



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 06:57 PM EST

PDB ID : 3AIC
Title : Crystal Structure of Glucansucrase from Streptococcus mutans
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.
Deposited on : 2010-05-12
Resolution : 3.11 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

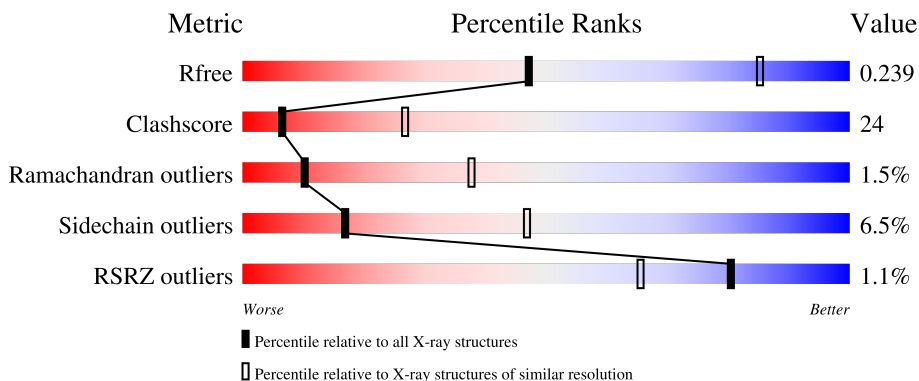
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



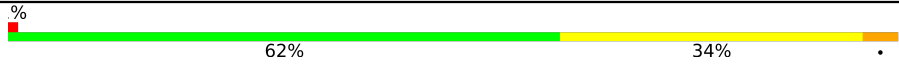

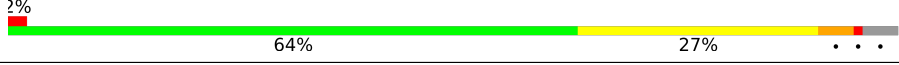





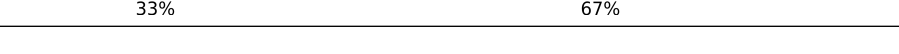


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	844	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">65% 31% •</p>
1	B	844	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">57% 29% • 11%</p>
1	C	844	<div style="display: flex; align-items: center;"> <div style="width: 66%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">66% 31% •</p>
1	D	844	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">63% 32% 5%</p>
1	E	844	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">66% 28% 5% •</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	844	 % 62% 34% .
1	G	844	 % 64% 31% .
1	H	844	 2% 64% 27% . . .
2	I	3	 33% 67%
2	J	3	 33% 67%
2	K	3	 33% 67%
2	L	3	 33% 67%
2	M	3	 33% 67%
2	N	3	 33% 67%
2	O	3	 33% 67%
2	P	3	 33% 67%

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
2	AC1	I	3	-	-	X	-
2	AC1	K	3	-	-	X	-
2	AC1	M	3	-	-	X	-
4	MES	F	5001	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52865 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 Glucosyltransferase-SI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	842	6643	4184	1141	1302	16	0	0	0
1	B	747	5854	3684	1005	1151	14	0	0	0
1	C	844	6660	4196	1143	1305	16	0	0	0
1	D	844	6660	4196	1143	1305	16	0	0	0
1	E	843	6654	4193	1142	1303	16	0	0	0
1	F	844	6660	4196	1143	1305	16	0	0	0
1	G	844	6660	4196	1143	1305	16	0	0	0
1	H	807	6372	4019	1093	1244	16	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ASN	SEE REMARK 999	UNP P13470
A	600	LYS	ARG	SEE REMARK 999	UNP P13470
A	727	ILE	THR	SEE REMARK 999	UNP P13470
A	734	VAL	ALA	SEE REMARK 999	UNP P13470
B	597	ASP	ASN	SEE REMARK 999	UNP P13470
B	600	LYS	ARG	SEE REMARK 999	UNP P13470
B	727	ILE	THR	SEE REMARK 999	UNP P13470
B	734	VAL	ALA	SEE REMARK 999	UNP P13470
C	597	ASP	ASN	SEE REMARK 999	UNP P13470
C	600	LYS	ARG	SEE REMARK 999	UNP P13470
C	727	ILE	THR	SEE REMARK 999	UNP P13470
C	734	VAL	ALA	SEE REMARK 999	UNP P13470
D	597	ASP	ASN	SEE REMARK 999	UNP P13470

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	600	LYS	ARG	SEE REMARK 999	UNP P13470
D	727	ILE	THR	SEE REMARK 999	UNP P13470
D	734	VAL	ALA	SEE REMARK 999	UNP P13470
E	597	ASP	ASN	SEE REMARK 999	UNP P13470
E	600	LYS	ARG	SEE REMARK 999	UNP P13470
E	727	ILE	THR	SEE REMARK 999	UNP P13470
E	734	VAL	ALA	SEE REMARK 999	UNP P13470
F	597	ASP	ASN	SEE REMARK 999	UNP P13470
F	600	LYS	ARG	SEE REMARK 999	UNP P13470
F	727	ILE	THR	SEE REMARK 999	UNP P13470
F	734	VAL	ALA	SEE REMARK 999	UNP P13470
G	597	ASP	ASN	SEE REMARK 999	UNP P13470
G	600	LYS	ARG	SEE REMARK 999	UNP P13470
G	727	ILE	THR	SEE REMARK 999	UNP P13470
G	734	VAL	ALA	SEE REMARK 999	UNP P13470
H	597	ASP	ASN	SEE REMARK 999	UNP P13470
H	600	LYS	ARG	SEE REMARK 999	UNP P13470
H	727	ILE	THR	SEE REMARK 999	UNP P13470
H	734	VAL	ALA	SEE REMARK 999	UNP P13470

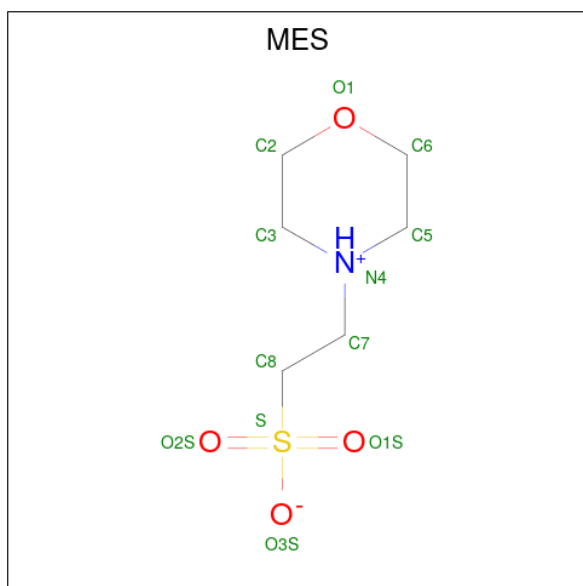
- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	J	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	K	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	L	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	M	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	N	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	O	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	P	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0
4	B	1	Total C N O S 12 6 1 4 1	0	0
4	C	1	Total C N O S 12 6 1 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

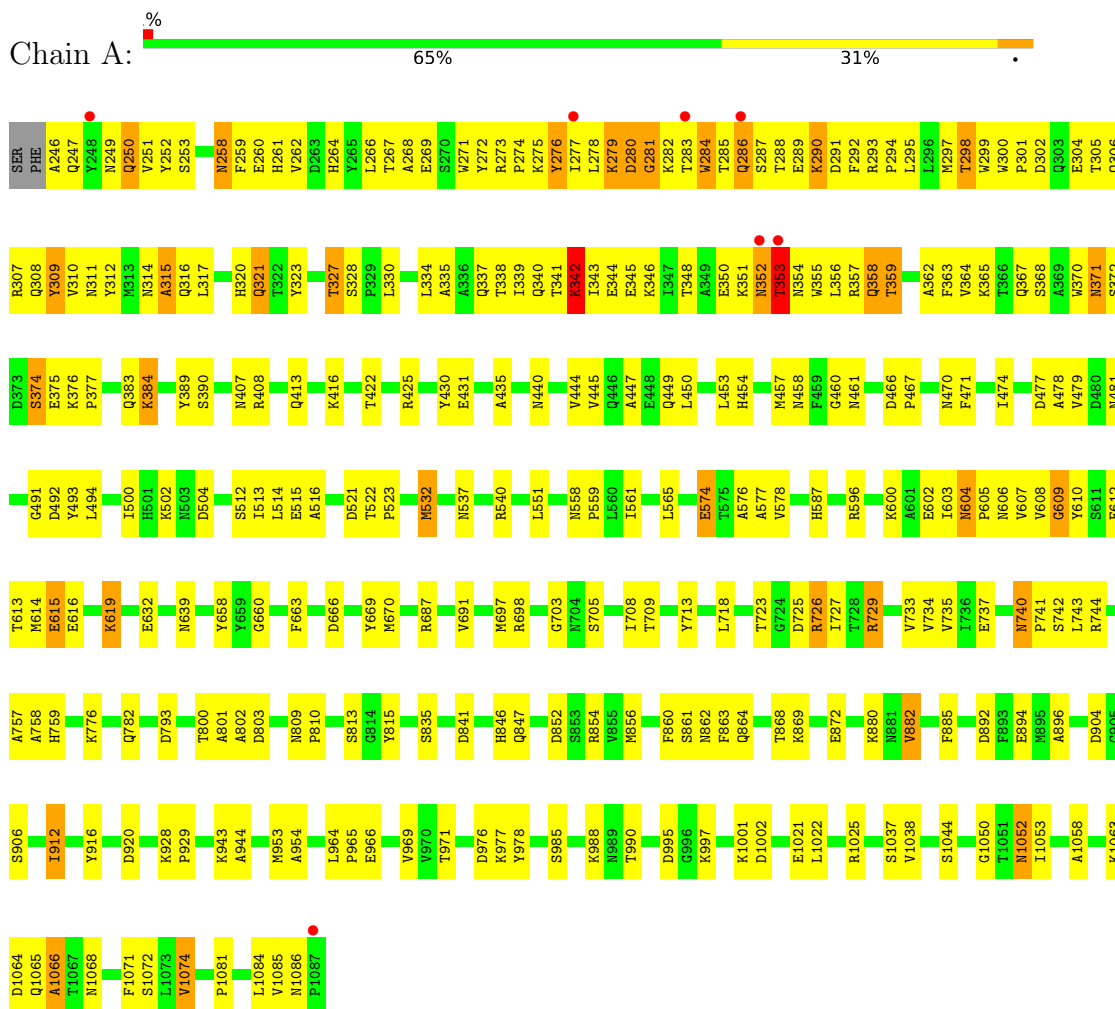
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	20	Total	O	0	0
			20	20		
5	C	32	Total	O	0	0
			32	32		
5	D	40	Total	O	0	0
			40	40		
5	E	48	Total	O	0	0
			48	48		
5	F	15	Total	O	0	0
			15	15		
5	G	34	Total	O	0	0
			34	34		
5	H	24	Total	O	0	0
			24	24		

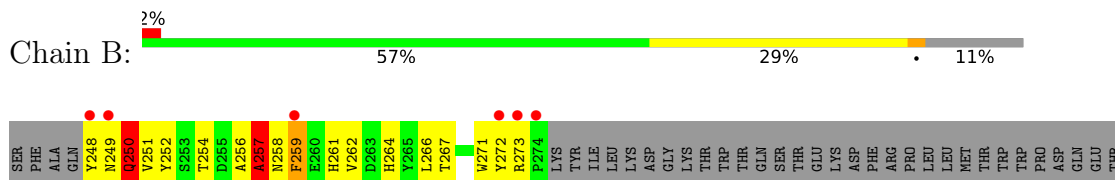
3 Residue-property plots [i](#)

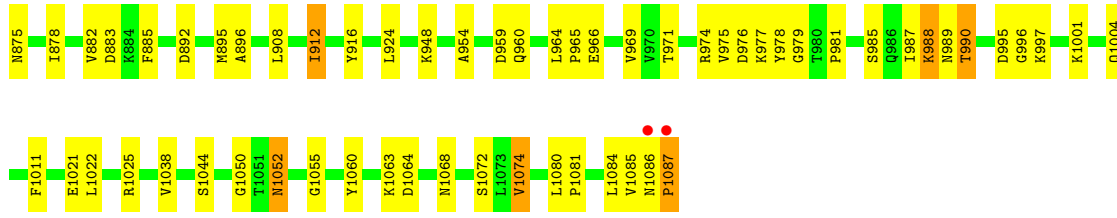
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucosyltransferase-SI

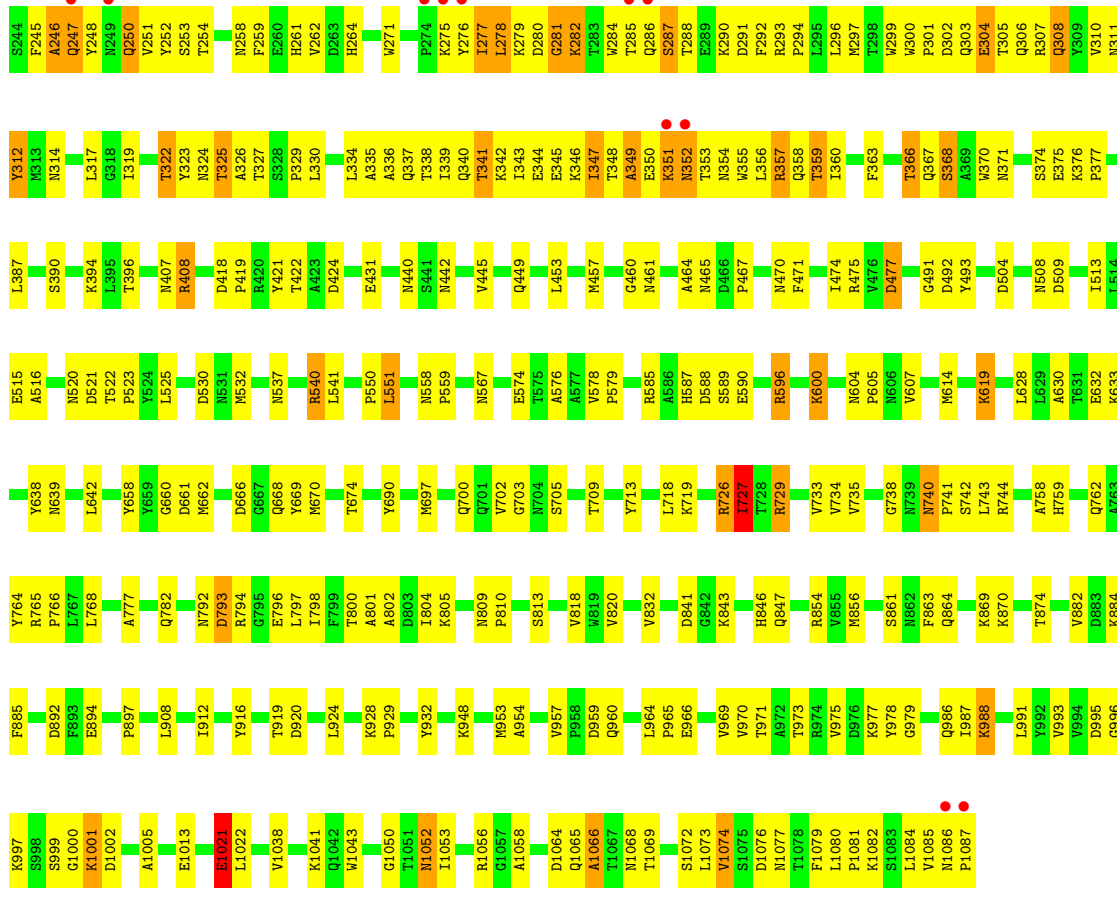


• Molecule 1: Glucosyltransferase-SI

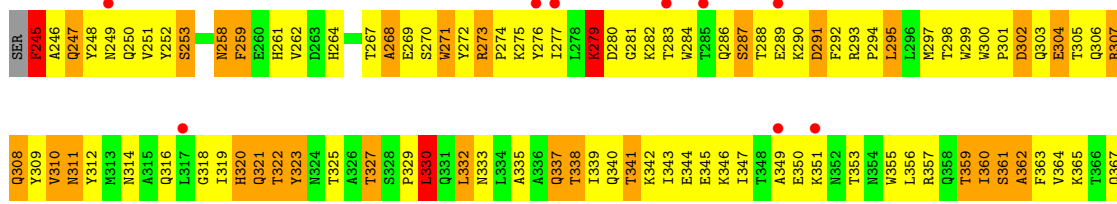


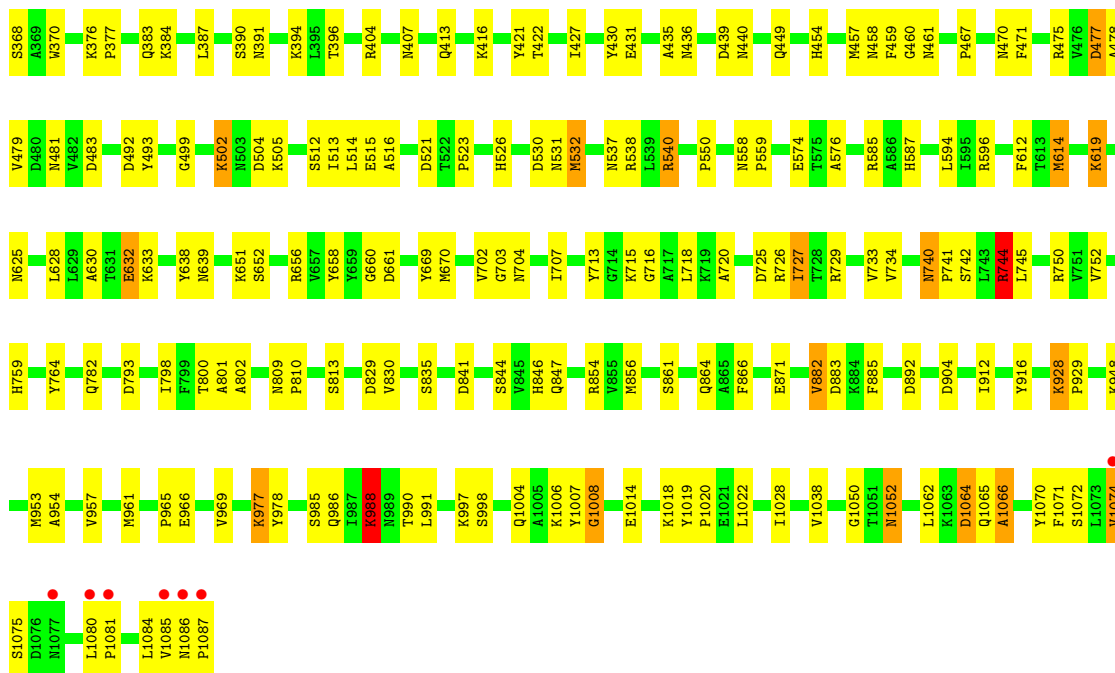


● Molecule 1: Glucosyltransferase-SI

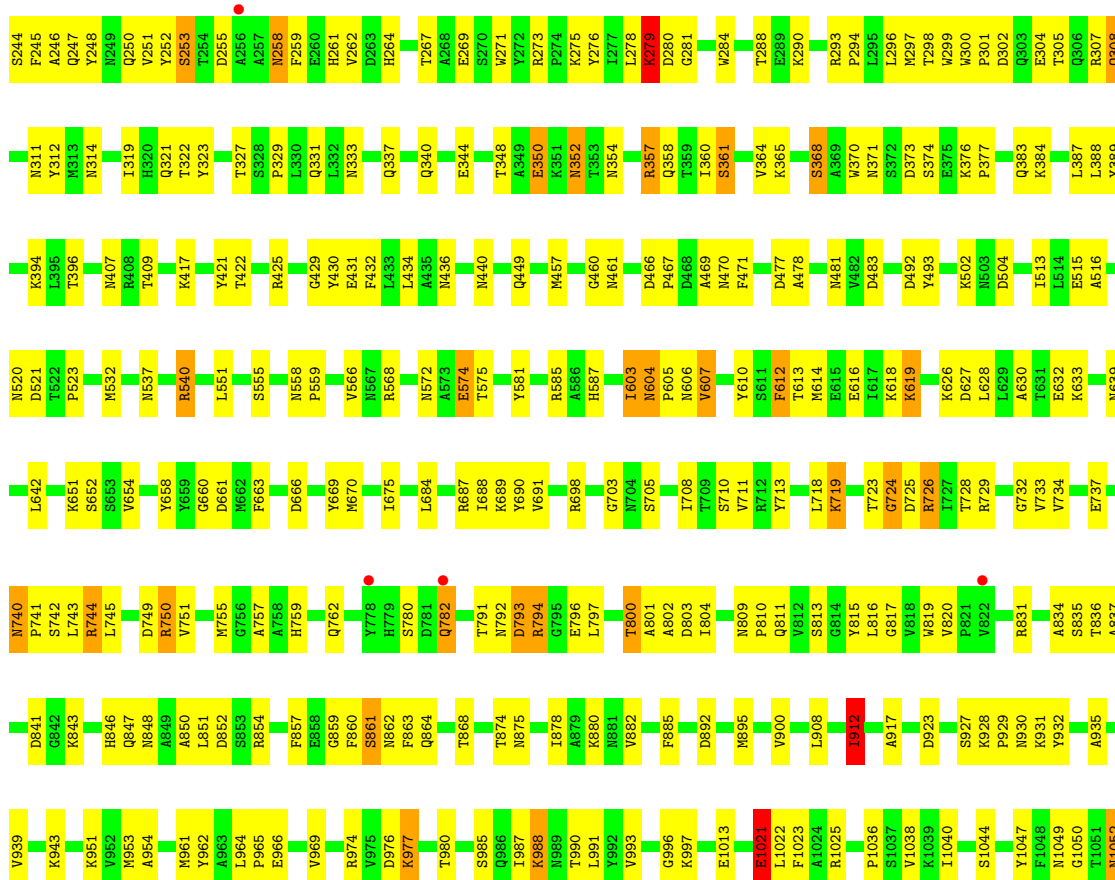


● Molecule 1: Glucosyltransferase-SI



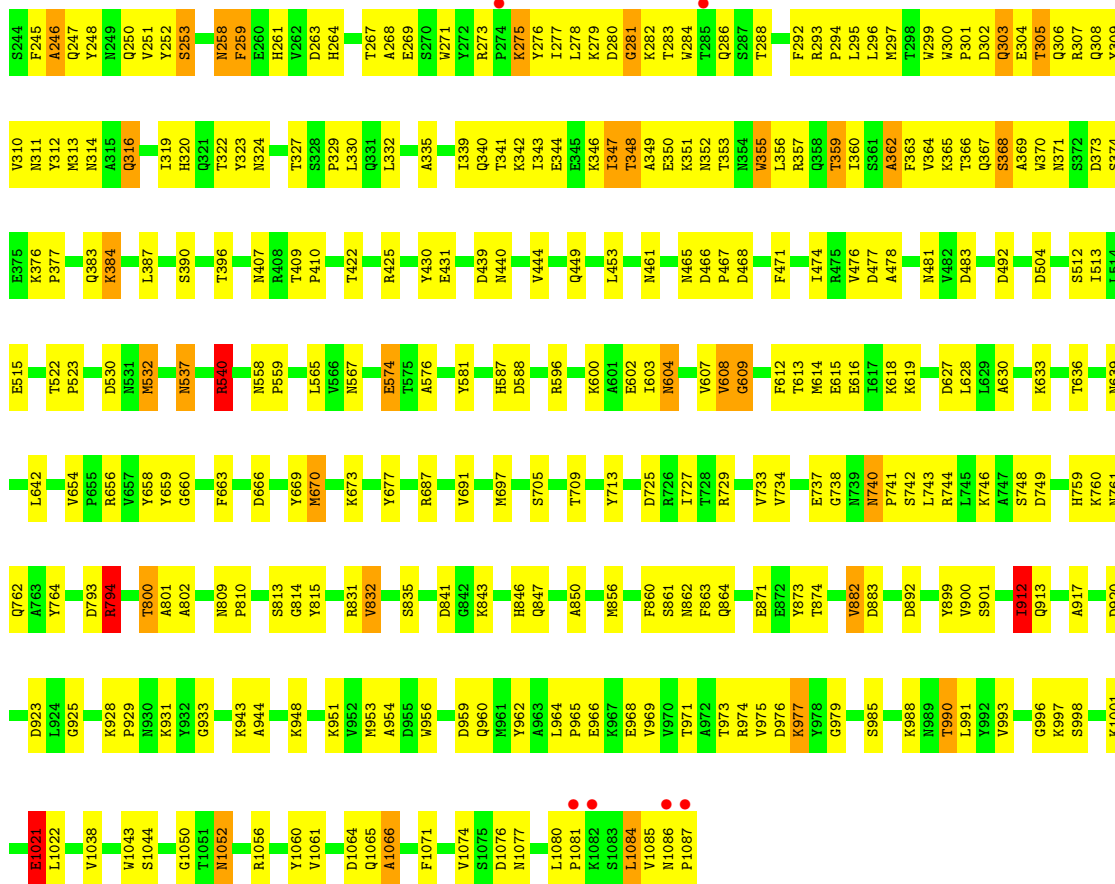


• Molecule 1: Glucosyltransferase-SI

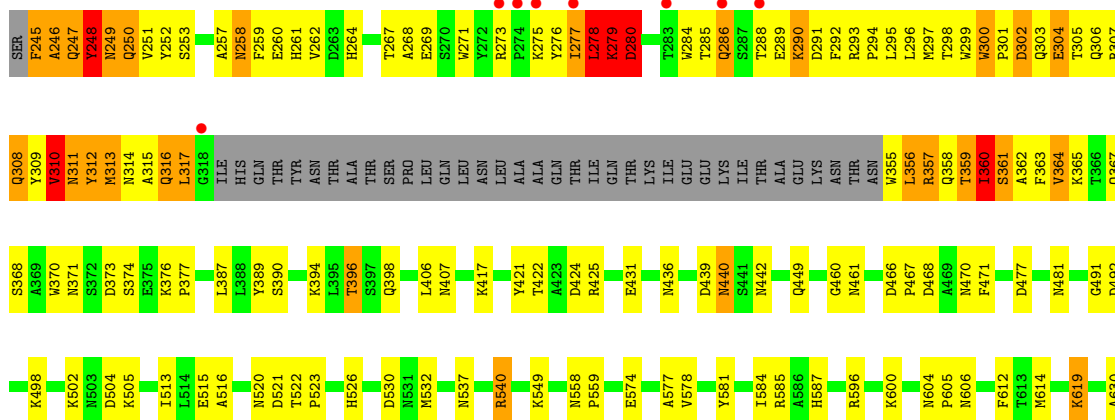


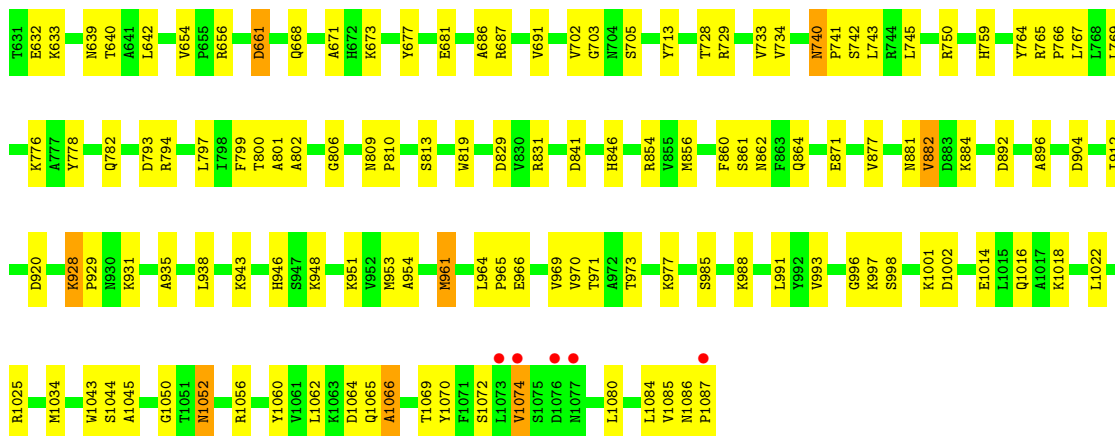


• Molecule 1: Glucosyltransferase-SI



• Molecule 1: Glucosyltransferase-SI





- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain I: 33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain J: 33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain K: 33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain L: 33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain M: 33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain N:  33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain O:  33% 67%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain P:  33% 67%

GLC1
GLC2
AC13

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	295.52Å 214.41Å 220.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.77 – 3.11 61.77 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.77-3.11) 95.3 (61.77-3.11)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.13Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.211 , 0.244 0.208 , 0.239	Depositor DCC
R_{free} test set	12026 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52865	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9554e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, CA, GLC, AC1

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	0.99	9/6784 (0.1%)	0.95	3/9213 (0.0%)
1	B	0.88	12/5976 (0.2%)	0.88	7/8113 (0.1%)
1	C	0.94	1/6802 (0.0%)	0.94	8/9237 (0.1%)
1	D	0.95	4/6802 (0.1%)	0.92	11/9237 (0.1%)
1	E	1.04	14/6796 (0.2%)	0.95	10/9229 (0.1%)
1	F	0.81	1/6802 (0.0%)	0.85	3/9237 (0.0%)
1	G	0.97	6/6802 (0.1%)	0.95	7/9237 (0.1%)
1	H	0.91	4/6510 (0.1%)	0.93	9/8837 (0.1%)
All	All	0.94	51/53274 (0.1%)	0.92	58/72340 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	HIS	CE1-NE2	14.48	1.66	1.32
1	E	245	PHE	N-CA	12.06	1.70	1.46
1	E	245	PHE	CE2-CZ	11.00	1.58	1.37
1	E	273	ARG	CZ-NH1	10.60	1.46	1.33
1	H	249	ASN	CG-OD1	10.12	1.46	1.24
1	E	245	PHE	CG-CD1	9.87	1.53	1.38
1	B	250	GLN	CD-NE2	9.80	1.57	1.32
1	E	279	LYS	CE-NZ	9.61	1.73	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1013	GLU	CD-OE1	9.29	1.35	1.25
1	A	290	LYS	CE-NZ	9.06	1.71	1.49
1	H	245	PHE	CD2-CE2	-8.69	1.21	1.39
1	B	729	ARG	CZ-NH1	-8.69	1.21	1.33
1	H	245	PHE	CD1-CE1	-8.28	1.22	1.39
1	B	249	ASN	CB-CG	8.12	1.69	1.51
1	D	282	LYS	CD-CE	8.10	1.71	1.51
1	A	320	HIS	CG-CD2	7.71	1.48	1.35
1	B	1084	LEU	C-O	7.65	1.37	1.23
1	G	1021	GLU	CD-OE1	7.45	1.33	1.25
1	E	271	TRP	CD2-CE2	-7.37	1.32	1.41
1	E	632	GLU	CD-OE1	6.96	1.33	1.25
1	B	271	TRP	CD2-CE3	6.96	1.50	1.40
1	G	279	LYS	CD-CE	6.92	1.68	1.51
1	B	271	TRP	CZ2-CH2	6.67	1.50	1.37
1	B	1087	PRO	N-CD	6.59	1.57	1.47
1	E	632	GLU	CB-CG	-6.51	1.39	1.52
1	E	279	LYS	CD-CE	6.47	1.67	1.51
1	H	245	PHE	CG-CD1	-6.45	1.29	1.38
1	B	1013	GLU	CD-OE1	6.42	1.32	1.25
1	A	574	GLU	CD-OE1	6.36	1.32	1.25
1	B	271	TRP	CE3-CZ3	6.21	1.49	1.38
1	C	1087	PRO	N-CD	-6.17	1.39	1.47
1	D	1082	LYS	CB-CG	5.97	1.68	1.52
1	B	257	ALA	CA-CB	5.86	1.64	1.52
1	E	323	TYR	CG-CD1	5.81	1.46	1.39
1	A	735	VAL	CB-CG1	-5.77	1.40	1.52
1	D	793	ASP	CB-CG	-5.77	1.39	1.51
1	E	726	ARG	CZ-NH1	5.73	1.40	1.33
1	G	1021	GLU	CG-CD	5.61	1.60	1.51
1	G	608	VAL	CB-CG1	5.59	1.64	1.52
1	A	1021	GLU	CG-CD	5.47	1.60	1.51
1	G	537	ASN	CB-CG	5.47	1.63	1.51
1	A	615	GLU	CD-OE1	5.27	1.31	1.25
1	B	1082	LYS	CE-NZ	5.25	1.62	1.49
1	E	988	LYS	CD-CE	5.23	1.64	1.51
1	E	720	ALA	CA-CB	-5.23	1.41	1.52
1	A	320	HIS	CG-ND1	5.22	1.50	1.38
1	E	323	TYR	CE2-CZ	5.17	1.45	1.38
1	D	1082	LYS	CE-NZ	5.15	1.61	1.49
1	B	1087	PRO	CA-C	5.15	1.63	1.52
1	A	284	TRP	CD2-CE3	5.09	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	794	ARG	CZ-NH1	5.05	1.39	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	245	PHE	CB-CG-CD1	-11.95	112.44	120.80
1	H	245	PHE	CG-CD2-CE2	-10.93	108.77	120.80
1	E	273	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	D	793	ASP	CB-CA-C	-8.51	93.38	110.40
1	E	727	ILE	CG1-CB-CG2	-8.07	93.64	111.40
1	E	245	PHE	CB-CG-CD2	-7.99	115.21	120.80
1	H	245	PHE	CD1-CG-CD2	7.94	128.63	118.30
1	G	912	ILE	CB-CA-C	-7.46	96.69	111.60
1	E	744	ARG	CB-CA-C	-7.35	95.71	110.40
1	B	250	GLN	OE1-CD-NE2	7.09	138.21	121.90
1	C	744	ARG	CB-CA-C	-7.04	96.31	110.40
1	E	330	LEU	CA-CB-CG	6.71	130.74	115.30
1	C	725	ASP	CB-CG-OD1	6.54	124.18	118.30
1	H	661	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	793	ASP	CB-CA-C	-6.10	98.20	110.40
1	B	250	GLN	CG-CD-NE2	-6.07	102.14	116.70
1	H	245	PHE	CD1-CE1-CZ	-5.88	113.05	120.10
1	B	912	ILE	CB-CA-C	-5.84	99.92	111.60
1	D	408	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	G	540	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	E	594	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	G	912	ILE	CG1-CB-CG2	-5.65	98.98	111.40
1	H	425	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	H	317	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	727	ILE	CG1-CB-CG2	-5.59	99.10	111.40
1	B	596	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	F	912	ILE	CB-CA-C	-5.53	100.55	111.60
1	D	596	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	250	GLN	CB-CA-C	-5.48	99.44	110.40
1	G	468	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	509	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	D	1021	GLU	CB-CG-CD	-5.42	99.56	114.20
1	D	995	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	727	ILE	CG1-CB-CG2	-5.41	99.50	111.40
1	E	538	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	D	1021	GLU	N-CA-C	5.34	125.43	111.00
1	H	540	ARG	NE-CZ-NH1	5.27	122.94	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	899	TYR	CA-CB-CG	-5.24	103.44	113.40
1	B	248	TYR	N-CA-CB	5.22	120.00	110.60
1	D	719	LYS	CD-CE-NZ	-5.22	99.70	111.70
1	A	793	ASP	CB-CA-C	-5.21	99.97	110.40
1	F	684	LEU	CA-CB-CG	-5.21	103.31	115.30
1	A	358	GLN	N-CA-CB	-5.21	101.23	110.60
1	B	544	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	C	406	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	C	317	LEU	CA-CB-CG	5.16	127.16	115.30
1	H	280	ASP	CB-CG-OD2	5.16	122.94	118.30
1	G	831	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	E	540	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	437	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	793	ASP	CB-CG-OD1	-5.12	113.70	118.30
1	G	793	ASP	CB-CA-C	-5.10	100.20	110.40
1	D	798	ILE	CB-CA-C	-5.10	101.41	111.60
1	E	279	LYS	CD-CE-NZ	-5.08	100.01	111.70
1	C	1087	PRO	CA-N-CD	5.06	118.78	111.70
1	C	495	LYS	CD-CE-NZ	-5.04	100.11	111.70
1	D	738	GLY	N-CA-C	-5.04	100.50	113.10
1	E	745	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	TRP	Peptide
1	H	245	PHE	Sidechain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6643	0	6475	332	0
1	B	5854	0	5691	243	0
1	C	6660	0	6489	258	0
1	D	6660	0	6489	323	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6654	0	6484	337	0
1	F	6660	0	6489	318	0
1	G	6660	0	6489	287	0
1	H	6372	0	6196	334	0
2	I	44	0	30	10	0
2	J	44	0	30	7	0
2	K	44	0	30	9	0
2	L	44	0	30	6	0
2	M	44	0	30	10	0
2	N	44	0	30	6	0
2	O	44	0	30	7	0
2	P	44	0	30	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	12	2	0
4	B	12	0	12	0	0
4	C	12	0	12	2	0
4	D	12	0	12	2	0
4	E	12	0	12	1	0
4	F	12	0	12	0	0
4	G	12	0	12	1	0
4	H	12	0	12	0	0
5	A	33	0	0	6	0
5	B	20	0	0	6	0
5	C	32	0	0	2	0
5	D	40	0	0	2	0
5	E	48	0	0	2	0
5	F	15	0	0	10	0
5	G	34	0	0	2	0
5	H	24	0	0	4	0
All	All	52865	0	51138	2464	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 24.

