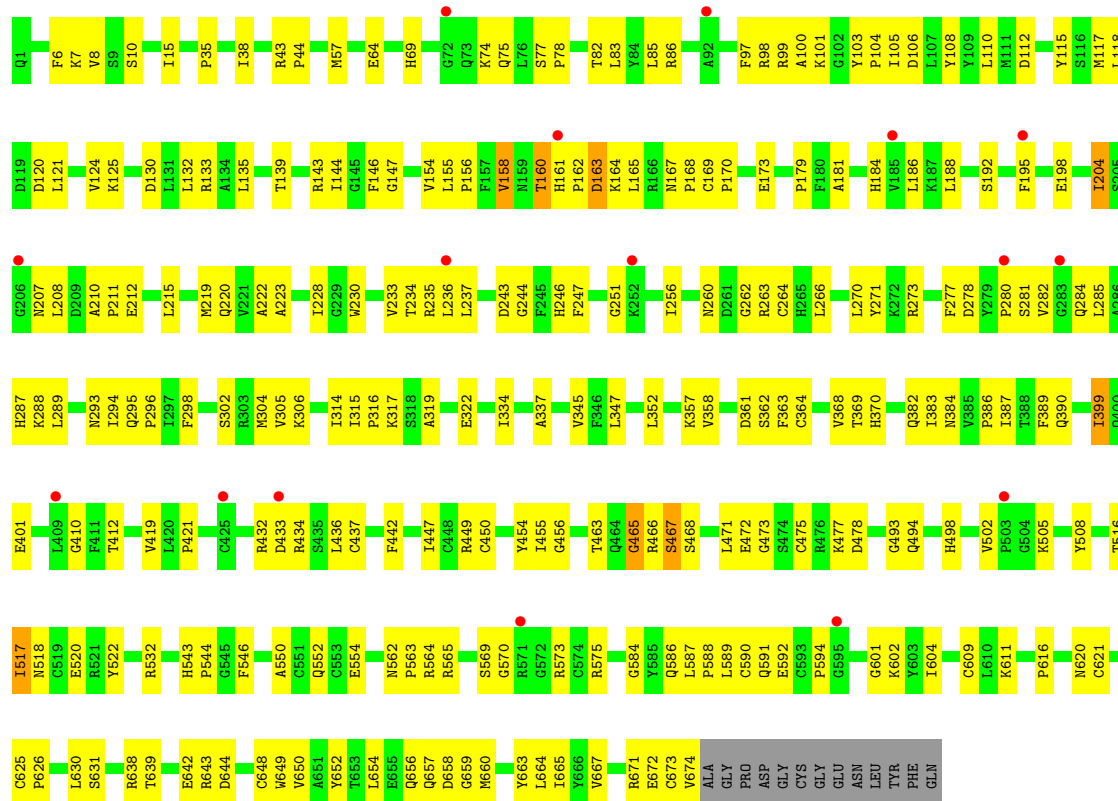


• Molecule 1: Integrin alpha-X



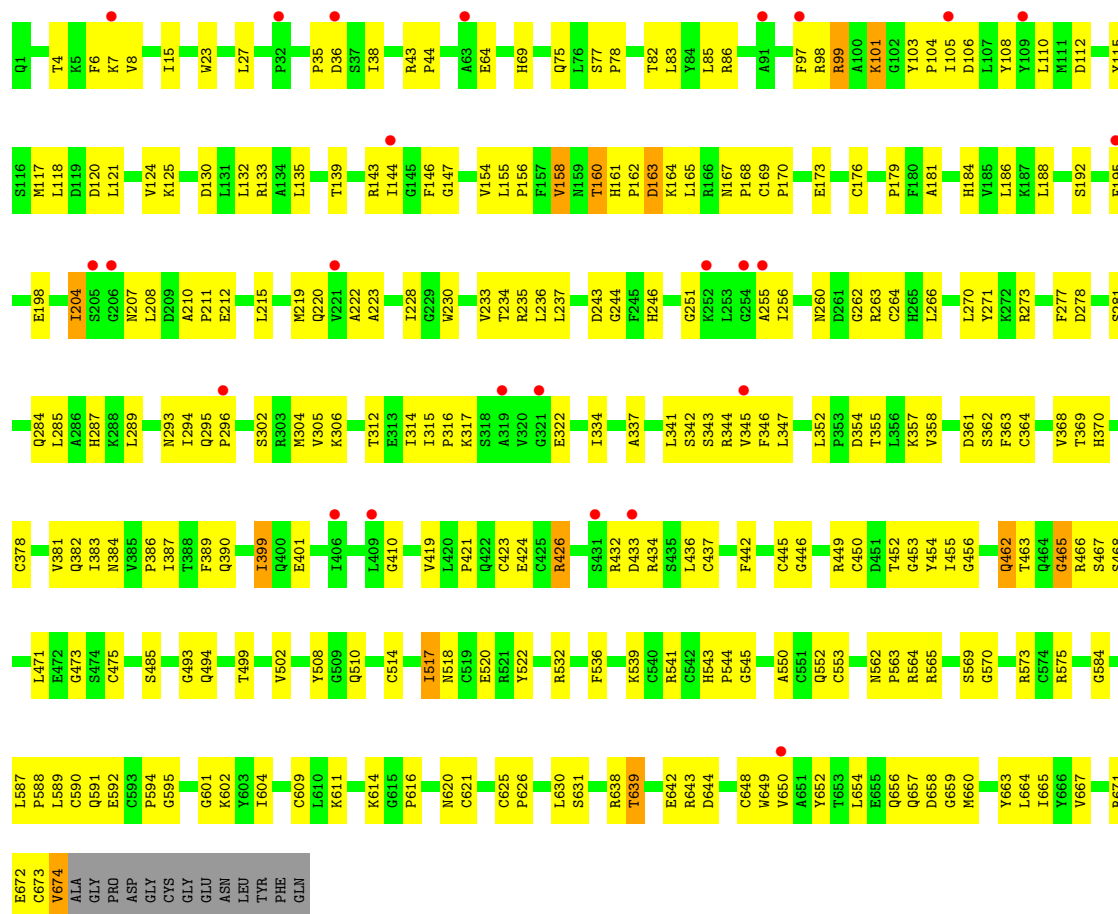


• Molecule 2: Integrin beta-2

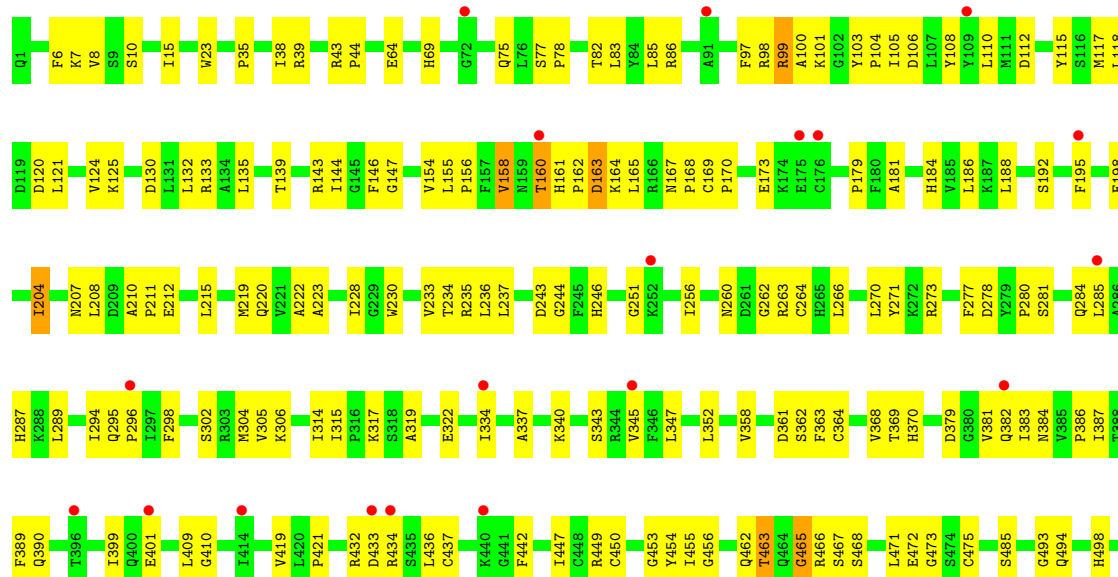


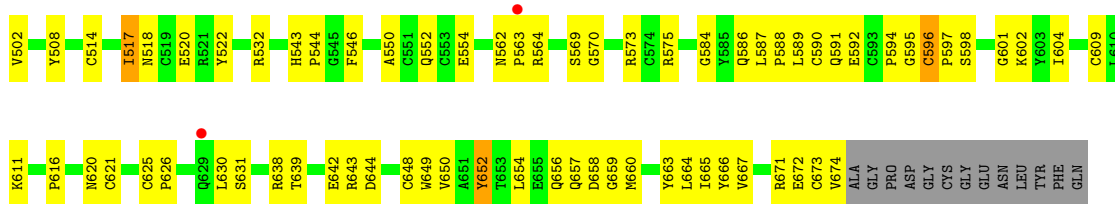
• Molecule 2: Integrin beta-2



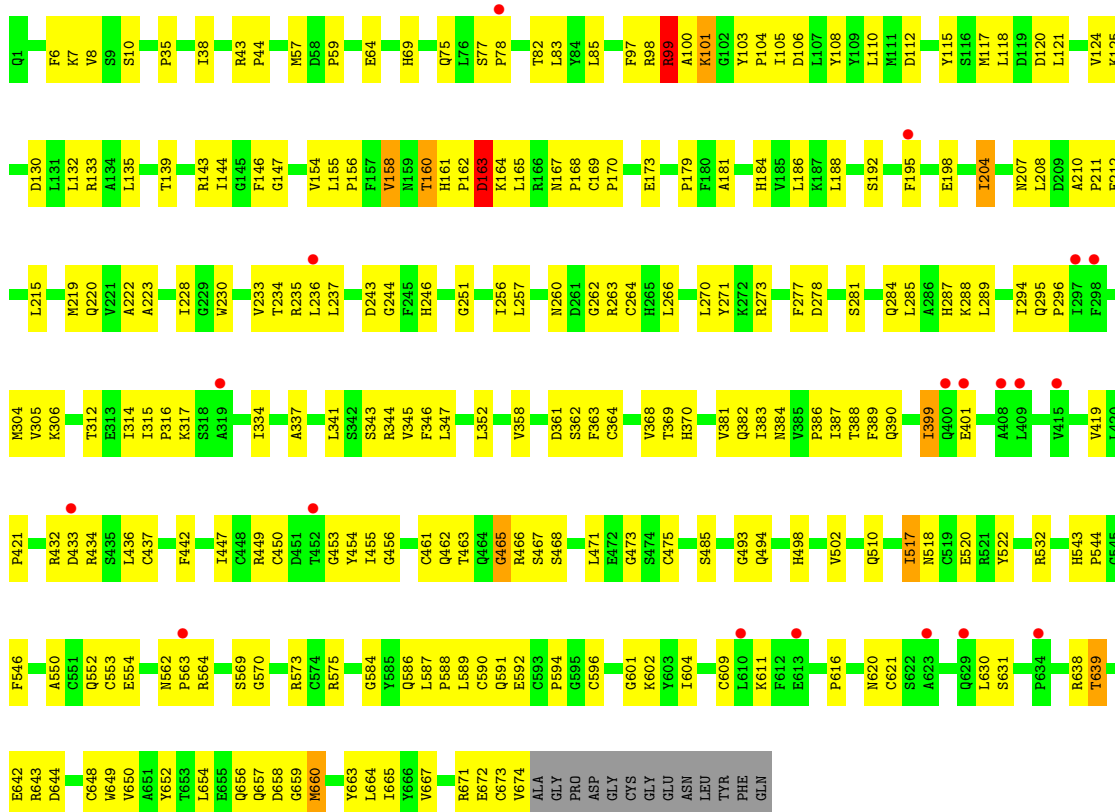


• Molecule 2: Integrin beta-2





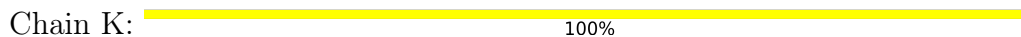
• Molecule 2: Integrin beta-2



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain L:  50% 50%

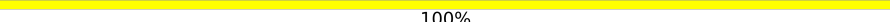


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



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

Chain N:  100%



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

Chain O:  50% 50%



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

Chain Q:  100%



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

Chain R:  50% 50%



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

Chain T:  100%

NAG1
NAG2

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

Chain J: 20% 80%

NAG1
NAG2
MAN3
MAN4
MAN5

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

Chain P: 100%

NAG1
NAG2
MAN3

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

Chain S: 100%

NAG1
NAG2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.09Å 163.56Å 536.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.50 48.61 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.61-3.50) 99.9 (48.61-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.297 , 0.335 (Not available) , 0.286	Depositor DCC
R_{free} test set	1536 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 198.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	50187	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.29	0/8579	0.74	5/11652 (0.0%)
1	C	0.29	0/6980	0.74	3/9494 (0.0%)
1	E	0.29	0/6974	0.74	3/9486 (0.0%)
1	G	0.29	0/6980	0.74	5/9494 (0.1%)
2	B	0.27	0/5280	0.73	2/7129 (0.0%)
2	D	0.29	0/5280	0.75	5/7129 (0.1%)
2	F	0.28	0/5280	0.73	4/7129 (0.1%)
2	H	0.27	0/5280	0.73	4/7129 (0.1%)
All	All	0.28	0/50633	0.74	31/68642 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	C	0	11
1	E	0	10
1	G	0	11
2	B	0	2
2	D	0	3
2	F	0	2
2	H	0	3
All	All	0	52

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	VAL	N-CA-C	9.60	120.52	110.05
1	C	821	GLN	N-CA-C	-9.44	97.80	111.30
1	A	625	VAL	CB-CA-C	-8.40	102.35	111.59
2	D	101	LYS	CB-CA-C	-8.13	107.19	116.63
1	C	622	GLU	N-CA-C	7.34	121.64	109.46
1	G	821	GLN	N-CA-C	-7.09	99.92	110.06
2	D	452	THR	N-CA-C	-6.76	103.98	111.82
1	E	491	LEU	N-CA-C	6.00	118.64	110.35
1	A	491	LEU	N-CA-C	5.92	118.52	110.35
1	A	821	GLN	N-CA-C	-5.92	98.19	110.80
1	C	491	LEU	N-CA-C	5.90	118.49	110.35
1	G	491	LEU	N-CA-C	5.84	118.41	110.35
1	E	625	VAL	CB-CA-C	-5.69	101.96	111.29
1	G	625	VAL	CB-CA-C	-5.68	101.97	111.29
2	F	596	CYS	CA-C-N	5.65	125.01	118.85
2	F	596	CYS	C-N-CA	5.65	125.01	118.85
2	H	596	CYS	CA-C-N	5.62	125.15	119.19
2	H	596	CYS	C-N-CA	5.62	125.15	119.19
1	G	625	VAL	N-CA-C	5.46	120.69	109.34
1	E	625	VAL	N-CA-C	5.41	120.60	109.34
2	F	434	ARG	N-CA-C	-5.31	106.58	113.16
1	G	820	GLY	N-CA-C	5.24	117.50	110.43
1	A	254	ILE	CB-CA-C	-5.22	108.74	113.70
2	D	452	THR	N-CA-CB	5.20	118.34	110.28
2	H	434	ARG	N-CA-C	-5.19	106.92	113.20
2	F	658	ASP	CB-CA-C	-5.14	110.23	117.23
2	D	658	ASP	CB-CA-C	-5.14	110.24	117.23
2	B	434	ARG	N-CA-C	-5.12	107.01	113.20
2	D	434	ARG	N-CA-C	-5.12	107.01	113.20
2	H	658	ASP	CB-CA-C	-5.11	110.28	117.23
2	B	658	ASP	CB-CA-C	-5.03	110.39	117.23

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	119	LEU	Peptide
1	A	488	ASP	Peptide
1	A	490	VAL	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
2	B	160	THR	Peptide
2	B	163	ASP	Peptide
1	C	118	ARG	Peptide
1	C	488	ASP	Peptide
1	C	490	VAL	Peptide
1	C	621	ARG	Peptide
1	C	622	GLU	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	817	GLN	Peptide
1	C	82	SER	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
2	D	160	THR	Peptide
2	D	163	ASP	Peptide
2	D	462	GLN	Peptide
1	E	118	ARG	Peptide
1	E	488	ASP	Peptide
1	E	490	VAL	Peptide
1	E	624	VAL	Peptide
1	E	625	VAL	Peptide
1	E	816	GLY	Peptide
1	E	817	GLN	Peptide
1	E	82	SER	Peptide
1	E	821	GLN	Peptide
1	E	824	SER	Peptide
2	F	160	THR	Peptide
2	F	163	ASP	Peptide
1	G	118	ARG	Peptide
1	G	488	ASP	Peptide
1	G	490	VAL	Peptide
1	G	624	VAL	Peptide
1	G	625	VAL	Peptide
1	G	816	GLY	Peptide
1	G	817	GLN	Peptide
1	G	819	GLN	Peptide
1	G	82	SER	Peptide
1	G	821	GLN	Peptide
1	G	824	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	H	160	THR	Peptide
2	H	163	ASP	Peptide
2	H	99	ARG	Peptide

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	8392	0	8227	531	0
1	C	6825	0	6685	486	0
1	E	6819	0	6680	461	0
1	G	6825	0	6685	468	0
2	B	5184	0	4975	227	0
2	D	5184	0	4975	265	0
2	F	5184	0	4975	236	0
2	H	5184	0	4975	226	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	4	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	T	28	0	25	1	0
4	J	61	0	52	10	0
5	P	39	0	34	6	0
5	S	39	0	34	6	0
6	A	11	0	10	4	0
7	A	28	0	25	0	0
7	B	14	0	13	0	0
7	C	28	0	25	1	0
7	D	14	0	13	0	0
7	E	28	0	25	0	0
7	F	14	0	13	0	0
7	G	28	0	24	1	0
7	H	14	0	13	0	0
8	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
8	C	3	0	0	0	0
8	D	1	0	0	0	0
8	E	3	0	0	0	0
8	F	1	0	0	0	0
8	G	3	0	0	0	0
8	H	1	0	0	0	0
9	A	1	0	0	0	0
10	A	3	0	0	0	0
All	All	50187	0	48683	2793	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 28.

