Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 02:54 PM EDT

PDB ID	:	3TOP
Title	:	Crystral Structure of the C-terminal Subunit of Human Maltase-Glucoamylase in Complex with Acarbose
Authors	:	Shen, Y.; Qin, X.H.; Ren, L.M.
Deposited on	:	2011-09-06
Resolution	:	2.88 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 (i) 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 (i)) were used in the production of this report:

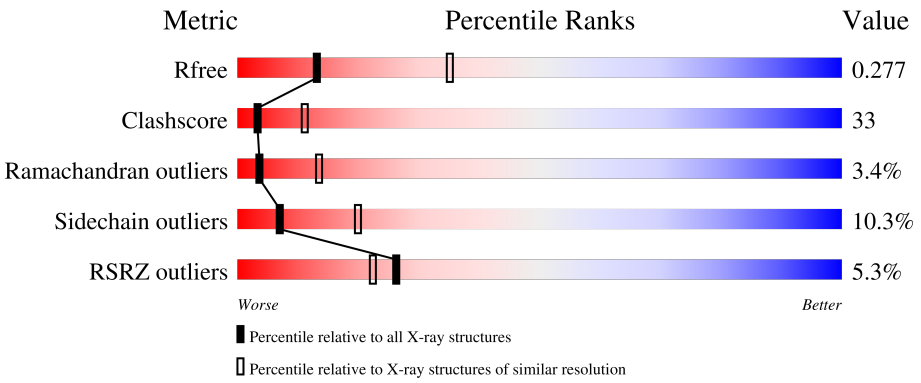
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 <=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	908	3%, 47%, 42%, 8%, •
1	B	908	7%, 47%, 43%, 8%, •
2	C	3	100%
2	D	3	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14388 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 Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	890	7131	4572	1190	1338	31	0	0	0
1	B	890	7131	4572	1190	1338	31	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	TRP	-	expression tag	UNP O43451
A	953	SER	-	expression tag	UNP O43451
A	954	HIS	-	expression tag	UNP O43451
A	955	PRO	-	expression tag	UNP O43451
A	956	GLN	-	expression tag	UNP O43451
A	957	PHE	-	expression tag	UNP O43451
A	958	GLU	-	expression tag	UNP O43451
A	959	LYS	-	expression tag	UNP O43451
A	1854	HIS	-	expression tag	UNP O43451
A	1855	HIS	-	expression tag	UNP O43451
A	1856	HIS	-	expression tag	UNP O43451
A	1857	HIS	-	expression tag	UNP O43451
A	1858	HIS	-	expression tag	UNP O43451
A	1859	HIS	-	expression tag	UNP O43451
B	952	TRP	-	expression tag	UNP O43451
B	953	SER	-	expression tag	UNP O43451
B	954	HIS	-	expression tag	UNP O43451
B	955	PRO	-	expression tag	UNP O43451
B	956	GLN	-	expression tag	UNP O43451
B	957	PHE	-	expression tag	UNP O43451
B	958	GLU	-	expression tag	UNP O43451
B	959	LYS	-	expression tag	UNP O43451
B	1854	HIS	-	expression tag	UNP O43451
B	1855	HIS	-	expression tag	UNP O43451
B	1856	HIS	-	expression tag	UNP O43451

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1857	HIS	-	expression tag	UNP O43451
B	1858	HIS	-	expression tag	UNP O43451
B	1859	HIS	-	expression tag	UNP O43451

- 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
			Total	C	N	O			
2	C	3	44	25	1	18	0	0	0
			Total	C	N	O			
2	D	3	44	25	1	18	0	0	0

- Molecule 3 is water.

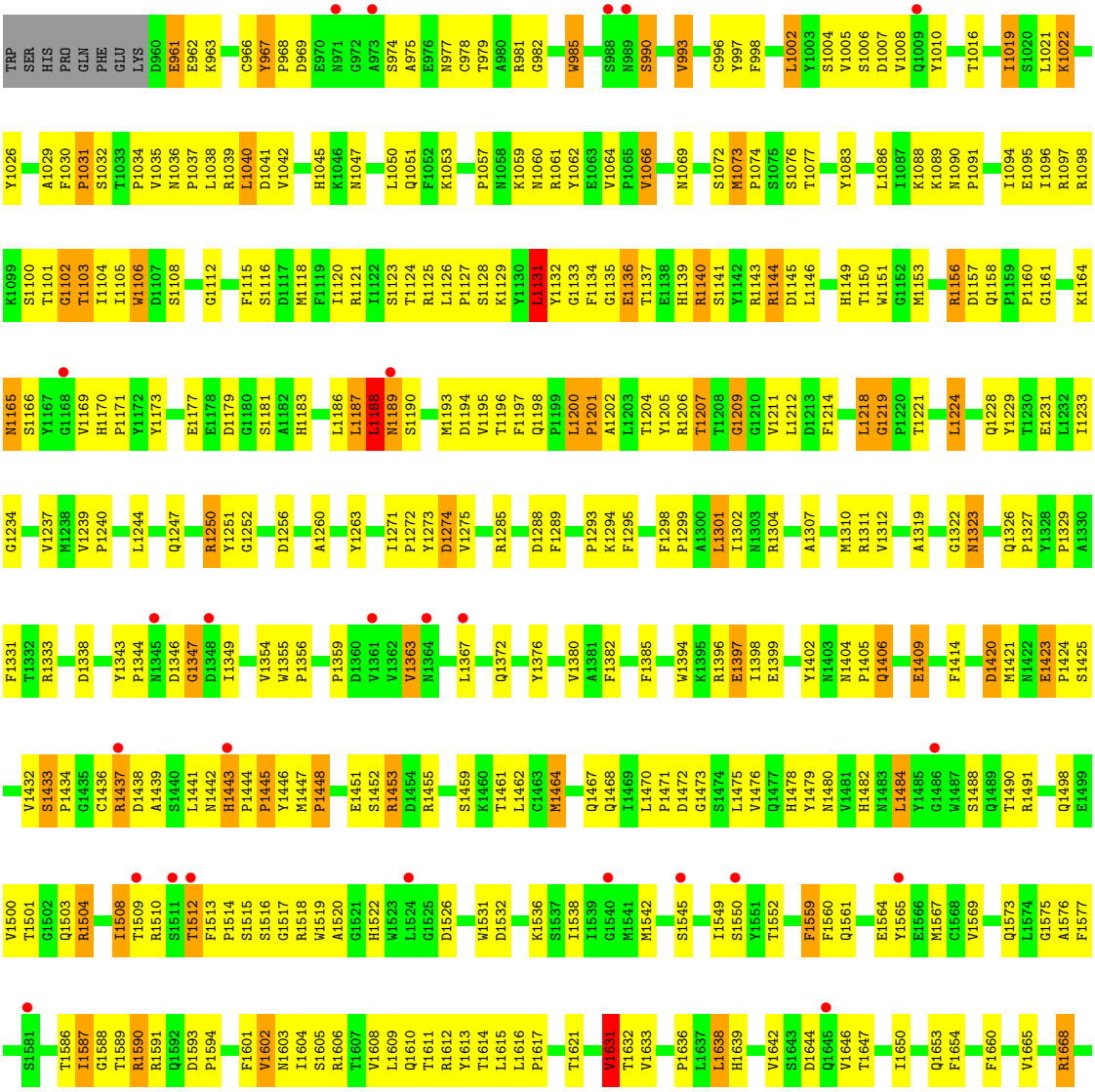
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	30	30	30	0	0
			Total	O		
3	B	8	8	8	0	0