All (2464) 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:E:245:PHE:N	1:E:245:PHE:CA	1.70	1.54
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.38	1.54
1:A:290:LYS:NZ	1:A:290:LYS:CE	1.71	1.53
1:E:279:LYS:NZ	1:E:279:LYS:CE	1.73	1.51
1:E:273:ARG:CD	1:E:287:SER:HB2	1.40	1.49
1:E:273:ARG:HD2	1:E:287:SER:CB	1.43	1.44
1:B:939:VAL:CG1	1:B:943:LYS:NZ	1.87	1.35
1:D:281:GLY:HA3	1:D:341:THR:CG2	1.56	1.33
1:E:271:TRP:NE1	1:E:294:PRO:HB3	1.46	1.28
1:G:355:TRP:O	1:G:359:THR:HG22	1.33	1.28
1:H:277:ILE:HD11	1:H:291:ASP:CB	1.63	1.26
2:L:2:GLC:H61	2:L:3:AC1:O5	1.36	1.25
2:K:2:GLC:H61	2:K:3:AC1:O5	1.36	1.24
2:P:2:GLC:H61	2:P:3:AC1:O5	1.36	1.24
1:E:280:ASP:O	1:E:282:LYS:HG3	1.38	1.23
1:E:300:TRP:CG	1:E:306:GLN:HB2	1.75	1.22
1:H:299:TRP:C	1:H:300:TRP:CE3	2.12	1.22
1:B:939:VAL:HG13	1:B:943:LYS:NZ	1.55	1.21
2:N:2:GLC:H61	2:N:3:AC1:O5	1.36	1.20
2:O:2:GLC:H61	2:O:3:AC1:O5	1.36	1.20
1:H:309:TYR:CD2	1:H:309:TYR:O	1.94	1.20
2:M:2:GLC:H61	2:M:3:AC1:O5	1.36	1.20
2:J:2:GLC:H61	2:J:3:AC1:O5	1.36	1.19
1:B:800:THR:HG22	1:B:802:ALA:N	1.59	1.18
1:H:294:PRO:HD2	1:H:297:MET:HE1	1.24	1.18
1:A:300:TRP:CD2	1:A:306:GLN:HG3	1.78	1.17
1:D:281:GLY:CA	1:D:341:THR:HG23	1.75	1.17
1:F:1021:GLU:CA	1:F:1021:GLU:OE1	1.92	1.16
1:H:277:ILE:CD1	1:H:291:ASP:HB3	1.75	1.16
1:B:743:LEU:O	1:B:744:ARG:HG2	1.43	1.16
1:E:346:LYS:HE2	1:E:350:GLU:OE2	1.46	1.15
1:H:466:ASP:OD2	1:H:943:LYS:HE2	1.44	1.15
1:E:277:ILE:HD11	1:E:291:ASP:CB	1.75	1.15
1:D:339:ILE:O	1:D:343:ILE:HG13	1.46	1.14
1:B:1083:SER:O	1:B:1087:PRO:HG3	1.46	1.14
1:H:862:ASN:O	1:H:912:ILE:HD13	1.46	1.14
1:G:800:THR:HG22	1:G:802:ALA:H	1.10	1.13
1:H:278:LEU:HA	1:H:284:TRP:HA	1.27	1.13
1:A:278:LEU:HG	1:A:281:GLY:HA2	1.21	1.13
1:B:743:LEU:C	1:B:744:ARG:HG2	1.64	1.13
1:F:250:GLN:HE21	1:F:275:LYS:CE	1.61	1.13
1:H:310:VAL:HG12	1:H:311:ASN:N	1.60	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:GLY:CA	1:D:341:THR:CG2	2.25	1.12
1:H:310:VAL:HG12	1:H:311:ASN:H	1.03	1.12
1:A:271:TRP:CZ2	1:A:357:ARG:HA	1.85	1.11
1:F:357:ARG:HH11	1:F:357:ARG:CG	1.60	1.11
1:E:277:ILE:HD12	1:E:291:ASP:HB3	1.16	1.10
1:G:339:ILE:O	1:G:343:ILE:HG13	1.51	1.10
1:E:304:GLU:OE1	1:E:304:GLU:HA	1.36	1.10
1:G:316:GLN:NE2	1:G:316:GLN:HA	1.51	1.10
1:A:271:TRP:HZ2	1:A:357:ARG:HA	1.09	1.10
1:A:346:LYS:O	1:A:350:GLU:HG2	1.48	1.10
1:E:277:ILE:CD1	1:E:291:ASP:CB	2.29	1.10
1:E:271:TRP:CD1	1:E:294:PRO:HA	1.87	1.09
1:F:357:ARG:HH11	1:F:357:ARG:HG2	1.10	1.09
1:H:248:TYR:HB3	1:H:276:TYR:HB2	1.33	1.08
1:H:277:ILE:HD12	1:H:291:ASP:OD2	1.51	1.08
1:C:800:THR:HG22	1:C:802:ALA:H	1.13	1.08
1:F:782:GLN:HE21	1:F:782:GLN:HA	0.99	1.08
1:H:252:TYR:HB3	1:H:258:ASN:HD21	1.12	1.08
1:F:250:GLN:HE21	1:F:275:LYS:HE3	1.05	1.07
1:D:800:THR:HG22	1:D:802:ALA:H	1.12	1.07
1:F:800:THR:HG22	1:F:802:ALA:H	1.17	1.06
1:E:246:ALA:HB3	1:E:247:GLN:HE21	1.21	1.06
1:F:862:ASN:O	1:F:912:ILE:HG21	1.56	1.06
1:E:300:TRP:CD1	1:E:306:GLN:HB2	1.89	1.06
1:B:1073:LEU:HD21	1:B:1080:LEU:HD21	1.37	1.05
1:D:281:GLY:HA3	1:D:341:THR:HG22	1.10	1.05
1:D:1021:GLU:OE1	1:D:1021:GLU:HA	1.28	1.05
1:H:288:THR:CG2	1:H:289:GLU:H	1.70	1.04
1:E:277:ILE:HD11	1:E:291:ASP:HB3	1.11	1.04
1:A:281:GLY:HA3	1:A:341:THR:HG23	1.08	1.04
1:A:800:THR:HG22	1:A:802:ALA:H	1.22	1.04
1:E:245:PHE:CA	1:E:248:TYR:HD2	1.70	1.04
1:H:300:TRP:CE3	1:H:300:TRP:N	2.26	1.04
1:F:713:TYR:O	1:F:759:HIS:HE1	1.40	1.03
1:A:339:ILE:O	1:A:343:ILE:HG13	1.56	1.03
1:E:800:THR:HG22	1:E:802:ALA:H	1.22	1.03
1:D:310:VAL:HG13	1:D:339:ILE:HD11	1.39	1.03
1:E:966:GLU:HB2	1:E:997:LYS:HB2	1.41	1.02
1:H:294:PRO:HD2	1:H:297:MET:CE	1.88	1.02
1:A:604:ASN:HD21	1:A:607:VAL:CA	1.73	1.01
1:A:604:ASN:ND2	1:A:607:VAL:HB	1.74	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:THR:CG2	1:B:802:ALA:H	1.73	1.01
1:D:280:ASP:OD1	1:D:345:GLU:HA	1.59	1.01
1:D:1021:GLU:OE1	1:D:1021:GLU:CA	2.08	1.01
1:H:1085:VAL:HG23	1:H:1086:ASN:H	1.25	1.01
1:C:639:ASN:HD21	1:C:813:SER:H	1.09	1.00
1:F:1021:GLU:OE1	1:F:1021:GLU:HA	1.21	1.00
1:C:252:TYR:HB3	1:C:258:ASN:HD21	1.23	1.00
1:H:288:THR:HG22	1:H:289:GLU:H	1.22	1.00
1:H:288:THR:HG22	1:H:289:GLU:N	1.74	1.00
1:D:323:TYR:HB3	1:D:327:THR:OG1	1.60	1.00
1:F:250:GLN:HB2	1:F:1084:LEU:O	1.62	1.00
1:F:782:GLN:HA	1:F:782:GLN:NE2	1.73	1.00
1:H:440:ASN:HD21	1:H:449:GLN:HE21	1.04	1.00
1:A:281:GLY:CA	1:A:341:THR:HG23	1.91	0.99
1:A:639:ASN:HD21	1:A:813:SER:H	1.05	0.99
1:D:740:ASN:ND2	1:D:742:SER:H	1.59	0.99
1:E:321:GLN:HG3	1:E:322:THR:H	1.26	0.99
1:E:639:ASN:HD21	1:E:813:SER:H	1.00	0.99
1:D:281:GLY:HA2	1:D:341:THR:HG23	1.38	0.99
1:C:1063:LYS:HE2	1:C:1068:ASN:ND2	1.78	0.99
1:E:440:ASN:HD21	1:E:449:GLN:HE21	1.06	0.98
1:E:861:SER:H	1:E:864:GLN:HE21	1.00	0.98
1:B:491:GLY:HA3	5:B:31:HOH:O	1.62	0.98
1:H:316:GLN:HG2	1:H:359:THR:HG21	1.42	0.98
1:F:252:TYR:HB3	1:F:258:ASN:HD21	1.24	0.98
1:F:261:HIS:HD2	1:F:264:HIS:H	0.99	0.98
1:F:311:ASN:HD21	1:F:323:TYR:H	1.10	0.98
1:H:861:SER:H	1:H:864:GLN:NE2	1.62	0.98
1:B:262:VAL:HG12	1:B:969:VAL:HG23	1.43	0.97
1:G:252:TYR:HA	1:G:275:LYS:HG2	1.45	0.97
1:G:316:GLN:NE2	1:G:316:GLN:CA	2.23	0.97
1:D:271:TRP:CD1	1:D:294:PRO:HA	1.99	0.97
1:G:252:TYR:HB3	1:G:258:ASN:HD21	1.27	0.97
1:G:316:GLN:HA	1:G:316:GLN:HE21	1.06	0.97
1:B:687:ARG:HA	1:B:691:VAL:CG2	1.94	0.97
1:E:245:PHE:HA	1:E:248:TYR:HD2	1.27	0.97
1:A:966:GLU:HB2	1:A:997:LYS:HB2	1.44	0.96
1:A:861:SER:H	1:A:864:GLN:HE21	1.12	0.96
1:F:360:ILE:O	1:F:364:VAL:HG23	1.65	0.96
1:H:311:ASN:O	1:H:314:ASN:HB2	1.65	0.96
1:H:639:ASN:HD21	1:H:813:SER:H	1.07	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:VAL:HG12	1:F:969:VAL:HG23	1.46	0.96
1:F:1085:VAL:HG23	1:F:1086:ASN:H	1.31	0.96
1:B:861:SER:H	1:B:864:GLN:HE21	1.01	0.95
1:A:440:ASN:HD21	1:A:449:GLN:NE2	1.64	0.95
1:G:440:ASN:HD21	1:G:449:GLN:HE21	1.11	0.95
1:G:912:ILE:HG22	1:G:912:ILE:O	1.66	0.95
1:A:271:TRP:HZ2	1:A:357:ARG:CA	1.78	0.95
1:C:460:GLY:H	1:C:470:ASN:HD22	1.11	0.95
1:D:740:ASN:HD22	1:D:742:SER:H	1.12	0.95
1:A:281:GLY:HA3	1:A:341:THR:CG2	1.96	0.95
1:E:252:TYR:CE2	1:E:273:ARG:NH2	2.34	0.95
1:D:276:TYR:HD1	1:D:285:THR:O	1.48	0.95
1:E:271:TRP:CE2	1:E:294:PRO:HB3	2.01	0.95
1:G:1052:ASN:H	1:G:1052:ASN:ND2	1.61	0.95
1:G:310:VAL:HG11	1:G:335:ALA:HB1	1.49	0.94
1:F:250:GLN:NE2	1:F:275:LYS:HE3	1.82	0.94
1:F:782:GLN:HE21	1:F:782:GLN:CA	1.71	0.94
1:E:346:LYS:O	1:E:350:GLU:HG3	1.67	0.94
1:H:300:TRP:N	1:H:300:TRP:HE3	1.64	0.94
1:A:278:LEU:CG	1:A:281:GLY:HA2	1.97	0.94
1:D:300:TRP:CD2	1:D:306:GLN:HG3	2.02	0.94
1:F:670:MET:HE1	1:F:885:PHE:HZ	1.30	0.94
1:E:245:PHE:HA	1:E:248:TYR:CD2	2.03	0.94
1:E:513:ILE:HG12	1:E:953:MET:HE2	1.49	0.94
1:H:800:THR:HG22	1:H:802:ALA:H	1.33	0.94
1:A:440:ASN:ND2	1:A:449:GLN:HE21	1.66	0.94
1:H:1052:ASN:HD22	1:H:1052:ASN:H	1.00	0.94
1:A:301:PRO:HG2	1:A:302:ASP:H	1.33	0.94
1:C:1052:ASN:HD22	1:C:1052:ASN:H	1.05	0.94
1:B:939:VAL:HG12	1:B:943:LYS:NZ	1.80	0.93
1:G:861:SER:H	1:G:864:GLN:HE21	1.05	0.93
1:D:297:MET:SD	1:D:340:GLN:HG3	2.08	0.93
1:F:800:THR:HG22	1:F:802:ALA:N	1.83	0.93
1:G:304:GLU:OE1	1:G:304:GLU:HA	1.64	0.93
1:B:939:VAL:HG13	1:B:943:LYS:HZ2	1.17	0.93
1:D:440:ASN:HD21	1:D:449:GLN:HE21	1.14	0.93
1:D:1052:ASN:H	1:D:1052:ASN:HD22	0.97	0.93
1:F:440:ASN:HD21	1:F:449:GLN:HE21	1.08	0.93
1:E:288:THR:HG22	1:E:289:GLU:H	1.30	0.93
1:D:1052:ASN:HD22	1:D:1052:ASN:N	1.66	0.92
1:G:862:ASN:O	1:G:912:ILE:HG21	1.68	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:GLN:O	1:E:309:TYR:HB3	1.69	0.92
1:C:440:ASN:HD21	1:C:449:GLN:HE21	1.11	0.92
1:H:260:GLU:OE1	1:H:271:TRP:HB2	1.69	0.92
1:B:939:VAL:CG1	1:B:943:LYS:HZ3	1.73	0.92
1:B:1052:ASN:H	1:B:1052:ASN:HD22	1.02	0.92
1:A:335:ALA:O	1:A:339:ILE:HG13	1.69	0.92
1:F:861:SER:H	1:F:864:GLN:HE21	1.00	0.92
1:E:271:TRP:NE1	1:E:294:PRO:CB	2.32	0.92
1:C:261:HIS:CD2	1:C:264:HIS:H	1.86	0.92
1:D:277:ILE:HG22	1:D:277:ILE:O	1.68	0.92
1:G:800:THR:HG22	1:G:802:ALA:N	1.83	0.92
1:D:492:ASP:HB3	1:D:1022:LEU:HD22	1.50	0.91
1:A:1052:ASN:H	1:A:1052:ASN:HD22	1.16	0.91
1:H:278:LEU:HB3	1:H:284:TRP:CE3	2.06	0.91
1:H:310:VAL:CG1	1:H:311:ASN:N	2.32	0.91
1:H:277:ILE:CD1	1:H:291:ASP:OD2	2.16	0.91
1:A:250:GLN:HB2	1:A:1084:LEU:O	1.71	0.91
1:A:740:ASN:HD22	1:A:740:ASN:C	1.73	0.91
1:H:1085:VAL:HG23	1:H:1086:ASN:N	1.82	0.91
1:D:861:SER:H	1:D:864:GLN:HE21	1.08	0.91
1:E:304:GLU:OE1	1:E:304:GLU:CA	2.19	0.91
1:F:861:SER:H	1:F:864:GLN:NE2	1.69	0.91
1:A:604:ASN:HD21	1:A:607:VAL:HA	1.34	0.91
1:H:360:ILE:HG22	1:H:361:SER:N	1.86	0.91
1:H:966:GLU:HB2	1:H:997:LYS:HB2	1.53	0.90
1:C:861:SER:H	1:C:864:GLN:NE2	1.68	0.90
1:C:861:SER:H	1:C:864:GLN:HE21	0.96	0.90
1:D:330:LEU:HD12	1:D:330:LEU:O	1.69	0.90
1:F:278:LEU:HD23	1:F:281:GLY:HA2	1.52	0.90
1:E:587:HIS:NE2	2:M:3:AC1:O3B	1.95	0.90
1:A:252:TYR:HB3	1:A:258:ASN:HD21	1.37	0.90
1:H:262:VAL:HG12	1:H:969:VAL:HG23	1.54	0.90
1:B:687:ARG:HA	1:B:691:VAL:HG23	1.52	0.90
2:I:2:GLC:H61	2:I:3:AC1:O5	1.71	0.89
1:E:320:HIS:O	1:E:321:GLN:O	1.90	0.89
1:G:349:ALA:O	1:G:350:GLU:HG2	1.71	0.89
1:E:245:PHE:N	1:E:248:TYR:CD2	2.41	0.89
1:B:939:VAL:CG1	1:B:943:LYS:HZ2	1.64	0.89
1:C:861:SER:N	1:C:864:GLN:HE21	1.70	0.89
1:G:1052:ASN:HD22	1:G:1052:ASN:N	1.70	0.89
1:E:279:LYS:O	1:E:279:LYS:HG2	1.71	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:TYR:HB3	1:B:258:ASN:ND2	1.88	0.88
1:D:276:TYR:CD1	1:D:285:THR:O	2.25	0.88
1:H:299:TRP:CA	1:H:300:TRP:CE3	2.56	0.88
1:C:261:HIS:HD2	1:C:264:HIS:N	1.71	0.88
1:E:347:ILE:HG12	1:E:353:THR:HB	1.54	0.88
1:F:669:TYR:CD2	1:F:670:MET:HG3	2.08	0.88
1:F:687:ARG:HA	1:F:691:VAL:CG2	2.02	0.88
1:C:740:ASN:C	1:C:740:ASN:HD22	1.77	0.88
1:H:246:ALA:O	1:H:247:GLN:C	2.10	0.88
1:F:350:GLU:HB3	1:F:352:ASN:ND2	1.88	0.88
1:E:346:LYS:CE	1:E:350:GLU:OE2	2.21	0.88
1:G:492:ASP:HB3	1:G:1022:LEU:HD22	1.55	0.88
1:A:251:VAL:HG21	1:A:259:PHE:CZ	2.09	0.87
1:C:261:HIS:HD2	1:C:264:HIS:H	0.93	0.87
1:D:639:ASN:HD21	1:D:813:SER:H	1.22	0.87
1:H:278:LEU:HD12	1:H:278:LEU:O	1.72	0.87
1:D:251:VAL:HG21	1:D:259:PHE:CZ	2.07	0.87
1:G:604:ASN:ND2	1:G:607:VAL:HB	1.90	0.87
1:F:261:HIS:HD2	1:F:264:HIS:N	1.73	0.87
1:A:316:GLN:HE21	1:A:359:THR:HG22	1.38	0.87
1:F:670:MET:CE	1:F:885:PHE:HZ	1.88	0.87
1:A:300:TRP:CE3	1:A:306:GLN:HG3	2.10	0.87
1:C:251:VAL:HG21	1:C:259:PHE:CZ	2.08	0.87
1:E:271:TRP:CD1	1:E:294:PRO:CA	2.58	0.87
1:H:861:SER:H	1:H:864:GLN:HE21	0.87	0.87
1:C:460:GLY:N	1:C:470:ASN:HD22	1.73	0.86
1:A:782:GLN:HE21	1:A:782:GLN:HA	1.40	0.86
1:F:248:TYR:HB3	1:F:276:TYR:HB2	1.57	0.86
1:F:250:GLN:OE1	1:F:1087:PRO:CG	2.24	0.86
1:G:740:ASN:ND2	1:G:742:SER:H	1.73	0.86
1:G:861:SER:N	1:G:864:GLN:HE21	1.72	0.86
1:A:440:ASN:HD21	1:A:449:GLN:HE21	0.88	0.86
1:H:309:TYR:O	1:H:309:TYR:CG	2.28	0.86
1:A:261:HIS:HD2	1:A:264:HIS:H	1.23	0.86
1:B:639:ASN:HD21	1:B:813:SER:H	1.22	0.86
1:A:376:LYS:HB3	1:A:377:PRO:HA	1.58	0.85
1:E:245:PHE:CA	1:E:248:TYR:CD2	2.59	0.85
1:A:604:ASN:ND2	1:A:607:VAL:CA	2.40	0.85
1:G:861:SER:H	1:G:864:GLN:NE2	1.73	0.85
1:B:658:TYR:CE2	1:B:660:GLY:HA3	2.12	0.85
1:A:302:ASP:OD1	1:A:304:GLU:HB3	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:HIS:NE2	2:L:3:AC1:O3B	2.09	0.85
1:G:794:ARG:NH1	1:G:794:ARG:HG2	1.91	0.85
1:C:376:LYS:HB3	1:C:377:PRO:HA	1.59	0.85
1:F:357:ARG:CG	1:F:357:ARG:NH1	2.34	0.85
1:D:271:TRP:CE2	1:D:294:PRO:HD3	2.12	0.85
1:F:669:TYR:HE2	1:F:670:MET:HE3	1.40	0.85
1:F:687:ARG:HA	1:F:691:VAL:HG23	1.57	0.85
1:H:861:SER:N	1:H:864:GLN:HE21	1.72	0.85
1:E:245:PHE:N	1:E:245:PHE:HD1	1.75	0.85
1:D:352:ASN:OD1	1:D:354:ASN:HB2	1.76	0.85
1:D:800:THR:HG22	1:D:802:ALA:N	1.91	0.85
1:E:245:PHE:N	1:E:245:PHE:CD1	2.44	0.85
1:B:466:ASP:OD2	1:B:943:LYS:HE3	1.77	0.85
1:C:639:ASN:ND2	1:C:813:SER:H	1.75	0.85
1:H:300:TRP:CD1	1:H:306:GLN:HA	2.12	0.85
1:A:604:ASN:ND2	1:A:607:VAL:CB	2.39	0.84
1:D:271:TRP:CZ2	1:D:294:PRO:HD3	2.12	0.84
1:G:261:HIS:HD2	1:G:264:HIS:H	1.25	0.84
1:F:713:TYR:O	1:F:759:HIS:CE1	2.30	0.84
1:F:357:ARG:HG2	1:F:357:ARG:NH1	1.89	0.84
1:F:1085:VAL:HG23	1:F:1086:ASN:N	1.92	0.84
1:C:740:ASN:ND2	1:C:742:SER:H	1.75	0.84
1:E:639:ASN:ND2	1:E:813:SER:H	1.74	0.84
1:F:321:GLN:OE1	1:F:321:GLN:HA	1.76	0.84
1:H:1052:ASN:H	1:H:1052:ASN:ND2	1.76	0.84
1:A:278:LEU:HG	1:A:281:GLY:CA	2.05	0.84
1:A:639:ASN:ND2	1:A:813:SER:H	1.76	0.84
1:D:782:GLN:HA	1:D:782:GLN:HE21	1.43	0.83
1:H:440:ASN:HD21	1:H:449:GLN:NE2	1.74	0.83
1:D:245:PHE:O	1:D:247:GLN:N	2.10	0.83
1:E:740:ASN:C	1:E:740:ASN:HD22	1.77	0.83
1:F:460:GLY:H	1:F:470:ASN:ND2	1.74	0.83
1:F:670:MET:HE1	1:F:885:PHE:CZ	2.12	0.83
1:F:261:HIS:CD2	1:F:264:HIS:H	1.91	0.83
1:D:293:ARG:HB3	1:D:297:MET:CE	2.08	0.83
1:D:460:GLY:H	1:D:470:ASN:HD22	1.25	0.83
1:G:966:GLU:HB2	1:G:997:LYS:HB2	1.61	0.83
1:G:303:GLN:OE1	1:G:329:PRO:HG3	1.79	0.83
1:A:861:SER:N	1:A:864:GLN:HE21	1.77	0.83
1:C:966:GLU:HB2	1:C:997:LYS:HB2	1.59	0.83
1:D:245:PHE:CE1	1:D:284:TRP:HZ2	1.97	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:ALA:HB3	1:E:247:GLN:NE2	1.93	0.83
1:F:964:LEU:HD12	1:F:996:GLY:HA2	1.61	0.83
2:K:2:GLC:H61	2:K:3:AC1:C1	2.09	0.83
2:P:2:GLC:H61	2:P:3:AC1:C1	2.09	0.83
1:B:440:ASN:HD21	1:B:449:GLN:HE21	1.27	0.83
1:E:271:TRP:HE1	1:E:294:PRO:HB3	1.41	0.83
1:G:1052:ASN:H	1:G:1052:ASN:HD22	0.86	0.83
1:B:1052:ASN:H	1:B:1052:ASN:ND2	1.77	0.83
1:H:304:GLU:OE1	1:H:304:GLU:O	1.95	0.82
1:F:1052:ASN:HD22	1:F:1052:ASN:H	1.26	0.82
1:H:277:ILE:CD1	1:H:291:ASP:CB	2.46	0.82
2:M:2:GLC:H61	2:M:3:AC1:C1	2.09	0.82
2:O:2:GLC:H61	2:O:3:AC1:C1	2.09	0.82
1:A:321:GLN:OE1	1:A:321:GLN:HA	1.76	0.82
1:E:587:HIS:HE2	2:M:3:AC1:HOB3	1.01	0.82
2:J:2:GLC:H61	2:J:3:AC1:C1	2.09	0.82
1:F:669:TYR:CE2	1:F:670:MET:HG3	2.15	0.82
2:N:2:GLC:H61	2:N:3:AC1:C1	2.09	0.82
1:E:262:VAL:HG12	1:E:969:VAL:HG23	1.60	0.82
1:H:740:ASN:C	1:H:740:ASN:HD22	1.82	0.82
1:E:321:GLN:HG3	1:E:322:THR:N	1.94	0.82
1:G:639:ASN:HD21	1:G:813:SER:H	1.27	0.82
1:G:355:TRP:O	1:G:359:THR:CG2	2.23	0.82
1:H:252:TYR:HB3	1:H:258:ASN:ND2	1.94	0.82
1:B:261:HIS:HD2	1:B:264:HIS:H	1.24	0.81
1:F:912:ILE:O	1:F:912:ILE:HG22	1.78	0.81
1:H:246:ALA:O	1:H:247:GLN:O	1.98	0.81
1:B:862:ASN:O	1:B:912:ILE:HG21	1.80	0.81
1:H:1085:VAL:CG2	1:H:1086:ASN:H	1.93	0.81
1:A:740:ASN:ND2	1:A:742:SER:H	1.77	0.81
1:D:1085:VAL:HG23	1:D:1086:ASN:H	1.43	0.81
1:E:261:HIS:HD2	1:E:264:HIS:H	1.26	0.81
1:G:740:ASN:C	1:G:740:ASN:HD22	1.83	0.81
2:L:2:GLC:H61	2:L:3:AC1:C1	2.09	0.81
1:G:251:VAL:HG21	1:G:259:PHE:CZ	2.15	0.81
1:H:278:LEU:CA	1:H:284:TRP:HA	2.09	0.81
1:H:360:ILE:HG22	1:H:361:SER:H	1.44	0.81
1:E:245:PHE:N	1:E:248:TYR:HD2	1.79	0.81
1:B:912:ILE:O	1:B:912:ILE:HG22	1.79	0.81
1:H:251:VAL:HG21	1:H:259:PHE:CZ	2.15	0.81
1:B:740:ASN:ND2	1:B:742:SER:H	1.77	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1080:LEU:HB2	1:H:1085:VAL:HG11	1.59	0.81
1:A:604:ASN:HD22	1:A:607:VAL:HB	1.42	0.81
1:A:782:GLN:HA	1:A:782:GLN:NE2	1.95	0.81
1:E:1052:ASN:HD22	1:E:1052:ASN:H	1.26	0.81
1:H:299:TRP:CA	1:H:300:TRP:CZ3	2.65	0.81
1:C:800:THR:HG22	1:C:802:ALA:N	1.93	0.80
1:B:740:ASN:HD22	1:B:742:SER:H	1.25	0.80
1:C:339:ILE:O	1:C:343:ILE:HG13	1.81	0.80
1:E:287:SER:HB3	1:E:291:ASP:HB2	1.64	0.80
1:C:407:ASN:HD21	1:C:431:GLU:H	1.30	0.80
1:D:920:ASP:OD2	1:D:1002:ASP:HB2	1.82	0.80
1:E:300:TRP:CD1	1:E:306:GLN:CB	2.65	0.80
1:D:355:TRP:CE3	1:D:359:THR:HG21	2.16	0.80
1:D:250:GLN:HB2	1:D:1084:LEU:O	1.82	0.79
1:D:300:TRP:CE3	1:D:306:GLN:HG3	2.17	0.79
1:F:782:GLN:NE2	1:F:782:GLN:CA	2.36	0.79
1:A:309:TYR:C	1:A:309:TYR:CD2	2.54	0.79
1:E:861:SER:N	1:E:864:GLN:HE21	1.80	0.79
1:H:466:ASP:OD2	1:H:943:LYS:CE	2.27	0.79
1:B:1052:ASN:HD22	1:B:1052:ASN:N	1.80	0.79
1:A:271:TRP:CZ2	1:A:357:ARG:CA	2.59	0.79
1:C:407:ASN:ND2	1:C:431:GLU:H	1.80	0.79
1:H:278:LEU:O	1:H:278:LEU:CG	2.31	0.79
1:F:279:LYS:O	1:F:280:ASP:HB3	1.82	0.79
1:C:587:HIS:NE2	2:K:3:AC1:O3B	2.16	0.79
1:D:966:GLU:HB2	1:D:997:LYS:HB2	1.64	0.79
1:E:252:TYR:HB3	1:E:258:ASN:HD21	1.47	0.79
1:H:278:LEU:O	1:H:278:LEU:CD1	2.30	0.79
2:I:2:GLC:C6	2:I:3:AC1:O5	2.30	0.79
1:D:666:ASP:HA	1:D:863:PHE:O	1.83	0.78
1:F:966:GLU:HB3	5:F:205:HOH:O	1.82	0.78
1:D:1052:ASN:H	1:D:1052:ASN:ND2	1.74	0.78
1:H:273:ARG:CZ	1:H:288:THR:O	2.31	0.78
1:C:1052:ASN:HD22	1:C:1052:ASN:N	1.79	0.78
1:D:293:ARG:HB3	1:D:297:MET:HE2	1.64	0.78
1:F:651:LYS:O	1:F:652:SER:HB2	1.80	0.78
1:D:310:VAL:HG13	1:D:339:ILE:CD1	2.13	0.78
1:G:1021:GLU:OE1	1:G:1021:GLU:HA	1.80	0.78
1:A:615:GLU:HA	1:A:615:GLU:OE1	1.81	0.78
1:H:312:TYR:CE2	1:H:363:PHE:HB2	2.18	0.78
1:D:861:SER:N	1:D:864:GLN:HE21	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:740:ASN:ND2	1:H:742:SER:H	1.80	0.78
1:A:251:VAL:HG21	1:A:259:PHE:HZ	1.46	0.77
1:F:639:ASN:HD22	1:F:642:LEU:HD13	1.48	0.77
1:H:309:TYR:CD2	1:H:309:TYR:C	2.56	0.77
1:H:705:SER:HB3	1:H:743:LEU:HD13	1.66	0.77
1:F:460:GLY:N	1:F:470:ASN:ND2	2.31	0.77
1:H:249:ASN:O	1:H:250:GLN:O	2.02	0.77
1:E:277:ILE:HD12	1:E:291:ASP:CB	2.07	0.77
1:A:687:ARG:HA	1:A:691:VAL:HG23	1.64	0.77
1:D:639:ASN:ND2	1:D:813:SER:H	1.81	0.77
1:D:841:ASP:OD1	1:D:846:HIS:HE1	1.67	0.77
1:D:1085:VAL:O	1:D:1087:PRO:HD3	1.84	0.77
1:E:337:GLN:O	1:E:340:GLN:N	2.16	0.77
1:G:300:TRP:CD2	1:G:306:GLN:HG3	2.18	0.77
1:G:368:SER:O	1:G:371:ASN:HB2	1.84	0.77
1:C:407:ASN:ND2	1:C:431:GLU:N	2.33	0.77
1:A:861:SER:H	1:A:864:GLN:NE2	1.83	0.77
1:H:285:THR:O	1:H:286:GLN:O	2.01	0.77
1:H:759:HIS:CD2	1:H:764:TYR:OH	2.37	0.77
1:F:492:ASP:HB3	1:F:1022:LEU:HD22	1.64	0.77
1:G:639:ASN:ND2	1:G:813:SER:H	1.82	0.77
1:A:276:TYR:HB3	1:A:285:THR:O	1.85	0.77
1:E:1064:ASP:HB2	1:E:1071:PHE:CE1	2.20	0.77
1:E:861:SER:H	1:E:864:GLN:NE2	1.81	0.76
1:G:359:THR:O	1:G:362:ALA:HB3	1.84	0.76
1:A:277:ILE:HD11	1:A:291:ASP:HB3	1.67	0.76
1:D:334:LEU:O	1:D:335:ALA:C	2.20	0.76
1:F:460:GLY:H	1:F:470:ASN:HD22	1.31	0.76
1:D:861:SER:H	1:D:864:GLN:NE2	1.82	0.76
1:H:277:ILE:HD11	1:H:291:ASP:HB3	0.82	0.76
1:C:669:TYR:HE2	1:C:670:MET:HE3	1.51	0.75
1:D:252:TYR:HB3	1:D:258:ASN:HD21	1.49	0.75
1:B:687:ARG:HA	1:B:691:VAL:HG21	1.67	0.75
1:B:939:VAL:HG13	1:B:943:LYS:HZ1	1.50	0.75
1:F:293:ARG:HG2	1:F:293:ARG:HH11	1.52	0.75
1:G:1085:VAL:HG23	1:G:1086:ASN:N	2.00	0.75
1:H:277:ILE:CD1	1:H:291:ASP:CG	2.55	0.75
1:A:252:TYR:HA	1:A:275:LYS:HG2	1.69	0.75
1:H:269:GLU:OE2	1:H:361:SER:HB3	1.85	0.75
1:A:287:SER:HA	1:A:291:ASP:OD2	1.86	0.75
1:H:376:LYS:HB3	1:H:377:PRO:HA	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:TRP:CG	1:E:294:PRO:HA	2.21	0.75
1:F:311:ASN:HD21	1:F:323:TYR:N	1.84	0.75
1:B:417:LYS:HE3	1:F:555:SER:HB3	1.67	0.74
1:B:809:ASN:HB2	1:B:810:PRO:HD2	1.68	0.74
1:D:800:THR:CG2	1:D:801:ALA:N	2.50	0.74
1:A:966:GLU:HB2	1:A:997:LYS:CB	2.16	0.74
1:A:1085:VAL:HG23	1:A:1086:ASN:N	2.00	0.74
1:F:965:PRO:HD2	1:F:997:LYS:O	1.86	0.74
1:E:716:GLY:HA2	5:E:33:HOH:O	1.87	0.74
1:C:1085:VAL:HG23	1:C:1086:ASN:N	2.02	0.74
1:E:329:PRO:HA	1:E:332:LEU:HD12	1.69	0.74
1:E:740:ASN:ND2	1:E:742:SER:H	1.85	0.74
1:F:587:HIS:NE2	2:N:3:AC1:O3B	2.19	0.74
1:C:350:GLU:O	1:C:352:ASN:N	2.21	0.73
1:E:321:GLN:CG	1:E:322:THR:N	2.51	0.73
1:F:966:GLU:HB2	1:F:997:LYS:HB2	1.69	0.73
1:B:252:TYR:HB3	1:B:258:ASN:HD21	1.51	0.73
1:B:966:GLU:HB2	1:B:997:LYS:HB2	1.69	0.73
1:H:311:ASN:O	1:H:314:ASN:CB	2.36	0.73
1:C:355:TRP:O	1:C:359:THR:HG22	1.88	0.73
1:B:861:SER:N	1:B:864:GLN:HE21	1.81	0.73
1:C:965:PRO:HD2	1:C:997:LYS:O	1.87	0.73
1:E:252:TYR:HD1	1:E:275:LYS:HG2	1.52	0.73
1:H:1085:VAL:CG2	1:H:1086:ASN:N	2.51	0.73
1:H:304:GLU:OE1	1:H:304:GLU:CA	2.36	0.73
1:D:334:LEU:O	1:D:336:ALA:N	2.21	0.73
1:F:251:VAL:HG21	1:F:259:PHE:CZ	2.24	0.73
1:H:587:HIS:NE2	2:P:3:AC1:O3B	2.21	0.73
1:F:352:ASN:HD22	1:F:352:ASN:H	1.36	0.73
1:E:299:TRP:CH2	1:E:301:PRO:HB3	2.24	0.73
1:F:740:ASN:HD22	1:F:741:PRO:N	1.87	0.73
1:F:740:ASN:HD22	1:F:741:PRO:CD	2.02	0.73
1:B:800:THR:CG2	1:B:801:ALA:N	2.51	0.73
1:G:310:VAL:HG11	1:G:335:ALA:CB	2.19	0.72
1:C:460:GLY:N	1:C:470:ASN:ND2	2.36	0.72
1:D:312:TYR:C	1:D:312:TYR:CD2	2.63	0.72
1:G:658:TYR:CE2	1:G:660:GLY:HA3	2.23	0.72
1:H:1052:ASN:HD22	1:H:1052:ASN:N	1.81	0.72
1:E:271:TRP:CE2	1:E:294:PRO:CB	2.71	0.72
1:G:335:ALA:O	1:G:339:ILE:HG13	1.88	0.72
1:H:639:ASN:ND2	1:H:813:SER:H	1.85	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HD12	1:A:330:LEU:O	1.90	0.72
1:D:347:ILE:HG12	1:D:353:THR:HG22	1.71	0.72
1:F:261:HIS:CD2	1:F:264:HIS:HA	2.24	0.72
1:G:346:LYS:HE3	1:G:355:TRP:CD2	2.24	0.72
1:E:752:VAL:HG22	1:E:798:ILE:HD13	1.72	0.72
1:F:861:SER:N	1:F:864:GLN:HE21	1.83	0.72
1:F:737:GLU:HA	1:F:815:TYR:O	1.90	0.72
1:E:330:LEU:O	1:E:333:ASN:HB2	1.89	0.71
1:F:669:TYR:CE1	1:F:874:THR:HG23	2.24	0.71
1:G:882:VAL:HG13	1:G:948:LYS:HG3	1.72	0.71
1:H:299:TRP:N	1:H:300:TRP:CZ3	2.58	0.71
1:E:280:ASP:O	1:E:282:LYS:CG	2.30	0.71
1:E:291:ASP:N	1:E:291:ASP:OD1	2.23	0.71
1:E:316:GLN:HG2	1:E:359:THR:CG2	2.20	0.71
1:H:278:LEU:O	1:H:278:LEU:HG	1.90	0.71
1:D:504:ASP:OD1	1:D:846:HIS:HD2	1.74	0.71
1:D:740:ASN:HD22	1:D:740:ASN:C	1.93	0.71
1:G:330:LEU:HD12	1:G:330:LEU:O	1.90	0.71
1:B:713:TYR:O	1:B:759:HIS:CE1	2.43	0.71
1:D:278:LEU:HB2	1:D:284:TRP:CH2	2.26	0.71
1:D:1085:VAL:HG23	1:D:1086:ASN:N	2.04	0.71
1:E:299:TRP:HH2	1:E:301:PRO:HB3	1.55	0.71
1:E:311:ASN:N	1:E:311:ASN:HD22	1.87	0.71
1:E:800:THR:HG22	1:E:802:ALA:N	2.02	0.71
1:C:614:MET:O	1:C:618:LYS:HG3	1.90	0.71
1:E:316:GLN:HG2	1:E:359:THR:HG21	1.72	0.71
1:A:352:ASN:O	1:A:353:THR:HG22	1.89	0.71
1:D:276:TYR:HD1	1:D:285:THR:C	1.94	0.71
1:D:278:LEU:HG	1:D:278:LEU:O	1.90	0.71
1:E:276:TYR:HB3	1:E:284:TRP:CE3	2.26	0.71
1:E:347:ILE:CG1	1:E:353:THR:HB	2.21	0.71
1:H:740:ASN:HD22	1:H:742:SER:H	1.38	0.71
1:D:513:ILE:HG12	1:D:953:MET:HE2	1.73	0.71
1:G:604:ASN:HD21	1:G:607:VAL:CA	2.04	0.71
1:D:809:ASN:HB2	1:D:810:PRO:CD	2.21	0.70
1:E:299:TRP:CZ2	1:E:301:PRO:HA	2.26	0.70
1:A:300:TRP:HB2	1:A:306:GLN:HB2	1.72	0.70
1:D:253:SER:H	1:D:258:ASN:ND2	1.89	0.70
1:D:303:GLN:HE22	1:D:329:PRO:HG3	1.56	0.70
1:E:440:ASN:HD21	1:E:449:GLN:NE2	1.84	0.70
1:G:259:PHE:N	1:G:259:PHE:CD2	2.59	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:VAL:CG1	1:B:943:LYS:HZ1	2.00	0.70
1:B:1063:LYS:HE2	1:B:1068:ASN:ND2	2.06	0.70
1:E:245:PHE:N	1:E:248:TYR:CE2	2.60	0.70
1:B:577:ALA:O	1:B:578:VAL:HG23	1.91	0.70
1:A:346:LYS:O	1:A:350:GLU:CG	2.37	0.70
1:C:669:TYR:CE2	1:C:670:MET:HE3	2.25	0.70
1:G:1021:GLU:OE1	1:G:1021:GLU:CA	2.38	0.70
1:H:299:TRP:HA	1:H:300:TRP:CE3	2.27	0.70
1:C:587:HIS:HE2	2:K:3:AC1:HOB3	1.40	0.70
1:C:306:GLN:O	1:C:310:VAL:HG23	1.91	0.70
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.05	0.70
1:F:612:PHE:CD2	1:F:612:PHE:N	2.57	0.70
1:H:504:ASP:OD1	1:H:846:HIS:HD2	1.74	0.70
1:F:250:GLN:OE1	1:F:1087:PRO:HG3	1.92	0.69
1:F:1085:VAL:CG2	1:F:1086:ASN:H	2.05	0.69
1:H:298:THR:C	1:H:300:TRP:CZ3	2.66	0.69
1:H:440:ASN:ND2	1:H:449:GLN:HE21	1.85	0.69
2:I:2:GLC:H61	2:I:3:AC1:C1	2.22	0.69
1:E:273:ARG:CG	1:E:287:SER:CB	2.71	0.69
1:D:251:VAL:HG21	1:D:259:PHE:HZ	1.56	0.69
1:E:883:ASP:OD1	1:E:948:LYS:HE3	1.93	0.69
1:G:271:TRP:CZ2	1:G:357:ARG:HD3	2.27	0.69
1:B:964:LEU:HD12	1:B:996:GLY:HA2	1.74	0.69
1:E:300:TRP:CD1	1:E:306:GLN:HA	2.27	0.69
1:F:440:ASN:HD21	1:F:449:GLN:NE2	1.87	0.69
1:F:800:THR:CG2	1:F:802:ALA:H	2.01	0.69
1:D:299:TRP:CH2	1:D:301:PRO:HA	2.28	0.69
1:E:323:TYR:HB3	1:E:327:THR:OG1	1.93	0.69
1:H:299:TRP:HA	1:H:300:TRP:CZ3	2.26	0.69
1:B:670:MET:HE1	1:B:885:PHE:CZ	2.27	0.69
1:C:1052:ASN:H	1:C:1052:ASN:ND2	1.80	0.69
1:C:516:ALA:HB1	1:C:521:ASP:OD2	1.92	0.69
1:D:460:GLY:N	1:D:470:ASN:HD22	1.89	0.69
1:F:639:ASN:ND2	1:F:642:LEU:HD13	2.07	0.69
1:F:669:TYR:CD1	1:F:874:THR:HG23	2.27	0.69
1:H:293:ARG:HB3	1:H:294:PRO:HD2	1.73	0.69
1:A:663:PHE:CZ	1:A:670:MET:HG2	2.28	0.69
1:C:262:VAL:HG12	1:C:969:VAL:HG23	1.74	0.69
1:E:330:LEU:O	1:E:333:ASN:N	2.24	0.69
1:F:1061:VAL:HG12	1:F:1070:TYR:CD1	2.28	0.69
1:G:800:THR:CG2	1:G:802:ALA:H	1.98	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:261:HIS:HD2	1:H:264:HIS:HA	1.56	0.69
1:A:300:TRP:CG	1:A:306:GLN:HG3	2.28	0.69
1:B:670:MET:HE1	1:B:885:PHE:CE1	2.28	0.69
1:F:250:GLN:HE21	1:F:275:LYS:HE2	1.56	0.69
1:H:360:ILE:CG2	1:H:361:SER:N	2.55	0.69
1:A:705:SER:HB3	1:A:743:LEU:HD13	1.75	0.69
1:B:540:ARG:HB2	5:B:106:HOH:O	1.92	0.69
1:D:245:PHE:CD1	1:D:284:TRP:HZ2	2.10	0.69
1:D:356:LEU:HA	1:D:359:THR:CG2	2.23	0.69
1:G:261:HIS:CD2	1:G:264:HIS:HA	2.28	0.68
1:H:733:VAL:HG22	1:H:734:VAL:N	2.07	0.68
2:P:2:GLC:C6	2:P:3:AC1:O5	2.30	0.68
1:A:273:ARG:HH12	1:A:289:GLU:HG2	1.58	0.68
1:G:440:ASN:ND2	1:G:449:GLN:HE21	1.88	0.68
1:H:304:GLU:OE1	1:H:304:GLU:HA	1.92	0.68
1:C:346:LYS:HB3	1:C:355:TRP:CZ2	2.28	0.68
1:C:440:ASN:HD21	1:C:449:GLN:NE2	1.86	0.68
1:H:304:GLU:OE1	1:H:304:GLU:C	2.32	0.68
1:A:613:THR:OG1	1:A:615:GLU:HB2	1.93	0.68
1:C:1085:VAL:HG23	1:C:1086:ASN:H	1.57	0.68
1:D:245:PHE:C	1:D:247:GLN:N	2.44	0.68
1:E:740:ASN:HD22	1:E:741:PRO:N	1.92	0.68
1:H:261:HIS:CD2	1:H:264:HIS:HA	2.28	0.68
1:C:537:ASN:OD1	1:C:540:ARG:NH1	2.26	0.68
1:C:670:MET:HE1	1:C:885:PHE:HZ	1.58	0.68
1:C:713:TYR:O	1:C:759:HIS:HE1	1.75	0.68
1:A:299:TRP:CH2	1:A:301:PRO:HA	2.28	0.68
1:B:368:SER:HA	1:B:371:ASN:HD22	1.58	0.68
1:E:513:ILE:HG12	1:E:953:MET:CE	2.23	0.68
1:G:492:ASP:HB3	1:G:1022:LEU:CD2	2.23	0.68
1:G:602:GLU:O	1:G:603:ILE:HG13	1.94	0.68
1:H:310:VAL:HG12	1:H:311:ASN:HD22	1.57	0.68
1:A:596:ARG:HB2	1:A:612:PHE:HZ	1.59	0.68
1:A:687:ARG:HA	1:A:691:VAL:CG2	2.23	0.68
1:F:312:TYR:C	1:F:312:TYR:CD2	2.66	0.68
1:A:301:PRO:HG2	1:A:302:ASP:N	2.07	0.68
1:A:457:MET:HE2	1:A:493:TYR:HE2	1.59	0.68
1:E:416:LYS:HD3	5:E:100:HOH:O	1.93	0.68
1:C:514:LEU:HD21	1:C:532:MET:HG3	1.76	0.68
1:C:1063:LYS:CE	1:C:1068:ASN:ND2	2.55	0.68
1:D:713:TYR:O	1:D:759:HIS:HE1	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:917:ALA:HA	1:F:962:TYR:CD1	2.29	0.68
1:H:1080:LEU:HB2	1:H:1085:VAL:CG1	2.24	0.68
1:B:526:HIS:HA	1:B:530:ASP:OD1	1.93	0.68
1:E:1052:ASN:H	1:E:1052:ASN:ND2	1.92	0.68
1:A:740:ASN:HD22	1:A:741:PRO:N	1.91	0.67
1:A:1052:ASN:H	1:A:1052:ASN:ND2	1.90	0.67
1:C:300:TRP:CD2	1:C:306:GLN:HG3	2.29	0.67
1:D:305:THR:HG23	1:D:367:GLN:HE21	1.59	0.67
1:C:740:ASN:HD22	1:C:742:SER:H	1.40	0.67
1:E:440:ASN:ND2	1:E:449:GLN:HE21	1.88	0.67
1:D:356:LEU:HD11	1:D:360:ILE:HD11	1.74	0.67
1:D:993:VAL:O	1:D:1056:ARG:NH1	2.27	0.67
1:F:250:GLN:NE2	1:F:275:LYS:CE	2.47	0.67
1:F:740:ASN:ND2	1:F:741:PRO:HD2	2.08	0.67
1:F:1022:LEU:HD23	1:F:1022:LEU:N	2.10	0.67
1:H:800:THR:HG22	1:H:801:ALA:N	2.09	0.67
2:O:2:GLC:C6	2:O:3:AC1:O5	2.30	0.67
1:B:1085:VAL:HG23	1:B:1086:ASN:N	2.08	0.67
1:H:585:ARG:HD3	1:H:661:ASP:OD1	1.94	0.67
1:B:988:LYS:O	1:B:989:ASN:HB2	1.94	0.67
1:H:931:LYS:HA	5:H:17:HOH:O	1.93	0.67
1:B:713:TYR:O	1:B:759:HIS:HE1	1.77	0.67
1:B:742:SER:O	1:B:744:ARG:HG3	1.94	0.67
1:C:248:TYR:HB3	1:C:276:TYR:HB2	1.76	0.67
1:B:939:VAL:HG12	1:B:943:LYS:HZ3	1.45	0.67
1:C:515:GLU:OE1	2:K:3:AC1:O3	2.12	0.67
1:D:261:HIS:HD2	1:D:264:HIS:H	1.43	0.67
1:A:271:TRP:CE2	1:A:294:PRO:HG3	2.30	0.67
1:F:248:TYR:HB2	1:F:284:TRP:CZ3	2.29	0.67
1:G:1085:VAL:CG2	1:G:1086:ASN:N	2.57	0.67
1:D:312:TYR:C	1:D:312:TYR:HD2	1.98	0.66
1:E:322:THR:CG2	1:E:323:TYR:N	2.57	0.66
1:H:800:THR:CG2	1:H:801:ALA:N	2.57	0.66
1:F:350:GLU:HB3	1:F:352:ASN:HD21	1.60	0.66
1:F:669:TYR:HE2	1:F:670:MET:CE	2.06	0.66
1:D:513:ILE:HG12	1:D:953:MET:CE	2.25	0.66
1:H:299:TRP:C	1:H:300:TRP:CD2	2.69	0.66
1:A:261:HIS:HD2	1:A:264:HIS:N	1.92	0.66
1:C:251:VAL:O	1:C:275:LYS:HE3	1.95	0.66
1:D:245:PHE:CE1	1:D:284:TRP:CZ2	2.84	0.66
1:F:658:TYR:CE2	1:F:660:GLY:HA3	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:LEU:O	1:B:744:ARG:CG	2.35	0.66
1:H:809:ASN:HB2	1:H:810:PRO:HD2	1.76	0.66
1:B:809:ASN:HB2	1:B:810:PRO:CD	2.25	0.66
1:F:368:SER:O	1:F:371:ASN:HB2	1.96	0.66
1:G:278:LEU:HG	1:G:281:GLY:HA2	1.78	0.66
1:G:376:LYS:HB3	1:G:377:PRO:HA	1.78	0.66
1:H:250:GLN:HB2	1:H:1084:LEU:O	1.96	0.66
1:A:279:LYS:N	1:A:283:THR:O	2.29	0.66
1:B:376:LYS:HB3	1:B:377:PRO:HA	1.77	0.66
1:G:310:VAL:CG1	1:G:335:ALA:HB1	2.24	0.66
1:A:250:GLN:HE21	1:A:275:LYS:HE3	1.60	0.66
1:G:740:ASN:HD22	1:G:741:PRO:N	1.93	0.66
1:A:342:LYS:O	1:A:346:LYS:HB2	1.95	0.66
1:B:759:HIS:CD2	1:B:764:TYR:OH	2.48	0.66
1:C:365:LYS:HE3	1:C:1055:GLY:O	1.96	0.66
1:C:800:THR:CG2	1:C:801:ALA:N	2.59	0.66
1:E:669:TYR:HE2	1:E:670:MET:HE3	1.61	0.66
1:E:809:ASN:HB2	1:E:810:PRO:CD	2.25	0.65
1:C:245:PHE:CE2	1:C:337:GLN:HB3	2.31	0.65
1:E:740:ASN:HD22	1:E:742:SER:H	1.44	0.65
1:F:740:ASN:HD22	1:F:741:PRO:HD2	1.61	0.65
1:F:329:PRO:O	1:F:333:ASN:ND2	2.29	0.65
1:A:317:LEU:HD13	1:A:342:LYS:HB3	1.76	0.65
1:B:261:HIS:HD2	1:B:264:HIS:N	1.95	0.65
1:D:440:ASN:HD21	1:D:449:GLN:NE2	1.91	0.65
1:G:297:MET:SD	1:G:340:GLN:HG3	2.37	0.65
1:A:309:TYR:HD2	1:A:310:VAL:N	1.94	0.65
1:B:639:ASN:ND2	1:B:813:SER:H	1.93	0.65
1:E:670:MET:HE1	1:E:885:PHE:HZ	1.61	0.65
1:F:1085:VAL:O	1:F:1087:PRO:HD3	1.96	0.65
1:E:800:THR:CG2	1:E:801:ALA:N	2.59	0.65
1:E:988:LYS:O	1:E:990:THR:HG23	1.97	0.65
1:F:860:PHE:HB2	1:F:864:GLN:HE22	1.61	0.65
1:H:276:TYR:HB3	1:H:284:TRP:HB3	1.78	0.65
1:A:327:THR:HG22	1:A:328:SER:O	1.97	0.65
1:B:466:ASP:OD2	1:B:943:LYS:CE	2.45	0.65
1:C:280:ASP:HB2	1:C:348:THR:OG1	1.97	0.65
1:D:277:ILE:O	1:D:277:ILE:CG2	2.37	0.65
1:H:294:PRO:HG2	1:H:297:MET:HB2	1.78	0.65
1:C:261:HIS:CD2	1:C:264:HIS:HA	2.31	0.65
1:C:705:SER:HB3	1:C:743:LEU:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:PHE:C	1:D:247:GLN:H	1.99	0.65
1:D:551:LEU:HD21	1:D:741:PRO:HG2	1.79	0.65
1:D:782:GLN:HA	1:D:782:GLN:NE2	2.11	0.65
1:E:271:TRP:CD2	1:E:357:ARG:NH1	2.64	0.65
1:E:297:MET:HG2	1:E:297:MET:O	1.96	0.65
1:F:750:ARG:HB2	5:F:55:HOH:O	1.96	0.65
1:G:809:ASN:HB2	1:G:810:PRO:CD	2.27	0.65
1:H:312:TYR:O	1:H:314:ASN:N	2.30	0.65
1:C:514:LEU:CD2	1:C:532:MET:HG3	2.27	0.65
1:G:917:ALA:HA	1:G:962:TYR:CD1	2.32	0.65
1:H:260:GLU:CD	1:H:271:TRP:HB2	2.17	0.65
1:E:504:ASP:OD1	1:E:846:HIS:HD2	1.80	0.65
1:F:516:ALA:HB1	1:F:521:ASP:OD2	1.97	0.65
1:G:252:TYR:HB3	1:G:258:ASN:ND2	2.06	0.65
1:B:551:LEU:HD12	1:B:551:LEU:O	1.97	0.64
1:C:311:ASN:HD21	1:C:323:TYR:H	1.43	0.64
2:M:2:GLC:C6	2:M:3:AC1:O5	2.30	0.64
1:E:303:GLN:O	1:E:304:GLU:C	2.36	0.64
1:E:740:ASN:C	1:E:740:ASN:ND2	2.50	0.64
1:F:537:ASN:OD1	1:F:540:ARG:NH1	2.29	0.64
1:C:245:PHE:N	1:C:245:PHE:CD1	2.63	0.64
1:E:279:LYS:NZ	1:E:279:LYS:HG3	2.11	0.64
1:G:740:ASN:HD22	1:G:742:SER:H	1.41	0.64
1:H:288:THR:HB	1:H:291:ASP:OD1	1.96	0.64
1:H:398:GLN:HG2	1:H:398:GLN:O	1.98	0.64
1:B:513:ILE:HG12	1:B:953:MET:CE	2.26	0.64
1:F:492:ASP:HB3	1:F:1022:LEU:CD2	2.27	0.64
1:E:299:TRP:CH2	1:E:301:PRO:CA	2.80	0.64
1:E:669:TYR:CE2	1:E:670:MET:HE3	2.31	0.64
1:B:587:HIS:NE2	2:J:3:AC1:O3B	2.29	0.64
1:B:939:VAL:O	1:B:943:LYS:HG3	1.97	0.64
1:E:273:ARG:HH11	1:E:288:THR:C	2.01	0.64
1:F:300:TRP:HB3	1:F:301:PRO:HD2	1.80	0.64
1:F:1052:ASN:HD22	1:F:1052:ASN:N	1.96	0.64
1:B:391:ASN:C	1:B:392:ASN:HD22	2.01	0.64
1:B:752:VAL:HG22	1:B:798:ILE:HG12	1.79	0.64
1:H:854:ARG:NH1	1:H:892:ASP:OD2	2.30	0.64
1:B:250:GLN:HA	1:B:1084:LEU:O	1.98	0.64
1:E:294:PRO:HG3	1:E:356:LEU:HD21	1.78	0.64
1:G:504:ASP:OD1	1:G:846:HIS:HD2	1.80	0.64
2:L:2:GLC:C6	2:L:3:AC1:O5	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ILE:HG12	1:B:953:MET:HE2	1.78	0.64
1:D:355:TRP:CG	1:D:356:LEU:N	2.66	0.64
1:G:371:ASN:HB3	1:G:373:ASP:H	1.63	0.64
1:A:740:ASN:C	1:A:740:ASN:ND2	2.47	0.64
1:C:407:ASN:ND2	1:C:431:GLU:HB2	2.13	0.64
1:D:334:LEU:C	1:D:336:ALA:N	2.46	0.64
1:D:1052:ASN:N	1:D:1052:ASN:ND2	2.35	0.64
1:F:357:ARG:HH11	1:F:357:ARG:HG3	1.57	0.64
1:F:513:ILE:HG12	1:F:953:MET:HE2	1.79	0.64
1:F:749:ASP:O	1:F:750:ARG:HG2	1.98	0.64
1:C:359:THR:HG23	1:C:360:ILE:H	1.63	0.63
1:G:350:GLU:O	1:G:352:ASN:ND2	2.22	0.63
1:A:928:LYS:HB2	1:A:929:PRO:HD2	1.79	0.63
1:B:406:LEU:HD22	1:B:431:GLU:HG2	1.80	0.63
1:C:364:VAL:HG13	1:C:370:TRP:CE3	2.33	0.63
1:C:687:ARG:HA	1:C:691:VAL:HG23	1.80	0.63
1:D:537:ASN:OD1	1:D:540:ARG:NH1	2.31	0.63
1:H:308:GLN:C	1:H:310:VAL:N	2.50	0.63
1:H:316:GLN:HG2	1:H:359:THR:CG2	2.22	0.63
1:A:290:LYS:NZ	1:A:290:LYS:CD	2.61	0.63
1:E:279:LYS:NZ	1:E:279:LYS:CD	2.60	0.63
1:B:733:VAL:HG22	1:B:734:VAL:N	2.13	0.63
1:E:306:GLN:O	1:E:309:TYR:N	2.31	0.63
1:E:346:LYS:HA	1:E:349:ALA:HB3	1.79	0.63
1:F:513:ILE:HG12	1:F:953:MET:CE	2.29	0.63
1:F:687:ARG:HA	1:F:691:VAL:HG21	1.79	0.63
1:G:912:ILE:O	1:G:912:ILE:CG2	2.45	0.63
1:G:1065:GLN:HG3	1:G:1066:ALA:N	2.13	0.63
1:H:299:TRP:CZ2	1:H:301:PRO:HA	2.34	0.63
1:B:743:LEU:C	1:B:744:ARG:CG	2.52	0.63
1:D:1080:LEU:HB3	1:D:1081:PRO:CD	2.28	0.63
1:A:356:LEU:O	1:A:357:ARG:C	2.37	0.63
1:A:516:ALA:HB1	1:A:521:ASP:OD2	1.99	0.63
1:B:764:TYR:CE1	1:B:821:PRO:HD3	2.33	0.63
2:J:2:GLC:C6	2:J:3:AC1:O5	2.30	0.63
1:A:250:GLN:CB	1:A:1084:LEU:O	2.45	0.63
1:B:571:ASP:OD2	1:B:651:LYS:HG2	1.99	0.62
1:D:1080:LEU:HB3	1:D:1081:PRO:HD2	1.80	0.62
1:E:713:TYR:O	1:E:759:HIS:HE1	1.82	0.62
1:F:917:ALA:HA	1:F:962:TYR:CE1	2.34	0.62
1:A:252:TYR:HB3	1:A:258:ASN:ND2	2.12	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:GLU:C	1:C:352:ASN:H	2.02	0.62
1:H:713:TYR:O	1:H:759:HIS:HE1	1.81	0.62
1:E:471:PHE:CG	1:E:954:ALA:HB2	2.35	0.62
1:A:281:GLY:H	1:A:344:GLU:HB2	1.65	0.62
1:D:305:THR:O	1:D:308:GLN:HB2	2.00	0.62
1:G:669:TYR:CE1	1:G:874:THR:HG23	2.34	0.62
1:H:300:TRP:HD1	1:H:306:GLN:HA	1.63	0.62
2:K:2:GLC:C6	2:K:3:AC1:O5	2.30	0.62
1:A:294:PRO:O	1:A:297:MET:HB3	2.00	0.62
1:A:854:ARG:NH1	1:A:892:ASP:OD2	2.32	0.62
1:B:761:ASN:ND2	1:B:761:ASN:N	2.47	0.62
1:D:280:ASP:O	1:D:282:LYS:N	2.32	0.62
1:E:271:TRP:CD1	1:E:294:PRO:HB3	2.30	0.62
1:F:606:ASN:O	1:F:607:VAL:C	2.38	0.62
1:F:724:GLY:HA3	1:F:728:THR:OG1	2.00	0.62
1:G:513:ILE:HG12	1:G:953:MET:HE2	1.81	0.62
1:H:284:TRP:O	1:H:285:THR:OG1	2.16	0.62
1:A:321:GLN:OE1	1:A:321:GLN:CA	2.48	0.62
1:E:279:LYS:NZ	1:E:279:LYS:CG	2.62	0.62
1:F:800:THR:CG2	1:F:801:ALA:N	2.63	0.62
1:A:261:HIS:CD2	1:A:264:HIS:HA	2.35	0.62
1:A:278:LEU:O	1:A:344:GLU:HG3	1.99	0.62
1:C:352:ASN:OD1	1:C:354:ASN:ND2	2.33	0.62
1:C:966:GLU:HB2	1:C:997:LYS:CB	2.27	0.62
1:B:259:PHE:N	1:B:259:PHE:CD2	2.68	0.62
1:B:861:SER:H	1:B:864:GLN:NE2	1.86	0.62
1:E:585:ARG:HD3	1:E:661:ASP:OD1	2.00	0.62
2:N:2:GLC:C6	2:N:3:AC1:O5	2.30	0.62
1:A:278:LEU:HD11	1:A:282:LYS:N	2.15	0.62
1:A:587:HIS:NE2	2:I:3:AC1:O3B	2.28	0.62
1:B:404:ARG:N	1:B:439:ASP:OD2	2.33	0.62
1:F:440:ASN:ND2	1:F:449:GLN:HE21	1.89	0.62
1:F:793:ASP:HB3	1:F:794:ARG:HG3	1.82	0.62
1:A:430:TYR:HB3	1:A:978:TYR:CE1	2.34	0.61
1:A:860:PHE:CG	1:A:896:ALA:HB2	2.34	0.61
1:F:250:GLN:OE1	1:F:1087:PRO:HG2	2.00	0.61
1:A:841:ASP:OD1	1:A:846:HIS:HE1	1.82	0.61
1:B:670:MET:CE	1:B:885:PHE:HZ	2.12	0.61
1:C:440:ASN:ND2	1:C:449:GLN:HE21	1.93	0.61
1:F:723:THR:HG22	1:F:757:ALA:HB1	1.81	0.61
1:G:348:THR:HG22	1:G:349:ALA:N	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ARG:HB3	1:A:297:MET:CE	2.30	0.61
1:D:551:LEU:CD2	1:D:741:PRO:HG2	2.30	0.61
1:E:454:HIS:CE1	1:E:458:ASN:ND2	2.67	0.61
1:E:587:HIS:CD2	2:M:3:AC1:HOB3	2.18	0.61
1:H:882:VAL:HG13	1:H:948:LYS:HG3	1.81	0.61
1:A:280:ASP:OD1	1:A:348:THR:HB	2.01	0.61
1:B:1052:ASN:ND2	1:B:1052:ASN:N	2.42	0.61
1:D:293:ARG:HB3	1:D:297:MET:HE1	1.80	0.61
1:A:307:ARG:HH11	1:A:307:ARG:CG	2.13	0.61
1:D:336:ALA:HA	1:D:339:ILE:HD12	1.83	0.61
1:G:604:ASN:ND2	1:G:607:VAL:CB	2.62	0.61
1:C:359:THR:HG23	1:C:360:ILE:N	2.15	0.61
1:C:874:THR:HG22	1:C:878:ILE:HD12	1.81	0.61
1:E:272:TYR:CD2	1:E:295:LEU:HD23	2.35	0.61
1:H:800:THR:HG22	1:H:802:ALA:N	2.12	0.61
1:A:478:ALA:HB2	2:I:3:AC1:O3	2.01	0.61
1:D:471:PHE:CG	1:D:954:ALA:HB2	2.35	0.61
1:E:460:GLY:H	1:E:470:ASN:HD22	1.48	0.61
1:G:794:ARG:HG2	1:G:794:ARG:HH11	1.60	0.61
1:H:596:ARG:NH2	1:H:600:LYS:HD2	2.15	0.61
1:C:740:ASN:HD22	1:C:741:PRO:N	1.97	0.61
1:D:245:PHE:CD1	1:D:284:TRP:CZ2	2.88	0.61
1:D:252:TYR:HB3	1:D:258:ASN:ND2	2.16	0.61
1:E:359:THR:O	1:E:362:ALA:HB3	2.00	0.61
1:H:1072:SER:OG	1:H:1074:VAL:CG1	2.48	0.61
1:D:277:ILE:HD13	1:D:293:ARG:NH2	2.15	0.61
1:G:515:GLU:OE1	2:O:3:AC1:O3	2.17	0.61
1:H:277:ILE:HD11	1:H:291:ASP:CG	2.17	0.61
1:D:278:LEU:HB2	1:D:284:TRP:CZ3	2.36	0.61
1:D:999:SER:O	1:D:1001:LYS:HG3	2.01	0.60
1:F:365:LYS:HE3	1:F:1055:GLY:O	2.01	0.60
1:A:740:ASN:HD22	1:A:742:SER:H	1.47	0.60
1:B:471:PHE:CG	1:B:954:ALA:HB2	2.35	0.60
1:D:639:ASN:HD21	1:D:813:SER:N	1.95	0.60
1:E:250:GLN:OE1	1:E:1087:PRO:CG	2.49	0.60
1:G:965:PRO:HD2	1:G:997:LYS:O	2.01	0.60
1:H:261:HIS:HD2	1:H:264:HIS:CA	2.14	0.60
1:D:908:LEU:O	1:D:912:ILE:HG13	2.00	0.60
1:H:310:VAL:O	1:H:311:ASN:C	2.39	0.60
1:H:356:LEU:HG	1:H:356:LEU:O	2.01	0.60
1:H:1072:SER:OG	1:H:1074:VAL:HG12	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:OG1	1:A:290:LYS:HD2	2.02	0.60
1:A:782:GLN:NE2	1:A:782:GLN:CA	2.58	0.60
1:D:740:ASN:HD22	1:D:742:SER:N	1.90	0.60
1:G:861:SER:HB3	1:G:864:GLN:HG3	1.82	0.60
1:B:577:ALA:O	1:B:578:VAL:CG2	2.49	0.60
1:B:670:MET:CE	1:B:885:PHE:CZ	2.84	0.60
1:C:630:ALA:O	1:C:633:LYS:NZ	2.35	0.60
1:C:860:PHE:CG	1:C:896:ALA:HB2	2.36	0.60
1:D:297:MET:SD	1:D:340:GLN:CG	2.86	0.60
1:A:316:GLN:HE21	1:A:359:THR:CG2	2.12	0.60
1:A:800:THR:HG22	1:A:802:ALA:N	2.05	0.60
1:H:307:ARG:O	1:H:310:VAL:HB	2.00	0.60
1:D:987:ILE:CG1	1:D:1058:ALA:HB2	2.32	0.60
1:G:261:HIS:HD2	1:G:264:HIS:N	1.96	0.60
1:H:993:VAL:O	1:H:1056:ARG:NH1	2.34	0.60
1:A:1052:ASN:HD22	1:A:1052:ASN:N	1.94	0.60
1:B:788:VAL:CG1	1:B:789:ARG:N	2.64	0.60
1:G:248:TYR:HB3	1:G:276:TYR:HB2	1.83	0.60
1:G:310:VAL:HG13	1:G:339:ILE:HD11	1.82	0.60
1:B:788:VAL:HG12	1:B:789:ARG:N	2.16	0.60
1:E:245:PHE:N	1:E:245:PHE:CB	2.62	0.60
1:A:460:GLY:N	1:A:470:ASN:HD22	1.99	0.60
1:E:300:TRP:CD1	1:E:306:GLN:CA	2.84	0.60
1:A:1085:VAL:CG2	1:A:1086:ASN:N	2.64	0.59
1:D:809:ASN:HB2	1:D:810:PRO:HD2	1.84	0.59
1:E:1085:VAL:HG23	1:E:1086:ASN:N	2.17	0.59
1:B:1040:ILE:HG12	1:B:1047:TYR:CE2	2.36	0.59
1:D:800:THR:HG22	1:D:801:ALA:N	2.16	0.59
1:E:306:GLN:O	1:E:309:TYR:CB	2.47	0.59
1:H:856:MET:HG3	1:H:892:ASP:HB2	1.84	0.59
1:A:276:TYR:CB	1:A:285:THR:O	2.50	0.59
1:A:576:ALA:HB3	1:A:847:GLN:HB3	1.83	0.59
1:B:585:ARG:HD3	1:B:661:ASP:OD1	2.02	0.59
1:D:302:ASP:OD1	1:D:304:GLU:HB3	2.01	0.59
1:D:957:VAL:O	1:D:957:VAL:HG12	2.01	0.59
1:A:274:PRO:HG2	1:A:277:ILE:HD13	1.84	0.59
1:A:301:PRO:CG	1:A:302:ASP:H	2.12	0.59
1:F:639:ASN:HD21	1:F:813:SER:H	1.50	0.59
1:G:1081:PRO:HG2	1:G:1084:LEU:HB2	1.84	0.59
1:H:513:ILE:HG12	1:H:953:MET:HE2	1.83	0.59
1:A:300:TRP:CD2	1:A:306:GLN:CG	2.72	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:GLY:N	1:D:470:ASN:ND2	2.51	0.59
1:E:273:ARG:NH1	1:E:288:THR:C	2.56	0.59
1:H:809:ASN:HB2	1:H:810:PRO:CD	2.32	0.59
1:C:809:ASN:HB2	1:C:810:PRO:CD	2.32	0.59
1:D:322:THR:O	1:D:322:THR:HG22	2.03	0.59
1:D:697:MET:HA	1:D:709:THR:O	2.03	0.59
1:H:782:GLN:HA	1:H:782:GLN:NE2	2.18	0.59
1:B:800:THR:HG22	1:B:802:ALA:H	0.76	0.59
1:D:733:VAL:HG22	1:D:734:VAL:N	2.17	0.59
1:E:272:TYR:CE2	1:E:295:LEU:HD23	2.38	0.59
1:G:307:ARG:HA	1:G:332:LEU:CD2	2.33	0.59
1:A:390:SER:HB2	1:A:971:THR:HB	1.85	0.59
1:C:551:LEU:HD12	1:C:551:LEU:O	2.02	0.59
1:C:733:VAL:HG22	1:C:734:VAL:N	2.17	0.59
1:D:491:GLY:HA3	5:D:36:HOH:O	2.03	0.59
1:E:965:PRO:HD2	1:E:997:LYS:O	2.02	0.59
1:F:614:MET:O	1:F:618:LYS:HG3	2.03	0.59
1:H:360:ILE:O	1:H:363:PHE:N	2.33	0.59
1:E:1064:ASP:HB2	1:E:1071:PHE:CZ	2.38	0.59
1:H:262:VAL:CG1	1:H:969:VAL:HG23	2.30	0.59
1:H:298:THR:O	1:H:300:TRP:HZ3	1.85	0.59
1:A:604:ASN:HD21	1:A:607:VAL:N	2.01	0.59
1:B:516:ALA:HB1	1:B:521:ASP:OD2	2.02	0.59
1:B:939:VAL:HG11	1:B:943:LYS:NZ	2.06	0.59
1:D:278:LEU:O	1:D:278:LEU:CG	2.51	0.59
1:E:271:TRP:CD1	1:E:294:PRO:CB	2.84	0.59
1:G:476:VAL:HG22	1:G:956:TRP:HE3	1.68	0.59
1:G:669:TYR:CD1	1:G:874:THR:HG23	2.37	0.59
1:D:250:GLN:HE21	1:D:275:LYS:CE	2.16	0.58
1:D:277:ILE:O	1:D:279:LYS:N	2.36	0.58
1:D:293:ARG:CB	1:D:297:MET:CE	2.80	0.58
1:A:323:TYR:HB3	1:A:327:THR:OG1	2.03	0.58
1:A:457:MET:HE2	1:A:493:TYR:CE2	2.37	0.58
1:D:300:TRP:HB2	1:D:306:GLN:HB2	1.84	0.58
1:D:440:ASN:ND2	1:D:449:GLN:HE21	1.95	0.58
1:H:303:GLN:O	1:H:304:GLU:C	2.38	0.58
1:H:308:GLN:C	1:H:310:VAL:H	2.04	0.58
1:G:430:TYR:CD1	1:G:977:LYS:HD2	2.38	0.58
1:H:526:HIS:HA	1:H:530:ASP:OD1	2.03	0.58
1:E:250:GLN:OE1	1:E:1087:PRO:HG2	2.03	0.58
1:E:271:TRP:CE2	1:E:294:PRO:HD3	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:TRP:CG	1:E:294:PRO:CA	2.83	0.58
1:F:780:SER:OG	1:F:782:GLN:HB3	2.04	0.58
1:F:1085:VAL:CG2	1:F:1086:ASN:N	2.64	0.58
1:H:277:ILE:HG12	1:H:293:ARG:HE	1.68	0.58
1:H:315:ALA:C	1:H:317:LEU:N	2.57	0.58
1:H:537:ASN:OD1	1:H:540:ARG:NH1	2.37	0.58
1:A:800:THR:CG2	1:A:801:ALA:N	2.67	0.58
1:E:261:HIS:HD2	1:E:264:HIS:N	1.99	0.58
1:F:457:MET:HE3	1:F:493:TYR:HE2	1.67	0.58
1:H:299:TRP:CH2	1:H:301:PRO:CA	2.87	0.58
1:H:299:TRP:CH2	1:H:301:PRO:HA	2.39	0.58
1:H:301:PRO:O	1:H:302:ASP:HB3	2.03	0.58
1:H:424:ASP:HB3	1:H:520:ASN:ND2	2.19	0.58
1:A:285:THR:HG22	1:A:286:GLN:O	2.03	0.58
1:B:800:THR:HG23	1:B:801:ALA:N	2.19	0.58
1:E:782:GLN:HA	1:E:782:GLN:NE2	2.18	0.58
1:F:705:SER:HB3	1:F:743:LEU:HD13	1.86	0.58
1:G:794:ARG:HH11	1:G:794:ARG:CG	2.16	0.58
1:H:829:ASP:OD1	1:H:831:ARG:HB2	2.04	0.58
1:A:277:ILE:HG21	1:A:293:ARG:NH2	2.19	0.58
1:H:363:PHE:O	1:H:365:LYS:N	2.36	0.58
1:E:339:ILE:CG2	1:E:343:ILE:HD11	2.34	0.58
1:E:871:GLU:H	1:E:871:GLU:CD	2.07	0.58
1:G:478:ALA:HB1	1:G:481:ASN:HD22	1.69	0.58
1:B:1016:GLN:HE21	1:G:748:SER:HA	1.69	0.57
1:C:729:ARG:HD2	1:C:758:ALA:O	2.03	0.57
1:F:311:ASN:ND2	1:F:323:TYR:H	1.91	0.57
1:G:251:VAL:HG21	1:G:259:PHE:HZ	1.66	0.57
1:H:288:THR:HG23	1:H:289:GLU:H	1.64	0.57
1:H:630:ALA:O	1:H:633:LYS:NZ	2.37	0.57
1:H:765:ARG:HB2	1:H:766:PRO:HD2	1.84	0.57
1:A:355:TRP:CE3	1:A:355:TRP:C	2.77	0.57
1:B:841:ASP:OD1	1:B:846:HIS:HE1	1.86	0.57
1:C:245:PHE:O	1:C:246:ALA:C	2.40	0.57
1:D:347:ILE:CG1	1:D:353:THR:HG22	2.34	0.57
1:D:854:ARG:NH1	1:D:892:ASP:OD2	2.33	0.57
1:E:271:TRP:CD2	1:E:294:PRO:HD3	2.38	0.57
1:E:457:MET:HE2	1:E:493:TYR:HE2	1.69	0.57
1:A:454:HIS:CE1	1:A:458:ASN:ND2	2.72	0.57
1:C:261:HIS:CD2	1:C:264:HIS:N	2.60	0.57
1:C:346:LYS:HE3	1:C:355:TRP:CE3	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:854:ARG:NH1	1:C:892:ASP:OD2	2.36	0.57
1:D:856:MET:HG3	1:D:892:ASP:HB2	1.86	0.57
1:D:874:THR:HB	1:D:932:TYR:HB3	1.85	0.57
1:G:269:GLU:HG3	1:G:364:VAL:HG21	1.85	0.57
1:A:596:ARG:HB2	1:A:612:PHE:CZ	2.38	0.57
1:B:709:THR:HG21	1:B:753:VAL:HG22	1.87	0.57
1:E:273:ARG:CG	1:E:287:SER:HB2	2.22	0.57
1:F:520:ASN:O	1:F:523:PRO:HG2	2.05	0.57
1:F:639:ASN:HB3	1:F:642:LEU:HB2	1.86	0.57
1:B:251:VAL:HG21	1:B:259:PHE:CZ	2.39	0.57
1:B:711:VAL:HG22	1:B:734:VAL:HG23	1.87	0.57
1:C:670:MET:HE1	1:C:885:PHE:CZ	2.38	0.57
1:E:651:LYS:O	1:E:652:SER:HB2	2.03	0.57
1:E:670:MET:HE1	1:E:885:PHE:CZ	2.40	0.57
1:F:252:TYR:HB3	1:F:258:ASN:ND2	2.08	0.57
1:F:874:THR:HG22	1:F:878:ILE:HD11	1.87	0.57
1:A:280:ASP:O	1:A:282:LYS:N	2.38	0.57
1:A:407:ASN:HD21	1:A:431:GLU:H	1.52	0.57
1:A:447:ALA:O	1:A:450:LEU:HB3	2.05	0.57
1:A:882:VAL:HG21	1:A:944:ALA:O	2.05	0.57
1:C:687:ARG:HA	1:C:691:VAL:CG2	2.34	0.57
1:D:308:GLN:HA	1:D:308:GLN:HE21	1.69	0.57
1:E:271:TRP:CZ2	1:E:294:PRO:HD3	2.40	0.57
1:E:457:MET:HE2	1:E:493:TYR:CE2	2.40	0.57
1:A:356:LEU:C	1:A:358:GLN:N	2.55	0.57
1:E:439:ASP:C	1:E:439:ASP:OD1	2.41	0.57
1:H:295:LEU:HD23	1:H:295:LEU:O	2.04	0.57
1:D:793:ASP:HB2	1:D:794:ARG:HG3	1.86	0.57
1:E:430:TYR:HB3	1:E:978:TYR:CE1	2.40	0.57
1:A:383:GLN:O	1:A:384:LYS:HB2	2.05	0.57
1:D:492:ASP:HB3	1:D:1022:LEU:CD2	2.31	0.57
1:G:301:PRO:O	1:G:302:ASP:HB3	2.05	0.57
1:A:334:LEU:O	1:A:335:ALA:C	2.43	0.56
1:A:367:GLN:O	1:A:371:ASN:HB3	2.05	0.56
1:C:288:THR:OG1	1:C:290:LYS:HB2	2.04	0.56
1:C:371:ASN:HB3	1:C:373:ASP:H	1.69	0.56
1:C:632:GLU:HG2	5:C:18:HOH:O	2.04	0.56
1:D:245:PHE:O	1:D:246:ALA:C	2.42	0.56
1:D:987:ILE:HG12	1:D:1058:ALA:HB2	1.85	0.56
1:E:323:TYR:CD1	1:E:327:THR:HG21	2.40	0.56
1:F:1052:ASN:H	1:F:1052:ASN:ND2	2.00	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:663:PHE:CZ	1:G:670:MET:HG2	2.40	0.56
1:H:841:ASP:OD1	1:H:846:HIS:HE1	1.88	0.56
1:A:300:TRP:CB	1:A:306:GLN:HB2	2.35	0.56
1:C:347:ILE:HG22	1:C:348:THR:N	2.19	0.56
1:E:245:PHE:O	1:E:249:ASN:HB2	2.04	0.56
1:E:271:TRP:CH2	1:E:356:LEU:HD23	2.40	0.56
1:E:299:TRP:CH2	1:E:301:PRO:CB	2.87	0.56
1:G:928:LYS:HB2	1:G:929:PRO:CD	2.33	0.56
1:H:293:ARG:HB3	1:H:297:MET:HE1	1.87	0.56
1:H:311:ASN:H	1:H:311:ASN:ND2	2.03	0.56
1:H:740:ASN:C	1:H:740:ASN:ND2	2.51	0.56
1:A:280:ASP:H	1:A:344:GLU:HB3	1.69	0.56
1:A:293:ARG:HB3	1:A:297:MET:HE2	1.86	0.56
1:A:309:TYR:CD2	1:A:310:VAL:N	2.73	0.56
1:B:531:ASN:ND2	1:B:844:SER:OG	2.38	0.56
1:B:740:ASN:HD22	1:B:740:ASN:C	2.09	0.56
1:B:742:SER:O	1:B:744:ARG:CG	2.53	0.56
1:C:619:LYS:O	1:C:622:GLU:HG3	2.05	0.56
1:D:356:LEU:HA	1:D:359:THR:HG23	1.86	0.56
1:D:363:PHE:O	1:D:366:THR:HG23	2.04	0.56
1:D:729:ARG:HD2	1:D:758:ALA:O	2.05	0.56
1:D:1085:VAL:CG2	1:D:1086:ASN:H	2.17	0.56
1:E:288:THR:HG22	1:E:289:GLU:N	2.11	0.56
1:E:335:ALA:O	1:E:339:ILE:HD12	2.05	0.56
1:E:361:SER:O	1:E:362:ALA:C	2.43	0.56
1:F:376:LYS:HB3	1:F:377:PRO:HA	1.88	0.56
1:F:478:ALA:HB1	1:F:481:ASN:HD22	1.69	0.56
1:F:862:ASN:O	1:F:912:ILE:CG2	2.43	0.56
1:G:928:LYS:HB2	1:G:929:PRO:HD2	1.86	0.56
1:H:363:PHE:O	1:H:364:VAL:C	2.44	0.56
1:A:374:SER:HB2	1:A:1058:ALA:HB2	1.87	0.56
1:A:610:TYR:HA	1:A:612:PHE:CE2	2.40	0.56
1:B:1085:VAL:CG2	1:B:1086:ASN:N	2.68	0.56
1:C:1085:VAL:CG2	1:C:1086:ASN:N	2.69	0.56
1:D:271:TRP:CD1	1:D:294:PRO:CA	2.83	0.56
1:E:957:VAL:HG12	1:E:957:VAL:O	2.04	0.56
1:G:809:ASN:HB2	1:G:810:PRO:HD3	1.85	0.56
1:H:261:HIS:HD2	1:H:264:HIS:H	1.51	0.56
1:A:408:ARG:HD2	1:A:413:GLN:O	2.06	0.56
1:C:317:LEU:HD13	1:C:342:LYS:HB3	1.88	0.56
1:E:314:ASN:ND2	1:E:321:GLN:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:856:MET:HG3	1:E:892:ASP:HB2	1.87	0.56
1:F:261:HIS:CD2	1:F:264:HIS:N	2.63	0.56
1:F:816:LEU:HD12	1:F:817:GLY:H	1.70	0.56
1:G:383:GLN:O	1:G:384:LYS:HB2	2.03	0.56
1:B:670:MET:HE3	1:B:885:PHE:HZ	1.70	0.56
1:C:1052:ASN:N	1:C:1052:ASN:ND2	2.43	0.56
1:D:368:SER:HA	1:D:371:ASN:HD22	1.71	0.56
1:D:1072:SER:OG	1:D:1074:VAL:HG12	2.05	0.56
1:H:271:TRP:HZ2	1:H:357:ARG:HA	1.71	0.56
1:H:278:LEU:CB	1:H:284:TRP:CE3	2.86	0.56
1:H:313:MET:O	1:H:317:LEU:HG	2.04	0.56
1:C:245:PHE:N	1:C:245:PHE:HD1	2.04	0.56
1:C:247:GLN:NE2	1:C:247:GLN:HA	2.21	0.56
1:C:355:TRP:CG	1:C:356:LEU:N	2.73	0.56
1:C:561:ILE:HG12	1:C:697:MET:HB3	1.87	0.56
1:D:310:VAL:HG11	1:D:335:ALA:HB1	1.88	0.56
1:D:461:ASN:OD1	1:D:467:PRO:HA	2.04	0.56
1:G:390:SER:HB2	1:G:971:THR:HB	1.86	0.56
1:H:311:ASN:N	1:H:311:ASN:HD22	2.02	0.56
1:D:740:ASN:HD22	1:D:741:PRO:N	2.03	0.56
1:E:656:ARG:HG3	1:E:856:MET:HB3	1.85	0.56
1:A:299:TRP:CD1	1:A:1081:PRO:HB3	2.41	0.56
1:A:856:MET:HG3	1:A:892:ASP:HB2	1.87	0.56
1:C:390:SER:HB2	1:C:971:THR:HB	1.88	0.56
1:D:355:TRP:CZ3	1:D:359:THR:HG21	2.41	0.56
1:E:343:ILE:HG23	1:E:355:TRP:CZ2	2.41	0.56
1:F:927:SER:OG	1:F:928:LYS:HG2	2.06	0.56
1:H:300:TRP:CD1	1:H:306:GLN:HG3	2.41	0.56
1:A:273:ARG:NH1	1:A:289:GLU:HG2	2.21	0.56
1:B:689:LYS:HD2	1:B:690:TYR:CE1	2.41	0.56
1:B:697:MET:HA	1:B:709:THR:O	2.05	0.56
1:C:555:SER:HB3	1:H:417:LYS:HE3	1.86	0.56
1:D:442:ASN:HB3	1:D:445:VAL:HG23	1.88	0.56
1:E:841:ASP:OD1	1:E:846:HIS:HE1	1.89	0.56
1:G:1052:ASN:ND2	1:G:1052:ASN:N	2.35	0.56
1:H:261:HIS:HD2	1:H:264:HIS:N	2.04	0.56
1:H:290:LYS:C	1:H:291:ASP:OD1	2.45	0.56
1:H:312:TYR:C	1:H:314:ASN:N	2.60	0.56
1:A:604:ASN:ND2	1:A:607:VAL:N	2.54	0.55
1:B:882:VAL:HG13	1:B:948:LYS:HG3	1.88	0.55
1:F:515:GLU:OE1	2:N:3:AC1:O3	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:733:VAL:CG2	1:H:734:VAL:N	2.70	0.55
1:B:537:ASN:OD1	1:B:540:ARG:NH1	2.36	0.55
1:D:288:THR:N	1:D:291:ASP:OD2	2.39	0.55
1:E:457:MET:CE	1:E:493:TYR:HE2	2.19	0.55
1:G:492:ASP:CB	1:G:1022:LEU:HD22	2.31	0.55
1:G:565:LEU:HD21	5:G:58:HOH:O	2.06	0.55
1:H:312:TYR:C	1:H:314:ASN:H	2.10	0.55
1:B:460:GLY:N	1:B:470:ASN:HD22	2.04	0.55
1:D:304:GLU:OE1	1:D:307:ARG:NH1	2.40	0.55
1:E:558:ASN:N	1:E:559:PRO:CD	2.70	0.55
1:E:670:MET:CE	1:E:885:PHE:HZ	2.18	0.55
1:F:843:LYS:HE2	5:F:84:HOH:O	2.05	0.55
1:H:315:ALA:C	1:H:317:LEU:H	2.08	0.55
1:B:1016:GLN:NE2	1:G:748:SER:HA	2.22	0.55
1:C:407:ASN:HD22	1:C:431:GLU:N	2.03	0.55
1:D:337:GLN:O	1:D:338:THR:C	2.44	0.55
1:D:355:TRP:CD2	1:D:356:LEU:N	2.75	0.55
1:B:558:ASN:N	1:B:559:PRO:HD2	2.22	0.55
1:D:250:GLN:HE21	1:D:275:LYS:HD2	1.72	0.55
1:E:269:GLU:OE2	1:E:361:SER:HB3	2.07	0.55
1:F:245:PHE:O	1:F:247:GLN:N	2.40	0.55
1:D:376:LYS:HB3	1:D:377:PRO:HA	1.89	0.55
1:F:912:ILE:HG22	1:F:931:LYS:HZ2	1.72	0.55
1:G:369:ALA:O	1:G:370:TRP:HD1	1.90	0.55
1:G:440:ASN:HD21	1:G:449:GLN:NE2	1.91	0.55
1:H:481:ASN:ND2	2:P:3:AC1:O2	2.39	0.55
1:A:513:ILE:HG12	1:A:953:MET:HE2	1.88	0.55
1:D:251:VAL:CG2	1:D:259:PHE:CZ	2.87	0.55
1:A:310:VAL:HG22	1:A:339:ILE:CD1	2.37	0.55
1:B:481:ASN:ND2	2:J:3:AC1:O2	2.39	0.55
1:C:576:ALA:HB3	1:C:847:GLN:HB3	1.88	0.55
1:D:323:TYR:HB3	1:D:327:THR:HG1	1.71	0.55
1:D:347:ILE:HG22	1:D:348:THR:N	2.21	0.55
1:E:515:GLU:OE1	2:M:3:AC1:O3	2.25	0.55
1:F:383:GLN:O	1:F:384:LYS:HB2	2.06	0.55
1:A:928:LYS:HB2	1:A:929:PRO:CD	2.37	0.55
1:B:740:ASN:ND2	1:B:741:PRO:HD2	2.22	0.55
1:F:321:GLN:OE1	1:F:321:GLN:CA	2.47	0.55
1:F:705:SER:HB3	1:F:743:LEU:CD1	2.36	0.55
1:F:848:ASN:OD1	1:F:850:ALA:HB3	2.06	0.55
1:F:1072:SER:OG	1:F:1074:VAL:CG1	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ASP:HA	1:A:863:PHE:O	2.05	0.54
1:B:368:SER:O	1:B:371:ASN:HB2	2.07	0.54
1:D:245:PHE:CZ	1:D:284:TRP:HZ2	2.24	0.54
1:D:352:ASN:C	1:D:352:ASN:ND2	2.61	0.54
1:E:460:GLY:N	1:E:470:ASN:HD22	2.05	0.54
1:F:371:ASN:HB3	1:F:373:ASP:H	1.72	0.54
1:G:746:LYS:HB2	1:G:749:ASP:OD2	2.07	0.54
1:H:522:THR:N	1:H:523:PRO:HD2	2.20	0.54
1:A:460:GLY:H	1:A:470:ASN:HD22	1.53	0.54
1:D:1069:THR:HB	1:D:1079:PHE:HE2	1.71	0.54
1:F:988:LYS:H	1:F:990:THR:HG23	1.72	0.54
1:G:346:LYS:HE3	1:G:355:TRP:CE2	2.42	0.54
1:H:300:TRP:NE1	1:H:306:GLN:HG3	2.22	0.54
1:A:280:ASP:O	1:A:281:GLY:C	2.45	0.54
1:B:392:ASN:HD22	1:B:392:ASN:N	2.06	0.54
1:C:809:ASN:HB2	1:C:810:PRO:HD3	1.88	0.54
1:D:293:ARG:CB	1:D:297:MET:HE1	2.36	0.54
1:D:330:LEU:HD12	1:D:330:LEU:C	2.28	0.54
1:E:271:TRP:CH2	1:E:294:PRO:HD3	2.42	0.54
1:G:863:PHE:CD2	1:G:912:ILE:HD11	2.42	0.54
1:H:273:ARG:NE	1:H:288:THR:O	2.40	0.54
1:H:293:ARG:HB3	1:H:294:PRO:CD	2.38	0.54
1:H:311:ASN:H	1:H:311:ASN:HD22	1.55	0.54
1:B:740:ASN:HD22	1:B:741:PRO:N	2.05	0.54
1:C:277:ILE:O	1:C:284:TRP:HA	2.07	0.54
1:D:342:LYS:O	1:D:346:LYS:HB2	2.08	0.54
1:E:277:ILE:HD13	1:E:293:ARG:NH2	2.23	0.54
1:G:299:TRP:CZ3	1:G:301:PRO:HD3	2.43	0.54
1:H:310:VAL:HG12	1:H:311:ASN:ND2	2.21	0.54
1:A:271:TRP:CH2	1:A:357:ARG:HG2	2.43	0.54
1:E:252:TYR:CD1	1:E:275:LYS:HG2	2.39	0.54
1:F:278:LEU:HD13	1:F:284:TRP:CE2	2.42	0.54
1:F:461:ASN:OD1	1:F:467:PRO:HA	2.07	0.54
1:G:369:ALA:O	1:G:370:TRP:CD1	2.60	0.54
1:H:315:ALA:O	1:H:317:LEU:N	2.40	0.54
1:H:277:ILE:O	1:H:277:ILE:HG22	2.06	0.54
1:B:658:TYR:CE2	1:B:660:GLY:CA	2.87	0.54
1:C:457:MET:HE2	1:C:493:TYR:HE2	1.73	0.54
1:E:299:TRP:CH2	1:E:301:PRO:HA	2.40	0.54
1:F:935:ALA:O	1:F:939:VAL:HG23	2.08	0.54
1:H:250:GLN:HG2	1:H:275:LYS:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:TYR:HA	1:D:285:THR:O	2.08	0.54
1:F:255:ASP:O	1:F:258:ASN:HB2	2.08	0.54
1:G:356:LEU:HA	1:G:359:THR:HG23	1.90	0.54
1:G:587:HIS:NE2	2:O:3:AC1:O3B	2.35	0.54
1:H:294:PRO:O	1:H:297:MET:N	2.29	0.54
1:H:966:GLU:HB2	1:H:997:LYS:CB	2.33	0.54
1:H:1069:THR:HG22	1:H:1070:TYR:O	2.08	0.54
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.71	0.54
1:A:310:VAL:HG22	1:A:339:ILE:HD12	1.88	0.54
1:A:407:ASN:ND2	1:A:431:GLU:N	2.55	0.54
1:A:920:ASP:OD2	1:A:1002:ASP:HB2	2.08	0.54
1:B:476:VAL:HB	1:B:514:LEU:HD22	1.90	0.54
1:B:492:ASP:HB3	1:B:1022:LEU:HD22	1.89	0.54
1:B:764:TYR:HE1	1:B:821:PRO:HD3	1.72	0.54
1:D:277:ILE:CD1	1:D:291:ASP:HB3	2.37	0.54
1:G:759:HIS:CD2	1:G:764:TYR:OH	2.61	0.54
1:H:596:ARG:HB2	1:H:612:PHE:HZ	1.71	0.54
1:A:311:ASN:HD22	1:A:311:ASN:N	2.06	0.54
1:A:461:ASN:H	1:A:470:ASN:HD21	1.53	0.54
1:A:916:TYR:HB3	2:I:3:AC1:HC61	1.89	0.54
1:B:809:ASN:OD1	1:B:812:VAL:N	2.33	0.54
1:C:1085:VAL:CG2	1:C:1086:ASN:H	2.21	0.54
1:H:251:VAL:HG21	1:H:259:PHE:HZ	1.69	0.54
1:B:266:LEU:HD21	1:B:1073:LEU:HD11	1.89	0.53
1:B:725:ASP:HB3	5:B:5:HOH:O	2.07	0.53
1:B:1083:SER:O	1:B:1087:PRO:CG	2.37	0.53
1:C:359:THR:O	1:C:362:ALA:HB3	2.08	0.53
1:C:1072:SER:OG	1:C:1074:VAL:CG1	2.56	0.53
1:D:297:MET:O	1:D:297:MET:HG2	2.07	0.53
1:D:516:ALA:HB1	1:D:521:ASP:OD2	2.08	0.53
1:F:863:PHE:CD2	1:F:912:ILE:HD11	2.43	0.53
1:G:300:TRP:CE3	1:G:306:GLN:HG3	2.43	0.53
1:G:471:PHE:CG	1:G:954:ALA:HB2	2.43	0.53
1:A:278:LEU:CD2	1:A:281:GLY:HA2	2.38	0.53
1:A:616:GLU:O	1:A:619:LYS:HB3	2.08	0.53
1:C:883:ASP:OD1	1:C:948:LYS:HE3	2.08	0.53
1:A:809:ASN:C	1:A:809:ASN:OD1	2.46	0.53
1:C:247:GLN:HA	1:C:247:GLN:HE21	1.73	0.53
1:D:271:TRP:CE2	1:D:294:PRO:CD	2.89	0.53
1:E:340:GLN:O	1:E:344:GLU:HG2	2.08	0.53
1:H:471:PHE:CG	1:H:954:ALA:HB2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:MET:HA	1:A:709:THR:O	2.08	0.53
1:A:713:TYR:O	1:A:759:HIS:HE1	1.91	0.53
1:C:670:MET:CE	1:C:885:PHE:HZ	2.22	0.53
1:E:782:GLN:HA	1:E:782:GLN:HE21	1.72	0.53
1:F:333:ASN:O	1:F:337:GLN:HG3	2.08	0.53
1:F:666:ASP:HA	1:F:863:PHE:O	2.08	0.53
1:F:1080:LEU:HB3	1:F:1081:PRO:HD2	1.90	0.53
1:G:316:GLN:NE2	1:G:316:GLN:N	2.56	0.53
1:G:316:GLN:N	1:G:316:GLN:CD	2.61	0.53
1:H:294:PRO:HD2	1:H:297:MET:HE2	1.86	0.53
1:H:316:GLN:CG	1:H:359:THR:HG21	2.26	0.53
1:H:390:SER:HB2	1:H:971:THR:HB	1.90	0.53
1:A:352:ASN:O	1:A:353:THR:CG2	2.56	0.53
1:C:250:GLN:HB2	1:C:1084:LEU:O	2.09	0.53
1:E:273:ARG:CD	1:E:287:SER:CB	2.28	0.53
1:F:471:PHE:CG	1:F:954:ALA:HB2	2.44	0.53
1:G:356:LEU:O	1:G:357:ARG:C	2.45	0.53
1:H:407:ASN:HD21	1:H:431:GLU:H	1.55	0.53
1:A:297:MET:HG2	1:A:298:THR:HG22	1.89	0.53
1:F:1023:PHE:CD1	1:F:1036:PRO:HG3	2.43	0.53
1:G:602:GLU:C	1:G:603:ILE:HG13	2.29	0.53
1:H:277:ILE:HG22	1:H:279:LYS:HD3	1.90	0.53
1:D:346:LYS:O	1:D:350:GLU:HG2	2.08	0.53
1:E:630:ALA:O	1:E:633:LYS:NZ	2.42	0.53
1:F:610:TYR:HA	1:F:612:PHE:CE2	2.43	0.53
1:G:917:ALA:HA	1:G:962:TYR:CE1	2.43	0.53
1:C:1063:LYS:HE2	1:C:1068:ASN:CG	2.28	0.53
1:E:729:ARG:O	1:E:729:ARG:HG3	2.09	0.53
1:E:991:LEU:HG	1:E:1070:TYR:CE2	2.44	0.53
1:F:250:GLN:CB	1:F:1084:LEU:O	2.47	0.53
1:F:261:HIS:CD2	1:F:264:HIS:CA	2.91	0.53
1:F:689:LYS:HB3	1:F:690:TYR:CD1	2.44	0.53
1:F:988:LYS:O	1:F:990:THR:HG22	2.08	0.53
1:G:347:ILE:HG12	1:G:353:THR:HG22	1.90	0.53
1:H:389:TYR:CE1	1:H:1050:GLY:HA2	2.44	0.53
1:C:461:ASN:H	1:C:470:ASN:HD21	1.56	0.53
1:C:648:LEU:O	1:C:687:ARG:HG3	2.08	0.53
1:D:299:TRP:NE1	1:D:1081:PRO:HB3	2.24	0.53
1:E:311:ASN:N	1:E:311:ASN:ND2	2.55	0.53
1:G:800:THR:CG2	1:G:801:ALA:N	2.72	0.53
1:G:1065:GLN:HG3	1:G:1066:ALA:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:406:LEU:HD22	1:H:431:GLU:HG2	1.91	0.53
1:B:581:TYR:HA	1:B:654:VAL:O	2.09	0.53
1:G:293:ARG:HB3	1:G:297:MET:CE	2.39	0.53
1:A:261:HIS:CD2	1:A:264:HIS:H	2.15	0.52
1:B:612:PHE:N	1:B:612:PHE:CD2	2.73	0.52
1:C:599:ILE:HG22	1:C:607:VAL:HG11	1.91	0.52
1:F:874:THR:HG22	1:F:878:ILE:CD1	2.40	0.52
1:G:973:THR:HG23	1:G:988:LYS:HA	1.90	0.52
1:A:460:GLY:N	1:A:470:ASN:ND2	2.56	0.52
1:B:577:ALA:C	1:B:578:VAL:HG23	2.29	0.52
1:C:478:ALA:HB1	1:C:481:ASN:HD22	1.73	0.52
1:C:639:ASN:HB3	1:C:642:LEU:HB2	1.91	0.52
1:C:740:ASN:C	1:C:740:ASN:ND2	2.51	0.52
1:D:334:LEU:C	1:D:336:ALA:H	2.11	0.52
1:D:964:LEU:HD12	1:D:996:GLY:HA2	1.91	0.52
1:E:279:LYS:HD2	1:E:283:THR:HG22	1.92	0.52
1:E:347:ILE:HG12	1:E:353:THR:CB	2.33	0.52
1:G:250:GLN:NE2	1:G:275:LYS:NZ	2.56	0.52
1:G:466:ASP:OD2	1:G:943:LYS:HD2	2.09	0.52
1:H:558:ASN:N	1:H:559:PRO:CD	2.73	0.52
1:A:491:GLY:HA3	5:A:1:HOH:O	2.09	0.52
1:D:335:ALA:O	1:D:339:ILE:HG13	2.10	0.52
1:D:607:VAL:HG13	1:D:607:VAL:O	2.08	0.52
1:D:997:LYS:HA	1:D:1043:TRP:O	2.09	0.52
1:G:363:PHE:CE1	1:G:367:GLN:OE1	2.62	0.52
1:G:537:ASN:OD1	1:G:540:ARG:NH1	2.39	0.52
1:H:304:GLU:O	1:H:307:ARG:HB3	2.10	0.52
1:H:491:GLY:HA3	5:H:196:HOH:O	2.09	0.52
1:A:276:TYR:N	1:A:276:TYR:CD2	2.77	0.52
1:A:494:LEU:HB3	1:A:500:ILE:HD13	1.90	0.52
1:B:585:ARG:NH2	1:B:624:TYR:OH	2.42	0.52
1:D:304:GLU:OE1	1:D:304:GLU:HA	2.09	0.52
1:D:407:ASN:ND2	1:D:431:GLU:H	2.06	0.52
1:D:669:TYR:CE2	1:D:670:MET:HE3	2.44	0.52
1:E:271:TRP:CE2	1:E:294:PRO:CD	2.92	0.52
1:E:387:LEU:O	1:E:1050:GLY:HA3	2.10	0.52
1:H:407:ASN:ND2	1:H:431:GLU:N	2.57	0.52
1:A:266:LEU:HD13	1:A:295:LEU:HD11	1.92	0.52
1:A:733:VAL:HG22	1:A:734:VAL:N	2.24	0.52
1:C:460:GLY:CA	1:C:470:ASN:ND2	2.72	0.52
1:C:551:LEU:HD22	1:C:741:PRO:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:ILE:O	1:E:363:PHE:N	2.41	0.52
1:G:245:PHE:O	1:G:246:ALA:C	2.48	0.52
1:G:250:GLN:NE2	1:G:275:LYS:HZ3	2.08	0.52
1:G:604:ASN:HD21	1:G:607:VAL:HA	1.74	0.52
1:C:346:LYS:HE3	1:C:355:TRP:CD2	2.44	0.52
1:E:430:TYR:CG	1:E:977:LYS:HD3	2.44	0.52
1:F:912:ILE:O	1:F:912:ILE:CG2	2.53	0.52
1:H:300:TRP:CD1	1:H:306:GLN:CA	2.90	0.52
1:A:603:ILE:CD1	1:A:619:LYS:HG3	2.40	0.52
1:B:504:ASP:OD1	1:B:846:HIS:HD2	1.92	0.52
1:B:733:VAL:CG2	1:B:734:VAL:N	2.72	0.52
1:E:271:TRP:CG	1:E:357:ARG:NH1	2.78	0.52
1:E:322:THR:HG23	1:E:323:TYR:N	2.24	0.52
1:H:363:PHE:C	1:H:365:LYS:N	2.60	0.52
1:A:327:THR:CG2	1:A:328:SER:N	2.73	0.52
1:B:272:TYR:CD1	1:B:273:ARG:N	2.78	0.52
1:B:610:TYR:HA	1:B:612:PHE:CE2	2.44	0.52
1:D:387:LEU:O	1:D:1050:GLY:HA3	2.10	0.52
1:E:271:TRP:CZ3	1:E:294:PRO:HD3	2.45	0.52
1:F:988:LYS:O	1:F:990:THR:CG2	2.57	0.52
1:H:871:GLU:H	1:H:871:GLU:CD	2.13	0.52
1:A:289:GLU:HG3	5:A:201:HOH:O	2.09	0.52
1:A:310:VAL:O	1:A:311:ASN:C	2.48	0.52
1:B:457:MET:HE2	1:B:493:TYR:HE2	1.75	0.52
1:B:924:LEU:HD12	1:B:924:LEU:N	2.24	0.52
1:D:308:GLN:HE21	1:D:308:GLN:CA	2.23	0.52
1:E:252:TYR:CD2	1:E:273:ARG:NH2	2.66	0.52
1:E:587:HIS:CD2	2:M:3:AC1:O3B	2.61	0.52
1:E:809:ASN:HB2	1:E:810:PRO:HD3	1.92	0.52
1:G:1076:ASP:OD2	1:G:1077:ASN:HB2	2.10	0.52
1:H:302:ASP:OD1	1:H:304:GLU:HB3	2.09	0.52
1:A:1052:ASN:ND2	1:A:1052:ASN:N	2.55	0.52
1:B:869:LYS:O	1:B:870:LYS:C	2.48	0.52
1:C:492:ASP:OD1	1:C:1025:ARG:NH1	2.43	0.52
1:D:297:MET:O	1:D:297:MET:CG	2.58	0.52
1:F:457:MET:HE3	1:F:493:TYR:CE2	2.45	0.52
1:F:740:ASN:HD22	1:F:740:ASN:C	2.12	0.52
1:G:271:TRP:HZ2	1:G:357:ARG:HA	1.75	0.52
1:A:352:ASN:C	1:A:353:THR:CG2	2.78	0.51
1:A:776:LYS:HE3	5:A:171:HOH:O	2.09	0.51
1:D:515:GLU:OE1	2:L:3:AC1:O3	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:928:LYS:HB2	1:D:929:PRO:CD	2.40	0.51
1:E:1085:VAL:CG2	1:E:1086:ASN:N	2.74	0.51
1:F:352:ASN:ND2	1:F:352:ASN:H	2.05	0.51
1:H:681:GLU:OE2	1:H:884:LYS:NZ	2.36	0.51
1:A:299:TRP:NE1	1:A:1081:PRO:HB3	2.26	0.51
1:A:504:ASP:OD1	1:A:846:HIS:HD2	1.93	0.51
1:A:603:ILE:HD13	1:A:619:LYS:HG3	1.91	0.51
1:D:735:VAL:HG22	1:D:818:VAL:HG22	1.91	0.51
1:E:882:VAL:HG13	1:E:948:LYS:HG3	1.91	0.51
1:H:673:LYS:HD3	1:H:677:TYR:CD2	2.45	0.51
1:A:271:TRP:HA	1:A:294:PRO:HA	1.92	0.51
1:C:321:GLN:OE1	1:C:321:GLN:HA	2.07	0.51
1:C:551:LEU:CD2	1:C:741:PRO:HG2	2.40	0.51
1:D:639:ASN:HD22	1:D:642:LEU:HD13	1.75	0.51
1:E:250:GLN:HB2	1:E:1084:LEU:O	2.10	0.51
1:E:297:MET:O	1:E:298:THR:HG22	2.10	0.51
1:E:337:GLN:O	1:E:338:THR:C	2.49	0.51
1:E:800:THR:HG22	1:E:801:ALA:N	2.26	0.51
1:F:860:PHE:HB2	1:F:864:GLN:NE2	2.26	0.51
1:H:271:TRP:CZ2	1:H:357:ARG:HA	2.45	0.51
1:H:293:ARG:HB3	1:H:297:MET:CE	2.41	0.51
1:A:301:PRO:CG	1:A:302:ASP:N	2.70	0.51
1:D:300:TRP:CB	1:D:306:GLN:HB2	2.40	0.51
1:E:273:ARG:HD3	1:E:288:THR:O	2.10	0.51
1:E:360:ILE:O	1:E:363:PHE:HB3	2.10	0.51
1:E:514:LEU:HD21	1:E:532:MET:HG3	1.93	0.51
1:G:368:SER:HA	1:G:371:ASN:HD22	1.75	0.51
1:G:687:ARG:HA	1:G:691:VAL:HG23	1.93	0.51
1:H:740:ASN:HD22	1:H:741:PRO:N	2.09	0.51
1:A:278:LEU:HG	1:A:278:LEU:O	2.11	0.51
1:A:304:GLU:OE1	1:A:304:GLU:HA	2.09	0.51
1:A:307:ARG:NH1	1:A:308:GLN:OE1	2.42	0.51
1:B:261:HIS:CD2	1:B:264:HIS:H	2.15	0.51
1:B:492:ASP:HB3	1:B:1022:LEU:CD2	2.41	0.51
1:B:515:GLU:OE1	2:J:3:AC1:O3	2.27	0.51
1:D:1005:ALA:O	1:D:1041:LYS:HD2	2.11	0.51
1:F:357:ARG:NH1	1:F:357:ARG:HG3	2.19	0.51
1:H:308:GLN:O	1:H:310:VAL:N	2.44	0.51
1:H:860:PHE:CG	1:H:896:ALA:HB2	2.45	0.51
1:A:251:VAL:CG2	1:A:259:PHE:CZ	2.90	0.51
1:B:442:ASN:HB3	1:B:445:VAL:CG2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:TYR:CD2	1:C:670:MET:HG3	2.46	0.51
1:E:344:GLU:C	1:E:346:LYS:H	2.14	0.51
1:E:916:TYR:HB3	2:M:3:AC1:HC61	1.93	0.51
1:F:568:ARG:HG3	1:F:568:ARG:HH11	1.75	0.51
1:F:750:ARG:CB	5:F:55:HOH:O	2.58	0.51
1:G:669:TYR:O	1:G:670:MET:HB2	2.10	0.51
1:H:407:ASN:ND2	1:H:431:GLU:H	2.09	0.51
1:C:313:MET:O	1:C:317:LEU:HG	2.11	0.51
1:G:246:ALA:HB1	1:G:1087:PRO:HB2	1.92	0.51
1:G:313:MET:HB2	1:G:339:ILE:HD13	1.93	0.51
1:G:658:TYR:CE2	1:G:660:GLY:CA	2.93	0.51
1:H:278:LEU:O	1:H:279:LYS:C	2.49	0.51
1:A:375:GLU:OE1	1:A:1053:ILE:HB	2.10	0.51
1:E:421:TYR:CD1	1:E:523:PRO:HB2	2.46	0.51
1:F:723:THR:HG22	1:F:757:ALA:CB	2.40	0.51
1:F:908:LEU:HD12	1:F:912:ILE:HG13	1.93	0.51
1:H:292:PHE:O	1:H:293:ARG:HG3	2.11	0.51
1:A:307:ARG:C	1:A:309:TYR:N	2.60	0.51
1:A:800:THR:HG22	1:A:801:ALA:N	2.24	0.51
1:B:1004:GLN:HG3	1:B:1004:GLN:O	2.11	0.51
1:C:585:ARG:HD3	1:C:661:ASP:OD1	2.11	0.51
1:E:271:TRP:CE3	1:E:294:PRO:HD3	2.46	0.51
1:E:347:ILE:CD1	1:E:353:THR:HB	2.40	0.51
1:F:278:LEU:CD1	1:F:284:TRP:CE2	2.94	0.51
1:F:300:TRP:CE3	1:F:300:TRP:N	2.79	0.51
1:H:300:TRP:CE2	1:H:306:GLN:HG3	2.46	0.51
1:A:278:LEU:HB2	1:A:284:TRP:CH2	2.46	0.51
1:C:261:HIS:CD2	1:C:264:HIS:CA	2.94	0.51
1:C:299:TRP:CD1	1:C:1081:PRO:HB3	2.46	0.51
1:C:333:ASN:O	1:C:337:GLN:HG3	2.11	0.51
1:F:269:GLU:OE2	1:F:361:SER:HB3	2.10	0.51
1:H:271:TRP:HZ3	1:H:294:PRO:HD3	1.75	0.51
1:D:305:THR:HG23	1:D:367:GLN:NE2	2.25	0.50
1:F:568:ARG:HG3	1:F:568:ARG:NH1	2.26	0.50
1:G:277:ILE:O	1:G:284:TRP:HA	2.11	0.50
1:H:965:PRO:HD2	1:H:998:SER:HA	1.93	0.50
1:E:251:VAL:HG21	1:E:259:PHE:CZ	2.46	0.50
1:E:281:GLY:HA2	1:E:341:THR:CG2	2.42	0.50
1:E:361:SER:O	1:E:364:VAL:N	2.44	0.50
1:E:430:TYR:CE2	1:E:977:LYS:HE2	2.46	0.50
1:F:800:THR:HG23	1:F:801:ALA:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:GLN:HG3	1:G:251:VAL:N	2.25	0.50
1:G:988:LYS:H	1:G:990:THR:HG23	1.74	0.50
1:H:355:TRP:CD2	1:H:356:LEU:N	2.80	0.50
1:D:668:GLN:OE1	1:D:668:GLN:HA	2.11	0.50
1:F:279:LYS:O	1:F:280:ASP:CB	2.52	0.50
1:F:847:GLN:NE2	1:F:852:ASP:OD1	2.34	0.50
1:G:355:TRP:CE3	1:G:359:THR:HG21	2.46	0.50
1:G:576:ALA:HB3	1:G:847:GLN:HB3	1.92	0.50
1:H:267:THR:C	1:H:269:GLU:H	2.14	0.50
1:H:389:TYR:CZ	1:H:1050:GLY:HA2	2.46	0.50
1:H:740:ASN:HD22	1:H:742:SER:N	2.07	0.50
1:D:407:ASN:ND2	1:D:431:GLU:N	2.59	0.50
1:E:310:VAL:HG22	1:E:339:ILE:HD11	1.94	0.50
1:F:348:THR:HB	5:F:59:HOH:O	2.10	0.50
1:F:670:MET:CE	1:F:885:PHE:CZ	2.79	0.50
1:F:1052:ASN:N	1:F:1052:ASN:ND2	2.59	0.50
1:G:666:ASP:HA	1:G:863:PHE:O	2.12	0.50
1:H:367:GLN:O	1:H:370:TRP:N	2.35	0.50
1:A:355:TRP:C	1:A:355:TRP:CD2	2.84	0.50
1:A:613:THR:HG1	1:A:615:GLU:HB2	1.77	0.50
1:B:417:LYS:HE2	1:B:425:ARG:O	2.12	0.50
1:C:800:THR:HG22	1:C:801:ALA:N	2.26	0.50
1:D:457:MET:CE	1:D:493:TYR:HE2	2.24	0.50
1:D:585:ARG:HD3	1:D:661:ASP:OD1	2.12	0.50
1:D:928:LYS:HB2	1:D:929:PRO:HD2	1.93	0.50
1:E:988:LYS:H	1:E:990:THR:HG23	1.76	0.50
1:G:293:ARG:HB3	1:G:297:MET:HE2	1.93	0.50
1:D:271:TRP:CH2	1:D:294:PRO:HD3	2.46	0.50
1:E:330:LEU:O	1:E:333:ASN:CB	2.57	0.50
1:E:988:LYS:C	1:E:990:THR:HG23	2.32	0.50
1:F:409:THR:HG21	1:F:429:GLY:HA3	1.94	0.50
1:G:1065:GLN:CG	1:G:1066:ALA:N	2.74	0.50
1:C:360:ILE:O	1:C:364:VAL:HG23	2.11	0.50
1:E:306:GLN:O	1:E:307:ARG:C	2.49	0.50
1:F:302:ASP:C	1:F:302:ASP:OD1	2.50	0.50
1:G:312:TYR:OH	1:G:362:ALA:HB1	2.11	0.50
1:H:1064:ASP:N	1:H:1069:THR:O	2.41	0.50
1:A:280:ASP:OD1	1:A:348:THR:CB	2.59	0.50
1:B:561:ILE:HG12	1:B:697:MET:HB3	1.94	0.50
1:C:686:ALA:CB	1:C:767:LEU:HD21	2.42	0.50
1:D:782:GLN:NE2	1:D:782:GLN:CA	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:PRO:HG3	1:D:916:TYR:CE1	2.46	0.50
1:E:988:LYS:O	1:E:990:THR:CG2	2.59	0.50
1:F:436:ASN:HB2	1:F:961:MET:O	2.12	0.50
1:G:407:ASN:ND2	1:G:431:GLU:H	2.10	0.50
1:B:453:LEU:CD1	1:B:474:ILE:HG21	2.41	0.50
1:B:492:ASP:OD1	1:B:1025:ARG:NH1	2.45	0.50
1:C:975:VAL:HB	1:C:979:GLY:HA2	1.94	0.50
1:D:271:TRP:NE1	1:D:294:PRO:HB3	2.27	0.50
1:D:662:MET:C	1:D:674:THR:HG23	2.32	0.50
1:C:424:ASP:HB3	1:C:520:ASN:ND2	2.27	0.49
1:D:294:PRO:HG2	1:D:297:MET:HB2	1.94	0.49
1:E:457:MET:CE	1:E:493:TYR:CE2	2.95	0.49
1:B:689:LYS:HG2	1:B:690:TYR:CE1	2.47	0.49
1:C:250:GLN:OE1	1:C:1087:PRO:CG	2.60	0.49
1:C:346:LYS:O	1:C:349:ALA:HB3	2.13	0.49
1:F:407:ASN:ND2	1:F:431:GLU:H	2.10	0.49
1:F:581:TYR:HA	1:F:654:VAL:O	2.11	0.49
1:G:250:GLN:CG	1:G:251:VAL:N	2.73	0.49
1:B:390:SER:HB2	1:B:971:THR:HB	1.93	0.49
1:B:996:GLY:O	1:B:1044:SER:HA	2.12	0.49
1:E:367:GLN:O	1:E:370:TRP:N	2.37	0.49
1:F:572:ASN:OD1	1:F:718:LEU:O	2.30	0.49
1:F:762:GLN:N	1:F:791:THR:OG1	2.37	0.49
1:G:307:ARG:HA	1:G:332:LEU:HD22	1.94	0.49
1:B:256:ALA:O	1:B:257:ALA:C	2.51	0.49
1:B:262:VAL:CG1	1:B:969:VAL:HG23	2.31	0.49
1:B:614:MET:O	1:B:618:LYS:HG3	2.12	0.49
1:C:868:THR:O	1:C:869:LYS:HB3	2.12	0.49
1:E:271:TRP:CD2	1:E:294:PRO:CD	2.96	0.49
1:E:273:ARG:HG3	1:E:287:SER:CB	2.42	0.49
1:F:809:ASN:HB2	1:F:810:PRO:CD	2.42	0.49
1:H:769:LEU:HD21	1:H:819:TRP:CZ2	2.47	0.49
1:B:460:GLY:H	1:B:470:ASN:HD22	1.58	0.49
1:C:407:ASN:ND2	1:C:431:GLU:CB	2.76	0.49
1:E:310:VAL:CG2	1:E:339:ILE:CD1	2.90	0.49
1:E:861:SER:HB3	1:E:864:GLN:HG3	1.94	0.49
1:G:912:ILE:HG22	1:G:931:LYS:HZ2	1.77	0.49
1:A:658:TYR:CE2	1:A:660:GLY:HA3	2.47	0.49
1:C:492:ASP:HB3	1:C:1022:LEU:CD2	2.42	0.49
1:E:383:GLN:O	1:E:384:LYS:HB2	2.13	0.49
1:F:612:PHE:N	1:F:612:PHE:HD2	2.08	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:862:ASN:O	1:F:912:ILE:HD12	2.12	0.49
1:D:285:THR:HG22	1:D:286:GLN:N	2.28	0.49
1:D:296:LEU:O	1:D:300:TRP:NE1	2.45	0.49
1:G:574:GLU:O	1:G:574:GLU:HG3	1.93	0.49
1:G:1064:ASP:HB2	1:G:1071:PHE:CE1	2.47	0.49
1:H:278:LEU:HA	1:H:284:TRP:CA	2.20	0.49
1:B:442:ASN:HB3	1:B:445:VAL:HG23	1.95	0.49
1:C:723:THR:HG22	1:C:757:ALA:HB1	1.94	0.49
1:E:407:ASN:HD21	1:E:431:GLU:H	1.59	0.49
1:F:271:TRP:CZ2	1:F:357:ARG:HG3	2.48	0.49
1:F:711:VAL:HG22	1:F:734:VAL:HG23	1.94	0.49
1:F:1072:SER:OG	1:F:1074:VAL:HG12	2.12	0.49
1:G:1065:GLN:CG	1:G:1066:ALA:H	2.26	0.49
2:I:3:AC1:O3	2:I:3:AC1:C1B	2.60	0.49
1:A:522:THR:N	1:A:523:PRO:HD2	2.28	0.49
1:D:800:THR:HG23	1:D:801:ALA:N	2.28	0.49
1:E:912:ILE:H	1:E:912:ILE:HG13	1.47	0.49
1:G:856:MET:HG3	1:G:892:ASP:HB2	1.95	0.49
1:H:249:ASN:ND2	1:H:298:THR:HG22	2.28	0.49
1:H:261:HIS:CD2	1:H:264:HIS:H	2.30	0.49
1:H:920:ASP:OD2	1:H:1002:ASP:HB2	2.12	0.49
1:A:862:ASN:O	1:A:912:ILE:HD13	2.13	0.49
1:B:1063:LYS:HE2	1:B:1068:ASN:CG	2.33	0.49
1:C:462:ILE:HD13	1:C:1011:PHE:CZ	2.48	0.49
1:D:475:ARG:NH1	1:D:477:ASP:HB2	2.27	0.49
1:D:604:ASN:C	1:D:604:ASN:OD1	2.49	0.49
1:F:908:LEU:CD1	1:F:912:ILE:HG13	2.42	0.49
1:F:928:LYS:HB2	1:F:929:PRO:CD	2.43	0.49
1:B:689:LYS:HG2	1:B:690:TYR:CD1	2.48	0.48
1:C:504:ASP:OD1	1:C:846:HIS:HD2	1.96	0.48
1:D:285:THR:CG2	1:D:286:GLN:N	2.76	0.48
1:D:312:TYR:CD2	1:D:312:TYR:O	2.66	0.48
1:E:271:TRP:CD2	1:E:294:PRO:N	2.81	0.48
1:F:387:LEU:O	1:F:1050:GLY:HA3	2.13	0.48
1:F:603:ILE:CD1	1:F:619:LYS:HG3	2.43	0.48
1:G:530:ASP:HB2	1:G:843:LYS:HB3	1.95	0.48
1:G:588:ASP:OD1	1:G:588:ASP:N	2.44	0.48
1:G:988:LYS:N	1:G:990:THR:HG23	2.28	0.48
1:H:294:PRO:CD	1:H:297:MET:CE	2.77	0.48
1:A:512:SER:O	1:A:532:MET:HB2	2.13	0.48
1:C:707:ILE:C	1:C:707:ILE:HD12	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:988:LYS:O	1:D:988:LYS:CG	2.60	0.48
1:E:537:ASN:OD1	1:E:540:ARG:NH1	2.38	0.48
1:F:669:TYR:O	1:F:670:MET:HB2	2.13	0.48
1:G:250:GLN:HB2	1:G:1084:LEU:O	2.13	0.48
1:G:513:ILE:HG12	1:G:953:MET:CE	2.42	0.48
1:G:608:VAL:O	1:G:609:GLY:C	2.50	0.48
1:G:997:LYS:HA	1:G:1043:TRP:O	2.14	0.48
1:H:686:ALA:HB2	1:H:767:LEU:HD21	1.96	0.48
1:C:484:ALA:O	1:C:485:ASP:C	2.49	0.48
1:F:663:PHE:CD1	1:F:670:MET:HA	2.49	0.48
1:F:703:GLY:HA3	1:F:744:ARG:O	2.13	0.48
1:F:930:ASN:O	1:F:932:TYR:N	2.46	0.48
1:G:344:GLU:OE1	1:G:344:GLU:HA	2.13	0.48
1:H:656:ARG:HG3	1:H:856:MET:HB3	1.96	0.48
1:H:793:ASP:HB3	1:H:794:ARG:HG3	1.96	0.48
1:A:277:ILE:HG21	1:A:293:ARG:HH21	1.77	0.48
1:A:292:PHE:O	1:A:293:ARG:HD3	2.14	0.48
1:A:965:PRO:HD2	1:A:997:LYS:O	2.12	0.48
1:C:376:LYS:HB3	1:C:377:PRO:CA	2.38	0.48
1:D:245:PHE:CZ	1:D:278:LEU:HD22	2.48	0.48
1:E:715:LYS:HD2	1:E:830:VAL:HB	1.95	0.48
1:G:387:LEU:O	1:G:1050:GLY:HA3	2.13	0.48
1:H:276:TYR:HD1	1:H:285:THR:N	2.12	0.48
1:B:723:THR:O	1:B:723:THR:OG1	2.29	0.48
1:C:251:VAL:HG21	1:C:259:PHE:HZ	1.72	0.48
1:D:323:TYR:CD1	1:D:327:THR:HG21	2.49	0.48
1:F:1021:GLU:OE1	1:F:1021:GLU:N	2.45	0.48
1:G:759:HIS:CD2	1:G:762:GLN:OE1	2.67	0.48
1:G:883:ASP:OD1	1:G:948:LYS:HE3	2.12	0.48
1:H:277:ILE:O	1:H:279:LYS:N	2.45	0.48
1:B:417:LYS:HE3	1:F:555:SER:CB	2.39	0.48
1:C:512:SER:O	1:C:532:MET:HB2	2.14	0.48
1:D:578:VAL:HG13	1:D:579:PRO:HD2	1.96	0.48
1:E:322:THR:HG22	1:E:323:TYR:N	2.29	0.48
1:F:504:ASP:HB3	1:F:834:ALA:HB1	1.96	0.48
1:F:745:LEU:N	1:F:745:LEU:HD12	2.28	0.48
1:A:352:ASN:OD1	1:A:354:ASN:HB2	2.14	0.48
1:B:430:TYR:CE2	1:B:977:LYS:HE2	2.47	0.48
1:C:383:GLN:O	1:C:384:LYS:HB2	2.13	0.48
1:C:533:ILE:HA	5:C:181:HOH:O	2.13	0.48
1:C:615:GLU:OE1	1:C:615:GLU:HA	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:LEU:O	1:D:357:ARG:C	2.52	0.48
1:E:300:TRP:CD2	1:E:306:GLN:HB2	2.41	0.48
1:E:658:TYR:CE2	1:E:660:GLY:HA3	2.49	0.48
1:H:361:SER:O	1:H:362:ALA:C	2.50	0.48
1:A:295:LEU:HD23	1:A:1084:LEU:HD11	1.96	0.48
1:A:703:GLY:HA3	1:A:744:ARG:O	2.13	0.48
1:B:454:HIS:ND1	1:B:1015:LEU:HD21	2.29	0.48
1:C:794:ARG:HG2	1:C:794:ARG:NH1	2.28	0.48
1:D:588:ASP:OD1	1:D:589:SER:N	2.43	0.48
1:E:245:PHE:CG	1:E:284:TRP:HZ2	2.31	0.48
1:E:516:ALA:HB1	1:E:521:ASP:OD2	2.13	0.48
1:H:687:ARG:HA	1:H:691:VAL:HG23	1.95	0.48
1:A:300:TRP:CD1	1:A:306:GLN:HA	2.48	0.48
1:E:965:PRO:HD2	1:E:998:SER:HA	1.95	0.48
1:F:725:ASP:C	1:F:725:ASP:OD1	2.52	0.48
1:H:247:GLN:O	1:H:249:ASN:N	2.47	0.48
1:H:359:THR:O	1:H:360:ILE:O	2.32	0.48
1:H:1065:GLN:O	1:H:1066:ALA:C	2.52	0.48
1:A:300:TRP:CG	1:A:306:GLN:CG	2.97	0.48
1:C:841:ASP:OD1	1:C:846:HIS:HE1	1.96	0.48
1:H:668:GLN:OE1	1:H:668:GLN:HA	2.14	0.48
1:A:278:LEU:HB2	1:A:284:TRP:CZ2	2.49	0.47
1:A:327:THR:HG22	1:A:328:SER:N	2.29	0.47
1:A:444:VAL:HG11	1:A:1038:VAL:HG22	1.96	0.47
1:A:723:THR:HG22	1:A:757:ALA:HB1	1.96	0.47
1:B:919:THR:O	1:B:961:MET:CE	2.62	0.47
1:E:252:TYR:HB3	1:E:258:ASN:ND2	2.23	0.47
1:F:675:ILE:O	1:F:811:GLN:NE2	2.47	0.47
1:F:974:ARG:HB2	1:F:985:SER:OG	2.14	0.47
1:G:324:ASN:OD1	1:G:324:ASN:C	2.52	0.47
1:G:341:THR:O	1:G:342:LYS:C	2.53	0.47
1:G:365:LYS:HD3	1:G:365:LYS:HA	1.81	0.47
1:G:407:ASN:ND2	1:G:431:GLU:N	2.61	0.47
1:G:453:LEU:CD1	1:G:474:ILE:HG21	2.44	0.47
1:G:959:ASP:OD2	1:G:960:GLN:OE1	2.31	0.47
1:H:292:PHE:O	1:H:293:ARG:CG	2.62	0.47
1:H:581:TYR:HA	1:H:654:VAL:O	2.14	0.47
1:H:935:ALA:O	1:H:938:LEU:HB3	2.13	0.47
1:A:278:LEU:HD11	1:A:281:GLY:C	2.34	0.47
1:A:492:ASP:HB3	1:A:1022:LEU:HD22	1.95	0.47
1:C:505:LYS:O	1:C:505:LYS:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:719:LYS:NZ	5:F:202:HOH:O	2.43	0.47
1:G:383:GLN:O	1:G:384:LYS:CB	2.62	0.47
1:G:740:ASN:ND2	1:G:740:ASN:C	2.58	0.47
1:G:975:VAL:HB	1:G:979:GLY:HA2	1.96	0.47
1:H:702:VAL:O	1:H:703:GLY:C	2.49	0.47
1:A:809:ASN:HB2	1:A:810:PRO:CD	2.44	0.47
1:B:861:SER:O	1:B:864:GLN:HG3	2.14	0.47
1:E:245:PHE:O	1:E:249:ASN:CB	2.62	0.47
1:E:281:GLY:HA2	1:E:341:THR:HG22	1.96	0.47
1:E:297:MET:O	1:E:297:MET:CG	2.63	0.47
1:E:308:GLN:HE21	1:E:308:GLN:HB3	1.45	0.47
1:E:461:ASN:OD1	1:E:467:PRO:HA	2.13	0.47
1:E:475:ARG:NH1	1:E:477:ASP:HB2	2.29	0.47
1:H:389:TYR:CD1	1:H:389:TYR:N	2.80	0.47
1:H:687:ARG:HA	1:H:691:VAL:CG2	2.45	0.47
1:A:298:THR:HA	1:A:300:TRP:CH2	2.50	0.47
1:A:669:TYR:O	1:A:670:MET:HB2	2.12	0.47
1:F:483:ASP:C	1:F:483:ASP:OD1	2.53	0.47
1:G:339:ILE:O	1:G:343:ILE:CG1	2.42	0.47
1:H:991:LEU:HG	1:H:1070:TYR:CE2	2.50	0.47
2:O:2:GLC:H61	2:O:3:AC1:C5	2.39	0.47
1:A:374:SER:HB2	1:A:1058:ALA:CB	2.44	0.47
1:C:614:MET:CE	1:C:866:PHE:HE2	2.27	0.47
1:C:875:ASN:OD1	1:C:895:MET:CE	2.63	0.47
1:C:988:LYS:O	1:C:989:ASN:HB2	2.15	0.47
1:D:669:TYR:HE2	1:D:670:MET:HE3	1.79	0.47
1:E:1006:LYS:HD3	1:E:1007:TYR:CZ	2.50	0.47
1:F:603:ILE:HD11	1:F:619:LYS:HG3	1.96	0.47
1:G:642:LEU:HD12	1:G:642:LEU:N	2.29	0.47
1:H:271:TRP:CZ2	1:H:357:ARG:HG2	2.50	0.47
1:H:604:ASN:OD1	1:H:604:ASN:C	2.53	0.47
1:H:1052:ASN:ND2	1:H:1052:ASN:N	2.46	0.47
1:A:272:TYR:HE2	1:A:295:LEU:HA	1.80	0.47
1:A:606:ASN:O	1:A:607:VAL:C	2.52	0.47
1:C:445:VAL:O	1:C:449:GLN:HG2	2.15	0.47
1:C:686:ALA:HB2	1:C:767:LEU:HD21	1.96	0.47
1:C:988:LYS:H	1:C:990:THR:HG23	1.80	0.47
1:D:733:VAL:CG2	1:D:734:VAL:N	2.77	0.47
1:E:435:ALA:HA	1:E:1052:ASN:ND2	2.29	0.47
1:F:259:PHE:CD2	1:F:259:PHE:N	2.82	0.47
1:F:928:LYS:HB2	1:F:929:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:PHE:C	1:H:365:LYS:H	2.18	0.47
1:H:948:LYS:HD3	1:H:948:LYS:HA	1.67	0.47
1:A:737:GLU:HA	1:A:815:TYR:O	2.14	0.47
1:B:440:ASN:ND2	1:B:449:GLN:HE21	2.05	0.47
1:C:356:LEU:HA	1:C:359:THR:CG2	2.45	0.47
1:C:561:ILE:HG12	1:C:697:MET:CB	2.44	0.47
1:D:250:GLN:HE21	1:D:275:LYS:CD	2.27	0.47
1:D:658:TYR:CE2	1:D:660:GLY:HA3	2.49	0.47
1:D:1064:ASP:O	1:D:1068:ASN:N	2.48	0.47
1:E:407:ASN:ND2	1:E:430:TYR:HA	2.30	0.47
1:E:526:HIS:HA	1:E:530:ASP:OD1	2.14	0.47
1:F:690:TYR:HB3	1:F:732:GLY:O	2.15	0.47
1:G:307:ARG:HG3	1:G:332:LEU:HD21	1.95	0.47
4:G:5001:MES:H52	4:G:5001:MES:O3S	2.14	0.47
1:H:311:ASN:O	1:H:314:ASN:N	2.45	0.47
1:H:577:ALA:C	1:H:578:VAL:HG23	2.35	0.47
1:H:585:ARG:CD	1:H:661:ASP:OD1	2.62	0.47
1:A:246:ALA:O	1:A:249:ASN:HB2	2.15	0.47
1:A:868:THR:O	1:A:869:LYS:HB3	2.15	0.47
1:B:261:HIS:CD2	1:B:264:HIS:HA	2.50	0.47
1:B:765:ARG:HB2	1:B:766:PRO:HD2	1.97	0.47
1:B:1076:ASP:OD2	1:B:1077:ASN:HB2	2.15	0.47
1:C:492:ASP:HB3	1:C:1022:LEU:HD22	1.97	0.47
1:C:610:TYR:HA	1:C:612:PHE:CE2	2.50	0.47
1:C:988:LYS:O	1:C:988:LYS:CG	2.63	0.47
1:D:551:LEU:CD2	1:D:741:PRO:CG	2.93	0.47
1:G:725:ASP:C	1:G:725:ASP:OD1	2.51	0.47
1:H:461:ASN:H	1:H:470:ASN:HD21	1.61	0.47
1:A:271:TRP:CD2	1:A:294:PRO:HG3	2.50	0.47
1:A:285:THR:CG2	1:A:286:GLN:N	2.78	0.47
1:A:1063:LYS:HE2	1:A:1068:ASN:ND2	2.29	0.47
1:B:457:MET:HE2	1:B:493:TYR:CE2	2.50	0.47
1:B:920:ASP:HB3	1:B:923:ASP:HB2	1.97	0.47
1:D:280:ASP:C	1:D:282:LYS:N	2.69	0.47
1:D:294:PRO:HG2	1:D:297:MET:CB	2.45	0.47
1:D:421:TYR:CD1	1:D:523:PRO:HB2	2.50	0.47
1:E:277:ILE:HD11	1:E:291:ASP:CA	2.38	0.47
1:E:344:GLU:C	1:E:346:LYS:N	2.68	0.47
1:F:299:TRP:C	1:F:300:TRP:CD2	2.88	0.47
1:G:363:PHE:CZ	1:G:367:GLN:OE1	2.68	0.47
1:G:613:THR:N	1:G:616:GLU:OE1	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:846:HIS:HA	5:H:11:HOH:O	2.14	0.47
1:A:515:GLU:O	1:A:515:GLU:HG2	2.15	0.47
1:A:725:ASP:O	1:A:726:ARG:C	2.53	0.47
1:D:442:ASN:HB3	1:D:445:VAL:CG2	2.45	0.47
1:E:514:LEU:CD2	1:E:532:MET:HG3	2.45	0.47
1:E:703:GLY:HA3	1:E:744:ARG:O	2.15	0.47
1:G:964:LEU:HD12	1:G:996:GLY:HA2	1.96	0.47
1:H:515:GLU:OE1	2:P:3:AC1:O3	2.34	0.47
1:A:341:THR:O	1:A:343:ILE:N	2.48	0.46
1:C:276:TYR:HA	1:C:285:THR:O	2.15	0.46
1:C:471:PHE:CG	1:C:954:ALA:HB2	2.49	0.46
1:D:690:TYR:CE2	1:D:820:VAL:HB	2.50	0.46
1:D:965:PRO:HD2	1:D:997:LYS:O	2.15	0.46
1:D:987:ILE:HG12	1:D:1058:ALA:CB	2.45	0.46
1:F:639:ASN:ND2	1:F:813:SER:H	2.13	0.46
1:H:360:ILE:HD13	1:H:360:ILE:HA	1.75	0.46
1:C:718:LEU:HA	1:C:718:LEU:HD23	1.57	0.46
1:D:352:ASN:C	1:D:352:ASN:HD22	2.18	0.46
1:D:1073:LEU:HD21	1:D:1080:LEU:HD21	1.96	0.46
1:E:261:HIS:CD2	1:E:264:HIS:HA	2.49	0.46
1:E:427:ILE:N	4:E:5001:MES:O3S	2.47	0.46
1:F:854:ARG:NH1	1:F:892:ASP:OD2	2.44	0.46
1:G:627:ASP:OD2	1:G:636:THR:HG23	2.16	0.46
1:H:1069:THR:HG22	1:H:1070:TYR:N	2.30	0.46
1:A:355:TRP:CD2	1:A:356:LEU:N	2.83	0.46
1:D:804:ILE:O	1:D:805:LYS:HB3	2.14	0.46
1:D:1022:LEU:N	1:D:1022:LEU:HD23	2.29	0.46
1:E:793:ASP:O	1:E:793:ASP:OD1	2.33	0.46
1:F:816:LEU:HD12	1:F:817:GLY:N	2.29	0.46
1:G:912:ILE:HG22	1:G:931:LYS:NZ	2.30	0.46
1:H:294:PRO:O	1:H:296:LEU:N	2.49	0.46
1:A:729:ARG:HD2	1:A:758:ALA:O	2.15	0.46
1:B:639:ASN:O	1:B:640:THR:C	2.53	0.46
1:B:824:ALA:N	5:B:195:HOH:O	2.48	0.46
1:C:697:MET:O	1:C:698:ARG:NH1	2.47	0.46
1:E:319:ILE:HD11	1:E:342:LYS:HD2	1.96	0.46
1:E:407:ASN:ND2	1:E:431:GLU:N	2.64	0.46
1:F:457:MET:CE	1:F:493:TYR:HE2	2.29	0.46
1:F:669:TYR:CE2	1:F:670:MET:HE3	2.31	0.46
1:F:734:VAL:HB	1:F:755:MET:SD	2.55	0.46
1:F:750:ARG:CA	5:F:55:HOH:O	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ALA:O	1:B:258:ASN:N	2.48	0.46
1:C:733:VAL:CG2	1:C:734:VAL:N	2.79	0.46
1:C:862:ASN:O	1:C:912:ILE:HD13	2.15	0.46
1:E:346:LYS:HD3	1:E:355:TRP:CZ2	2.51	0.46
1:E:512:SER:O	1:E:532:MET:HB2	2.15	0.46
1:F:912:ILE:HG22	1:F:931:LYS:NZ	2.30	0.46
1:G:355:TRP:CD2	1:G:356:LEU:N	2.83	0.46
1:G:604:ASN:HD21	1:G:607:VAL:CB	2.27	0.46
1:H:439:ASP:OD1	1:H:439:ASP:C	2.51	0.46
1:H:877:VAL:HG12	1:H:881:ASN:HD22	1.81	0.46
1:A:250:GLN:NE2	1:A:275:LYS:HE3	2.29	0.46
1:A:278:LEU:O	1:A:281:GLY:N	2.48	0.46
1:A:354:ASN:O	1:A:357:ARG:HB2	2.16	0.46
1:B:1064:ASP:HB2	1:B:1071:PHE:CZ	2.51	0.46
1:C:874:THR:HG22	1:C:878:ILE:CD1	2.46	0.46
1:C:912:ILE:H	1:C:912:ILE:HG13	1.55	0.46
1:D:726:ARG:HE	1:D:726:ARG:HB3	1.26	0.46
1:D:740:ASN:ND2	1:D:740:ASN:C	2.61	0.46
1:D:1065:GLN:HG3	1:D:1066:ALA:H	1.81	0.46
1:D:1076:ASP:OD2	1:D:1077:ASN:HB2	2.15	0.46
1:E:454:HIS:CE1	1:E:458:ASN:HD21	2.33	0.46
1:F:630:ALA:O	1:F:633:LYS:NZ	2.48	0.46
1:G:258:ASN:C	1:G:259:PHE:CD2	2.89	0.46
1:G:920:ASP:OD2	1:G:923:ASP:HB2	2.16	0.46
1:B:987:ILE:HG13	1:B:1058:ALA:HB2	1.98	0.46
1:C:280:ASP:OD1	1:C:345:GLU:HA	2.15	0.46
1:C:297:MET:SD	1:C:340:GLN:HG3	2.56	0.46
1:C:1021:GLU:HG2	1:C:1022:LEU:N	2.29	0.46
1:E:298:THR:O	1:E:300:TRP:CZ3	2.68	0.46
1:F:352:ASN:OD1	1:F:354:ASN:ND2	2.48	0.46
1:H:733:VAL:HG23	1:H:819:TRP:O	2.16	0.46
2:I:3:AC1:O3	2:I:3:AC1:HCB1	2.15	0.46
1:B:604:ASN:HD21	1:B:607:VAL:HA	1.81	0.46
1:C:300:TRP:CE3	1:C:306:GLN:HG3	2.51	0.46
1:D:919:THR:O	1:D:919:THR:HG22	2.16	0.46
1:F:384:LYS:HA	5:F:149:HOH:O	2.16	0.46
1:G:252:TYR:CB	1:G:273:ARG:HG2	2.46	0.46
1:H:299:TRP:HH2	1:H:301:PRO:HB3	1.81	0.46
1:A:492:ASP:OD2	1:A:1025:ARG:NH1	2.42	0.46
1:C:387:LEU:O	1:C:1050:GLY:HA3	2.16	0.46
1:C:669:TYR:CE2	1:C:670:MET:CE	2.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:GLU:OE1	1:E:344:GLU:HA	2.16	0.46
1:E:1065:GLN:O	1:E:1066:ALA:C	2.54	0.46
1:F:551:LEU:HD22	1:F:741:PRO:HG2	1.97	0.46
1:G:396:THR:HG21	1:G:969:VAL:HG12	1.98	0.46
1:G:901:SER:OG	1:G:913:GLN:HA	2.16	0.46
1:H:299:TRP:O	1:H:300:TRP:CD2	2.69	0.46
1:H:436:ASN:HB2	1:H:961:MET:O	2.16	0.46
1:B:457:MET:CE	1:B:493:TYR:HE2	2.28	0.46
1:B:939:VAL:HG12	1:B:943:LYS:HZ2	1.53	0.46
1:D:407:ASN:HD21	1:D:431:GLU:H	1.63	0.46
1:E:250:GLN:HB3	1:E:1087:PRO:HG3	1.98	0.46
1:F:912:ILE:HG23	1:F:912:ILE:HD13	1.46	0.46
1:A:841:ASP:OD1	1:A:846:HIS:CE1	2.67	0.45
1:B:267:THR:HB	1:B:1060:TYR:CE2	2.51	0.45
1:B:555:SER:HB3	1:F:417:LYS:HE3	1.98	0.45
1:C:365:LYS:HD3	1:C:365:LYS:HA	1.70	0.45
1:F:558:ASN:N	1:F:559:PRO:CD	2.79	0.45
1:F:851:LEU:HD12	1:F:851:LEU:HA	1.81	0.45
1:F:951:LYS:HD3	1:F:951:LYS:HA	1.65	0.45
1:G:267:THR:O	1:G:269:GLU:N	2.49	0.45
1:B:625:ASN:O	1:B:628:LEU:HB2	2.16	0.45
1:B:1084:LEU:HD23	1:B:1084:LEU:N	2.29	0.45
1:C:1080:LEU:HB3	1:C:1081:PRO:HD2	1.97	0.45
1:D:245:PHE:O	1:D:248:TYR:N	2.48	0.45
1:D:356:LEU:HD12	1:D:360:ILE:HG12	1.98	0.45
1:F:809:ASN:HB2	1:F:810:PRO:HD2	1.97	0.45
1:H:296:LEU:N	1:H:296:LEU:HD12	2.32	0.45
1:A:262:VAL:HG12	1:A:969:VAL:HG23	1.99	0.45
1:A:276:TYR:HA	1:A:285:THR:O	2.16	0.45
1:A:312:TYR:OH	1:A:362:ALA:HB3	2.16	0.45
1:C:615:GLU:OE1	1:C:615:GLU:CA	2.64	0.45
1:C:669:TYR:HE2	1:C:670:MET:CE	2.25	0.45
1:D:280:ASP:C	1:D:282:LYS:H	2.19	0.45
1:D:869:LYS:O	1:D:870:LYS:C	2.55	0.45
1:D:948:LYS:NZ	5:D:226:HOH:O	2.49	0.45
1:E:337:GLN:O	1:E:339:ILE:N	2.49	0.45
1:F:278:LEU:HD13	1:F:284:TRP:CZ2	2.51	0.45
1:F:719:LYS:HE3	1:F:719:LYS:HB2	1.70	0.45
1:G:347:ILE:HA	1:G:355:TRP:HE1	1.82	0.45
1:H:371:ASN:HB3	1:H:373:ASP:H	1.81	0.45
1:B:725:ASP:C	1:B:725:ASP:OD1	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:ASP:OD1	1:D:846:HIS:CD2	2.62	0.45
1:F:407:ASN:ND2	1:F:431:GLU:N	2.64	0.45
1:F:604:ASN:OD1	1:F:604:ASN:C	2.55	0.45
1:F:613:THR:OG1	1:F:616:GLU:HG3	2.16	0.45
1:G:483:ASP:C	1:G:483:ASP:OD1	2.55	0.45
1:H:289:GLU:O	1:H:289:GLU:HG3	2.17	0.45
1:A:274:PRO:O	1:A:287:SER:HB3	2.16	0.45
1:A:376:LYS:CB	1:A:377:PRO:HA	2.31	0.45
1:C:1072:SER:OG	1:C:1074:VAL:HG13	2.16	0.45
1:F:1040:ILE:HG12	1:F:1047:TYR:CE2	2.52	0.45
2:J:2:GLC:H61	2:J:3:AC1:C5	2.39	0.45
1:A:355:TRP:CE3	1:A:355:TRP:O	2.69	0.45
1:B:658:TYR:CZ	1:B:660:GLY:HA3	2.50	0.45
1:C:430:TYR:HB3	1:C:978:TYR:CE1	2.51	0.45
1:C:744:ARG:HA	1:C:744:ARG:HD3	1.37	0.45
1:D:576:ALA:HB3	1:D:847:GLN:HB3	1.98	0.45
1:D:619:LYS:HD2	1:D:619:LYS:HA	1.75	0.45
1:D:800:THR:HG23	1:D:801:ALA:H	1.82	0.45
1:F:293:ARG:HH11	1:F:293:ARG:CG	2.21	0.45
1:F:627:ASP:O	1:F:628:LEU:C	2.54	0.45
1:G:512:SER:O	1:G:532:MET:HB2	2.16	0.45
1:G:604:ASN:ND2	1:G:607:VAL:CA	2.77	0.45
1:G:841:ASP:OD1	1:G:846:HIS:HE1	2.00	0.45
1:G:1080:LEU:HB3	1:G:1081:PRO:HD2	1.99	0.45
1:H:300:TRP:HE3	1:H:300:TRP:H	1.55	0.45
1:H:516:ALA:HB1	1:H:521:ASP:OD2	2.15	0.45
1:H:705:SER:HB3	1:H:743:LEU:CD1	2.43	0.45
1:A:537:ASN:OD1	1:A:540:ARG:NH1	2.49	0.45
1:A:1085:VAL:CG2	1:A:1086:ASN:H	2.30	0.45
1:B:439:ASP:C	1:B:439:ASP:OD1	2.55	0.45
1:B:510:HIS:CE1	5:B:197:HOH:O	2.68	0.45
1:C:315:ALA:O	1:C:317:LEU:N	2.50	0.45
1:F:585:ARG:HD3	1:F:661:ASP:OD1	2.17	0.45
1:F:690:TYR:CE2	1:F:820:VAL:HB	2.51	0.45
1:G:628:LEU:HD23	1:G:636:THR:HG21	1.98	0.45
1:G:809:ASN:CB	1:G:810:PRO:CD	2.93	0.45
1:H:298:THR:O	1:H:300:TRP:CZ3	2.66	0.45
1:A:312:TYR:O	1:A:315:ALA:HB3	2.17	0.45
1:C:252:TYR:HB2	1:C:273:ARG:HG2	1.99	0.45
1:C:312:TYR:OH	1:C:362:ALA:HB1	2.17	0.45
1:C:666:ASP:HA	1:C:863:PHE:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:SER:O	1:E:295:LEU:HB2	2.16	0.45
1:E:301:PRO:O	1:E:302:ASP:HB3	2.17	0.45
1:E:531:ASN:ND2	1:E:844:SER:OG	2.50	0.45
1:F:278:LEU:HB3	1:F:344:GLU:HG3	1.98	0.45
1:F:280:ASP:HA	1:F:348:THR:OG1	2.17	0.45
1:F:733:VAL:HG22	1:F:734:VAL:N	2.32	0.45
1:G:263:ASP:OD2	1:G:968:GLU:HA	2.16	0.45
1:G:296:LEU:HA	1:G:296:LEU:HD23	1.62	0.45
1:G:705:SER:HB3	1:G:743:LEU:HD13	1.98	0.45
1:A:273:ARG:NH1	1:A:289:GLU:HA	2.32	0.45
1:A:481:ASN:ND2	2:I:3:AC1:O2	2.50	0.45
1:B:471:PHE:CD1	1:B:954:ALA:HB2	2.52	0.45
1:B:688:ILE:HD11	1:B:889:GLY:CA	2.47	0.45
1:B:761:ASN:N	1:B:761:ASN:HD22	2.15	0.45
1:C:312:TYR:C	1:C:312:TYR:CD2	2.90	0.45
1:D:368:SER:O	1:D:371:ASN:HB2	2.17	0.45
1:E:293:ARG:HB3	1:E:294:PRO:HD2	1.98	0.45
1:E:725:ASP:C	1:E:725:ASP:OD1	2.55	0.45
1:F:604:ASN:O	1:F:604:ASN:CG	2.55	0.45
1:F:740:ASN:ND2	1:F:742:SER:H	2.15	0.45
1:F:988:LYS:N	1:F:990:THR:HG23	2.30	0.45
1:H:249:ASN:O	1:H:250:GLN:C	2.55	0.45
1:H:279:LYS:O	1:H:280:ASP:C	2.55	0.45
1:H:312:TYR:CD2	1:H:363:PHE:HB2	2.51	0.45
1:A:558:ASN:N	1:A:559:PRO:CD	2.79	0.45
1:A:561:ILE:HD13	1:A:561:ILE:HG21	1.71	0.45
1:C:581:TYR:HA	1:C:654:VAL:O	2.17	0.45
1:C:875:ASN:OD1	1:C:895:MET:HE3	2.17	0.45
4:C:5001:MES:H51	4:C:5001:MES:H81	1.48	0.45
1:D:339:ILE:HG22	1:D:343:ILE:HD11	1.99	0.45
1:D:700:GLN:HG2	1:D:702:VAL:HG13	1.99	0.45
1:E:1014:GLU:CG	1:E:1018:LYS:HE3	2.47	0.45
1:G:759:HIS:HD2	1:G:762:GLN:OE1	2.00	0.45
1:A:847:GLN:NE2	1:A:852:ASP:OD1	2.39	0.44
1:B:1086:ASN:N	1:B:1087:PRO:HD3	2.32	0.44
1:C:314:ASN:HB3	1:C:319:ILE:O	2.17	0.44
1:D:703:GLY:HA3	1:D:744:ARG:O	2.17	0.44
1:D:705:SER:HB3	1:D:743:LEU:HD13	1.99	0.44
1:E:279:LYS:N	1:E:283:THR:O	2.50	0.44
1:E:407:ASN:ND2	1:E:431:GLU:H	2.14	0.44
1:E:576:ALA:HB3	1:E:847:GLN:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:566:VAL:HG21	1:F:652:SER:HB3	1.99	0.44
1:G:733:VAL:HG22	1:G:734:VAL:N	2.32	0.44
2:K:2:GLC:H61	2:K:3:AC1:C5	2.39	0.44
1:A:281:GLY:N	1:A:344:GLU:HB2	2.31	0.44
1:B:430:TYR:CD2	1:B:977:LYS:HE2	2.52	0.44
1:C:869:LYS:O	1:C:870:LYS:C	2.55	0.44
1:E:928:LYS:HE3	1:E:928:LYS:HB2	1.63	0.44
1:F:300:TRP:N	1:F:300:TRP:CD2	2.86	0.44
1:H:291:ASP:OD1	1:H:291:ASP:N	2.51	0.44
1:H:421:TYR:CD1	1:H:523:PRO:HB2	2.52	0.44
1:H:686:ALA:CB	1:H:767:LEU:HD21	2.47	0.44
1:A:363:PHE:O	1:A:364:VAL:C	2.56	0.44
1:B:391:ASN:OD1	1:B:404:ARG:HD2	2.17	0.44
1:C:350:GLU:C	1:C:352:ASN:N	2.66	0.44
1:C:352:ASN:C	1:C:353:THR:CG2	2.86	0.44
1:C:376:LYS:HA	1:C:377:PRO:C	2.38	0.44
1:D:281:GLY:H	1:D:344:GLU:HB2	1.81	0.44
1:D:765:ARG:HB2	1:D:766:PRO:HD2	1.99	0.44
4:D:5001:MES:H82	4:D:5001:MES:H52	1.74	0.44
1:E:391:ASN:OD1	1:E:404:ARG:HD2	2.18	0.44
1:G:713:TYR:O	1:G:759:HIS:HE1	2.00	0.44
1:G:860:PHE:HB2	1:G:864:GLN:HE22	1.81	0.44
1:G:862:ASN:O	1:G:912:ILE:HD12	2.16	0.44
1:H:299:TRP:CH2	1:H:301:PRO:HB3	2.52	0.44
1:A:551:LEU:HD22	1:A:741:PRO:HG2	1.98	0.44
1:B:697:MET:O	1:B:698:ARG:NH1	2.43	0.44
1:C:247:GLN:NE2	1:C:247:GLN:CA	2.81	0.44
1:E:303:GLN:O	1:E:307:ARG:N	2.47	0.44
1:G:639:ASN:HD21	1:G:813:SER:N	2.05	0.44
1:A:310:VAL:CG1	1:A:314:ASN:ND2	2.81	0.44
1:A:577:ALA:C	1:A:578:VAL:HG23	2.38	0.44
1:A:776:LYS:CE	5:A:171:HOH:O	2.64	0.44
1:C:320:HIS:O	1:C:321:GLN:HB2	2.17	0.44
1:D:978:TYR:CE1	4:D:5001:MES:H81	2.53	0.44
1:E:718:LEU:HD23	1:E:718:LEU:HA	1.80	0.44
1:G:760:LYS:O	1:G:761:ASN:C	2.55	0.44
1:A:776:LYS:NZ	5:A:171:HOH:O	2.50	0.44
1:A:860:PHE:CD2	1:A:896:ALA:HB2	2.53	0.44
1:E:287:SER:HA	1:E:291:ASP:OD2	2.18	0.44
1:E:345:GLU:O	1:E:349:ALA:HB2	2.16	0.44
1:E:1019:TYR:N	1:E:1020:PRO:CD	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:604:ASN:HA	1:F:605:PRO:HD2	1.77	0.44
1:F:606:ASN:HB3	5:F:228:HOH:O	2.17	0.44
1:G:357:ARG:HD3	1:G:357:ARG:HA	1.78	0.44
1:H:668:GLN:HB2	1:H:671:ALA:HB2	1.98	0.44
1:C:908:LEU:O	1:C:912:ILE:HG13	2.18	0.44
1:E:1004:GLN:O	1:E:1008:GLY:N	2.46	0.44
1:F:900:VAL:HG23	1:F:923:ASP:O	2.17	0.44
1:G:299:TRP:CD1	1:G:1081:PRO:HB2	2.53	0.44
1:G:311:ASN:HD21	1:G:323:TYR:H	1.66	0.44
1:G:630:ALA:O	1:G:633:LYS:NZ	2.51	0.44
1:H:741:PRO:O	1:H:806:GLY:HA3	2.17	0.44
1:H:951:LYS:HA	1:H:951:LYS:HD3	1.76	0.44
1:A:280:ASP:OD1	1:A:345:GLU:HA	2.18	0.44
1:A:513:ILE:HG12	1:A:953:MET:CE	2.47	0.44
1:C:615:GLU:HB2	1:C:616:GLU:H	1.37	0.44
1:C:916:TYR:HB3	2:K:3:AC1:HC61	1.98	0.44
1:D:390:SER:HB2	1:D:971:THR:HB	2.00	0.44
1:D:973:THR:HG23	1:D:988:LYS:HA	1.98	0.44
1:G:294:PRO:O	1:G:297:MET:HB3	2.18	0.44
1:G:976:ASP:OD1	1:G:976:ASP:C	2.56	0.44
1:B:488:GLN:OE1	1:B:1028:ILE:HD12	2.18	0.44
1:B:951:LYS:HA	1:B:951:LYS:HD3	1.89	0.44
1:C:457:MET:CE	1:C:493:TYR:HE2	2.29	0.44
1:D:287:SER:HA	1:D:291:ASP:OD2	2.17	0.44
1:D:445:VAL:O	1:D:449:GLN:HG2	2.18	0.44
1:D:596:ARG:NH2	1:D:600:LYS:HD2	2.32	0.44
1:D:1065:GLN:HG3	1:D:1066:ALA:N	2.32	0.44
1:E:436:ASN:HB2	1:E:961:MET:O	2.18	0.44
1:G:280:ASP:O	1:G:282:LYS:N	2.51	0.44
1:A:371:ASN:OD1	1:A:372:SER:N	2.51	0.43
1:A:912:ILE:H	1:A:912:ILE:HG13	1.54	0.43
1:C:466:ASP:HA	1:C:467:PRO:HD2	1.79	0.43
1:C:604:ASN:ND2	1:C:607:VAL:HB	2.32	0.43
1:C:621:PHE:O	1:C:625:ASN:ND2	2.51	0.43
1:C:988:LYS:O	1:C:988:LYS:HG2	2.17	0.43
1:D:292:PHE:C	1:D:293:ARG:HG2	2.39	0.43
1:D:457:MET:HE3	1:D:493:TYR:HE2	1.83	0.43
1:D:541:LEU:HD23	1:D:541:LEU:HA	1.85	0.43
1:D:718:LEU:HA	1:D:718:LEU:HD23	1.73	0.43
1:D:894:GLU:HA	1:D:953:MET:HB3	1.99	0.43
1:E:245:PHE:HA	1:E:248:TYR:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:GLU:O	1:E:307:ARG:HB3	2.18	0.43
1:F:492:ASP:CB	1:F:1022:LEU:HD22	2.43	0.43
1:F:733:VAL:HG23	1:F:819:TRP:O	2.17	0.43
1:F:841:ASP:OD1	1:F:846:HIS:HE1	2.01	0.43
1:H:294:PRO:CD	1:H:297:MET:HE1	2.17	0.43
1:H:1034:MET:CE	5:H:198:HOH:O	2.66	0.43
1:A:278:LEU:CD1	1:A:282:LYS:N	2.81	0.43
1:B:460:GLY:N	1:B:470:ASN:ND2	2.66	0.43
1:D:530:ASP:HB2	1:D:843:LYS:HB3	2.00	0.43
1:E:733:VAL:HG22	1:E:734:VAL:N	2.33	0.43
1:F:421:TYR:CD1	1:F:523:PRO:HB2	2.53	0.43
1:G:355:TRP:CE3	1:G:355:TRP:C	2.91	0.43
1:H:278:LEU:HD22	1:H:284:TRP:CH2	2.53	0.43
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.58	0.43
1:A:310:VAL:HG13	1:A:339:ILE:HD11	2.00	0.43
1:A:551:LEU:CD2	1:A:741:PRO:HG2	2.48	0.43
1:B:797:LEU:HA	1:B:797:LEU:HD23	1.85	0.43
1:C:612:PHE:CD2	1:C:612:PHE:N	2.84	0.43
1:D:262:VAL:HG12	1:D:969:VAL:HG23	1.99	0.43
1:E:1072:SER:OG	1:E:1074:VAL:HG12	2.17	0.43
1:G:409:THR:O	1:G:410:PRO:C	2.55	0.43
1:G:871:GLU:H	1:G:871:GLU:CD	2.21	0.43
1:A:604:ASN:ND2	1:A:607:VAL:HA	2.13	0.43
1:B:252:TYR:HD2	1:B:258:ASN:HD21	1.66	0.43
1:B:368:SER:HA	1:B:371:ASN:ND2	2.29	0.43
1:C:278:LEU:HD13	1:C:284:TRP:CE2	2.53	0.43
1:C:389:TYR:CE1	1:C:1050:GLY:HA2	2.53	0.43
1:E:413:GLN:HG2	1:E:1028:ILE:HG22	1.99	0.43
1:G:314:ASN:ND2	1:G:319:ILE:HG22	2.33	0.43
1:G:371:ASN:HB3	1:G:373:ASP:HB2	2.00	0.43
1:G:522:THR:N	1:G:523:PRO:HD2	2.33	0.43
1:A:299:TRP:CZ2	1:A:301:PRO:HA	2.53	0.43
1:A:1065:GLN:HG3	1:A:1066:ALA:N	2.32	0.43
1:B:722:ASP:O	1:B:757:ALA:HB3	2.19	0.43
1:C:613:THR:OG1	1:C:615:GLU:HG2	2.18	0.43
1:D:317:LEU:HD13	1:D:342:LYS:HB3	2.00	0.43
1:D:670:MET:HE1	1:D:885:PHE:HZ	1.83	0.43
1:E:310:VAL:HG22	1:E:339:ILE:CD1	2.48	0.43
1:E:1080:LEU:HB2	1:E:1085:VAL:HG11	1.99	0.43
1:F:991:LEU:HG	1:F:1070:TYR:CE2	2.53	0.43
1:H:278:LEU:CB	1:H:284:TRP:HA	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:642:LEU:N	1:H:642:LEU:HD12	2.34	0.43
1:B:725:ASP:OD1	1:B:727:ILE:N	2.51	0.43
1:C:526:HIS:HA	1:C:530:ASP:OD1	2.18	0.43
1:C:924:LEU:HD12	1:C:924:LEU:N	2.33	0.43
1:D:669:TYR:HE2	1:D:670:MET:CE	2.31	0.43
1:D:884:LYS:HD3	1:D:884:LYS:HA	1.85	0.43
1:E:483:ASP:C	1:E:483:ASP:OD1	2.57	0.43
1:E:550:PRO:HA	1:E:638:TYR:CE2	2.53	0.43
1:F:749:ASP:C	1:F:750:ARG:CG	2.86	0.43
1:G:293:ARG:CG	1:G:297:MET:HE1	2.49	0.43
1:G:430:TYR:CG	1:G:977:LYS:HD2	2.53	0.43
1:A:272:TYR:CE2	1:A:295:LEU:HA	2.53	0.43
1:A:602:GLU:C	1:A:603:ILE:HG13	2.39	0.43
1:A:964:LEU:HB2	1:A:995:ASP:O	2.18	0.43
1:B:771:THR:O	1:B:772:ASP:C	2.56	0.43
1:C:1072:SER:HG	1:C:1074:VAL:HG13	1.84	0.43
1:E:478:ALA:HB1	1:E:481:ASN:HD22	1.83	0.43
1:E:499:GLY:O	1:E:502:LYS:HG3	2.19	0.43
1:F:273:ARG:NE	1:F:288:THR:O	2.51	0.43
1:F:278:LEU:CD2	1:F:281:GLY:HA2	2.35	0.43
1:F:340:GLN:O	1:F:344:GLU:HG2	2.18	0.43
1:F:750:ARG:N	5:F:55:HOH:O	2.52	0.43
1:G:271:TRP:CZ2	1:G:357:ARG:HA	2.53	0.43
1:G:407:ASN:HD21	1:G:431:GLU:H	1.65	0.43
1:A:453:LEU:CD1	1:A:474:ILE:HG21	2.49	0.43
1:A:461:ASN:OD1	1:A:467:PRO:HA	2.19	0.43
1:A:1085:VAL:HG23	1:A:1086:ASN:H	1.77	0.43
1:B:530:ASP:HB2	1:B:843:LYS:HB3	2.00	0.43
1:B:567:ASN:C	1:B:567:ASN:OD1	2.57	0.43
1:B:800:THR:HG22	1:B:801:ALA:N	2.24	0.43
1:B:874:THR:HB	1:B:932:TYR:HB3	2.00	0.43
1:C:524:TYR:C	1:C:524:TYR:CD2	2.91	0.43
1:D:259:PHE:CD2	1:D:259:PHE:N	2.85	0.43
1:D:271:TRP:CG	1:D:294:PRO:HA	2.50	0.43
1:D:669:TYR:CE2	1:D:670:MET:CE	3.01	0.43
1:D:700:GLN:HE21	1:D:702:VAL:CG1	2.32	0.43
1:D:759:HIS:HD2	1:D:762:GLN:OE1	2.01	0.43
1:E:310:VAL:HG21	1:E:335:ALA:HB1	2.01	0.43
1:E:356:LEU:O	1:E:357:ARG:C	2.56	0.43
1:F:253:SER:H	1:F:258:ASN:ND2	2.16	0.43
1:F:304:GLU:O	1:F:308:GLN:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:841:ASP:OD2	1:F:846:HIS:HE1	2.00	0.43
1:G:912:ILE:HG21	1:G:912:ILE:HD12	1.55	0.43
1:G:943:LYS:HB3	1:G:943:LYS:HE3	1.89	0.43
1:H:267:THR:C	1:H:1062:LEU:HD11	2.39	0.43
1:H:1022:LEU:N	1:H:1022:LEU:HD23	2.33	0.43
1:A:330:LEU:HD12	1:A:330:LEU:C	2.35	0.43
1:A:613:THR:OG1	1:A:616:GLU:HG3	2.18	0.43
1:B:709:THR:HG22	1:B:736:ILE:HG12	2.01	0.43
1:B:800:THR:C	1:B:802:ALA:N	2.72	0.43
1:B:920:ASP:HB3	1:B:923:ASP:CB	2.49	0.43
1:C:976:ASP:C	1:C:976:ASP:OD1	2.57	0.43
1:D:639:ASN:ND2	1:D:642:LEU:HD13	2.34	0.43
1:E:277:ILE:CG2	1:E:293:ARG:HH21	2.31	0.43
1:E:707:ILE:C	1:E:707:ILE:HD12	2.39	0.43
1:E:759:HIS:CD2	1:E:764:TYR:OH	2.72	0.43
1:F:857:PHE:CE2	1:F:859:GLY:HA2	2.52	0.43
1:F:930:ASN:C	1:F:932:TYR:H	2.22	0.43
1:F:1063:LYS:HE2	1:F:1068:ASN:ND2	2.33	0.43
1:G:481:ASN:ND2	2:O:3:AC1:O2	2.47	0.43
1:G:639:ASN:HB3	1:G:642:LEU:HB2	2.00	0.43
1:H:492:ASP:OD2	1:H:1025:ARG:NH1	2.40	0.43
1:A:281:GLY:C	1:A:341:THR:HG23	2.37	0.43
1:B:565:LEU:HD23	1:B:565:LEU:HA	1.91	0.43
1:B:610:TYR:O	1:B:908:LEU:HB2	2.19	0.43
1:B:922:TYR:HB2	1:B:1003:GLN:HB3	1.99	0.43
1:C:996:GLY:O	1:C:1044:SER:HA	2.19	0.43
1:D:304:GLU:OE1	1:D:304:GLU:CA	2.67	0.43
1:D:314:ASN:O	1:D:319:ILE:N	2.52	0.43
1:E:273:ARG:HG2	1:E:274:PRO:O	2.19	0.43
1:E:322:THR:HG23	1:E:323:TYR:H	1.81	0.43
1:E:596:ARG:HB2	1:E:612:PHE:HZ	1.84	0.43
1:E:854:ARG:NH1	1:E:892:ASP:OD2	2.42	0.43
1:F:841:ASP:OD2	1:F:846:HIS:CE1	2.72	0.43
1:G:614:MET:O	1:G:618:LYS:HG3	2.19	0.43
1:H:288:THR:CG2	1:H:289:GLU:N	2.34	0.43
1:D:551:LEU:HD12	1:D:551:LEU:O	2.19	0.42
1:E:1080:LEU:HB3	1:E:1081:PRO:HD2	2.01	0.42
1:F:988:LYS:H	1:F:990:THR:CG2	2.32	0.42
1:G:988:LYS:H	1:G:990:THR:CG2	2.32	0.42
2:L:2:GLC:H61	2:L:3:AC1:C5	2.39	0.42
1:A:988:LYS:C	1:A:990:THR:HG23	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ILE:HD13	1:B:1011:PHE:CZ	2.54	0.42
1:B:558:ASN:N	1:B:559:PRO:CD	2.82	0.42
1:B:698:ARG:HA	1:B:698:ARG:HD3	1.86	0.42
1:C:455:PHE:CD2	1:C:455:PHE:C	2.92	0.42
1:C:712:ARG:HA	1:C:712:ARG:HD2	1.84	0.42
1:D:567:ASN:C	1:D:567:ASN:OD1	2.56	0.42
1:E:321:GLN:CG	1:E:322:THR:H	2.05	0.42
1:E:339:ILE:HG22	1:E:343:ILE:HD11	2.00	0.42
1:E:458:ASN:O	1:E:459:PHE:C	2.56	0.42
1:E:734:VAL:O	1:E:734:VAL:HG13	2.19	0.42
1:F:875:ASN:OD1	1:F:895:MET:CE	2.67	0.42
1:G:267:THR:C	1:G:269:GLU:N	2.73	0.42
1:G:303:GLN:O	1:G:304:GLU:C	2.57	0.42
1:G:873:TYR:CD1	1:G:933:GLY:HA2	2.54	0.42
1:G:966:GLU:HB2	1:G:997:LYS:CB	2.42	0.42
1:B:871:GLU:H	1:B:871:GLU:CD	2.21	0.42
1:B:928:LYS:HE3	1:B:928:LYS:HB2	1.89	0.42
1:B:991:LEU:HD12	1:B:1061:VAL:HG11	2.01	0.42
1:E:268:ALA:HA	1:E:1062:LEU:HD11	2.02	0.42
1:E:619:LYS:HD2	1:E:619:LYS:HA	1.91	0.42
1:G:697:MET:HA	1:G:709:THR:O	2.19	0.42
1:H:1014:GLU:O	1:H:1018:LYS:HG3	2.19	0.42
1:A:293:ARG:CB	1:A:297:MET:CE	2.97	0.42
1:A:471:PHE:CG	1:A:954:ALA:HB2	2.54	0.42
4:A:5001:MES:H51	4:A:5001:MES:H81	1.82	0.42
4:A:5001:MES:H51	4:A:5001:MES:O2S	2.20	0.42
1:B:741:PRO:HB3	1:B:807:TYR:O	2.20	0.42
1:C:533:ILE:HD13	1:C:533:ILE:HG21	1.83	0.42
1:C:964:LEU:HD12	1:C:996:GLY:HA2	2.02	0.42
1:C:1072:SER:OG	1:C:1074:VAL:HG12	2.18	0.42
1:D:352:ASN:OD1	1:D:354:ASN:CB	2.59	0.42
1:D:550:PRO:HA	1:D:638:TYR:CE2	2.54	0.42
1:D:628:LEU:HD23	1:D:628:LEU:HA	1.83	0.42
1:E:376:LYS:HB3	1:E:377:PRO:HA	1.99	0.42
1:F:304:GLU:OE2	1:F:307:ARG:NH1	2.52	0.42
1:G:673:LYS:HD3	1:G:677:TYR:CD2	2.54	0.42
1:G:991:LEU:HD12	1:G:1061:VAL:HG11	2.00	0.42
1:H:251:VAL:HG13	1:H:251:VAL:O	2.20	0.42
1:H:604:ASN:OD1	1:H:606:ASN:N	2.50	0.42
1:H:782:GLN:HA	1:H:782:GLN:HE21	1.84	0.42
1:H:797:LEU:HD23	1:H:797:LEU:HA	1.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2:GLC:C6	2:I:3:AC1:C1	2.93	0.42
1:A:389:TYR:CZ	1:A:1050:GLY:HA2	2.54	0.42
1:A:466:ASP:OD2	1:A:943:LYS:HD2	2.20	0.42
1:C:296:LEU:HD23	1:C:296:LEU:HA	1.72	0.42
1:C:299:TRP:NE1	1:C:1081:PRO:HB3	2.33	0.42
1:D:418:ASP:OD1	1:D:419:PRO:HD2	2.20	0.42
1:D:461:ASN:H	1:D:470:ASN:HD21	1.67	0.42
1:E:310:VAL:HG23	1:E:339:ILE:CD1	2.49	0.42
1:E:479:VAL:HG21	1:E:514:LEU:HB3	2.01	0.42
1:E:614:MET:CE	1:E:866:PHE:HE2	2.32	0.42
1:H:267:THR:HB	1:H:1060:TYR:CE2	2.55	0.42
1:H:612:PHE:CD2	1:H:612:PHE:N	2.85	0.42
1:A:299:TRP:CH2	1:A:301:PRO:CA	3.02	0.42
1:A:355:TRP:O	1:A:355:TRP:HE3	2.02	0.42
1:A:479:VAL:HG21	1:A:514:LEU:HB3	2.02	0.42
1:A:670:MET:CE	1:A:885:PHE:CZ	3.02	0.42
1:C:533:ILE:HG13	1:C:533:ILE:O	2.19	0.42
1:C:964:LEU:O	1:C:995:ASP:HB3	2.19	0.42
1:D:408:ARG:HA	1:D:408:ARG:HD3	1.74	0.42
1:D:797:LEU:HD23	1:D:797:LEU:HA	1.78	0.42
1:E:288:THR:H	1:E:291:ASP:CG	2.22	0.42
1:E:316:GLN:C	1:E:318:GLY:H	2.23	0.42
1:F:364:VAL:HG13	1:F:370:TRP:CE3	2.54	0.42
1:F:797:LEU:HD23	1:F:797:LEU:HA	1.82	0.42
1:G:604:ASN:HD22	1:G:607:VAL:HB	1.81	0.42
1:G:738:GLY:O	1:G:814:GLY:HA3	2.19	0.42
1:G:973:THR:HG22	1:G:974:ARG:N	2.35	0.42
1:H:355:TRP:CG	1:H:356:LEU:N	2.87	0.42
1:H:442:ASN:OD1	1:H:442:ASN:C	2.58	0.42
1:H:460:GLY:H	1:H:470:ASN:HD22	1.66	0.42
1:A:894:GLU:HA	1:A:953:MET:HB3	2.02	0.42
1:B:603:ILE:HG22	1:B:604:ASN:N	2.33	0.42
1:B:658:TYR:O	1:B:659:TYR:C	2.58	0.42
1:B:719:LYS:HB2	1:B:719:LYS:HE3	1.66	0.42
1:B:1012:LEU:HD23	1:B:1012:LEU:HA	1.83	0.42
1:C:304:GLU:OE1	1:C:304:GLU:HA	2.20	0.42
1:C:457:MET:HE2	1:C:493:TYR:CE2	2.52	0.42
1:C:492:ASP:CG	1:C:1025:ARG:HH11	2.22	0.42
1:D:277:ILE:HD11	1:D:291:ASP:HB3	2.02	0.42
1:D:311:ASN:HD21	1:D:323:TYR:H	1.68	0.42
1:D:792:ASN:HD21	1:D:796:GLU:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1085:VAL:CG2	1:D:1086:ASN:N	2.73	0.42
1:G:449:GLN:HA	1:G:449:GLN:OE1	2.20	0.42
1:G:461:ASN:OD1	1:G:467:PRO:HA	2.19	0.42
1:G:951:LYS:HA	1:G:951:LYS:HD3	1.83	0.42
1:H:312:TYR:O	1:H:313:MET:C	2.58	0.42
1:H:461:ASN:OD1	1:H:467:PRO:HA	2.20	0.42
1:H:513:ILE:HG23	1:H:953:MET:HE1	2.01	0.42
1:H:860:PHE:HB2	1:H:864:GLN:HE22	1.84	0.42
1:A:273:ARG:HB2	1:A:292:PHE:CE2	2.55	0.42
1:B:267:THR:HA	1:B:1060:TYR:O	2.19	0.42
1:C:551:LEU:HD22	1:C:741:PRO:CG	2.49	0.42
1:D:630:ALA:O	1:D:633:LYS:NZ	2.53	0.42
1:D:727:ILE:HD12	1:D:727:ILE:HA	1.78	0.42
1:E:267:THR:C	1:E:269:GLU:H	2.23	0.42
1:E:297:MET:C	1:E:298:THR:CG2	2.88	0.42
1:E:367:GLN:HE21	1:E:367:GLN:HB3	1.60	0.42
1:F:312:TYR:C	1:F:312:TYR:HD2	2.20	0.42
1:F:432:PHE:HB2	1:F:977:LYS:HA	2.01	0.42
1:G:293:ARG:HG3	1:G:297:MET:HE1	2.02	0.42
1:G:476:VAL:HG22	1:G:956:TRP:CE3	2.51	0.42
1:G:656:ARG:HG3	1:G:856:MET:HB3	2.01	0.42
1:H:248:TYR:O	1:H:275:LYS:HB2	2.20	0.42
1:H:928:LYS:HB2	1:H:929:PRO:HD2	2.02	0.42
1:A:454:HIS:CE1	1:A:458:ASN:HD21	2.38	0.42
1:C:427:ILE:HG12	4:C:5001:MES:O2S	2.19	0.42
1:C:734:VAL:O	1:C:734:VAL:HG13	2.19	0.42
1:C:959:ASP:OD2	1:C:960:GLN:OE1	2.37	0.42
1:D:809:ASN:CB	1:D:810:PRO:CD	2.93	0.42
1:E:1080:LEU:HB2	1:E:1085:VAL:CG1	2.50	0.42
1:F:740:ASN:ND2	1:F:741:PRO:CD	2.73	0.42
1:F:1021:GLU:HB3	1:F:1022:LEU:H	1.73	0.42
1:G:355:TRP:CZ3	1:G:359:THR:HG21	2.54	0.42
1:G:604:ASN:HD21	1:G:607:VAL:N	2.17	0.42
1:G:917:ALA:HB1	1:G:962:TYR:CG	2.55	0.42
1:H:267:THR:C	1:H:269:GLU:N	2.72	0.42
1:H:387:LEU:HA	1:H:973:THR:O	2.19	0.42
1:H:797:LEU:HB3	1:H:799:PHE:CE2	2.54	0.42
1:A:304:GLU:OE1	1:A:304:GLU:CA	2.68	0.42
1:B:258:ASN:C	1:B:259:PHE:CD2	2.93	0.42
1:B:409:THR:O	1:B:410:PRO:C	2.56	0.42
1:C:1004:GLN:O	1:C:1004:GLN:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:TRP:CH2	1:D:301:PRO:CA	3.00	0.42
1:E:303:GLN:H	1:E:303:GLN:HG2	1.64	0.42
1:E:360:ILE:HG22	1:E:361:SER:N	2.34	0.42
1:E:928:LYS:HB2	1:E:929:PRO:CD	2.50	0.42
1:F:323:TYR:HB3	1:F:327:THR:OG1	2.20	0.42
1:G:323:TYR:HB3	1:G:327:THR:OG1	2.20	0.42
1:G:669:TYR:O	1:G:670:MET:CB	2.66	0.42
1:H:782:GLN:NE2	1:H:782:GLN:CA	2.83	0.42
1:A:267:THR:C	1:A:269:GLU:H	2.24	0.41
1:A:307:ARG:O	1:A:308:GLN:C	2.57	0.41
1:A:460:GLY:CA	1:A:470:ASN:ND2	2.83	0.41
1:A:698:ARG:O	1:A:708:ILE:HA	2.20	0.41
1:B:424:ASP:C	1:B:424:ASP:OD1	2.58	0.41
1:B:884:LYS:HA	1:B:884:LYS:HD3	1.77	0.41
1:B:912:ILE:HG23	1:B:912:ILE:HD13	1.58	0.41
1:B:987:ILE:CG1	1:B:1058:ALA:HB2	2.49	0.41
1:C:429:GLY:HA3	1:C:480:ASP:HB3	2.02	0.41
1:C:603:ILE:CD1	1:C:619:LYS:HG3	2.50	0.41
1:C:775:ILE:HD13	1:C:775:ILE:HG21	1.83	0.41
1:D:424:ASP:HB3	1:D:520:ASN:ND2	2.35	0.41
1:G:615:GLU:H	1:G:615:GLU:HG2	1.51	0.41
1:G:993:VAL:O	1:G:1056:ARG:NH1	2.48	0.41
1:H:300:TRP:HB3	1:H:301:PRO:HD2	2.02	0.41
1:H:355:TRP:CE3	1:H:356:LEU:N	2.88	0.41
1:A:261:HIS:HD2	1:A:264:HIS:CA	2.33	0.41
1:A:297:MET:HG2	1:A:298:THR:CG2	2.50	0.41
1:A:339:ILE:HG22	1:A:343:ILE:HD11	2.02	0.41
1:A:868:THR:OG1	1:A:872:GLU:OE1	2.34	0.41
1:A:976:ASP:OD1	1:A:976:ASP:C	2.58	0.41
1:B:259:PHE:N	1:B:259:PHE:HD2	2.16	0.41
1:B:628:LEU:HD23	1:B:628:LEU:HA	1.83	0.41
1:C:460:GLY:HA3	1:C:470:ASN:ND2	2.35	0.41
1:C:974:ARG:O	1:C:981:PRO:HA	2.20	0.41
1:D:258:ASN:O	1:D:292:PHE:HE1	2.02	0.41
1:D:278:LEU:HB2	1:D:284:TRP:CZ2	2.54	0.41
1:D:324:ASN:C	1:D:326:ALA:H	2.23	0.41
1:D:375:GLU:OE1	1:D:1053:ILE:HB	2.20	0.41
1:D:457:MET:CE	1:D:493:TYR:CE2	3.02	0.41
1:F:293:ARG:HB3	1:F:294:PRO:CD	2.49	0.41
1:F:327:THR:HG22	1:F:331:GLN:HB2	2.01	0.41
1:H:359:THR:O	1:H:360:ILE:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:639:ASN:O	1:H:640:THR:C	2.56	0.41
1:H:965:PRO:HD2	1:H:997:LYS:O	2.19	0.41
1:A:416:LYS:HD3	5:A:217:HOH:O	2.19	0.41
1:A:445:VAL:O	1:A:449:GLN:HG2	2.20	0.41
1:B:368:SER:HA	1:B:371:ASN:HB2	2.02	0.41
1:C:255:ASP:O	1:C:258:ASN:HB2	2.20	0.41
1:E:253:SER:H	1:E:258:ASN:ND2	2.17	0.41
1:E:279:LYS:O	1:E:279:LYS:CG	2.54	0.41
1:E:339:ILE:HG22	1:E:343:ILE:CD1	2.49	0.41
1:F:434:LEU:HD13	1:F:962:TYR:OH	2.19	0.41
1:F:619:LYS:HA	1:F:619:LYS:HD2	1.90	0.41
1:H:584:ILE:O	1:H:584:ILE:HG13	2.19	0.41
1:A:276:TYR:CA	1:A:285:THR:O	2.68	0.41
1:A:854:ARG:HH11	1:A:854:ARG:HD3	1.74	0.41
1:B:695:GLN:HA	1:B:711:VAL:O	2.21	0.41
1:C:503:ASN:HA	1:C:839:SER:OG	2.20	0.41
1:D:349:ALA:C	1:D:351:LYS:H	2.22	0.41
1:E:280:ASP:O	1:E:282:LYS:N	2.53	0.41
1:E:280:ASP:C	1:E:282:LYS:N	2.73	0.41
1:F:800:THR:O	1:F:801:ALA:C	2.58	0.41
1:F:912:ILE:HG21	1:F:912:ILE:HD12	1.56	0.41
1:G:267:THR:O	1:G:268:ALA:C	2.58	0.41
1:G:832:VAL:HG12	1:G:850:ALA:HA	2.02	0.41
1:A:305:THR:C	1:A:307:ARG:N	2.74	0.41
1:A:1072:SER:OG	1:A:1074:VAL:CG1	2.68	0.41
1:B:666:ASP:HA	1:B:863:PHE:O	2.20	0.41
1:B:1014:GLU:HG3	1:B:1018:LYS:HE3	2.02	0.41
1:C:352:ASN:OD1	1:C:354:ASN:HB2	2.20	0.41
1:C:737:GLU:HA	1:C:815:TYR:O	2.20	0.41
1:D:464:ALA:O	1:D:465:ASN:CB	2.67	0.41
1:E:413:GLN:HG2	1:E:1028:ILE:CG2	2.51	0.41
1:E:504:ASP:OD1	1:E:846:HIS:CD2	2.68	0.41
1:E:625:ASN:O	1:E:628:LEU:HB2	2.21	0.41
1:F:358:GLN:O	1:F:358:GLN:HG2	2.18	0.41
1:F:977:LYS:H	1:F:977:LYS:HG3	1.60	0.41
1:G:309:TYR:O	1:G:310:VAL:C	2.58	0.41
1:G:596:ARG:HB2	1:G:612:PHE:HZ	1.84	0.41
1:H:299:TRP:C	1:H:300:TRP:HE3	1.89	0.41
1:A:260:GLU:OE2	1:A:357:ARG:NH2	2.37	0.41
1:A:300:TRP:HB3	1:A:301:PRO:HD2	2.01	0.41
1:B:252:TYR:CB	1:B:273:ARG:HG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:TRP:HB2	1:B:921:ARG:NH2	2.36	0.41
1:B:546:SER:HB2	1:B:560:LEU:HD21	2.01	0.41
1:B:682:THR:HG22	1:B:767:LEU:HD11	2.02	0.41
1:D:337:GLN:O	1:D:340:GLN:N	2.46	0.41
1:D:522:THR:N	1:D:523:PRO:HD2	2.36	0.41
1:D:999:SER:O	1:D:1001:LYS:N	2.53	0.41
1:E:492:ASP:HB3	1:E:1022:LEU:HD22	2.01	0.41
1:E:752:VAL:HG22	1:E:798:ILE:CD1	2.45	0.41
1:E:1080:LEU:HB3	1:E:1081:PRO:CD	2.51	0.41
1:F:296:LEU:HD23	1:F:296:LEU:HA	1.97	0.41
1:G:367:GLN:O	1:G:370:TRP:N	2.39	0.41
1:G:687:ARG:HA	1:G:691:VAL:CG2	2.50	0.41
1:H:516:ALA:HB1	1:H:521:ASP:CB	2.50	0.41
1:A:718:LEU:HD23	1:A:718:LEU:HA	1.85	0.41
1:B:461:ASN:OD1	1:B:467:PRO:HB3	2.21	0.41
1:B:614:MET:HG3	1:B:618:LYS:HE3	2.01	0.41
1:C:334:LEU:O	1:C:335:ALA:C	2.57	0.41
1:D:959:ASP:OD2	1:D:960:GLN:OE1	2.39	0.41
1:D:975:VAL:HB	1:D:979:GLY:HA2	2.02	0.41
1:F:604:ASN:HD21	1:F:607:VAL:HA	1.85	0.41
1:F:688:ILE:HG12	1:F:831:ARG:CZ	2.50	0.41
1:G:280:ASP:OD1	1:G:348:THR:HB	2.20	0.41
1:G:466:ASP:HA	1:G:467:PRO:HD2	1.86	0.41
1:G:900:VAL:HG23	1:G:925:GLY:H	1.84	0.41
2:N:2:GLC:H61	2:N:3:AC1:C5	2.39	0.41
1:A:608:VAL:O	1:A:609:GLY:C	2.59	0.41
1:B:939:VAL:HG11	1:B:943:LYS:HZ3	1.70	0.41
1:C:561:ILE:HG22	1:C:562:THR:HG23	2.02	0.41
1:D:271:TRP:CH2	1:D:357:ARG:HD3	2.56	0.41
1:D:370:TRP:HA	1:D:1056:ARG:O	2.21	0.41
1:F:267:THR:HB	1:F:1060:TYR:CE2	2.55	0.41
1:F:293:ARG:HG2	1:F:293:ARG:NH1	2.27	0.41
1:F:389:TYR:CE1	1:F:1050:GLY:HA2	2.56	0.41
1:F:1064:ASP:O	1:F:1068:ASN:N	2.54	0.41
1:G:581:TYR:HA	1:G:654:VAL:O	2.21	0.41
1:H:619:LYS:HD2	1:H:619:LYS:HA	1.74	0.41
1:H:912:ILE:H	1:H:912:ILE:HG13	1.75	0.41
1:H:928:LYS:HB2	1:H:928:LYS:HE3	1.79	0.41
1:A:267:THR:C	1:A:269:GLU:N	2.74	0.41
1:A:293:ARG:HB3	1:A:297:MET:HE1	2.02	0.41
1:A:365:LYS:HD3	1:A:365:LYS:HA	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ALA:HA	1:A:1052:ASN:ND2	2.36	0.41
1:B:737:GLU:HA	1:B:815:TYR:O	2.21	0.41
1:C:267:THR:HB	1:C:1060:TYR:CE2	2.56	0.41
1:C:355:TRP:CD2	1:C:356:LEU:N	2.89	0.41
1:C:558:ASN:N	1:C:559:PRO:CD	2.84	0.41
1:D:589:SER:O	1:D:590:GLU:HB2	2.21	0.41
1:D:768:LEU:HD23	1:D:777:ALA:HA	2.01	0.41
1:D:970:VAL:O	1:D:991:LEU:HA	2.21	0.41
1:E:829:ASP:C	1:E:829:ASP:OD1	2.58	0.41
1:F:297:MET:HE3	1:F:298:THR:CG2	2.50	0.41
1:F:407:ASN:HD21	1:F:431:GLU:H	1.69	0.41
1:F:430:TYR:O	1:F:481:ASN:HA	2.21	0.41
1:F:585:ARG:NH1	1:F:661:ASP:OD1	2.40	0.41
1:F:836:THR:O	1:F:837:ALA:C	2.57	0.41
1:F:969:VAL:HG22	1:F:993:VAL:HG22	2.03	0.41
1:G:245:PHE:O	1:G:247:GLN:N	2.53	0.41
1:G:302:ASP:OD1	1:G:305:THR:OG1	2.36	0.41
1:G:376:LYS:HA	1:G:377:PRO:C	2.40	0.41
1:G:558:ASN:N	1:G:559:PRO:CD	2.84	0.41
1:G:737:GLU:HA	1:G:815:TYR:O	2.21	0.41
1:G:1076:ASP:OD2	1:G:1077:ASN:N	2.54	0.41
1:H:278:LEU:CD2	1:H:284:TRP:CZ3	3.04	0.41
1:H:387:LEU:O	1:H:1050:GLY:HA3	2.21	0.41
1:H:745:LEU:N	1:H:745:LEU:HD12	2.36	0.41
1:H:964:LEU:HA	1:H:965:PRO:HD3	1.92	0.41
1:H:996:GLY:O	1:H:1044:SER:HA	2.21	0.41
1:A:305:THR:C	1:A:307:ARG:H	2.23	0.41
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.21	0.41
1:B:408:ARG:HA	1:B:408:ARG:HD3	1.85	0.41
1:B:464:ALA:HA	5:B:27:HOH:O	2.22	0.41
1:C:245:PHE:CZ	1:C:337:GLN:HB3	2.56	0.41
1:C:376:LYS:CB	1:C:377:PRO:CA	2.99	0.41
1:D:276:TYR:CA	1:D:285:THR:O	2.69	0.41
1:D:558:ASN:N	1:D:559:PRO:CD	2.84	0.41
1:E:276:TYR:HB3	1:E:284:TRP:HE3	1.84	0.41
1:E:704:ASN:OD1	1:E:704:ASN:N	2.54	0.41
1:F:388:LEU:HD12	1:F:1049:ASN:O	2.21	0.41
1:F:726:ARG:O	1:F:729:ARG:HB3	2.20	0.41
1:F:792:ASN:ND2	1:F:796:GLU:HB2	2.36	0.41
1:G:360:ILE:O	1:G:364:VAL:HG23	2.20	0.41
1:H:364:VAL:HG13	1:H:370:TRP:CE3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:THR:HG21	1:H:970:VAL:HA	2.03	0.41
1:H:460:GLY:N	1:H:470:ASN:HD22	2.18	0.41
1:H:498:LYS:HA	1:H:498:LYS:HD3	1.89	0.41
2:M:2:GLC:H61	2:M:3:AC1:C5	2.39	0.41
1:A:279:LYS:O	1:A:280:ASP:HB2	2.22	0.40
1:A:337:GLN:O	1:A:338:THR:C	2.59	0.40
1:B:1025:ARG:O	1:B:1033:PRO:HA	2.21	0.40
1:C:651:LYS:O	1:C:652:SER:HB2	2.21	0.40
1:F:314:ASN:HB3	1:F:319:ILE:O	2.20	0.40
1:F:469:ALA:CB	1:F:939:VAL:HG13	2.51	0.40
1:F:698:ARG:O	1:F:708:ILE:HA	2.20	0.40
1:F:751:VAL:HG21	1:F:804:ILE:CD1	2.51	0.40
1:F:976:ASP:C	1:F:976:ASP:OD1	2.59	0.40
1:F:1078:THR:HG22	1:F:1079:PHE:N	2.36	0.40
1:G:247:GLN:O	1:G:248:TYR:C	2.59	0.40
1:G:267:THR:HB	1:G:1060:TYR:CE2	2.56	0.40
1:G:603:ILE:CD1	1:G:619:LYS:HG3	2.51	0.40
1:G:912:ILE:HG23	1:G:912:ILE:HD13	1.42	0.40
1:H:305:THR:C	1:H:307:ARG:N	2.73	0.40
1:H:549:LYS:HA	1:H:549:LYS:HD3	1.92	0.40
1:H:1086:ASN:HA	1:H:1087:PRO:HD3	1.92	0.40
1:A:310:VAL:O	1:A:314:ASN:N	2.47	0.40
1:A:337:GLN:O	1:A:340:GLN:N	2.52	0.40
1:A:615:GLU:OE1	1:A:615:GLU:CA	2.54	0.40
1:B:965:PRO:HD2	1:B:997:LYS:O	2.21	0.40
1:D:330:LEU:C	1:D:330:LEU:CD1	2.89	0.40
1:D:342:LYS:O	1:D:346:LYS:CB	2.69	0.40
1:D:504:ASP:O	1:D:508:ASN:HB2	2.21	0.40
1:D:525:LEU:HD12	1:D:525:LEU:HA	1.93	0.40
1:D:759:HIS:CD2	1:D:764:TYR:OH	2.74	0.40
1:D:809:ASN:HB2	1:D:810:PRO:HD3	2.03	0.40
1:D:924:LEU:N	1:D:924:LEU:HD12	2.36	0.40
1:E:396:THR:HG21	1:E:969:VAL:O	2.20	0.40
1:E:800:THR:HG23	1:E:801:ALA:N	2.36	0.40
1:F:321:GLN:HG3	1:F:323:TYR:CZ	2.56	0.40
1:F:466:ASP:OD2	1:F:943:LYS:HD2	2.20	0.40
1:F:574:GLU:HG3	1:F:575:THR:N	2.35	0.40
1:F:606:ASN:O	1:F:607:VAL:O	2.39	0.40
1:F:987:ILE:CG1	1:F:1058:ALA:HB2	2.50	0.40
1:G:273:ARG:HB2	1:G:292:PHE:CE2	2.56	0.40
1:G:439:ASP:C	1:G:439:ASP:OD1	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:658:TYR:O	1:G:659:TYR:C	2.59	0.40
1:H:300:TRP:CD1	1:H:306:GLN:CB	3.05	0.40
1:H:997:LYS:HA	1:H:1043:TRP:O	2.20	0.40
1:A:279:LYS:O	1:A:280:ASP:CB	2.69	0.40
1:A:882:VAL:HG21	1:A:944:ALA:C	2.42	0.40
1:B:744:ARG:HE	1:B:744:ARG:HB3	1.24	0.40
1:B:874:THR:HG22	1:B:875:ASN:N	2.36	0.40
1:C:481:ASN:ND2	2:K:3:AC1:O2	2.50	0.40
1:C:782:GLN:NE2	1:C:782:GLN:HA	2.35	0.40
1:C:974:ARG:HG2	1:C:987:ILE:HB	2.03	0.40
1:G:407:ASN:ND2	1:G:430:TYR:HA	2.37	0.40
1:G:965:PRO:HD2	1:G:998:SER:HA	2.02	0.40
1:G:1076:ASP:CG	1:G:1077:ASN:N	2.75	0.40
1:H:468:ASP:O	1:H:946:HIS:ND1	2.48	0.40
1:H:604:ASN:HA	1:H:605:PRO:HD2	1.67	0.40
1:H:877:VAL:CG1	1:H:881:ASN:ND2	2.85	0.40
1:A:272:TYR:O	1:A:293:ARG:N	2.50	0.40
1:A:285:THR:HG22	1:A:286:GLN:N	2.35	0.40
1:A:341:THR:O	1:A:344:GLU:N	2.54	0.40
1:A:565:LEU:HA	1:A:565:LEU:HD23	1.80	0.40
1:A:613:THR:C	1:A:615:GLU:N	2.74	0.40
1:A:1064:ASP:HB2	1:A:1071:PHE:CE1	2.56	0.40
1:C:788:VAL:HG12	1:C:789:ARG:N	2.36	0.40
1:D:339:ILE:O	1:D:343:ILE:CG1	2.40	0.40
1:D:453:LEU:CD1	1:D:474:ILE:HG21	2.52	0.40
1:F:759:HIS:HA	1:F:762:GLN:OE1	2.21	0.40
1:G:444:VAL:HG23	5:G:208:HOH:O	2.21	0.40
1:G:565:LEU:HA	1:G:565:LEU:HD23	1.87	0.40
1:G:996:GLY:O	1:G:1044:SER:HA	2.21	0.40
1:A:293:ARG:HD3	1:A:293:ARG:HH11	1.74	0.40
1:A:299:TRP:C	1:A:300:TRP:CD2	2.95	0.40
1:A:904:ASP:OD2	1:A:906:SER:OG	2.30	0.40
1:B:430:TYR:O	1:B:481:ASN:HA	2.20	0.40
1:C:326:ALA:O	1:C:327:THR:C	2.59	0.40
1:C:530:ASP:HB2	1:C:843:LYS:HB3	2.03	0.40
1:D:250:GLN:NE2	1:D:275:LYS:HD2	2.37	0.40
1:D:324:ASN:O	1:D:326:ALA:N	2.54	0.40
1:E:245:PHE:N	1:E:245:PHE:CG	2.90	0.40
1:F:250:GLN:CG	1:F:275:LYS:HE2	2.51	0.40
1:F:504:ASP:OD1	1:F:846:HIS:HD2	2.04	0.40
1:F:988:LYS:C	1:F:990:THR:HG23	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:567:ASN:OD1	1:G:567:ASN:C	2.59	0.40
1:G:882:VAL:HG21	1:G:944:ALA:C	2.42	0.40
1:H:776:LYS:HG2	1:H:778:TYR:CZ	2.57	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	840/844 (100%)	772 (92%)	57 (7%)	11 (1%)	12	41
1	B	743/844 (88%)	678 (91%)	53 (7%)	12 (2%)	9	36
1	C	842/844 (100%)	777 (92%)	57 (7%)	8 (1%)	15	48
1	D	842/844 (100%)	763 (91%)	66 (8%)	13 (2%)	10	38
1	E	841/844 (100%)	758 (90%)	70 (8%)	13 (2%)	10	38
1	F	842/844 (100%)	771 (92%)	65 (8%)	6 (1%)	22	56
1	G	842/844 (100%)	776 (92%)	56 (7%)	10 (1%)	13	43
1	H	803/844 (95%)	717 (89%)	62 (8%)	24 (3%)	4	23
All	All	6595/6752 (98%)	6012 (91%)	486 (7%)	97 (2%)	10	38