All (2793) 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:A:985:ALA:CB	1:C:621:ARG:HB2	1.81	1.11
1:A:985:ALA:HB2	1:C:621:ARG:CB	1.90	1.01
1:A:985:ALA:HB2	1:C:621:ARG:CD	1.91	1.00
1:C:484:ARG:NH2	1:C:1021:GLN:HA	1.81	0.95
1:A:985:ALA:HB2	1:C:621:ARG:HB2	1.42	0.94
1:A:957:GLU:CB	1:C:621:ARG:HH22	1.81	0.93
1:E:923:GLU:HB2	1:E:1080:LYS:HB3	1.51	0.93
1:G:923:GLU:HB2	1:G:1080:LYS:HB3	1.51	0.92
1:A:484:ARG:HD2	2:B:586:GLN:HG3	1.52	0.91
1:C:923:GLU:HB2	1:C:1080:LYS:HB3	1.51	0.90
1:A:480:ARG:HG2	1:A:1021:GLN:HB3	1.54	0.89
1:A:923:GLU:HB2	1:A:1080:LYS:HB3	1.51	0.89
2:D:455:ILE:CG2	2:D:494:GLN:NE2	2.36	0.89
6:A:3378:MAN:C1	4:J:5:MAN:H4	2.02	0.88
1:A:491:LEU:HD11	1:A:545:ILE:HG12	1.56	0.88
1:C:491:LEU:HD11	1:C:545:ILE:HG12	1.55	0.88
1:A:625:VAL:HG21	1:A:627:GLU:HG3	1.54	0.88
1:G:491:LEU:HD11	1:G:545:ILE:HG12	1.55	0.88
1:C:822:LEU:HG	1:C:823:ARG:H	1.37	0.87
2:D:570:GLY:HA2	2:D:659:GLY:HA2	1.57	0.87
1:E:491:LEU:HD11	1:E:545:ILE:HG12	1.56	0.86
1:C:650:ARG:HD3	1:C:729:ASN:HB3	1.58	0.85
1:G:119:LEU:N	1:G:120:PRO:HA	1.91	0.85
1:E:119:LEU:N	1:E:120:PRO:HA	1.91	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:N	1:C:120:PRO:HA	1.92	0.85
1:C:486:TRP:HH2	1:C:1021:GLN:HG2	1.42	0.85
1:E:650:ARG:HD3	1:E:729:ASN:HB3	1.59	0.84
1:A:650:ARG:HD3	1:A:729:ASN:HB3	1.58	0.84
1:E:822:LEU:HG	1:E:823:ARG:H	1.42	0.84
1:C:630:LEU:HD21	1:G:653:GLN:HB2	1.60	0.83
1:G:650:ARG:HD3	1:G:729:ASN:HB3	1.61	0.82
1:G:816:GLY:O	1:G:818:LYS:N	2.13	0.82
1:A:985:ALA:CB	1:C:621:ARG:CD	2.57	0.82
2:D:455:ILE:HG22	2:D:494:GLN:NE2	1.94	0.82
5:S:2:NAG:O3	5:S:3:MAN:H2	1.79	0.82
1:A:822:LEU:HG	1:A:823:ARG:H	1.43	0.82
1:E:816:GLY:O	1:E:818:LYS:N	2.12	0.82
5:P:2:NAG:O3	5:P:3:MAN:H2	1.80	0.82
1:A:985:ALA:CB	1:C:621:ARG:HD2	2.10	0.81
2:D:160:THR:O	2:D:165:LEU:HD22	1.80	0.81
2:F:160:THR:O	2:F:165:LEU:HD22	1.80	0.81
2:H:160:THR:O	2:H:165:LEU:HD22	1.80	0.81
1:C:908:VAL:HG11	2:D:595:GLY:HA3	1.62	0.81
1:E:789:TRP:CZ2	1:G:772:LYS:HA	2.16	0.81
2:B:160:THR:O	2:B:165:LEU:HD22	1.80	0.80
1:A:119:LEU:O	1:A:363:TYR:CE1	2.35	0.80
2:D:455:ILE:CG2	2:D:494:GLN:HE22	1.94	0.79
1:A:985:ALA:HB2	1:C:621:ARG:HD3	1.64	0.79
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.65	0.79
4:J:2:NAG:O3	4:J:3:MAN:H2	1.81	0.79
1:G:597:ARG:HB3	1:G:731:ARG:O	1.83	0.79
2:F:210:ALA:HB3	2:F:211:PRO:HD3	1.65	0.79
1:A:194:LEU:HD22	1:A:197:LEU:HD12	1.66	0.78
1:C:491:LEU:HD11	1:C:545:ILE:CG1	2.14	0.78
1:G:721:GLY:C	1:G:723:PRO:HD3	2.09	0.78
2:D:317:LYS:HA	2:D:344:ARG:HD2	1.66	0.77
1:E:721:GLY:C	1:E:723:PRO:HD3	2.09	0.77
1:G:491:LEU:HD11	1:G:545:ILE:CG1	2.14	0.77
1:A:480:ARG:CG	1:A:1021:GLN:HB3	2.14	0.77
1:C:484:ARG:NH1	1:C:939:ASN:HB2	1.99	0.77
1:C:721:GLY:C	1:C:723:PRO:HD3	2.09	0.77
1:E:491:LEU:HD11	1:E:545:ILE:CG1	2.14	0.77
2:H:210:ALA:HB3	2:H:211:PRO:HD3	1.65	0.77
1:A:721:GLY:C	1:A:723:PRO:HD3	2.09	0.77
1:A:118:ARG:HA	1:A:120:PRO:HA	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:ALA:HB3	2:D:211:PRO:HD3	1.65	0.77
1:A:491:LEU:HD11	1:A:545:ILE:CG1	2.14	0.76
1:G:597:ARG:HD2	1:G:731:ARG:O	1.86	0.76
1:A:484:ARG:HD3	2:B:594:PRO:HG2	1.67	0.76
1:C:486:TRP:CH2	1:C:1021:GLN:HG2	2.20	0.76
1:C:1032:LEU:HD21	1:C:1078:LEU:HD21	1.68	0.76
1:A:484:ARG:CD	2:B:594:PRO:HG2	2.15	0.76
1:A:957:GLU:HB3	1:C:621:ARG:HH22	1.51	0.76
1:A:1032:LEU:HD21	1:A:1078:LEU:HD21	1.68	0.76
1:A:1063:LEU:HD12	1:A:1064:PRO:N	2.01	0.76
1:E:1032:LEU:HD21	1:E:1078:LEU:HD21	1.68	0.76
1:A:119:LEU:N	1:A:120:PRO:HA	2.01	0.75
1:G:822:LEU:HG	1:G:823:ARG:H	1.51	0.75
1:A:623:GLN:O	1:A:624:VAL:HG22	1.86	0.75
1:G:597:ARG:HG3	1:G:731:ARG:HG2	1.68	0.75
1:E:1063:LEU:HD12	1:E:1064:PRO:N	2.02	0.75
1:G:1032:LEU:HD21	1:G:1078:LEU:HD21	1.68	0.75
1:A:957:GLU:CB	1:C:621:ARG:NH2	2.50	0.75
1:G:625:VAL:HG21	1:G:627:GLU:HG3	1.67	0.75
1:C:490:VAL:HG12	1:C:491:LEU:CA	2.17	0.75
1:E:625:VAL:HG21	1:E:627:GLU:HG3	1.68	0.75
1:A:490:VAL:HG12	1:A:491:LEU:CA	2.17	0.75
1:C:848:HIS:HB2	2:D:485:SER:HB3	1.69	0.75
1:E:490:VAL:HG12	1:E:491:LEU:CA	2.17	0.75
1:C:1063:LEU:HD12	1:C:1064:PRO:N	2.02	0.74
1:G:490:VAL:HG12	1:G:491:LEU:CA	2.17	0.74
2:H:532:ARG:HD3	2:H:554:GLU:CD	2.12	0.74
1:G:490:VAL:HG12	1:G:491:LEU:N	2.02	0.74
1:A:816:GLY:O	1:A:818:LYS:N	2.20	0.74
1:C:119:LEU:H	1:C:120:PRO:HA	1.53	0.74
2:F:455:ILE:HG13	2:F:463:THR:CG2	2.16	0.74
1:G:1063:LEU:HD12	1:G:1064:PRO:N	2.02	0.74
2:F:570:GLY:HA2	2:F:659:GLY:HA2	1.70	0.74
1:G:623:GLN:O	1:G:624:VAL:HG22	1.87	0.74
1:C:490:VAL:HG12	1:C:491:LEU:N	2.02	0.74
1:A:164:ARG:HB2	1:A:165:PRO:HA	1.70	0.73
1:E:490:VAL:HG12	1:E:491:LEU:N	2.02	0.73
1:E:623:GLN:O	1:E:624:VAL:HG22	1.88	0.73
1:E:908:VAL:HG11	2:F:595:GLY:HA3	1.69	0.73
2:B:317:LYS:HE3	2:B:410:GLY:HA3	1.70	0.73
1:E:731:ARG:O	1:E:731:ARG:HG3	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:CZ2	1:A:1021:GLN:OE1	2.42	0.73
1:G:119:LEU:O	1:G:363:TYR:CE1	2.41	0.73
1:G:731:ARG:O	1:G:731:ARG:HG3	1.89	0.73
1:A:490:VAL:HG12	1:A:491:LEU:N	2.02	0.73
1:E:119:LEU:O	1:E:363:TYR:CE1	2.41	0.73
1:G:1064:PRO:HG3	1:G:1067:GLU:CD	2.14	0.73
1:C:119:LEU:O	1:C:363:TYR:CE1	2.41	0.72
1:C:731:ARG:HG3	1:C:731:ARG:O	1.89	0.72
1:A:1064:PRO:HG3	1:A:1067:GLU:CD	2.14	0.72
1:C:1064:PRO:HG3	1:C:1067:GLU:CD	2.14	0.72
1:A:731:ARG:HG3	1:A:731:ARG:O	1.88	0.72
6:A:3378:MAN:C1	4:J:5:MAN:C4	2.67	0.72
1:E:121:VAL:O	1:E:121:VAL:HG12	1.90	0.72
2:F:455:ILE:CG1	2:F:463:THR:HG23	2.19	0.72
2:H:100:ALA:O	2:H:101:LYS:HB2	1.90	0.72
1:E:119:LEU:H	1:E:120:PRO:HA	1.52	0.72
1:A:957:GLU:HB2	1:C:621:ARG:HH22	1.53	0.71
2:F:455:ILE:HG12	2:F:463:THR:HG23	1.72	0.71
1:A:121:VAL:O	1:A:121:VAL:HG12	1.90	0.71
1:A:194:LEU:CD2	1:A:197:LEU:HD12	2.20	0.71
1:G:119:LEU:H	1:G:120:PRO:HA	1.52	0.71
1:G:121:VAL:O	1:G:121:VAL:HG12	1.90	0.71
1:E:1064:PRO:HG3	1:E:1067:GLU:CD	2.15	0.71
1:A:772:LYS:HA	1:C:789:TRP:CZ2	2.26	0.71
1:C:121:VAL:O	1:C:121:VAL:HG12	1.90	0.70
1:G:928:GLU:HG3	1:G:929:SER:N	2.07	0.70
1:G:598:PRO:CG	1:G:650:ARG:NH1	2.54	0.70
1:E:772:LYS:HA	1:G:789:TRP:CZ2	2.25	0.70
1:E:928:GLU:HG3	1:E:929:SER:N	2.06	0.70
1:C:928:GLU:HG3	1:C:929:SER:N	2.07	0.70
2:F:532:ARG:HD3	2:F:554:GLU:CD	2.16	0.70
1:A:662:LEU:HD11	1:A:673:PHE:CZ	2.27	0.70
1:A:953:TRP:CH2	1:C:755:ASP:HA	2.26	0.70
2:B:532:ARG:HD3	2:B:554:GLU:CD	2.16	0.70
2:H:99:ARG:HG2	2:H:100:ALA:H	1.55	0.70
1:C:662:LEU:HD11	1:C:673:PHE:CZ	2.27	0.69
1:A:928:GLU:HG3	1:A:929:SER:N	2.07	0.69
1:G:662:LEU:HD11	1:G:673:PHE:CZ	2.27	0.69
1:E:662:LEU:HD11	1:E:673:PHE:CZ	2.27	0.69
1:C:630:LEU:HD21	1:G:653:GLN:CB	2.22	0.69
2:F:472:GLU:HA	2:F:475:CYS:CB	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:472:GLU:HA	2:F:475:CYS:HB3	1.74	0.69
1:C:622:GLU:C	1:C:623:GLN:HG2	2.18	0.69
2:D:316:PRO:HB3	2:D:346:PHE:CZ	2.27	0.68
2:F:15:ILE:HG23	2:F:86:ARG:CZ	2.23	0.68
1:A:1064:PRO:HG3	1:A:1067:GLU:HG3	1.76	0.68
1:E:871:LEU:HD11	1:E:901:VAL:HG21	1.76	0.68
1:A:957:GLU:HB3	1:C:621:ARG:NH2	2.07	0.68
1:G:657:THR:HG23	1:G:720:VAL:HB	1.76	0.68
1:G:1064:PRO:HG3	1:G:1067:GLU:HG3	1.75	0.68
1:A:871:LEU:HD11	1:A:901:VAL:HG21	1.76	0.68
1:E:756:HIS:O	1:E:757:ILE:HG22	1.94	0.68
1:A:395:TRP:HZ2	1:A:1021:GLN:OE1	1.76	0.67
1:A:953:TRP:CZ2	1:C:755:ASP:HA	2.29	0.67
1:C:871:LEU:HD11	1:C:901:VAL:HG21	1.76	0.67
1:E:657:THR:HG23	1:E:720:VAL:HB	1.76	0.67
1:A:957:GLU:HB2	1:C:621:ARG:NH2	2.09	0.67
1:A:657:THR:HG23	1:A:720:VAL:HB	1.76	0.67
1:C:657:THR:HG23	1:C:720:VAL:HB	1.76	0.67
1:E:1064:PRO:HG3	1:E:1067:GLU:HG3	1.76	0.67
1:A:919:LEU:HB2	1:A:1079:GLU:HB3	1.76	0.67
1:E:812:TYR:CD2	1:E:814:ALA:HB2	2.30	0.67
1:A:789:TRP:CZ2	1:C:772:LYS:HA	2.29	0.67
1:C:816:GLY:O	1:C:818:LYS:N	2.28	0.67
1:G:362:LEU:HD23	1:G:363:TYR:N	2.10	0.67
1:G:673:PHE:CG	1:G:681:LEU:HD23	2.30	0.67
1:G:871:LEU:HD11	1:G:901:VAL:HG21	1.76	0.67
1:C:919:LEU:HB2	1:C:1079:GLU:HB3	1.76	0.67
1:E:362:LEU:HD23	1:E:363:TYR:N	2.10	0.67
1:G:919:LEU:HB2	1:G:1079:GLU:HB3	1.76	0.67
1:C:1064:PRO:HG3	1:C:1067:GLU:HG3	1.76	0.67
1:A:650:ARG:HD3	1:A:729:ASN:CB	2.25	0.66
1:E:812:TYR:CE2	1:E:814:ALA:HB2	2.29	0.66
1:A:362:LEU:HD23	1:A:363:TYR:N	2.10	0.66
1:E:673:PHE:CG	1:E:681:LEU:HD23	2.31	0.66
1:E:919:LEU:HB2	1:E:1079:GLU:HB3	1.76	0.66
1:G:650:ARG:HD3	1:G:729:ASN:CB	2.26	0.66
1:C:650:ARG:HD3	1:C:729:ASN:CB	2.24	0.66
1:E:650:ARG:HD3	1:E:729:ASN:CB	2.26	0.66
2:F:10:SER:HB3	2:F:449:ARG:CZ	2.25	0.66
1:A:311:LYS:HG3	1:A:312:GLU:N	2.10	0.66
1:A:673:PHE:CG	1:A:681:LEU:HD23	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:PHE:CG	1:C:681:LEU:HD23	2.30	0.66
1:G:118:ARG:HA	1:G:120:PRO:HA	1.78	0.66
1:C:118:ARG:HA	1:C:120:PRO:HA	1.78	0.66
1:C:362:LEU:HD23	1:C:363:TYR:N	2.10	0.66
2:H:455:ILE:HG12	2:H:463:THR:HG23	1.76	0.66
1:G:756:HIS:O	1:G:757:ILE:HG22	1.96	0.66
2:D:471:LEU:O	2:D:493:GLY:HA2	1.96	0.65
1:E:118:ARG:HA	1:E:120:PRO:HA	1.78	0.65
1:A:273:PHE:HB2	1:A:296:LYS:HD2	1.78	0.65
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.32	0.65
2:B:75:GLN:O	2:B:97:PHE:HA	1.97	0.65
1:C:665:GLY:HA2	2:D:499:THR:O	1.95	0.65
1:C:1063:LEU:HD12	1:C:1064:PRO:CA	2.27	0.65
1:E:721:GLY:C	1:E:723:PRO:CD	2.70	0.65
2:F:587:LEU:HB3	2:F:588:PRO:HA	1.79	0.65
1:A:562:LEU:HD11	1:A:590:GLN:HG2	1.79	0.65
1:A:721:GLY:C	1:A:723:PRO:CD	2.70	0.65
1:A:985:ALA:HB2	1:C:621:ARG:CG	2.27	0.65
1:C:622:GLU:HG3	1:C:623:GLN:HB3	1.79	0.65
1:G:812:TYR:CE2	1:G:814:ALA:HB2	2.31	0.65
1:E:1063:LEU:HD12	1:E:1064:PRO:CA	2.27	0.64
2:F:75:GLN:O	2:F:97:PHE:HA	1.97	0.64
2:H:75:GLN:O	2:H:97:PHE:HA	1.97	0.64
1:A:1063:LEU:HD12	1:A:1064:PRO:CA	2.27	0.64
1:G:562:LEU:HD11	1:G:590:GLN:HG2	1.80	0.64
1:G:721:GLY:C	1:G:723:PRO:CD	2.70	0.64
1:G:1063:LEU:HD12	1:G:1064:PRO:CA	2.27	0.64
1:A:531:ARG:HA	1:A:563:GLN:O	1.98	0.64
1:C:531:ARG:HA	1:C:563:GLN:O	1.98	0.64
2:D:456:GLY:HA2	2:D:494:GLN:OE1	1.97	0.64
1:A:985:ALA:HB1	1:C:621:ARG:HD2	1.79	0.64
1:E:531:ARG:HA	1:E:563:GLN:O	1.98	0.64
2:B:15:ILE:HG23	2:B:86:ARG:CZ	2.28	0.64
2:B:161:HIS:HB3	2:B:162:PRO:HA	1.80	0.64
1:C:94:HIS:NE2	2:D:155:LEU:HD21	2.12	0.64
2:D:6:PHE:CE1	2:D:541:ARG:HD2	2.33	0.64
2:D:75:GLN:O	2:D:97:PHE:HA	1.97	0.64
2:F:161:HIS:HB3	2:F:162:PRO:HA	1.80	0.64
2:H:587:LEU:HB3	2:H:588:PRO:HA	1.79	0.64
1:C:623:GLN:O	1:C:624:VAL:HG22	1.98	0.64
1:E:609:ILE:HB	1:E:610:PRO:HD3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CE1	1:A:209:THR:HA	2.32	0.64
2:B:587:LEU:HB3	2:B:588:PRO:HA	1.79	0.64
1:C:812:TYR:CE2	1:C:814:ALA:HB2	2.32	0.64
1:C:721:GLY:C	1:C:723:PRO:CD	2.70	0.63
1:A:469:ARG:NH2	2:B:287:HIS:HB2	2.13	0.63
2:H:471:LEU:O	2:H:493:GLY:HA2	1.98	0.63
2:D:161:HIS:HB3	2:D:162:PRO:HA	1.80	0.63
1:E:562:LEU:HD11	1:E:590:GLN:HG2	1.79	0.63
2:F:289:LEU:HD21	2:F:296:PRO:CD	2.29	0.63
2:D:587:LEU:HB3	2:D:588:PRO:HA	1.79	0.63
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.80	0.63
1:G:531:ARG:HA	1:G:563:GLN:O	1.98	0.63
2:H:161:HIS:HB3	2:H:162:PRO:HA	1.80	0.63
1:A:625:VAL:CG2	1:A:627:GLU:HG3	2.29	0.63
1:A:756:HIS:O	1:A:757:ILE:HG22	1.98	0.63
2:B:289:LEU:HD21	2:B:296:PRO:CD	2.29	0.63
2:B:468:SER:HB2	2:B:471:LEU:HG	1.81	0.63
1:A:44:THR:HG22	1:A:71:MET:HG2	1.81	0.63
1:A:250:TYR:HA	1:A:253:VAL:HG22	1.81	0.63
2:F:455:ILE:CG1	2:F:463:THR:CG2	2.76	0.63
2:D:468:SER:HB2	2:D:471:LEU:HG	1.81	0.62
1:G:18:PHE:CE2	1:G:32:VAL:HG21	2.34	0.62
1:E:44:THR:HG22	1:E:71:MET:HG2	1.81	0.62
1:G:812:TYR:CD2	1:G:814:ALA:HB2	2.34	0.62
1:C:18:PHE:CE2	1:C:32:VAL:HG21	2.34	0.62
1:G:119:LEU:N	1:G:120:PRO:CA	2.62	0.62
1:G:609:ILE:HB	1:G:610:PRO:HD3	1.80	0.62
1:A:985:ALA:HB3	1:C:621:ARG:HB2	1.80	0.62
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.80	0.62
1:A:953:TRP:CE2	1:C:755:ASP:HB2	2.35	0.62
1:C:756:HIS:O	1:C:757:ILE:HG22	1.99	0.62
2:H:289:LEU:HD21	2:H:296:PRO:CD	2.29	0.62
1:C:1064:PRO:HG3	1:C:1067:GLU:CG	2.30	0.62
2:D:289:LEU:HD21	2:D:296:PRO:CD	2.29	0.62
1:E:822:LEU:CG	1:E:823:ARG:H	2.10	0.62
1:A:18:PHE:CE2	1:A:32:VAL:HG21	2.34	0.62
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.35	0.62
1:E:18:PHE:CE2	1:E:32:VAL:HG21	2.34	0.62
1:G:406:PRO:HB3	1:G:438:TYR:CE2	2.35	0.62
2:B:115:TYR:HA	2:B:204:ILE:HD13	1.82	0.62
1:E:406:PRO:HB3	1:E:438:TYR:CE2	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:PRO:HG3	1:A:1067:GLU:CG	2.30	0.62
2:D:115:TYR:HA	2:D:204:ILE:HD13	1.82	0.62
2:D:355:THR:HA	2:D:544:PRO:CB	2.29	0.62
2:H:468:SER:HB2	2:H:471:LEU:HG	1.82	0.62
1:C:44:THR:HG22	1:C:71:MET:HG2	1.81	0.61
1:C:406:PRO:HB3	1:C:438:TYR:CE2	2.35	0.61
1:C:562:LEU:HD11	1:C:590:GLN:HG2	1.79	0.61
2:F:468:SER:HB2	2:F:471:LEU:HG	1.81	0.61
1:G:94:HIS:NE2	2:H:155:LEU:HD21	2.15	0.61
2:D:562:ASN:HB2	2:D:563:PRO:HD2	1.82	0.61
6:A:3378:MAN:C1	4:J:5:MAN:O3	2.48	0.61
1:G:44:THR:HG22	1:G:71:MET:HG2	1.81	0.61
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.36	0.61
5:S:2:NAG:C3	5:S:3:MAN:H2	2.30	0.61
2:F:115:TYR:HA	2:F:204:ILE:HD13	1.82	0.61
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.00	0.61
1:C:620:CYS:HB3	1:C:702:SER:C	2.26	0.61
2:D:155:LEU:HB2	2:D:156:PRO:HA	1.83	0.61
1:A:103:LEU:HD11	2:B:155:LEU:HD13	1.82	0.61
1:A:822:LEU:CG	1:A:823:ARG:H	2.10	0.61
2:D:220:GLN:HA	2:D:264:CYS:HB3	1.83	0.61
1:E:1064:PRO:HG3	1:E:1067:GLU:CG	2.30	0.61
2:D:155:LEU:H	2:D:160:THR:HG21	1.66	0.61
2:F:508:TYR:CZ	2:F:514:CYS:HB3	2.36	0.61
1:G:1064:PRO:HG3	1:G:1067:GLU:CG	2.30	0.61
2:H:115:TYR:HA	2:H:204:ILE:HD13	1.82	0.61
2:B:220:GLN:HA	2:B:264:CYS:HB3	1.83	0.61
1:C:491:LEU:C	1:C:491:LEU:HD12	2.26	0.61
1:E:119:LEU:N	1:E:120:PRO:CA	2.63	0.61
1:A:812:TYR:CD2	1:A:814:ALA:HB2	2.35	0.61
2:D:98:ARG:O	2:D:98:ARG:HG2	2.01	0.61
2:F:155:LEU:H	2:F:160:THR:HG21	1.66	0.61
2:H:220:GLN:HA	2:H:264:CYS:HB3	1.83	0.61
2:B:155:LEU:H	2:B:160:THR:HG21	1.66	0.60
2:H:155:LEU:H	2:H:160:THR:HG21	1.66	0.60
2:B:155:LEU:HB2	2:B:156:PRO:HA	1.83	0.60
2:B:562:ASN:HB2	2:B:563:PRO:HD2	1.82	0.60
1:E:599:VAL:HG23	1:E:599:VAL:O	2.01	0.60
2:H:155:LEU:HB2	2:H:156:PRO:HA	1.83	0.60
1:A:491:LEU:C	1:A:491:LEU:HD12	2.26	0.60
1:A:630:LEU:HD21	1:E:653:GLN:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:491:LEU:C	1:E:491:LEU:HD12	2.26	0.60
2:F:220:GLN:HA	2:F:264:CYS:HB3	1.83	0.60
1:G:822:LEU:CG	1:G:823:ARG:H	2.15	0.60
1:A:825:LEU:HD12	1:A:859:PHE:HB3	1.83	0.60
1:G:491:LEU:HD12	1:G:491:LEU:C	2.26	0.60
2:F:98:ARG:O	2:F:98:ARG:HG2	2.02	0.60
2:H:442:PHE:CZ	2:H:449:ARG:HB2	2.36	0.60
2:H:562:ASN:HB2	2:H:563:PRO:HD2	1.83	0.60
1:A:181:HIS:CE1	1:A:200:VAL:HG13	2.37	0.60
2:B:357:LYS:HG3	2:B:544:PRO:HB2	1.83	0.60
2:B:562:ASN:HB3	2:B:589:LEU:HD13	1.84	0.60
2:D:27:LEU:CD2	2:D:446:GLY:HA2	2.32	0.60
2:F:522:TYR:CD1	2:F:552:GLN:HA	2.36	0.60
2:F:562:ASN:HB2	2:F:563:PRO:HD2	1.82	0.60
1:G:825:LEU:HD12	1:G:859:PHE:HB3	1.84	0.60
1:A:715:LEU:HD12	1:A:715:LEU:O	2.02	0.60
1:A:472:GLN:NE2	1:A:492:TYR:HB2	2.17	0.60
2:B:364:CYS:HB2	2:B:368:VAL:HB	1.84	0.60
2:B:442:PHE:CZ	2:B:449:ARG:HB2	2.36	0.60
1:C:1029:LYS:CE	1:E:113:THR:HG22	2.32	0.60
2:D:442:PHE:CZ	2:D:449:ARG:HB2	2.36	0.60
1:A:1020:VAL:HG12	1:A:1021:GLN:HG3	1.84	0.60
2:D:293:ASN:HA	2:D:410:GLY:HA2	1.82	0.60
1:G:715:LEU:O	1:G:715:LEU:HD12	2.02	0.60
2:B:98:ARG:HG2	2:B:98:ARG:O	2.01	0.59
2:D:357:LYS:HE3	2:D:545:GLY:HA2	1.83	0.59
1:E:825:LEU:HD12	1:E:859:PHE:HB3	1.83	0.59
1:E:986:PRO:CB	1:E:987:PRO:HD2	2.32	0.59
1:A:81:THR:O	1:A:82:SER:C	2.45	0.59
1:A:797:GLY:CA	1:A:884:GLU:HB2	2.32	0.59
1:C:822:LEU:CG	1:C:823:ARG:H	2.07	0.59
1:C:986:PRO:CB	1:C:987:PRO:HD2	2.32	0.59
1:C:1064:PRO:CG	1:C:1067:GLU:HG3	2.32	0.59
2:F:155:LEU:HB2	2:F:156:PRO:HA	1.83	0.59
2:F:562:ASN:HB3	2:F:589:LEU:HD13	1.84	0.59
1:G:797:GLY:CA	1:G:884:GLU:HB2	2.32	0.59
1:A:1064:PRO:CG	1:A:1067:GLU:HG3	2.32	0.59
1:C:472:GLN:NE2	1:C:492:TYR:HB2	2.17	0.59
2:D:343:SER:HA	2:D:381:VAL:O	2.03	0.59
2:F:364:CYS:HB2	2:F:368:VAL:HB	1.84	0.59
1:G:513:ASN:HA	1:G:599:VAL:HG22	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:599:VAL:HG23	1:G:599:VAL:O	2.01	0.59
5:P:2:NAG:C3	5:P:3:MAN:H2	2.32	0.59
2:D:162:PRO:O	2:D:164:LYS:N	2.35	0.59
1:E:103:LEU:HD11	2:F:155:LEU:HD13	1.82	0.59
2:F:162:PRO:O	2:F:164:LYS:N	2.35	0.59
2:B:162:PRO:O	2:B:164:LYS:N	2.35	0.59
1:C:812:TYR:CD2	1:C:814:ALA:HB2	2.36	0.59
1:C:825:LEU:HD12	1:C:859:PHE:HB3	1.85	0.59
1:E:681:LEU:C	1:E:681:LEU:HD12	2.28	0.59
2:F:442:PHE:CZ	2:F:449:ARG:HB2	2.37	0.59
1:A:986:PRO:CB	1:A:987:PRO:HD2	2.32	0.59
1:C:484:ARG:CZ	1:C:1021:GLN:HA	2.31	0.59
2:D:27:LEU:HD21	2:D:446:GLY:O	2.03	0.59
1:G:918:TYR:HA	2:H:643:ARG:NH2	2.18	0.59
1:G:986:PRO:CB	1:G:987:PRO:HD2	2.32	0.59
2:H:616:PRO:HB2	2:H:620:ASN:HA	1.84	0.59
2:D:616:PRO:HB2	2:D:620:ASN:HA	1.85	0.59
2:H:364:CYS:HB2	2:H:368:VAL:HB	1.84	0.59
2:D:364:CYS:HB2	2:D:368:VAL:HB	1.84	0.59
1:E:1020:VAL:HG12	1:E:1021:GLN:HG3	1.85	0.59
1:G:1020:VAL:HG12	1:G:1021:GLN:HG3	1.85	0.59
1:G:1064:PRO:CG	1:G:1067:GLU:HG3	2.31	0.59
1:A:674:GLN:HB2	1:A:699:LEU:HD11	1.85	0.59
1:C:81:THR:O	1:C:82:SER:C	2.45	0.59
1:C:681:LEU:C	1:C:681:LEU:HD12	2.28	0.59
1:E:472:GLN:NE2	1:E:492:TYR:HB2	2.17	0.59
1:A:604:VAL:HG11	1:A:742:PHE:CD2	2.38	0.59
1:C:797:GLY:CA	1:C:884:GLU:HB2	2.33	0.59
1:A:599:VAL:HG23	1:A:599:VAL:O	2.01	0.58
2:B:616:PRO:HB2	2:B:620:ASN:HA	1.84	0.58
1:C:374:MET:HG3	1:C:381:MET:SD	2.43	0.58
2:D:6:PHE:HE1	2:D:536:PHE:CB	2.15	0.58
1:E:797:GLY:CA	1:E:884:GLU:HB2	2.32	0.58
1:G:472:GLN:NE2	1:G:492:TYR:HB2	2.17	0.58
1:G:722:LYS:N	1:G:723:PRO:CD	2.66	0.58
2:H:103:TYR:HB3	2:H:104:PRO:HD2	1.85	0.58
1:C:599:VAL:O	1:C:599:VAL:HG23	2.01	0.58
2:D:562:ASN:HB3	2:D:589:LEU:HD13	1.84	0.58
1:E:674:GLN:HB2	1:E:699:LEU:HD11	1.84	0.58
2:F:135:LEU:HD11	2:F:139:THR:HB	1.85	0.58
1:G:604:VAL:HG11	1:G:742:PHE:CD2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:PRO:O	2:H:164:LYS:N	2.36	0.58
1:A:119:LEU:N	1:A:120:PRO:CA	2.66	0.58
1:A:430:VAL:HG21	1:A:487:CYS:SG	2.43	0.58
2:B:471:LEU:O	2:B:493:GLY:HA2	2.03	0.58
1:C:722:LYS:N	1:C:723:PRO:CD	2.66	0.58
1:E:604:VAL:HG11	1:E:742:PHE:CD2	2.39	0.58
1:E:722:LYS:N	1:E:723:PRO:CD	2.66	0.58
1:E:994:HIS:CG	1:E:1005:ILE:HD11	2.38	0.58
2:F:616:PRO:HB2	2:F:620:ASN:HA	1.85	0.58
2:H:98:ARG:HG2	2:H:98:ARG:O	2.02	0.58
2:H:399:ILE:HG13	2:H:421:PRO:HG3	1.85	0.58
2:B:399:ILE:HG13	2:B:421:PRO:HG3	1.85	0.58
1:C:43:GLN:HA	1:C:70:ASN:H	1.68	0.58
1:E:1064:PRO:CG	1:E:1067:GLU:HG3	2.32	0.58
1:G:674:GLN:HB2	1:G:699:LEU:HD11	1.84	0.58
2:H:562:ASN:HB3	2:H:589:LEU:HD13	1.84	0.58
1:A:681:LEU:C	1:A:681:LEU:HD12	2.28	0.58
2:B:468:SER:HB2	2:B:471:LEU:CG	2.34	0.58
1:C:430:VAL:HG21	1:C:487:CYS:SG	2.43	0.58
1:C:715:LEU:HD12	1:C:715:LEU:O	2.03	0.58
2:D:468:SER:HB2	2:D:471:LEU:CG	2.34	0.58
1:E:81:THR:O	1:E:82:SER:C	2.45	0.58
1:E:715:LEU:HD12	1:E:715:LEU:O	2.03	0.58
1:C:604:VAL:HG11	1:C:742:PHE:CD2	2.38	0.58
1:C:674:GLN:HB2	1:C:699:LEU:HD11	1.84	0.58
2:F:103:TYR:HB3	2:F:104:PRO:HD2	1.86	0.58
1:G:81:THR:O	1:G:82:SER:C	2.46	0.58
1:G:833:PRO:HA	1:G:840:TRP:CB	2.34	0.58
1:A:374:MET:HG3	1:A:381:MET:SD	2.44	0.58
1:A:833:PRO:HA	1:A:840:TRP:CB	2.34	0.58
2:B:74:LYS:HD3	2:B:103:TYR:OH	2.04	0.58
2:B:135:LEU:HD11	2:B:139:THR:HB	1.85	0.58
2:F:399:ILE:HG13	2:F:421:PRO:HG3	1.85	0.58
2:H:468:SER:HB2	2:H:471:LEU:CG	2.34	0.58
1:A:953:TRP:CE2	1:C:755:ASP:CB	2.87	0.58
1:A:1044:LYS:HA	1:A:1079:GLU:HB2	1.86	0.58
1:C:1020:VAL:HG12	1:C:1021:GLN:HG3	1.86	0.58
1:G:994:HIS:CG	1:G:1005:ILE:HD11	2.38	0.58
1:A:43:GLN:HA	1:A:70:ASN:H	1.68	0.58
1:A:490:VAL:HG12	1:A:491:LEU:HB3	1.86	0.58
1:C:964:TRP:CB	1:C:1032:LEU:HA	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:LYS:HA	1:C:1079:GLU:HB2	1.86	0.58
2:D:316:PRO:HB3	2:D:346:PHE:CE1	2.38	0.58
1:E:833:PRO:HA	1:E:840:TRP:CB	2.34	0.58
2:H:295:GLN:HG3	2:H:317:LYS:HE2	1.86	0.58
1:C:615:ARG:HA	1:C:618:PHE:HB2	1.86	0.58
1:C:833:PRO:HA	1:C:840:TRP:CB	2.34	0.58
1:A:119:LEU:H	1:A:120:PRO:HA	1.68	0.57
1:A:722:LYS:N	1:A:723:PRO:CD	2.67	0.57
1:A:964:TRP:CB	1:A:1032:LEU:HA	2.34	0.57
1:C:625:VAL:HG23	1:C:626:SER:C	2.29	0.57
1:E:374:MET:HG3	1:E:381:MET:SD	2.44	0.57
1:E:430:VAL:HG21	1:E:487:CYS:SG	2.44	0.57
2:F:155:LEU:H	2:F:160:THR:CG2	2.17	0.57
1:G:681:LEU:HD12	1:G:681:LEU:C	2.29	0.57
1:G:964:TRP:CB	1:G:1032:LEU:HA	2.33	0.57
1:A:253:VAL:HG23	1:A:254:ILE:N	2.18	0.57
2:B:103:TYR:HB3	2:B:104:PRO:HD2	1.84	0.57
2:D:155:LEU:H	2:D:160:THR:CG2	2.18	0.57
2:D:399:ILE:HG13	2:D:421:PRO:HG3	1.85	0.57
1:E:418:THR:HG21	1:E:482:TRP:CZ2	2.39	0.57
2:F:295:GLN:HG3	2:F:317:LYS:HE2	1.86	0.57
1:G:739:GLN:HB2	1:G:742:PHE:CZ	2.39	0.57
1:A:994:HIS:CG	1:A:1005:ILE:HD11	2.39	0.57
2:B:289:LEU:HD21	2:B:296:PRO:HD3	1.86	0.57
2:D:23:TRP:HE1	2:D:445:CYS:HB3	1.70	0.57
2:D:36:ASP:H	2:D:510:GLN:NE2	2.02	0.57
2:D:312:THR:CG2	2:D:344:ARG:HH22	2.16	0.57
2:H:135:LEU:HD11	2:H:139:THR:HB	1.85	0.57
1:A:657:THR:HG22	1:A:684:VAL:HG22	1.87	0.57
2:B:295:GLN:HG3	2:B:317:LYS:HE2	1.86	0.57
1:C:418:THR:HG21	1:C:482:TRP:CZ2	2.39	0.57
1:E:490:VAL:HG12	1:E:491:LEU:HB3	1.86	0.57
1:E:657:THR:HG22	1:E:684:VAL:HG22	1.87	0.57
1:G:430:VAL:HG21	1:G:487:CYS:SG	2.44	0.57
1:G:490:VAL:HG12	1:G:491:LEU:HB3	1.86	0.57
2:H:289:LEU:HD21	2:H:296:PRO:HD3	1.86	0.57
1:A:444:CYS:HB2	1:A:506:LEU:CD1	2.35	0.57
1:C:739:GLN:HB2	1:C:742:PHE:CZ	2.39	0.57
1:G:1044:LYS:HA	1:G:1079:GLU:HB2	1.86	0.57
1:A:93:VAL:O	1:A:103:LEU:HA	2.05	0.57
2:F:453:GLY:O	2:F:462:GLN:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:GLN:HB2	1:A:742:PHE:CZ	2.39	0.57
2:B:155:LEU:H	2:B:160:THR:CG2	2.18	0.57
2:B:347:LEU:HD22	2:B:389:PHE:CD1	2.39	0.57
1:C:89:CYS:C	1:C:91:PRO:HD3	2.30	0.57
2:D:6:PHE:CE1	2:D:536:PHE:CB	2.88	0.57
2:D:6:PHE:CE1	2:D:536:PHE:HB3	2.40	0.57
2:D:295:GLN:HG3	2:D:317:LYS:HE2	1.86	0.57
2:D:587:LEU:HD12	2:D:587:LEU:N	2.20	0.57
1:G:374:MET:HG3	1:G:381:MET:SD	2.44	0.57
1:G:598:PRO:HG3	1:G:650:ARG:NH1	2.19	0.57
2:H:155:LEU:H	2:H:160:THR:CG2	2.17	0.57
1:A:89:CYS:C	1:A:91:PRO:HD3	2.30	0.57
1:E:444:CYS:HB2	1:E:506:LEU:CD1	2.35	0.57
1:E:513:ASN:HA	1:E:599:VAL:CG2	2.35	0.57
2:F:468:SER:HB2	2:F:471:LEU:CG	2.34	0.57
2:H:312:THR:CG2	2:H:344:ARG:HH22	2.18	0.57
2:H:455:ILE:CG1	2:H:463:THR:HG23	2.34	0.57
2:H:455:ILE:HG13	2:H:463:THR:CG2	2.34	0.57
1:A:418:THR:HG21	1:A:482:TRP:CZ2	2.39	0.57
2:B:454:TYR:O	2:B:455:ILE:HD13	2.05	0.57
1:C:119:LEU:N	1:C:120:PRO:CA	2.63	0.57
1:C:490:VAL:HG12	1:C:491:LEU:HB3	1.86	0.57
2:D:341:LEU:C	2:D:343:SER:H	2.13	0.57
1:E:89:CYS:C	1:E:91:PRO:HD3	2.30	0.57
1:E:739:GLN:HB2	1:E:742:PHE:CZ	2.39	0.57
1:E:848:HIS:HB2	2:F:485:SER:HB3	1.86	0.57
1:A:756:HIS:HA	1:C:1052:GLU:OE1	2.04	0.57
1:C:1065:GLY:C	1:C:1066:GLN:HG3	2.30	0.57
1:E:117:GLN:HB3	1:E:121:VAL:HG21	1.86	0.57
1:E:964:TRP:CB	1:E:1032:LEU:HA	2.34	0.57
1:E:1044:LYS:HA	1:E:1079:GLU:HB2	1.86	0.57
1:E:1065:GLY:C	1:E:1066:GLN:HG3	2.30	0.57
1:A:1054:THR:HG21	1:C:757:ILE:HG21	1.87	0.56
1:C:362:LEU:HD23	1:C:362:LEU:C	2.30	0.56
1:G:418:THR:HG21	1:G:482:TRP:CZ2	2.39	0.56
1:G:597:ARG:NH2	1:G:730:LEU:HD12	2.18	0.56
1:E:468:THR:HG23	1:E:498:PRO:HG3	1.87	0.56
2:F:10:SER:HA	2:F:447:ILE:HD11	1.87	0.56
2:F:587:LEU:N	2:F:587:LEU:HD12	2.20	0.56
1:G:117:GLN:HB3	1:G:121:VAL:HG21	1.86	0.56
2:H:75:GLN:CD	2:H:98:ARG:O	2.48	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:SER:HB3	2:B:449:ARG:CZ	2.35	0.56
1:C:93:VAL:O	1:C:103:LEU:HA	2.05	0.56
1:C:117:GLN:HB3	1:C:121:VAL:HG21	1.86	0.56
1:C:444:CYS:HB2	1:C:506:LEU:CD1	2.35	0.56
1:C:468:THR:HG23	1:C:498:PRO:HG3	1.87	0.56
1:C:755:ASP:O	1:C:756:HIS:HB3	2.05	0.56
2:D:103:TYR:HB3	2:D:104:PRO:HD2	1.86	0.56
2:D:355:THR:HG22	2:D:544:PRO:HG2	1.86	0.56
1:E:43:GLN:HA	1:E:70:ASN:H	1.68	0.56
1:E:93:VAL:O	1:E:103:LEU:HA	2.05	0.56
1:E:789:TRP:NE1	1:G:772:LYS:HB3	2.20	0.56
1:G:1:PHE:CE2	1:G:599:VAL:HG11	2.40	0.56
1:G:94:HIS:CD2	2:H:155:LEU:HD21	2.40	0.56
1:G:444:CYS:HB2	1:G:506:LEU:CD1	2.35	0.56
1:A:117:GLN:HB3	1:A:121:VAL:HG21	1.86	0.56
2:B:587:LEU:HD12	2:B:587:LEU:N	2.20	0.56
2:D:135:LEU:HD11	2:D:139:THR:HB	1.85	0.56
1:E:364:PRO:CB	1:E:365:PRO:HD2	2.36	0.56
1:G:89:CYS:C	1:G:91:PRO:HD3	2.30	0.56
1:G:747:PRO:HB3	1:G:884:GLU:HG2	1.87	0.56
2:H:587:LEU:N	2:H:587:LEU:HD12	2.20	0.56
1:C:394:LEU:HD23	1:C:395:TRP:N	2.20	0.56
1:E:598:PRO:HB3	1:E:650:ARG:NH1	2.20	0.56
2:F:23:TRP:CH2	2:F:447:ILE:HD13	2.41	0.56
1:G:362:LEU:HD23	1:G:362:LEU:C	2.30	0.56
2:D:75:GLN:CD	2:D:98:ARG:O	2.49	0.56
1:E:394:LEU:HD23	1:E:395:TRP:N	2.21	0.56
1:E:963:VAL:HA	1:E:1036:TRP:CD1	2.41	0.56
2:F:289:LEU:HD21	2:F:296:PRO:HD3	1.86	0.56
1:G:394:LEU:HD23	1:G:395:TRP:N	2.21	0.56
1:G:468:THR:HG23	1:G:498:PRO:HG3	1.87	0.56
2:D:456:GLY:CA	2:D:494:GLN:OE1	2.53	0.56
1:E:362:LEU:HD23	1:E:362:LEU:C	2.30	0.56
1:E:741:TYR:CD2	2:F:502:VAL:HG22	2.41	0.56
1:G:598:PRO:HB3	1:G:650:ARG:NH1	2.21	0.56
2:H:295:GLN:CG	2:H:317:LYS:HE2	2.36	0.56
1:A:156:ARG:HB3	1:A:197:LEU:HD13	1.87	0.56
1:C:908:VAL:O	1:C:938:VAL:HG23	2.06	0.56
1:C:941:LEU:N	1:C:941:LEU:HD12	2.21	0.56
1:E:32:VAL:HG11	1:E:591:VAL:HG11	1.88	0.56
2:F:10:SER:HB3	2:F:449:ARG:NE	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:PRO:CB	1:G:365:PRO:HD2	2.36	0.56
1:G:833:PRO:HA	1:G:840:TRP:HB2	1.88	0.56
1:G:908:VAL:O	1:G:938:VAL:HG23	2.06	0.56
1:A:394:LEU:HD23	1:A:395:TRP:N	2.21	0.56
2:D:289:LEU:HD21	2:D:296:PRO:HD3	1.86	0.56
1:E:919:LEU:O	2:F:643:ARG:NH1	2.35	0.56
2:F:454:TYR:O	2:F:455:ILE:HD13	2.06	0.56
1:G:43:GLN:HA	1:G:70:ASN:H	1.68	0.56
1:A:32:VAL:HG11	1:A:591:VAL:HG11	1.88	0.56
1:A:963:VAL:HA	1:A:1036:TRP:CD1	2.41	0.56
2:B:146:PHE:HB2	2:B:195:PHE:CZ	2.41	0.56
1:C:332:MET:SD	2:D:208:LEU:HD13	2.45	0.56
1:C:994:HIS:CG	1:C:1005:ILE:HD11	2.41	0.56
1:G:93:VAL:O	1:G:103:LEU:HA	2.06	0.56
1:G:578:ASP:OD2	1:G:595:ARG:HD2	2.06	0.56
1:G:657:THR:HG22	1:G:684:VAL:HG22	1.87	0.56
1:C:578:ASP:OD2	1:C:595:ARG:HD2	2.06	0.55
1:E:575:LEU:HD12	1:E:576:THR:N	2.22	0.55
1:G:333:ALA:HB1	1:G:350:ALA:HB1	1.89	0.55
1:G:597:ARG:HG3	1:G:731:ARG:CG	2.36	0.55
1:G:941:LEU:HD12	1:G:941:LEU:N	2.21	0.55
1:A:362:LEU:HD23	1:A:362:LEU:C	2.30	0.55
2:B:75:GLN:CD	2:B:98:ARG:O	2.49	0.55
1:E:363:TYR:CD1	1:E:369:PRO:HB3	2.41	0.55
1:E:824:SER:H	1:E:825:LEU:HG	1.72	0.55
2:F:260:ASN:HA	2:F:277:PHE:CE2	2.42	0.55
2:H:146:PHE:HB2	2:H:195:PHE:CZ	2.41	0.55
1:A:122:SER:O	1:A:123:ARG:C	2.50	0.55
1:C:364:PRO:CB	1:C:365:PRO:HD2	2.36	0.55
1:E:416:ILE:HD11	1:E:485:TRP:CZ2	2.42	0.55
1:E:578:ASP:OD2	1:E:595:ARG:HD2	2.06	0.55
2:H:10:SER:HB3	2:H:449:ARG:CZ	2.36	0.55
1:A:169:PHE:HB2	1:A:187:PHE:CE1	2.41	0.55
1:C:32:VAL:HG11	1:C:591:VAL:HG11	1.88	0.55
1:C:479:PRO:HD2	1:C:485:TRP:CD1	2.42	0.55
1:E:446:VAL:HG21	1:E:520:VAL:CG1	2.37	0.55
1:E:941:LEU:N	1:E:941:LEU:HD12	2.21	0.55
1:G:963:VAL:HA	1:G:1036:TRP:CD1	2.41	0.55
1:G:1065:GLY:C	1:G:1066:GLN:HG3	2.30	0.55
1:C:786:VAL:HG11	1:C:859:PHE:CZ	2.42	0.55
1:C:1029:LYS:HE2	1:E:113:THR:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:THR:HG21	2:D:539:LYS:NZ	2.21	0.55
1:E:786:VAL:HG11	1:E:859:PHE:CZ	2.42	0.55
1:E:908:VAL:O	1:E:938:VAL:HG23	2.05	0.55
2:F:295:GLN:CG	2:F:317:LYS:HE2	2.36	0.55
1:G:32:VAL:HG11	1:G:591:VAL:HG11	1.88	0.55
1:G:513:ASN:HB2	1:G:599:VAL:HG21	1.87	0.55
1:A:363:TYR:CD1	1:A:369:PRO:HB3	2.41	0.55
1:A:513:ASN:HA	1:A:599:VAL:HG21	1.89	0.55
1:A:908:VAL:O	1:A:938:VAL:HG23	2.06	0.55
1:C:68:ALA:HB1	1:C:71:MET:HE2	1.89	0.55
1:E:122:SER:O	1:E:123:ARG:C	2.50	0.55
2:F:146:PHE:HB2	2:F:195:PHE:CZ	2.41	0.55
1:G:786:VAL:HG11	1:G:859:PHE:CZ	2.42	0.55
2:H:260:ASN:HA	2:H:277:PHE:CE2	2.42	0.55
1:A:416:ILE:HD11	1:A:485:TRP:CZ2	2.42	0.55
1:A:468:THR:HG23	1:A:498:PRO:HG3	1.87	0.55
1:A:575:LEU:HD12	1:A:576:THR:N	2.22	0.55
1:A:615:ARG:HA	1:A:618:PHE:HB2	1.88	0.55
1:C:416:ILE:HD11	1:C:485:TRP:CZ2	2.42	0.55
1:C:963:VAL:HA	1:C:1036:TRP:CD1	2.41	0.55
2:D:347:LEU:HD22	2:D:389:PHE:CD1	2.42	0.55
1:E:333:ALA:HB1	1:E:350:ALA:HB1	1.88	0.55
1:G:513:ASN:HA	1:G:599:VAL:CG2	2.36	0.55
1:G:575:LEU:HD12	1:G:576:THR:N	2.21	0.55
1:A:618:PHE:CE2	1:A:619:GLU:HG3	2.42	0.55
1:A:786:VAL:HG11	1:A:859:PHE:CZ	2.42	0.55
2:B:295:GLN:CG	2:B:317:LYS:HE2	2.36	0.55
1:C:446:VAL:HG21	1:C:520:VAL:CG1	2.37	0.55
1:C:657:THR:HG22	1:C:684:VAL:HG22	1.87	0.55
1:C:716:ASN:C	1:C:716:ASN:OD1	2.50	0.55
2:D:260:ASN:HA	2:D:277:PHE:CE2	2.42	0.55
2:D:355:THR:HA	2:D:544:PRO:HB3	1.89	0.55
1:E:68:ALA:HB1	1:E:71:MET:HE2	1.89	0.55
1:A:941:LEU:HD12	1:A:941:LEU:N	2.21	0.55
2:D:295:GLN:CG	2:D:317:LYS:HE2	2.36	0.55
1:E:479:PRO:HD2	1:E:485:TRP:CD1	2.42	0.55
1:E:716:ASN:C	1:E:716:ASN:OD1	2.50	0.55
1:E:833:PRO:HA	1:E:840:TRP:HB2	1.89	0.55
1:A:364:PRO:CB	1:A:365:PRO:HD2	2.36	0.55
1:A:917:LYS:HE3	1:A:1077:VAL:CG2	2.37	0.55
1:A:1065:GLY:C	1:A:1066:GLN:HG3	2.30	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:ASN:HA	2:B:277:PHE:CE2	2.42	0.55
1:C:363:TYR:CD1	1:C:369:PRO:HB3	2.41	0.55
2:F:75:GLN:CD	2:F:98:ARG:O	2.49	0.55
2:F:347:LEU:HD22	2:F:389:PHE:CD1	2.42	0.55
1:G:70:ASN:HB3	1:G:94:HIS:ND1	2.22	0.55
1:G:122:SER:O	1:G:123:ARG:C	2.50	0.55
1:G:363:TYR:CD1	1:G:369:PRO:HB3	2.41	0.55
2:H:673:CYS:O	2:H:674:VAL:C	2.50	0.55
1:A:479:PRO:HD2	1:A:485:TRP:CD1	2.42	0.54
2:B:161:HIS:HB3	2:B:162:PRO:CA	2.37	0.54
1:C:70:ASN:HB3	1:C:94:HIS:ND1	2.22	0.54
1:C:876:LEU:HD12	1:C:876:LEU:C	2.32	0.54
2:D:146:PHE:HB2	2:D:195:PHE:CZ	2.41	0.54
1:E:615:ARG:HA	1:E:618:PHE:HB2	1.88	0.54
1:C:333:ALA:HB1	1:C:350:ALA:HB1	1.88	0.54
1:C:619:GLU:O	1:C:620:CYS:SG	2.65	0.54
2:D:161:HIS:HB3	2:D:162:PRO:CA	2.37	0.54
1:E:70:ASN:HB3	1:E:94:HIS:ND1	2.22	0.54
1:E:459:ILE:HD12	1:E:487:CYS:SG	2.47	0.54
2:F:115:TYR:CD1	2:F:170:PRO:HD2	2.43	0.54
1:A:459:ILE:HD12	1:A:487:CYS:SG	2.48	0.54
1:C:741:TYR:CD2	2:D:502:VAL:HG13	2.42	0.54
2:F:161:HIS:HB3	2:F:162:PRO:CA	2.37	0.54
1:G:528:GLU:HB2	1:G:531:ARG:HB2	1.90	0.54
1:G:716:ASN:C	1:G:716:ASN:OD1	2.50	0.54
2:H:161:HIS:HB3	2:H:162:PRO:CA	2.37	0.54
1:A:70:ASN:HB3	1:A:94:HIS:ND1	2.22	0.54
2:B:115:TYR:CD1	2:B:170:PRO:HD2	2.43	0.54
2:D:426:ARG:CZ	2:D:426:ARG:HB3	2.37	0.54
1:G:416:ILE:HD11	1:G:485:TRP:CZ2	2.42	0.54
1:G:615:ARG:HA	1:G:618:PHE:HB2	1.89	0.54
1:A:68:ALA:HB1	1:A:71:MET:HE2	1.90	0.54
2:B:654:LEU:HD13	2:B:665:ILE:HG13	1.90	0.54
1:C:917:LYS:HE3	1:C:1077:VAL:CG2	2.37	0.54
1:E:624:VAL:HG23	1:E:625:VAL:H	1.73	0.54
1:G:68:ALA:HB1	1:G:71:MET:HE2	1.89	0.54
1:G:917:LYS:HE3	1:G:1077:VAL:CG2	2.38	0.54
2:H:520:GLU:HB3	2:H:550:ALA:HB2	1.90	0.54
1:A:578:ASP:OD2	1:A:595:ARG:HD2	2.07	0.54
1:A:986:PRO:CB	1:A:987:PRO:CD	2.86	0.54
2:H:110:LEU:HD11	2:H:237:LEU:HD23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:GLU:O	2:B:594:PRO:HD3	2.08	0.54
1:C:459:ILE:HD12	1:C:487:CYS:SG	2.47	0.54
1:C:575:LEU:HD12	1:C:576:THR:N	2.22	0.54
1:E:917:LYS:HE3	1:E:1077:VAL:CG2	2.38	0.54
1:G:2:ASN:HB2	1:G:597:ARG:O	2.08	0.54
1:G:459:ILE:HD12	1:G:487:CYS:SG	2.48	0.54
1:G:479:PRO:HD2	1:G:485:TRP:CD1	2.42	0.54
1:G:876:LEU:C	1:G:876:LEU:HD12	2.33	0.54
2:H:454:TYR:O	2:H:455:ILE:HD13	2.08	0.54
1:A:716:ASN:C	1:A:716:ASN:OD1	2.49	0.54
1:A:833:PRO:HA	1:A:840:TRP:HB2	1.88	0.54
1:C:650:ARG:CD	1:C:729:ASN:CB	2.86	0.54
2:F:520:GLU:HB3	2:F:550:ALA:HB2	1.89	0.54
1:A:333:ALA:HB1	1:A:350:ALA:HB1	1.89	0.54
1:A:804:HIS:HB2	1:A:808:LEU:HD11	1.90	0.54
2:D:520:GLU:HB3	2:D:550:ALA:HB2	1.89	0.54
1:E:491:LEU:HD11	1:E:545:ILE:CD1	2.38	0.54
1:E:876:LEU:C	1:E:876:LEU:HD12	2.33	0.54
1:E:905:VAL:HG11	1:E:946:LEU:HD21	1.90	0.54
2:F:100:ALA:C	2:F:101:LYS:HG3	2.32	0.54
2:H:347:LEU:HD22	2:H:389:PHE:CD1	2.43	0.54
2:H:455:ILE:CG1	2:H:463:THR:CG2	2.86	0.54
1:C:833:PRO:HA	1:C:840:TRP:HB2	1.89	0.54
1:G:446:VAL:HG21	1:G:520:VAL:CG1	2.37	0.54
1:G:816:GLY:O	1:G:818:LYS:CA	2.56	0.54
2:H:115:TYR:CD1	2:H:170:PRO:HD2	2.43	0.54
2:H:562:ASN:HB2	2:H:563:PRO:CD	2.38	0.54
2:H:654:LEU:HD13	2:H:665:ILE:HG13	1.90	0.54
1:A:741:TYR:CD2	2:B:502:VAL:HG22	2.43	0.53
1:A:905:VAL:HG11	1:A:946:LEU:HD21	1.90	0.53
2:B:562:ASN:HB2	2:B:563:PRO:CD	2.38	0.53
1:C:25:TYR:CE1	1:C:86:LEU:HB2	2.44	0.53
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.42	0.53
1:G:624:VAL:HG23	1:G:625:VAL:H	1.73	0.53
4:J:1:NAG:H3	4:J:2:NAG:N2	2.22	0.53
1:A:513:ASN:HA	1:A:599:VAL:CG2	2.38	0.53
1:A:876:LEU:C	1:A:876:LEU:HD12	2.33	0.53
1:C:122:SER:O	1:C:123:ARG:C	2.50	0.53
1:E:908:VAL:HG13	1:E:1069:PHE:HB3	1.90	0.53
1:G:80:THR:HB	1:G:341:PHE:CG	2.43	0.53
1:G:602:VAL:HG23	1:G:638:TYR:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLU:HB2	1:A:531:ARG:HB2	1.90	0.53
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.91	0.53
1:A:908:VAL:HG13	1:A:1069:PHE:HB3	1.90	0.53
2:B:110:LEU:HD11	2:B:237:LEU:HD23	1.90	0.53
1:C:908:VAL:HG13	1:C:1069:PHE:HB3	1.90	0.53
2:D:454:TYR:CE2	2:D:462:GLN:HG3	2.43	0.53
1:E:81:THR:O	1:E:82:SER:O	2.26	0.53
1:E:453:SER:O	1:E:454:THR:C	2.51	0.53
2:H:453:GLY:O	2:H:462:GLN:HG3	2.07	0.53
1:A:446:VAL:HG21	1:A:520:VAL:CG1	2.37	0.53
1:A:484:ARG:HD2	2:B:594:PRO:HG2	1.87	0.53
1:A:602:VAL:HG23	1:A:638:TYR:O	2.09	0.53
2:B:520:GLU:HB3	2:B:550:ALA:HB2	1.89	0.53
1:C:725:LEU:HG	1:C:726:ALA:N	2.23	0.53
2:D:6:PHE:HE1	2:D:536:PHE:HB2	1.73	0.53
2:D:35:PRO:CB	2:D:510:GLN:HE22	2.21	0.53
2:D:211:PRO:HB2	2:D:246:HIS:CE1	2.44	0.53
1:E:804:HIS:HB2	1:E:808:LEU:HD11	1.90	0.53
1:G:597:ARG:CG	1:G:731:ARG:HG2	2.37	0.53
1:G:725:LEU:HG	1:G:726:ALA:N	2.24	0.53
1:G:804:HIS:HB2	1:G:808:LEU:HD11	1.90	0.53
1:G:905:VAL:HG21	1:G:946:LEU:HD22	1.91	0.53
1:A:80:THR:HB	1:A:341:PHE:CG	2.43	0.53
1:A:559:SER:O	1:A:560:SER:C	2.52	0.53
1:C:780:LEU:O	1:C:865:VAL:HG12	2.09	0.53
1:E:618:PHE:CE2	1:E:619:GLU:HG3	2.44	0.53
5:P:1:NAG:H3	5:P:2:NAG:N2	2.23	0.53
1:A:81:THR:O	1:A:82:SER:O	2.27	0.53
1:C:80:THR:HB	1:C:341:PHE:CG	2.43	0.53
1:C:475:VAL:HG11	1:C:491:LEU:HG	1.90	0.53
1:C:491:LEU:HD11	1:C:545:ILE:CD1	2.38	0.53
1:C:710:PRO:HG3	1:C:884:GLU:OE2	2.09	0.53
2:D:363:PHE:CE2	2:D:369:THR:HG23	2.44	0.53
1:E:80:THR:HB	1:E:341:PHE:CG	2.43	0.53
1:E:94:HIS:NE2	2:F:155:LEU:HD21	2.24	0.53
1:E:528:GLU:HB2	1:E:531:ARG:HB2	1.90	0.53
1:E:905:VAL:HG21	1:E:946:LEU:HD22	1.91	0.53
1:E:920:ASN:OD1	1:E:1080:LYS:HE2	2.09	0.53
1:G:600:LEU:HD12	1:G:600:LEU:O	2.09	0.53
1:A:491:LEU:HD11	1:A:545:ILE:CD1	2.38	0.53
1:A:506:LEU:HA	1:A:569:LEU:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:PHE:CE2	2:B:369:THR:HG23	2.44	0.53
1:C:528:GLU:HB2	1:C:531:ARG:HB2	1.90	0.53
2:D:15:ILE:HG23	2:D:86:ARG:CZ	2.39	0.53
2:D:562:ASN:HB2	2:D:563:PRO:CD	2.38	0.53
1:E:465:TYR:CG	1:E:469:ARG:HG3	2.44	0.53
1:G:559:SER:O	1:G:560:SER:C	2.52	0.53
2:H:363:PHE:CE2	2:H:369:THR:HG23	2.44	0.53
1:C:908:VAL:HG11	2:D:595:GLY:CA	2.36	0.53
1:E:506:LEU:HA	1:E:569:LEU:HD11	1.91	0.53
1:E:725:LEU:HG	1:E:726:ALA:N	2.23	0.53
1:E:756:HIS:O	1:E:756:HIS:CG	2.61	0.53
2:F:562:ASN:HB2	2:F:563:PRO:CD	2.38	0.53
2:F:604:ILE:HD11	2:F:642:GLU:HB2	1.91	0.53
1:G:491:LEU:HD11	1:G:545:ILE:CD1	2.38	0.53
1:C:476:CYS:CB	1:C:487:CYS:HA	2.39	0.53
1:C:559:SER:O	1:C:560:SER:C	2.52	0.53
1:C:624:VAL:HG23	1:C:625:VAL:N	2.24	0.53
1:C:986:PRO:CB	1:C:987:PRO:CD	2.87	0.53
2:F:110:LEU:HD11	2:F:237:LEU:HD23	1.90	0.53
2:F:363:PHE:CE2	2:F:369:THR:HG23	2.44	0.53
1:G:905:VAL:HG11	1:G:946:LEU:HD21	1.91	0.53
1:A:25:TYR:CE1	1:A:86:LEU:HB2	2.43	0.53
2:B:83:LEU:HD13	2:B:85:LEU:HB2	1.91	0.53
1:C:94:HIS:CD2	2:D:155:LEU:HD21	2.44	0.53
2:D:289:LEU:HD23	2:D:315:ILE:HD11	1.91	0.53
1:E:25:TYR:CE1	1:E:86:LEU:HB2	2.43	0.53
1:E:559:SER:O	1:E:560:SER:C	2.52	0.53
1:G:453:SER:O	1:G:454:THR:C	2.51	0.53
1:A:475:VAL:HG11	1:A:491:LEU:HG	1.90	0.52
1:E:789:TRP:CZ2	1:G:771:LEU:O	2.61	0.52
1:E:986:PRO:CB	1:E:987:PRO:CD	2.87	0.52
2:F:592:GLU:O	2:F:594:PRO:HD3	2.09	0.52
1:G:25:TYR:O	1:G:26:ALA:C	2.52	0.52
1:G:506:LEU:HA	1:G:569:LEU:HD11	1.91	0.52
1:G:756:HIS:O	1:G:756:HIS:CG	2.62	0.52
1:A:47:LEU:HB2	1:A:60:ILE:HG21	1.91	0.52
1:A:465:TYR:CG	1:A:469:ARG:HG3	2.44	0.52
2:B:285:LEU:O	2:B:289:LEU:HB3	2.09	0.52
2:B:401:GLU:HA	2:B:421:PRO:HD3	1.92	0.52
1:C:47:LEU:HB2	1:C:60:ILE:HG21	1.91	0.52
1:C:453:SER:O	1:C:454:THR:C	2.51	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:TYR:CG	1:C:469:ARG:HG3	2.44	0.52
2:D:654:LEU:HD13	2:D:665:ILE:HG13	1.90	0.52
2:F:104:PRO:HD2	2:F:233:VAL:HG11	1.91	0.52
2:H:83:LEU:HD13	2:H:85:LEU:HB2	1.91	0.52
1:A:453:SER:O	1:A:454:THR:C	2.52	0.52
1:A:920:ASN:OD1	1:A:1080:LYS:HE2	2.09	0.52
2:B:105:ILE:HG21	2:B:135:LEU:HD13	1.91	0.52
2:B:211:PRO:HB2	2:B:246:HIS:CE1	2.44	0.52
2:B:455:ILE:HG12	2:B:463:THR:HG23	1.91	0.52
1:C:600:LEU:HD12	1:C:600:LEU:O	2.10	0.52
1:C:602:VAL:HG23	1:C:638:TYR:O	2.09	0.52
1:E:47:LEU:HB2	1:E:60:ILE:HG21	1.91	0.52
2:F:105:ILE:HG12	2:F:106:ASP:N	2.24	0.52
1:G:465:TYR:CG	1:G:469:ARG:HG3	2.44	0.52
1:G:475:VAL:HG11	1:G:491:LEU:HG	1.90	0.52
2:H:43:ARG:HB3	2:H:44:PRO:HD3	1.92	0.52
2:H:285:LEU:O	2:H:289:LEU:HB3	2.10	0.52
2:H:570:GLY:HA2	2:H:659:GLY:HA2	1.91	0.52
2:H:592:GLU:O	2:H:594:PRO:HD3	2.09	0.52
1:A:465:TYR:HB3	1:A:469:ARG:HA	1.91	0.52
1:A:824:SER:H	1:A:825:LEU:HG	1.74	0.52
2:B:317:LYS:HE3	2:B:410:GLY:CA	2.40	0.52
2:B:505:LYS:HA	2:B:517:ILE:CG2	2.40	0.52
1:C:364:PRO:HB3	1:C:365:PRO:HD2	1.92	0.52
2:D:43:ARG:HB3	2:D:44:PRO:HD3	1.91	0.52
1:E:82:SER:CB	1:E:83:PRO:CD	2.88	0.52
1:E:476:CYS:CB	1:E:487:CYS:HA	2.40	0.52
1:E:671:ALA:HB2	1:E:700:LEU:HD23	1.92	0.52
1:E:780:LEU:O	1:E:865:VAL:HG12	2.10	0.52
2:F:591:GLN:HG2	2:F:592:GLU:N	2.25	0.52
1:G:47:LEU:HB2	1:G:60:ILE:HG21	1.91	0.52
1:A:624:VAL:HG23	1:A:625:VAL:H	1.74	0.52
2:B:295:GLN:CD	2:B:317:LYS:HE2	2.35	0.52
1:C:804:HIS:HB2	1:C:808:LEU:HD11	1.90	0.52
2:D:654:LEU:CD1	2:D:665:ILE:HG13	2.40	0.52
2:F:211:PRO:HB2	2:F:246:HIS:CE1	2.44	0.52
1:G:598:PRO:CB	1:G:650:ARG:NH1	2.73	0.52
1:A:82:SER:CB	1:A:83:PRO:CD	2.88	0.52
1:A:713:LEU:HD23	1:A:713:LEU:C	2.35	0.52
2:B:289:LEU:HD23	2:B:315:ILE:HD11	1.91	0.52
1:C:928:GLU:HG3	1:C:929:SER:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:PRO:HB3	2:D:510:GLN:OE1	2.09	0.52
1:E:475:VAL:HG11	1:E:491:LEU:HG	1.90	0.52
1:E:566:GLY:O	1:E:567:GLN:C	2.53	0.52
1:E:602:VAL:HG23	1:E:638:TYR:O	2.09	0.52
1:E:619:GLU:O	1:E:620:CYS:SG	2.68	0.52
2:F:654:LEU:HD13	2:F:665:ILE:HG13	1.90	0.52
1:G:490:VAL:HG12	1:G:491:LEU:CB	2.39	0.52
1:G:671:ALA:HB2	1:G:700:LEU:HD23	1.92	0.52
1:G:908:VAL:HG13	1:G:1069:PHE:HB3	1.90	0.52
2:H:104:PRO:HD2	2:H:233:VAL:HG11	1.91	0.52
1:A:333:ALA:HA	1:A:352:GLY:H	1.75	0.52
1:A:656:VAL:HG21	1:A:687:LEU:CD1	2.40	0.52
1:C:465:TYR:HB3	1:C:469:ARG:HA	1.91	0.52
1:C:905:VAL:HG21	1:C:946:LEU:HD22	1.91	0.52
2:D:105:ILE:HG12	2:D:106:ASP:N	2.24	0.52
2:D:592:GLU:O	2:D:594:PRO:HD3	2.09	0.52
1:G:364:PRO:HB3	1:G:365:PRO:HD2	1.92	0.52
1:G:484:ARG:HH12	2:H:586:GLN:HG3	1.75	0.52
5:S:1:NAG:H3	5:S:2:NAG:N2	2.24	0.52
1:A:1055:PHE:CE2	1:A:1070:MET:HE1	2.45	0.52
2:B:105:ILE:HG12	2:B:106:ASP:N	2.25	0.52
1:C:81:THR:O	1:C:82:SER:O	2.27	0.52
1:C:566:GLY:O	1:C:567:GLN:C	2.53	0.52
2:D:83:LEU:HD13	2:D:85:LEU:HB2	1.91	0.52
2:D:110:LEU:HD11	2:D:237:LEU:HD23	1.90	0.52
2:D:285:LEU:O	2:D:289:LEU:HB3	2.09	0.52
1:E:44:THR:CG2	1:E:71:MET:HE3	2.40	0.52
1:A:44:THR:CG2	1:A:71:MET:HE3	2.40	0.52
1:A:490:VAL:HG12	1:A:491:LEU:CB	2.39	0.52
1:A:650:ARG:CD	1:A:729:ASN:CB	2.87	0.52
2:B:345:VAL:HG11	2:B:387:ILE:CD1	2.40	0.52
1:C:565:PHE:HB2	1:C:587:ALA:HB2	1.92	0.52
1:C:905:VAL:HG11	1:C:946:LEU:HD21	1.90	0.52
1:C:920:ASN:OD1	1:C:1080:LYS:HE2	2.09	0.52
2:D:105:ILE:HG21	2:D:135:LEU:HD13	1.91	0.52
2:D:270:LEU:HD23	2:D:271:TYR:O	2.10	0.52
2:D:450:CYS:HB2	2:D:454:TYR:O	2.10	0.52
1:E:25:TYR:O	1:E:26:ALA:C	2.52	0.52
1:E:465:TYR:HB3	1:E:469:ARG:HA	1.91	0.52
1:E:650:ARG:CD	1:E:729:ASN:HB3	2.36	0.52
1:E:912:HIS:ND1	1:E:935:ARG:HD2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:289:LEU:HD23	2:F:315:ILE:HD11	1.91	0.52
1:G:476:CYS:CB	1:G:487:CYS:HA	2.40	0.52
1:G:619:GLU:O	1:G:620:CYS:SG	2.67	0.52
1:G:824:SER:H	1:G:825:LEU:HG	1.74	0.52
2:H:270:LEU:HD23	2:H:271:TYR:O	2.10	0.52
2:H:289:LEU:HD23	2:H:315:ILE:HD11	1.91	0.52
1:A:600:LEU:O	1:A:600:LEU:HD12	2.09	0.52
1:A:665:GLY:HA3	2:B:498:HIS:HB3	1.92	0.52
1:A:671:ALA:HB2	1:A:700:LEU:HD23	1.92	0.52
1:A:878:THR:HG22	1:A:896:GLN:HB3	1.92	0.52
2:B:104:PRO:HD2	2:B:233:VAL:HG11	1.91	0.52
2:B:270:LEU:HD23	2:B:271:TYR:O	2.11	0.52
1:C:82:SER:CB	1:C:83:PRO:CD	2.88	0.52
1:C:333:ALA:HA	1:C:352:GLY:H	1.75	0.52
1:C:490:VAL:HG12	1:C:491:LEU:CB	2.39	0.52
1:C:506:LEU:HA	1:C:569:LEU:HD11	1.91	0.52
2:D:401:GLU:HA	2:D:421:PRO:HD3	1.92	0.52
2:D:454:TYR:O	2:D:455:ILE:HD13	2.10	0.52
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.45	0.52
2:D:591:GLN:HG2	2:D:592:GLU:N	2.25	0.52
2:D:604:ILE:HD11	2:D:642:GLU:HB2	1.91	0.52
1:E:82:SER:HB2	1:E:83:PRO:CD	2.40	0.52
2:F:285:LEU:O	2:F:289:LEU:HB3	2.10	0.52
1:G:565:PHE:HB2	1:G:587:ALA:HB2	1.92	0.52
2:H:316:PRO:HB3	2:H:346:PHE:CE1	2.44	0.52
2:H:654:LEU:CD1	2:H:665:ILE:HG13	2.40	0.52
1:A:25:TYR:O	1:A:26:ALA:C	2.52	0.51
1:A:82:SER:HB2	1:A:83:PRO:CD	2.40	0.51
1:A:725:LEU:HG	1:A:726:ALA:N	2.25	0.51
2:B:591:GLN:HG2	2:B:592:GLU:N	2.25	0.51
1:C:44:THR:CG2	1:C:71:MET:HE3	2.40	0.51
1:C:364:PRO:CB	1:C:365:PRO:CD	2.89	0.51
1:E:565:PHE:HB2	1:E:587:ALA:HB2	1.92	0.51
2:F:83:LEU:HD13	2:F:85:LEU:HB2	1.91	0.51
1:G:637:LEU:HD11	1:G:658:LEU:HD21	1.92	0.51
1:G:650:ARG:CD	1:G:729:ASN:CB	2.88	0.51
1:G:656:VAL:HG21	1:G:687:LEU:CD1	2.40	0.51
1:G:780:LEU:O	1:G:865:VAL:HG12	2.09	0.51
1:G:912:HIS:ND1	1:G:935:ARG:HD2	2.25	0.51
2:H:105:ILE:HG21	2:H:135:LEU:HD13	1.91	0.51
1:A:364:PRO:HB3	1:A:365:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:SER:O	1:A:650:ARG:HB3	2.11	0.51