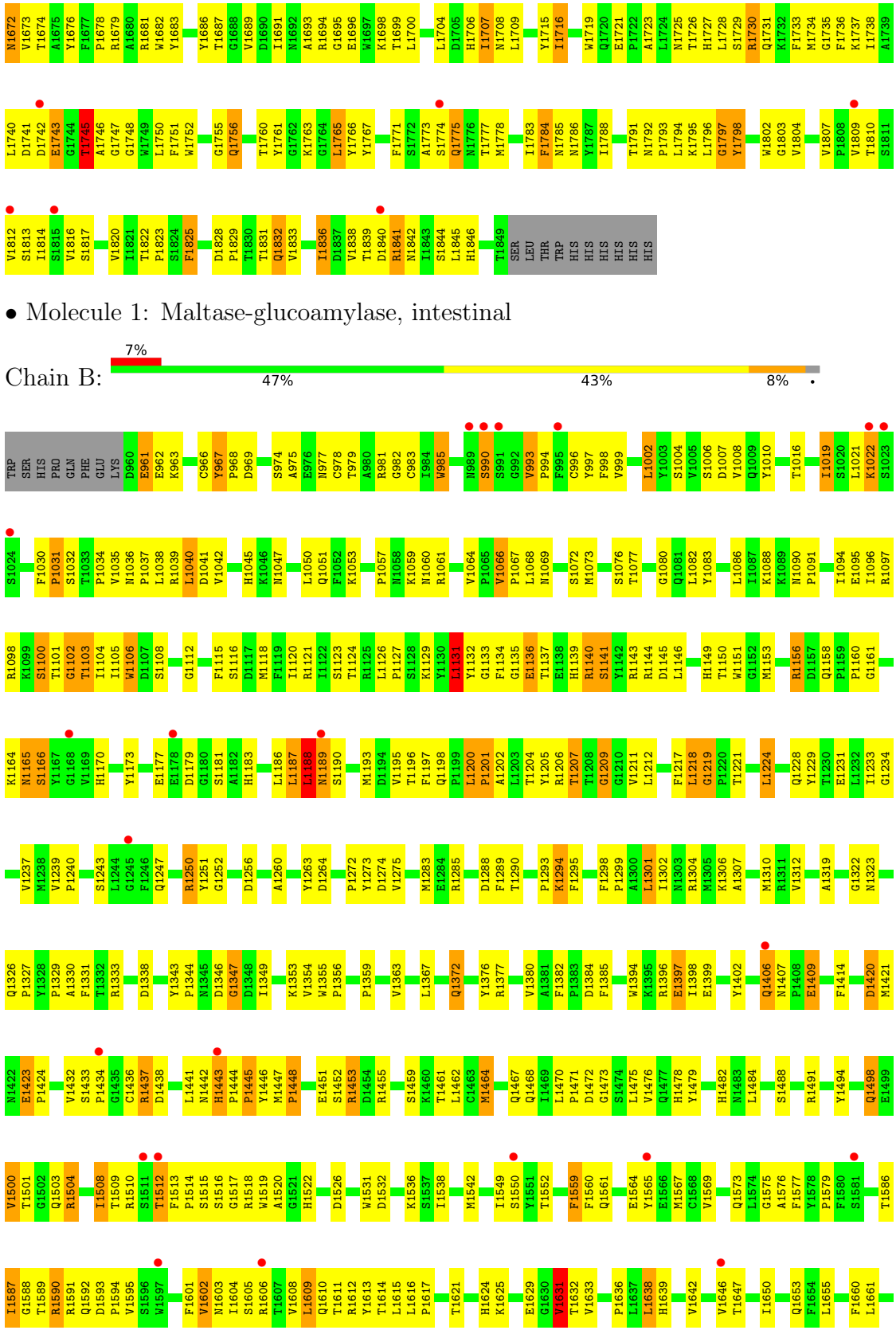
3 Residue-property plots (i)

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: Maltase-glucoamylase, intestinal

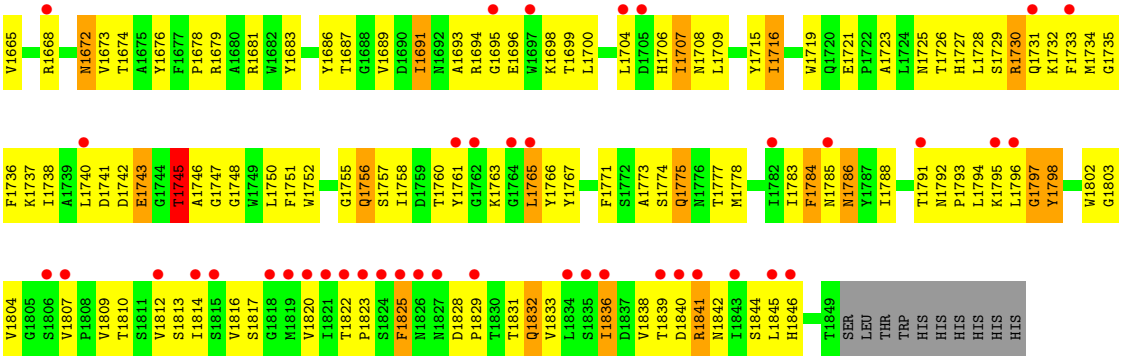
Chain A: 3% 47% 42% 8%





• Molecule 1: Maltase-glucoamylase, intestinal

Chain B: 7% 47% 43% 8%



• Molecule 2: 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

Chain C: 100%

• Molecule 2: 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

Chain D: 100%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.50Å 105.50Å 516.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.45 – 2.88 36.45 – 2.88	Depositor EDS
% Data completeness (in resolution range)	82.3 (36.45-2.88) 87.9 (36.45-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.218 , 0.284 0.217 , 0.277	Depositor DCC
R_{free} test set	3014 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14388	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.44	2/7350 (0.0%)	0.63	2/10031 (0.0%)
1	B	0.44	0/7350	0.63	2/10031 (0.0%)
All	All	0.44	2/14700 (0.0%)	0.63	4/20062 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1144	ARG	CB-CG	6.16	1.69	1.52
1	A	1323	ASN	CB-CG	5.42	1.63	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1219	GLY	N-CA-C	-6.06	97.95	113.10
1	A	1131	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	1219	GLY	N-CA-C	-5.73	98.77	113.10
1	B	1131	LEU	CA-CB-CG	5.69	128.38	115.30

There are no chirality outliers.

There are no planarity outliers.

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	7131	0	6766	461	0
1	B	7131	0	6766	454	0
2	C	44	0	30	7	0
2	D	44	0	30	0	0
3	A	30	0	0	1	0
3	B	8	0	0	1	0
All	All	14388	0	13592	915	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 33.