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	GLN
1	C	321	GLN
1	C	327	THR
1	C	351	LYS
1	D	278	LEU
1	D	281	GLY
1	D	351	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	320	HIS
1	E	321	GLN
1	E	1066	ALA
1	F	246	ALA
1	F	1021	GLU
1	G	246	ALA
1	H	247	GLN
1	H	250	GLN
1	H	277	ILE
1	H	286	GLN
1	H	302	ASP
1	H	311	ASN
1	H	313	MET
1	H	360	ILE
1	A	247	GLN
1	A	281	GLY
1	A	315	ALA
1	B	257	ALA
1	B	724	GLY
1	B	761	ASN
1	B	1066	ALA
1	C	316	GLN
1	D	246	ALA
1	D	349	ALA
1	D	1021	GLU
1	D	1066	ALA
1	E	268	ALA
1	E	312	TYR
1	E	337	GLN
1	E	360	ILE
1	F	724	GLY
1	G	281	GLY
1	G	1021	GLU
1	H	246	ALA
1	H	248	TYR
1	H	279	LYS
1	H	280	ASP
1	A	327	THR
1	A	351	LYS
1	B	384	LYS
1	B	1000	GLY
1	B	1045	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	268	ALA
1	C	315	ALA
1	D	304	GLU
1	D	325	THR
1	E	338	THR
1	E	351	LYS
1	F	279	LYS
1	G	253	SER
1	G	348	THR
1	G	351	LYS
1	G	362	ALA
1	G	1066	ALA
1	H	268	ALA
1	H	278	LEU
1	H	1045	ALA
1	H	1066	ALA
1	A	353	THR
1	A	1066	ALA
1	D	254	THR
1	E	302	ASP
1	E	307	ARG
1	G	609	GLY
1	H	257	ALA
1	H	316	GLN
1	A	342	LYS
1	B	870	LYS
1	D	250	GLN
1	D	357	ARG
1	D	1000	GLY
1	E	362	ALA
1	H	312	TYR
1	H	357	ARG
1	H	358	GLN
1	H	364	VAL
1	A	268	ALA
1	A	384	LYS
1	B	614	MET
1	C	381	HIS
1	C	870	LYS
1	F	607	VAL
1	G	384	LYS
1	H	440	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	556	GLY
1	E	1008	GLY
1	A	609	GLY
1	H	310	VAL
1	B	882	VAL
1	F	603	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	713/715 (100%)	669 (94%)	44 (6%)	18 48
1	B	627/715 (88%)	596 (95%)	31 (5%)	25 57
1	C	715/715 (100%)	671 (94%)	44 (6%)	18 48
1	D	715/715 (100%)	671 (94%)	44 (6%)	18 48
1	E	714/715 (100%)	658 (92%)	56 (8%)	12 40
1	F	715/715 (100%)	662 (93%)	53 (7%)	13 41
1	G	715/715 (100%)	666 (93%)	49 (7%)	15 44
1	H	682/715 (95%)	640 (94%)	42 (6%)	18 48
All	All	5596/5720 (98%)	5233 (94%)	363 (6%)	17 47