2:B:43:ARG:HB3	2:B:44:PRO:HD3	1.92	0.51
2:B:654:LEU:CD1	2:B:665:ILE:HG13	2.40	0.51
1:C:624:VAL:HG23	1:C:625:VAL:H	1.75	0.51
2:D:295:GLN:CD	2:D:317:LYS:HE2	2.36	0.51
1:E:780:LEU:C	1:E:780:LEU:HD23	2.35	0.51
2:F:135:LEU:CD1	2:F:139:THR:HB	2.41	0.51
1:G:333:ALA:HA	1:G:352:GLY:H	1.75	0.51
2:H:211:PRO:HB2	2:H:246:HIS:CE1	2.44	0.51
1:A:566:GLY:O	1:A:567:GLN:C	2.53	0.51
1:A:637:LEU:HD11	1:A:658:LEU:HD21	1.93	0.51
1:A:780:LEU:O	1:A:865:VAL:HG12	2.09	0.51
1:C:491:LEU:HD12	1:C:492:TYR:N	2.26	0.51
1:C:637:LEU:HD11	1:C:658:LEU:HD21	1.92	0.51
1:E:469:ARG:NH2	2:F:287:HIS:HB2	2.24	0.51
1:E:600:LEU:HD12	1:E:600:LEU:O	2.09	0.51
1:E:637:LEU:HD11	1:E:658:LEU:HD21	1.93	0.51
2:F:6:PHE:O	2:F:8:VAL:HG23	2.11	0.51
2:F:184:HIS:CE1	2:F:228:ILE:HG23	2.46	0.51
2:F:508:TYR:CE1	2:F:514:CYS:HB3	2.46	0.51
1:G:44:THR:CG2	1:G:71:MET:HE3	2.41	0.51
1:G:465:TYR:HB3	1:G:469:ARG:HA	1.91	0.51
1:G:920:ASN:OD1	1:G:1080:LYS:HE2	2.09	0.51
1:G:986:PRO:CB	1:G:987:PRO:CD	2.87	0.51
1:G:986:PRO:HB3	1:G:987:PRO:HD2	1.93	0.51
2:H:105:ILE:HG12	2:H:106:ASP:N	2.24	0.51
4:J:2:NAG:C3	4:J:3:MAN:H2	2.39	0.51
1:A:532:GLY:HA3	1:A:565:PHE:HD2	1.76	0.51
2:B:98:ARG:O	2:B:99:ARG:C	2.53	0.51
2:B:184:HIS:CE1	2:B:228:ILE:HG23	2.46	0.51
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.45	0.51
1:C:756:HIS:O	1:C:756:HIS:CG	2.63	0.51
1:E:650:ARG:CD	1:E:729:ASN:CB	2.88	0.51
1:E:713:LEU:C	1:E:713:LEU:HD23	2.35	0.51
2:F:105:ILE:HG21	2:F:135:LEU:HD13	1.91	0.51
2:F:522:TYR:CE1	2:F:552:GLN:HA	2.46	0.51
1:G:532:GLY:HA3	1:G:565:PHE:HD2	1.76	0.51
1:G:649:SER:O	1:G:650:ARG:HB3	2.10	0.51
2:H:343:SER:HA	2:H:381:VAL:O	2.10	0.51
2:H:591:GLN:HG2	2:H:592:GLU:N	2.25	0.51
1:A:211:THR:HA	1:A:248:LEU:HD12	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:LEU:HD23	1:C:992:LEU:C	2.36	0.51
2:D:104:PRO:HD2	2:D:233:VAL:HG11	1.92	0.51
1:E:94:HIS:CD2	2:F:155:LEU:HD21	2.45	0.51
1:E:364:PRO:HB3	1:E:365:PRO:HD2	1.92	0.51
2:F:270:LEU:HD23	2:F:271:TYR:O	2.10	0.51
2:F:654:LEU:CD1	2:F:665:ILE:HG13	2.40	0.51
2:H:341:LEU:C	2:H:343:SER:H	2.17	0.51
1:A:912:HIS:ND1	1:A:935:ARG:HD2	2.25	0.51
1:C:907:THR:CG2	1:C:1053:ILE:HD13	2.41	0.51
1:E:649:SER:O	1:E:650:ARG:HB3	2.10	0.51
1:E:986:PRO:HB3	1:E:987:PRO:HD2	1.93	0.51
2:F:121:LEU:O	2:F:125:LYS:HB3	2.11	0.51
1:G:25:TYR:CE1	1:G:86:LEU:HB2	2.45	0.51
2:B:505:LYS:HA	2:B:517:ILE:HG21	1.93	0.51
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.46	0.51
2:B:604:ILE:HD11	2:B:642:GLU:HB2	1.91	0.51
1:C:622:GLU:O	1:C:623:GLN:HG2	2.10	0.51
2:D:362:SER:HB2	2:D:370:HIS:HB2	1.93	0.51
1:E:532:GLY:HA3	1:E:565:PHE:HD2	1.76	0.51
1:E:710:PRO:HG3	1:E:884:GLU:OE2	2.10	0.51
2:F:43:ARG:HB3	2:F:44:PRO:HD3	1.92	0.51
2:F:295:GLN:CD	2:F:317:LYS:HE2	2.35	0.51
1:G:713:LEU:HD23	1:G:713:LEU:C	2.35	0.51
1:G:907:THR:CG2	1:G:1053:ILE:HD13	2.41	0.51
2:H:604:ILE:HD11	2:H:642:GLU:HB2	1.91	0.51
1:C:685:ARG:CZ	1:G:685:ARG:NH2	2.74	0.51
1:E:725:LEU:HG	1:E:726:ALA:H	1.76	0.51
1:E:907:THR:CG2	1:E:1053:ILE:HD13	2.41	0.51
1:G:364:PRO:CB	1:G:365:PRO:CD	2.89	0.51
1:G:928:GLU:HG3	1:G:929:SER:H	1.74	0.51
1:A:156:ARG:HG3	1:A:157:ALA:N	2.26	0.51
2:B:6:PHE:O	2:B:8:VAL:HG23	2.11	0.51
2:B:143:ARG:C	2:B:144:ILE:HD12	2.36	0.51
1:C:649:SER:O	1:C:650:ARG:HB3	2.10	0.51
1:C:873:ASP:C	1:C:901:VAL:HG12	2.36	0.51
1:C:919:LEU:CD1	2:D:643:ARG:NH1	2.74	0.51
2:D:354:ASP:O	2:D:544:PRO:HB2	2.11	0.51
1:E:121:VAL:O	1:E:121:VAL:CG1	2.59	0.51
1:E:656:VAL:HG21	1:E:687:LEU:CD1	2.40	0.51
1:G:780:LEU:HD23	1:G:780:LEU:C	2.36	0.51
1:A:907:THR:CG2	1:A:1053:ILE:HD13	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:VAL:HG21	1:C:687:LEU:CD1	2.40	0.51
1:C:671:ALA:HB2	1:C:700:LEU:HD23	1.92	0.51
1:E:446:VAL:HG22	1:E:447:ASP:H	1.76	0.51
1:E:490:VAL:HG12	1:E:491:LEU:CB	2.39	0.51
1:G:81:THR:O	1:G:82:SER:O	2.28	0.51
1:G:82:SER:CB	1:G:83:PRO:CD	2.88	0.51
1:G:121:VAL:O	1:G:121:VAL:CG1	2.59	0.51
1:G:822:LEU:HG	1:G:823:ARG:N	2.23	0.51
2:H:184:HIS:CE1	2:H:228:ILE:HG23	2.46	0.51
2:H:401:GLU:HA	2:H:421:PRO:HD3	1.92	0.51
1:A:311:LYS:CG	1:A:312:GLU:N	2.74	0.50
1:A:364:PRO:CB	1:A:365:PRO:CD	2.88	0.50
2:B:135:LEU:CD1	2:B:139:THR:HB	2.41	0.50
1:C:623:GLN:O	1:C:624:VAL:CG2	2.58	0.50
2:D:6:PHE:O	2:D:8:VAL:HG23	2.11	0.50
2:D:121:LEU:O	2:D:125:LYS:HB3	2.11	0.50
2:D:638:ARG:HB2	2:D:654:LEU:O	2.12	0.50
1:G:7:GLU:HB2	1:G:730:LEU:HD13	1.92	0.50
1:G:618:PHE:CE2	1:G:619:GLU:HG3	2.46	0.50
1:G:725:LEU:HG	1:G:726:ALA:H	1.77	0.50
2:H:121:LEU:O	2:H:125:LYS:HB3	2.11	0.50
1:A:420:VAL:HB	1:A:423:GLN:HB2	1.93	0.50
1:A:476:CYS:CB	1:A:487:CYS:HA	2.40	0.50
1:C:484:ARG:HH11	1:C:939:ASN:HB2	1.73	0.50
1:C:713:LEU:HD23	1:C:713:LEU:C	2.36	0.50
1:C:1055:PHE:CE2	1:C:1070:MET:HE1	2.46	0.50
2:D:184:HIS:CE1	2:D:228:ILE:HG23	2.46	0.50
1:E:333:ALA:HA	1:E:352:GLY:H	1.75	0.50
1:E:1009:LEU:HD22	1:E:1011:PHE:CE1	2.47	0.50
2:F:143:ARG:C	2:F:144:ILE:HD12	2.36	0.50
1:G:446:VAL:HG22	1:G:447:ASP:H	1.76	0.50
1:G:465:TYR:CG	1:G:469:ARG:CG	2.94	0.50
1:A:126:CYS:HB3	1:A:127:PRO:CD	2.41	0.50
1:A:565:PHE:HB2	1:A:587:ALA:HB2	1.92	0.50
1:A:606:MET:HE3	1:A:715:LEU:HD23	1.93	0.50
2:B:121:LEU:O	2:B:125:LYS:HB3	2.11	0.50
2:B:546:PHE:CD2	2:B:554:GLU:O	2.64	0.50
2:B:673:CYS:O	2:B:674:VAL:C	2.54	0.50
1:C:82:SER:HB2	1:C:83:PRO:CD	2.40	0.50
1:C:532:GLY:HA3	1:C:565:PHE:HD2	1.76	0.50
1:C:986:PRO:HB3	1:C:987:PRO:HD2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:491:LEU:HD12	1:E:492:TYR:N	2.26	0.50
1:E:817:GLN:O	1:E:818:LYS:HG2	2.12	0.50
1:G:886:ASN:O	1:G:888:PRO:HD3	2.12	0.50
2:H:35:PRO:HG2	2:H:510:GLN:CD	2.37	0.50
2:H:135:LEU:CD1	2:H:139:THR:HB	2.41	0.50
2:H:295:GLN:CD	2:H:317:LYS:HE2	2.35	0.50
2:H:638:ARG:HB2	2:H:654:LEU:O	2.11	0.50
2:B:631:SER:HB3	2:B:664:LEU:HD11	1.94	0.50
1:C:31:VAL:HG21	1:C:86:LEU:HD13	1.94	0.50
1:C:420:VAL:HB	1:C:423:GLN:HB2	1.93	0.50
1:C:878:THR:HG22	1:C:896:GLN:HB3	1.93	0.50
2:D:135:LEU:CD1	2:D:139:THR:HB	2.41	0.50
2:D:143:ARG:C	2:D:144:ILE:HD12	2.36	0.50
2:F:210:ALA:HB3	2:F:211:PRO:CD	2.39	0.50
2:F:345:VAL:HG11	2:F:387:ILE:CD1	2.42	0.50
2:F:401:GLU:HA	2:F:421:PRO:HD3	1.92	0.50
1:G:420:VAL:HB	1:G:423:GLN:HB2	1.93	0.50
1:G:499:TRP:CZ2	2:H:284:GLN:HG3	2.46	0.50
1:G:650:ARG:CD	1:G:729:ASN:HB3	2.38	0.50
1:A:94:HIS:CD2	2:B:155:LEU:HD21	2.47	0.50
1:A:491:LEU:HD12	1:A:492:TYR:N	2.26	0.50
1:A:650:ARG:CD	1:A:729:ASN:HB3	2.35	0.50
1:A:1009:LEU:HD22	1:A:1011:PHE:CE1	2.46	0.50
1:C:912:HIS:ND1	1:C:935:ARG:HD2	2.25	0.50
1:E:364:PRO:CB	1:E:365:PRO:CD	2.89	0.50
1:E:606:MET:HE3	1:E:715:LEU:HD23	1.93	0.50
1:G:31:VAL:HG21	1:G:86:LEU:HD13	1.94	0.50
1:G:491:LEU:HD12	1:G:492:TYR:N	2.26	0.50
1:G:878:THR:HG22	1:G:896:GLN:HB3	1.93	0.50
2:H:6:PHE:O	2:H:8:VAL:HG23	2.11	0.50
1:A:987:PRO:O	1:A:988:ALA:HB3	2.10	0.50
1:C:650:ARG:CD	1:C:729:ASN:HB3	2.35	0.50
2:D:35:PRO:HB3	2:D:510:GLN:HE22	1.76	0.50
3:M:1:NAG:H3	3:M:2:NAG:N2	2.27	0.50
1:A:121:VAL:O	1:A:121:VAL:CG1	2.59	0.50
1:A:304:LYS:O	1:A:307:GLN:HB3	2.11	0.50
1:A:772:LYS:HG3	1:A:772:LYS:O	2.12	0.50
1:A:928:GLU:HG3	1:A:929:SER:H	1.75	0.50
1:A:964:TRP:HB2	1:A:1032:LEU:HA	1.93	0.50
1:C:44:THR:HG21	1:C:71:MET:HE3	1.94	0.50
1:E:465:TYR:CG	1:E:469:ARG:CG	2.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:ARG:NH1	2:F:586:GLN:HG3	2.26	0.50
1:E:850:ILE:HG22	1:E:851:PHE:N	2.26	0.50
1:G:1055:PHE:CE2	1:G:1070:MET:HE1	2.46	0.50
2:H:10:SER:HA	2:H:447:ILE:HD11	1.94	0.50
1:A:499:TRP:CZ2	2:B:284:GLN:HG3	2.46	0.50
1:A:623:GLN:O	1:A:624:VAL:CG2	2.58	0.50
1:A:756:HIS:O	1:A:756:HIS:CG	2.64	0.50
1:A:886:ASN:O	1:A:888:PRO:HD3	2.12	0.50
1:C:364:PRO:HD2	1:C:369:PRO:HA	1.93	0.50
1:C:964:TRP:HB2	1:C:1032:LEU:HA	1.93	0.50
1:G:625:VAL:CG2	1:G:627:GLU:HG3	2.40	0.50
1:G:772:LYS:HG3	1:G:772:LYS:O	2.12	0.50
1:G:952:PHE:HB2	1:G:1011:PHE:HB2	1.94	0.50
1:A:446:VAL:HG22	1:A:447:ASP:H	1.76	0.50
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.94	0.50
2:B:638:ARG:HB2	2:B:654:LEU:O	2.12	0.50
1:C:25:TYR:O	1:C:26:ALA:C	2.52	0.50
1:C:465:TYR:CG	1:C:469:ARG:CG	2.94	0.50
1:E:772:LYS:HG3	1:E:772:LYS:O	2.12	0.50
1:E:1055:PHE:CE2	1:E:1070:MET:HE1	2.46	0.50
1:G:566:GLY:O	1:G:567:GLN:C	2.53	0.50
2:H:143:ARG:C	2:H:144:ILE:HD12	2.36	0.50
2:H:181:ALA:HB3	2:H:271:TYR:CZ	2.47	0.50
1:A:110:LEU:N	1:A:110:LEU:HD12	2.27	0.49
1:C:430:VAL:HG22	1:C:485:TRP:HZ3	1.77	0.49
1:C:446:VAL:HG22	1:C:447:ASP:H	1.76	0.49
1:C:685:ARG:NH2	1:G:685:ARG:CZ	2.75	0.49
1:C:725:LEU:HG	1:C:726:ALA:H	1.76	0.49
1:C:780:LEU:HD23	1:C:780:LEU:C	2.36	0.49
1:E:364:PRO:HD2	1:E:369:PRO:HA	1.93	0.49
1:E:873:ASP:C	1:E:901:VAL:HG12	2.37	0.49
1:A:465:TYR:CG	1:A:469:ARG:CG	2.94	0.49
1:A:766:PHE:CZ	1:A:877:LEU:CD1	2.95	0.49
1:A:766:PHE:CZ	1:A:877:LEU:HD12	2.47	0.49
1:A:850:ILE:HG22	1:A:851:PHE:N	2.27	0.49
1:A:873:ASP:C	1:A:901:VAL:HG12	2.37	0.49
1:C:766:PHE:CZ	1:C:877:LEU:HD12	2.47	0.49
1:C:850:ILE:HG22	1:C:851:PHE:N	2.28	0.49
2:D:317:LYS:HG3	2:D:346:PHE:HE1	1.77	0.49
2:D:673:CYS:O	2:D:674:VAL:C	2.55	0.49
1:E:766:PHE:CZ	1:E:877:LEU:HD12	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:766:PHE:CZ	1:E:877:LEU:CD1	2.95	0.49
1:G:82:SER:HB2	1:G:83:PRO:CD	2.40	0.49
1:G:446:VAL:HG12	1:G:456:LEU:CD1	2.42	0.49
1:G:873:ASP:C	1:G:901:VAL:HG12	2.37	0.49
1:A:174:PHE:CG	1:A:174:PHE:O	2.65	0.49
1:A:243:LYS:HG3	1:A:243:LYS:O	2.12	0.49
1:A:263:ILE:HD12	1:A:317:ILE:CD1	2.42	0.49
1:A:364:PRO:HD2	1:A:369:PRO:HA	1.94	0.49
2:B:210:ALA:HB3	2:B:211:PRO:CD	2.39	0.49
1:C:598:PRO:HB3	1:C:650:ARG:NH1	2.27	0.49
1:C:806:ALA:HA	1:C:840:TRP:NE1	2.27	0.49
2:D:35:PRO:CA	2:D:510:GLN:HE22	2.25	0.49
2:D:237:LEU:HD13	2:D:294:ILE:HG23	1.94	0.49
2:D:631:SER:HB3	2:D:664:LEU:HD11	1.93	0.49
1:E:107:CYS:SG	1:E:348:LEU:HD21	2.52	0.49
2:F:638:ARG:HB2	2:F:654:LEU:O	2.11	0.49
1:G:766:PHE:CZ	1:G:877:LEU:HD12	2.47	0.49
1:G:1009:LEU:HD22	1:G:1011:PHE:CE1	2.46	0.49
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.91	0.49
1:A:456:LEU:HA	1:A:477:PRO:HA	1.94	0.49
1:C:886:ASN:O	1:C:888:PRO:HD3	2.13	0.49
1:E:430:VAL:HG22	1:E:485:TRP:HZ3	1.78	0.49
1:E:771:LEU:HD11	1:E:774:LEU:HB2	1.94	0.49
1:E:878:THR:HG22	1:E:896:GLN:HB3	1.93	0.49
1:G:469:ARG:NH2	2:H:287:HIS:HB2	2.26	0.49
1:G:964:TRP:HB2	1:G:1032:LEU:HA	1.93	0.49
1:A:430:VAL:HG22	1:A:485:TRP:HZ3	1.78	0.49
1:A:780:LEU:HD23	1:A:780:LEU:C	2.36	0.49
1:C:1009:LEU:HD22	1:C:1011:PHE:CE1	2.47	0.49
2:D:426:ARG:CZ	2:D:426:ARG:CB	2.91	0.49
2:D:455:ILE:HG22	2:D:494:GLN:CD	2.37	0.49
1:E:71:MET:HG3	1:E:90:GLY:HA3	1.95	0.49
1:E:110:LEU:HD12	1:E:110:LEU:N	2.27	0.49
1:E:420:VAL:HB	1:E:423:GLN:HB2	1.93	0.49
2:F:472:GLU:HA	2:F:475:CYS:HB2	1.92	0.49
1:G:364:PRO:HD2	1:G:369:PRO:HA	1.94	0.49
1:A:480:ARG:HB3	1:A:1021:GLN:HG2	1.95	0.49
1:C:446:VAL:HG12	1:C:456:LEU:CD1	2.42	0.49
1:E:73:LEU:C	1:E:73:LEU:HD12	2.38	0.49
1:E:446:VAL:HG12	1:E:456:LEU:CD1	2.42	0.49
1:E:499:TRP:CZ2	2:F:284:GLN:HG3	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:755:ASP:O	1:E:756:HIS:HB3	2.12	0.49
1:E:886:ASN:O	1:E:888:PRO:HD3	2.12	0.49
1:E:992:LEU:C	1:E:992:LEU:HD23	2.37	0.49
2:F:181:ALA:HB3	2:F:271:TYR:CZ	2.47	0.49
1:G:71:MET:HG3	1:G:90:GLY:HA3	1.95	0.49
1:G:771:LEU:HD11	1:G:774:LEU:HB2	1.95	0.49
2:H:455:ILE:HG22	2:H:456:GLY:N	2.27	0.49
1:A:31:VAL:HG21	1:A:86:LEU:HD13	1.94	0.49
1:A:1024:LEU:HD23	1:A:1024:LEU:C	2.38	0.49
2:B:98:ARG:HB2	2:B:386:PRO:HG3	1.94	0.49
1:C:71:MET:HG3	1:C:90:GLY:HA3	1.95	0.49
1:C:73:LEU:C	1:C:73:LEU:HD12	2.38	0.49
1:C:121:VAL:O	1:C:121:VAL:CG1	2.59	0.49
1:C:771:LEU:HD11	1:C:774:LEU:HB2	1.94	0.49
2:D:98:ARG:O	2:D:99:ARG:C	2.56	0.49
2:D:181:ALA:HB3	2:D:271:TYR:CZ	2.48	0.49
2:D:465:GLY:O	2:D:466:ARG:HG2	2.13	0.49
2:F:212:GLU:HG2	2:F:243:ASP:HB2	1.95	0.49
1:G:987:PRO:O	1:G:988:ALA:HB3	2.11	0.49
2:H:450:CYS:HB2	2:H:454:TYR:O	2.12	0.49
1:A:171:LEU:HB3	1:A:182:PHE:CE1	2.48	0.49
1:A:771:LEU:HD11	1:A:774:LEU:HB2	1.94	0.49
1:A:986:PRO:HB3	1:A:987:PRO:HD2	1.95	0.49
2:B:181:ALA:HB3	2:B:271:TYR:CZ	2.47	0.49
1:C:110:LEU:HD12	1:C:110:LEU:N	2.27	0.49
1:C:126:CYS:HB3	1:C:127:PRO:CD	2.43	0.49
1:C:772:LYS:O	1:C:772:LYS:HG3	2.12	0.49
1:C:952:PHE:HB2	1:C:1011:PHE:HB2	1.94	0.49
2:D:77:SER:HA	2:D:78:PRO:C	2.37	0.49
1:E:126:CYS:HB3	1:E:127:PRO:CD	2.42	0.49
1:E:816:GLY:O	1:E:818:LYS:CA	2.61	0.49
1:E:1024:LEU:C	1:E:1024:LEU:HD23	2.38	0.49
1:G:44:THR:HG21	1:G:71:MET:HE3	1.95	0.49
1:G:71:MET:CG	1:G:90:GLY:HA3	2.43	0.49
1:G:108:PHE:HD1	1:G:117:GLN:HG2	1.78	0.49
1:G:597:ARG:NH2	1:G:730:LEU:CD1	2.76	0.49
1:G:1069:PHE:CE2	2:H:584:GLY:HA3	2.47	0.49
2:H:77:SER:HA	2:H:78:PRO:C	2.37	0.49
2:H:212:GLU:HG2	2:H:243:ASP:HB2	1.95	0.49
1:A:470:GLY:HA2	1:A:497:HIS:O	2.13	0.49
2:B:237:LEU:HD13	2:B:294:ILE:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:952:PHE:HB2	1:E:1011:PHE:HB2	1.94	0.49
1:G:25:TYR:CD1	1:G:86:LEU:HB2	2.48	0.49
1:G:26:ALA:O	1:G:28:SER:N	2.45	0.49
1:G:107:CYS:SG	1:G:348:LEU:HD21	2.53	0.49
1:G:850:ILE:HG22	1:G:851:PHE:N	2.28	0.49
1:A:44:THR:HG21	1:A:71:MET:HE3	1.94	0.49
1:A:269:VAL:HG11	1:A:300:PHE:CE2	2.48	0.49
1:A:446:VAL:HG12	1:A:456:LEU:CD1	2.43	0.49
1:C:606:MET:HE3	1:C:715:LEU:HD23	1.93	0.49
1:C:987:PRO:O	1:C:988:ALA:HB3	2.13	0.49
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.48	0.49
1:E:470:GLY:HA2	1:E:497:HIS:O	2.13	0.49
2:F:465:GLY:O	2:F:466:ARG:HG2	2.13	0.49
1:G:806:ALA:HA	1:G:840:TRP:NE1	2.27	0.49
1:G:964:TRP:HB3	1:G:1032:LEU:HA	1.95	0.49
1:G:1024:LEU:HD23	1:G:1024:LEU:C	2.38	0.49
1:A:94:HIS:NE2	2:B:155:LEU:HD21	2.28	0.48
1:A:159:ILE:HD12	1:A:197:LEU:HD11	1.94	0.48
2:B:77:SER:HA	2:B:78:PRO:C	2.37	0.48
1:C:711:ILE:HD11	1:C:746:LEU:HD13	1.95	0.48
1:C:766:PHE:CZ	1:C:877:LEU:CD1	2.95	0.48
1:C:1029:LYS:HE3	1:E:113:THR:HG22	1.95	0.48
1:E:31:VAL:HG21	1:E:86:LEU:HD13	1.94	0.48
2:F:98:ARG:HB2	2:F:386:PRO:HG3	1.94	0.48
1:G:110:LEU:N	1:G:110:LEU:HD12	2.27	0.48
1:G:766:PHE:CZ	1:G:877:LEU:CD1	2.95	0.48
2:H:522:TYR:CD1	2:H:552:GLN:HA	2.48	0.48
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.77	0.48
2:B:450:CYS:HB2	2:B:454:TYR:O	2.13	0.48
2:B:570:GLY:HA2	2:B:659:GLY:HA2	1.95	0.48
1:C:26:ALA:O	1:C:28:SER:N	2.46	0.48
2:D:98:ARG:HB2	2:D:386:PRO:HG3	1.94	0.48
2:D:355:THR:HA	2:D:544:PRO:CG	2.44	0.48
1:E:26:ALA:O	1:E:28:SER:N	2.46	0.48
1:E:964:TRP:HB2	1:E:1032:LEU:HA	1.94	0.48
1:A:26:ALA:O	1:A:28:SER:N	2.46	0.48
1:A:107:CYS:SG	1:A:348:LEU:HD21	2.53	0.48
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.91	0.48
1:E:44:THR:HG21	1:E:71:MET:HE3	1.94	0.48
1:E:456:LEU:HA	1:E:477:PRO:HA	1.94	0.48
1:E:761:ASN:ND2	1:E:791:ASP:HB2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:471:LEU:O	2:F:493:GLY:HA2	2.13	0.48
1:G:126:CYS:HB3	1:G:127:PRO:CD	2.43	0.48
1:A:254:ILE:N	1:A:255:PRO:CD	2.76	0.48
1:A:354:PHE:CG	4:J:1:NAG:H62	2.48	0.48
1:A:761:ASN:ND2	1:A:791:ASP:HB2	2.29	0.48
1:A:806:ALA:HA	1:A:840:TRP:NE1	2.27	0.48
2:B:212:GLU:HG2	2:B:243:ASP:HB2	1.95	0.48
1:C:25:TYR:CD1	1:C:86:LEU:HB2	2.48	0.48
1:C:107:CYS:SG	1:C:348:LEU:HD21	2.53	0.48
2:D:64:GLU:HB3	2:D:82:THR:HB	1.96	0.48
1:E:806:ALA:HA	1:E:840:TRP:NE1	2.27	0.48
2:F:98:ARG:O	2:F:99:ARG:C	2.57	0.48
2:F:317:LYS:HZ1	2:F:409:LEU:HB3	1.77	0.48
1:G:430:VAL:HG22	1:G:485:TRP:HZ3	1.78	0.48
2:H:237:LEU:HD13	2:H:294:ILE:HG23	1.94	0.48
2:B:644:ASP:HB3	2:B:650:VAL:HG23	1.96	0.48
1:C:351:VAL:HG23	1:C:352:GLY:N	2.29	0.48
1:C:456:LEU:HA	1:C:477:PRO:HA	1.94	0.48
1:C:609:ILE:CB	1:C:610:PRO:HD3	2.44	0.48
1:C:816:GLY:O	1:C:818:LYS:HA	2.14	0.48
2:D:455:ILE:HG21	2:D:494:GLN:NE2	2.25	0.48
1:E:764:ILE:CD1	1:E:800:ILE:HD11	2.44	0.48
1:E:964:TRP:HB3	1:E:1032:LEU:HA	1.95	0.48
2:F:186:LEU:HD13	2:F:195:PHE:CD1	2.49	0.48
1:G:490:VAL:CG1	1:G:491:LEU:N	2.68	0.48
1:G:606:MET:HE3	1:G:715:LEU:HD23	1.94	0.48
1:G:761:ASN:ND2	1:G:791:ASP:HB2	2.28	0.48
1:A:108:PHE:HD1	1:A:117:GLN:HG2	1.78	0.48
1:A:725:LEU:HG	1:A:726:ALA:H	1.79	0.48
2:B:362:SER:HB2	2:B:370:HIS:HB2	1.96	0.48
1:C:108:PHE:HD1	1:C:117:GLN:HG2	1.78	0.48
1:C:824:SER:H	1:C:825:LEU:HG	1.77	0.48
1:C:848:HIS:O	1:C:849:LEU:HB3	2.14	0.48
1:C:930:HIS:O	1:C:931:VAL:C	2.57	0.48
2:F:154:VAL:HA	2:F:160:THR:HG22	1.96	0.48
1:G:470:GLY:HA2	1:G:497:HIS:O	2.13	0.48
1:G:609:ILE:CB	1:G:610:PRO:HD3	2.44	0.48
1:G:623:GLN:O	1:G:624:VAL:CG2	2.59	0.48
1:G:772:LYS:O	1:G:773:SER:HB3	2.14	0.48
1:G:934:HIS:ND1	1:G:1074:THR:CG2	2.76	0.48
2:H:656:GLN:HG2	2:H:657:GLN:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:LYS:HB3	1:E:609:ILE:HD11	1.96	0.48
1:A:711:ILE:HD11	1:A:746:LEU:HD13	1.95	0.48
2:B:64:GLU:HB3	2:B:82:THR:HB	1.96	0.48
1:C:484:ARG:NH2	1:C:1021:GLN:CA	2.67	0.48
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.76	0.48
1:E:25:TYR:CD1	1:E:86:LEU:HB2	2.48	0.48
1:E:711:ILE:HD11	1:E:746:LEU:HD13	1.96	0.48
2:F:237:LEU:HD13	2:F:294:ILE:HG23	1.95	0.48
2:F:455:ILE:HG22	2:F:456:GLY:N	2.29	0.48
1:G:444:CYS:CB	1:G:506:LEU:CD1	2.91	0.48
1:G:764:ILE:CD1	1:G:800:ILE:HD11	2.44	0.48
1:A:73:LEU:C	1:A:73:LEU:HD12	2.38	0.48
1:A:351:VAL:HG23	1:A:352:GLY:N	2.29	0.48
1:A:964:TRP:HB3	1:A:1032:LEU:HA	1.95	0.48
1:C:376:GLN:HB2	3:M:1:NAG:O4	2.14	0.48
1:C:1024:LEU:HD23	1:C:1024:LEU:C	2.38	0.48
2:D:154:VAL:HA	2:D:160:THR:HG22	1.96	0.48
2:D:212:GLU:HG2	2:D:243:ASP:HB2	1.95	0.48
2:D:273:ARG:O	2:D:277:PHE:HB3	2.14	0.48
2:D:644:ASP:HB3	2:D:650:VAL:HG23	1.95	0.48
1:E:71:MET:CG	1:E:90:GLY:HA3	2.43	0.48
1:E:513:ASN:HA	1:E:599:VAL:HG22	1.95	0.48
1:E:623:GLN:O	1:E:624:VAL:CG2	2.60	0.48
2:F:10:SER:CB	2:F:449:ARG:CZ	2.91	0.48
2:F:64:GLU:HB3	2:F:82:THR:HB	1.95	0.48
1:G:971:HIS:CE1	1:G:974:ASN:HB2	2.49	0.48
1:C:71:MET:CG	1:C:90:GLY:HA3	2.43	0.48
1:E:108:PHE:HD1	1:E:117:GLN:HG2	1.78	0.48
2:F:77:SER:HA	2:F:78:PRO:C	2.37	0.48
1:G:73:LEU:HD12	1:G:73:LEU:C	2.38	0.48
1:G:456:LEU:HA	1:G:477:PRO:HA	1.95	0.48
1:G:662:LEU:HD11	1:G:673:PHE:CE1	2.49	0.48
2:H:98:ARG:HB2	2:H:386:PRO:HG3	1.95	0.48
2:H:465:GLY:O	2:H:466:ARG:HG2	2.13	0.48
1:A:25:TYR:CD1	1:A:86:LEU:HB2	2.48	0.48
1:A:764:ILE:CD1	1:A:800:ILE:HD11	2.44	0.48
1:A:971:HIS:CE1	1:A:974:ASN:HB2	2.49	0.48
1:A:1058:SER:O	1:A:1059:VAL:HB	2.14	0.48
1:A:1063:LEU:HG	1:A:1064:PRO:HD3	1.96	0.48
2:B:98:ARG:HD2	2:B:384:ASN:OD1	2.14	0.48
1:C:411:THR:HG22	1:C:435:ILE:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLY:HA2	1:C:497:HIS:O	2.13	0.48
2:D:357:LYS:CE	2:D:545:GLY:HA2	2.43	0.48
1:E:444:CYS:CB	1:E:506:LEU:CD1	2.91	0.48
1:E:565:PHE:CD2	1:E:565:PHE:C	2.92	0.48
1:E:848:HIS:O	1:E:849:LEU:HB3	2.14	0.48
1:E:930:HIS:O	1:E:931:VAL:C	2.57	0.48
1:E:971:HIS:CE1	1:E:974:ASN:HB2	2.49	0.48
2:F:362:SER:HB2	2:F:370:HIS:HB2	1.96	0.48
1:G:354:PHE:CG	5:S:1:NAG:H62	2.49	0.48
1:A:71:MET:HG3	1:A:90:GLY:HA3	1.95	0.47
1:A:365:PRO:C	1:A:367:MET:H	2.22	0.47
2:B:455:ILE:HG22	2:B:456:GLY:N	2.29	0.47
2:D:317:LYS:N	2:D:344:ARG:HH11	2.12	0.47
1:E:490:VAL:CG1	1:E:491:LEU:N	2.68	0.47
1:E:598:PRO:CB	1:E:650:ARG:NH1	2.77	0.47
1:E:772:LYS:O	1:E:773:SER:HB3	2.14	0.47
1:E:928:GLU:HG3	1:E:929:SER:H	1.74	0.47
2:H:118:LEU:HD21	2:H:204:ILE:CD1	2.44	0.47
1:A:71:MET:CG	1:A:90:GLY:HA3	2.43	0.47
1:A:597:ARG:HG3	1:A:731:ARG:HE	1.79	0.47
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.97	0.47
2:B:118:LEU:HD21	2:B:204:ILE:CD1	2.44	0.47
1:C:662:LEU:HD11	1:C:673:PHE:CE1	2.49	0.47
2:D:186:LEU:HD13	2:D:195:PHE:CD1	2.49	0.47
1:E:676:THR:HG23	1:E:678:ASN:H	1.79	0.47
1:E:934:HIS:ND1	1:E:1074:THR:CG2	2.76	0.47
2:F:118:LEU:HD21	2:F:204:ILE:CD1	2.44	0.47
1:G:411:THR:HG22	1:G:435:ILE:HA	1.96	0.47
1:A:181:HIS:CE1	1:A:200:VAL:CG1	2.96	0.47
1:A:930:HIS:O	1:A:931:VAL:C	2.57	0.47
1:A:1028:LEU:HD12	1:A:1028:LEU:O	2.14	0.47
2:B:212:GLU:HG2	2:B:243:ASP:CB	2.45	0.47
1:C:43:GLN:HG2	1:C:44:THR:HG23	1.97	0.47
1:C:761:ASN:ND2	1:C:791:ASP:HB2	2.28	0.47
1:C:840:TRP:CD1	1:C:840:TRP:N	2.83	0.47
1:C:964:TRP:HB3	1:C:1032:LEU:HA	1.95	0.47
2:D:212:GLU:HG2	2:D:243:ASP:CB	2.45	0.47
2:D:453:GLY:O	2:D:463:THR:HG23	2.13	0.47
1:E:598:PRO:CG	1:E:650:ARG:NH1	2.77	0.47
1:E:831:SER:CB	1:E:842:THR:HG22	2.45	0.47
2:F:118:LEU:HD21	2:F:204:ILE:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:365:PRO:C	1:G:367:MET:H	2.23	0.47
1:G:711:ILE:HD11	1:G:746:LEU:HD13	1.95	0.47
1:A:221:PHE:CE1	1:A:233:LYS:HD2	2.50	0.47
2:B:347:LEU:HD22	2:B:389:PHE:CG	2.49	0.47
1:G:406:PRO:HB3	1:G:438:TYR:CD2	2.50	0.47
1:G:831:SER:CB	1:G:842:THR:HG22	2.44	0.47
2:H:64:GLU:HB3	2:H:82:THR:HB	1.96	0.47
2:H:473:GLY:C	2:H:475:CYS:H	2.22	0.47
1:C:565:PHE:CD2	1:C:565:PHE:C	2.92	0.47
1:C:831:SER:CB	1:C:842:THR:HG22	2.45	0.47
1:C:906:TYR:CE2	1:C:1067:GLU:OE1	2.68	0.47
1:C:1058:SER:O	1:C:1059:VAL:HB	2.14	0.47
1:E:365:PRO:C	1:E:367:MET:H	2.22	0.47
1:E:465:TYR:HB3	1:E:469:ARG:HG2	1.97	0.47
1:E:918:TYR:C	2:F:643:ARG:HH22	2.22	0.47
1:E:1028:LEU:HD12	1:E:1028:LEU:O	2.15	0.47
1:E:1063:LEU:HG	1:E:1064:PRO:HD3	1.96	0.47
2:F:260:ASN:ND2	2:F:277:PHE:HZ	2.13	0.47
2:F:644:ASP:HB3	2:F:650:VAL:HG23	1.95	0.47
1:G:465:TYR:HB3	1:G:469:ARG:HG2	1.97	0.47
1:G:906:TYR:CE2	1:G:1067:GLU:OE1	2.68	0.47
1:G:1028:LEU:HD12	1:G:1028:LEU:O	2.14	0.47
1:G:1058:SER:O	1:G:1059:VAL:HB	2.14	0.47
1:G:1063:LEU:HG	1:G:1064:PRO:HD3	1.96	0.47
2:H:273:ARG:O	2:H:277:PHE:HB3	2.14	0.47
1:A:618:PHE:CD2	1:A:619:GLU:N	2.82	0.47
1:A:906:TYR:CE2	1:A:1067:GLU:OE1	2.68	0.47
2:B:118:LEU:HD21	2:B:204:ILE:HD13	1.97	0.47
2:B:186:LEU:HD13	2:B:195:PHE:CD1	2.49	0.47
2:B:352:LEU:CD2	2:B:358:VAL:HG23	2.45	0.47
2:B:465:GLY:O	2:B:466:ARG:HG2	2.13	0.47
1:C:365:PRO:C	1:C:367:MET:H	2.23	0.47
1:C:465:TYR:HB3	1:C:469:ARG:HG2	1.97	0.47
1:C:764:ILE:CD1	1:C:800:ILE:HD11	2.44	0.47
2:D:98:ARG:HD2	2:D:384:ASN:OD1	2.14	0.47
2:D:343:SER:O	2:D:378:CYS:O	2.33	0.47
2:D:609:CYS:SG	2:D:616:PRO:HB3	2.55	0.47
1:E:609:ILE:CB	1:E:610:PRO:HD3	2.44	0.47
1:G:662:LEU:CD1	1:G:673:PHE:CE1	2.98	0.47
1:G:670:ARG:HG2	1:G:711:ILE:CG2	2.45	0.47
1:G:930:HIS:O	1:G:931:VAL:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLY:O	1:A:105:GLY:HA2	2.15	0.47
1:A:253:VAL:CG2	1:A:254:ILE:N	2.78	0.47
1:A:376:GLN:HB2	4:J:1:NAG:O4	2.15	0.47
1:A:465:TYR:HB3	1:A:469:ARG:HG2	1.97	0.47
1:A:840:TRP:N	1:A:840:TRP:CD1	2.83	0.47
1:A:848:HIS:O	1:A:849:LEU:HB3	2.14	0.47
2:B:154:VAL:HA	2:B:160:THR:HG22	1.96	0.47
2:B:630:LEU:HD12	2:B:665:ILE:HB	1.97	0.47
1:C:478:LEU:HA	1:C:485:TRP:HE1	1.80	0.47
1:C:971:HIS:CE1	1:C:974:ASN:HB2	2.49	0.47
1:C:980:SER:HB3	1:C:1012:ARG:HB3	1.97	0.47
1:C:1063:LEU:HG	1:C:1064:PRO:HD3	1.96	0.47
2:D:43:ARG:N	2:D:44:PRO:CD	2.78	0.47
2:D:118:LEU:HD21	2:D:204:ILE:HD13	1.97	0.47
1:E:41:ALA:O	1:E:42:ASN:C	2.58	0.47
1:E:351:VAL:HG23	1:E:352:GLY:N	2.29	0.47
1:E:662:LEU:CD1	1:E:673:PHE:CE1	2.97	0.47
1:E:920:ASN:O	1:E:1080:LYS:HG2	2.14	0.47
2:F:121:LEU:O	2:F:121:LEU:HD23	2.15	0.47
2:F:609:CYS:SG	2:F:616:PRO:HB3	2.55	0.47
2:F:630:LEU:HD12	2:F:665:ILE:HB	1.97	0.47
1:G:351:VAL:HG23	1:G:352:GLY:N	2.29	0.47
1:G:565:PHE:C	1:G:565:PHE:CD2	2.93	0.47
1:G:920:ASN:O	1:G:1080:LYS:HG2	2.15	0.47
1:G:980:SER:HB3	1:G:1012:ARG:HB3	1.97	0.47
1:G:992:LEU:HD23	1:G:992:LEU:C	2.39	0.47
2:H:98:ARG:HD2	2:H:384:ASN:OD1	2.14	0.47
2:H:234:THR:CG2	2:H:236:LEU:HD13	2.45	0.47
2:H:644:ASP:HB3	2:H:650:VAL:HG23	1.96	0.47
3:T:1:NAG:H4	3:T:2:NAG:H2	1.70	0.47
1:A:43:GLN:HG2	1:A:44:THR:HG23	1.97	0.47
1:A:158:VAL:O	1:A:158:VAL:HG12	2.15	0.47
1:A:609:ILE:CB	1:A:610:PRO:HD3	2.44	0.47
1:A:772:LYS:O	1:A:773:SER:HB3	2.14	0.47
1:A:953:TRP:NE1	1:C:755:ASP:HB2	2.30	0.47
2:B:273:ARG:O	2:B:277:PHE:HB3	2.14	0.47
1:E:411:THR:HG22	1:E:435:ILE:HA	1.96	0.47
1:E:662:LEU:HD11	1:E:673:PHE:CE1	2.49	0.47
2:F:273:ARG:O	2:F:277:PHE:HB3	2.14	0.47
1:G:41:ALA:O	1:G:42:ASN:C	2.58	0.47
1:G:741:TYR:CD2	2:H:502:VAL:HG22	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:840:TRP:N	1:G:840:TRP:CD1	2.83	0.47
1:G:848:HIS:O	1:G:849:LEU:HB3	2.14	0.47
2:H:154:VAL:HA	2:H:160:THR:HG22	1.96	0.47
2:H:352:LEU:CD2	2:H:358:VAL:HG23	2.45	0.47
1:A:411:THR:HG22	1:A:435:ILE:HA	1.96	0.47
1:C:119:LEU:CD2	1:C:124:GLN:NE2	2.78	0.47
2:D:234:THR:CG2	2:D:236:LEU:HD13	2.45	0.47
2:D:260:ASN:ND2	2:D:277:PHE:HZ	2.13	0.47
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.49	0.47
1:E:597:ARG:HB3	1:E:731:ARG:O	2.14	0.47
1:E:598:PRO:HB3	1:E:650:ARG:HH12	1.79	0.47
2:F:98:ARG:HD2	2:F:384:ASN:OD1	2.14	0.47
2:F:450:CYS:HB2	2:F:454:TYR:O	2.15	0.47
1:G:376:GLN:HB2	5:S:1:NAG:O4	2.15	0.47
1:G:514:GLY:CA	1:G:644:LYS:HD3	2.45	0.47
2:H:121:LEU:O	2:H:121:LEU:HD23	2.15	0.47
2:H:305:VAL:HG13	2:H:306:LYS:N	2.30	0.47
2:H:609:CYS:SG	2:H:616:PRO:HB3	2.55	0.47
2:H:630:LEU:HD12	2:H:665:ILE:HB	1.97	0.47
1:A:565:PHE:CD2	1:A:565:PHE:C	2.92	0.47
1:A:676:THR:HG23	1:A:678:ASN:H	1.80	0.47
1:A:831:SER:CB	1:A:842:THR:HG22	2.45	0.47
2:B:656:GLN:HG2	2:B:657:GLN:N	2.29	0.47
1:C:119:LEU:O	1:C:363:TYR:HE1	1.97	0.47
1:C:479:PRO:HB3	1:C:1021:GLN:CD	2.39	0.47
1:C:601:TRP:HZ2	1:C:641:LYS:HD3	1.80	0.47
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.98	0.47
1:C:772:LYS:O	1:C:773:SER:HB3	2.14	0.47
1:E:119:LEU:CD2	1:E:124:GLN:NE2	2.78	0.47
1:E:816:GLY:C	1:E:818:LYS:N	2.73	0.47
1:E:840:TRP:N	1:E:840:TRP:CD1	2.83	0.47
2:H:43:ARG:N	2:H:44:PRO:CD	2.78	0.47
2:H:186:LEU:HD13	2:H:195:PHE:CD1	2.49	0.47
2:H:212:GLU:HG2	2:H:243:ASP:CB	2.45	0.47
2:H:631:SER:HB3	2:H:664:LEU:HD11	1.97	0.47
1:A:102:TYR:HA	1:A:332:MET:HE3	1.98	0.46
1:A:799:THR:HA	1:A:845:ARG:HA	1.98	0.46
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.46
2:B:234:THR:CG2	2:B:236:LEU:HD13	2.45	0.46
1:C:406:PRO:HB3	1:C:438:TYR:CD2	2.50	0.46
1:E:90:GLY:O	1:E:105:GLY:HA2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:TYR:HA	1:E:332:MET:HE3	1.97	0.46
1:E:376:GLN:HB2	5:P:1:NAG:O4	2.15	0.46
1:E:906:TYR:CE2	1:E:1067:GLU:OE1	2.68	0.46
1:E:987:PRO:O	1:E:988:ALA:HB3	2.14	0.46
1:E:1058:SER:O	1:E:1059:VAL:HB	2.14	0.46
1:G:465:TYR:CD1	1:G:469:ARG:HG2	2.50	0.46
1:G:476:CYS:HB3	1:G:487:CYS:HA	1.97	0.46
1:G:676:THR:HG23	1:G:678:ASN:H	1.80	0.46
1:G:918:TYR:O	1:G:919:LEU:C	2.58	0.46
1:A:174:PHE:HB2	1:A:212:ALA:HB2	1.96	0.46
1:A:478:LEU:HA	1:A:485:TRP:HE1	1.80	0.46
1:A:601:TRP:HZ2	1:A:641:LYS:HD3	1.81	0.46
1:A:662:LEU:HD11	1:A:673:PHE:CE1	2.49	0.46
2:B:334:ILE:HA	2:B:337:ALA:CB	2.45	0.46
1:C:476:CYS:HB3	1:C:487:CYS:HA	1.97	0.46
1:C:920:ASN:O	1:C:1080:LYS:HG2	2.14	0.46
2:D:352:LEU:CD2	2:D:358:VAL:HG23	2.45	0.46
2:D:630:LEU:HD12	2:D:665:ILE:HB	1.97	0.46
1:E:406:PRO:HB3	1:E:438:TYR:CD2	2.50	0.46
1:E:909:VAL:HG12	1:E:1069:PHE:O	2.15	0.46
2:F:340:LYS:HD2	2:F:379:ASP:OD1	2.16	0.46
1:G:797:GLY:N	1:G:884:GLU:HB2	2.31	0.46
1:G:831:SER:HA	1:G:842:THR:HG22	1.97	0.46
1:A:619:GLU:O	1:A:620:CYS:SG	2.73	0.46
1:A:920:ASN:O	1:A:1080:LYS:HG2	2.14	0.46
2:B:121:LEU:O	2:B:121:LEU:HD23	2.15	0.46
1:C:676:THR:HG23	1:C:678:ASN:H	1.80	0.46
1:C:698:LEU:N	1:C:698:LEU:HD12	2.30	0.46
2:D:7:LYS:HD2	2:D:508:TYR:CD1	2.49	0.46
2:D:210:ALA:HB3	2:D:211:PRO:CD	2.40	0.46
2:F:43:ARG:N	2:F:44:PRO:CD	2.78	0.46
2:F:158:VAL:HA	2:F:208:LEU:HG	1.97	0.46
2:F:161:HIS:CB	2:F:162:PRO:HA	2.43	0.46
2:F:465:GLY:O	2:F:466:ARG:CG	2.63	0.46
2:F:656:GLN:HG2	2:F:657:GLN:N	2.29	0.46
1:G:119:LEU:CD2	1:G:124:GLN:NE2	2.78	0.46
1:G:799:THR:HA	1:G:845:ARG:HA	1.97	0.46
2:H:210:ALA:HB3	2:H:211:PRO:CD	2.39	0.46
1:A:670:ARG:HG2	1:A:711:ILE:CG2	2.45	0.46
1:C:465:TYR:CD1	1:C:469:ARG:HG2	2.50	0.46
1:C:609:ILE:HD11	1:G:690:LYS:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:PRO:HB3	2:D:510:GLN:NE2	2.29	0.46
2:D:118:LEU:HD21	2:D:204:ILE:CD1	2.44	0.46
2:D:361:ASP:HB2	2:D:390:GLN:HB3	1.97	0.46
1:E:354:PHE:CG	5:P:1:NAG:H62	2.50	0.46
1:E:465:TYR:CD1	1:E:469:ARG:HG2	2.50	0.46
1:E:763:GLY:C	1:E:789:TRP:HE3	2.24	0.46
1:E:799:THR:HA	1:E:845:ARG:HA	1.98	0.46
2:F:39:ARG:HD2	2:F:447:ILE:CG2	2.45	0.46
2:F:212:GLU:HG2	2:F:243:ASP:CB	2.45	0.46
2:F:643:ARG:NH2	2:F:649:TRP:CZ2	2.84	0.46
2:H:118:LEU:HD21	2:H:204:ILE:HD13	1.97	0.46
2:H:334:ILE:HA	2:H:337:ALA:CB	2.45	0.46
2:H:461:CYS:SG	2:H:466:ARG:CD	3.04	0.46
1:A:406:PRO:HB3	1:A:438:TYR:CD2	2.50	0.46
1:A:698:LEU:HD12	1:A:698:LEU:N	2.30	0.46
1:A:797:GLY:N	1:A:884:GLU:HB2	2.31	0.46
1:C:609:ILE:HB	1:C:610:PRO:CD	2.45	0.46
1:C:964:TRP:HB3	1:C:1032:LEU:HG	1.98	0.46
2:D:158:VAL:HA	2:D:208:LEU:HG	1.97	0.46
2:D:562:ASN:OD1	2:D:564:ARG:HB2	2.15	0.46
2:D:652:TYR:HB3	2:D:667:VAL:HA	1.97	0.46
1:E:698:LEU:N	1:E:698:LEU:HD12	2.31	0.46
1:E:1052:GLU:OE1	1:G:756:HIS:HA	2.16	0.46
2:F:305:VAL:HG13	2:F:306:LYS:N	2.31	0.46
2:F:562:ASN:OD1	2:F:564:ARG:HB2	2.16	0.46
2:F:597:PRO:O	2:F:598:SER:CB	2.63	0.46
2:H:75:GLN:HG3	2:H:98:ARG:O	2.15	0.46
2:H:260:ASN:ND2	2:H:277:PHE:HZ	2.13	0.46
1:A:151:MET:SD	1:A:238:ILE:HG21	2.56	0.46
1:A:164:ARG:CB	1:A:165:PRO:HA	2.44	0.46
1:A:598:PRO:HB3	1:A:650:ARG:NH1	2.31	0.46
1:A:755:ASP:O	1:A:756:HIS:HB3	2.14	0.46
2:B:260:ASN:ND2	2:B:277:PHE:HZ	2.13	0.46
1:C:670:ARG:HG2	1:C:711:ILE:CG2	2.46	0.46
2:D:130:ASP:HA	2:D:133:ARG:HB3	1.98	0.46
1:E:618:PHE:CD2	1:E:619:GLU:N	2.84	0.46
2:F:75:GLN:HG3	2:F:98:ARG:O	2.16	0.46
2:F:361:ASP:HB2	2:F:390:GLN:HB3	1.97	0.46
1:G:90:GLY:O	1:G:105:GLY:HA2	2.15	0.46
1:G:119:LEU:H	1:G:120:PRO:CA	2.25	0.46
1:G:478:LEU:HA	1:G:485:TRP:HE1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:TYR:HB3	2:H:233:VAL:HG11	1.98	0.46
1:A:41:ALA:O	1:A:42:ASN:C	2.59	0.46
1:A:119:LEU:CD2	1:A:124:GLN:NE2	2.78	0.46
1:A:181:HIS:CG	1:A:200:VAL:HG21	2.50	0.46
1:A:385:TYR:CE2	1:A:407:ARG:HD3	2.51	0.46
1:A:827:LEU:HD13	1:A:829:CYS:SG	2.56	0.46
1:A:992:LEU:HD23	1:A:992:LEU:C	2.40	0.46
1:A:1057:THR:HG21	1:C:760:ASP:O	2.16	0.46
2:B:305:VAL:HG13	2:B:306:LYS:N	2.31	0.46
1:C:90:GLY:O	1:C:105:GLY:HA2	2.15	0.46
1:C:831:SER:HA	1:C:842:THR:HG22	1.98	0.46
2:D:121:LEU:O	2:D:121:LEU:HD23	2.15	0.46
2:F:39:ARG:CD	2:F:447:ILE:HG23	2.46	0.46
2:F:665:ILE:HD12	2:F:665:ILE:N	2.31	0.46
1:G:827:LEU:CD1	1:G:829:CYS:SG	3.04	0.46
2:H:361:ASP:HB2	2:H:390:GLN:HB3	1.97	0.46
1:A:300:PHE:O	1:A:303:LEU:HB3	2.15	0.46
1:A:894:THR:O	1:C:874:ARG:NH2	2.48	0.46
2:B:43:ARG:N	2:B:44:PRO:CD	2.78	0.46
2:B:158:VAL:HA	2:B:208:LEU:HG	1.97	0.46
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.97	0.46
2:B:609:CYS:SG	2:B:616:PRO:HB3	2.55	0.46
2:D:99:ARG:NH1	2:D:101:LYS:O	2.49	0.46
1:E:43:GLN:HG2	1:E:44:THR:HG23	1.97	0.46
1:E:416:ILE:HG22	1:E:427:LYS:HD3	1.98	0.46
1:E:476:CYS:HB3	1:E:487:CYS:HA	1.97	0.46
1:E:564:TYR:CZ	1:E:588:ARG:HD2	2.51	0.46
1:E:827:LEU:HD13	1:E:829:CYS:SG	2.56	0.46
2:F:352:LEU:CD2	2:F:358:VAL:HG23	2.45	0.46
1:G:698:LEU:HD12	1:G:698:LEU:N	2.30	0.46
1:G:827:LEU:HD13	1:G:829:CYS:SG	2.55	0.46
2:H:130:ASP:HA	2:H:133:ARG:HB3	1.98	0.46
2:H:362:SER:HB2	2:H:370:HIS:HB2	1.96	0.46
1:A:25:TYR:CG	1:A:26:ALA:N	2.84	0.46
1:A:448:VAL:HA	1:A:518:THR:HG22	1.98	0.46
2:B:120:ASP:O	2:B:124:VAL:HB	2.16	0.46
2:B:293:ASN:OD1	2:B:412:THR:HG22	2.16	0.46
1:C:25:TYR:CG	1:C:26:ALA:N	2.84	0.46
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.04	0.46
1:E:68:ALA:CB	1:E:71:MET:HE2	2.46	0.46
2:H:120:ASP:O	2:H:124:VAL:HB	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:VAL:HA	2:H:208:LEU:HG	1.97	0.46
1:A:263:ILE:HD12	1:A:317:ILE:HD12	1.98	0.46
1:A:430:VAL:HG13	1:A:485:TRP:CE3	2.51	0.46
1:A:465:TYR:CD1	1:A:469:ARG:HG2	2.50	0.46
1:A:752:CYS:SG	1:A:758:CYS:N	2.89	0.46
1:C:909:VAL:HG12	1:C:1069:PHE:O	2.16	0.46
1:C:1028:LEU:HD12	1:C:1028:LEU:O	2.16	0.46
2:D:465:GLY:O	2:D:466:ARG:CG	2.64	0.46
1:E:625:VAL:CG2	1:E:627:GLU:HG3	2.40	0.46
1:E:797:GLY:N	1:E:884:GLU:HB2	2.31	0.46
1:E:827:LEU:CD1	1:E:829:CYS:SG	3.04	0.46
2:F:23:TRP:HH2	2:F:447:ILE:HD13	1.81	0.46
2:F:334:ILE:HA	2:F:337:ALA:CB	2.46	0.46
1:G:43:GLN:HG2	1:G:44:THR:HG23	1.97	0.46
1:G:119:LEU:O	1:G:363:TYR:HE1	1.96	0.46
1:G:564:TYR:CZ	1:G:588:ARG:HD2	2.51	0.46
1:G:663:ASP:N	1:G:664:PRO:HD3	2.31	0.46
1:G:1063:LEU:N	1:G:1064:PRO:CD	2.79	0.46
2:H:465:GLY:O	2:H:466:ARG:CG	2.64	0.46
1:A:308:ASN:O	1:A:311:LYS:HD3	2.17	0.45
1:A:354:PHE:CE2	4:J:1:NAG:O5	2.69	0.45
1:A:564:TYR:CZ	1:A:588:ARG:HD2	2.51	0.45
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.04	0.45
1:A:980:SER:HB3	1:A:1012:ARG:HB3	1.97	0.45
1:C:763:GLY:C	1:C:789:TRP:HE3	2.24	0.45
1:C:797:GLY:N	1:C:884:GLU:HB2	2.31	0.45
1:C:1063:LEU:N	1:C:1064:PRO:CD	2.79	0.45
2:D:334:ILE:HA	2:D:337:ALA:CB	2.45	0.45
1:E:959:ASN:O	1:E:960:GLN:HB3	2.16	0.45
1:G:430:VAL:HG13	1:G:485:TRP:CE3	2.51	0.45
1:G:448:VAL:HA	1:G:518:THR:HG22	1.98	0.45
2:H:643:ARG:NH2	2:H:649:TRP:CZ2	2.84	0.45
2:H:665:ILE:N	2:H:665:ILE:HD12	2.31	0.45
1:A:739:GLN:HB2	1:A:742:PHE:CE1	2.51	0.45
1:A:757:ILE:HG21	1:C:1054:THR:HG21	1.97	0.45
1:A:763:GLY:C	1:A:789:TRP:HE3	2.24	0.45
1:A:1020:VAL:O	1:A:1021:GLN:HB2	2.16	0.45
1:A:1048:VAL:HG22	1:A:1075:THR:HB	1.99	0.45
2:B:465:GLY:O	2:B:466:ARG:CG	2.64	0.45
2:B:562:ASN:OD1	2:B:564:ARG:HB2	2.16	0.45
1:C:430:VAL:HG13	1:C:485:TRP:CE3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:LEU:HD12	1:C:576:THR:CG2	2.47	0.45
1:C:938:VAL:HG12	1:C:1024:LEU:O	2.16	0.45
2:D:120:ASP:O	2:D:124:VAL:HB	2.16	0.45
2:D:305:VAL:HG13	2:D:306:LYS:N	2.31	0.45
2:D:345:VAL:HG11	2:D:387:ILE:CD1	2.46	0.45
2:F:652:TYR:HB3	2:F:667:VAL:HA	1.98	0.45
1:G:1023:GLU:O	1:G:1024:LEU:C	2.59	0.45
1:A:271:LEU:C	1:A:273:PHE:N	2.75	0.45
1:A:402:VAL:HG22	1:A:416:ILE:HG23	1.98	0.45
1:A:476:CYS:HB3	1:A:487:CYS:HA	1.97	0.45
1:A:663:ASP:N	1:A:664:PRO:HD3	2.31	0.45
1:A:959:ASN:O	1:A:960:GLN:HB3	2.16	0.45
2:B:601:GLY:O	2:B:602:LYS:HB2	2.17	0.45
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.85	0.45
1:C:18:PHE:CZ	1:C:32:VAL:HG21	2.51	0.45
1:C:68:ALA:CB	1:C:71:MET:HE2	2.46	0.45
1:C:613:ILE:HD12	1:C:748:PHE:CD2	2.52	0.45
2:D:665:ILE:HD12	2:D:665:ILE:N	2.31	0.45
1:E:402:VAL:HG22	1:E:416:ILE:HG23	1.98	0.45
1:E:437:SER:HA	1:E:463:HIS:O	2.17	0.45
1:E:670:ARG:HG2	1:E:711:ILE:CG2	2.45	0.45
1:E:681:LEU:HD12	1:E:682:SER:N	2.32	0.45
1:E:698:LEU:C	1:E:699:LEU:HD12	2.42	0.45
1:E:739:GLN:HB2	1:E:742:PHE:CE1	2.52	0.45
1:E:789:TRP:NE1	1:G:772:LYS:CB	2.79	0.45
1:E:1023:GLU:O	1:E:1024:LEU:C	2.60	0.45
2:F:83:LEU:HD12	2:F:83:LEU:O	2.16	0.45
2:F:234:THR:CG2	2:F:236:LEU:HD13	2.45	0.45
2:F:271:TYR:O	2:F:271:TYR:CG	2.69	0.45
1:G:108:PHE:CD1	1:G:117:GLN:HG2	2.52	0.45
1:G:964:TRP:HB3	1:G:1032:LEU:HG	1.98	0.45
1:A:108:PHE:CD1	1:A:117:GLN:HG2	2.52	0.45
1:A:565:PHE:CD2	1:A:565:PHE:O	2.69	0.45
1:A:909:VAL:HG12	1:A:1069:PHE:O	2.16	0.45
1:C:448:VAL:HA	1:C:518:THR:HG22	1.98	0.45
1:C:775:LEU:CD1	1:C:904:ALA:HB2	2.46	0.45
1:C:799:THR:HG22	1:C:845:ARG:CB	2.47	0.45
1:C:827:LEU:HD13	1:C:829:CYS:SG	2.56	0.45
2:D:83:LEU:O	2:D:83:LEU:HD12	2.17	0.45
2:D:656:GLN:HG2	2:D:657:GLN:N	2.29	0.45
1:E:25:TYR:CG	1:E:26:ALA:N	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:GLN:C	1:E:378:ASN:N	2.75	0.45
1:E:385:TYR:CE2	1:E:407:ARG:HD3	2.51	0.45
1:E:448:VAL:HA	1:E:518:THR:HG22	1.98	0.45
1:E:478:LEU:HA	1:E:485:TRP:HE1	1.80	0.45
1:E:964:TRP:HB3	1:E:1032:LEU:HG	1.98	0.45
2:F:130:ASP:HA	2:F:133:ARG:HB3	1.98	0.45
1:G:68:ALA:CB	1:G:71:MET:HE2	2.46	0.45
1:G:959:ASN:O	1:G:960:GLN:HB3	2.16	0.45
2:H:652:TYR:HB3	2:H:667:VAL:HA	1.98	0.45
1:A:18:PHE:CZ	1:A:32:VAL:HG21	2.51	0.45
2:B:130:ASP:HA	2:B:133:ARG:HB3	1.98	0.45
2:B:652:TYR:HB3	2:B:667:VAL:HA	1.98	0.45
1:C:816:GLY:O	1:C:818:LYS:CA	2.65	0.45
2:D:186:LEU:HD21	2:D:198:GLU:CB	2.47	0.45
1:E:491:LEU:HD11	1:E:545:ILE:HD11	1.99	0.45
1:E:575:LEU:HD12	1:E:576:THR:CG2	2.47	0.45
1:E:663:ASP:N	1:E:664:PRO:HD3	2.31	0.45
1:E:822:LEU:HG	1:E:823:ARG:N	2.22	0.45
2:F:186:LEU:HD21	2:F:198:GLU:CB	2.47	0.45
2:F:382:GLN:HG3	2:F:383:ILE:H	1.81	0.45
2:F:532:ARG:O	2:F:543:HIS:HB2	2.17	0.45
1:G:103:LEU:HD12	2:H:156:PRO:HB3	1.96	0.45
1:G:437:SER:HA	1:G:463:HIS:O	2.16	0.45
1:G:475:VAL:HG12	1:G:491:LEU:O	2.16	0.45
1:G:609:ILE:HB	1:G:610:PRO:CD	2.45	0.45
1:G:909:VAL:HG12	1:G:1069:PHE:O	2.15	0.45
1:G:1048:VAL:HG22	1:G:1075:THR:HB	1.98	0.45
1:A:436:GLY:C	2:B:282:VAL:HG11	2.42	0.45
1:A:491:LEU:HD11	1:A:545:ILE:HD11	1.99	0.45
1:A:799:THR:HG22	1:A:845:ARG:CB	2.47	0.45
1:A:831:SER:HA	1:A:842:THR:HG22	1.98	0.45
1:A:938:VAL:HG12	1:A:1024:LEU:O	2.17	0.45
1:A:986:PRO:HG3	1:A:1003:CYS:O	2.17	0.45
1:A:1069:PHE:CZ	2:B:584:GLY:HA3	2.52	0.45
2:B:75:GLN:HG3	2:B:98:ARG:O	2.16	0.45
2:B:382:GLN:HG3	2:B:383:ILE:H	1.81	0.45
2:B:616:PRO:HB2	2:B:620:ASN:CA	2.47	0.45
1:C:486:TRP:C	1:C:488:ASP:H	2.24	0.45
1:C:663:ASP:N	1:C:664:PRO:HD3	2.31	0.45
1:C:681:LEU:HD12	1:C:682:SER:N	2.32	0.45
1:C:698:LEU:C	1:C:699:LEU:HD12	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1048:VAL:HG22	1:C:1075:THR:HB	1.98	0.45
2:D:522:TYR:C	2:D:522:TYR:CD2	2.95	0.45
1:E:565:PHE:CD2	1:E:565:PHE:O	2.69	0.45
1:E:629:THR:CG2	1:E:630:LEU:N	2.80	0.45
1:E:799:THR:HG22	1:E:845:ARG:CB	2.47	0.45
1:E:1048:VAL:HG22	1:E:1075:THR:HB	1.98	0.45
2:F:120:ASP:O	2:F:124:VAL:HB	2.16	0.45
2:F:285:LEU:C	2:F:287:HIS:N	2.74	0.45
1:G:18:PHE:CZ	1:G:32:VAL:HG21	2.51	0.45
1:G:102:TYR:HA	1:G:332:MET:HE3	1.97	0.45
1:G:569:LEU:HD12	1:G:569:LEU:O	2.17	0.45
1:G:601:TRP:HZ2	1:G:641:LYS:HD3	1.81	0.45
1:G:797:GLY:H	1:G:884:GLU:HB2	1.81	0.45
1:A:416:ILE:HG22	1:A:427:LYS:HD3	1.98	0.45
2:B:168:PRO:CG	2:B:179:PRO:HG3	2.47	0.45
2:B:665:ILE:N	2:B:665:ILE:HD12	2.31	0.45
1:C:102:TYR:HA	1:C:332:MET:HE3	1.97	0.45
1:C:385:TYR:CE2	1:C:407:ARG:HD3	2.51	0.45
1:C:739:GLN:HB2	1:C:742:PHE:CE1	2.52	0.45
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.45
2:D:75:GLN:HG3	2:D:98:ARG:O	2.16	0.45
1:E:18:PHE:CZ	1:E:32:VAL:HG21	2.51	0.45
1:E:348:LEU:N	1:E:348:LEU:HD12	2.32	0.45
1:E:938:VAL:HG12	1:E:1024:LEU:O	2.16	0.45
2:F:83:LEU:HD11	2:F:419:VAL:HG13	1.99	0.45
1:G:491:LEU:HD11	1:G:545:ILE:HD11	1.99	0.45
1:G:575:LEU:HD12	1:G:576:THR:CG2	2.47	0.45
2:H:168:PRO:CG	2:H:179:PRO:HG3	2.47	0.45
2:H:382:GLN:HG3	2:H:383:ILE:H	1.81	0.45
2:H:562:ASN:OD1	2:H:564:ARG:HB2	2.16	0.45
1:A:527:GLU:HG3	1:A:533:ALA:CB	2.47	0.45
1:A:608:PHE:O	1:A:609:ILE:C	2.59	0.45
1:A:609:ILE:HD12	1:A:632:GLN:OE1	2.17	0.45
2:B:186:LEU:HD21	2:B:198:GLU:CB	2.47	0.45
1:C:354:PHE:CG	3:M:1:NAG:H62	2.51	0.45
1:C:444:CYS:HB2	1:C:506:LEU:HD12	1.99	0.45
1:C:491:LEU:HD11	1:C:545:ILE:HD11	1.99	0.45
1:C:959:ASN:O	1:C:960:GLN:HB3	2.16	0.45
1:C:961:GLU:HG2	1:C:1036:TRP:HA	1.99	0.45
2:D:154:VAL:HA	2:D:160:THR:CG2	2.47	0.45
1:E:831:SER:HA	1:E:842:THR:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:918:TYR:O	1:E:919:LEU:C	2.58	0.45
2:F:546:PHE:CD2	2:F:554:GLU:O	2.69	0.45
1:G:444:CYS:HB2	1:G:506:LEU:HD12	1.99	0.45
1:G:629:THR:CG2	1:G:630:LEU:N	2.80	0.45
1:G:679:ARG:C	1:G:679:ARG:HD3	2.42	0.45
1:G:681:LEU:HD12	1:G:682:SER:N	2.32	0.45
1:G:698:LEU:C	1:G:699:LEU:HD12	2.41	0.45
1:G:801:THR:HG22	1:G:843:SER:CB	2.47	0.45
2:H:154:VAL:HA	2:H:160:THR:CG2	2.47	0.45
2:H:601:GLY:O	2:H:602:LYS:HB2	2.17	0.45
1:A:243:LYS:HB2	1:A:246:ASP:HB2	1.98	0.45
1:A:269:VAL:HA	1:A:297:VAL:O	2.17	0.45
1:A:606:MET:HE3	1:A:715:LEU:CD2	2.47	0.45
1:A:613:ILE:HD12	1:A:748:PHE:CD2	2.52	0.45
1:A:653:GLN:HB2	1:E:630:LEU:HD21	1.99	0.45
1:A:801:THR:HG22	1:A:843:SER:CB	2.47	0.45
1:A:1063:LEU:N	1:A:1064:PRO:CD	2.79	0.45
1:C:41:ALA:O	1:C:42:ASN:C	2.58	0.45
1:C:52:TYR:O	1:C:53:SER:C	2.60	0.45
1:C:565:PHE:CD2	1:C:565:PHE:O	2.69	0.45
1:C:1069:PHE:CE2	2:D:584:GLY:HA3	2.52	0.45
2:D:285:LEU:C	2:D:287:HIS:N	2.74	0.45
2:D:347:LEU:HD22	2:D:389:PHE:CG	2.52	0.45
1:E:430:VAL:HG13	1:E:485:TRP:CE3	2.51	0.45
1:E:918:TYR:C	2:F:643:ARG:NH2	2.75	0.45
1:E:980:SER:HB3	1:E:1012:ARG:HB3	1.97	0.45
1:E:1063:LEU:N	1:E:1064:PRO:CD	2.79	0.45
2:F:188:LEU:HD12	2:F:230:TRP:HA	1.99	0.45
1:G:486:TRP:C	1:G:488:ASP:H	2.24	0.45
1:G:527:GLU:HG3	1:G:533:ALA:CB	2.47	0.45
1:G:613:ILE:HD12	1:G:748:PHE:CD2	2.52	0.45
1:G:799:THR:HG22	1:G:845:ARG:CB	2.47	0.45
2:H:83:LEU:HD11	2:H:419:VAL:HG13	1.99	0.45
2:H:100:ALA:O	2:H:101:LYS:CB	2.62	0.45
2:H:285:LEU:C	2:H:287:HIS:N	2.74	0.45
2:H:532:ARG:O	2:H:543:HIS:HB2	2.17	0.45
2:H:552:GLN:HG3	2:H:553:CYS:H	1.82	0.45
1:A:137:ILE:HD13	1:A:152:MET:SD	2.57	0.45
1:A:418:THR:HB	1:A:427:LYS:CG	2.47	0.45
1:A:475:VAL:HG12	1:A:491:LEU:O	2.17	0.45
1:A:609:ILE:HB	1:A:610:PRO:CD	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:THR:CG2	1:A:630:LEU:N	2.79	0.45
1:A:657:THR:HG23	1:A:720:VAL:CB	2.45	0.45
2:B:154:VAL:HA	2:B:160:THR:CG2	2.47	0.45
1:C:416:ILE:HG22	1:C:427:LYS:HD3	1.98	0.45
1:C:801:THR:HG22	1:C:843:SER:CB	2.47	0.45
1:E:606:MET:HE3	1:E:715:LEU:CD2	2.47	0.45
1:E:764:ILE:HD12	1:E:800:ILE:HD13	1.99	0.45
1:E:801:THR:HG22	1:E:843:SER:CB	2.47	0.45
2:F:154:VAL:HA	2:F:160:THR:CG2	2.47	0.45
1:G:25:TYR:CG	1:G:26:ALA:N	2.84	0.45
1:G:763:GLY:C	1:G:789:TRP:HE3	2.24	0.45
2:H:57:MET:HE2	2:H:57:MET:HA	1.99	0.45
1:A:303:LEU:O	1:A:306:ILE:HG12	2.17	0.44
1:A:437:SER:HA	1:A:463:HIS:O	2.17	0.44
1:A:464:TYR:HD2	1:A:472:GLN:HB2	1.82	0.44
1:A:486:TRP:C	1:A:488:ASP:H	2.24	0.44
1:A:822:LEU:HG	1:A:823:ARG:N	2.21	0.44
6:A:3378:MAN:C1	4:J:5:MAN:C3	2.95	0.44
2:B:532:ARG:O	2:B:543:HIS:HB2	2.16	0.44
1:C:108:PHE:CD1	1:C:117:GLN:HG2	2.52	0.44
1:C:464:TYR:HD2	1:C:472:GLN:HB2	1.82	0.44
1:C:529:GLU:C	1:C:531:ARG:H	2.26	0.44
1:C:764:ILE:HD12	1:C:800:ILE:HD13	1.99	0.44
1:C:956:VAL:HG12	1:C:957:GLU:N	2.32	0.44
2:D:36:ASP:N	2:D:510:GLN:HE22	2.15	0.44
2:D:453:GLY:HA2	2:D:463:THR:HG21	1.99	0.44
2:D:601:GLY:O	2:D:602:LYS:HB2	2.16	0.44
1:E:797:GLY:H	1:E:884:GLU:HB2	1.82	0.44
1:E:956:VAL:HG12	1:E:957:GLU:N	2.32	0.44
2:F:305:VAL:HG13	2:F:306:LYS:HG3	1.99	0.44
2:F:522:TYR:C	2:F:522:TYR:CD2	2.95	0.44