All (915) 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:B:1734:MET:HE3	1:B:1794:LEU:HD21	1.29	1.10
1:A:1542:MET:HE1	1:A:1636:PRO:CB	1.81	1.10
1:B:967:TYR:CE2	1:B:1030:PHE:HZ	1.72	1.08
1:B:1542:MET:HE1	1:B:1636:PRO:HB3	1.09	1.06
1:B:1542:MET:HE1	1:B:1636:PRO:CB	1.85	1.06
1:A:1734:MET:HE3	1:A:1794:LEU:HD21	1.31	1.05
1:A:1765:LEU:H	1:A:1765:LEU:HD23	1.16	1.05
1:B:981:ARG:NH1	1:B:1030:PHE:HB2	1.71	1.04
1:B:1441:LEU:HD12	1:B:1464:MET:HB2	1.40	1.04
1:B:1765:LEU:HD23	1:B:1765:LEU:H	1.16	1.03
1:A:1542:MET:HE1	1:A:1636:PRO:HB3	1.04	1.02
1:A:967:TYR:CE2	1:A:1030:PHE:HZ	1.78	1.00
1:A:981:ARG:NH1	1:A:1030:PHE:HB2	1.77	1.00
1:A:1047:ASN:HD21	1:A:1077:THR:H	1.08	0.98
1:A:1681:ARG:HH11	1:A:1742:ASP:H	1.07	0.98
1:B:1047:ASN:HD21	1:B:1077:THR:H	1.12	0.96
1:A:1441:LEU:HD12	1:A:1464:MET:HB2	1.46	0.95
1:B:1681:ARG:HH11	1:B:1742:ASP:H	1.07	0.95
1:A:1538:ILE:O	1:A:1542:MET:HG3	1.68	0.92
1:B:1538:ILE:O	1:B:1542:MET:HG3	1.69	0.92
1:A:1030:PHE:CD2	1:A:1031:PRO:HD2	2.05	0.91
1:B:1030:PHE:CD2	1:B:1031:PRO:HD2	2.06	0.91
1:A:1542:MET:CE	1:A:1636:PRO:HB3	1.99	0.90
1:B:1030:PHE:HD2	1:B:1031:PRO:HD2	1.36	0.89
1:A:1050:LEU:HD21	1:A:1083:TYR:CE1	2.07	0.88
1:B:1441:LEU:CD1	1:B:1464:MET:H	1.87	0.88
1:B:1542:MET:CE	1:B:1636:PRO:HB3	2.02	0.88
1:A:1030:PHE:HD2	1:A:1031:PRO:HD2	1.37	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:LEU:CD1	1:A:1464:MET:H	1.86	0.87
1:A:1784:PHE:HE2	1:A:1786:ASN:HB2	1.41	0.86
1:A:1035:VAL:HG23	1:A:1038:LEU:HD21	1.57	0.86
1:A:1636:PRO:HG2	1:A:1639:HIS:CD2	2.10	0.86
1:A:1156:ARG:HH11	1:A:1158:GLN:HG2	1.40	0.86
1:B:967:TYR:CE2	1:B:1030:PHE:CZ	2.62	0.86
1:B:1035:VAL:HG23	1:B:1038:LEU:HD21	1.57	0.85
1:B:1120:ILE:HG21	1:B:1212:LEU:HD21	1.58	0.85
1:A:1021:LEU:HB2	1:A:1036:ASN:HD21	1.40	0.85
1:B:1816:VAL:HG22	1:B:1820:VAL:HG22	1.58	0.85
1:A:961:GLU:HB3	1:A:1200:LEU:HB3	1.59	0.85
1:B:1256:ASP:HB2	1:B:1295:PHE:HA	1.58	0.85
1:B:1823:PRO:HB3	1:B:1841:ARG:HH21	1.41	0.85
1:B:1021:LEU:HB2	1:B:1036:ASN:HD21	1.39	0.85
1:B:1526:ASP:HB3	1:B:1560:PHE:CE2	2.12	0.85
1:A:1716:ILE:HG12	1:A:1748:GLY:HA3	1.59	0.85
1:A:1716:ILE:HG22	1:A:1738:ILE:HA	1.59	0.85
1:B:1587:ILE:HG23	1:B:1588:GLY:H	1.41	0.84
1:B:1636:PRO:HG2	1:B:1639:HIS:CD2	2.11	0.84
1:B:1716:ILE:HG12	1:B:1748:GLY:HA3	1.55	0.84
1:B:1156:ARG:HH11	1:B:1158:GLN:HG2	1.42	0.84
1:A:1256:ASP:HB2	1:A:1295:PHE:HA	1.60	0.83
1:B:961:GLU:HB3	1:B:1200:LEU:HB3	1.61	0.83
1:B:1784:PHE:HE2	1:B:1786:ASN:HB2	1.43	0.83
1:B:1716:ILE:HG22	1:B:1738:ILE:HA	1.58	0.82
1:A:1526:ASP:HB3	1:A:1560:PHE:CE2	2.13	0.82
1:A:1681:ARG:HD3	1:A:1741:ASP:HA	1.59	0.82
1:B:1681:ARG:HD3	1:B:1741:ASP:HA	1.60	0.82
1:A:1587:ILE:HG23	1:A:1588:GLY:H	1.44	0.82
1:B:1468:GLN:NE2	1:B:1478:HIS:HD2	1.76	0.82
1:B:1726:THR:O	1:B:1730:ARG:HG2	1.81	0.81
1:A:1517:GLY:HA3	1:A:1549:ILE:HG12	1.62	0.81
1:A:1816:VAL:HG22	1:A:1820:VAL:HG22	1.63	0.81
1:A:1343:TYR:HB3	1:A:1344:PRO:HD2	1.63	0.80
1:A:967:TYR:CE2	1:A:1030:PHE:CZ	2.67	0.80
1:A:1165:ASN:HD21	1:A:1451:GLU:H	1.29	0.80
1:A:1823:PRO:HB3	1:A:1841:ARG:HH21	1.46	0.80
1:B:1517:GLY:HA3	1:B:1549:ILE:HG12	1.64	0.80
1:B:1050:LEU:HD21	1:B:1083:TYR:CE1	2.18	0.79
1:A:1120:ILE:HG21	1:A:1212:LEU:HD21	1.62	0.79
1:A:1468:GLN:NE2	1:A:1478:HIS:HD2	1.79	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1098:ARG:NH1	1:B:1181:SER:HB3	1.97	0.78
1:B:1165:ASN:HD21	1:B:1451:GLU:H	1.31	0.78
1:A:1726:THR:O	1:A:1730:ARG:HG2	1.84	0.78
1:B:1617:PRO:O	1:B:1621:THR:HG23	1.84	0.78
1:A:981:ARG:HG3	1:A:981:ARG:HH11	1.47	0.77
1:A:1088:LYS:HE2	1:A:1095:GLU:HB2	1.64	0.77
1:B:1765:LEU:HD23	1:B:1765:LEU:N	1.99	0.77
1:A:1617:PRO:O	1:A:1621:THR:HG23	1.85	0.77
1:B:1219:GLY:H	1:B:1228:GLN:HE22	1.30	0.77
1:B:1468:GLN:HE21	1:B:1478:HIS:HD2	1.31	0.77
1:B:981:ARG:HH12	1:B:1030:PHE:HB2	1.49	0.76
1:A:1665:VAL:HG22	1:A:1673:VAL:HG11	1.67	0.75
1:A:1219:GLY:H	1:A:1228:GLN:HE22	1.30	0.75
1:A:1039:ARG:HB3	1:A:1057:PRO:HG3	1.66	0.75
1:B:1088:LYS:HE2	1:B:1095:GLU:HB2	1.67	0.75
1:A:1165:ASN:ND2	1:A:1451:GLU:H	1.84	0.75
1:B:1765:LEU:H	1:B:1765:LEU:CD2	1.97	0.75
1:A:1765:LEU:HD23	1:A:1765:LEU:N	1.99	0.75
1:B:1343:TYR:HB3	1:B:1344:PRO:HD2	1.66	0.75
1:A:1559:PHE:CE2	1:A:1586:THR:HB	2.22	0.74
1:B:1039:ARG:HB3	1:B:1057:PRO:HG3	1.70	0.74
1:A:1653:GLN:HE22	1:A:1676:TYR:H	1.36	0.74
1:B:1723:ALA:HB1	1:B:1728:LEU:HB2	1.69	0.74
1:A:1665:VAL:HG22	1:A:1673:VAL:CG1	2.17	0.74
1:B:981:ARG:HH11	1:B:981:ARG:HG3	1.52	0.74