All (363) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	253	SER
1	A	258	ASN
1	A	276	TYR
1	A	279	LYS
1	A	280	ASP
1	A	286	GLN
1	A	298	THR
1	A	309	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	321	GLN
1	A	342	LYS
1	A	352	ASN
1	A	353	THR
1	A	359	THR
1	A	368	SER
1	A	371	ASN
1	A	374	SER
1	A	422	THR
1	A	425	ARG
1	A	477	ASP
1	A	502	LYS
1	A	532	MET
1	A	574	GLU
1	A	600	LYS
1	A	604	ASN
1	A	605	PRO
1	A	614	MET
1	A	619	LYS
1	A	632	GLU
1	A	726	ARG
1	A	729	ARG
1	A	740	ASN
1	A	803	ASP
1	A	835	SER
1	A	880	LYS
1	A	882	VAL
1	A	912	ILE
1	A	977	LYS
1	A	985	SER
1	A	1001	LYS
1	A	1037	SER
1	A	1044	SER
1	A	1052	ASN
1	A	1074	VAL
1	B	254	THR
1	B	259	PHE
1	B	390	SER
1	B	392	ASN
1	B	394	LYS
1	B	422	THR
1	B	425	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	501	HIS
1	B	502	LYS
1	B	505	LYS
1	B	532	MET
1	B	540	ARG
1	B	574	GLU
1	B	600	LYS
1	B	604	ASN
1	B	612	PHE
1	B	632	GLU
1	B	726	ARG
1	B	740	ASN
1	B	744	ARG
1	B	761	ASN
1	B	793	ASP
1	B	835	SER
1	B	882	VAL
1	B	977	LYS
1	B	985	SER
1	B	988	LYS
1	B	1001	LYS
1	B	1038	VAL
1	B	1052	ASN
1	B	1074	VAL
1	C	247	GLN
1	C	253	SER
1	C	258	ASN
1	C	275	LYS
1	C	283	THR
1	C	285	THR
1	C	286	GLN
1	C	290	LYS
1	C	308	GLN
1	C	321	GLN
1	C	342	LYS
1	C	350	GLU
1	C	352	ASN
1	C	353	THR
1	C	368	SER
1	C	374	SER
1	C	390	SER
1	C	394	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	422	THR
1	C	425	ARG
1	C	532	MET
1	C	574	GLU
1	C	604	ASN
1	C	612	PHE
1	C	614	MET
1	C	619	LYS
1	C	629	LEU
1	C	632	GLU
1	C	702	VAL
1	C	726	ARG
1	C	740	ASN
1	C	744	ARG
1	C	835	SER
1	C	882	VAL
1	C	912	ILE
1	C	977	LYS
1	C	985	SER
1	C	988	LYS
1	C	990	THR
1	C	1001	LYS
1	C	1038	VAL
1	C	1052	ASN
1	C	1064	ASP
1	C	1074	VAL
1	D	247	GLN
1	D	277	ILE
1	D	287	SER
1	D	290	LYS
1	D	308	GLN
1	D	312	TYR
1	D	322	THR
1	D	325	THR
1	D	341	THR
1	D	347	ILE
1	D	352	ASN
1	D	358	GLN
1	D	359	THR
1	D	366	THR
1	D	368	SER
1	D	374	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	394	LYS
1	D	396	THR
1	D	422	THR
1	D	477	ASP
1	D	532	MET
1	D	540	ARG
1	D	551	LEU
1	D	574	GLU
1	D	600	LYS
1	D	605	PRO
1	D	614	MET
1	D	619	LYS
1	D	632	GLU
1	D	726	ARG
1	D	727	ILE
1	D	729	ARG
1	D	740	ASN
1	D	832	VAL
1	D	882	VAL
1	D	977	LYS
1	D	986	GLN
1	D	988	LYS
1	D	1001	LYS
1	D	1013	GLU
1	D	1021	GLU
1	D	1038	VAL
1	D	1052	ASN
1	D	1074	VAL
1	E	245	PHE
1	E	247	GLN
1	E	253	SER
1	E	258	ASN
1	E	259	PHE
1	E	279	LYS
1	E	286	GLN
1	E	287	SER
1	E	290	LYS
1	E	291	ASP
1	E	292	PHE
1	E	295	LEU
1	E	304	GLU
1	E	305	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	308	GLN
1	E	310	VAL
1	E	311	ASN
1	E	322	THR
1	E	325	THR
1	E	327	THR
1	E	330	LEU
1	E	332	LEU
1	E	341	THR
1	E	359	THR
1	E	361	SER
1	E	365	LYS
1	E	368	SER
1	E	390	SER
1	E	394	LYS
1	E	422	THR
1	E	477	ASP
1	E	502	LYS
1	E	505	LYS
1	E	532	MET
1	E	574	GLU
1	E	614	MET
1	E	619	LYS
1	E	632	GLU
1	E	702	VAL
1	E	727	ILE
1	E	740	ASN
1	E	744	ARG
1	E	750	ARG
1	E	835	SER
1	E	882	VAL
1	E	904	ASP
1	E	928	LYS
1	E	977	LYS
1	E	985	SER
1	E	986	GLN
1	E	988	LYS
1	E	1038	VAL
1	E	1052	ASN
1	E	1064	ASP
1	E	1074	VAL
1	E	1075	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	244	SER
1	F	253	SER
1	F	258	ASN
1	F	279	LYS
1	F	290	LYS
1	F	305	THR
1	F	308	GLN
1	F	322	THR
1	F	350	GLU
1	F	352	ASN
1	F	357	ARG
1	F	361	SER
1	F	368	SER
1	F	374	SER
1	F	394	LYS
1	F	396	THR
1	F	422	THR
1	F	425	ARG
1	F	477	ASP
1	F	502	LYS
1	F	532	MET
1	F	540	ARG
1	F	574	GLU
1	F	604	ASN
1	F	612	PHE
1	F	619	LYS
1	F	626	LYS
1	F	632	GLU
1	F	710	SER
1	F	719	LYS
1	F	726	ARG
1	F	740	ASN
1	F	744	ARG
1	F	750	ARG
1	F	782	GLN
1	F	794	ARG
1	F	800	THR
1	F	803	ASP
1	F	835	SER
1	F	861	SER
1	F	868	THR
1	F	880	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	882	VAL
1	F	912	ILE
1	F	977	LYS
1	F	980	THR
1	F	988	LYS
1	F	1021	GLU
1	F	1025	ARG
1	F	1038	VAL
1	F	1044	SER
1	F	1052	ASN
1	F	1074	VAL
1	G	253	SER
1	G	258	ASN
1	G	259	PHE
1	G	275	LYS
1	G	283	THR
1	G	286	GLN
1	G	288	THR
1	G	295	LEU
1	G	303	GLN
1	G	305	THR
1	G	308	GLN
1	G	316	GLN
1	G	320	HIS
1	G	322	THR
1	G	347	ILE
1	G	355	TRP
1	G	359	THR
1	G	366	THR
1	G	368	SER
1	G	374	SER
1	G	422	THR
1	G	425	ARG
1	G	465	ASN
1	G	477	ASP
1	G	532	MET
1	G	540	ARG
1	G	574	GLU
1	G	600	LYS
1	G	604	ASN
1	G	670	MET
1	G	727	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	729	ARG
1	G	740	ASN
1	G	744	ARG
1	G	794	ARG
1	G	800	THR
1	G	832	VAL
1	G	835	SER
1	G	882	VAL
1	G	912	ILE
1	G	977	LYS
1	G	985	SER
1	G	990	THR
1	G	1001	LYS
1	G	1021	GLU
1	G	1038	VAL
1	G	1052	ASN
1	G	1074	VAL
1	G	1084	LEU
1	H	248	TYR
1	H	253	SER
1	H	258	ASN
1	H	278	LEU
1	H	279	LYS
1	H	290	LYS
1	H	300	TRP
1	H	304	GLU
1	H	308	GLN
1	H	310	VAL
1	H	356	LEU
1	H	359	THR
1	H	360	ILE
1	H	361	SER
1	H	368	SER
1	H	374	SER
1	H	394	LYS
1	H	396	THR
1	H	422	THR
1	H	477	ASP
1	H	502	LYS
1	H	505	LYS
1	H	532	MET
1	H	574	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	614	MET
1	H	619	LYS
1	H	632	GLU
1	H	728	THR
1	H	729	ARG
1	H	740	ASN
1	H	750	ARG
1	H	882	VAL
1	H	904	ASP
1	H	928	LYS
1	H	961	MET
1	H	977	LYS
1	H	985	SER
1	H	988	LYS
1	H	1001	LYS
1	H	1016	GLN
1	H	1052	ASN
1	H	1074	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	261	HIS
1	A	303	GLN
1	A	311	ASN
1	A	316	GLN
1	A	407	ASN
1	A	440	ASN
1	A	458	ASN
1	A	461	ASN
1	A	470	ASN
1	A	481	ASN
1	A	531	ASN
1	A	572	ASN
1	A	604	ASN
1	A	639	ASN
1	A	740	ASN
1	A	759	HIS
1	A	782	GLN
1	A	846	HIS
1	A	864	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1003	GLN
1	A	1052	ASN
1	A	1068	ASN
1	B	250	GLN
1	B	258	ASN
1	B	261	HIS
1	B	371	ASN
1	B	392	ASN
1	B	407	ASN
1	B	440	ASN
1	B	470	ASN
1	B	481	ASN
1	B	531	ASN
1	B	572	ASN
1	B	625	ASN
1	B	639	ASN
1	B	740	ASN
1	B	759	HIS
1	B	761	ASN
1	B	782	GLN
1	B	846	HIS
1	B	864	GLN
1	B	881	ASN
1	B	1016	GLN
1	B	1052	ASN
1	C	247	GLN
1	C	258	ASN
1	C	261	HIS
1	C	311	ASN
1	C	371	ASN
1	C	407	ASN
1	C	440	ASN
1	C	458	ASN
1	C	470	ASN
1	C	481	ASN
1	C	531	ASN
1	C	572	ASN
1	C	625	ASN
1	C	639	ASN
1	C	700	GLN
1	C	740	ASN
1	C	759	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	782	GLN
1	C	846	HIS
1	C	864	GLN
1	C	1052	ASN
1	C	1068	ASN
1	D	258	ASN
1	D	261	HIS
1	D	303	GLN
1	D	308	GLN
1	D	311	ASN
1	D	367	GLN
1	D	407	ASN
1	D	440	ASN
1	D	470	ASN
1	D	481	ASN
1	D	531	ASN
1	D	572	ASN
1	D	639	ASN
1	D	700	GLN
1	D	740	ASN
1	D	759	HIS
1	D	782	GLN
1	D	846	HIS
1	D	864	GLN
1	D	881	ASN
1	D	1003	GLN
1	D	1052	ASN
1	E	247	GLN
1	E	258	ASN
1	E	261	HIS
1	E	306	GLN
1	E	308	GLN
1	E	311	ASN
1	E	333	ASN
1	E	354	ASN
1	E	367	GLN
1	E	407	ASN
1	E	440	ASN
1	E	458	ASN
1	E	470	ASN
1	E	481	ASN
1	E	531	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	639	ASN
1	E	740	ASN
1	E	759	HIS
1	E	782	GLN
1	E	846	HIS
1	E	864	GLN
1	E	1052	ASN
1	F	258	ASN
1	F	261	HIS
1	F	308	GLN
1	F	311	ASN
1	F	333	ASN
1	F	337	GLN
1	F	354	ASN
1	F	367	GLN
1	F	407	ASN
1	F	440	ASN
1	F	470	ASN
1	F	481	ASN
1	F	531	ASN
1	F	572	ASN
1	F	625	ASN
1	F	639	ASN
1	F	740	ASN
1	F	759	HIS
1	F	782	GLN
1	F	846	HIS
1	F	864	GLN
1	F	881	ASN
1	F	913	GLN
1	F	1052	ASN
1	F	1068	ASN
1	G	250	GLN
1	G	258	ASN
1	G	261	HIS
1	G	308	GLN
1	G	311	ASN
1	G	316	GLN
1	G	367	GLN
1	G	407	ASN
1	G	440	ASN
1	G	470	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	481	ASN
1	G	531	ASN
1	G	572	ASN
1	G	604	ASN
1	G	639	ASN
1	G	740	ASN
1	G	759	HIS
1	G	782	GLN
1	G	846	HIS
1	G	864	GLN
1	G	881	ASN
1	G	1052	ASN
1	H	258	ASN
1	H	261	HIS
1	H	303	GLN
1	H	308	GLN
1	H	311	ASN
1	H	367	GLN
1	H	407	ASN
1	H	440	ASN
1	H	458	ASN
1	H	470	ASN
1	H	481	ASN
1	H	531	ASN
1	H	639	ASN
1	H	740	ASN
1	H	759	HIS
1	H	782	GLN
1	H	846	HIS
1	H	864	GLN
1	H	881	ASN
1	H	1052	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	I	1	2	12,12,12	0.69	0	17,17,17	2.03	6 (35%)
2	GLC	I	2	2	11,11,12	1.19	0	15,15,17	2.72	5 (33%)
2	AC1	I	3	2	21,22,23	1.48	5 (23%)	22,32,34	2.28	4 (18%)
2	GLC	J	1	2	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	GLC	J	2	2	11,11,12	1.15	1 (9%)	15,15,17	2.33	5 (33%)
2	AC1	J	3	2	21,22,23	1.35	2 (9%)	22,32,34	1.97	4 (18%)
2	GLC	K	1	2	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	GLC	K	2	2	11,11,12	1.14	1 (9%)	15,15,17	2.34	5 (33%)
2	AC1	K	3	2	21,22,23	1.34	2 (9%)	22,32,34	1.98	4 (18%)
2	GLC	L	1	2	12,12,12	0.80	0	17,17,17	1.92	5 (29%)
2	GLC	L	2	2	11,11,12	1.14	1 (9%)	15,15,17	2.33	5 (33%)
2	AC1	L	3	2	21,22,23	1.35	2 (9%)	22,32,34	1.98	4 (18%)
2	GLC	M	1	2	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	GLC	M	2	2	11,11,12	1.15	1 (9%)	15,15,17	2.33	5 (33%)
2	AC1	M	3	2	21,22,23	1.36	3 (14%)	22,32,34	1.97	4 (18%)
2	GLC	N	1	2	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	GLC	N	2	2	11,11,12	1.15	1 (9%)	15,15,17	2.33	5 (33%)
2	AC1	N	3	2	21,22,23	1.34	2 (9%)	22,32,34	1.98	4 (18%)
2	GLC	O	1	2	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	GLC	O	2	2	11,11,12	1.13	1 (9%)	15,15,17	2.34	5 (33%)
2	AC1	O	3	2	21,22,23	1.35	2 (9%)	22,32,34	1.97	4 (18%)
2	GLC	P	1	2	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	GLC	P	2	2	11,11,12	1.14	1 (9%)	15,15,17	2.33	5 (33%)
2	AC1	P	3	2	21,22,23	1.35	2 (9%)	22,32,34	1.97	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	AC1	I	3	2	-	3/6/43/46	0/2/2/2
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	2/2/19/22	0/1/1/1
2	AC1	J	3	2	-	3/6/43/46	0/2/2/2
2	GLC	K	1	2	-	2/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	AC1	K	3	2	-	3/6/43/46	0/2/2/2
2	GLC	L	1	2	-	2/2/22/22	0/1/1/1
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1
2	AC1	L	3	2	-	3/6/43/46	0/2/2/2
2	GLC	M	1	2	-	2/2/22/22	0/1/1/1
2	GLC	M	2	2	-	2/2/19/22	0/1/1/1
2	AC1	M	3	2	-	3/6/43/46	0/2/2/2
2	GLC	N	1	2	-	2/2/22/22	0/1/1/1
2	GLC	N	2	2	-	2/2/19/22	0/1/1/1
2	AC1	N	3	2	-	3/6/43/46	0/2/2/2
2	GLC	O	1	2	-	2/2/22/22	0/1/1/1
2	GLC	O	2	2	-	2/2/19/22	0/1/1/1
2	AC1	O	3	2	-	3/6/43/46	0/2/2/2
2	GLC	P	1	2	-	2/2/22/22	0/1/1/1
2	GLC	P	2	2	-	2/2/19/22	0/1/1/1
2	AC1	P	3	2	-	3/6/43/46	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	AC1	C4A-C5B	-3.16	1.48	1.51
2	L	3	AC1	C4A-C5B	-2.73	1.49	1.51
2	J	3	AC1	C4A-C5B	-2.71	1.49	1.51
2	M	3	AC1	C4A-C5B	-2.70	1.49	1.51
2	P	3	AC1	C4A-C5B	-2.70	1.49	1.51
2	O	3	AC1	C4A-C5B	-2.62	1.49	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	3	AC1	C4A-C5B	-2.61	1.49	1.51
2	K	3	AC1	C4A-C5B	-2.57	1.49	1.51
2	I	3	AC1	C2B-C1B	-2.55	1.49	1.52
2	N	3	AC1	C3-C4	-2.55	1.48	1.53
2	M	3	AC1	C3-C4	-2.53	1.48	1.53
2	O	3	AC1	C3-C4	-2.53	1.48	1.53
2	P	3	AC1	C3-C4	-2.53	1.48	1.53
2	L	3	AC1	C3-C4	-2.53	1.48	1.53
2	J	3	AC1	C3-C4	-2.53	1.48	1.53
2	K	3	AC1	C3-C4	-2.52	1.48	1.53
2	N	2	GLC	O5-C1	-2.44	1.39	1.43
2	J	2	GLC	O5-C1	-2.44	1.39	1.43
2	M	2	GLC	O5-C1	-2.42	1.39	1.43
2	I	3	AC1	O5-C1	-2.40	1.39	1.43
2	P	2	GLC	O5-C1	-2.39	1.39	1.43
2	L	2	GLC	O5-C1	-2.39	1.39	1.43
2	K	2	GLC	O5-C1	-2.38	1.39	1.43
2	O	2	GLC	O5-C1	-2.37	1.39	1.43
2	I	3	AC1	C4-N4A	-2.19	1.43	1.47
2	I	3	AC1	C3-C4	-2.07	1.49	1.53
2	M	3	AC1	O5-C1	-2.00	1.40	1.43