1:G:52:TYR:O	1:G:53:SER:C	2.60	0.44
1:G:376:GLN:C	1:G:378:ASN:N	2.75	0.44
1:G:385:TYR:CE2	1:G:407:ARG:HD3	2.51	0.44
1:G:608:PHE:O	1:G:609:ILE:C	2.60	0.44
1:G:902:LYS:C	1:G:903:TYR:CD2	2.95	0.44
1:G:1001:LEU:O	1:G:1001:LEU:HD23	2.18	0.44
2:H:305:VAL:HG13	2:H:306:LYS:HG3	1.99	0.44
1:A:52:TYR:O	1:A:53:SER:C	2.60	0.44
1:A:376:GLN:C	1:A:378:ASN:N	2.75	0.44
1:A:407:ARG:HG2	2:B:247:PHE:CZ	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:C	1:A:699:LEU:HD12	2.41	0.44
1:A:797:GLY:H	1:A:884:GLU:HB2	1.82	0.44
2:B:83:LEU:HD12	2:B:83:LEU:O	2.17	0.44
2:B:188:LEU:HD12	2:B:230:TRP:HA	1.99	0.44
2:B:432:ARG:O	2:B:433:ASP:HB2	2.17	0.44
2:B:436:LEU:O	2:B:437:CYS:HB2	2.17	0.44
1:C:418:THR:HB	1:C:427:LYS:CG	2.48	0.44
1:C:534:VAL:HG23	1:C:565:PHE:CE2	2.53	0.44
1:C:608:PHE:O	1:C:609:ILE:C	2.59	0.44
2:D:587:LEU:N	2:D:587:LEU:CD1	2.80	0.44
1:E:71:MET:O	1:E:72:SER:C	2.60	0.44
1:E:486:TRP:C	1:E:488:ASP:H	2.24	0.44
1:E:569:LEU:HD12	1:E:569:LEU:O	2.17	0.44
1:E:717:PHE:CE1	1:E:740:ARG:HA	2.52	0.44
1:E:752:CYS:SG	1:E:758:CYS:N	2.90	0.44
1:E:986:PRO:HG3	1:E:1003:CYS:O	2.17	0.44
2:F:317:LYS:HE3	2:F:410:GLY:HA3	1.99	0.44
2:F:616:PRO:HB2	2:F:620:ASN:CA	2.47	0.44
1:G:71:MET:O	1:G:72:SER:C	2.60	0.44
1:G:89:CYS:O	1:G:91:PRO:HD3	2.18	0.44
1:G:348:LEU:N	1:G:348:LEU:HD12	2.32	0.44
1:G:598:PRO:HG2	1:G:650:ARG:HD2	1.99	0.44
2:H:188:LEU:HD12	2:H:230:TRP:HA	2.00	0.44
1:A:68:ALA:CB	1:A:71:MET:HE2	2.46	0.44
2:B:522:TYR:CD2	2:B:522:TYR:C	2.95	0.44
1:C:116:THR:HG22	1:C:118:ARG:HG3	1.99	0.44
1:C:348:LEU:HD12	1:C:348:LEU:N	2.32	0.44
1:C:402:VAL:HG22	1:C:416:ILE:HG23	1.98	0.44
1:C:475:VAL:HG12	1:C:491:LEU:O	2.16	0.44
1:C:527:GLU:HG3	1:C:533:ALA:CB	2.47	0.44
1:C:564:TYR:CZ	1:C:588:ARG:HD2	2.52	0.44
1:C:797:GLY:H	1:C:884:GLU:HB2	1.82	0.44
2:D:382:GLN:HG3	2:D:383:ILE:H	1.82	0.44
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.85	0.44
1:E:108:PHE:CD1	1:E:117:GLN:HG2	2.52	0.44
1:E:475:VAL:HG12	1:E:491:LEU:O	2.17	0.44
1:E:601:TRP:HZ2	1:E:641:LYS:HD3	1.81	0.44
1:E:897:LEU:C	1:E:897:LEU:HD12	2.43	0.44
1:E:919:LEU:CB	1:E:1079:GLU:HB3	2.46	0.44
2:F:103:TYR:HB3	2:F:233:VAL:HG11	1.99	0.44
2:F:601:GLY:O	2:F:602:LYS:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:418:THR:HB	1:G:427:LYS:CG	2.48	0.44
1:G:565:PHE:CD2	1:G:565:PHE:O	2.70	0.44
1:G:717:PHE:CE1	1:G:740:ARG:HA	2.52	0.44
1:G:739:GLN:HB2	1:G:742:PHE:CE1	2.52	0.44
1:G:938:VAL:HG12	1:G:1024:LEU:O	2.17	0.44
2:H:436:LEU:O	2:H:437:CYS:HB2	2.17	0.44
1:A:679:ARG:HD3	1:A:679:ARG:C	2.43	0.44
1:A:717:PHE:CE1	1:A:740:ARG:HA	2.53	0.44
1:A:897:LEU:C	1:A:897:LEU:HD12	2.42	0.44
2:B:271:TYR:O	2:B:271:TYR:CG	2.70	0.44
1:C:71:MET:O	1:C:72:SER:C	2.60	0.44
2:D:103:TYR:HB3	2:D:233:VAL:HG11	1.99	0.44
2:D:168:PRO:CG	2:D:179:PRO:HG3	2.47	0.44
2:D:305:VAL:HG13	2:D:306:LYS:HG3	1.99	0.44
1:E:354:PHE:CE2	5:P:1:NAG:O5	2.70	0.44
1:E:609:ILE:HB	1:E:610:PRO:CD	2.45	0.44
2:F:75:GLN:CG	2:F:98:ARG:O	2.66	0.44
2:F:112:ASP:O	2:F:117:MET:HG3	2.17	0.44
2:F:144:ILE:HG22	2:F:195:PHE:CZ	2.53	0.44
2:F:631:SER:HB3	2:F:664:LEU:HD11	1.99	0.44
1:G:416:ILE:HG22	1:G:427:LYS:HD3	1.98	0.44
1:G:598:PRO:HB3	1:G:650:ARG:HH12	1.82	0.44
1:G:897:LEU:C	1:G:897:LEU:HD12	2.43	0.44
1:G:956:VAL:HG12	1:G:957:GLU:N	2.32	0.44
2:H:186:LEU:HD21	2:H:198:GLU:CB	2.47	0.44
1:A:134:VAL:O	1:A:235:LEU:HD12	2.17	0.44
1:A:444:CYS:HB2	1:A:506:LEU:HD12	1.98	0.44
1:A:553:ILE:HG23	1:A:557:GLN:HG3	2.00	0.44
1:A:569:LEU:HD12	1:A:569:LEU:O	2.17	0.44
2:B:144:ILE:HG22	2:B:195:PHE:CZ	2.53	0.44
1:C:89:CYS:O	1:C:91:PRO:HD3	2.18	0.44
1:C:569:LEU:HD12	1:C:569:LEU:O	2.17	0.44
1:C:766:PHE:HZ	1:C:877:LEU:HD12	1.83	0.44
1:C:897:LEU:C	1:C:897:LEU:HD12	2.42	0.44
2:D:75:GLN:CG	2:D:98:ARG:O	2.66	0.44
1:E:116:THR:HG22	1:E:118:ARG:HG3	2.00	0.44
1:E:444:CYS:HB2	1:E:506:LEU:HD12	1.99	0.44
2:F:436:LEU:O	2:F:437:CYS:HB2	2.17	0.44
1:G:565:PHE:HB2	1:G:587:ALA:CB	2.48	0.44
1:G:961:GLU:HG2	1:G:1036:TRP:HA	1.99	0.44
2:H:158:VAL:HB	2:H:207:ASN:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:TYR:O	2:H:271:TYR:CG	2.70	0.44
2:H:522:TYR:CE1	2:H:552:GLN:HA	2.53	0.44
1:A:71:MET:O	1:A:72:SER:C	2.60	0.44
1:A:964:TRP:HB3	1:A:1032:LEU:HG	1.99	0.44
1:A:1001:LEU:HD23	1:A:1001:LEU:O	2.18	0.44
1:A:1023:GLU:O	1:A:1024:LEU:C	2.60	0.44
2:B:345:VAL:HG11	2:B:387:ILE:HD11	1.99	0.44
1:C:717:PHE:CE1	1:C:740:ARG:HA	2.52	0.44
1:C:799:THR:HA	1:C:845:ARG:HA	1.98	0.44
1:C:986:PRO:HG3	1:C:1003:CYS:O	2.17	0.44
2:D:168:PRO:HG2	2:D:179:PRO:HG3	1.99	0.44
1:E:52:TYR:O	1:E:53:SER:C	2.60	0.44
1:E:89:CYS:O	1:E:91:PRO:HD3	2.18	0.44
1:E:418:THR:HB	1:E:427:LYS:CG	2.47	0.44
1:E:527:GLU:HG3	1:E:533:ALA:CB	2.47	0.44
2:F:158:VAL:HB	2:F:207:ASN:HB2	1.99	0.44
1:G:4:ASP:OD2	1:G:597:ARG:NH2	2.51	0.44
2:H:75:GLN:CG	2:H:98:ARG:O	2.65	0.44
2:H:83:LEU:HD12	2:H:83:LEU:O	2.16	0.44
2:H:345:VAL:HG11	2:H:387:ILE:CD1	2.47	0.44
1:A:110:LEU:HG	1:A:115:LEU:CD2	2.48	0.44
1:A:116:THR:HG22	1:A:118:ARG:HG3	2.00	0.44
1:A:254:ILE:HG23	1:A:264:ARG:NH2	2.32	0.44
1:A:534:VAL:HG12	1:A:535:TYR:N	2.33	0.44
1:A:953:TRP:CD2	1:C:755:ASP:HB3	2.52	0.44
2:B:158:VAL:HB	2:B:207:ASN:HB2	1.99	0.44
1:C:908:VAL:CG1	2:D:595:GLY:HA3	2.41	0.44
1:E:534:VAL:HG23	1:E:565:PHE:CE2	2.53	0.44
1:E:608:PHE:O	1:E:609:ILE:C	2.59	0.44
2:F:368:VAL:HG11	2:F:370:HIS:CE1	2.53	0.44
1:G:402:VAL:HG22	1:G:416:ILE:HG23	1.98	0.44
2:H:522:TYR:CD2	2:H:522:TYR:C	2.95	0.44
1:A:270:GLY:O	1:A:271:LEU:HB3	2.18	0.44
1:A:367:MET:HG2	1:A:368:SER:O	2.18	0.44
1:A:529:GLU:C	1:A:531:ARG:H	2.26	0.44
1:A:575:LEU:HD12	1:A:576:THR:CG2	2.47	0.44
1:A:816:GLY:O	1:A:818:LYS:CA	2.66	0.44
1:A:1081:TYR:O	1:A:1082:LYS:HB2	2.18	0.44
2:B:103:TYR:HB3	2:B:233:VAL:HG11	1.98	0.44
2:B:368:VAL:HG11	2:B:370:HIS:CE1	2.53	0.44
1:C:119:LEU:HD23	1:C:124:GLN:HE21	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:LYS:HG3	2:D:346:PHE:CE1	2.53	0.44
2:D:436:LEU:O	2:D:437:CYS:HB2	2.17	0.44
1:E:119:LEU:O	1:E:363:TYR:HE1	1.97	0.44
1:E:553:ILE:HG23	1:E:557:GLN:HG3	2.00	0.44
1:E:565:PHE:HB2	1:E:587:ALA:CB	2.48	0.44
1:E:679:ARG:C	1:E:679:ARG:HD3	2.42	0.44
1:E:1020:VAL:O	1:E:1021:GLN:HB2	2.18	0.44
1:E:1071:ARG:HH12	1:G:755:ASP:CG	2.26	0.44
1:G:20:ASP:OD1	2:H:257:LEU:HD22	2.18	0.44
1:G:529:GLU:C	1:G:531:ARG:H	2.26	0.44
1:G:609:ILE:HD12	1:G:632:GLN:OE1	2.18	0.44
2:H:112:ASP:O	2:H:117:MET:HG3	2.17	0.44
1:A:565:PHE:HB2	1:A:587:ALA:CB	2.48	0.44
1:A:961:GLU:HG2	1:A:1036:TRP:HA	1.99	0.44
2:B:75:GLN:CG	2:B:98:ARG:O	2.66	0.44
2:B:99:ARG:O	2:B:383:ILE:O	2.36	0.44
2:B:112:ASP:O	2:B:117:MET:HG3	2.17	0.44
2:B:289:LEU:HD12	2:B:294:ILE:HB	2.00	0.44
2:B:587:LEU:N	2:B:587:LEU:CD1	2.80	0.44
1:C:22:VAL:HG22	1:C:23:VAL:N	2.33	0.44
2:D:112:ASP:O	2:D:117:MET:HG3	2.17	0.44
2:D:277:PHE:CE1	2:D:278:ASP:O	2.71	0.44
2:D:368:VAL:HG11	2:D:370:HIS:CE1	2.53	0.44
1:E:22:VAL:HG22	1:E:23:VAL:N	2.33	0.44
1:E:529:GLU:C	1:E:531:ARG:H	2.26	0.44
1:G:119:LEU:HD23	1:G:124:GLN:HE21	1.83	0.44
1:G:525:PRO:HA	1:G:532:GLY:HA2	2.00	0.44
1:G:534:VAL:HG23	1:G:565:PHE:CE2	2.53	0.44
1:G:534:VAL:HG12	1:G:535:TYR:N	2.33	0.44
1:G:822:LEU:CG	1:G:823:ARG:N	2.81	0.44
2:H:108:TYR:CE2	2:H:147:GLY:HA3	2.53	0.44
2:H:289:LEU:HD12	2:H:294:ILE:HB	2.00	0.44
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.00	0.43
1:A:681:LEU:HD12	1:A:682:SER:N	2.32	0.43
1:A:956:VAL:HG12	1:A:957:GLU:N	2.32	0.43
2:B:305:VAL:HG13	2:B:306:LYS:HG3	1.99	0.43
1:C:103:LEU:HD11	2:D:155:LEU:HD13	2.00	0.43
1:C:367:MET:HG2	1:C:368:SER:O	2.18	0.43
1:C:525:PRO:HA	1:C:532:GLY:HA2	2.00	0.43
1:C:560:SER:C	1:C:561:ARG:HG3	2.43	0.43
1:C:565:PHE:HB2	1:C:587:ALA:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:ARG:C	1:C:679:ARG:HD3	2.43	0.43
1:C:1001:LEU:O	1:C:1001:LEU:HD23	2.18	0.43
1:C:1023:GLU:O	1:C:1024:LEU:C	2.60	0.43
2:D:532:ARG:O	2:D:543:HIS:HB2	2.17	0.43
1:E:367:MET:HG2	1:E:368:SER:O	2.18	0.43
1:G:22:VAL:HG22	1:G:23:VAL:N	2.33	0.43
2:H:144:ILE:HG22	2:H:195:PHE:CZ	2.53	0.43
2:H:461:CYS:SG	2:H:466:ARG:NE	2.91	0.43
1:A:348:LEU:HD12	1:A:348:LEU:N	2.32	0.43
1:A:419:GLN:HA	1:A:424:TRP:HA	2.00	0.43
1:A:970:SER:C	1:A:972:PRO:HD3	2.43	0.43
2:B:108:TYR:CE2	2:B:147:GLY:HA3	2.53	0.43
2:B:277:PHE:CE1	2:B:278:ASP:O	2.71	0.43
1:C:1020:VAL:C	1:C:1021:GLN:HG3	2.43	0.43
2:F:168:PRO:CG	2:F:179:PRO:HG3	2.47	0.43
2:F:347:LEU:HD22	2:F:389:PHE:CG	2.52	0.43
1:G:553:ILE:HG23	1:G:557:GLN:HG3	2.00	0.43
1:G:986:PRO:HG3	1:G:1003:CYS:O	2.17	0.43
2:H:277:PHE:CE1	2:H:278:ASP:O	2.71	0.43
1:A:323:THR:O	1:A:324:SER:C	2.61	0.43
1:A:361:PHE:CE2	1:A:371:PHE:CE1	3.06	0.43
1:A:764:ILE:HD12	1:A:800:ILE:HD13	1.99	0.43
1:A:915:PHE:CZ	1:A:917:LYS:HB2	2.53	0.43
2:B:671:ARG:C	2:B:672:GLU:HG3	2.43	0.43
1:C:103:LEU:HD12	2:D:156:PRO:HB3	2.00	0.43
1:C:110:LEU:HG	1:C:115:LEU:CD2	2.48	0.43
1:C:437:SER:HA	1:C:463:HIS:O	2.17	0.43
1:C:534:VAL:HG12	1:C:535:TYR:N	2.33	0.43
1:C:917:LYS:HE3	1:C:1077:VAL:HG23	2.00	0.43
2:D:108:TYR:CE2	2:D:147:GLY:HA3	2.53	0.43
2:D:354:ASP:O	2:D:544:PRO:CB	2.66	0.43
2:D:552:GLN:HG3	2:D:553:CYS:H	1.83	0.43
1:E:71:MET:SD	1:E:90:GLY:HA3	2.59	0.43
1:E:597:ARG:HA	1:E:598:PRO:HD3	1.88	0.43
1:E:613:ILE:HD12	1:E:748:PHE:CD2	2.52	0.43
1:E:639:ILE:HG13	1:E:689:LEU:HA	2.00	0.43
1:G:333:ALA:O	1:G:334:GLN:C	2.61	0.43
1:G:354:PHE:CE2	5:S:1:NAG:O5	2.71	0.43
1:G:764:ILE:HD12	1:G:800:ILE:HD13	1.99	0.43
2:H:103:TYR:HB3	2:H:104:PRO:CD	2.48	0.43
2:H:347:LEU:HD22	2:H:389:PHE:CG	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:368:VAL:HG11	2:H:370:HIS:CE1	2.53	0.43
2:H:616:PRO:HB2	2:H:620:ASN:CA	2.47	0.43
2:H:671:ARG:C	2:H:672:GLU:HG3	2.43	0.43
1:A:634:ASN:HB2	1:A:695:ASN:HB3	2.01	0.43
1:A:799:THR:HG22	1:A:845:ARG:HB3	2.00	0.43
2:B:10:SER:HA	2:B:447:ILE:HD11	2.01	0.43
2:B:57:MET:HE2	2:B:57:MET:HA	2.00	0.43
1:C:553:ILE:HG23	1:C:557:GLN:HG3	2.00	0.43
1:C:606:MET:HE3	1:C:715:LEU:CD2	2.47	0.43
1:C:970:SER:C	1:C:972:PRO:HD3	2.43	0.43
2:D:83:LEU:HD11	2:D:419:VAL:HG13	1.99	0.43
2:D:289:LEU:HD12	2:D:294:ILE:HB	2.00	0.43
2:D:671:ARG:C	2:D:672:GLU:HG3	2.43	0.43
1:E:665:GLY:HA3	2:F:498:HIS:HB3	1.99	0.43
1:E:766:PHE:CD1	1:E:766:PHE:C	2.96	0.43
1:E:799:THR:HG22	1:E:845:ARG:HB3	2.00	0.43
2:F:345:VAL:HG11	2:F:387:ILE:HD11	1.99	0.43
1:G:116:THR:HG22	1:G:118:ARG:HG3	2.00	0.43
1:G:934:HIS:ND1	1:G:1074:THR:HB	2.33	0.43
1:A:234:ILE:HD13	1:A:314:ILE:HG23	2.00	0.43
1:A:310:LEU:O	1:A:311:LYS:C	2.61	0.43
1:A:534:VAL:HG23	1:A:565:PHE:CE2	2.53	0.43
1:A:766:PHE:CD1	1:A:766:PHE:C	2.97	0.43
2:B:616:PRO:HB3	2:B:621:CYS:SG	2.58	0.43
1:C:656:VAL:HG13	1:C:718:THR:O	2.18	0.43
1:C:919:LEU:CB	1:C:1079:GLU:HB3	2.46	0.43
2:D:251:GLY:HA3	2:D:278:ASP:OD1	2.19	0.43
1:E:534:VAL:HG12	1:E:535:TYR:N	2.33	0.43
1:E:657:THR:HG23	1:E:720:VAL:CB	2.45	0.43
1:E:915:PHE:CZ	1:E:917:LYS:HB2	2.53	0.43
1:E:961:GLU:HG2	1:E:1036:TRP:HA	1.99	0.43
1:E:970:SER:C	1:E:972:PRO:HD3	2.43	0.43
1:E:1045:VAL:HG22	1:E:1046:SER:N	2.34	0.43
2:F:289:LEU:HD12	2:F:294:ILE:HB	2.00	0.43
2:F:432:ARG:O	2:F:433:ASP:HB2	2.17	0.43
1:G:402:VAL:HG12	1:G:443:LEU:HD22	2.00	0.43
1:G:606:MET:HE3	1:G:715:LEU:CD2	2.48	0.43
2:H:611:LYS:HG2	2:H:667:VAL:HB	2.01	0.43
1:A:282:LEU:HB3	1:A:294:ILE:HD13	1.99	0.43
1:A:631:VAL:HG11	1:A:746:LEU:CD1	2.49	0.43
1:A:790:ASN:O	1:A:853:GLY:O	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:PHE:CG	2:B:7:LYS:N	2.86	0.43
1:C:71:MET:SD	1:C:90:GLY:HA3	2.59	0.43
1:C:376:GLN:C	1:C:378:ASN:N	2.75	0.43
1:C:629:THR:CG2	1:C:630:LEU:N	2.80	0.43
1:C:919:LEU:HG	2:D:643:ARG:NH1	2.33	0.43
2:D:158:VAL:HB	2:D:207:ASN:HB2	2.00	0.43
2:D:611:LYS:HG2	2:D:667:VAL:HB	2.01	0.43
2:D:616:PRO:HB2	2:D:620:ASN:CA	2.47	0.43
1:E:1:PHE:CE2	1:E:599:VAL:HG11	2.54	0.43
1:E:361:PHE:CE2	1:E:371:PHE:CE1	3.07	0.43
1:E:464:TYR:HD2	1:E:472:GLN:HB2	1.83	0.43
1:E:663:ASP:HB3	1:E:666:ARG:HD3	2.01	0.43
1:E:771:LEU:O	1:G:789:TRP:CZ2	2.71	0.43
1:E:893:THR:HG23	1:E:893:THR:O	2.19	0.43
2:F:75:GLN:O	2:F:97:PHE:CD1	2.72	0.43
2:F:251:GLY:HA3	2:F:278:ASP:OD1	2.18	0.43
1:G:110:LEU:HG	1:G:115:LEU:CD2	2.48	0.43
1:G:657:THR:HG23	1:G:720:VAL:CB	2.45	0.43
2:H:168:PRO:HG2	2:H:179:PRO:HG3	2.00	0.43
2:H:334:ILE:HA	2:H:337:ALA:HB2	2.00	0.43
2:H:587:LEU:N	2:H:587:LEU:CD1	2.80	0.43
1:A:103:LEU:CD1	2:B:156:PRO:HG3	2.49	0.43
1:A:822:LEU:CG	1:A:823:ARG:N	2.81	0.43
1:A:956:VAL:O	1:A:963:VAL:HG23	2.19	0.43
2:B:83:LEU:HD11	2:B:419:VAL:HG13	1.99	0.43
2:B:219:MET:CE	2:B:262:GLY:HA2	2.48	0.43
1:C:36:GLN:HE21	2:D:255:ALA:HB1	1.83	0.43
1:C:915:PHE:CZ	1:C:917:LYS:HB2	2.53	0.43
1:E:110:LEU:HG	1:E:115:LEU:CD2	2.48	0.43
1:E:790:ASN:O	1:E:853:GLY:O	2.36	0.43
1:E:934:HIS:ND1	1:E:1074:THR:HB	2.34	0.43
1:E:1001:LEU:O	1:E:1001:LEU:HD23	2.18	0.43
2:F:108:TYR:CE2	2:F:147:GLY:HA3	2.53	0.43
2:F:340:LYS:HA	2:F:343:SER:HB2	2.00	0.43
2:F:616:PRO:HB3	2:F:621:CYS:SG	2.59	0.43
1:G:917:LYS:HE3	1:G:1077:VAL:HG23	2.00	0.43
1:A:402:VAL:CG1	1:A:443:LEU:HD22	2.49	0.43
1:A:484:ARG:NH1	2:B:586:GLN:NE2	2.67	0.43
1:A:766:PHE:HZ	1:A:877:LEU:HD12	1.83	0.43
2:B:466:ARG:O	2:B:467:SER:CB	2.65	0.43
2:B:565:ARG:HA	2:B:565:ARG:HD3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:VAL:HG23	1:C:565:PHE:CZ	2.54	0.43
2:D:27:LEU:HD21	2:D:446:GLY:C	2.43	0.43
2:D:186:LEU:HD21	2:D:198:GLU:HB2	2.01	0.43
2:D:188:LEU:HD12	2:D:230:TRP:HA	1.99	0.43
2:D:345:VAL:HG11	2:D:387:ILE:HD11	2.01	0.43
2:D:432:ARG:O	2:D:433:ASP:HB2	2.18	0.43
1:E:918:TYR:C	1:E:918:TYR:CD1	2.96	0.43
2:F:132:LEU:HA	2:F:135:LEU:HB3	2.01	0.43
2:F:277:PHE:CE1	2:F:278:ASP:O	2.71	0.43
2:F:587:LEU:N	2:F:587:LEU:CD1	2.80	0.43
1:G:402:VAL:CG1	1:G:443:LEU:HD22	2.49	0.43
1:G:1020:VAL:O	1:G:1021:GLN:HB2	2.18	0.43
1:G:1081:TYR:O	1:G:1082:LYS:HB2	2.18	0.43
2:H:6:PHE:CG	2:H:7:LYS:N	2.86	0.43
1:A:137:ILE:HG22	1:A:151:MET:HE3	2.00	0.43
1:A:317:ILE:HG23	1:A:317:ILE:O	2.18	0.43
1:A:333:ALA:O	1:A:334:GLN:C	2.62	0.43
1:A:656:VAL:HG13	1:A:718:THR:O	2.19	0.43
1:A:919:LEU:CB	1:A:1079:GLU:HB3	2.46	0.43
2:B:75:GLN:O	2:B:97:PHE:CD1	2.72	0.43
2:B:508:TYR:HE2	2:B:516:THR:HG23	1.83	0.43
1:C:402:VAL:CG1	1:C:443:LEU:HD22	2.49	0.43
1:C:790:ASN:O	1:C:853:GLY:O	2.37	0.43
2:D:161:HIS:CB	2:D:162:PRO:HA	2.44	0.43
2:D:543:HIS:HB3	2:D:544:PRO:HD2	2.00	0.43
1:E:333:ALA:O	1:E:334:GLN:C	2.62	0.43
1:E:609:ILE:HD12	1:E:632:GLN:OE1	2.19	0.43
1:E:987:PRO:HA	1:G:619:GLU:CD	2.43	0.43
2:F:6:PHE:CG	2:F:7:LYS:N	2.86	0.43
1:G:893:THR:HG23	1:G:893:THR:O	2.19	0.43
1:G:956:VAL:O	1:G:963:VAL:HG23	2.19	0.43
1:G:970:SER:C	1:G:972:PRO:HD3	2.43	0.43
2:H:132:LEU:HD22	2:H:192:SER:HB3	2.01	0.43
2:H:251:GLY:HA3	2:H:278:ASP:OD1	2.19	0.43
1:A:93:VAL:HB	1:A:104:THR:CG2	2.49	0.43
1:A:119:LEU:HD23	1:A:124:GLN:HE21	1.84	0.43
1:A:297:VAL:HG12	1:A:298:GLU:N	2.34	0.43
1:A:525:PRO:HA	1:A:532:GLY:HA2	2.00	0.43
1:A:1063:LEU:HD12	1:A:1064:PRO:HA	2.01	0.43
1:C:484:ARG:HH21	1:C:1021:GLN:HA	1.73	0.43
1:C:622:GLU:HG3	1:C:623:GLN:CB	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:ASP:HB3	1:C:666:ARG:HD3	2.01	0.43
1:C:816:GLY:O	1:C:817:GLN:C	2.62	0.43
2:D:75:GLN:O	2:D:97:PHE:CD1	2.72	0.43
2:D:271:TYR:O	2:D:271:TYR:CG	2.69	0.43
1:E:93:VAL:HB	1:E:104:THR:CG2	2.49	0.43
1:E:119:LEU:HD23	1:E:124:GLN:HE21	1.83	0.43
1:E:513:ASN:HA	1:E:599:VAL:HG21	1.99	0.43
1:E:797:GLY:HA3	1:E:884:GLU:HB2	2.01	0.43
2:F:168:PRO:HG2	2:F:179:PRO:HG3	1.99	0.43
2:F:169:CYS:HA	2:F:170:PRO:HD3	1.83	0.43
2:F:219:MET:CE	2:F:262:GLY:HA2	2.48	0.43
2:F:671:ARG:C	2:F:672:GLU:HG3	2.43	0.43
1:G:419:GLN:HA	1:G:424:TRP:HA	2.00	0.43
1:G:513:ASN:CB	1:G:599:VAL:HG21	2.49	0.43
1:G:618:PHE:CD2	1:G:619:GLU:N	2.87	0.43
1:G:790:ASN:O	1:G:853:GLY:O	2.36	0.43
1:G:915:PHE:CZ	1:G:917:LYS:HB2	2.53	0.43
2:H:75:GLN:O	2:H:97:PHE:CD1	2.72	0.43
2:H:132:LEU:HA	2:H:135:LEU:HB3	2.01	0.43
1:A:22:VAL:HG22	1:A:23:VAL:N	2.32	0.42
1:A:534:VAL:HG23	1:A:565:PHE:CZ	2.54	0.42
1:A:656:VAL:HG21	1:A:687:LEU:HD11	2.01	0.42
2:B:168:PRO:HG2	2:B:179:PRO:HG3	1.99	0.42
2:B:234:THR:HG22	2:B:235:ARG:N	2.34	0.42
1:C:8:LEU:C	1:C:8:LEU:HD12	2.44	0.42
1:C:361:PHE:CE2	1:C:371:PHE:CE1	3.06	0.42
1:C:639:ILE:HG13	1:C:689:LEU:HA	2.01	0.42
1:C:956:VAL:O	1:C:963:VAL:HG23	2.19	0.42
1:E:107:CYS:SG	1:E:348:LEU:CD2	3.07	0.42
1:E:534:VAL:HG23	1:E:565:PHE:CZ	2.54	0.42
1:E:634:ASN:HB2	1:E:695:ASN:HB3	2.01	0.42
1:E:656:VAL:HG13	1:E:718:THR:O	2.19	0.42
2:F:215:LEU:HD12	2:F:246:HIS:O	2.19	0.42
2:F:543:HIS:HB3	2:F:544:PRO:HD2	2.00	0.42
1:G:361:PHE:CE2	1:G:371:PHE:CE1	3.06	0.42
1:G:367:MET:HG2	1:G:368:SER:O	2.18	0.42
1:G:597:ARG:CD	1:G:731:ARG:HG2	2.49	0.42
1:G:631:VAL:HG11	1:G:746:LEU:CD1	2.49	0.42
1:G:639:ILE:HG13	1:G:689:LEU:HA	2.01	0.42
1:G:755:ASP:O	1:G:756:HIS:HB3	2.18	0.42
2:H:219:MET:CE	2:H:262:GLY:HA2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:317:LYS:HA	2:H:344:ARG:HD2	2.00	0.42
2:H:345:VAL:HG11	2:H:387:ILE:HD11	2.02	0.42
2:H:643:ARG:NH2	2:H:649:TRP:HZ2	2.17	0.42
1:A:151:MET:SD	1:A:238:ILE:CG2	3.08	0.42
1:A:402:VAL:HG12	1:A:443:LEU:HD22	2.00	0.42
1:A:491:LEU:HD21	1:A:545:ILE:O	2.19	0.42
1:A:893:THR:HG23	1:A:893:THR:O	2.19	0.42
1:A:934:HIS:ND1	1:A:1074:THR:HB	2.34	0.42
2:B:251:GLY:HA3	2:B:278:ASP:OD1	2.18	0.42
1:C:461:ALA:N	1:C:462:PRO:HD3	2.34	0.42
1:C:491:LEU:HD21	1:C:545:ILE:O	2.19	0.42
1:C:833:PRO:HA	1:C:840:TRP:HB3	2.01	0.42
2:D:6:PHE:CG	2:D:7:LYS:N	2.87	0.42
2:D:352:LEU:HD22	2:D:358:VAL:HG23	2.01	0.42
1:E:490:VAL:HG12	1:E:491:LEU:HA	1.99	0.42
1:E:631:VAL:HG11	1:E:746:LEU:CD1	2.49	0.42
1:G:534:VAL:HG23	1:G:565:PHE:CZ	2.54	0.42
1:G:656:VAL:HG13	1:G:718:THR:O	2.19	0.42
2:H:186:LEU:HD21	2:H:198:GLU:HB2	2.01	0.42
2:H:215:LEU:HD12	2:H:246:HIS:O	2.19	0.42
1:A:218:HIS:NE2	1:A:256:MET:SD	2.90	0.42
2:B:215:LEU:HD12	2:B:246:HIS:O	2.19	0.42
2:B:611:LYS:HG2	2:B:667:VAL:HB	2.01	0.42
1:C:119:LEU:H	1:C:120:PRO:CA	2.26	0.42
1:C:402:VAL:HG12	1:C:443:LEU:HD22	2.00	0.42
1:C:631:VAL:HG11	1:C:746:LEU:CD1	2.49	0.42
1:C:890:THR:HG22	1:C:891:SER:N	2.34	0.42
1:C:908:VAL:HG12	1:C:909:VAL:N	2.35	0.42
2:D:144:ILE:HG22	2:D:195:PHE:CZ	2.53	0.42
2:D:219:MET:CE	2:D:262:GLY:HA2	2.48	0.42
2:D:234:THR:HG22	2:D:235:ARG:N	2.34	0.42
1:E:374:MET:SD	1:E:417:PHE:CZ	3.13	0.42
1:E:491:LEU:HD21	1:E:545:ILE:O	2.19	0.42
1:G:634:ASN:HB2	1:G:695:ASN:HB3	2.01	0.42
1:A:89:CYS:O	1:A:91:PRO:HD3	2.18	0.42
1:A:160:SER:C	1:A:162:PHE:N	2.77	0.42
1:A:833:PRO:HA	1:A:840:TRP:HB3	2.01	0.42
2:B:256:ILE:O	2:B:256:ILE:HG13	2.19	0.42
2:B:569:SER:HB2	2:B:590:CYS:O	2.19	0.42
1:C:107:CYS:SG	1:C:348:LEU:CD2	3.08	0.42
1:C:656:VAL:HG21	1:C:687:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:PHE:CD1	1:C:766:PHE:C	2.97	0.42
1:C:813:VAL:HG23	1:C:823:ARG:NH1	2.34	0.42
1:C:832:ALA:O	1:C:840:TRP:HB2	2.19	0.42
2:D:256:ILE:O	2:D:256:ILE:HG13	2.20	0.42
1:E:956:VAL:O	1:E:963:VAL:HG23	2.19	0.42
2:F:569:SER:HB2	2:F:590:CYS:O	2.19	0.42
1:G:464:TYR:HD2	1:G:472:GLN:HB2	1.82	0.42
1:G:663:ASP:HB3	1:G:666:ARG:HD3	2.01	0.42
1:G:799:THR:HG22	1:G:845:ARG:HB3	2.00	0.42
1:G:918:TYR:CD1	1:G:918:TYR:C	2.97	0.42
1:G:1045:VAL:HG22	1:G:1046:SER:N	2.35	0.42
2:H:432:ARG:O	2:H:433:ASP:HB2	2.18	0.42
2:H:648:CYS:SG	2:H:673:CYS:N	2.92	0.42
1:A:175:SER:HB2	1:A:204:GLN:O	2.20	0.42
1:A:461:ALA:N	1:A:462:PRO:HD3	2.34	0.42
1:A:609:ILE:HD11	1:E:690:LYS:HB3	2.00	0.42
1:A:639:ILE:HG13	1:A:689:LEU:HA	2.01	0.42
1:A:710:PRO:HG3	1:A:884:GLU:OE2	2.19	0.42
1:A:917:LYS:HE3	1:A:1077:VAL:HG23	2.00	0.42
2:B:352:LEU:HD22	2:B:358:VAL:HG23	2.01	0.42
1:C:419:GLN:HA	1:C:424:TRP:HA	2.01	0.42
1:C:799:THR:HG22	1:C:845:ARG:HB3	2.00	0.42
1:C:893:THR:HG23	1:C:893:THR:O	2.19	0.42
2:D:132:LEU:HD22	2:D:192:SER:HB3	2.01	0.42
2:D:244:GLY:HA2	2:D:304:MET:CE	2.50	0.42
1:E:525:PRO:HA	1:E:532:GLY:HA2	2.00	0.42
1:E:689:LEU:C	1:E:689:LEU:HD12	2.45	0.42
2:F:352:LEU:HD22	2:F:358:VAL:HG23	2.01	0.42
1:G:656:VAL:HG21	1:G:687:LEU:HD11	2.02	0.42
1:G:832:ALA:O	1:G:840:TRP:HB2	2.20	0.42
1:G:890:THR:HG22	1:G:891:SER:N	2.34	0.42
2:H:99:ARG:CG	2:H:100:ALA:H	2.27	0.42
2:H:352:LEU:HD22	2:H:358:VAL:HG23	2.01	0.42
1:A:71:MET:SD	1:A:90:GLY:HA3	2.59	0.42
1:A:438:TYR:HD2	1:A:441:ALA:HB2	1.85	0.42
1:A:790:ASN:O	1:A:854:GLY:HA2	2.20	0.42
2:B:334:ILE:HA	2:B:337:ALA:HB2	2.00	0.42
2:B:643:ARG:NH2	2:B:649:TRP:HZ2	2.18	0.42
1:C:333:ALA:O	1:C:334:GLN:C	2.61	0.42
1:C:695:ASN:O	1:G:686:VAL:CG1	2.67	0.42
1:C:797:GLY:HA3	1:C:884:GLU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:ASP:N	2:D:510:GLN:NE2	2.65	0.42
2:D:223:ALA:HB1	2:D:263:ARG:HA	2.02	0.42
2:D:455:ILE:HG22	2:D:456:GLY:N	2.35	0.42
2:D:473:GLY:C	2:D:475:CYS:H	2.28	0.42
2:D:616:PRO:HB3	2:D:621:CYS:SG	2.59	0.42
1:E:560:SER:C	1:E:561:ARG:HG3	2.45	0.42
1:E:656:VAL:HG21	1:E:687:LEU:HD11	2.02	0.42
1:E:908:VAL:HG11	2:F:595:GLY:CA	2.45	0.42
2:F:234:THR:HG22	2:F:235:ARG:N	2.34	0.42
1:G:86:LEU:HD23	1:G:87:LEU:N	2.34	0.42
1:G:107:CYS:SG	1:G:348:LEU:CD2	3.08	0.42
1:G:562:LEU:HD23	1:G:562:LEU:HA	1.85	0.42
1:G:817:GLN:O	1:G:818:LYS:HG2	2.19	0.42
2:H:234:THR:HG22	2:H:235:ARG:N	2.34	0.42
2:H:656:GLN:HB2	2:H:663:TYR:CE1	2.55	0.42
1:A:119:LEU:H	1:A:120:PRO:CA	2.31	0.42
1:A:119:LEU:CD2	1:A:124:GLN:HE21	2.33	0.42
2:B:244:GLY:HA2	2:B:304:MET:CE	2.50	0.42
2:B:315:ILE:HA	2:B:316:PRO:HD3	1.88	0.42
1:C:438:TYR:HD2	1:C:441:ALA:HB2	1.85	0.42
1:C:817:GLN:O	1:C:818:LYS:HG2	2.19	0.42
1:C:1081:TYR:O	1:C:1082:LYS:HB2	2.18	0.42
1:E:86:LEU:HD23	1:E:87:LEU:N	2.35	0.42
2:F:466:ARG:HE	2:F:466:ARG:HB3	1.81	0.42
2:H:256:ILE:HG13	2:H:256:ILE:O	2.19	0.42
2:H:616:PRO:HB3	2:H:621:CYS:SG	2.59	0.42
1:A:208:TYR:CD1	1:A:246:ASP:HA	2.55	0.42
1:A:374:MET:SD	1:A:417:PHE:CZ	3.13	0.42
1:A:560:SER:C	1:A:561:ARG:HG3	2.45	0.42
1:A:597:ARG:CD	1:A:731:ARG:HG2	2.50	0.42
1:A:890:THR:HG22	1:A:891:SER:N	2.34	0.42
1:A:1045:VAL:HG22	1:A:1046:SER:N	2.35	0.42
2:B:74:LYS:CD	2:B:103:TYR:OH	2.68	0.42
2:B:573:ARG:NH2	2:B:575:ARG:HD3	2.35	0.42
2:B:656:GLN:HB2	2:B:663:TYR:CE1	2.55	0.42
1:C:575:LEU:HD11	1:C:593:LEU:HD13	2.02	0.42
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.68	0.42
2:D:103:TYR:HB3	2:D:104:PRO:CD	2.49	0.42
1:E:372:ILE:O	1:E:372:ILE:HG13	2.20	0.42
1:E:402:VAL:CG1	1:E:443:LEU:HD22	2.49	0.42
1:E:419:GLN:HA	1:E:424:TRP:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:610:PRO:O	1:E:611:ALA:C	2.63	0.42
1:E:624:VAL:HG23	1:E:625:VAL:N	2.35	0.42
1:E:890:THR:HG22	1:E:891:SER:N	2.34	0.42
2:F:573:ARG:NH2	2:F:575:ARG:HD3	2.35	0.42
2:F:611:LYS:HG2	2:F:667:VAL:HB	2.01	0.42
1:G:93:VAL:HB	1:G:104:THR:CG2	2.49	0.42
1:G:352:GLY:HA2	1:G:356:TRP:HA	2.02	0.42
1:G:372:ILE:HG13	1:G:372:ILE:O	2.19	0.42
1:G:374:MET:SD	1:G:417:PHE:CZ	3.12	0.42
1:G:750:LYS:HG2	1:G:796:TYR:CE1	2.54	0.42
1:G:833:PRO:HA	1:G:840:TRP:HB3	2.01	0.42
2:H:543:HIS:HB3	2:H:544:PRO:HD2	2.00	0.42
1:A:832:ALA:O	1:A:840:TRP:HB2	2.20	0.42
2:B:543:HIS:HB3	2:B:544:PRO:HD2	2.00	0.42
1:C:450:SER:HB3	1:E:978:ARG:HH22	1.85	0.42
1:C:634:ASN:HB2	1:C:695:ASN:HB3	2.01	0.42
1:C:1020:VAL:O	1:C:1021:GLN:HB2	2.19	0.42
2:D:334:ILE:HA	2:D:337:ALA:HB2	2.00	0.42
2:D:656:GLN:HB2	2:D:663:TYR:CE1	2.54	0.42
1:E:23:VAL:HG22	1:E:24:GLN:N	2.35	0.42
1:E:832:ALA:O	1:E:840:TRP:HB2	2.19	0.42
1:E:1003:CYS:HB3	1:E:1008:CYS:HB2	1.89	0.42
2:F:256:ILE:HG13	2:F:256:ILE:O	2.20	0.42
2:F:648:CYS:SG	2:F:673:CYS:N	2.93	0.42
2:F:656:GLN:HB2	2:F:663:TYR:CE1	2.55	0.42
1:G:491:LEU:HD21	1:G:545:ILE:O	2.20	0.42
2:H:105:ILE:HG21	2:H:135:LEU:CD1	2.50	0.42
2:H:118:LEU:HD23	2:H:204:ILE:HG21	2.02	0.42
2:H:244:GLY:HA2	2:H:304:MET:CE	2.50	0.42
2:H:546:PHE:CD2	2:H:554:GLU:HG2	2.55	0.42
1:A:413:LYS:HG3	1:A:430:VAL:O	2.20	0.42
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.68	0.42
2:B:100:ALA:C	2:B:101:LYS:HG3	2.45	0.42
2:B:285:LEU:C	2:B:287:HIS:N	2.74	0.42
1:C:93:VAL:HB	1:C:104:THR:CG2	2.49	0.42
1:C:630:LEU:CD2	1:G:653:GLN:OE1	2.67	0.42
2:D:517:ILE:HD12	2:D:518:ASN:N	2.35	0.42
1:E:119:LEU:CD2	1:E:124:GLN:HE21	2.33	0.42
1:E:491:LEU:CD2	1:E:545:ILE:O	2.68	0.42
1:E:917:LYS:HE3	1:E:1077:VAL:HG23	2.00	0.42
2:F:118:LEU:HD23	2:F:204:ILE:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:611:LYS:CB	2:F:667:VAL:HB	2.50	0.42
1:G:71:MET:SD	1:G:90:GLY:HA3	2.59	0.42
1:G:119:LEU:CD2	1:G:124:GLN:HE21	2.33	0.42
1:G:766:PHE:HZ	1:G:877:LEU:HD12	1.83	0.42
2:H:468:SER:HB2	2:H:471:LEU:HD12	2.01	0.42
3:Q:1:NAG:H4	3:Q:2:NAG:H2	1.69	0.42
1:A:673:PHE:HE1	1:A:680:SER:HA	1.84	0.41
1:A:918:TYR:CD1	1:A:918:TYR:C	2.97	0.41
1:A:985:ALA:CB	1:C:621:ARG:HD3	2.38	0.41
1:A:1003:CYS:HB3	1:A:1008:CYS:HB2	1.89	0.41
2:B:132:LEU:HA	2:B:135:LEU:HB3	2.01	0.41
2:B:517:ILE:HD12	2:B:518:ASN:N	2.35	0.41
1:C:374:MET:SD	1:C:417:PHE:CZ	3.13	0.41
2:D:342:SER:O	2:D:382:GLN:HA	2.20	0.41
2:D:611:LYS:CB	2:D:667:VAL:HB	2.50	0.41
1:E:8:LEU:C	1:E:8:LEU:HD12	2.45	0.41
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.02	0.41
1:E:402:VAL:HG12	1:E:443:LEU:HD22	2.01	0.41
1:E:673:PHE:HE1	1:E:680:SER:HA	1.85	0.41
2:F:186:LEU:HD21	2:F:198:GLU:HB2	2.01	0.41
2:F:222:ALA:CB	2:F:294:ILE:HD12	2.50	0.41
1:G:438:TYR:HD2	1:G:441:ALA:HB2	1.85	0.41
1:G:560:SER:C	1:G:561:ARG:HG3	2.45	0.41
1:G:673:PHE:HE1	1:G:680:SER:HA	1.84	0.41
1:G:790:ASN:O	1:G:854:GLY:HA2	2.20	0.41
1:G:1020:VAL:C	1:G:1021:GLN:HG3	2.45	0.41
2:H:222:ALA:CB	2:H:294:ILE:HD12	2.50	0.41
1:A:352:GLY:HA2	1:A:356:TRP:HA	2.02	0.41
1:A:490:VAL:HG12	1:A:491:LEU:HA	1.99	0.41
1:A:772:LYS:HB3	1:C:789:TRP:NE1	2.35	0.41
2:B:105:ILE:HG21	2:B:135:LEU:CD1	2.50	0.41
1:C:391:GLU:HG2	1:C:445:SER:H	1.85	0.41
1:C:533:ALA:HA	1:C:554:ALA:HA	2.02	0.41
1:C:625:VAL:CG2	1:C:627:GLU:HG3	2.50	0.41
1:C:934:HIS:ND1	1:C:1074:THR:HB	2.34	0.41
2:D:169:CYS:HB2	2:D:173:GLU:HA	2.02	0.41
2:D:423:CYS:O	2:D:424:GLU:C	2.63	0.41
1:E:766:PHE:HZ	1:E:877:LEU:HD12	1.83	0.41
2:F:132:LEU:HD22	2:F:192:SER:HB3	2.01	0.41
2:F:244:GLY:HA2	2:F:304:MET:CE	2.50	0.41
1:G:20:ASP:CG	2:H:257:LEU:HD22	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:VAL:HG22	1:G:24:GLN:N	2.35	0.41
1:G:461:ALA:N	1:G:462:PRO:HD3	2.34	0.41
1:G:490:VAL:HG12	1:G:491:LEU:HA	1.99	0.41
1:G:575:LEU:HD11	1:G:593:LEU:HD13	2.02	0.41
1:G:905:VAL:CG1	1:G:946:LEU:HD21	2.50	0.41
1:A:800:ILE:HG22	1:A:844:CYS:O	2.21	0.41
2:B:118:LEU:HD23	2:B:204:ILE:HG21	2.02	0.41
2:B:471:LEU:C	2:B:473:GLY:H	2.28	0.41
1:C:47:LEU:HB2	1:C:60:ILE:CG2	2.51	0.41
1:C:372:ILE:O	1:C:372:ILE:HG13	2.20	0.41
1:C:800:ILE:HG22	1:C:844:CYS:O	2.20	0.41
2:D:35:PRO:O	2:D:38:ILE:HG12	2.20	0.41
2:D:118:LEU:HD23	2:D:204:ILE:HG21	2.02	0.41
2:D:155:LEU:N	2:D:160:THR:CG2	2.84	0.41
2:D:643:ARG:NH2	2:D:649:TRP:HZ2	2.18	0.41
1:E:391:GLU:HG2	1:E:445:SER:H	1.85	0.41
1:E:1032:LEU:CD2	1:E:1078:LEU:HD21	2.46	0.41
2:F:223:ALA:HB1	2:F:263:ARG:HA	2.02	0.41
2:F:471:LEU:C	2:F:473:GLY:H	2.28	0.41
2:F:508:TYR:CE1	2:F:514:CYS:CB	3.03	0.41
2:F:643:ARG:NH2	2:F:649:TRP:HZ2	2.17	0.41
1:G:82:SER:HB2	1:G:83:PRO:HD2	2.03	0.41
1:G:446:VAL:CG1	1:G:456:LEU:HD11	2.50	0.41
1:G:464:TYR:O	1:G:465:TYR:HB3	2.21	0.41
1:G:491:LEU:CD2	1:G:545:ILE:O	2.69	0.41
1:G:597:ARG:CG	1:G:731:ARG:CG	2.99	0.41
1:G:678:ASN:ND2	7:G:3678:NAG:C7	2.79	0.41
1:G:787:MET:HA	1:G:858:THR:HG22	2.02	0.41
1:A:107:CYS:SG	1:A:348:LEU:CD2	3.08	0.41
1:A:689:LEU:C	1:A:689:LEU:HD12	2.45	0.41
1:A:800:ILE:HG23	1:A:800:ILE:O	2.21	0.41
2:B:132:LEU:HD22	2:B:192:SER:HB3	2.01	0.41
2:B:222:ALA:CB	2:B:294:ILE:HD12	2.50	0.41
2:B:223:ALA:HB1	2:B:263:ARG:HA	2.02	0.41
1:C:352:GLY:HA2	1:C:356:TRP:HA	2.02	0.41
1:C:384:SER:HB2	1:C:405:ALA:HB1	2.02	0.41
1:C:578:ASP:O	1:C:579:GLY:C	2.64	0.41
1:C:917:LYS:HE3	1:C:1077:VAL:HG21	2.02	0.41
2:D:132:LEU:HA	2:D:135:LEU:HB3	2.01	0.41
2:D:215:LEU:HD12	2:D:246:HIS:O	2.19	0.41
1:E:1020:VAL:O	1:E:1021:GLN:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:442:PHE:CE1	2:F:449:ARG:HD3	2.55	0.41
1:G:662:LEU:O	1:G:663:ASP:C	2.63	0.41
2:H:35:PRO:O	2:H:38:ILE:HG12	2.21	0.41
2:H:468:SER:HB2	2:H:471:LEU:CD1	2.51	0.41
2:H:573:ARG:NH2	2:H:575:ARG:HD3	2.35	0.41
1:A:82:SER:HB2	1:A:83:PRO:HD2	2.03	0.41
1:A:194:LEU:HD23	1:A:197:LEU:HD12	2.00	0.41
1:A:469:ARG:HH22	2:B:287:HIS:HB2	1.85	0.41
1:A:491:LEU:CD2	1:A:545:ILE:O	2.68	0.41
1:A:533:ALA:HA	1:A:554:ALA:HA	2.03	0.41
1:A:663:ASP:HB3	1:A:666:ARG:HD3	2.01	0.41
1:A:797:GLY:HA3	1:A:884:GLU:HB2	2.01	0.41
2:B:473:GLY:C	2:B:475:CYS:H	2.28	0.41
1:C:119:LEU:CD2	1:C:124:GLN:HE21	2.33	0.41
1:C:354:PHE:CE2	3:M:1:NAG:O5	2.73	0.41
1:C:621:ARG:HG2	1:C:622:GLU:H	1.86	0.41
1:C:753:GLY:C	1:C:755:ASP:H	2.28	0.41
1:C:790:ASN:O	1:C:854:GLY:HA2	2.19	0.41
1:C:1045:VAL:HG22	1:C:1046:SER:N	2.35	0.41
2:D:35:PRO:HB3	2:D:510:GLN:CD	2.46	0.41
2:D:468:SER:HB2	2:D:471:LEU:HD12	2.01	0.41
1:E:354:PHE:HB2	1:E:355:THR:H	1.67	0.41
1:E:533:ALA:HA	1:E:554:ALA:HA	2.03	0.41
1:E:772:LYS:HB3	1:G:789:TRP:NE1	2.35	0.41
2:F:105:ILE:HG21	2:F:135:LEU:CD1	2.50	0.41
2:F:169:CYS:CB	2:F:173:GLU:HA	2.50	0.41
2:F:517:ILE:HD12	2:F:518:ASN:N	2.35	0.41
1:G:438:TYR:CD2	1:G:441:ALA:HB2	2.56	0.41
1:G:752:CYS:SG	1:G:758:CYS:N	2.93	0.41
1:G:917:LYS:HE3	1:G:1077:VAL:HG21	2.03	0.41
2:H:223:ALA:HB1	2:H:263:ARG:HA	2.02	0.41
2:H:266:LEU:HD12	2:H:266:LEU:C	2.46	0.41
2:H:639:THR:O	2:H:639:THR:HG23	2.21	0.41
1:A:372:ILE:HG13	1:A:372:ILE:O	2.20	0.41
1:A:714:ARG:C	1:A:714:ARG:HD2	2.46	0.41
2:B:35:PRO:O	2:B:38:ILE:HG12	2.20	0.41
2:B:611:LYS:CB	2:B:667:VAL:HB	2.51	0.41
1:C:82:SER:HB2	1:C:83:PRO:HD2	2.02	0.41
1:C:610:PRO:O	1:C:611:ALA:C	2.64	0.41
1:C:662:LEU:HD21	1:C:698:LEU:HD23	2.03	0.41
2:D:99:ARG:O	2:D:383:ILE:O	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:SER:HB3	2:D:322:GLU:CG	2.51	0.41
2:D:569:SER:HB2	2:D:590:CYS:O	2.20	0.41
1:E:103:LEU:HD13	1:E:334:GLN:NE2	2.36	0.41
1:E:358:GLY:HA3	1:E:386:LEU:HB3	2.03	0.41
1:E:413:LYS:HG3	1:E:430:VAL:O	2.21	0.41
1:E:446:VAL:CG1	1:E:456:LEU:HD11	2.51	0.41
1:E:602:VAL:HG23	1:E:638:TYR:C	2.46	0.41
1:E:833:PRO:HA	1:E:840:TRP:HB3	2.01	0.41
1:E:917:LYS:HE3	1:E:1077:VAL:HG21	2.02	0.41
2:F:334:ILE:HA	2:F:337:ALA:HB2	2.00	0.41
2:F:468:SER:HB2	2:F:471:LEU:CD1	2.50	0.41
1:G:430:VAL:HG23	1:G:430:VAL:O	2.20	0.41
1:G:662:LEU:HD21	1:G:698:LEU:HD23	2.02	0.41
1:G:720:VAL:HG22	1:G:721:GLY:N	2.36	0.41
1:G:797:GLY:HA3	1:G:884:GLU:HB2	2.01	0.41
1:G:1003:CYS:HB3	1:G:1008:CYS:HB2	1.89	0.41
2:H:155:LEU:N	2:H:160:THR:CG2	2.84	0.41
1:A:103:LEU:HD13	1:A:334:GLN:NE2	2.36	0.41
1:A:391:GLU:HG2	1:A:445:SER:H	1.85	0.41
1:A:816:GLY:O	1:A:817:GLN:C	2.63	0.41
2:B:186:LEU:HD21	2:B:198:GLU:HB2	2.01	0.41
2:B:468:SER:HB2	2:B:471:LEU:CD1	2.51	0.41
1:C:60:ILE:HD11	1:C:110:LEU:CD2	2.51	0.41
1:C:328:PHE:O	1:C:354:PHE:HA	2.21	0.41
1:C:637:LEU:CD1	1:C:658:LEU:HD21	2.51	0.41
1:C:689:LEU:C	1:C:689:LEU:HD12	2.45	0.41
1:C:714:ARG:HD2	1:C:714:ARG:C	2.46	0.41
1:C:752:CYS:SG	1:C:758:CYS:N	2.94	0.41
2:D:468:SER:HB2	2:D:471:LEU:CD1	2.51	0.41
2:D:614:LYS:HE3	2:D:614:LYS:HB2	1.87	0.41
1:E:438:TYR:HD2	1:E:441:ALA:HB2	1.85	0.41
1:E:461:ALA:N	1:E:462:PRO:HD3	2.35	0.41
1:E:822:LEU:CG	1:E:823:ARG:N	2.82	0.41
2:F:35:PRO:O	2:F:38:ILE:HG12	2.20	0.41
2:F:188:LEU:CD1	2:F:230:TRP:HA	2.51	0.41
1:G:30:VAL:O	1:G:30:VAL:HG13	2.21	0.41
1:G:800:ILE:HG22	1:G:844:CYS:O	2.20	0.41
1:G:848:HIS:HB2	2:H:485:SER:HB3	2.01	0.41
2:H:169:CYS:CB	2:H:173:GLU:HA	2.51	0.41
2:H:471:LEU:C	2:H:473:GLY:H	2.29	0.41
2:H:569:SER:HB2	2:H:590:CYS:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD23	1:A:87:LEU:N	2.35	0.41
1:A:135:PHE:HZ	1:A:158:VAL:HB	1.86	0.41
1:A:221:PHE:CD1	1:A:233:LYS:HD2	2.56	0.41
1:A:560:SER:C	1:A:561:ARG:CG	2.94	0.41
1:A:602:VAL:HG23	1:A:638:TYR:C	2.46	0.41
1:A:610:PRO:O	1:A:611:ALA:C	2.63	0.41
1:A:811:ARG:HD3	1:A:864:ASP:OD2	2.21	0.41
1:A:905:VAL:CG1	1:A:946:LEU:HD21	2.50	0.41
1:A:986:PRO:HB3	1:A:987:PRO:CD	2.51	0.41
2:B:266:LEU:C	2:B:266:LEU:HD12	2.46	0.41
2:B:289:LEU:HD11	2:B:294:ILE:HG22	2.03	0.41
2:B:648:CYS:SG	2:B:673:CYS:N	2.94	0.41
1:C:413:LYS:HG3	1:C:430:VAL:O	2.20	0.41
1:C:630:LEU:HD22	1:G:653:GLN:OE1	2.21	0.41
1:C:657:THR:HG23	1:C:720:VAL:CB	2.45	0.41
1:C:686:VAL:HG11	1:G:695:ASN:O	2.20	0.41
1:C:876:LEU:HB3	1:C:898:GLU:HG3	2.03	0.41
1:C:918:TYR:CD1	1:C:918:TYR:C	2.97	0.41
1:C:931:VAL:HG23	1:C:1030:GLY:H	1.86	0.41
1:C:970:SER:O	1:C:1026:PHE:HB2	2.21	0.41
1:C:985:ALA:HA	1:C:986:PRO:HD3	1.94	0.41
2:D:281:SER:OG	2:D:284:GLN:HB2	2.21	0.41
1:E:676:THR:O	1:E:677:LYS:CB	2.69	0.41
1:E:876:LEU:HB3	1:E:898:GLU:HG3	2.03	0.41
1:E:970:SER:O	1:E:1026:PHE:HB2	2.21	0.41
1:E:1068:ALA:C	1:E:1070:MET:H	2.29	0.41
1:E:1081:TYR:O	1:E:1082:LYS:HB2	2.20	0.41
2:F:302:SER:HB3	2:F:322:GLU:CG	2.51	0.41
2:F:352:LEU:C	2:F:352:LEU:HD12	2.46	0.41
1:G:8:LEU:C	1:G:8:LEU:HD12	2.45	0.41
1:G:766:PHE:CD1	1:G:766:PHE:C	2.97	0.41
1:G:931:VAL:HG23	1:G:1030:GLY:H	1.86	0.41
2:H:546:PHE:CE2	2:H:554:GLU:HG2	2.56	0.41
1:A:8:LEU:C	1:A:8:LEU:HD12	2.45	0.41
1:A:23:VAL:HG22	1:A:24:GLN:N	2.35	0.41
1:A:181:HIS:CG	1:A:200:VAL:CG2	3.04	0.41
1:A:243:LYS:HD3	1:A:250:TYR:CE2	2.56	0.41
1:A:384:SER:HB2	1:A:405:ALA:HB1	2.02	0.41
1:A:438:TYR:CD2	1:A:441:ALA:HB2	2.56	0.41
1:A:813:VAL:HG23	1:A:823:ARG:NH1	2.36	0.41
2:B:169:CYS:CB	2:B:173:GLU:HA	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:SER:OG	2:B:284:GLN:HB2	2.21	0.41
2:B:442:PHE:CE1	2:B:449:ARG:HD3	2.56	0.41
2:B:468:SER:HB2	2:B:471:LEU:HD12	2.02	0.41
2:B:472:GLU:HA	2:B:475:CYS:CB	2.50	0.41
2:B:648:CYS:HA	2:B:672:GLU:O	2.21	0.41
1:C:23:VAL:HG22	1:C:24:GLN:N	2.35	0.41
1:C:86:LEU:HD23	1:C:87:LEU:N	2.35	0.41
1:C:490:VAL:HG12	1:C:491:LEU:HA	1.99	0.41
1:C:609:ILE:HD12	1:C:632:GLN:OE1	2.21	0.41
1:C:720:VAL:HG22	1:C:721:GLY:N	2.36	0.41
2:D:105:ILE:HG21	2:D:135:LEU:CD1	2.50	0.41
2:D:352:LEU:C	2:D:352:LEU:HD12	2.46	0.41
2:D:455:ILE:HG23	2:D:494:GLN:HE22	1.82	0.41
2:D:471:LEU:C	2:D:473:GLY:H	2.28	0.41
2:D:573:ARG:NH2	2:D:575:ARG:HD3	2.35	0.41
2:D:648:CYS:SG	2:D:673:CYS:N	2.94	0.41
1:E:25:TYR:HD2	1:E:29:TRP:HB2	1.86	0.41
1:E:119:LEU:H	1:E:120:PRO:CA	2.26	0.41
1:E:420:VAL:HG12	1:E:421:SER:N	2.36	0.41
1:E:714:ARG:C	1:E:714:ARG:HD2	2.46	0.41
1:E:905:VAL:CG1	1:E:946:LEU:HD21	2.50	0.41
1:E:986:PRO:HB3	1:E:987:PRO:CD	2.51	0.41
2:F:155:LEU:N	2:F:160:THR:CG2	2.83	0.41
2:F:281:SER:OG	2:F:284:GLN:HB2	2.21	0.41
2:F:468:SER:HB2	2:F:471:LEU:HD12	2.01	0.41
2:F:648:CYS:HA	2:F:672:GLU:O	2.21	0.41
1:G:103:LEU:CD1	2:H:156:PRO:HG3	2.50	0.41
1:G:103:LEU:HD11	2:H:155:LEU:HD13	2.02	0.41
1:G:384:SER:HB2	1:G:405:ALA:HB1	2.02	0.41
1:G:533:ALA:HA	1:G:554:ALA:HA	2.03	0.41
1:G:611:ALA:HB1	1:G:886:ASN:ND2	2.36	0.41
1:G:665:GLY:HA3	2:H:498:HIS:HB3	2.01	0.41
1:G:800:ILE:O	1:G:800:ILE:HG23	2.21	0.41
1:G:908:VAL:HG12	1:G:909:VAL:N	2.35	0.41
1:G:1020:VAL:O	1:G:1021:GLN:CB	2.68	0.41
2:H:289:LEU:HD11	2:H:294:ILE:HG22	2.03	0.41
2:H:517:ILE:HD12	2:H:518:ASN:N	2.35	0.41
1:A:764:ILE:HD12	1:A:800:ILE:CD1	2.51	0.41
1:A:876:LEU:HB3	1:A:898:GLU:HG3	2.03	0.41
1:C:420:VAL:HG12	1:C:421:SER:N	2.36	0.41
1:C:446:VAL:CG1	1:C:456:LEU:HD11	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:MET:HA	1:C:858:THR:HG22	2.02	0.41
2:D:222:ALA:CB	2:D:294:ILE:HD12	2.50	0.41
1:E:642:ARG:O	1:E:644:LYS:N	2.54	0.41
1:E:790:ASN:O	1:E:854:GLY:HA2	2.20	0.41
1:E:908:VAL:HG12	1:E:909:VAL:N	2.35	0.41
1:E:1020:VAL:C	1:E:1021:GLN:HG3	2.46	0.41
2:F:298:PHE:HB2	2:F:319:ALA:O	2.21	0.41
2:F:343:SER:HA	2:F:381:VAL:O	2.21	0.41
1:G:358:GLY:HA3	1:G:386:LEU:HB3	2.03	0.41
1:G:637:LEU:CD1	1:G:658:LEU:HD21	2.51	0.41
1:G:764:ILE:HD12	1:G:800:ILE:CD1	2.51	0.41
1:G:876:LEU:HB3	1:G:898:GLU:HG3	2.03	0.41
1:G:919:LEU:CB	1:G:1079:GLU:HB3	2.46	0.41
2:H:219:MET:HE1	2:H:288:LYS:HG2	2.03	0.41
2:H:546:PHE:HA	2:H:554:GLU:O	2.21	0.41
1:A:119:LEU:O	1:A:363:TYR:HE1	1.97	0.40
1:A:446:VAL:CG1	1:A:456:LEU:HD11	2.51	0.40
1:A:575:LEU:HD11	1:A:593:LEU:HD13	2.02	0.40
1:A:648:GLY:O	1:A:649:SER:C	2.64	0.40
2:B:103:TYR:HB3	2:B:104:PRO:CD	2.48	0.40
2:B:164:LYS:O	2:B:167:ASN:C	2.64	0.40
2:B:625:CYS:N	2:B:626:PRO:CD	2.84	0.40
1:C:464:TYR:O	1:C:465:TYR:HB3	2.21	0.40
1:C:586:GLY:HA2	1:C:591:VAL:HG23	2.04	0.40
1:C:673:PHE:HE1	1:C:680:SER:HA	1.85	0.40
2:D:164:LYS:O	2:D:167:ASN:C	2.64	0.40
2:D:169:CYS:CB	2:D:173:GLU:HA	2.51	0.40
2:D:266:LEU:C	2:D:266:LEU:HD12	2.46	0.40
1:E:47:LEU:HB2	1:E:60:ILE:CG2	2.51	0.40
1:E:60:ILE:HD11	1:E:110:LEU:CD2	2.51	0.40
1:E:335:GLU:OE2	1:E:361:PHE:HB2	2.21	0.40
1:E:438:TYR:CD2	1:E:441:ALA:HB2	2.56	0.40
1:E:560:SER:C	1:E:561:ARG:CG	2.94	0.40
1:E:575:LEU:HD11	1:E:593:LEU:HD13	2.02	0.40
1:E:776:VAL:HG12	1:E:867:PRO:O	2.21	0.40
1:G:578:ASP:O	1:G:579:GLY:C	2.64	0.40
1:G:642:ARG:O	1:G:644:LYS:N	2.54	0.40
1:G:1032:LEU:CD2	1:G:1078:LEU:HD21	2.46	0.40
2:H:648:CYS:HA	2:H:672:GLU:O	2.21	0.40
1:A:47:LEU:HB2	1:A:60:ILE:CG2	2.51	0.40
1:A:273:PHE:CB	1:A:296:LYS:HD2	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:O	1:A:663:ASP:C	2.63	0.40
1:A:908:VAL:HG12	1:A:909:VAL:N	2.35	0.40
1:A:1075:THR:HG23	1:A:1075:THR:O	2.21	0.40
1:C:25:TYR:HD2	1:C:29:TRP:HB2	1.86	0.40
1:C:103:LEU:HD13	1:C:334:GLN:NE2	2.36	0.40
1:C:560:SER:C	1:C:561:ARG:CG	2.93	0.40
1:C:618:PHE:CD2	1:C:619:GLU:HG3	2.57	0.40
1:C:746:LEU:HD23	1:C:746:LEU:C	2.46	0.40
1:C:776:VAL:HG12	1:C:867:PRO:O	2.21	0.40
2:D:565:ARG:HA	2:D:565:ARG:HD3	1.83	0.40
2:D:639:THR:HG23	2:D:639:THR:O	2.21	0.40
1:E:332:MET:SD	2:F:208:LEU:HD13	2.61	0.40
1:E:430:VAL:O	1:E:430:VAL:HG23	2.21	0.40
1:E:478:LEU:HG	1:E:478:LEU:O	2.21	0.40
1:E:662:LEU:HD21	1:E:698:LEU:HD23	2.02	0.40
1:E:746:LEU:HD23	1:E:746:LEU:C	2.46	0.40
2:F:230:TRP:CZ3	2:F:235:ARG:HB3	2.56	0.40
2:F:260:ASN:OD1	2:F:260:ASN:C	2.65	0.40
2:F:266:LEU:C	2:F:266:LEU:HD12	2.46	0.40
2:F:532:ARG:CD	2:F:554:GLU:HG3	2.51	0.40
2:F:596:CYS:HA	2:F:597:PRO:HD3	1.85	0.40
2:F:625:CYS:N	2:F:626:PRO:CD	2.85	0.40
1:G:25:TYR:HD2	1:G:29:TRP:HB2	1.85	0.40
2:H:164:LYS:O	2:H:167:ASN:C	2.64	0.40
1:A:578:ASP:O	1:A:579:GLY:C	2.64	0.40
1:A:630:LEU:HD21	1:E:653:GLN:CB	2.51	0.40
1:A:637:LEU:CD1	1:A:658:LEU:HD21	2.51	0.40
1:A:766:PHE:CE1	1:A:877:LEU:HD11	2.57	0.40
1:A:776:VAL:HG12	1:A:867:PRO:O	2.21	0.40
2:B:169:CYS:HA	2:B:170:PRO:HD3	1.82	0.40
2:B:219:MET:HE1	2:B:288:LYS:HG2	2.04	0.40
2:B:352:LEU:C	2:B:352:LEU:HD12	2.46	0.40
1:C:438:TYR:CD2	1:C:441:ALA:HB2	2.56	0.40
1:C:478:LEU:O	1:C:478:LEU:HG	2.21	0.40
1:C:631:VAL:HG11	1:C:746:LEU:HD11	2.04	0.40
1:C:678:ASN:ND2	7:C:3678:NAG:C7	2.78	0.40
1:C:800:ILE:O	1:C:800:ILE:HG23	2.21	0.40
1:C:1032:LEU:CD2	1:C:1078:LEU:HD21	2.46	0.40
2:D:97:PHE:O	2:D:387:ILE:HG12	2.22	0.40
2:D:169:CYS:HA	2:D:170:PRO:HD3	1.83	0.40
2:D:341:LEU:C	2:D:343:SER:N	2.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:442:PHE:CE1	2:D:449:ARG:HD3	2.56	0.40
1:E:342:THR:OG1	1:E:343:PRO:HD2	2.21	0.40
1:E:720:VAL:HG22	1:E:721:GLY:N	2.36	0.40
1:E:800:ILE:HG22	1:E:844:CYS:O	2.20	0.40
2:F:99:ARG:O	2:F:383:ILE:O	2.39	0.40
2:F:169:CYS:HB2	2:F:173:GLU:HA	2.02	0.40
2:F:665:ILE:HG22	2:F:666:TYR:N	2.36	0.40
2:F:673:CYS:O	2:F:674:VAL:C	2.64	0.40
1:G:586:GLY:HA2	1:G:591:VAL:HG23	2.04	0.40
1:G:676:THR:O	1:G:677:LYS:CB	2.69	0.40
1:G:714:ARG:HD2	1:G:714:ARG:C	2.46	0.40
2:H:97:PHE:O	2:H:387:ILE:HG12	2.22	0.40
2:H:163:ASP:C	2:H:165:LEU:N	2.79	0.40
2:H:442:PHE:CE1	2:H:449:ARG:HD3	2.56	0.40
2:H:611:LYS:CB	2:H:667:VAL:HB	2.50	0.40
1:A:137:ILE:CG2	1:A:151:MET:HE3	2.51	0.40
1:A:270:GLY:C	1:A:272:ALA:H	2.30	0.40
1:A:335:GLU:OE2	1:A:361:PHE:HB2	2.21	0.40
1:A:631:VAL:HG11	1:A:746:LEU:HD11	2.04	0.40
1:A:642:ARG:O	1:A:644:LYS:N	2.54	0.40
1:A:746:LEU:C	1:A:746:LEU:HD23	2.46	0.40
2:B:106:ASP:OD2	2:B:188:LEU:HD13	2.22	0.40
2:B:169:CYS:HB2	2:B:173:GLU:HA	2.03	0.40
2:B:260:ASN:ND2	2:B:280:PRO:HG3	2.37	0.40
2:B:302:SER:HB3	2:B:322:GLU:CG	2.51	0.40
1:C:335:GLU:OE2	1:C:361:PHE:HB2	2.21	0.40
1:C:958:LEU:O	1:C:959:ASN:HB3	2.21	0.40
1:C:1076:THR:CG2	1:C:1077:VAL:N	2.85	0.40
2:D:176:CYS:HB2	2:D:204:ILE:O	2.22	0.40
2:D:260:ASN:OD1	2:D:260:ASN:C	2.65	0.40
2:D:289:LEU:HD11	2:D:294:ILE:HG22	2.03	0.40
1:E:82:SER:HB2	1:E:83:PRO:HD2	2.02	0.40
1:E:464:TYR:O	1:E:465:TYR:HB3	2.21	0.40
1:E:637:LEU:CD1	1:E:658:LEU:HD21	2.51	0.40
1:E:812:TYR:HE2	1:E:814:ALA:HB2	1.85	0.40
2:F:164:LYS:O	2:F:167:ASN:C	2.64	0.40
1:G:60:ILE:HD11	1:G:110:LEU:CD2	2.51	0.40
1:G:103:LEU:HD13	1:G:334:GLN:NE2	2.36	0.40
1:G:970:SER:O	1:G:1026:PHE:HB2	2.21	0.40
1:G:1076:THR:HG22	1:G:1077:VAL:N	2.36	0.40
2:H:352:LEU:C	2:H:352:LEU:HD12	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:363:PHE:HB2	2:H:388:THR:HB	2.04	0.40
1:A:342:THR:OG1	1:A:343:PRO:HD2	2.22	0.40
1:A:676:THR:O	1:A:677:LYS:CB	2.69	0.40
1:A:917:LYS:HE3	1:A:1077:VAL:HG21	2.03	0.40
2:B:298:PHE:HB2	2:B:319:ALA:O	2.22	0.40
2:B:477:LYS:HG3	2:B:478:ASP:N	2.37	0.40
2:D:625:CYS:N	2:D:626:PRO:CD	2.84	0.40
2:D:648:CYS:HA	2:D:672:GLU:O	2.21	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.02	0.40
1:E:662:LEU:O	1:E:663:ASP:C	2.63	0.40
1:E:787:MET:HA	1:E:858:THR:HG22	2.03	0.40
1:E:800:ILE:HG23	1:E:800:ILE:O	2.21	0.40
1:E:813:VAL:HG23	1:E:823:ARG:NH1	2.36	0.40
1:E:1069:PHE:CE2	2:F:584:GLY:HA3	2.56	0.40
2:F:260:ASN:ND2	2:F:280:PRO:HG3	2.37	0.40
1:G:4:ASP:CG	1:G:597:ARG:NH2	2.80	0.40
1:G:335:GLU:OE2	1:G:361:PHE:HB2	2.21	0.40
1:G:971:HIS:N	1:G:972:PRO:HD3	2.37	0.40
2:H:158:VAL:CG2	2:H:207:ASN:HA	2.52	0.40
2:H:169:CYS:HB2	2:H:173:GLU:HA	2.02	0.40
2:H:281:SER:OG	2:H:284:GLN:HB2	2.21	0.40
2:H:659:GLY:O	2:H:660:MET: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 X-ray entries followed by that with respect to entries of similar resolution.