1:B:1165:ASN:ND2	1:B:1451:GLU:H	1.86	0.73
1:B:1665:VAL:HG22	1:B:1673:VAL:HG11	1.69	0.73
1:A:1468:GLN:HE21	1:A:1478:HIS:HD2	1.36	0.73
1:A:1004:SER:OG	1:A:1022:LYS:HG2	1.87	0.73
1:A:1030:PHE:CB	1:A:1031:PRO:HD2	2.18	0.73
1:B:1606:ARG:O	1:B:1610:GLN:HG3	1.88	0.73
1:B:1653:GLN:HE22	1:B:1676:TYR:H	1.37	0.72
1:A:1030:PHE:HD2	1:A:1031:PRO:CD	2.01	0.72
1:A:1123:SER:OG	1:A:1204:THR:HG23	1.89	0.72
1:B:1665:VAL:HG22	1:B:1673:VAL:CG1	2.19	0.72
1:A:962:GLU:HG3	1:A:1200:LEU:HD22	1.70	0.72
1:B:1030:PHE:HD2	1:B:1031:PRO:CD	2.02	0.72
1:B:1423:GLU:N	1:B:1424:PRO:HA	2.05	0.72
1:B:1559:PHE:CE2	1:B:1586:THR:HB	2.25	0.71
1:A:1120:ILE:HB	1:A:1207:THR:HG22	1.72	0.71
1:B:1146:LEU:HA	1:B:1197:PHE:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1399:GLU:HA	1:B:1500:VAL:HG21	1.71	0.71
1:B:1614:THR:HG23	1:B:1719:TRP:HE3	1.55	0.71
1:A:1723:ALA:HB1	1:A:1728:LEU:HB2	1.72	0.71
1:A:1399:GLU:HA	1:A:1500:VAL:HG21	1.73	0.71
1:A:1721:GLU:OE1	1:A:1733:PHE:HB2	1.90	0.71
1:A:1437:ARG:O	1:A:1437:ARG:HG2	1.90	0.71
1:A:1647:THR:HA	1:A:1650:ILE:HG22	1.73	0.71
1:B:1467:GLN:NE2	1:B:1475:LEU:HD13	2.06	0.71
1:B:1681:ARG:HH11	1:B:1742:ASP:N	1.85	0.70
1:B:1004:SER:OG	1:B:1022:LYS:HG2	1.91	0.70
1:B:1251:TYR:CD1	1:B:1587:ILE:HB	2.27	0.70
1:A:1251:TYR:CD1	1:A:1587:ILE:HB	2.27	0.70
1:A:1681:ARG:HH11	1:A:1742:ASP:N	1.85	0.70
1:B:1437:ARG:O	1:B:1437:ARG:HG2	1.92	0.70
1:B:1129:LYS:HD2	1:B:1201:PRO:HG3	1.74	0.70
1:B:1120:ILE:HB	1:B:1207:THR:HG22	1.72	0.70
1:A:1606:ARG:O	1:A:1610:GLN:HG3	1.91	0.70
1:B:1035:VAL:CG2	1:B:1038:LEU:HD21	2.21	0.70
1:B:1444:PRO:O	1:B:1446:TYR:N	2.25	0.70
1:A:1098:ARG:NH1	1:A:1181:SER:HB3	2.07	0.69
1:A:1614:THR:HG23	1:A:1719:TRP:HE3	1.57	0.69
1:B:1083:TYR:HD2	1:B:1218:LEU:HD11	1.58	0.69
1:A:1047:ASN:HD21	1:A:1077:THR:N	1.87	0.69
1:A:1804:VAL:HG22	1:A:1832:GLN:O	1.93	0.69
1:B:1647:THR:HA	1:B:1650:ILE:HG22	1.72	0.69
1:A:1803:GLY:H	1:A:1832:GLN:HB2	1.56	0.69
1:B:1803:GLY:H	1:B:1832:GLN:HB2	1.59	0.68
1:A:981:ARG:HH12	1:A:1030:PHE:HB2	1.54	0.68
1:B:1804:VAL:HG22	1:B:1832:GLN:O	1.93	0.68
1:A:1030:PHE:HB3	1:A:1031:PRO:HD2	1.75	0.68
1:A:1765:LEU:H	1:A:1765:LEU:CD2	1.97	0.68
1:A:1035:VAL:CG2	1:A:1038:LEU:HD21	2.22	0.68
1:A:1807:VAL:HG23	1:A:1807:VAL:O	1.94	0.68
1:B:962:GLU:HG3	1:B:1200:LEU:HD22	1.76	0.67
1:B:1021:LEU:HB2	1:B:1036:ASN:ND2	2.09	0.67
1:A:1771:PHE:HB3	1:A:1778:MET:HE2	1.75	0.67
1:B:1030:PHE:CB	1:B:1031:PRO:HD2	2.24	0.67
1:A:1083:TYR:HD2	1:A:1218:LEU:HD11	1.59	0.67
1:B:1587:ILE:HG23	1:B:1588:GLY:N	2.10	0.67
1:A:1423:GLU:N	1:A:1424:PRO:HA	2.10	0.67
1:A:1587:ILE:HG23	1:A:1588:GLY:N	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:GLU:C	1:A:963:LYS:H	1.98	0.67
1:A:1503:GLN:HE22	1:A:1756:GLN:CD	1.97	0.67
1:B:1503:GLN:HE22	1:B:1756:GLN:CD	1.99	0.66
1:A:1129:LYS:HD2	1:A:1201:PRO:HG3	1.76	0.66
1:B:1251:TYR:O	1:B:1587:ILE:HA	1.94	0.66
1:B:1721:GLU:OE1	1:B:1733:PHE:HB2	1.95	0.66
1:A:1674:THR:HG22	1:A:1699:THR:OG1	1.95	0.66
1:B:1120:ILE:CG2	1:B:1212:LEU:HD21	2.25	0.66
1:B:1326:GLN:HB3	1:B:1327:PRO:HD2	1.77	0.66
1:A:1687:THR:OG1	1:A:1689:VAL:HG12	1.95	0.65
1:A:1139:HIS:CD2	1:A:1144:ARG:HD2	2.32	0.65
1:B:1733:PHE:CD1	1:B:1795:LYS:HB3	2.31	0.65
1:A:1131:LEU:HD22	1:A:1173:TYR:CD1	2.32	0.65
1:B:1139:HIS:CG	1:B:1144:ARG:HD2	2.31	0.65
1:A:1437:ARG:O	1:A:1438:ASP:HB2	1.96	0.65
1:B:1302:ILE:HD12	1:B:1312:VAL:HG21	1.77	0.65
1:B:1771:PHE:HB3	1:B:1778:MET:HE2	1.78	0.65
1:B:1437:ARG:O	1:B:1438:ASP:HB2	1.95	0.65
1:A:1146:LEU:HA	1:A:1197:PHE:HB3	1.76	0.65
1:A:1139:HIS:CG	1:A:1144:ARG:HD2	2.32	0.65
1:A:1733:PHE:CD1	1:A:1795:LYS:HB3	2.31	0.65
1:B:1200:LEU:O	1:B:1200:LEU:HG	1.97	0.64
1:A:1135:GLY:HA3	1:A:1170:HIS:H	1.61	0.64
1:B:961:GLU:C	1:B:963:LYS:H	2.00	0.64
1:B:1047:ASN:HD21	1:B:1077:THR:N	1.89	0.64
1:A:1021:LEU:HB2	1:A:1036:ASN:ND2	2.11	0.64
1:B:1687:THR:OG1	1:B:1689:VAL:HG12	1.98	0.64
1:A:1467:GLN:NE2	1:A:1475:LEU:HD13	2.13	0.64
1:B:1719:TRP:NE1	1:B:1735:GLY:HA3	2.12	0.64
1:A:1745:THR:HB	1:A:1773:ALA:O	1.98	0.64
1:B:963:LYS:HE2	1:B:997:TYR:CE2	2.33	0.64
1:A:1120:ILE:CG2	1:A:1212:LEU:HD21	2.28	0.63
1:A:1251:TYR:O	1:A:1587:ILE:HA	1.97	0.63
1:B:1098:ARG:CG	1:B:1100:SER:HB3	2.28	0.63
1:B:1135:GLY:HA3	1:B:1170:HIS:H	1.64	0.63
1:B:1467:GLN:HE22	1:B:1475:LEU:HD13	1.63	0.63
1:A:1289:PHE:CZ	1:A:1397:GLU:HB3	2.34	0.63
1:B:1745:THR:HB	1:B:1773:ALA:O	1.97	0.63
1:A:1433:SER:HB3	1:A:1434:PRO:HD3	1.81	0.62