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	AC1	C1-C2-C3	8.17	119.71	109.67
2	L	3	AC1	C2-C3-C4	-6.23	105.13	110.63
2	K	3	AC1	C2-C3-C4	-6.20	105.16	110.63
2	N	3	AC1	C2-C3-C4	-6.20	105.17	110.63
2	P	3	AC1	C2-C3-C4	-6.18	105.18	110.63
2	M	3	AC1	C2-C3-C4	-6.18	105.18	110.63
2	O	3	AC1	C2-C3-C4	-6.17	105.19	110.63
2	J	3	AC1	C2-C3-C4	-6.14	105.22	110.63
2	I	2	GLC	C1-O5-C5	6.01	120.34	112.19
2	I	2	GLC	O2-C2-C1	-5.70	97.49	109.15
2	I	1	GLC	C3-C4-C5	-4.70	101.85	110.24
2	J	2	GLC	C6-C5-C4	-4.52	102.42	113.00
2	K	2	GLC	C6-C5-C4	-4.51	102.43	113.00
2	O	2	GLC	C6-C5-C4	-4.51	102.44	113.00
2	L	2	GLC	C6-C5-C4	-4.51	102.44	113.00
2	N	2	GLC	C6-C5-C4	-4.50	102.46	113.00
2	M	2	GLC	C6-C5-C4	-4.50	102.47	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	GLC	C6-C5-C4	-4.50	102.47	113.00
2	K	2	GLC	O2-C2-C1	-4.42	100.10	109.15
2	N	2	GLC	O2-C2-C1	-4.42	100.12	109.15
2	O	2	GLC	O2-C2-C1	-4.41	100.12	109.15
2	J	2	GLC	O2-C2-C1	-4.41	100.13	109.15
2	P	2	GLC	O2-C2-C1	-4.41	100.14	109.15
2	L	2	GLC	O2-C2-C1	-4.40	100.16	109.15
2	M	2	GLC	O2-C2-C1	-4.38	100.18	109.15
2	N	1	GLC	C3-C4-C5	-4.35	102.49	110.24
2	L	1	GLC	C3-C4-C5	-4.34	102.50	110.24
2	O	1	GLC	C3-C4-C5	-4.33	102.51	110.24
2	J	1	GLC	C3-C4-C5	-4.31	102.54	110.24
2	P	1	GLC	C3-C4-C5	-4.31	102.54	110.24
2	M	1	GLC	C3-C4-C5	-4.31	102.55	110.24
2	K	1	GLC	C3-C4-C5	-4.31	102.56	110.24
2	O	3	AC1	O3-C3-C2	4.10	117.84	109.99
2	M	3	AC1	O3-C3-C2	4.09	117.82	109.99
2	J	3	AC1	O3-C3-C2	4.09	117.82	109.99
2	N	3	AC1	O3-C3-C2	4.08	117.82	109.99
2	L	3	AC1	O3-C3-C2	4.08	117.81	109.99
2	K	3	AC1	O3-C3-C2	4.07	117.79	109.99
2	P	3	AC1	O3-C3-C2	4.06	117.77	109.99
2	O	2	GLC	C1-C2-C3	3.95	114.53	109.67
2	P	2	GLC	C1-C2-C3	3.94	114.51	109.67
2	M	2	GLC	C1-C2-C3	3.94	114.51	109.67
2	K	2	GLC	C1-C2-C3	3.93	114.50	109.67
2	J	2	GLC	C1-C2-C3	3.93	114.50	109.67
2	N	2	GLC	C1-C2-C3	3.92	114.48	109.67
2	L	2	GLC	C1-C2-C3	3.90	114.46	109.67
2	I	2	GLC	O3-C3-C4	-3.75	101.67	110.35
2	I	2	GLC	C6-C5-C4	-3.74	104.24	113.00
2	M	1	GLC	C4-C3-C2	-3.45	104.81	110.82
2	L	1	GLC	C4-C3-C2	-3.43	104.83	110.82
2	K	1	GLC	C4-C3-C2	-3.43	104.84	110.82
2	J	1	GLC	C4-C3-C2	-3.42	104.85	110.82
2	N	1	GLC	C4-C3-C2	-3.41	104.86	110.82
2	P	1	GLC	C4-C3-C2	-3.41	104.87	110.82
2	O	1	GLC	C4-C3-C2	-3.40	104.88	110.82
2	O	2	GLC	O3-C3-C4	-3.38	102.53	110.35
2	P	2	GLC	O3-C3-C4	-3.37	102.55	110.35
2	N	2	GLC	O3-C3-C4	-3.37	102.55	110.35
2	J	2	GLC	O3-C3-C4	-3.37	102.56	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	AC1	O3-C3-C4	-3.37	102.86	109.66
2	K	2	GLC	O3-C3-C4	-3.37	102.56	110.35
2	L	2	GLC	O3-C3-C4	-3.36	102.58	110.35
2	M	2	GLC	O3-C3-C4	-3.36	102.58	110.35
2	I	2	GLC	O5-C5-C6	-3.22	102.16	107.20
2	I	1	GLC	C1-C2-C3	3.15	116.84	110.31
2	I	1	GLC	O5-C5-C4	-3.09	104.09	109.69
2	M	1	GLC	O2-C2-C1	-2.84	102.56	109.16
2	N	1	GLC	O2-C2-C1	-2.84	102.57	109.16
2	P	1	GLC	O2-C2-C1	-2.83	102.59	109.16
2	O	1	GLC	O2-C2-C1	-2.83	102.60	109.16
2	J	1	GLC	O2-C2-C1	-2.83	102.60	109.16
2	K	1	GLC	O2-C2-C1	-2.83	102.60	109.16
2	L	1	GLC	O2-C2-C1	-2.83	102.61	109.16
2	I	1	GLC	O5-C1-C2	2.78	115.25	110.28
2	K	3	AC1	O4-C4A-C3B	-2.44	105.48	110.53
2	J	3	AC1	O4-C4A-C3B	-2.44	105.50	110.53
2	N	3	AC1	O4-C4A-C3B	-2.44	105.50	110.53
2	P	3	AC1	O4-C4A-C3B	-2.43	105.51	110.53
2	L	3	AC1	O4-C4A-C3B	-2.43	105.51	110.53
2	O	3	AC1	O4-C4A-C3B	-2.43	105.52	110.53
2	M	3	AC1	O4-C4A-C3B	-2.42	105.53	110.53
2	I	3	AC1	O5-C1-C2	2.40	114.48	110.77
2	P	3	AC1	O6B-C6B-C5B	-2.32	106.94	112.50
2	K	3	AC1	O6B-C6B-C5B	-2.32	106.96	112.50
2	M	3	AC1	O6B-C6B-C5B	-2.31	106.96	112.50
2	N	3	AC1	O6B-C6B-C5B	-2.31	106.97	112.50
2	J	3	AC1	O6B-C6B-C5B	-2.31	106.97	112.50
2	L	3	AC1	O6B-C6B-C5B	-2.31	106.98	112.50
2	O	3	AC1	O6B-C6B-C5B	-2.31	106.98	112.50
2	P	1	GLC	O1-C1-O5	-2.30	103.47	110.38
2	K	1	GLC	O1-C1-O5	-2.30	103.48	110.38
2	J	1	GLC	O1-C1-O5	-2.30	103.48	110.38
2	L	1	GLC	O1-C1-O5	-2.30	103.48	110.38
2	O	1	GLC	O1-C1-O5	-2.29	103.50	110.38
2	M	1	GLC	O1-C1-O5	-2.29	103.51	110.38
2	I	3	AC1	O6B-C6B-C5B	-2.29	107.03	112.50
2	N	1	GLC	O1-C1-O5	-2.28	103.55	110.38
2	I	1	GLC	O2-C2-C1	-2.15	104.17	109.16
2	P	2	GLC	O5-C5-C6	-2.14	103.85	107.20
2	K	2	GLC	O5-C5-C6	-2.14	103.85	107.20
2	L	2	GLC	O5-C5-C6	-2.13	103.86	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	GLC	C4-C3-C2	-2.13	107.11	110.82
2	J	2	GLC	O5-C5-C6	-2.13	103.87	107.20
2	M	2	GLC	O5-C5-C6	-2.13	103.87	107.20
2	O	2	GLC	O5-C5-C6	-2.12	103.88	107.20
2	J	1	GLC	O4-C4-C5	-2.11	104.06	109.30
2	N	2	GLC	O5-C5-C6	-2.11	103.90	107.20
2	K	1	GLC	O4-C4-C5	-2.10	104.08	109.30
2	N	1	GLC	O4-C4-C5	-2.10	104.08	109.30
2	M	1	GLC	O4-C4-C5	-2.10	104.08	109.30
2	O	1	GLC	O4-C4-C5	-2.10	104.09	109.30
2	L	1	GLC	O4-C4-C5	-2.09	104.11	109.30
2	P	1	GLC	O4-C4-C5	-2.08	104.12	109.30