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	1080/1095 (99%)	839 (78%)	215 (20%)	26 (2%)	4	29
1	C	881/1095 (80%)	663 (75%)	194 (22%)	24 (3%)	4	27
1	E	880/1095 (80%)	665 (76%)	190 (22%)	25 (3%)	4	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	881/1095 (80%)	666 (76%)	191 (22%)	24 (3%)	4	27
2	B	672/687 (98%)	514 (76%)	147 (22%)	11 (2%)	7	36
2	D	672/687 (98%)	515 (77%)	145 (22%)	12 (2%)	6	34
2	F	672/687 (98%)	514 (76%)	145 (22%)	13 (2%)	6	33
2	H	672/687 (98%)	512 (76%)	146 (22%)	14 (2%)	5	31
All	All	6410/7128 (90%)	4888 (76%)	1373 (21%)	149 (2%)	5	30

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	120	PRO
1	A	757	ILE
1	C	82	SER
1	C	757	ILE
1	E	82	SER
1	E	757	ILE
1	E	817	GLN
1	G	82	SER
1	G	757	ILE
1	G	817	GLN
2	H	99	ARG
1	A	27	ASN
1	A	490	VAL
1	A	624	VAL
1	A	817	GLN
1	A	818	LYS
1	A	847	ASN
1	A	931	VAL
1	A	956	VAL
2	B	163	ASP
2	B	465	GLY
1	C	27	ASN
1	C	490	VAL
1	C	818	LYS
1	C	847	ASN
1	C	931	VAL
1	C	956	VAL
2	D	163	ASP
2	D	465	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	27	ASN
1	E	490	VAL
1	E	624	VAL
1	E	818	LYS
1	E	847	ASN
1	E	931	VAL
1	E	956	VAL
2	F	163	ASP
2	F	465	GLY
1	G	27	ASN
1	G	490	VAL
1	G	624	VAL
1	G	847	ASN
1	G	931	VAL
1	G	956	VAL
2	H	101	LYS
2	H	163	ASP
2	H	465	GLY
1	A	649	SER
2	B	158	VAL
2	B	314	ILE
2	B	467	SER
1	C	649	SER
1	C	817	GLN
2	D	158	VAL
2	D	314	ILE
2	D	467	SER
1	E	649	SER
2	F	158	VAL
2	F	314	ILE
2	F	467	SER
1	G	649	SER
1	G	818	LYS
2	H	158	VAL
2	H	314	ILE
2	H	467	SER
1	A	70	ASN
1	A	123	ARG
1	A	124	GLN
1	A	209	THR
1	A	246	ASP
1	A	643	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	654	SER
2	B	69	HIS
1	C	123	ARG
1	C	124	GLN
1	C	454	THR
1	C	624	VAL
1	C	643	SER
1	C	654	SER
1	C	816	GLY
2	D	69	HIS
1	E	123	ARG
1	E	124	GLN
1	E	454	THR
1	E	654	SER
1	E	758	CYS
2	F	69	HIS
2	F	463	THR
1	G	123	ARG
1	G	124	GLN
1	G	643	SER
1	G	654	SER
2	H	69	HIS
1	A	454	THR
1	A	579	GLY
1	A	816	GLY
2	B	639	THR
1	C	70	ASN
1	C	579	GLY
2	D	99	ARG
1	E	70	ASN
1	E	579	GLY
1	E	643	SER
1	E	722	LYS
2	F	99	ARG
2	F	639	THR
1	G	70	ASN
1	G	454	THR
1	G	579	GLY
2	H	639	THR
1	A	722	LYS
1	A	773	SER
2	B	660	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	722	LYS
1	C	773	SER
2	D	639	THR
2	D	660	MET
1	E	773	SER
1	E	816	GLY
2	F	652	TYR
2	F	660	MET
1	G	722	LYS
1	G	773	SER
1	G	816	GLY
2	H	660	MET
1	A	540	VAL
1	C	540	VAL
1	C	846	ILE
1	E	540	VAL
1	E	846	ILE
1	G	540	VAL
1	A	846	ILE
1	G	846	ILE
2	H	59	PRO
2	B	517	ILE
2	D	517	ILE
2	F	517	ILE
2	H	399	ILE
2	H	517	ILE
2	B	204	ILE
2	B	399	ILE
2	D	204	ILE
2	D	399	ILE
2	F	204	ILE
2	H	204	ILE
1	C	120	PRO
1	E	120	PRO
1	G	120	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 X-ray entries followed by that with respect to entries of similar resolution.