1:B:1237:VAL:HG22	1:B:1518:ARG:C	2.19	0.62
1:A:1237:VAL:HG22	1:A:1518:ARG:C	2.19	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1433:SER:HB3	1:B:1434:PRO:HD3	1.80	0.62
1:A:1444:PRO:O	1:A:1446:TYR:N	2.31	0.62
1:A:1513:PHE:CD2	1:A:1514:PRO:HD2	2.34	0.62
1:B:1532:ASP:O	1:B:1536:LYS:HG2	1.99	0.62
1:B:1123:SER:OG	1:B:1204:THR:HG23	1.99	0.62
1:A:1200:LEU:HG	1:A:1200:LEU:O	1.99	0.62
1:B:1550:SER:HB2	1:B:1633:VAL:HG21	1.82	0.62
1:A:1730:ARG:HH12	1:A:1755:GLY:HA3	1.65	0.62
1:B:1030:PHE:HB3	1:B:1031:PRO:HD2	1.82	0.62
1:B:1726:THR:O	1:B:1730:ARG:CG	2.48	0.62
2:C:1:GLC:H62	2:C:2:GLC:O2	2.00	0.62
1:A:981:ARG:NH1	1:A:981:ARG:HG3	2.15	0.61
1:A:1804:VAL:H	1:A:1832:GLN:HB3	1.63	0.61
1:B:1047:ASN:ND2	1:B:1077:THR:H	1.91	0.61
1:B:1531:TRP:CH2	1:B:1567:MET:HA	2.35	0.61
1:A:1513:PHE:H	1:A:1516:SER:HB2	1.65	0.61
1:A:1135:GLY:HA2	1:A:1170:HIS:HB2	1.81	0.61
1:B:1298:PHE:N	1:B:1299:PRO:CD	2.63	0.61
1:A:963:LYS:HE2	1:A:997:TYR:CE2	2.35	0.61
1:A:961:GLU:HG2	1:A:1200:LEU:N	2.15	0.61
1:A:1326:GLN:HB3	1:A:1327:PRO:HD2	1.81	0.61
1:B:1135:GLY:HA2	1:B:1170:HIS:HB2	1.82	0.61
1:B:1614:THR:HG23	1:B:1719:TRP:CE3	2.35	0.61
1:B:1694:ARG:H	1:B:1696:GLU:HG3	1.66	0.61
1:A:1298:PHE:N	1:A:1299:PRO:CD	2.64	0.61
1:A:1726:THR:O	1:A:1730:ARG:CG	2.49	0.61
1:A:966:CYS:SG	1:A:981:ARG:HD3	2.41	0.60
1:A:1022:LYS:HD2	1:A:1022:LYS:O	2.01	0.60
1:B:966:CYS:SG	1:B:981:ARG:HD3	2.41	0.60
1:B:1139:HIS:CD2	1:B:1144:ARG:HD2	2.37	0.60
1:B:1804:VAL:H	1:B:1832:GLN:HB3	1.65	0.60
1:A:1083:TYR:CD2	1:A:1218:LEU:HD11	2.37	0.60
1:A:1105:ILE:HG23	1:A:1183:HIS:CD2	2.36	0.60
1:A:1631:VAL:HG13	1:A:1632:THR:N	2.16	0.60
1:A:1461:THR:OG1	1:A:1462:LEU:N	2.33	0.60
1:B:1285:ARG:NH2	1:B:1359:PRO:HA	2.17	0.60
1:B:1611:THR:O	1:B:1614:THR:HB	2.02	0.60
1:B:1740:LEU:HA	1:B:1745:THR:O	2.02	0.60
2:C:1:GLC:O3	2:C:2:GLC:H5	2.02	0.60
1:B:1040:LEU:HD12	1:B:1041:ASP:N	2.17	0.60
1:A:1512:THR:HG22	1:A:1516:SER:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1550:SER:HB2	1:A:1633:VAL:HG21	1.84	0.60
1:A:1719:TRP:NE1	1:A:1735:GLY:HA3	2.16	0.60
1:B:1382:PHE:CD2	1:B:1462:LEU:HD21	2.37	0.60
1:A:1694:ARG:H	1:A:1696:GLU:HG3	1.67	0.59
1:B:1674:THR:HG22	1:B:1699:THR:OG1	2.00	0.59
1:B:1838:VAL:HG12	1:B:1838:VAL:O	2.00	0.59
1:B:1135:GLY:CA	1:B:1170:HIS:H	2.15	0.59
1:A:1813:SER:HG	1:A:1825:PHE:HE2	1.50	0.59
1:B:966:CYS:HB3	1:B:996:CYS:SG	2.42	0.59
1:B:1513:PHE:CD2	1:B:1514:PRO:HD2	2.37	0.59
1:B:1064:VAL:HG13	1:B:1066:VAL:HG13	1.84	0.59
1:A:1136:GLU:OE1	1:A:1522:HIS:HE1	1.85	0.59
1:A:1803:GLY:HA2	1:A:1832:GLN:HG3	1.84	0.59
1:B:961:GLU:HG2	1:B:1200:LEU:N	2.18	0.59
1:B:1101:THR:O	1:B:1103:THR:N	2.36	0.59
1:A:1740:LEU:HA	1:A:1745:THR:O	2.02	0.59
1:B:1807:VAL:HG23	1:B:1807:VAL:O	2.01	0.59
1:A:1098:ARG:CG	1:A:1100:SER:HB3	2.32	0.59
1:B:1396:ARG:O	1:B:1399:GLU:HB3	2.03	0.59
1:B:1120:ILE:HG21	1:B:1212:LEU:CD2	2.33	0.59
1:B:1136:GLU:OE1	1:B:1522:HIS:HE1	1.85	0.59
1:B:1512:THR:HG22	1:B:1516:SER:HB3	1.85	0.59
1:B:1289:PHE:CZ	1:B:1397:GLU:HB3	2.38	0.59
1:A:1207:THR:HG23	1:A:1209:GLY:H	1.68	0.58
1:B:1823:PRO:HB3	1:B:1841:ARG:NH2	2.15	0.58
1:A:1302:ILE:HD12	1:A:1312:VAL:HG21	1.84	0.58
1:A:1040:LEU:HD12	1:A:1041:ASP:N	2.17	0.58
1:A:1135:GLY:CA	1:A:1170:HIS:H	2.15	0.58
1:B:1686:TYR:CE2	1:B:1706:HIS:HE1	2.22	0.58
1:A:1614:THR:HG23	1:A:1719:TRP:CE3	2.37	0.58
1:B:1186:LEU:HD12	1:B:1187:LEU:N	2.18	0.58
1:B:1576:ALA:O	1:B:1612:ARG:HD2	2.03	0.58
1:B:1621:THR:HG22	1:B:1751:PHE:H	1.67	0.58
1:B:1745:THR:HG21	1:B:1774:SER:O	2.04	0.58
1:A:1382:PHE:CD2	1:A:1462:LEU:HD21	2.37	0.58
1:B:1083:TYR:CD2	1:B:1218:LEU:HD11	2.36	0.58
2:C:1:GLC:H4	2:C:2:GLC:O2	2.03	0.58
1:A:1621:THR:HG22	1:A:1751:PHE:H	1.67	0.58
1:A:1838:VAL:HG12	1:A:1838:VAL:O	2.03	0.58
1:B:1040:LEU:HD11	1:B:1042:VAL:HG23	1.86	0.58
1:B:1472:ASP:OD1	1:B:1473:GLY:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:ALA:HB2	1:A:1301:LEU:HD11	1.86	0.58
1:B:1104:ILE:O	1:B:1127:PRO:HB3	2.03	0.58
1:B:1615:LEU:HD11	1:B:1660:PHE:CZ	2.39	0.58
1:A:1798:TYR:N	1:A:1798:TYR:CD2	2.71	0.58
1:B:968:PRO:HB3	1:B:1206:ARG:NH1	2.19	0.58
1:A:966:CYS:HB3	1:A:996:CYS:SG	2.44	0.58
1:B:1461:THR:OG1	1:B:1462:LEU:N	2.33	0.58
1:A:1101:THR:O	1:A:1103:THR:N	2.36	0.57
1:B:1470:LEU:HD21	1:B:1476:VAL:HG21	1.86	0.57
1:A:1823:PRO:HB3	1:A:1841:ARG:NH2	2.18	0.57
1:B:1156:ARG:HD3	1:B:1158:GLN:CG	2.34	0.57
1:B:1784:PHE:CE2	1:B:1786:ASN:HB2	2.33	0.57