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	AC1	C7B-C1B-N4A-C4
2	I	3	AC1	C4A-C5B-C6B-O6B
2	I	3	AC1	C7B-C5B-C6B-O6B
2	J	3	AC1	C7B-C1B-N4A-C4
2	J	3	AC1	C4A-C5B-C6B-O6B
2	J	3	AC1	C7B-C5B-C6B-O6B
2	K	3	AC1	C7B-C1B-N4A-C4
2	K	3	AC1	C4A-C5B-C6B-O6B
2	K	3	AC1	C7B-C5B-C6B-O6B
2	L	3	AC1	C7B-C1B-N4A-C4
2	L	3	AC1	C4A-C5B-C6B-O6B
2	L	3	AC1	C7B-C5B-C6B-O6B
2	M	3	AC1	C7B-C1B-N4A-C4
2	M	3	AC1	C4A-C5B-C6B-O6B
2	M	3	AC1	C7B-C5B-C6B-O6B
2	N	3	AC1	C7B-C1B-N4A-C4
2	N	3	AC1	C4A-C5B-C6B-O6B
2	N	3	AC1	C7B-C5B-C6B-O6B
2	O	3	AC1	C7B-C1B-N4A-C4
2	O	3	AC1	C4A-C5B-C6B-O6B
2	O	3	AC1	C7B-C5B-C6B-O6B
2	P	3	AC1	C7B-C1B-N4A-C4
2	P	3	AC1	C4A-C5B-C6B-O6B
2	P	3	AC1	C7B-C5B-C6B-O6B
2	J	1	GLC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	1	GLC	O5-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	M	1	GLC	O5-C5-C6-O6
2	N	1	GLC	O5-C5-C6-O6
2	O	1	GLC	O5-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	J	2	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	L	2	GLC	O5-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
2	N	2	GLC	O5-C5-C6-O6
2	O	2	GLC	O5-C5-C6-O6
2	P	2	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	J	1	GLC	C4-C5-C6-O6
2	K	1	GLC	C4-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	M	1	GLC	C4-C5-C6-O6
2	N	1	GLC	C4-C5-C6-O6
2	O	1	GLC	C4-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	J	2	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
2	L	2	GLC	C4-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	O	2	GLC	C4-C5-C6-O6
2	P	2	GLC	C4-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 61 short contacts:

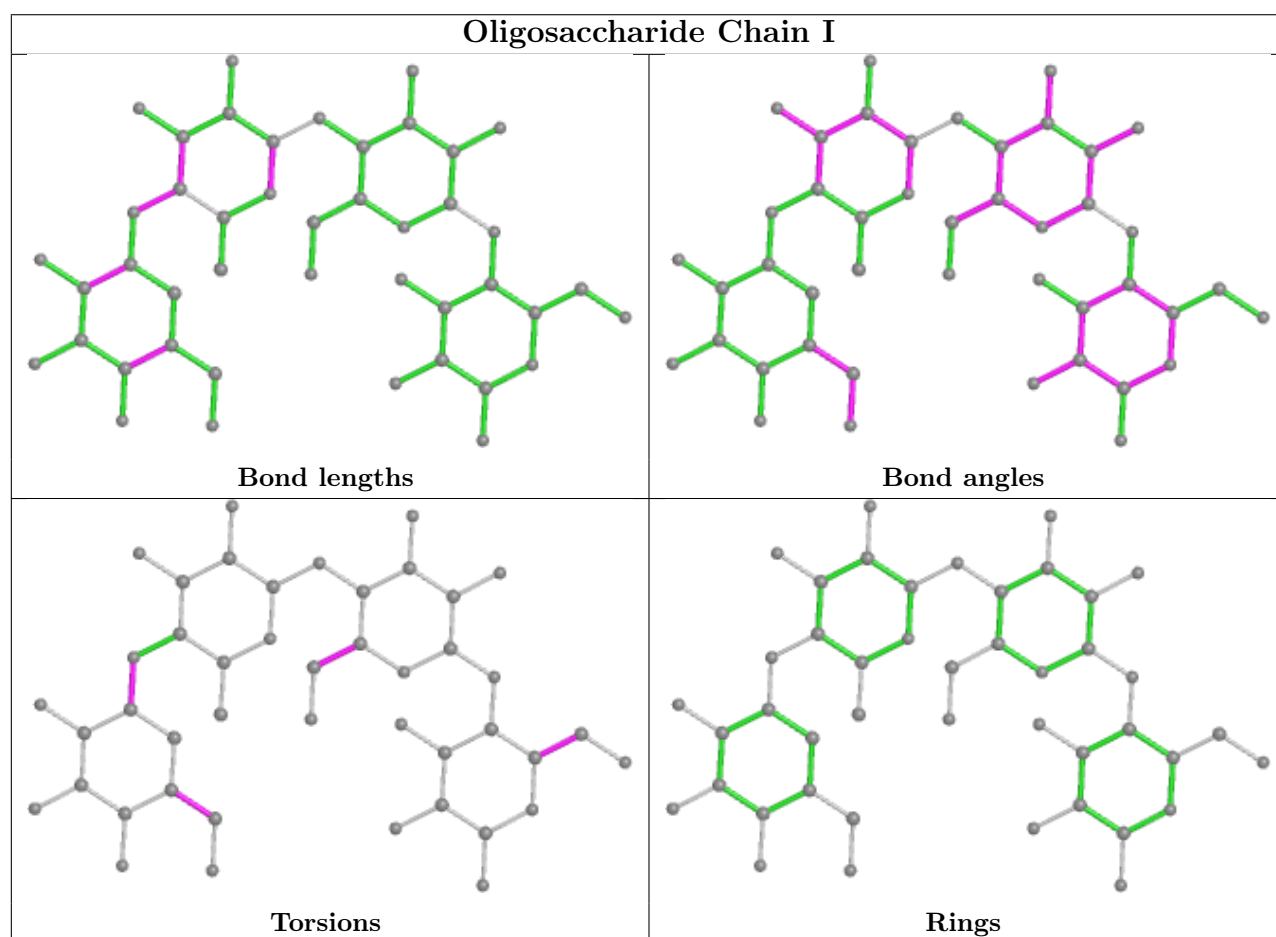
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	AC1	6	0
2	K	3	AC1	9	0
2	N	2	GLC	4	0
2	O	2	GLC	4	0
2	P	2	GLC	3	0
2	O	3	AC1	7	0

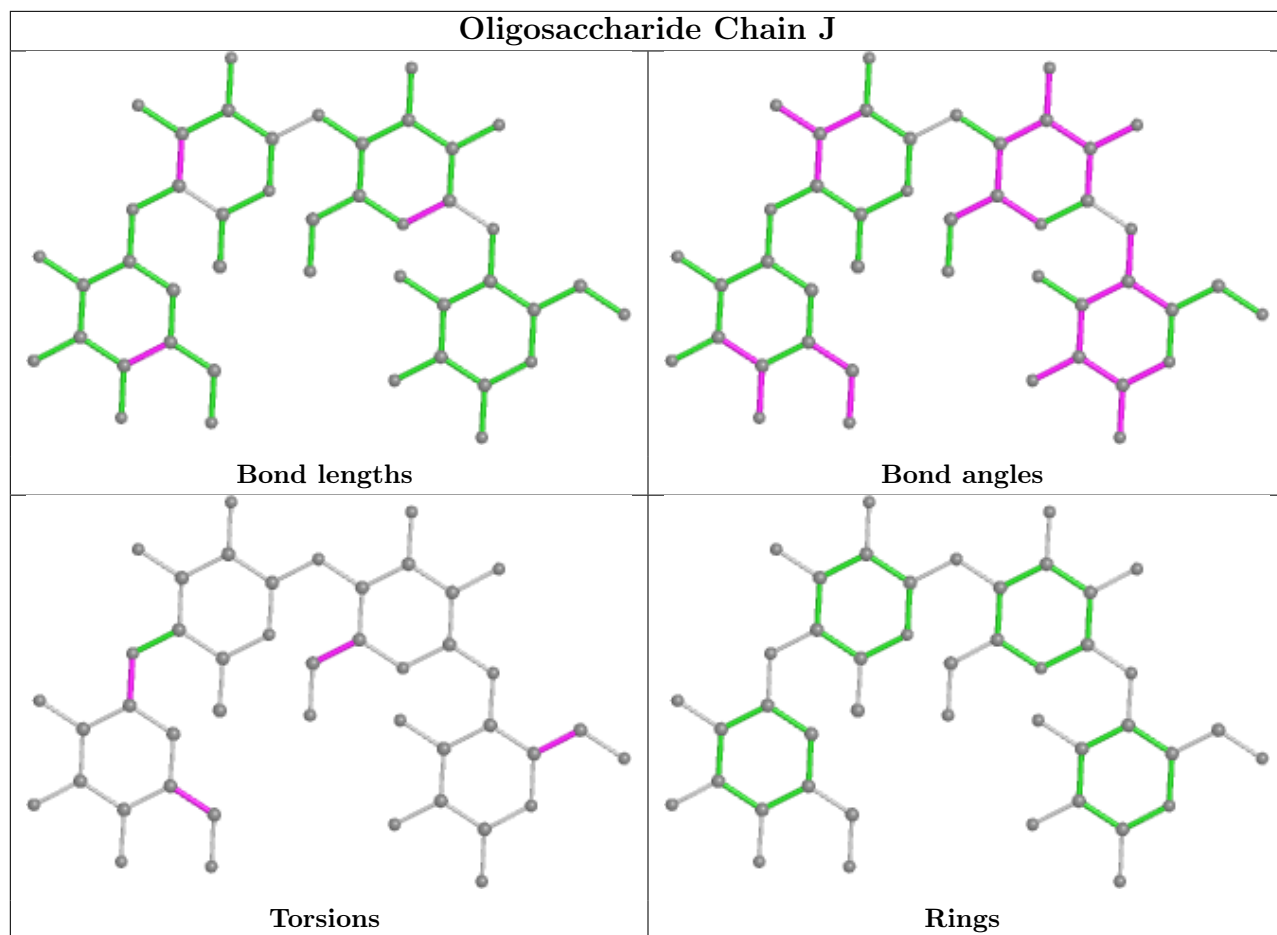
Continued on next page...

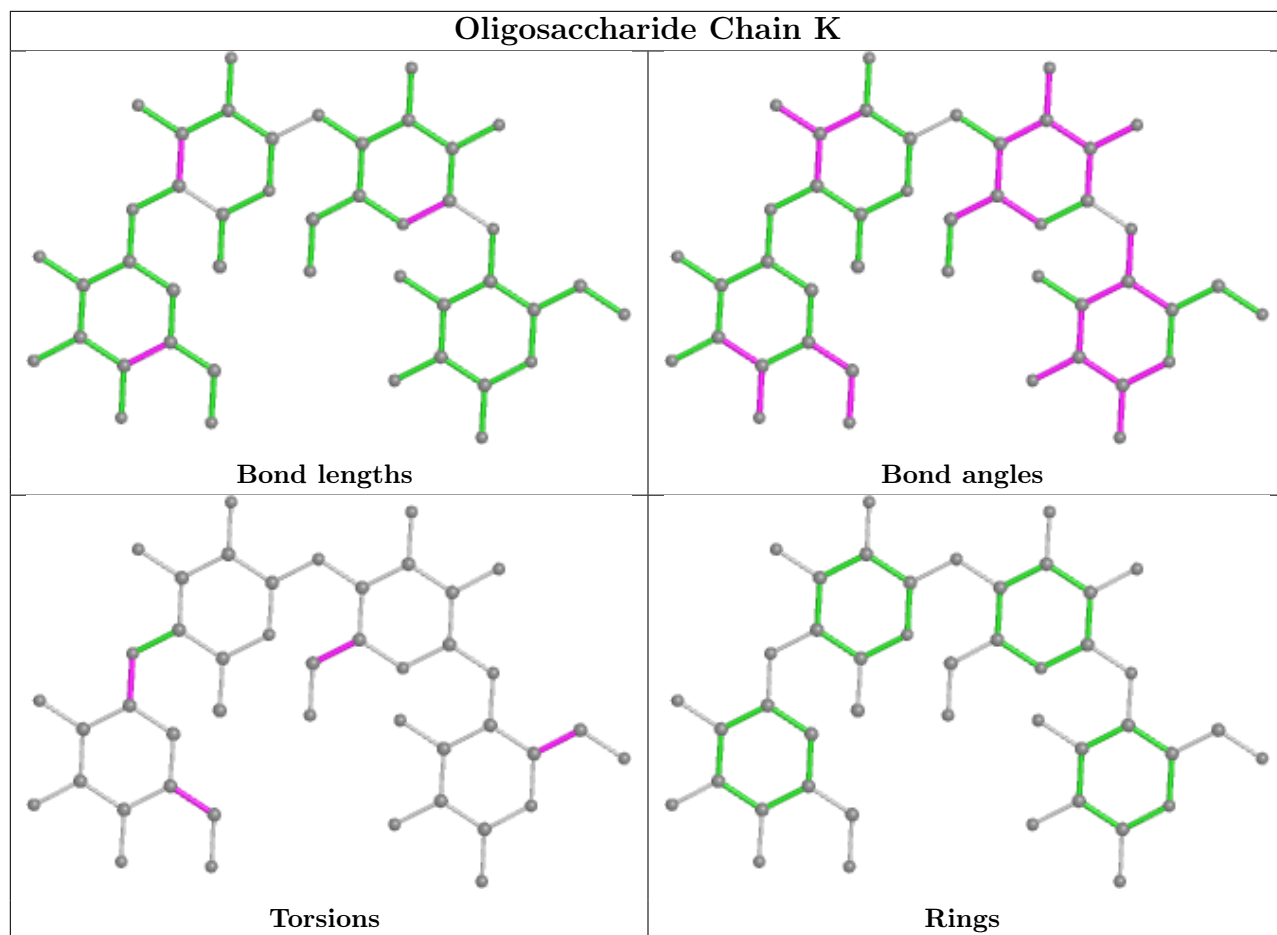
Continued from previous page...

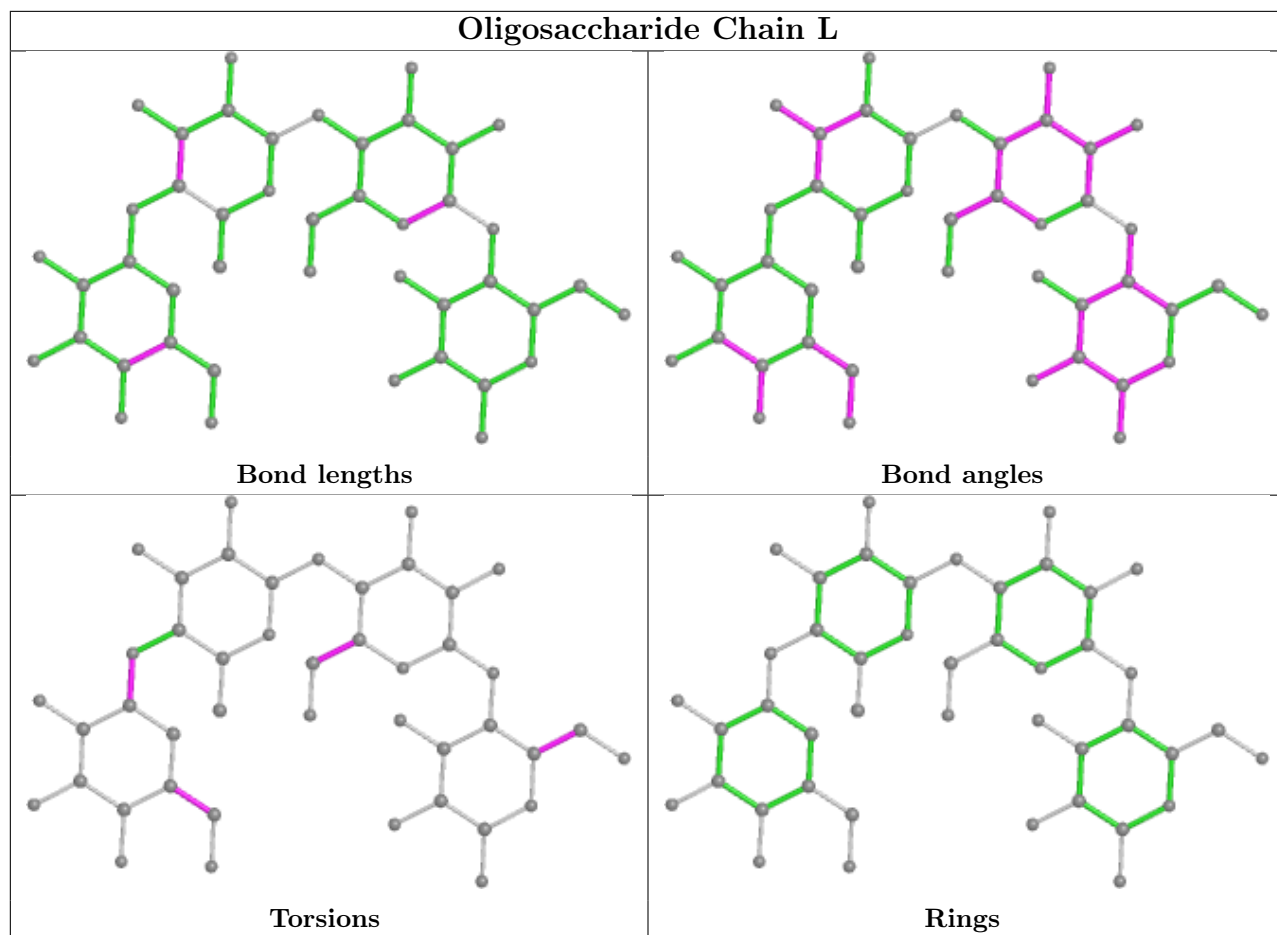
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	3	AC1	7	0
2	K	2	GLC	4	0
2	I	3	AC1	10	0
2	P	3	AC1	6	0
2	L	2	GLC	4	0
2	J	2	GLC	4	0
2	M	2	GLC	4	0
2	I	2	GLC	4	0
2	N	3	AC1	6	0
2	M	3	AC1	10	0

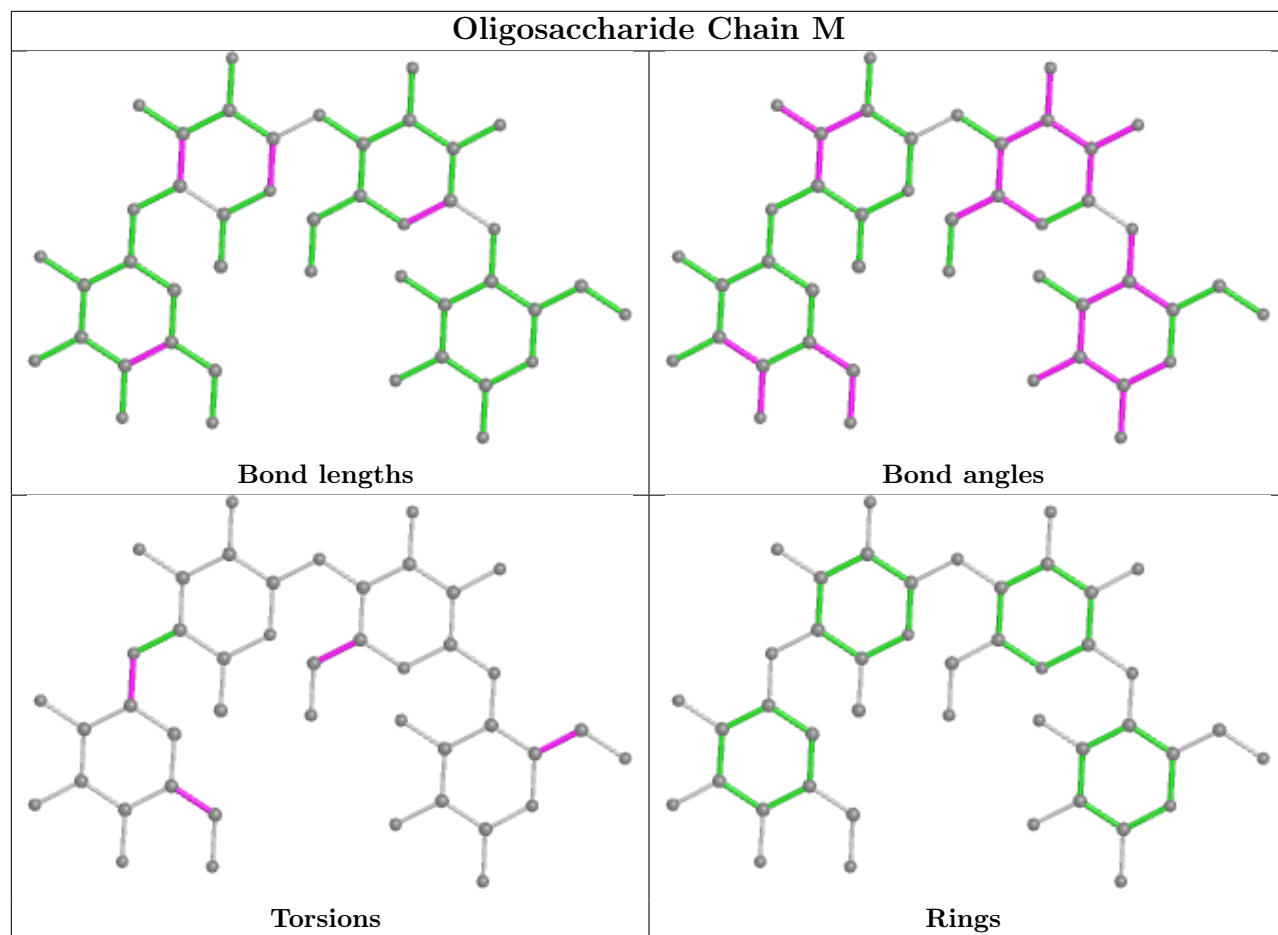
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