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	924/934 (99%)	914 (99%)	10 (1%)	65	74
1	C	754/934 (81%)	743 (98%)	11 (2%)	57	71
1	E	753/934 (81%)	743 (99%)	10 (1%)	61	72
1	G	754/934 (81%)	744 (99%)	10 (1%)	61	72
2	B	583/592 (98%)	582 (100%)	1 (0%)	87	85
2	D	583/592 (98%)	581 (100%)	2 (0%)	86	83
2	F	583/592 (98%)	582 (100%)	1 (0%)	87	85
2	H	583/592 (98%)	582 (100%)	1 (0%)	87	85
All	All	5517/6104 (90%)	5471 (99%)	46 (1%)	73	77

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	565	PHE
1	A	567	GLN
1	A	578	ASP
1	A	643	SER
1	A	681	LEU
1	A	731	ARG
1	A	840	TRP
1	A	915	PHE
1	A	933	MET
2	B	494	GLN
1	C	119	LEU
1	C	565	PHE
1	C	567	GLN
1	C	578	ASP
1	C	625	VAL
1	C	643	SER
1	C	681	LEU
1	C	731	ARG
1	C	840	TRP
1	C	915	PHE
1	C	933	MET
2	D	426	ARG
2	D	674	VAL
1	E	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	565	PHE
1	E	567	GLN
1	E	578	ASP
1	E	643	SER
1	E	681	LEU
1	E	731	ARG
1	E	840	TRP
1	E	915	PHE
1	E	933	MET
2	F	494	GLN
1	G	119	LEU
1	G	565	PHE
1	G	567	GLN
1	G	578	ASP
1	G	643	SER
1	G	681	LEU
1	G	731	ARG
1	G	840	TRP
1	G	915	PHE
1	G	933	MET
2	H	494	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	HIS
1	A	472	GLN
1	A	495	GLN
1	A	549	HIS
1	A	567	GLN
2	B	123	ASN
2	B	194	GLN
1	C	334	GLN
1	C	472	GLN
1	C	495	GLN
1	C	549	HIS
1	C	567	GLN
1	C	697	ASN
1	C	1039	GLN
2	D	123	ASN
2	D	194	GLN
2	D	293	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	462	GLN
2	D	510	GLN
2	D	552	GLN
1	E	124	GLN
1	E	463	HIS
1	E	472	GLN
1	E	495	GLN
1	E	549	HIS
1	E	567	GLN
1	E	623	GLN
1	E	674	GLN
2	F	123	ASN
2	F	194	GLN
2	F	293	ASN
1	G	463	HIS
1	G	472	GLN
1	G	495	GLN
1	G	549	HIS
1	G	567	GLN
1	G	886	ASN
2	H	123	ASN
2	H	194	GLN
2	H	464	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

29 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	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.53	0	17,19,21	0.61	0
3	NAG	I	2	3	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.50	0	17,19,21	1.18	2 (11%)
4	NAG	J	2	4	14,14,15	0.56	0	17,19,21	1.77	3 (17%)
4	MAN	J	3	4	11,11,12	0.44	0	15,15,17	1.80	4 (26%)
4	MAN	J	4	4	11,11,12	0.75	0	15,15,17	1.03	1 (6%)
4	MAN	J	5	4	11,11,12	0.62	0	15,15,17	1.53	2 (13%)
3	NAG	K	1	1,3	14,14,15	0.60	0	17,19,21	1.78	2 (11%)
3	NAG	K	2	3	14,14,15	0.54	0	17,19,21	1.58	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.54	0	17,19,21	0.59	0
3	NAG	L	2	3	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.48	0	17,19,21	1.16	2 (11%)
3	NAG	M	2	3	14,14,15	0.52	0	17,19,21	1.54	1 (5%)
3	NAG	N	1	1,3	14,14,15	0.55	0	17,19,21	1.97	2 (11%)
3	NAG	N	2	3	14,14,15	0.59	0	17,19,21	1.53	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.54	0	17,19,21	0.60	0
3	NAG	O	2	3	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.49	0	17,19,21	1.16	2 (11%)
5	NAG	P	2	5	14,14,15	0.57	0	17,19,21	1.73	2 (11%)
5	MAN	P	3	5	11,11,12	0.48	0	15,15,17	1.33	2 (13%)
3	NAG	Q	1	1,3	14,14,15	0.55	0	17,19,21	1.88	2 (11%)
3	NAG	Q	2	3	14,14,15	0.57	0	17,19,21	1.42	1 (5%)
3	NAG	R	1	1,3	14,14,15	0.53	0	17,19,21	0.61	0
3	NAG	R	2	3	14,14,15	0.59	0	17,19,21	1.02	1 (5%)
5	NAG	S	1	1,5	14,14,15	0.47	0	17,19,21	1.15	2 (11%)
5	NAG	S	2	5	14,14,15	0.56	0	17,19,21	1.77	2 (11%)
5	MAN	S	3	5	11,11,12	0.50	0	15,15,17	1.34	2 (13%)
3	NAG	T	1	1,3	14,14,15	0.56	0	17,19,21	1.95	2 (11%)
3	NAG	T	2	3	14,14,15	0.57	0	17,19,21	1.48	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	MAN	J	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	MAN	P	3	5	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
5	NAG	S	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	MAN	S	3	5	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C1-O5-C5	6.81	121.31	112.19
3	T	1	NAG	C1-O5-C5	6.67	121.13	112.19
3	Q	1	NAG	C1-O5-C5	6.46	120.85	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C1-O5-C5	6.15	120.43	112.19
3	K	2	NAG	C1-O5-C5	5.75	119.89	112.19
3	N	2	NAG	C1-O5-C5	5.55	119.63	112.19
3	T	2	NAG	C1-O5-C5	5.35	119.35	112.19
3	M	2	NAG	C1-O5-C5	5.33	119.33	112.19
3	Q	2	NAG	C1-O5-C5	5.11	119.04	112.19
5	S	2	NAG	C1-O5-C5	5.08	119.00	112.19
4	J	2	NAG	C1-O5-C5	5.02	118.91	112.19
5	P	2	NAG	C1-O5-C5	4.91	118.77	112.19
4	J	5	MAN	C1-O5-C5	3.59	117.00	112.19
3	T	1	NAG	O5-C1-C2	3.39	116.53	111.29
4	J	3	MAN	O3-C3-C2	3.36	116.91	110.05
3	N	1	NAG	O5-C1-C2	3.28	116.37	111.29
4	J	3	MAN	C2-C3-C4	-3.24	105.16	110.86
3	Q	1	NAG	O5-C1-C2	3.13	116.13	111.29
3	K	1	NAG	O5-C1-C2	3.02	115.97	111.29
3	R	2	NAG	C1-O5-C5	2.99	116.19	112.19
5	S	3	MAN	C2-C3-C4	-2.94	105.70	110.86
3	I	2	NAG	C1-O5-C5	2.93	116.11	112.19
3	L	2	NAG	C1-O5-C5	2.87	116.04	112.19
5	S	2	NAG	O4-C4-C3	2.85	117.11	110.38
5	P	3	MAN	C2-C3-C4	-2.81	105.91	110.86
3	O	2	NAG	C1-O5-C5	2.81	115.95	112.19
5	P	2	NAG	O4-C4-C3	2.77	116.91	110.38
4	J	5	MAN	C6-C5-C4	-2.76	106.24	113.02
4	J	2	NAG	O4-C4-C3	2.75	116.86	110.38
4	J	4	MAN	C1-O5-C5	-2.72	108.54	112.19
4	J	1	NAG	O5-C1-C2	2.67	115.42	111.29
5	S	1	NAG	O5-C1-C2	2.60	115.32	111.29
5	P	1	NAG	O5-C1-C2	2.56	115.25	111.29
5	P	3	MAN	O5-C5-C6	2.48	112.49	107.66
5	P	1	NAG	C1-O5-C5	2.47	115.50	112.19
4	J	1	NAG	C1-O5-C5	2.44	115.45	112.19
3	M	1	NAG	O5-C1-C2	2.41	115.03	111.29
5	S	3	MAN	O5-C5-C6	2.40	112.33	107.66
4	J	3	MAN	C3-C4-C5	-2.33	106.01	110.23
5	S	1	NAG	C1-O5-C5	2.32	115.30	112.19
3	M	1	NAG	C1-O5-C5	2.26	115.22	112.19
4	J	3	MAN	C1-O5-C5	2.16	115.09	112.19
4	J	2	NAG	O3-C3-C2	-2.10	105.04	109.40

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	1	NAG	C1
4	J	1	NAG	C1
4	J	3	MAN	C1
5	P	1	NAG	C1
5	P	3	MAN	C1
5	S	1	NAG	C1
5	S	3	MAN	C1

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C3-C2-N2-C7
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C3-C2-N2-C7
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
4	J	3	MAN	O5-C5-C6-O6
5	P	3	MAN	O5-C5-C6-O6
5	S	3	MAN	O5-C5-C6-O6
4	J	3	MAN	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
5	P	3	MAN	C4-C5-C6-O6
5	S	3	MAN	C4-C5-C6-O6
3	O	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

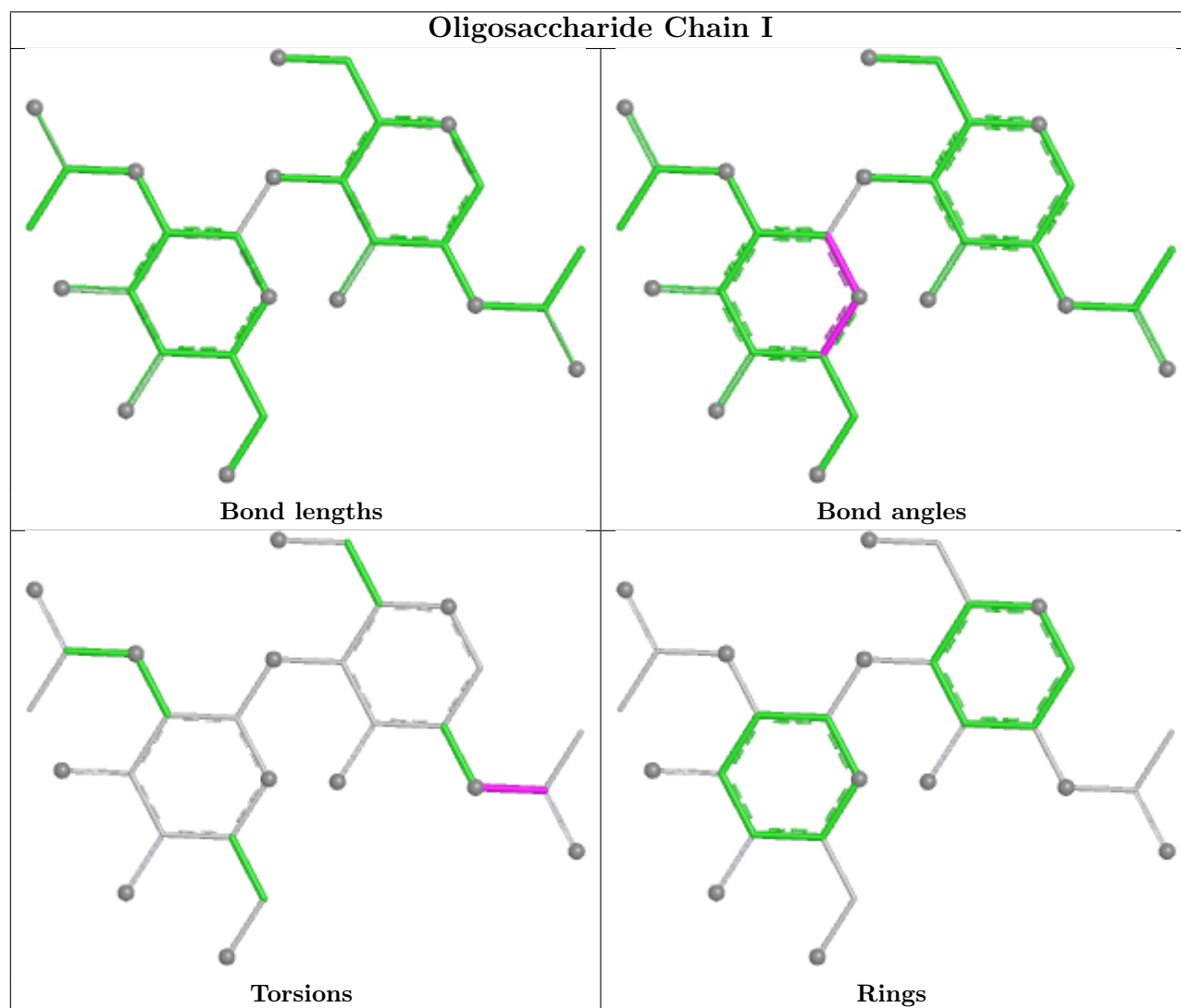
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
5	P	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
4	J	4	MAN	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C8-C7-N2-C2
3	M	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O7-C7-N2-C2
5	P	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6

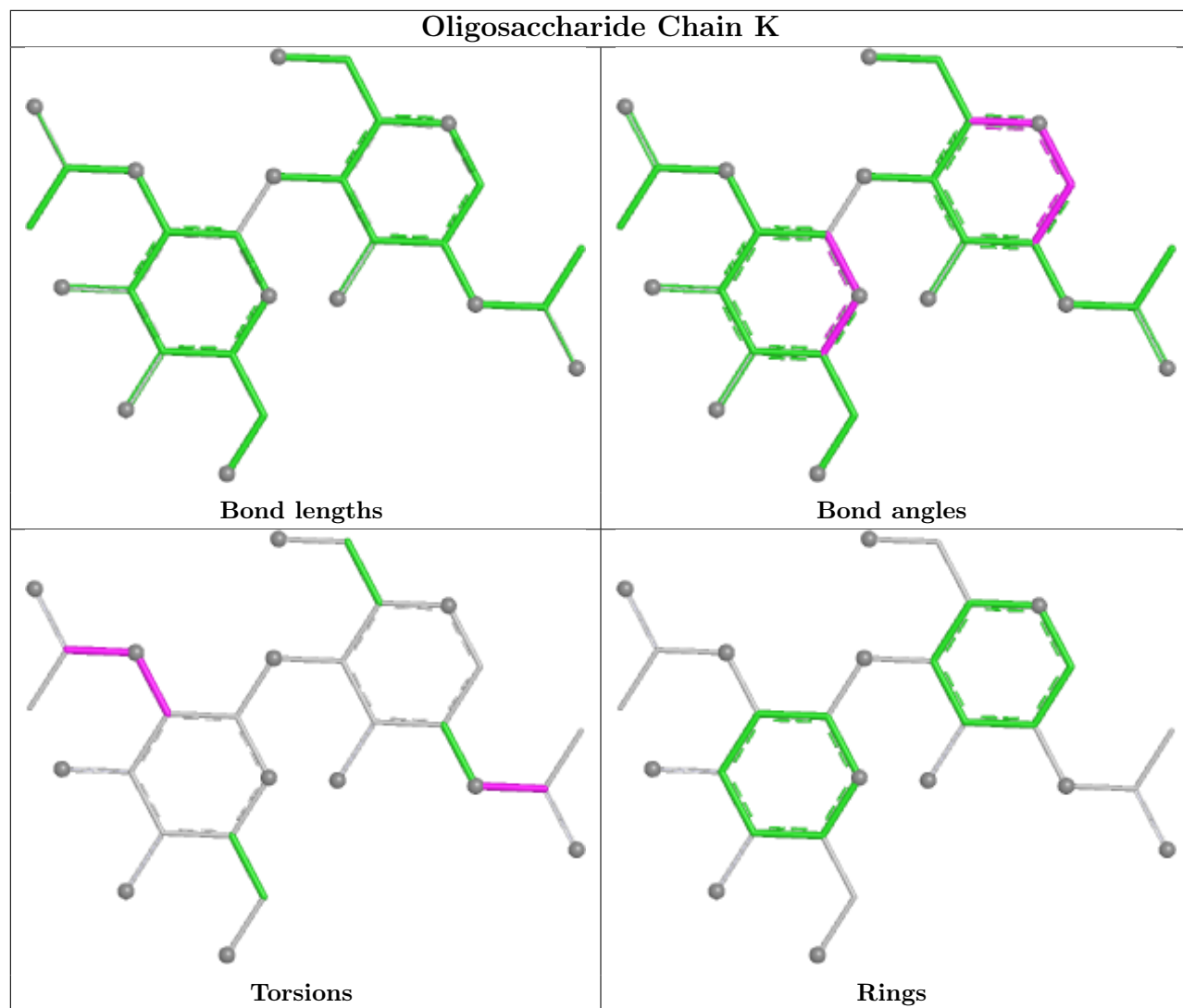
There are no ring outliers.