1:B:1803:GLY:HA2	1:B:1832:GLN:HG3	1.86	0.57
1:B:1813:SER:HG	1:B:1825:PHE:HE2	1.52	0.57
1:A:1784:PHE:C	1:A:1784:PHE:CD2	2.77	0.57
1:B:1367:LEU:HD12	1:B:1376:TYR:OH	2.05	0.57
1:A:1047:ASN:ND2	1:A:1077:THR:H	1.90	0.57
1:B:1098:ARG:HG2	1:B:1100:SER:HB3	1.85	0.57
1:A:1715:TYR:HA	1:A:1747:GLY:O	2.04	0.57
1:B:961:GLU:OE1	1:B:961:GLU:N	2.37	0.57
1:B:1022:LYS:HD2	1:B:1022:LYS:O	2.05	0.57
1:B:1716:ILE:CG1	1:B:1748:GLY:HA3	2.30	0.57
1:A:1784:PHE:CE2	1:A:1786:ASN:HB2	2.31	0.57
1:A:1156:ARG:HD3	1:A:1158:GLN:CG	2.35	0.57
1:A:1298:PHE:CZ	1:A:1302:ILE:HD11	2.40	0.57
1:A:1576:ALA:O	1:A:1612:ARG:HD2	2.05	0.57
1:A:1098:ARG:HG2	1:A:1100:SER:HB3	1.86	0.56
1:A:1532:ASP:O	1:A:1536:LYS:HG2	2.03	0.56
1:B:1131:LEU:HD22	1:B:1173:TYR:CD1	2.40	0.56
1:B:1715:TYR:HA	1:B:1747:GLY:O	2.04	0.56
1:A:1441:LEU:HD13	1:A:1464:MET:H	1.70	0.56
1:A:1531:TRP:CH2	1:A:1567:MET:HA	2.39	0.56
1:A:1086:LEU:HD22	1:B:1097:ARG:CZ	2.36	0.56
1:A:1745:THR:HG21	1:A:1774:SER:O	2.05	0.56
1:B:1035:VAL:CG2	1:B:1115:PHE:CD2	2.89	0.56
1:B:1750:LEU:HD21	1:B:1752:TRP:HD1	1.71	0.56
1:A:968:PRO:HB3	1:A:1206:ARG:NH1	2.21	0.56
1:B:1432:VAL:HG13	1:B:1433:SER:N	2.19	0.56
1:A:967:TYR:CD2	1:A:1030:PHE:HZ	2.22	0.56
1:A:1040:LEU:HD11	1:A:1042:VAL:HG23	1.88	0.56
1:B:981:ARG:NH1	1:B:981:ARG:HG3	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1794:LEU:HD22	1:B:1845:LEU:HD23	1.88	0.56
1:A:1219:GLY:N	1:A:1228:GLN:HE22	2.02	0.56
1:A:1250:ARG:NH2	1:A:1589:THR:HG23	2.21	0.56
1:A:1022:LYS:O	1:A:1022:LYS:CD	2.54	0.56
1:A:1464:MET:HG3	1:A:1479:TYR:HA	1.88	0.56
1:A:1686:TYR:CE2	1:A:1706:HIS:HE1	2.23	0.56
1:A:961:GLU:HB3	1:A:1200:LEU:CB	2.34	0.55
1:A:1784:PHE:C	1:A:1784:PHE:HD2	2.09	0.55
1:B:1513:PHE:H	1:B:1516:SER:HB2	1.70	0.55
1:B:1399:GLU:HA	1:B:1500:VAL:CG2	2.34	0.55
1:A:1064:VAL:HG13	1:A:1066:VAL:HG13	1.87	0.55
1:B:1153:MET:HE3	1:B:1193:MET:CG	2.35	0.55
1:B:1385:PHE:HB2	1:B:1488:SER:OG	2.05	0.55
1:B:1522:HIS:O	1:B:1552:THR:HA	2.06	0.55
1:A:1059:LYS:HD3	1:A:1060:ASN:H	1.72	0.55
1:B:1784:PHE:C	1:B:1784:PHE:CD2	2.78	0.55
1:A:1590:ARG:HD3	1:A:1591:ARG:O	2.07	0.55
1:B:1333:ARG:NH2	1:B:1396:ARG:HD3	2.21	0.55
1:A:1399:GLU:HA	1:A:1500:VAL:CG2	2.36	0.55
1:B:1406:GLN:HE21	1:B:1406:GLN:HA	1.72	0.55
1:B:961:GLU:HB3	1:B:1200:LEU:CB	2.34	0.55
1:A:981:ARG:HG2	1:A:982:GLY:H	1.72	0.55
1:A:1165:ASN:H	1:A:1165:ASN:HD22	1.54	0.55
1:A:1467:GLN:HE22	1:A:1475:LEU:HD13	1.71	0.55
1:A:1526:ASP:HB3	1:A:1560:PHE:HE2	1.71	0.55
1:B:1590:ARG:HD3	1:B:1591:ARG:O	2.07	0.55
1:A:1794:LEU:HD22	1:A:1845:LEU:HD23	1.89	0.55
1:B:1237:VAL:HG21	1:B:1520:ALA:N	2.22	0.55
1:A:1237:VAL:HG21	1:A:1520:ALA:N	2.22	0.55
1:A:1716:ILE:CG2	1:A:1738:ILE:HG23	2.37	0.55
1:B:1707:ILE:HD13	1:B:1709:LEU:HD21	1.87	0.55
1:A:1153:MET:HE3	1:A:1193:MET:CG	2.37	0.54
1:A:1333:ARG:NH2	1:A:1396:ARG:HD3	2.22	0.54
1:A:1406:GLN:HE21	1:A:1406:GLN:HA	1.71	0.54
2:C:1:GLC:O3	2:C:2:GLC:C5	2.55	0.54
1:A:1621:THR:HG21	1:A:1750:LEU:HA	1.89	0.54
1:A:961:GLU:O	1:A:963:LYS:N	2.40	0.54
1:A:1707:ILE:HG12	1:A:1708:ASN:N	2.22	0.54
1:B:1621:THR:HG21	1:B:1750:LEU:HA	1.89	0.54
1:B:1730:ARG:HH12	1:B:1755:GLY:HA3	1.73	0.54
1:B:1784:PHE:C	1:B:1784:PHE:HD2	2.10	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:HIS:CE1	1:A:1051:GLN:HG2	2.43	0.54
1:A:1145:ASP:O	1:A:1146:LEU:HB2	2.08	0.54
1:A:1611:THR:O	1:A:1614:THR:HB	2.08	0.54
1:B:961:GLU:O	1:B:963:LYS:N	2.40	0.54
1:A:1030:PHE:CG	1:A:1031:PRO:HD2	2.42	0.54
1:B:1681:ARG:NH1	1:B:1742:ASP:HB2	2.23	0.54
1:A:1441:LEU:HD12	1:A:1464:MET:H	1.71	0.54
1:A:1467:GLN:NE2	1:A:1475:LEU:HB3	2.23	0.54
1:B:1036:ASN:OD1	1:B:1037:PRO:HA	2.07	0.54
1:B:1647:THR:HA	1:B:1650:ILE:CG2	2.38	0.54
1:B:1273:TYR:HA	1:B:1613:TYR:OH	2.08	0.54
1:B:1423:GLU:OE2	1:B:1510:ARG:NH2	2.38	0.54
1:A:981:ARG:HB2	1:A:1030:PHE:CE1	2.44	0.53
1:B:1250:ARG:NH2	1:B:1589:THR:HG23	2.23	0.53
1:B:1560:PHE:O	1:B:1561:GLN:HB2	2.08	0.53
1:A:961:GLU:HG2	1:A:1200:LEU:H	1.74	0.53
1:A:1120:ILE:HG21	1:A:1212:LEU:CD2	2.36	0.53
1:A:1319:ALA:HB1	1:A:1380:VAL:CG2	2.38	0.53
1:B:1526:ASP:HB3	1:B:1560:PHE:HE2	1.69	0.53
1:B:1141:SER:HB3	3:B:31:HOH:O	2.09	0.53
1:A:1396:ARG:O	1:A:1399:GLU:HB3	2.08	0.53
1:A:1432:VAL:HG13	1:A:1433:SER:N	2.24	0.53
1:A:1750:LEU:HD21	1:A:1752:TRP:HD1	1.73	0.53
1:B:1187:LEU:HD12	1:B:1205:TYR:CD2	2.43	0.53
1:A:1560:PHE:O	1:A:1561:GLN:HB2	2.07	0.53
1:B:1022:LYS:O	1:B:1022:LYS:CD	2.57	0.53
1:B:1260:ALA:HB2	1:B:1301:LEU:HD11	1.90	0.53