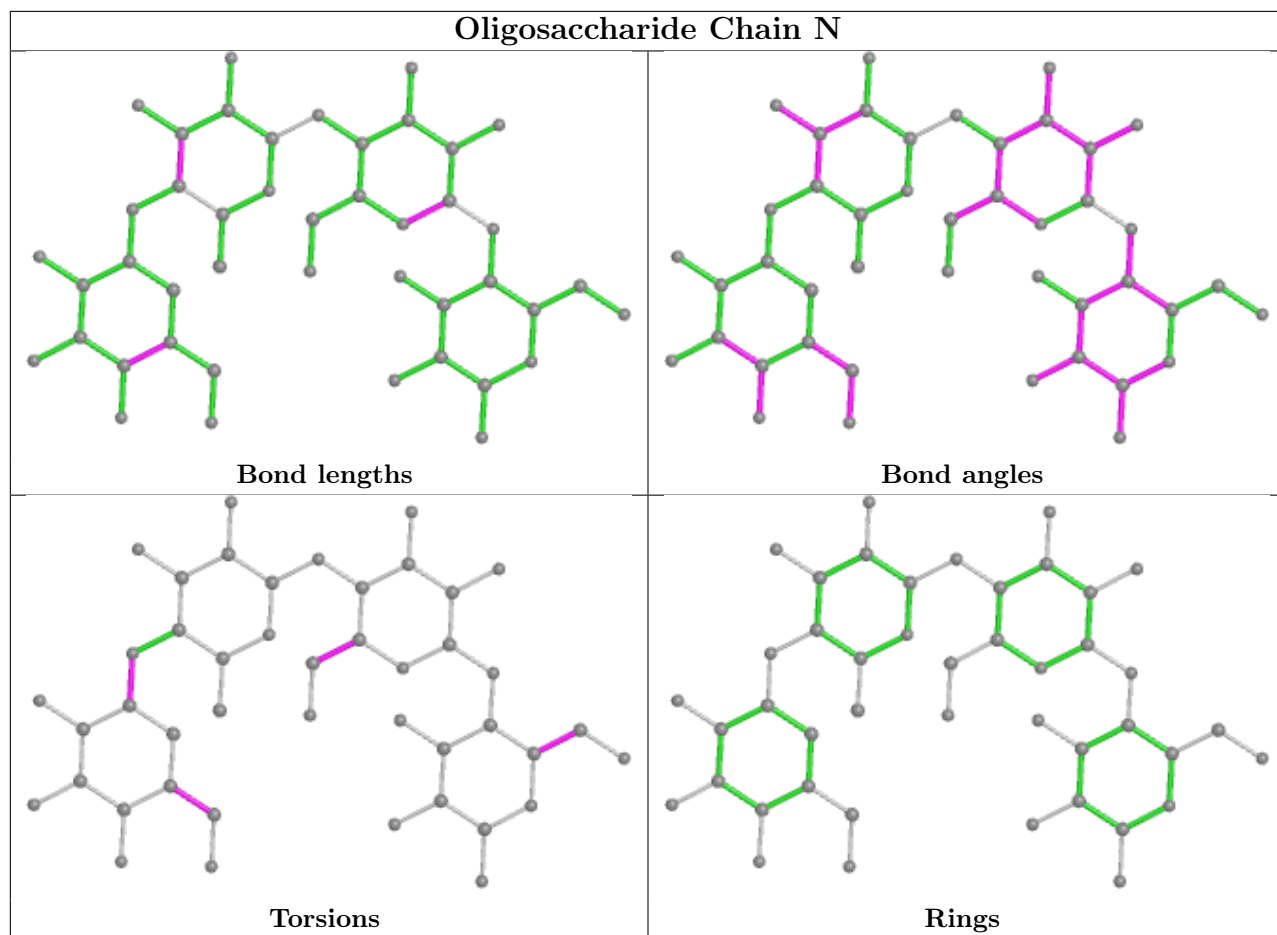


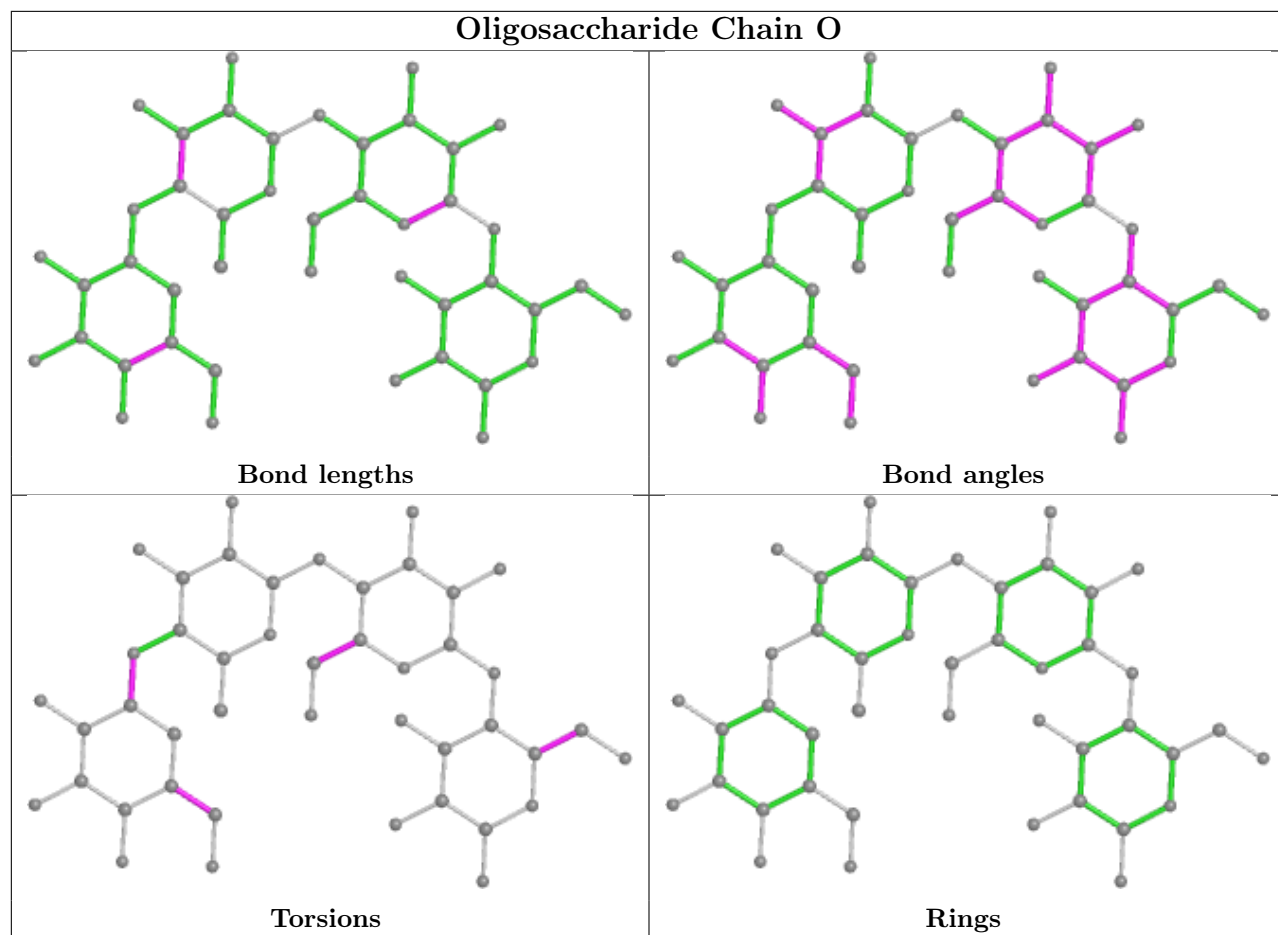


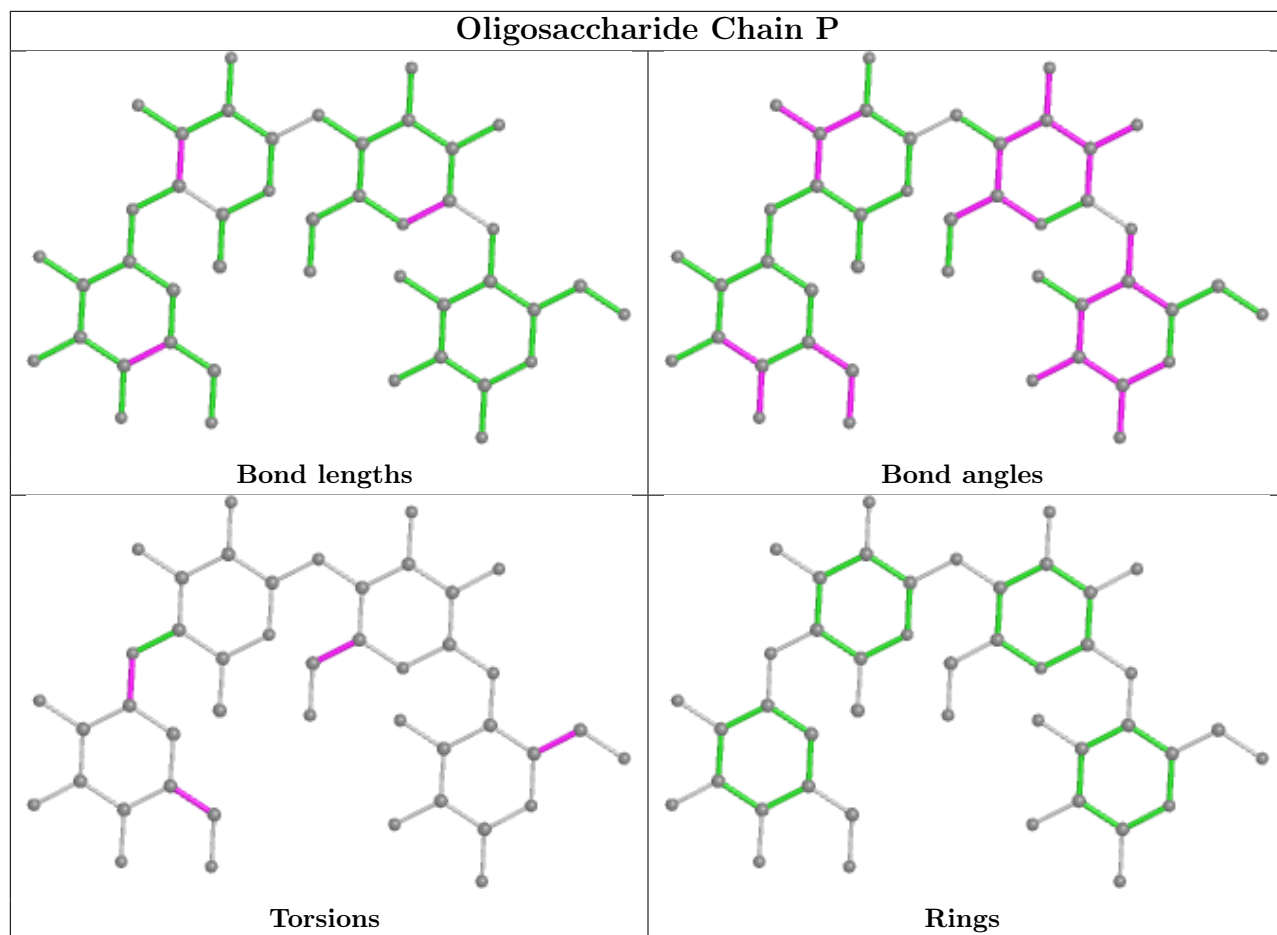












5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
4	MES	A	5001	-	12,12,12	1.49	2 (16%)	14,16,16	8.44	10 (71%)
4	MES	E	5001	-	12,12,12	1.38	4 (33%)	14,16,16	7.57	11 (78%)
4	MES	B	5001	-	12,12,12	1.68	4 (33%)	14,16,16	8.11	11 (78%)
4	MES	H	5001	-	12,12,12	1.05	0	14,16,16	7.36	11 (78%)
4	MES	D	5001	-	12,12,12	1.39	2 (16%)	14,16,16	6.50	9 (64%)
4	MES	F	5001	-	12,12,12	1.84	3 (25%)	14,16,16	7.65	11 (78%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	G	5001	-	12,12,12	1.44	2 (16%)	14,16,16	7.31	10 (71%)
4	MES	C	5001	-	12,12,12	1.49	3 (25%)	14,16,16	6.95	9 (64%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	5001	-	-	2/6/14/14	0/1/1/1
4	MES	E	5001	-	-	1/6/14/14	0/1/1/1
4	MES	B	5001	-	-	2/6/14/14	0/1/1/1
4	MES	H	5001	-	-	1/6/14/14	0/1/1/1
4	MES	D	5001	-	-	5/6/14/14	0/1/1/1
4	MES	F	5001	-	-	4/6/14/14	0/1/1/1
4	MES	G	5001	-	-	5/6/14/14	0/1/1/1
4	MES	C	5001	-	-	4/6/14/14	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5001	MES	C8-S	-4.00	1.71	1.77
4	A	5001	MES	O2S-S	3.67	1.55	1.45
4	B	5001	MES	C8-S	-3.27	1.72	1.77
4	B	5001	MES	O2S-S	3.04	1.54	1.45
4	F	5001	MES	O1S-S	2.81	1.53	1.45
4	C	5001	MES	O2S-S	2.73	1.53	1.45
4	C	5001	MES	O3S-S	2.72	1.57	1.47
4	E	5001	MES	C8-S	-2.68	1.73	1.77
4	F	5001	MES	O2S-S	2.65	1.52	1.45
4	G	5001	MES	O1S-S	2.64	1.52	1.45
4	G	5001	MES	C8-S	-2.36	1.74	1.77
4	D	5001	MES	C7-C8	2.35	1.58	1.52
4	B	5001	MES	O1S-S	2.24	1.51	1.45
4	D	5001	MES	O1S-S	2.20	1.51	1.45
4	C	5001	MES	O1S-S	2.19	1.51	1.45
4	E	5001	MES	O3S-S	2.16	1.55	1.47
4	A	5001	MES	O1S-S	2.11	1.51	1.45
4	E	5001	MES	O2S-S	2.03	1.51	1.45
4	B	5001	MES	O3S-S	2.01	1.54	1.47
4	E	5001	MES	O1S-S	2.01	1.50	1.45

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5001	MES	O2S-S-C8	-26.11	75.47	106.92
4	B	5001	MES	O1S-S-C8	-21.78	80.69	106.92
4	F	5001	MES	O2S-S-C8	-18.51	84.62	106.92
4	C	5001	MES	O1S-S-C8	-18.46	84.69	106.92
4	E	5001	MES	O2S-S-C8	-18.26	84.93	106.92
4	H	5001	MES	O1S-S-C8	-18.00	85.24	106.92
4	E	5001	MES	O1S-S-C8	-16.97	86.48	106.92
4	B	5001	MES	O2S-S-C8	-16.57	86.97	106.92
4	G	5001	MES	O1S-S-C8	-16.11	87.52	106.92
4	D	5001	MES	O3S-S-C8	-15.76	80.28	105.77
4	C	5001	MES	O2S-S-C8	-14.71	89.20	106.92
4	H	5001	MES	O2S-S-C8	-14.56	89.39	106.92
4	G	5001	MES	O3S-S-C8	-14.23	82.76	105.77
4	A	5001	MES	O1S-S-C8	-14.08	89.96	106.92
4	D	5001	MES	O1S-S-C8	-13.88	90.20	106.92
4	F	5001	MES	O1S-S-C8	-13.80	90.29	106.92
4	G	5001	MES	O2S-S-C8	-12.75	91.56	106.92
4	F	5001	MES	O3S-S-C8	-12.24	85.98	105.77
4	H	5001	MES	O3S-S-C8	-9.83	89.88	105.77
4	E	5001	MES	O3S-S-C8	-8.06	92.73	105.77
4	B	5001	MES	O3S-S-C8	-7.95	92.91	105.77
4	D	5001	MES	O2S-S-C8	-7.28	98.15	106.92
4	E	5001	MES	C5-N4-C3	6.51	123.47	108.83
4	C	5001	MES	C5-N4-C3	6.33	123.07	108.83
4	H	5001	MES	C6-C5-N4	-6.05	100.94	110.10
4	G	5001	MES	O3S-S-O1S	5.99	125.92	111.27
4	C	5001	MES	O3S-S-C8	-5.79	96.40	105.77
4	F	5001	MES	C2-C3-N4	-5.72	101.43	110.10
4	A	5001	MES	C5-N4-C3	5.51	121.24	108.83
4	G	5001	MES	C7-N4-C5	5.27	124.70	111.23
4	F	5001	MES	C7-N4-C3	5.14	124.38	111.23
4	D	5001	MES	O3S-S-O1S	5.01	123.50	111.27
4	A	5001	MES	O3S-S-C8	-4.91	97.83	105.77
4	B	5001	MES	C5-N4-C3	4.84	119.72	108.83
4	F	5001	MES	C6-C5-N4	-4.73	102.93	110.10
4	H	5001	MES	C5-N4-C3	4.42	118.77	108.83
4	B	5001	MES	C2-C3-N4	-4.29	103.59	110.10
4	F	5001	MES	C5-N4-C3	4.29	118.49	108.83
4	A	5001	MES	C6-C5-N4	-4.25	103.65	110.10
4	E	5001	MES	O3S-S-O2S	4.17	121.46	111.27
4	F	5001	MES	O3S-S-O2S	4.12	121.33	111.27
4	D	5001	MES	C7-N4-C5	3.94	121.32	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5001	MES	C7-N4-C3	3.92	121.27	111.23
4	D	5001	MES	C5-N4-C3	3.90	117.61	108.83
4	G	5001	MES	C6-C5-N4	-3.85	104.26	110.10
4	H	5001	MES	C2-C3-N4	-3.85	104.26	110.10
4	D	5001	MES	C7-N4-C3	3.84	121.06	111.23
4	B	5001	MES	C6-C5-N4	-3.80	104.33	110.10
4	E	5001	MES	C2-C3-N4	-3.80	104.34	110.10
4	B	5001	MES	C7-N4-C5	3.75	120.83	111.23
4	H	5001	MES	C7-N4-C3	3.73	120.78	111.23
4	A	5001	MES	C7-N4-C5	3.62	120.49	111.23
4	H	5001	MES	C7-N4-C5	3.60	120.44	111.23
4	C	5001	MES	O3S-S-O2S	3.59	120.05	111.27
4	G	5001	MES	O3S-S-O2S	3.38	119.53	111.27
4	H	5001	MES	O3S-S-O2S	3.22	119.14	111.27
4	D	5001	MES	O3S-S-O2S	3.22	119.13	111.27
4	B	5001	MES	C7-N4-C3	3.20	119.41	111.23
4	B	5001	MES	O3S-S-O2S	3.18	119.06	111.27
4	E	5001	MES	C7-N4-C3	3.16	119.32	111.23
4	G	5001	MES	C2-C3-N4	-3.07	105.45	110.10
4	A	5001	MES	O2S-S-O1S	3.01	124.36	113.95
4	A	5001	MES	O3S-S-O1S	3.01	118.62	111.27
4	B	5001	MES	O3S-S-O1S	3.00	118.61	111.27
4	C	5001	MES	C7-N4-C5	2.95	118.77	111.23
4	H	5001	MES	O3S-S-O1S	2.88	118.32	111.27
4	E	5001	MES	O1-C2-C3	-2.80	105.64	111.80
4	D	5001	MES	C6-C5-N4	-2.77	105.90	110.10
4	E	5001	MES	O2S-S-O1S	2.74	123.44	113.95
4	A	5001	MES	C7-N4-C3	2.74	118.23	111.23
4	C	5001	MES	C7-N4-C3	2.71	118.16	111.23
4	E	5001	MES	C6-C5-N4	2.66	114.13	110.10
4	C	5001	MES	O2S-S-O1S	2.57	122.84	113.95
4	F	5001	MES	O2S-S-O1S	2.47	122.51	113.95
4	H	5001	MES	O2S-S-O1S	2.39	122.23	113.95
4	C	5001	MES	O3S-S-O1S	2.39	117.11	111.27
4	E	5001	MES	C7-N4-C5	2.33	117.19	111.23
4	G	5001	MES	C5-N4-C3	2.30	114.02	108.83
4	F	5001	MES	C7-N4-C5	2.30	117.13	111.23
4	B	5001	MES	O2S-S-O1S	2.15	121.40	113.95
4	A	5001	MES	O3S-S-O2S	2.13	116.47	111.27
4	F	5001	MES	O1-C6-C5	-2.09	107.20	111.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5001	MES	C8-C7-N4-C5
4	A	5001	MES	N4-C7-C8-S
4	B	5001	MES	C8-C7-N4-C5
4	B	5001	MES	N4-C7-C8-S
4	C	5001	MES	C8-C7-N4-C5
4	C	5001	MES	C7-C8-S-O2S
4	C	5001	MES	C7-C8-S-O3S
4	D	5001	MES	C8-C7-N4-C5
4	D	5001	MES	N4-C7-C8-S
4	E	5001	MES	C8-C7-N4-C5
4	F	5001	MES	C8-C7-N4-C5
4	G	5001	MES	N4-C7-C8-S
4	G	5001	MES	C7-C8-S-O1S
4	G	5001	MES	C7-C8-S-O2S
4	H	5001	MES	C8-C7-N4-C5
4	F	5001	MES	C7-C8-S-O3S
4	G	5001	MES	C7-C8-S-O3S
4	D	5001	MES	C7-C8-S-O3S
4	G	5001	MES	C8-C7-N4-C3
4	C	5001	MES	C7-C8-S-O1S
4	D	5001	MES	C7-C8-S-O1S
4	F	5001	MES	C7-C8-S-O1S
4	F	5001	MES	C7-C8-S-O2S
4	D	5001	MES	C7-C8-S-O2S

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5001	MES	2	0
4	E	5001	MES	1	0
4	D	5001	MES	2	0
4	G	5001	MES	1	0
4	C	5001	MES	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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	842/844 (99%)	-0.19	7 (0%) 86 74	23, 38, 90, 113	0
1	B	747/844 (88%)	-0.11	15 (2%) 65 45	31, 50, 88, 136	0
1	C	844/844 (100%)	-0.31	2 (0%) 95 91	24, 35, 60, 70	0
1	D	844/844 (100%)	-0.23	11 (1%) 77 60	26, 39, 83, 101	0
1	E	843/844 (99%)	-0.18	16 (1%) 66 47	22, 36, 101, 126	0
1	F	844/844 (100%)	-0.17	6 (0%) 87 77	37, 53, 73, 89	0
1	G	844/844 (100%)	-0.26	6 (0%) 87 77	24, 35, 68, 79	0
1	H	807/844 (95%)	-0.19	13 (1%) 72 52	24, 42, 95, 139	0
All	All	6615/6752 (97%)	-0.21	76 (1%) 80 65	22, 40, 83, 139	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1087	PRO	5.8
1	A	1087	PRO	5.3
1	G	1087	PRO	5.0
1	E	285	THR	4.7
1	H	1087	PRO	4.0
1	B	1086	ASN	3.9
1	B	248	TYR	3.7
1	E	1085	VAL	3.6
1	F	1087	PRO	3.6
1	F	1086	ASN	3.5
1	D	275	LYS	3.5
1	G	1086	ASN	3.3
1	A	283	THR	3.3
1	H	277	ILE	3.3
1	B	274	PRO	3.2
1	C	1087	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	276	TYR	3.1
1	D	247	GLN	3.1
1	B	249	ASN	3.0
1	E	317	LEU	2.9
1	C	1086	ASN	2.8
1	E	1087	PRO	2.8
1	A	352	ASN	2.7
1	E	1077	ASN	2.7
1	B	1085	VAL	2.7
1	G	1081	PRO	2.7
1	A	353	THR	2.7
1	D	1086	ASN	2.6
1	E	1086	ASN	2.6
1	B	272	TYR	2.6
1	B	259	PHE	2.6
1	H	1074	VAL	2.6
1	E	1080	LEU	2.5
1	D	285	THR	2.5
1	B	1083	SER	2.5
1	D	274	PRO	2.5
1	E	277	ILE	2.5
1	A	277	ILE	2.5
1	E	1074	VAL	2.5
1	H	318	GLY	2.5
1	D	249	ASN	2.4
1	B	1081	PRO	2.4
1	H	274	PRO	2.4
1	H	288	THR	2.4
1	E	1081	PRO	2.4
1	D	1087	PRO	2.4
1	B	1073	LEU	2.4
1	E	276	TYR	2.3
1	G	285	THR	2.3
1	H	286	GLN	2.3
1	D	352	ASN	2.3
1	E	289	GLU	2.3
1	B	1072	SER	2.2
1	H	283	THR	2.2
1	G	1082	LYS	2.2
1	E	249	ASN	2.2
1	A	286	GLN	2.2
1	A	248	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	275	LYS	2.2
1	D	286	GLN	2.2
1	H	1077	ASN	2.1
1	H	273	ARG	2.1
1	E	283	THR	2.1
1	D	351	LYS	2.1
1	B	273	ARG	2.1
1	F	256	ALA	2.1
1	G	274	PRO	2.0
1	F	782	GLN	2.0
1	E	351	LYS	2.0
1	E	349	ALA	2.0
1	B	1071	PHE	2.0
1	H	1073	LEU	2.0
1	H	1076	ASP	2.0
1	B	1080	LEU	2.0
1	F	778	TYR	2.0
1	F	822	VAL	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.

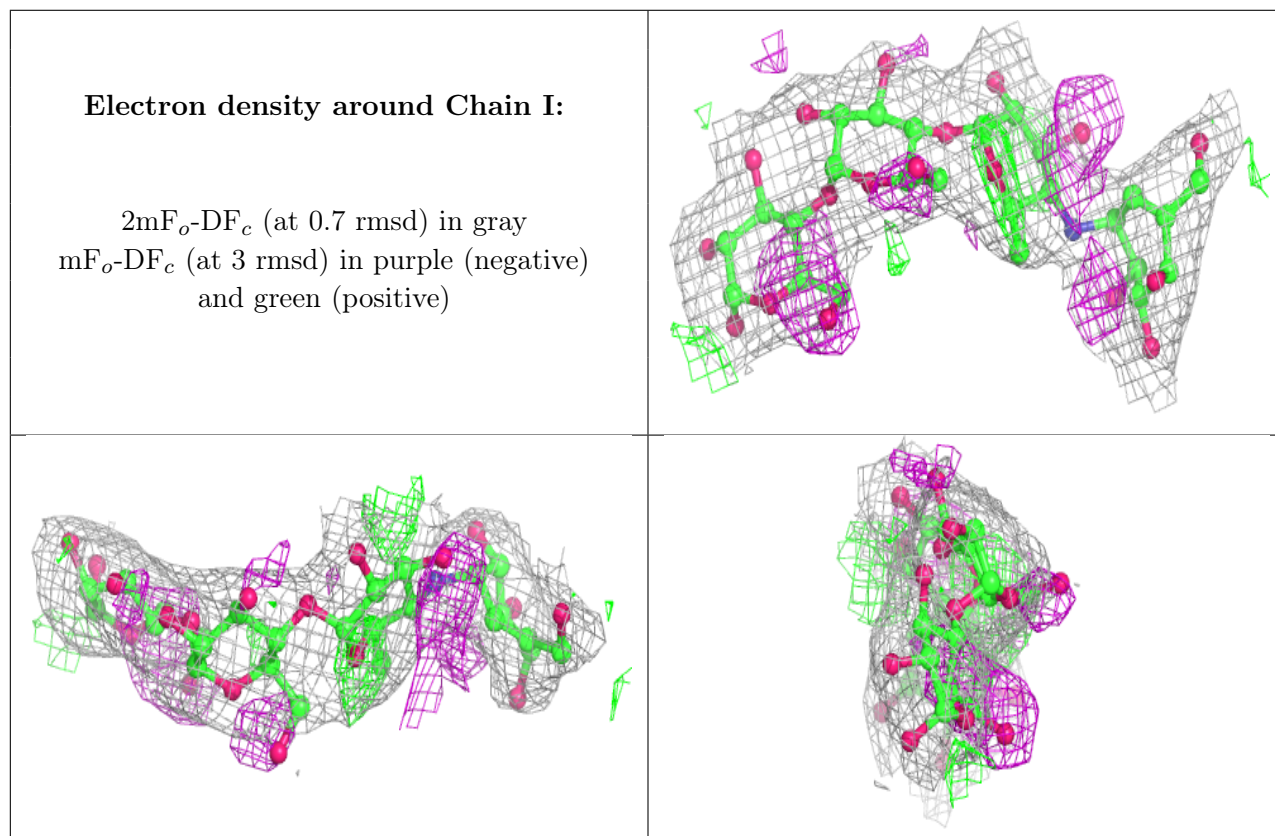
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	L	1	12/12	0.80	0.28	48,49,49,50	0
2	GLC	M	1	12/12	0.81	0.30	48,49,49,50	0
2	GLC	N	1	12/12	0.83	0.26	48,49,49,50	0
2	GLC	O	1	12/12	0.83	0.23	48,49,49,50	0
2	GLC	N	2	11/12	0.84	0.28	46,47,47,47	0
2	GLC	K	1	12/12	0.86	0.25	48,49,49,50	0
2	GLC	O	2	11/12	0.86	0.26	46,47,47,47	0
2	GLC	P	1	12/12	0.86	0.26	48,49,49,50	0
2	GLC	M	2	11/12	0.87	0.27	46,47,47,47	0
2	AC1	M	3	21/22	0.89	0.29	35,50,53,53	0

Continued on next page...

Continued from previous page...

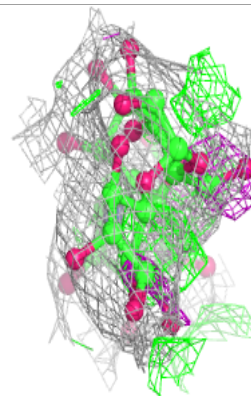
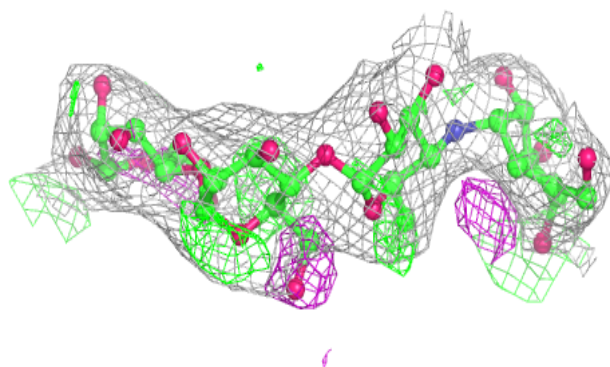
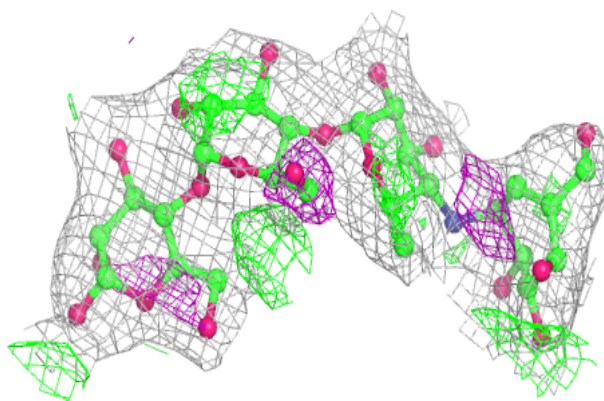
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	J	1	12/12	0.89	0.21	48,49,49,50	0
2	GLC	J	2	11/12	0.89	0.22	46,47,47,47	0
2	GLC	L	2	11/12	0.90	0.23	46,47,47,47	0
2	GLC	I	1	12/12	0.90	0.21	48,49,49,50	0
2	AC1	N	3	21/22	0.90	0.28	35,50,53,53	0
2	AC1	K	3	21/22	0.91	0.27	35,50,53,53	0
2	GLC	I	2	11/12	0.91	0.20	46,47,47,47	0
2	GLC	K	2	11/12	0.91	0.27	46,47,47,47	0
2	GLC	P	2	11/12	0.91	0.22	46,47,47,47	0
2	AC1	I	3	21/22	0.92	0.24	35,50,53,53	0
2	AC1	P	3	21/22	0.92	0.22	35,50,53,53	0
2	AC1	L	3	21/22	0.94	0.24	35,50,53,53	0
2	AC1	J	3	21/22	0.94	0.23	35,50,53,53	0
2	AC1	O	3	21/22	0.95	0.26	35,50,53,53	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.

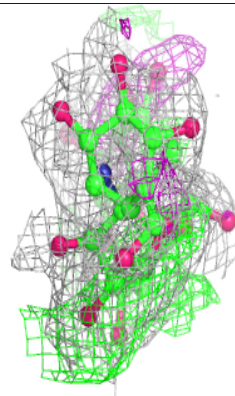
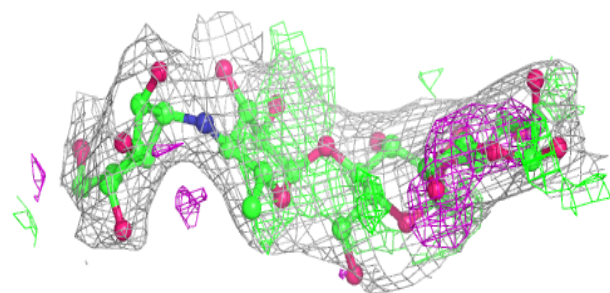
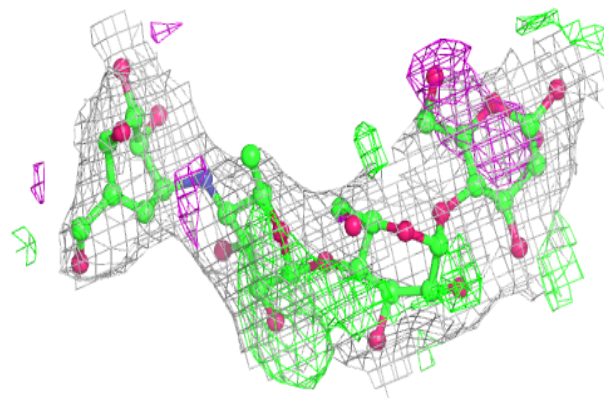


Electron density around Chain J:

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

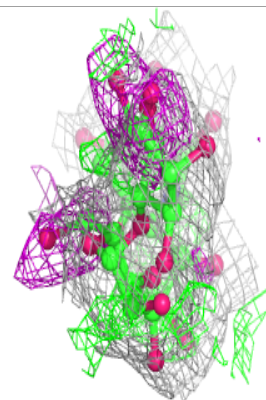
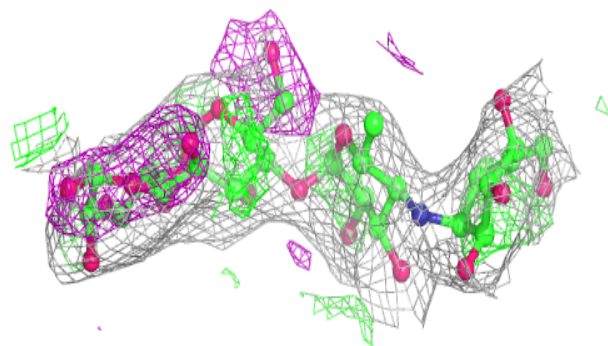
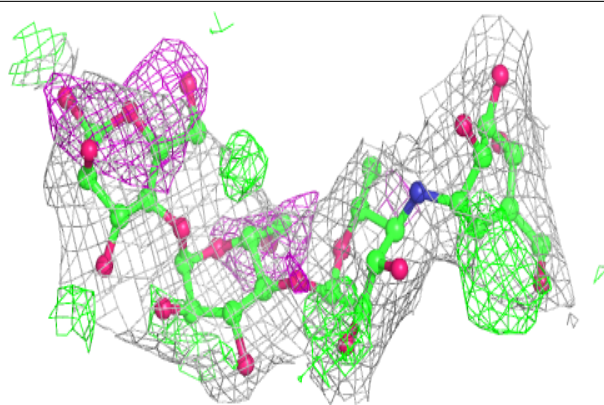
**Electron density around Chain K:**

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

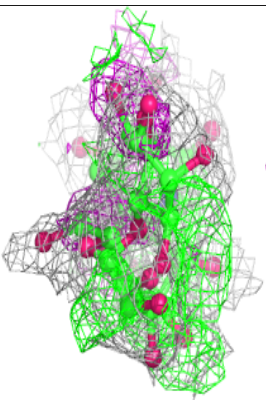
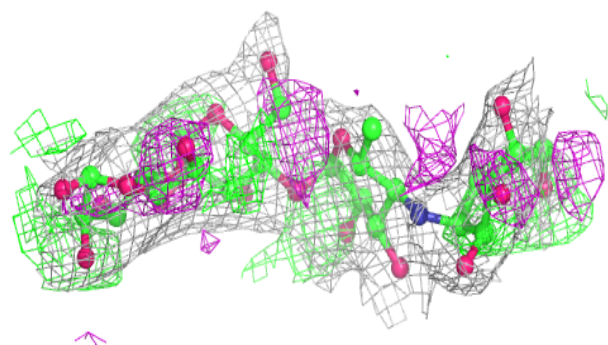
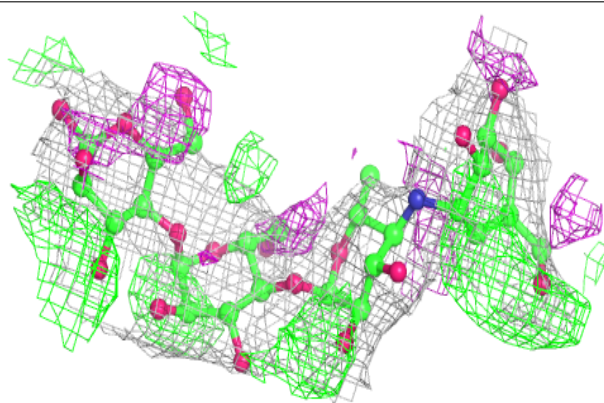


Electron density around Chain L:

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

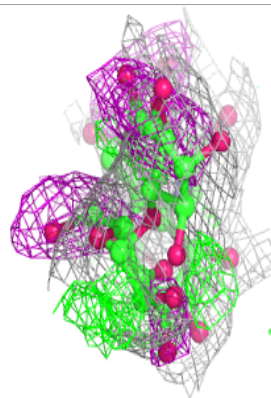
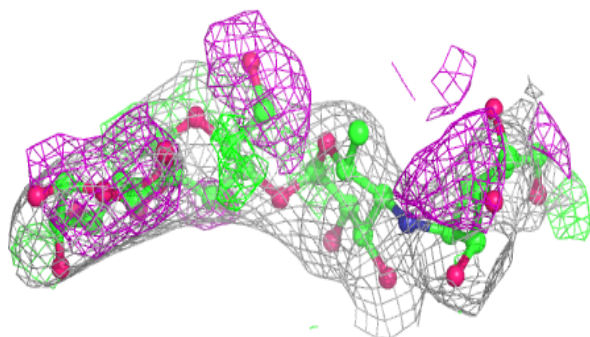
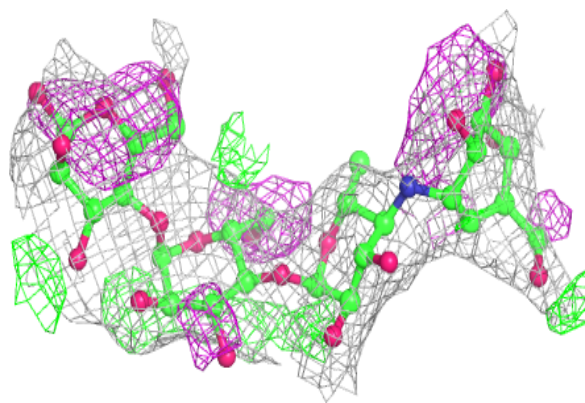
**Electron density around Chain M:**

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

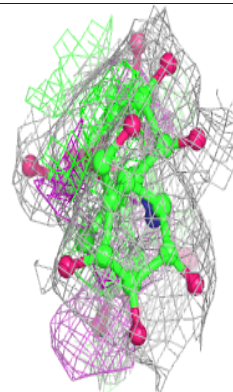
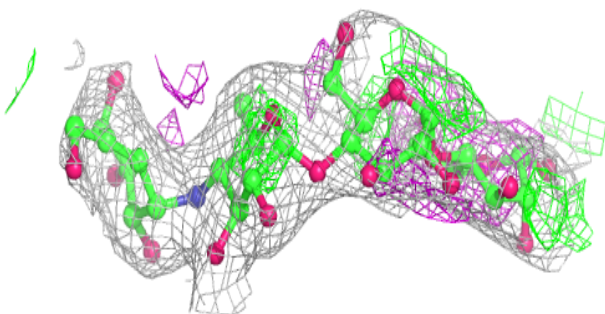
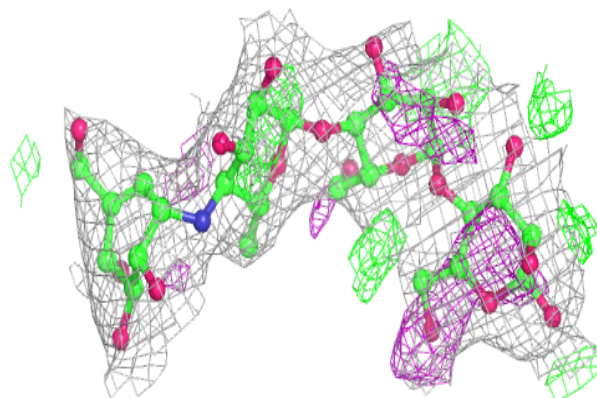


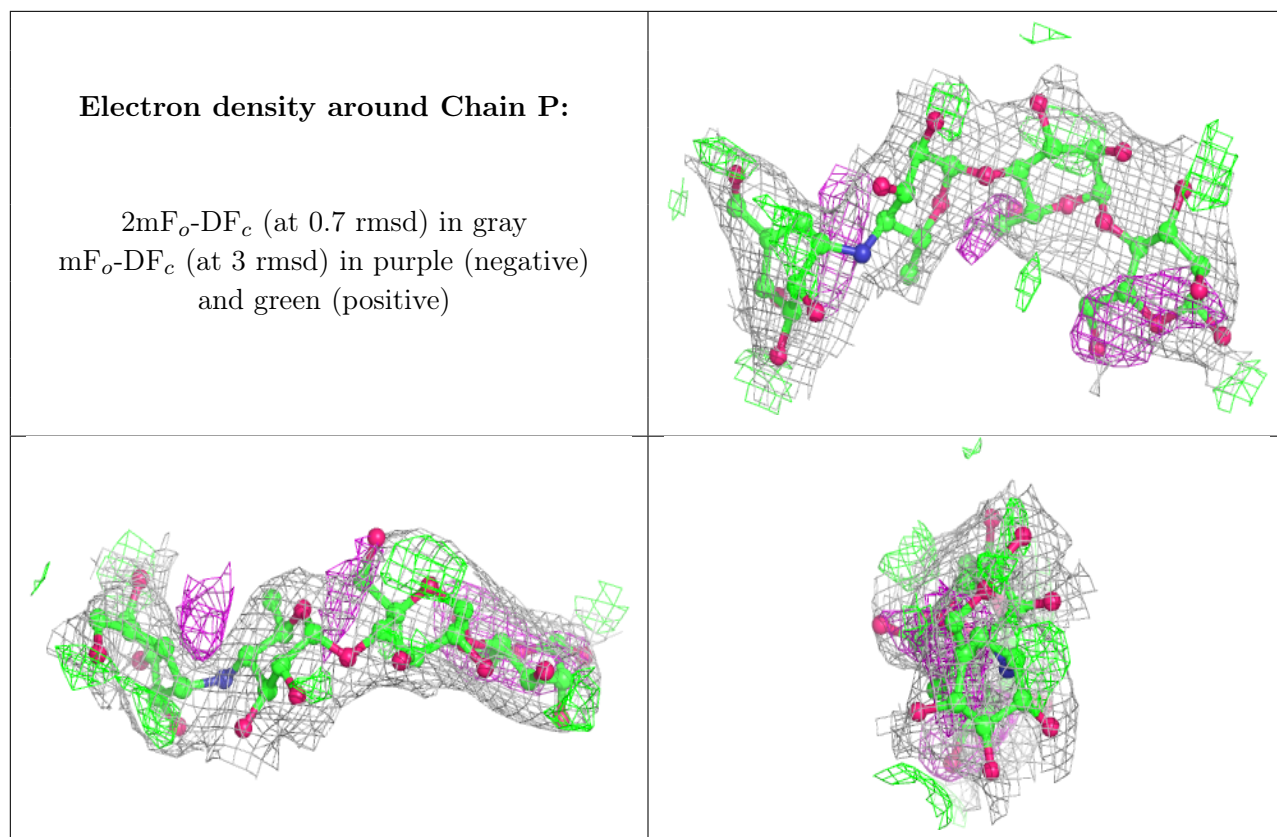
Electron density around Chain N:

$2mF_o-DF_c$ (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)





6.4 Ligands [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(\AA^2)	Q<0.9
3	CA	F	4001	1/1	0.94	0.15	38,38,38,38	0
4	MES	A	5001	12/12	0.94	0.20	29,31,33,33	0
4	MES	B	5001	12/12	0.94	0.18	39,41,43,44	0
4	MES	F	5001	12/12	0.94	0.17	36,37,37,37	0
4	MES	C	5001	12/12	0.95	0.16	29,31,32,32	0
4	MES	D	5001	12/12	0.96	0.16	31,33,35,35	0
4	MES	E	5001	12/12	0.96	0.18	30,33,35,36	0
3	CA	A	4001	1/1	0.96	0.16	28,28,28,28	0
4	MES	G	5001	12/12	0.96	0.15	30,31,33,33	0
3	CA	B	4001	1/1	0.97	0.14	33,33,33,33	0
4	MES	H	5001	12/12	0.97	0.17	28,30,32,32	0
3	CA	D	4001	1/1	0.98	0.16	32,32,32,32	0
3	CA	E	4001	1/1	0.98	0.18	32,32,32,32	0
3	CA	C	4001	1/1	0.98	0.13	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	G	4001	1/1	0.98	0.14	28,28,28,28	0
3	CA	H	4001	1/1	0.99	0.17	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.