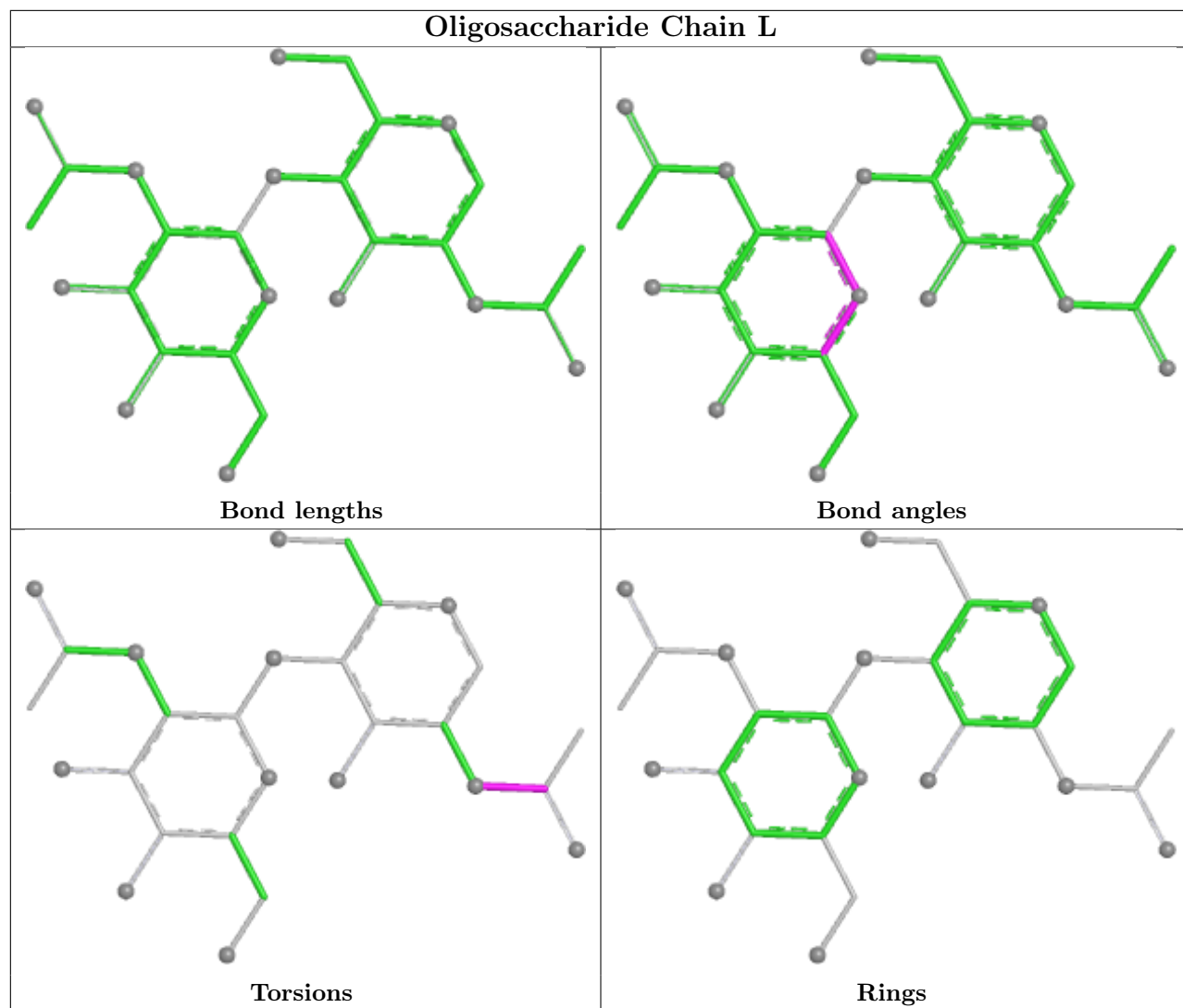
16 monomers are involved in 28 short contacts:

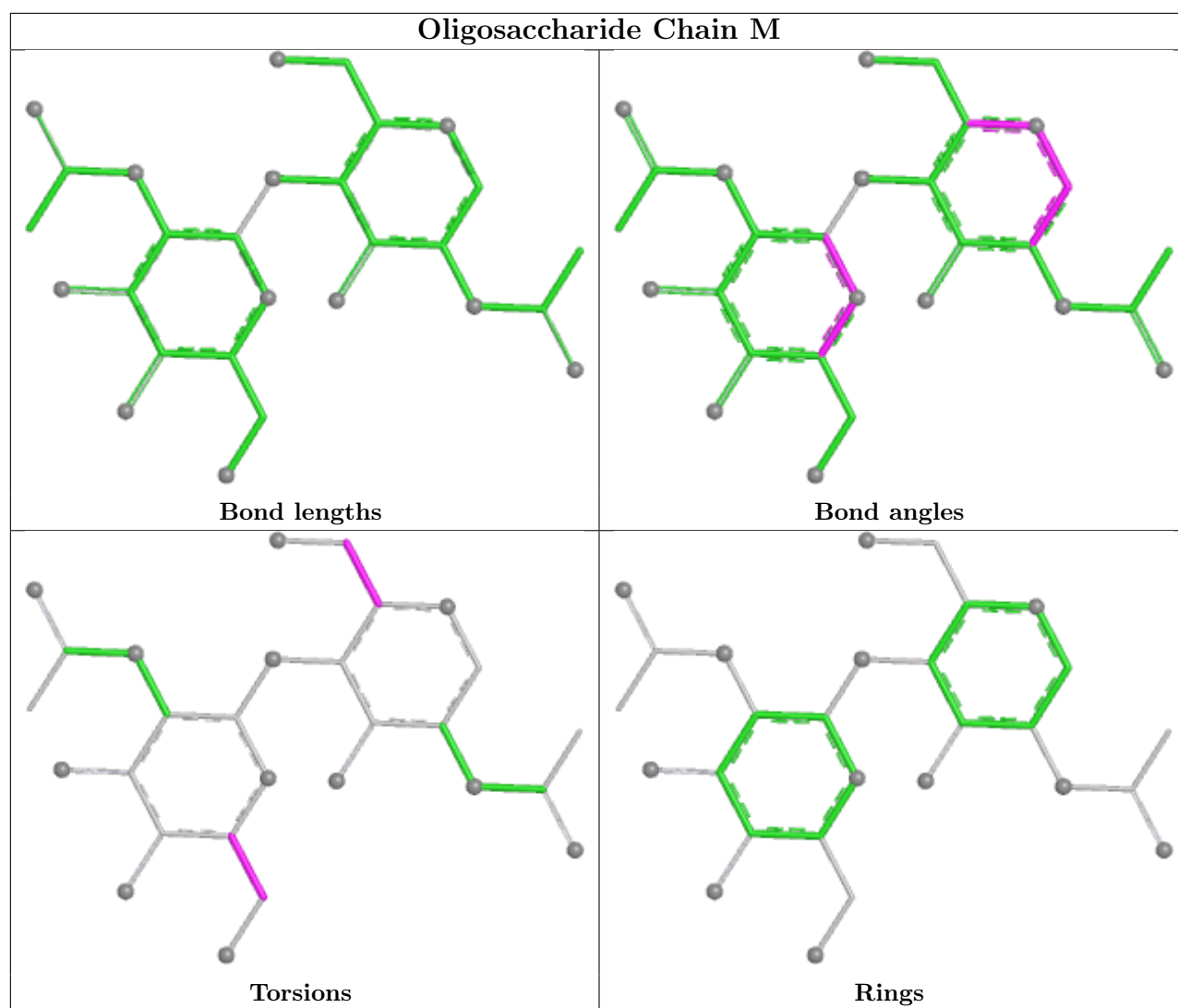
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	1	NAG	4	0
5	P	3	MAN	2	0
4	J	3	MAN	2	0
3	T	2	NAG	1	0
3	Q	2	NAG	1	0
4	J	5	MAN	4	0
5	S	3	MAN	2	0
4	J	1	NAG	4	0
5	P	2	NAG	3	0
3	Q	1	NAG	1	0
3	M	2	NAG	1	0
4	J	2	NAG	3	0
5	P	1	NAG	4	0
3	T	1	NAG	1	0
5	S	2	NAG	3	0
3	M	1	NAG	4	0

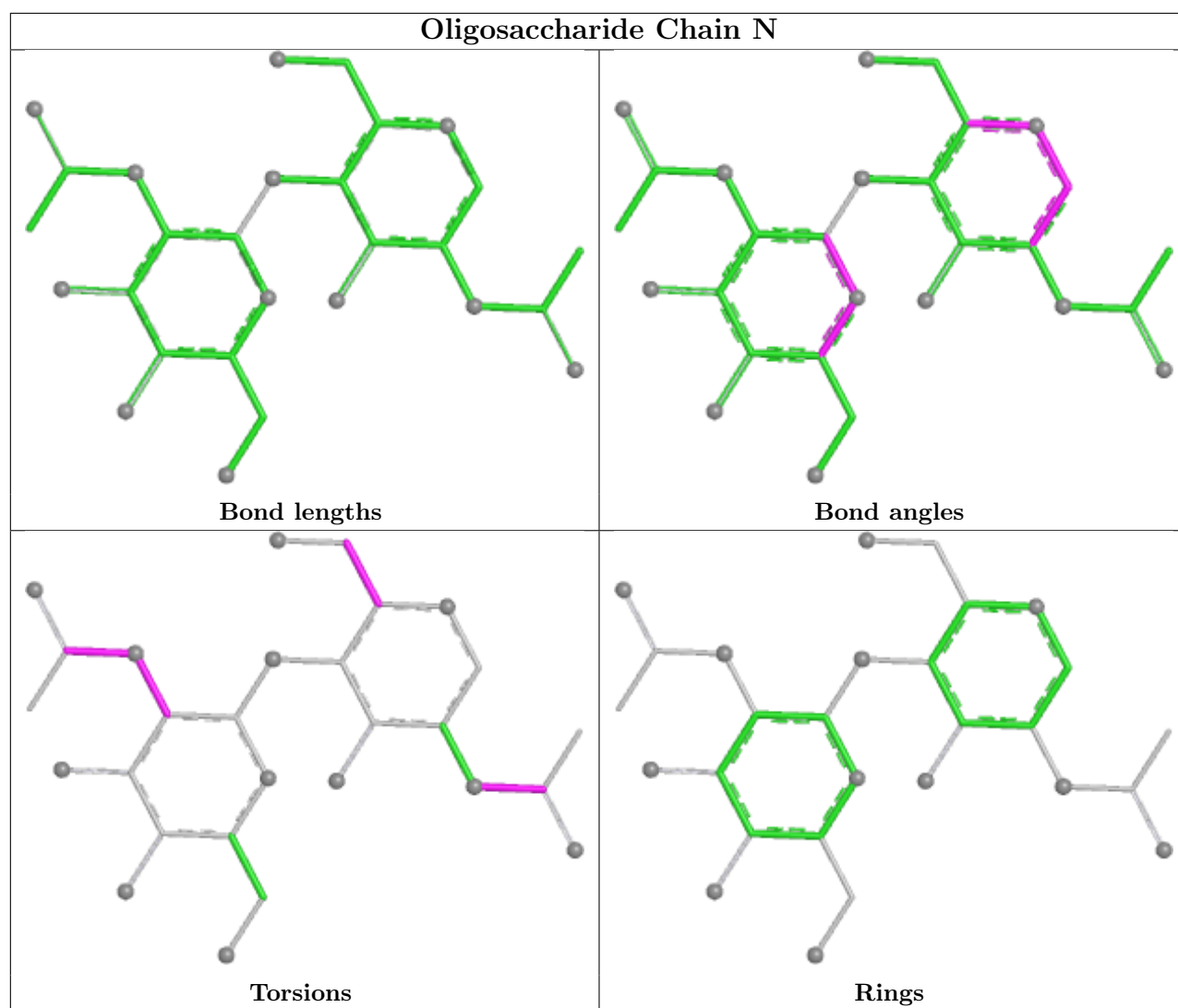
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

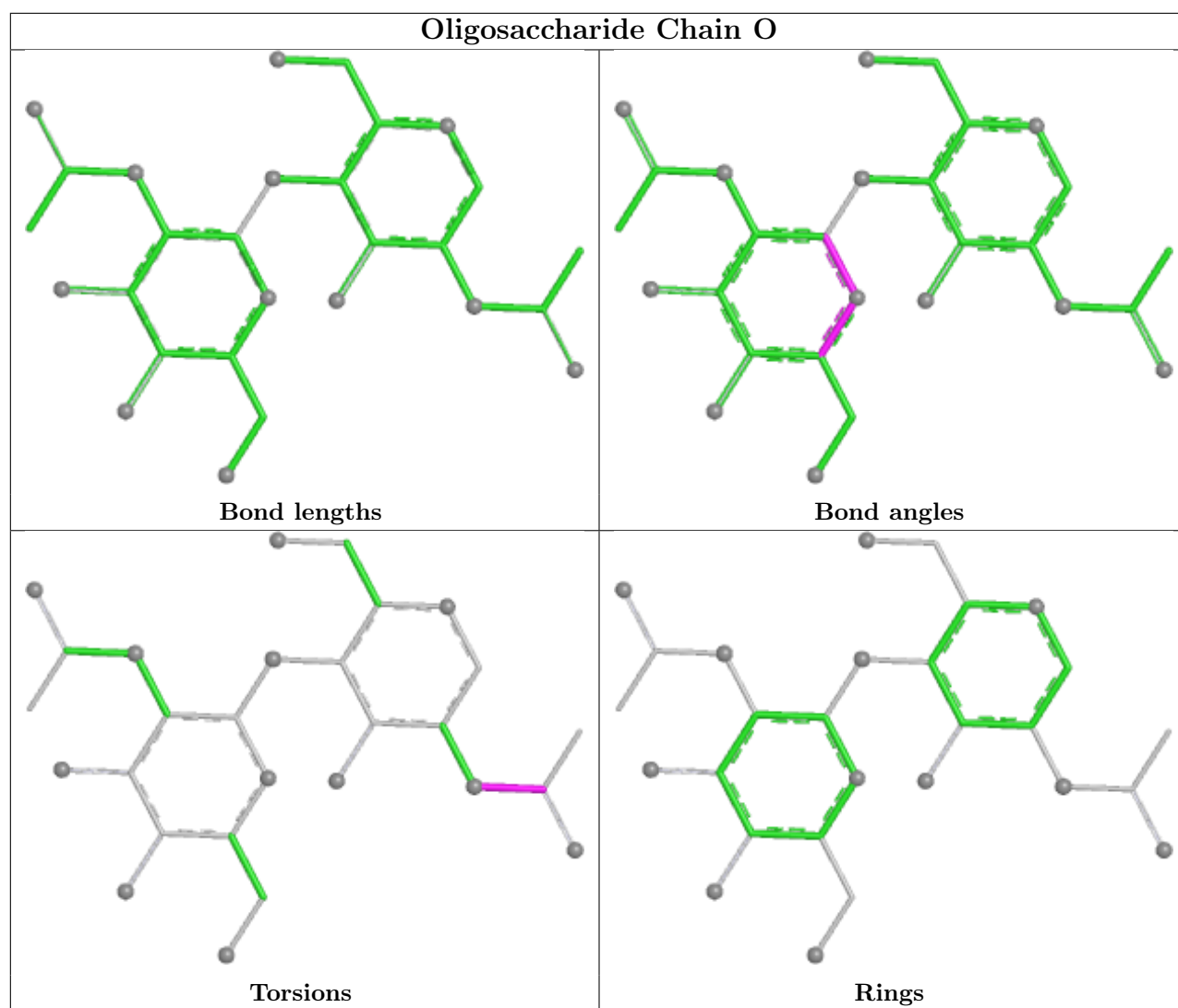


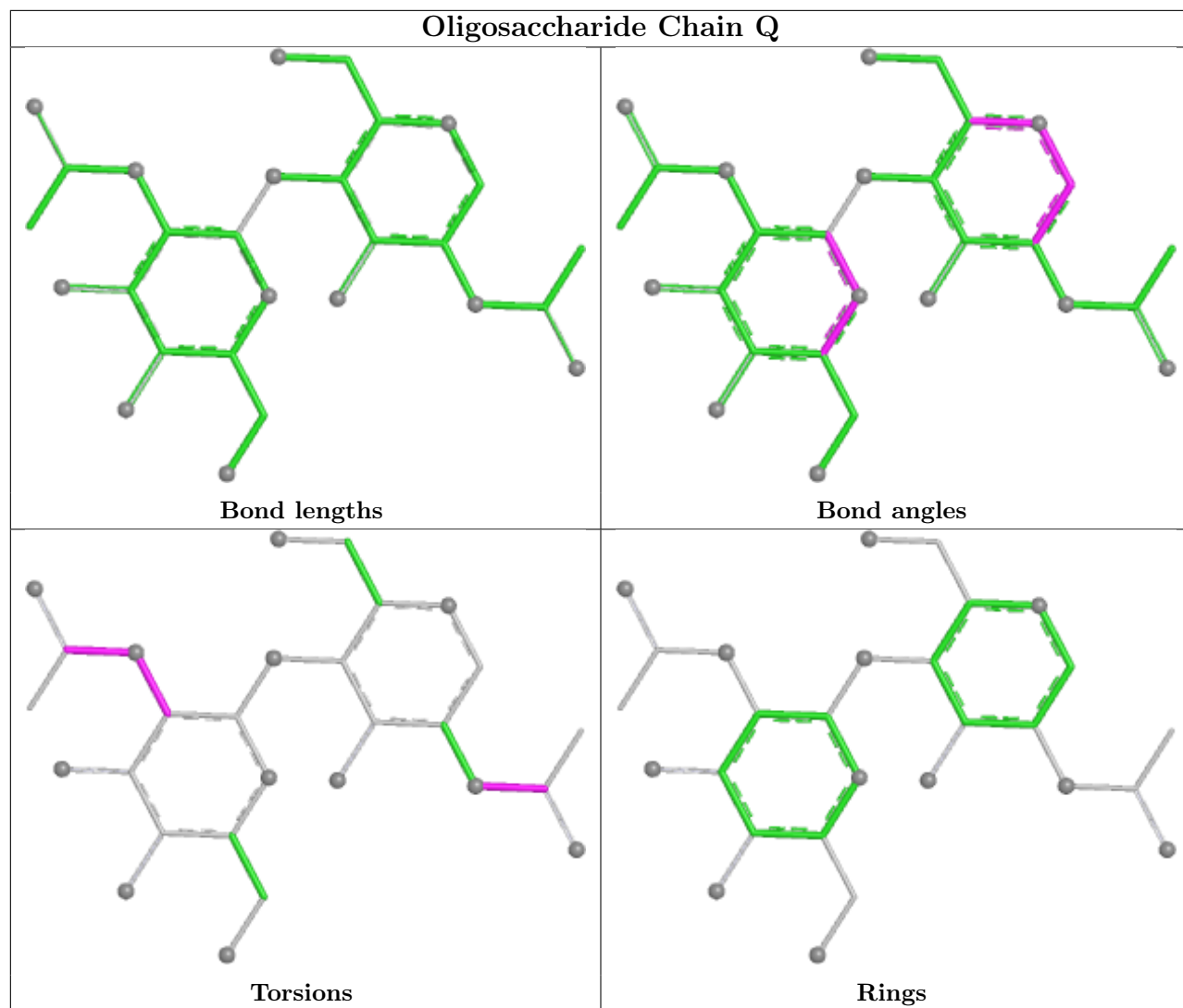


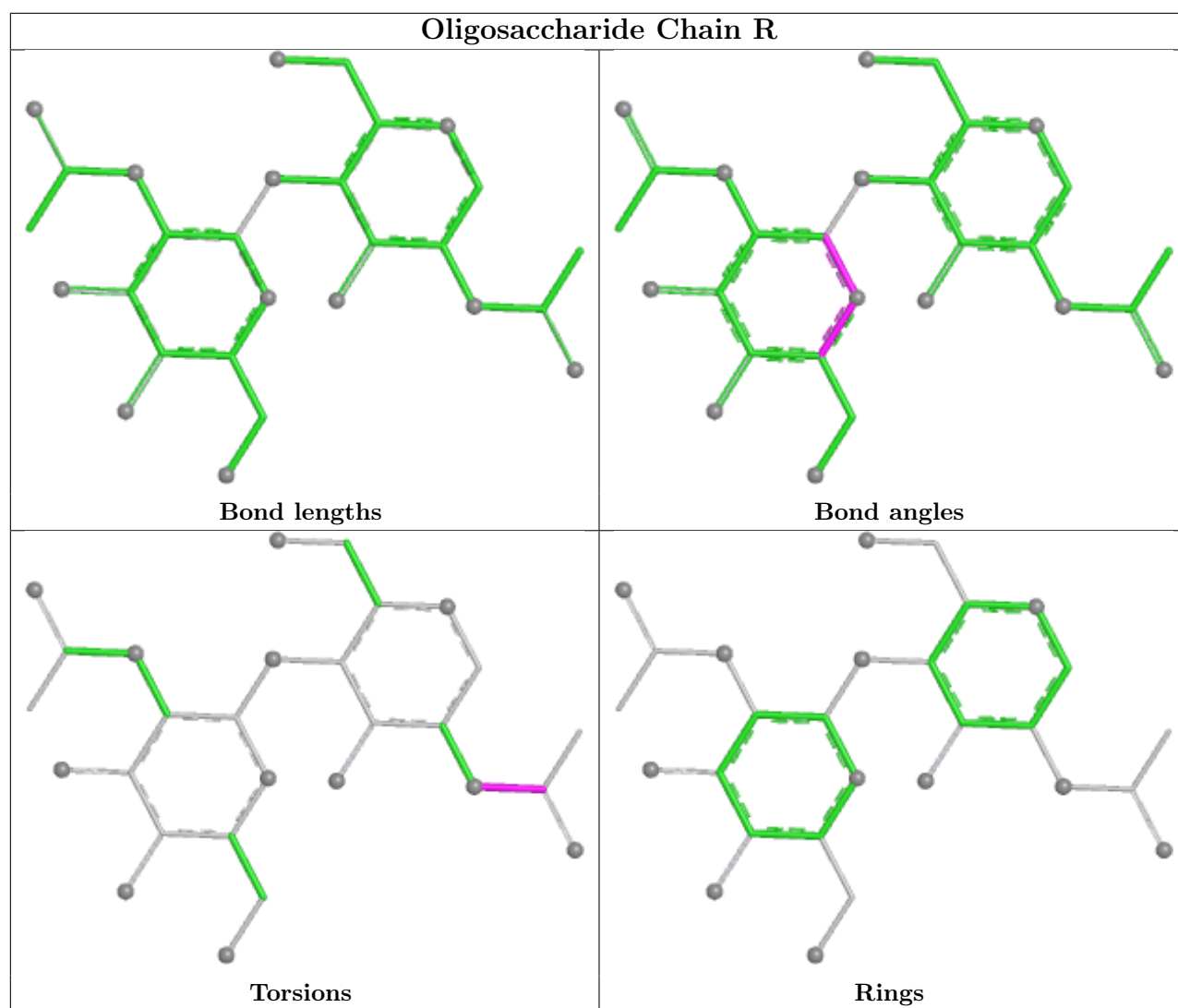


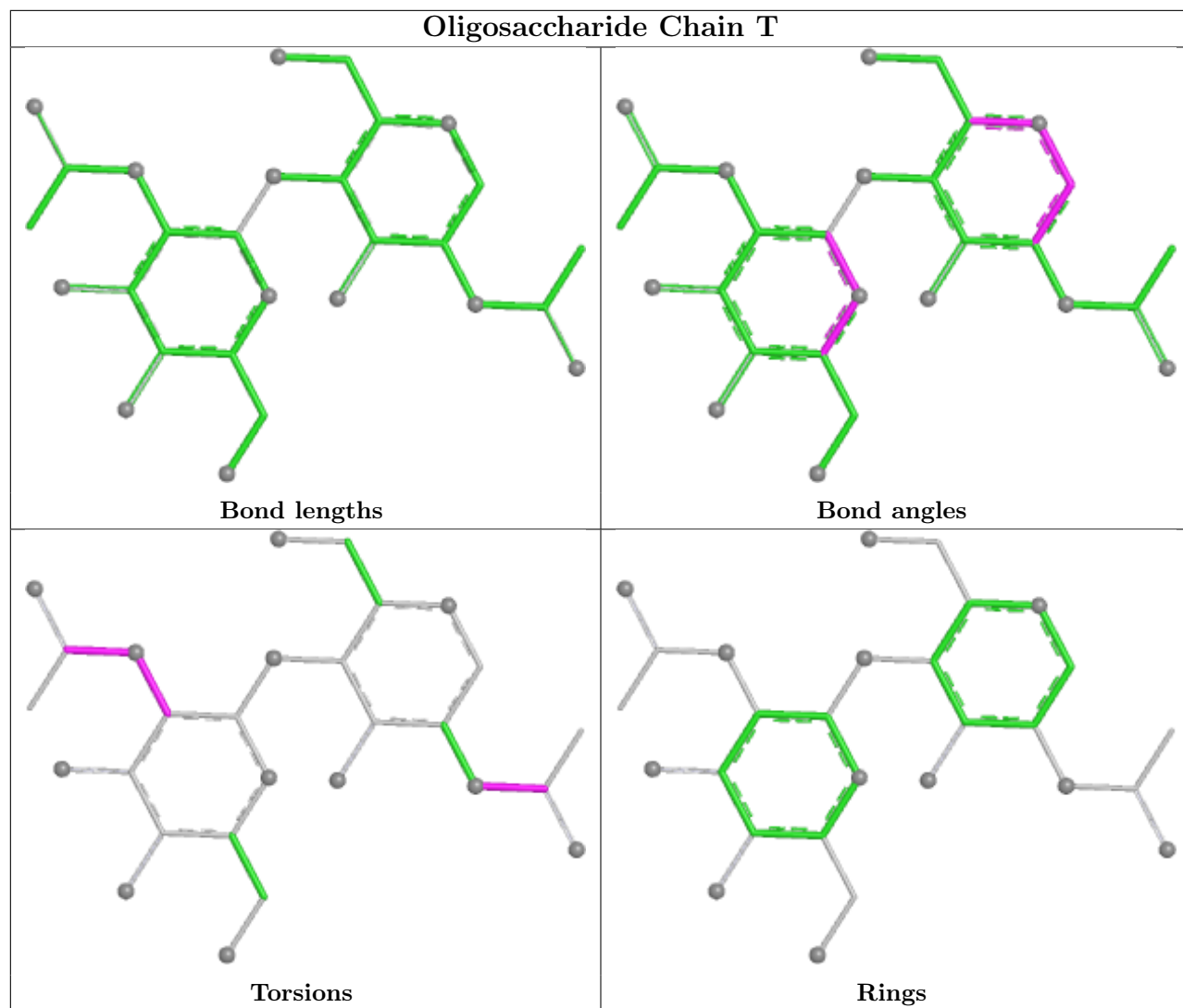


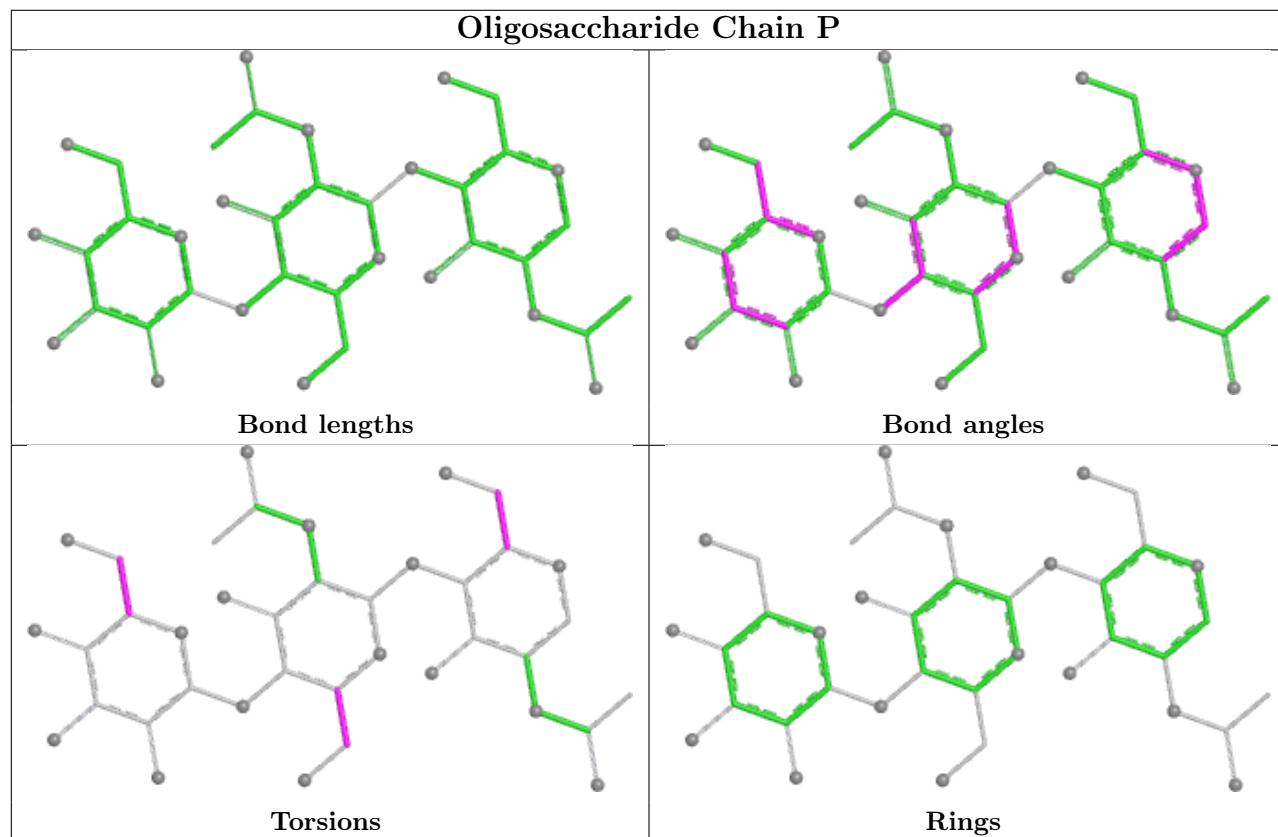
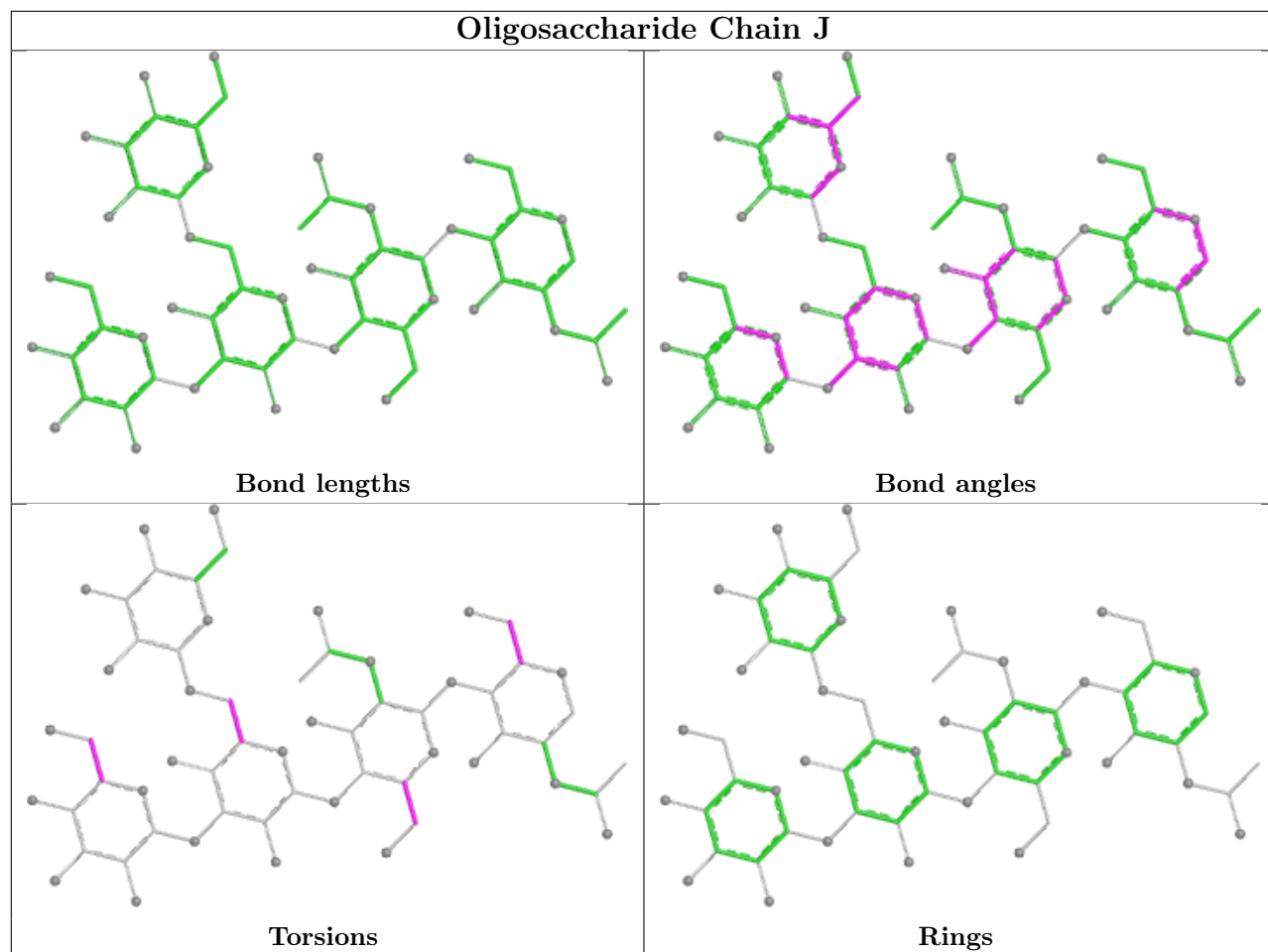


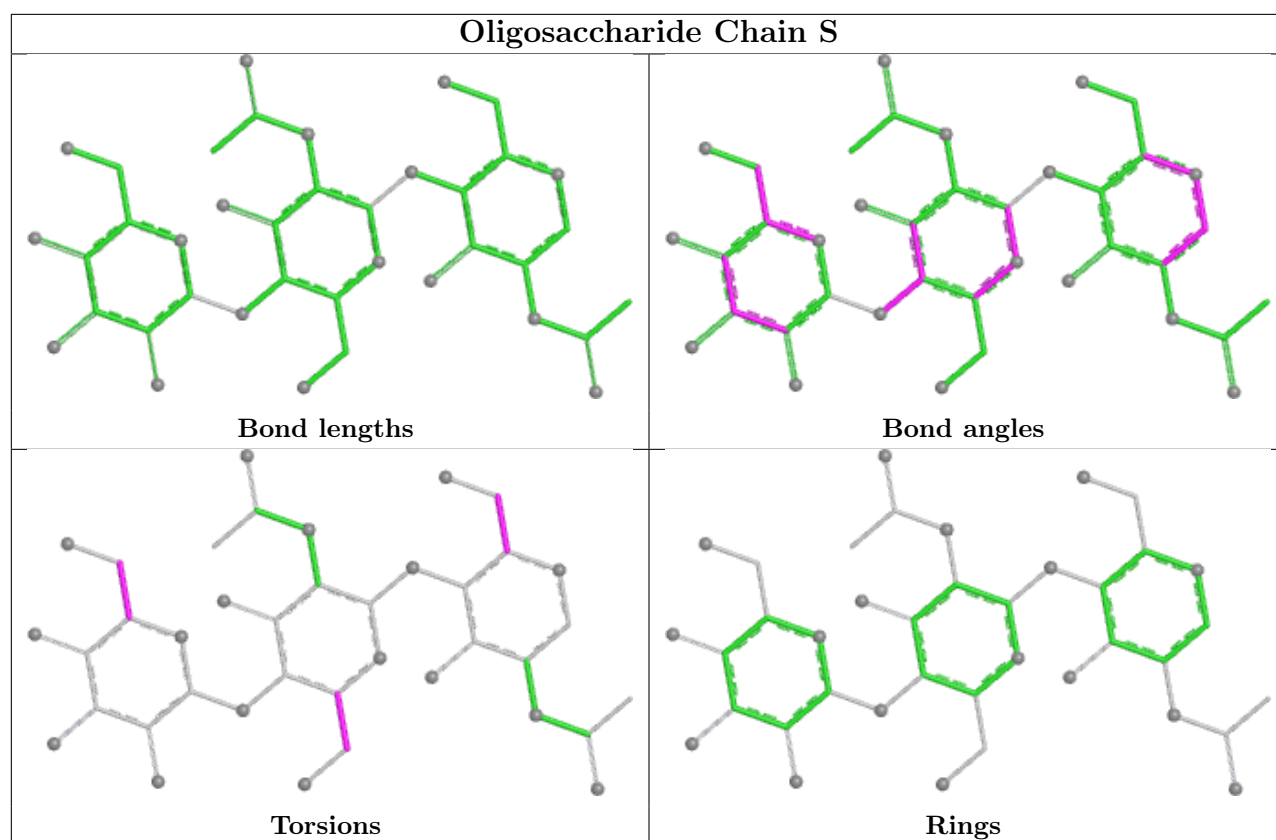












5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 17 are monoatomic - leaving 13 for Mogul analysis.