1:A:961:GLU:N	1:A:961:GLU:OE1	2.39	0.53
1:A:1237:VAL:HG21	1:A:1519:TRP:C	2.29	0.53
1:B:1263:TYR:CE1	1:B:1310:MET:HG3	2.44	0.53
1:B:1741:ASP:C	1:B:1743:GLU:N	2.61	0.53
1:A:1470:LEU:HD21	1:A:1476:VAL:HG21	1.91	0.53
1:B:1646:VAL:HG11	1:B:1676:TYR:CE1	2.43	0.53
1:B:1716:ILE:CG2	1:B:1738:ILE:HG23	2.39	0.53
1:B:1814:ILE:CB	1:B:1822:THR:HG22	2.39	0.53
1:A:1035:VAL:CG2	1:A:1115:PHE:CD2	2.92	0.52
1:A:1707:ILE:HD13	1:A:1709:LEU:HD21	1.91	0.52
1:A:1247:GLN:HG2	1:A:1275:VAL:HB	1.90	0.52
1:B:967:TYR:CD2	1:B:1030:PHE:HZ	2.21	0.52
1:B:981:ARG:HG2	1:B:982:GLY:H	1.74	0.52
1:B:1423:GLU:N	1:B:1424:PRO:CA	2.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1707:ILE:HG12	1:B:1708:ASN:N	2.23	0.52
1:B:1512:THR:HG21	1:B:1549:ILE:CD1	2.39	0.52
1:B:981:ARG:HB2	1:B:1030:PHE:CE1	2.44	0.52
1:A:1097:ARG:CZ	1:B:1086:LEU:HD22	2.40	0.52
1:B:1177:GLU:O	1:B:1179:ASP:O	2.27	0.52
1:A:1647:THR:HA	1:A:1650:ILE:CG2	2.39	0.52
1:B:1032:SER:HB3	1:B:1116:SER:HB3	1.92	0.52
1:B:1145:ASP:O	1:B:1146:LEU:HB2	2.08	0.52
1:B:1550:SER:HB2	1:B:1633:VAL:CG2	2.38	0.52
1:A:1298:PHE:N	1:A:1299:PRO:HD2	2.25	0.52
1:A:1322:GLY:HA3	1:A:1331:PHE:CE2	2.45	0.52
1:A:1472:ASP:OD1	1:A:1473:GLY:N	2.42	0.52
1:B:975:ALA:HA	1:B:985:TRP:CG	2.45	0.52
1:B:1322:GLY:HA3	1:B:1331:PHE:CE2	2.44	0.52
1:A:1542:MET:CE	1:A:1636:PRO:CB	2.73	0.52
1:A:1615:LEU:HD11	1:A:1660:PHE:CZ	2.46	0.52
1:B:1219:GLY:N	1:B:1228:GLN:HE22	2.03	0.52
1:A:1200:LEU:O	1:A:1201:PRO:C	2.49	0.51
1:B:1040:LEU:HD22	1:B:1094:ILE:HD11	1.92	0.51
1:A:1716:ILE:CG2	1:A:1738:ILE:HG12	2.40	0.51
1:B:1237:VAL:HG21	1:B:1519:TRP:C	2.30	0.51
1:A:981:ARG:HD2	1:A:1030:PHE:CD1	2.46	0.51
1:B:1420:ASP:CG	1:B:1421:MET:N	2.63	0.51
1:B:1047:ASN:ND2	1:B:1076:SER:HA	2.25	0.51
1:B:1105:ILE:HG23	1:B:1183:HIS:CD2	2.45	0.51
1:B:1247:GLN:HG2	1:B:1275:VAL:HB	1.92	0.51
1:B:1298:PHE:CZ	1:B:1302:ILE:HD11	2.46	0.51
1:B:1441:LEU:HD13	1:B:1464:MET:H	1.69	0.51
1:B:1513:PHE:CG	1:B:1514:PRO:HD2	2.46	0.51
1:A:1186:LEU:HD12	1:A:1187:LEU:N	2.25	0.51
1:A:1423:GLU:OE2	1:A:1510:ARG:NH2	2.36	0.51
1:B:1030:PHE:CG	1:B:1031:PRO:HD2	2.46	0.51
1:B:1045:HIS:CE1	1:B:1051:GLN:HG2	2.46	0.51
1:B:1165:ASN:HD22	1:B:1165:ASN:H	1.57	0.51
1:B:1464:MET:HG3	1:B:1479:TYR:HA	1.92	0.51
1:A:1059:LYS:HD3	1:A:1060:ASN:N	2.26	0.51
1:A:1420:ASP:CG	1:A:1421:MET:N	2.64	0.51
1:A:1638:LEU:HD12	1:A:1638:LEU:O	2.10	0.51
1:B:1156:ARG:HD3	1:B:1158:GLN:HG2	1.93	0.51
1:A:1034:PRO:HA	1:A:1116:SER:HA	1.92	0.51
1:A:1187:LEU:HD12	1:A:1205:TYR:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1613:TYR:HA	1:A:1616:LEU:HG	1.93	0.51
1:A:1668:ARG:HD2	3:A:12:HOH:O	2.11	0.51
1:B:1035:VAL:HG21	1:B:1115:PHE:CD2	2.45	0.51
1:B:1433:SER:HB3	1:B:1434:PRO:CD	2.40	0.51
2:C:1:GLC:C4	2:C:2:GLC:O2	2.59	0.51
1:A:1737:LYS:HD3	1:A:1802:TRP:CH2	2.46	0.51
1:A:1050:LEU:HD21	1:A:1083:TYR:CZ	2.45	0.51
1:A:1513:PHE:CG	1:A:1514:PRO:HD2	2.45	0.51
1:B:1765:LEU:N	1:B:1765:LEU:CD2	2.67	0.51
1:A:1032:SER:HB3	1:A:1116:SER:HB3	1.92	0.51
1:A:1522:HIS:O	1:A:1552:THR:HA	2.11	0.51
1:A:1814:ILE:CB	1:A:1822:THR:HG22	2.40	0.51
1:B:1200:LEU:O	1:B:1201:PRO:C	2.49	0.51
1:B:1478:HIS:CE1	1:B:1482:HIS:ND1	2.79	0.51
1:A:1150:THR:OG1	1:A:1196:THR:HG23	2.12	0.50
1:A:1177:GLU:O	1:A:1179:ASP:O	2.29	0.50
1:A:1302:ILE:HD12	1:A:1312:VAL:HG11	1.93	0.50
1:A:1601:PHE:O	1:A:1602:VAL:C	2.50	0.50
1:A:1731:GLN:O	1:A:1795:LYS:HE3	2.11	0.50
1:B:961:GLU:HG2	1:B:1200:LEU:H	1.76	0.50
1:B:1613:TYR:HA	1:B:1616:LEU:HG	1.92	0.50
1:A:1367:LEU:HD12	1:A:1376:TYR:OH	2.11	0.50
1:B:1761:TYR:HA	1:B:1766:TYR:CD1	2.47	0.50
1:A:1421:MET:HE3	2:C:3:AC1:C7B	2.41	0.50
1:B:1491:ARG:HG3	1:B:1519:TRP:CE3	2.47	0.50
1:A:1550:SER:HB2	1:A:1633:VAL:CG2	2.42	0.50
1:B:1402:TYR:CD2	1:B:1500:VAL:HG13	2.46	0.50
1:B:1441:LEU:CD1	1:B:1464:MET:HB2	2.26	0.50
1:B:1683:TYR:CE2	1:B:1740:LEU:O	2.64	0.50
1:A:1681:ARG:NH1	1:A:1742:ASP:HB2	2.25	0.50
1:A:1700:LEU:HD12	1:A:1700:LEU:N	2.27	0.50
1:B:1272:PRO:HB2	1:B:1613:TYR:CE2	2.47	0.50
1:B:1638:LEU:HD12	1:B:1638:LEU:O	2.11	0.50
1:B:1775:GLN:O	1:B:1777:THR:HG23	2.10	0.50
1:A:1097:ARG:NH1	1:B:1086:LEU:HD22	2.26	0.50
1:A:1273:TYR:HA	1:A:1613:TYR:OH	2.11	0.50
1:A:1285:ARG:NH2	1:A:1359:PRO:HA	2.27	0.50
1:A:1716:ILE:HG22	1:A:1738:ILE:CA	2.38	0.50
1:B:1229:TYR:CZ	1:B:1233:ILE:HD13	2.47	0.50
1:B:1731:GLN:O	1:B:1795:LYS:HE3	2.11	0.50
1:B:1798:TYR:CD2	1:B:1798:TYR:N	2.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:ALA:HA	1:A:985:TRP:CG	2.47	0.50