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	3678	1	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
7	NAG	A	3880	1	14,14,15	0.42	0	17,19,21	1.18	1 (5%)
7	NAG	B	3094	2	14,14,15	0.48	0	17,19,21	0.72	0
7	NAG	E	3678	1	14,14,15	0.52	0	17,19,21	1.02	2 (11%)
7	NAG	H	3094	2	14,14,15	0.50	0	17,19,21	0.71	0
7	NAG	A	3678	1	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
7	NAG	E	3880	1	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
7	NAG	D	3094	2	14,14,15	0.51	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	3880	1	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
7	NAG	G	3678	1	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
7	NAG	C	3880	1	14,14,15	0.42	0	17,19,21	1.08	1 (5%)
6	MAN	A	3378	-	11,11,12	1.06	0	15,15,17	5.12	4 (26%)
7	NAG	F	3094	2	14,14,15	0.48	0	17,19,21	0.71	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
7	NAG	C	3678	1	-	2/6/23/26	0/1/1/1
7	NAG	A	3880	1	-	4/6/23/26	0/1/1/1
7	NAG	B	3094	2	-	2/6/23/26	0/1/1/1
7	NAG	E	3678	1	-	2/6/23/26	0/1/1/1
7	NAG	H	3094	2	-	1/6/23/26	0/1/1/1
7	NAG	A	3678	1	-	2/6/23/26	0/1/1/1
7	NAG	E	3880	1	-	3/6/23/26	0/1/1/1
7	NAG	D	3094	2	-	1/6/23/26	0/1/1/1
7	NAG	G	3880	1	-	3/6/23/26	0/1/1/1
7	NAG	G	3678	1	-	2/6/23/26	0/1/1/1
7	NAG	C	3880	1	-	3/6/23/26	0/1/1/1
6	MAN	A	3378	-	-	2/2/19/22	0/1/1/1
7	NAG	F	3094	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3378	MAN	C1-C2-C3	-14.75	88.17	109.64
6	A	3378	MAN	C1-O5-C5	-11.61	96.63	112.19
6	A	3378	MAN	C3-C4-C5	4.70	118.76	110.23
7	A	3880	NAG	C1-O5-C5	3.59	117.00	112.19
7	E	3880	NAG	C1-O5-C5	3.52	116.90	112.19
7	C	3880	NAG	C1-O5-C5	3.19	116.46	112.19
7	E	3678	NAG	C1-O5-C5	3.05	116.28	112.19
7	G	3880	NAG	C1-O5-C5	3.02	116.24	112.19
7	A	3678	NAG	C1-O5-C5	2.94	116.12	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	3678	NAG	C1-O5-C5	2.89	116.06	112.19
7	C	3678	NAG	C1-O5-C5	2.81	115.96	112.19
7	E	3678	NAG	O5-C1-C2	2.12	114.56	111.29
6	A	3378	MAN	O3-C3-C2	2.02	114.18	110.05

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3880	NAG	C8-C7-N2-C2
7	A	3880	NAG	O7-C7-N2-C2
7	C	3880	NAG	C8-C7-N2-C2
7	C	3880	NAG	O7-C7-N2-C2
7	E	3880	NAG	C8-C7-N2-C2
7	E	3880	NAG	O7-C7-N2-C2
7	G	3880	NAG	C8-C7-N2-C2
7	G	3880	NAG	O7-C7-N2-C2
6	A	3378	MAN	O5-C5-C6-O6
7	A	3880	NAG	O5-C5-C6-O6
7	C	3880	NAG	O5-C5-C6-O6
7	G	3880	NAG	O5-C5-C6-O6
7	E	3880	NAG	O5-C5-C6-O6
6	A	3378	MAN	C4-C5-C6-O6
7	C	3678	NAG	C4-C5-C6-O6
7	A	3678	NAG	C4-C5-C6-O6
7	B	3094	NAG	C4-C5-C6-O6
7	E	3678	NAG	C4-C5-C6-O6
7	G	3678	NAG	C4-C5-C6-O6
7	C	3678	NAG	O5-C5-C6-O6
7	H	3094	NAG	C4-C5-C6-O6
7	A	3880	NAG	C4-C5-C6-O6
7	A	3678	NAG	O5-C5-C6-O6
7	G	3678	NAG	O5-C5-C6-O6
7	E	3678	NAG	O5-C5-C6-O6
7	D	3094	NAG	C4-C5-C6-O6
7	F	3094	NAG	C4-C5-C6-O6
7	B	3094	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	3678	NAG	1	0
7	G	3678	NAG	1	0
6	A	3378	MAN	4	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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	1082/1095 (98%)	0.43	27 (2%)	58	35	61, 153, 256, 362	0
1	C	885/1095 (80%)	0.44	28 (3%)	50	29	67, 172, 280, 410	0
1	E	883/1095 (80%)	0.37	23 (2%)	57	33	65, 157, 258, 337	0
1	G	883/1095 (80%)	0.45	28 (3%)	50	29	74, 150, 266, 342	0
2	B	674/687 (98%)	0.42	16 (2%)	59	35	54, 205, 286, 421	2 (0%)
2	D	674/687 (98%)	0.58	25 (3%)	45	25	76, 229, 313, 416	2 (0%)
2	F	674/687 (98%)	0.49	21 (3%)	51	29	57, 207, 289, 374	2 (0%)
2	H	674/687 (98%)	0.45	19 (2%)	55	32	61, 210, 293, 390	2 (0%)
All	All	6429/7128 (90%)	0.45	187 (2%)	53	31	54, 185, 283, 421	8 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	92	ALA	4.7
2	B	206	GLY	4.2
1	E	433	THR	4.1
1	A	651	ASP	3.8
1	G	651	ASP	3.8
2	F	195	PHE	3.7
2	D	32	PRO	3.7
1	A	488	ASP	3.7
1	G	650	ARG	3.6
1	A	548	SER	3.6
2	B	280	PRO	3.5
2	D	144	ILE	3.5
2	H	195	PHE	3.5
2	D	431	SER	3.5
1	G	465	TYR	3.4
2	B	433	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	619	GLU	3.4
2	B	195	PHE	3.3
1	G	919	LEU	3.3
1	A	492	TYR	3.2
1	G	918	TYR	3.2
2	F	109	TYR	3.2
2	F	345	VAL	3.2
1	E	465	TYR	3.2
2	F	176	CYS	3.1
2	H	623	ALA	3.1
1	A	383	ASP	3.0
2	F	91	ALA	3.0
1	G	1000	VAL	3.0
1	A	8	LEU	3.0
1	C	106	LEU	3.0
2	F	296	PRO	2.9
1	G	618	PHE	2.9
1	A	398	VAL	2.9
1	C	335	GLU	2.9
1	A	465	TYR	2.8
1	G	490	VAL	2.7
1	A	436	GLY	2.7
1	G	466	GLU	2.7
1	A	933	MET	2.7
1	E	106	LEU	2.7
1	A	653	GLN	2.7
2	F	414	ILE	2.7
2	H	433	ASP	2.7
2	F	160	THR	2.7
2	D	409	LEU	2.7
2	B	283	GLY	2.6
2	D	195	PHE	2.6
2	F	382	GLN	2.6
2	D	97	PHE	2.6
1	C	833	PRO	2.6
1	G	489	ALA	2.6
2	B	72	GLY	2.6
1	G	41	ALA	2.6
1	A	919	LEU	2.6
2	F	629	GLN	2.6
2	H	563	PRO	2.6
2	D	109	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	297	ILE	2.5
1	G	796	TYR	2.5
1	G	1063	LEU	2.5
2	H	401	GLU	2.5
2	B	425	CYS	2.5
2	D	7	LYS	2.5
1	G	994	HIS	2.5
2	D	319	ALA	2.5
1	A	355	THR	2.5
1	C	529	GLU	2.5
2	F	334	ILE	2.5
1	E	651	ASP	2.5
1	G	488	ASP	2.5
2	F	433	ASP	2.5
2	H	236	LEU	2.5
2	B	185	VAL	2.5
2	D	205	SER	2.4
1	G	930	HIS	2.4
2	B	161	HIS	2.4
2	D	105	ILE	2.4
2	D	63	ALA	2.4
2	D	206	GLY	2.4
1	A	463	HIS	2.4
1	C	688	GLY	2.4
2	D	406	ILE	2.4
1	A	335	GLU	2.4
1	C	621	ARG	2.4
1	A	504	ALA	2.4
1	C	618	PHE	2.4
1	A	490	VAL	2.4
1	C	814	ALA	2.4
1	C	703	CYS	2.3
1	E	543	PRO	2.3
1	G	436	GLY	2.3
2	F	563	PRO	2.3
2	D	650	VAL	2.3
2	H	634	PRO	2.3
2	D	91	ALA	2.3
1	E	398	VAL	2.3
1	G	362	LEU	2.3
1	C	1079	GLU	2.3
1	E	848	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	917	LYS	2.3
1	C	435	ILE	2.3
2	D	255	ALA	2.3
1	E	488	ASP	2.3
2	H	415	VAL	2.3
1	A	930	HIS	2.3
2	H	409	LEU	2.3
1	A	592	LEU	2.2
1	C	592	LEU	2.2
1	E	504	ALA	2.2
1	A	399	GLN	2.2
2	B	571	ARG	2.2
2	D	345	VAL	2.2
2	H	400	GLN	2.2
1	A	559	SER	2.2
1	C	773	SER	2.2
1	G	627	GLU	2.2
2	B	236	LEU	2.2
2	B	503	PRO	2.2
2	H	610	LEU	2.2
2	D	321	GLY	2.2
2	H	613	GLU	2.2
1	A	543	PRO	2.2
1	A	847	ASN	2.2
1	C	760	ASP	2.2
1	C	735	ALA	2.2
1	C	1078	LEU	2.2
2	B	409	LEU	2.2
2	D	36	ASP	2.2
1	C	332	MET	2.2
1	C	831	SER	2.2
2	H	629	GLN	2.2
1	E	688	GLY	2.2
1	G	1040	ILE	2.2
2	B	252	LYS	2.2
1	E	652	LEU	2.2
1	C	463	HIS	2.1
1	G	124	GLN	2.1
1	G	463	HIS	2.1
2	D	433	ASP	2.1
1	G	542	GLY	2.1
2	H	78	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	650	ARG	2.1
1	E	38	ILE	2.1
1	E	796	TYR	2.1
2	F	175	GLU	2.1
1	C	504	ALA	2.1
1	E	751	ASN	2.1
1	E	540	VAL	2.1
2	D	252	LYS	2.1
1	C	796	TYR	2.1
1	G	638	TYR	2.1
2	F	72	GLY	2.1
2	H	298	PHE	2.1
1	C	492	TYR	2.1
1	E	486	TRP	2.1
1	E	755	ASP	2.1
1	E	542	GLY	2.1
2	B	595	GLY	2.1
2	H	452	THR	2.1
1	A	278	SER	2.1
2	F	252	LYS	2.1
1	C	623	GLN	2.1
1	A	1000	VAL	2.1
2	D	221	VAL	2.1
1	A	261	GLY	2.1
1	G	127	PRO	2.1
1	C	433	THR	2.1
1	G	118	ARG	2.1
1	C	32	VAL	2.1
1	E	448	VAL	2.1
2	F	285	LEU	2.1
2	D	254	GLY	2.0
2	F	396	THR	2.0
2	F	440	LYS	2.0
1	C	723	PRO	2.0
1	E	1016	PRO	2.0
2	D	296	PRO	2.0
2	F	434	ARG	2.0
2	H	319	ALA	2.0
1	C	398	VAL	2.0
1	A	688	GLY	2.0
1	E	463	HIS	2.0
1	C	651	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	478	LEU	2.0
2	F	401	GLU	2.0
2	H	408	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

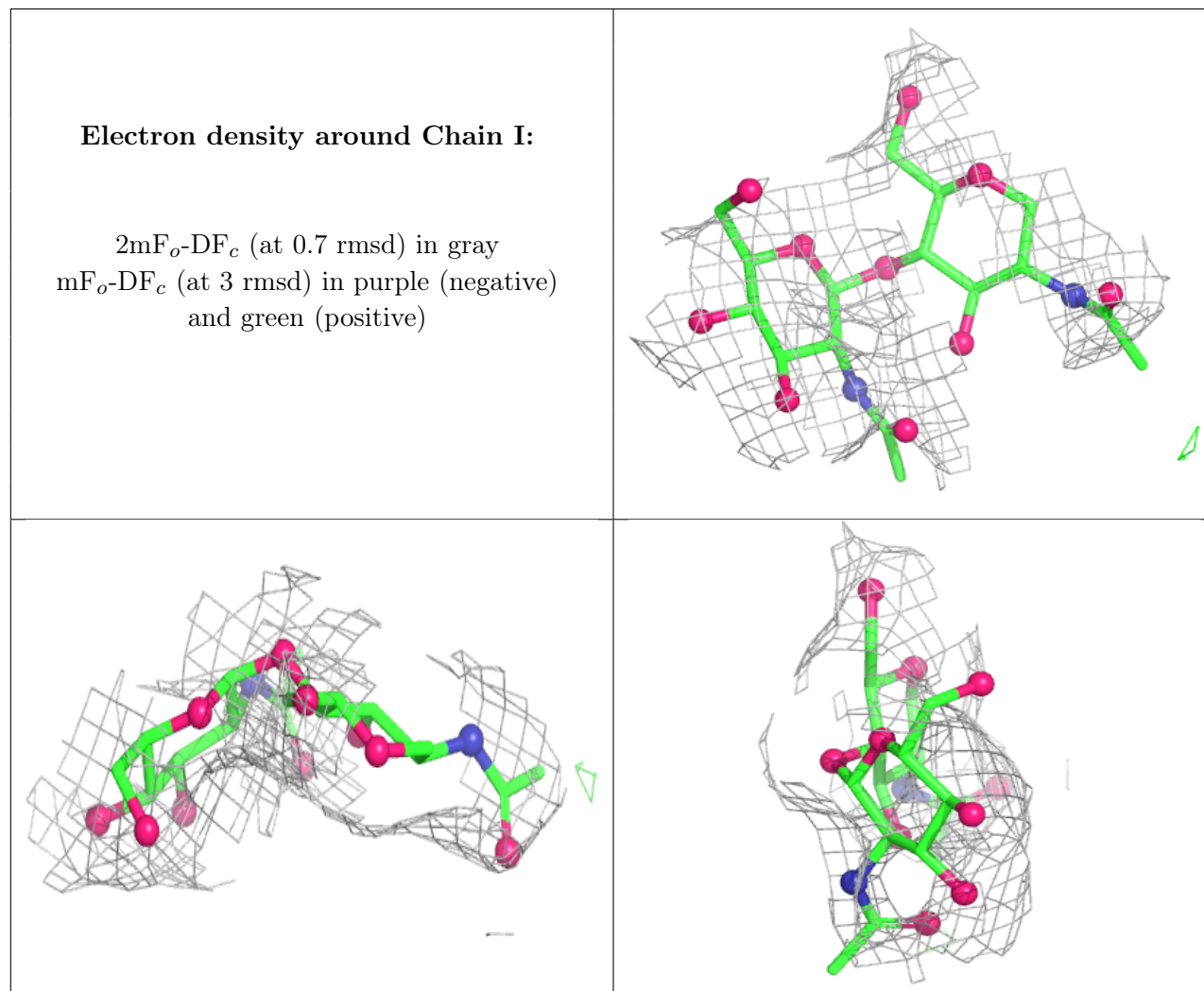
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	O	2	14/15	-0.00	0.12	183,310,366,378	0
3	NAG	M	2	14/15	0.16	0.15	136,238,359,434	0
3	NAG	L	2	14/15	0.16	0.14	179,305,351,363	0
3	NAG	R	2	14/15	0.28	0.13	176,248,297,317	0
3	NAG	N	2	14/15	0.30	0.20	224,297,342,395	0
5	MAN	P	3	11/12	0.36	0.13	171,251,305,311	0
5	NAG	S	2	14/15	0.36	0.12	136,261,326,367	0
5	MAN	S	3	11/12	0.38	0.13	173,208,309,351	0
3	NAG	M	1	14/15	0.39	0.14	198,292,381,425	0
3	NAG	T	2	14/15	0.43	0.12	192,216,305,376	0
3	NAG	L	1	14/15	0.52	0.11	150,232,327,335	0
3	NAG	I	2	14/15	0.54	0.13	80,233,327,333	0
3	NAG	K	2	14/15	0.55	0.15	185,218,319,381	0
3	NAG	Q	2	14/15	0.56	0.16	117,240,280,337	0
4	NAG	J	2	14/15	0.56	0.14	91,240,362,435	0
4	MAN	J	4	11/12	0.56	0.10	114,259,296,316	0
5	NAG	P	2	14/15	0.67	0.09	201,279,352,410	0
3	NAG	O	1	14/15	0.69	0.09	198,249,285,287	0
3	NAG	I	1	14/15	0.72	0.10	133,175,235,244	0
4	MAN	J	5	11/12	0.74	0.11	99,256,308,331	0
5	NAG	P	1	14/15	0.74	0.14	146,324,390,464	0
4	NAG	J	1	14/15	0.78	0.15	136,261,376,443	0
4	MAN	J	3	11/12	0.79	0.10	140,207,283,324	0
3	NAG	R	1	14/15	0.81	0.12	193,244,274,279	0
5	NAG	S	1	14/15	0.82	0.11	106,265,384,401	0

Continued on next page...

Continued from previous page...

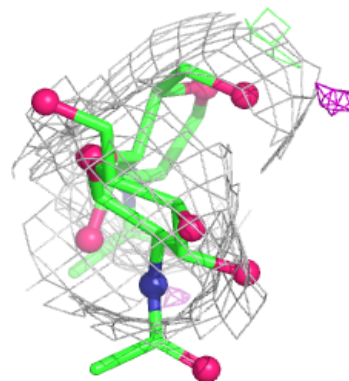
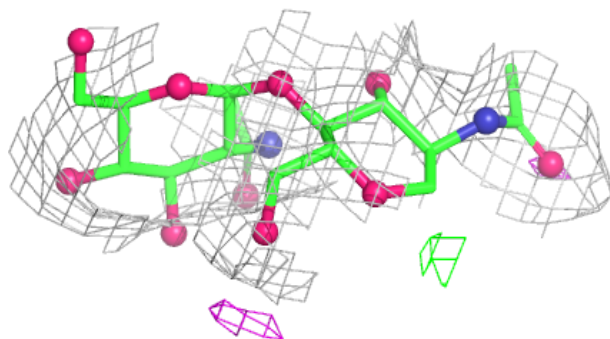
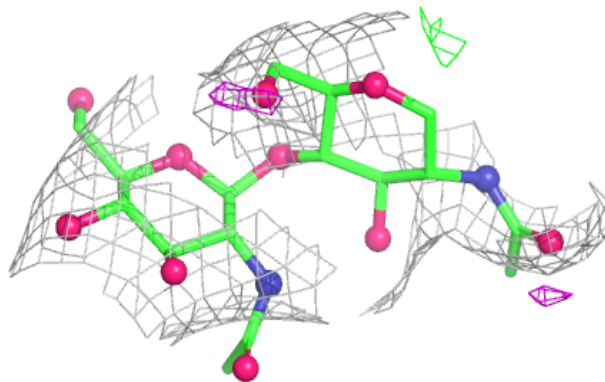
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	T	1	14/15	0.88	0.12	77,188,300,303	0
3	NAG	Q	1	14/15	0.89	0.14	49,184,277,297	0
3	NAG	N	1	14/15	0.92	0.11	60,167,211,249	0
3	NAG	K	1	14/15	0.94	0.11	28,156,272,274	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



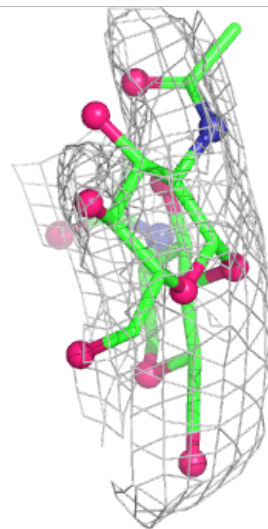
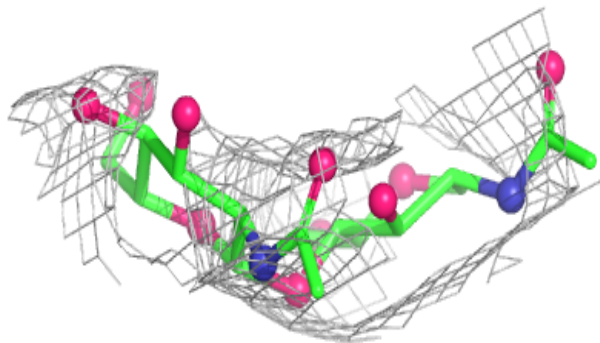
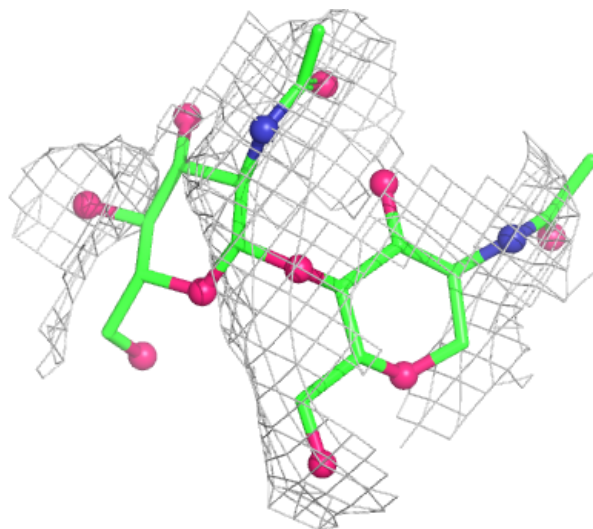
Electron density around Chain K:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



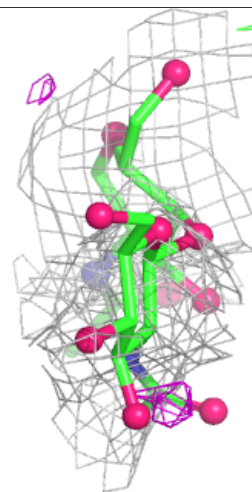
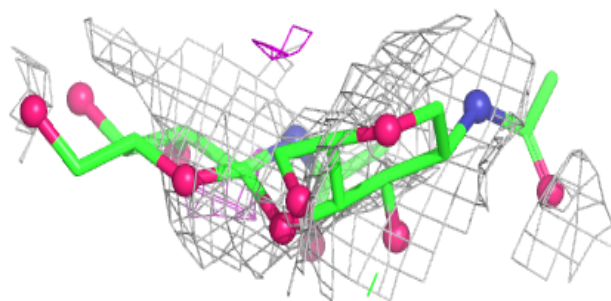
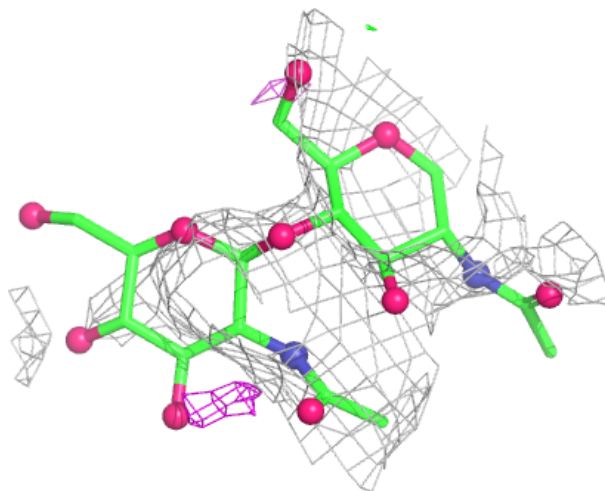
Electron density around Chain L:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



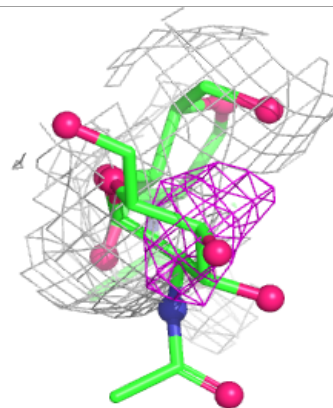
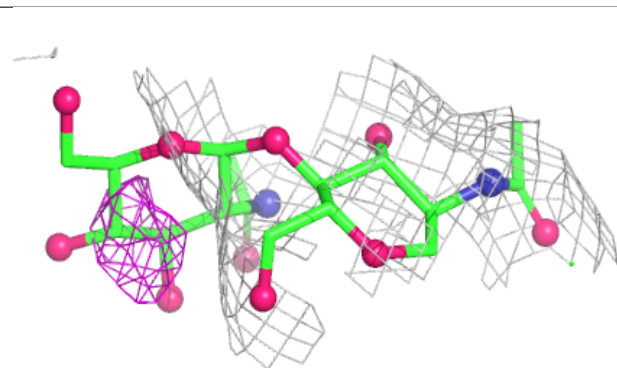
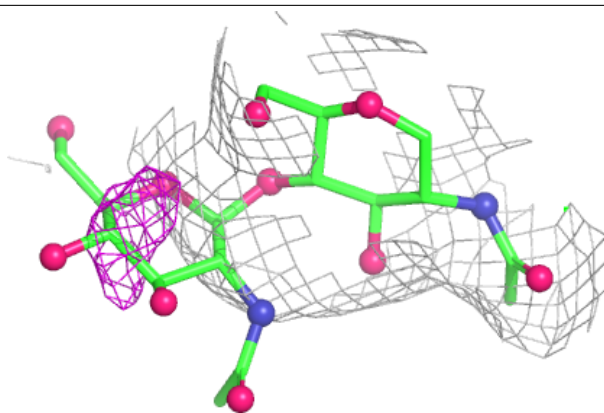
Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



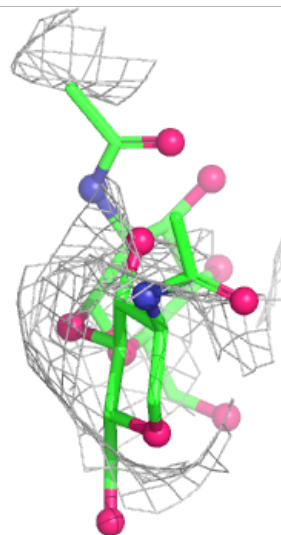
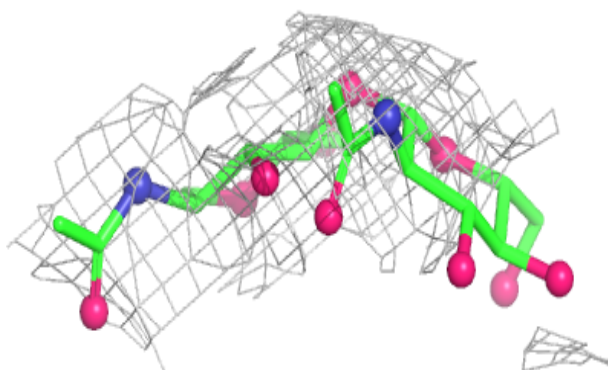
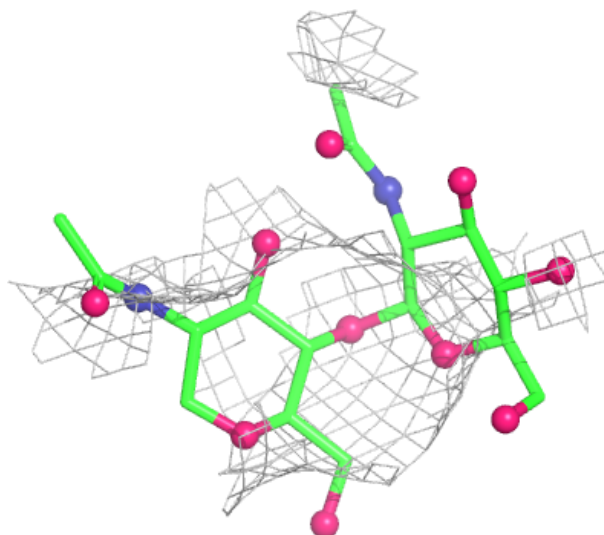
Electron density around Chain N:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



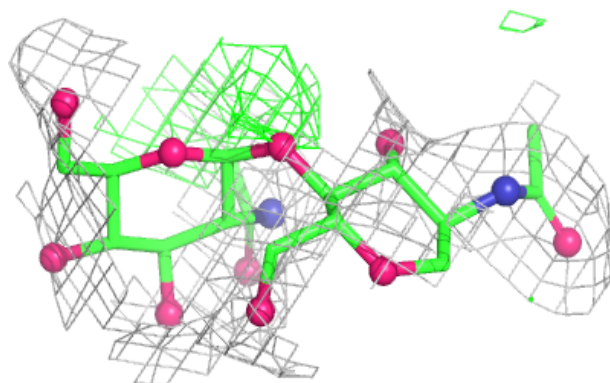
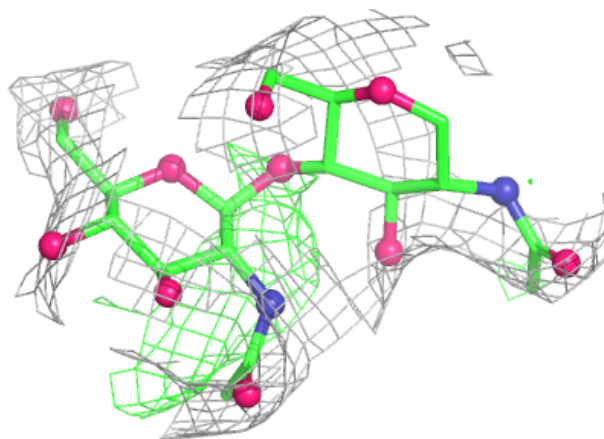
Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



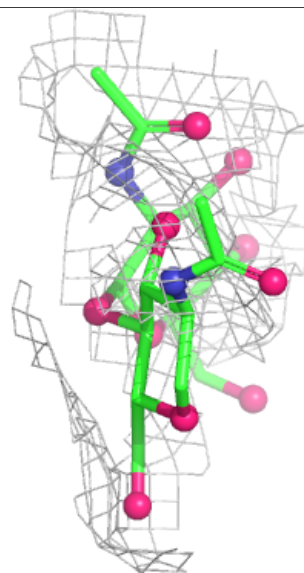
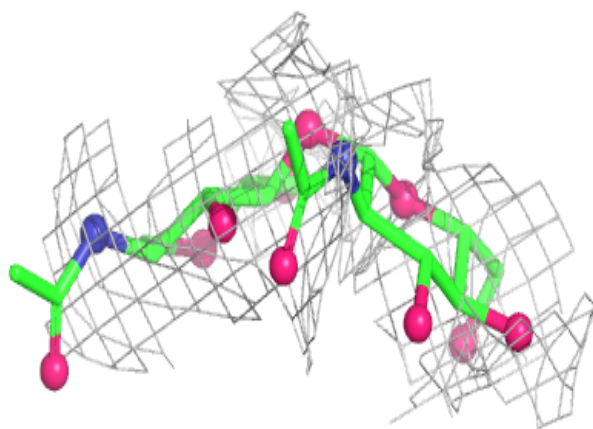
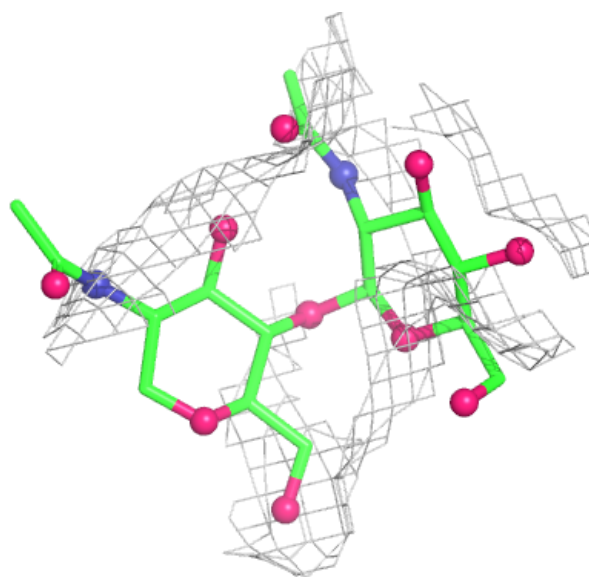
Electron density around Chain Q:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



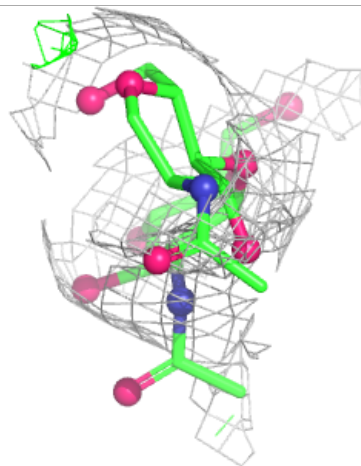
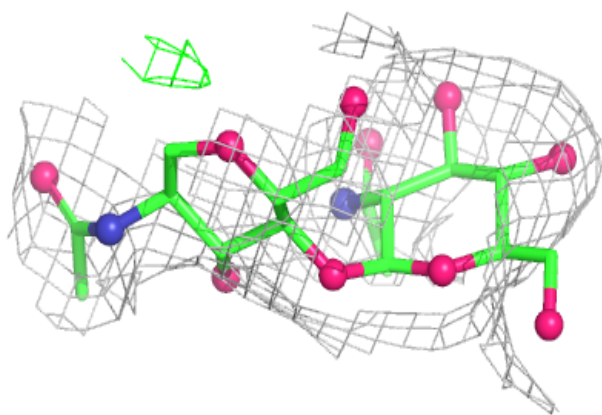
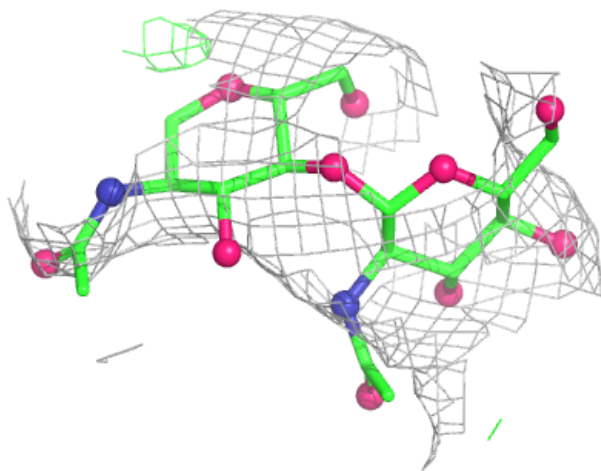
Electron density around Chain R:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



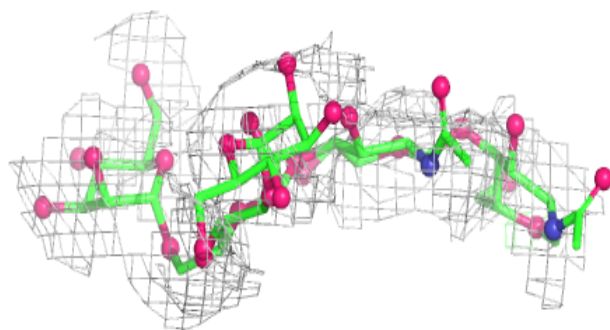
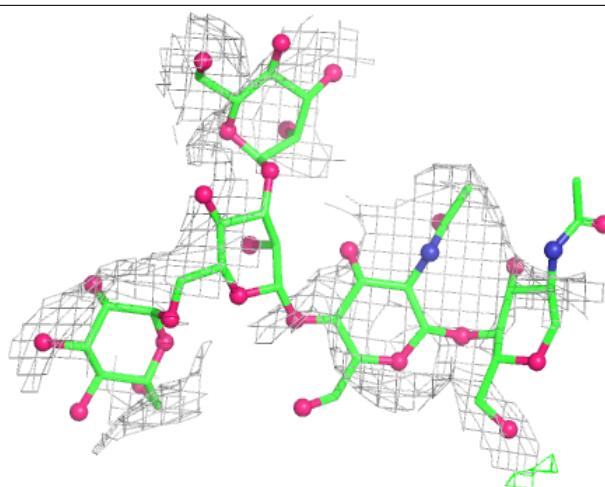
Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



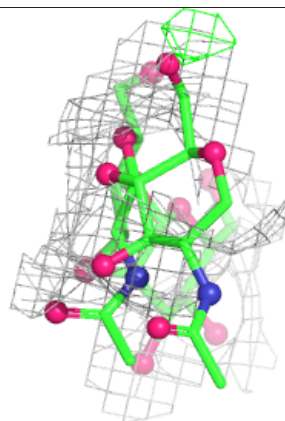
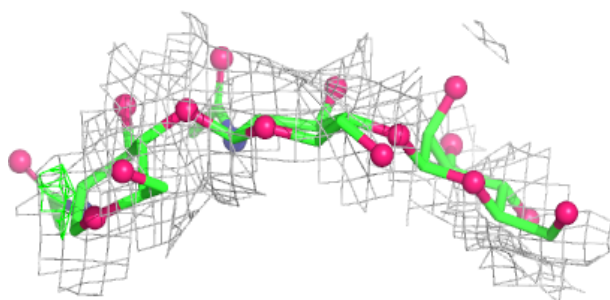
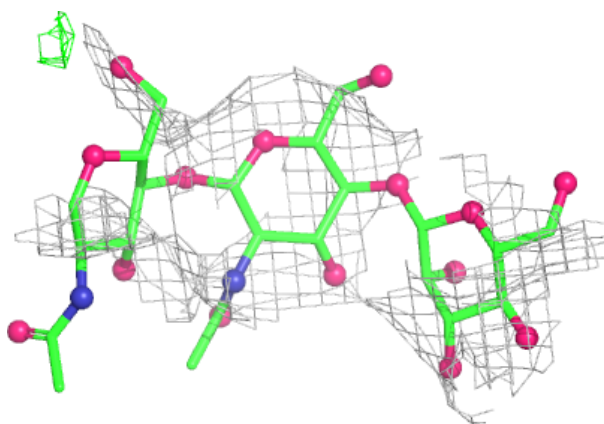
Electron density around Chain J:

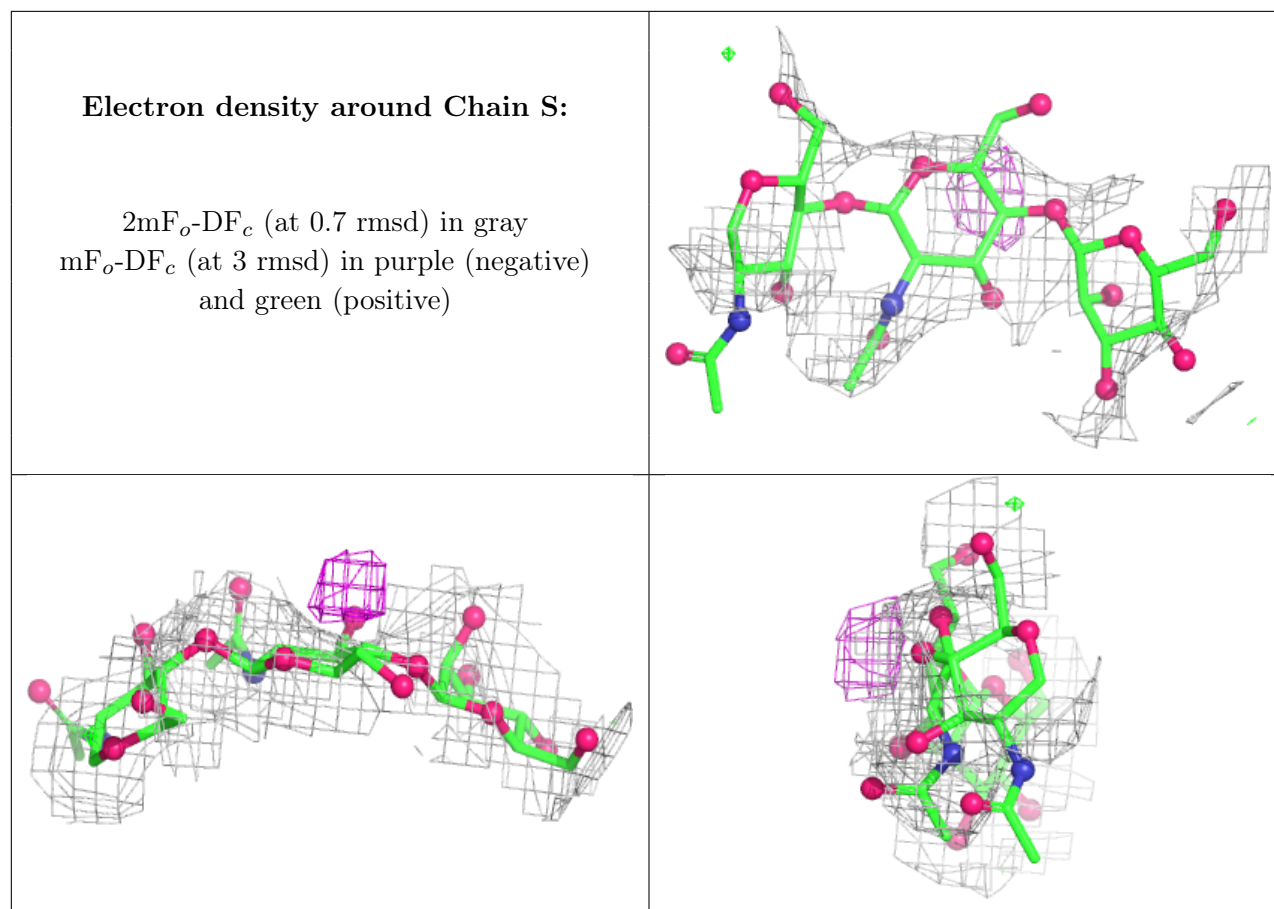
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	3678	14/15	0.25	0.17	125,245,317,319	0
7	NAG	A	3678	14/15	0.39	0.15	117,269,324,327	0
7	NAG	D	3094	14/15	0.41	0.12	189,258,296,299	0
6	MAN	A	3378	11/12	0.48	0.14	171,186,272,293	0
7	NAG	G	3678	14/15	0.48	0.11	132,218,244,251	0
7	NAG	H	3094	14/15	0.62	0.11	148,232,292,297	0
8	CA	D	2002	1/1	0.65	0.10	547,547,547,547	0
7	NAG	B	3094	14/15	0.67	0.12	107,197,277,325	0
7	NAG	E	3678	14/15	0.68	0.12	104,227,276,317	0
8	CA	H	2002	1/1	0.68	0.08	510,510,510,510	0
7	NAG	F	3094	14/15	0.78	0.09	124,217,266,291	0
9	MG	A	2009	1/1	0.79	0.08	367,367,367,367	0
8	CA	F	2002	1/1	0.86	0.09	578,578,578,578	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	B	2002	1/1	0.87	0.06	535,535,535,535	0
7	NAG	A	3880	14/15	0.89	0.11	105,143,196,220	0
7	NAG	C	3880	14/15	0.89	0.11	60,171,245,293	0
7	NAG	G	3880	14/15	0.89	0.15	84,176,236,252	0
7	NAG	E	3880	14/15	0.90	0.11	80,160,189,194	0
8	CA	A	2005	1/1	0.91	0.07	145,145,145,145	0
8	CA	C	2007	1/1	0.93	0.05	206,206,206,206	0
8	CA	E	2005	1/1	0.94	0.07	176,176,176,176	0
8	CA	C	2006	1/1	0.94	0.07	125,125,125,125	0
8	CA	A	2007	1/1	0.95	0.05	181,181,181,181	0
8	CA	G	2006	1/1	0.96	0.05	95,95,95,95	0
8	CA	E	2007	1/1	0.96	0.05	188,188,188,188	0
8	CA	E	2006	1/1	0.96	0.04	137,137,137,137	0
8	CA	C	2005	1/1	0.97	0.04	200,200,200,200	0
8	CA	G	2007	1/1	0.97	0.04	150,150,150,150	0
8	CA	A	2006	1/1	0.98	0.03	107,107,107,107	0
8	CA	G	2005	1/1	0.99	0.03	139,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.