1:A:1040:LEU:HD22	1:A:1094:ILE:HD11	1.94	0.50
1:A:1137:THR:HG21	1:A:1151:TRP:CE3	2.47	0.50
1:B:1468:GLN:HE21	1:B:1478:HIS:CD2	2.21	0.50
1:A:1559:PHE:CD2	1:A:1586:THR:HB	2.47	0.50
1:B:1513:PHE:O	1:B:1516:SER:HB2	2.12	0.50
1:B:1783:ILE:HD12	1:B:1783:ILE:H	1.76	0.50
1:A:1189:ASN:HD22	1:A:1190:SER:N	2.10	0.49
1:A:1433:SER:HB3	1:A:1434:PRO:CD	2.42	0.49
1:A:1478:HIS:CE1	1:A:1482:HIS:ND1	2.80	0.49
1:A:1765:LEU:N	1:A:1765:LEU:CD2	2.67	0.49
1:B:1775:GLN:C	1:B:1777:THR:H	2.15	0.49
1:A:990:SER:O	1:A:993:VAL:HG22	2.12	0.49
1:A:1402:TYR:CD2	1:A:1500:VAL:HG13	2.47	0.49
1:B:1467:GLN:NE2	1:B:1475:LEU:HB3	2.27	0.49
1:A:1106:TRP:CZ3	1:A:1108:SER:HB3	2.47	0.49
1:A:1455:ARG:HB2	1:A:1459:SER:HB2	1.94	0.49
1:B:1376:TYR:N	1:B:1376:TYR:CD2	2.79	0.49
1:A:1221:THR:OG1	1:A:1224:LEU:HD23	2.12	0.49
1:A:1447:MET:O	1:A:1453:ARG:HD3	2.13	0.49
1:A:1621:THR:CG2	1:A:1751:PHE:H	2.25	0.49
1:A:1831:THR:O	1:A:1833:VAL:N	2.45	0.49
1:A:1587:ILE:CG2	1:A:1588:GLY:H	2.22	0.49
1:B:1207:THR:HG23	1:B:1209:GLY:H	1.76	0.49
1:B:1455:ARG:HB2	1:B:1459:SER:HB2	1.93	0.49
1:A:961:GLU:C	1:A:963:LYS:N	2.64	0.49
1:A:1145:ASP:HB3	1:A:1149:HIS:HD2	1.77	0.49
1:B:1189:ASN:HD22	1:B:1190:SER:H	1.60	0.49
1:B:1621:THR:CG2	1:B:1751:PHE:H	2.26	0.49
1:A:1104:ILE:O	1:A:1127:PRO:HB3	2.11	0.49
1:A:1161:GLY:HA3	1:A:1164:LYS:HD2	1.95	0.49
1:A:1250:ARG:HG3	1:A:1251:TYR:N	2.25	0.49
1:B:990:SER:O	1:B:993:VAL:HG22	2.13	0.49
1:B:1161:GLY:HA3	1:B:1164:LYS:HD2	1.95	0.49
1:A:1086:LEU:HD22	1:B:1097:ARG:NH1	2.27	0.49
1:B:1828:ASP:OD1	1:B:1829:PRO:HD2	2.13	0.49
1:A:1038:LEU:HD11	1:A:1115:PHE:HB3	1.95	0.49
1:A:1761:TYR:HA	1:A:1766:TYR:CD1	2.47	0.49
1:A:1035:VAL:HG21	1:A:1115:PHE:CD2	2.47	0.48
1:A:1036:ASN:OD1	1:A:1037:PRO:HA	2.12	0.48
1:B:1603:ASN:HA	1:B:1606:ARG:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1716:ILE:CG2	1:B:1738:ILE:HG12	2.44	0.48
1:B:1237:VAL:HG22	1:B:1518:ARG:O	2.12	0.48
1:A:1132:TYR:CE1	1:A:1143:ARG:HB2	2.47	0.48
1:A:1603:ASN:HA	1:A:1606:ARG:HD3	1.95	0.48
1:A:1716:ILE:CG1	1:A:1748:GLY:HA3	2.35	0.48
1:A:1394:TRP:O	1:A:1398:ILE:HG12	2.12	0.48
1:B:961:GLU:C	1:B:963:LYS:N	2.66	0.48
1:B:1187:LEU:O	1:B:1189:ASN:N	2.42	0.48
1:A:1156:ARG:HD3	1:A:1158:GLN:HG2	1.95	0.48
1:A:1260:ALA:HB2	1:A:1301:LEU:CD1	2.43	0.48
1:A:1513:PHE:O	1:A:1516:SER:HB2	2.14	0.48
1:A:1691:ILE:O	1:A:1698:LYS:NZ	2.46	0.48
1:A:1784:PHE:HD2	1:A:1785:ASN:N	2.11	0.48
1:B:1189:ASN:HD22	1:B:1190:SER:N	2.11	0.48
1:B:1319:ALA:HB1	1:B:1380:VAL:CG2	2.44	0.48
1:B:1716:ILE:HG22	1:B:1738:ILE:CA	2.38	0.48
1:A:1145:ASP:HB3	1:A:1149:HIS:CD2	2.48	0.48
1:A:1189:ASN:HD22	1:A:1190:SER:H	1.59	0.48
1:A:1512:THR:HG21	1:A:1549:ILE:CD1	2.44	0.48
1:A:1775:GLN:C	1:A:1777:THR:H	2.17	0.48
1:B:1038:LEU:HD11	1:B:1115:PHE:HB3	1.95	0.48
1:B:1059:LYS:HD3	1:B:1060:ASN:H	1.79	0.48
1:A:1061:ARG:HD3	1:A:1211:VAL:HG12	1.96	0.48
1:A:1237:VAL:HG22	1:A:1518:ARG:O	2.14	0.48
1:A:1274:ASP:OD1	1:A:1726:THR:HG23	2.14	0.48
1:A:1606:ARG:CB	1:A:1606:ARG:HH11	2.27	0.48
1:A:1784:PHE:CD2	1:A:1785:ASN:N	2.82	0.48
1:B:981:ARG:HD2	1:B:1030:PHE:CD1	2.48	0.48
1:A:1229:TYR:CZ	1:A:1233:ILE:HD13	2.49	0.48
1:A:1683:TYR:CE2	1:A:1740:LEU:O	2.66	0.48
1:A:1019:ILE:HB	1:A:1038:LEU:HB2	1.96	0.48
1:B:1252:GLY:CA	1:B:1587:ILE:HD12	2.44	0.48
1:B:1509:THR:O	1:B:1522:HIS:HD2	1.96	0.48
1:B:1470:LEU:HB3	1:B:1471:PRO:CD	2.44	0.48
1:B:1542:MET:HE1	1:B:1636:PRO:CA	2.43	0.48
1:B:1831:THR:O	1:B:1833:VAL:N	2.47	0.48
1:A:1083:TYR:CD1	1:A:1083:TYR:C	2.87	0.47
1:A:1442:ASN:C	1:A:1444:PRO:CD	2.82	0.47
1:A:1446:TYR:O	1:A:1448:PRO:HD3	2.14	0.47
1:B:1145:ASP:HB3	1:B:1149:HIS:HD2	1.79	0.47
1:B:1631:VAL:HG13	1:B:1632:THR:N	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:HIS:O	1:A:1444:PRO:C	2.52	0.47
1:B:1034:PRO:HA	1:B:1116:SER:HA	1.95	0.47
1:B:1137:THR:HG21	1:B:1151:TRP:CE3	2.49	0.47
1:B:1737:LYS:HD3	1:B:1802:TRP:CH2	2.48	0.47
1:A:1423:GLU:N	1:A:1424:PRO:CA	2.76	0.47
1:A:1565:TYR:O	1:A:1569:VAL:HG23	2.14	0.47
1:B:1053:LYS:HA	1:B:1212:LEU:O	2.15	0.47
1:B:1478:HIS:HE1	1:B:1482:HIS:ND1	2.13	0.47
1:A:1047:ASN:ND2	1:A:1076:SER:HA	2.29	0.47
1:A:1134:PHE:CE1	1:A:1195:VAL:HG11	2.48	0.47
1:A:1542:MET:HE1	1:A:1636:PRO:CA	2.43	0.47
1:B:1798:TYR:HE2	1:B:1839:THR:CG2	2.27	0.47
1:A:1683:TYR:HE2	1:A:1740:LEU:O	1.97	0.47
1:B:1030:PHE:CD2	1:B:1031:PRO:CD	2.86	0.47
1:B:1302:ILE:HD12	1:B:1312:VAL:HG11	1.96	0.47
1:B:1446:TYR:O	1:B:1448:PRO:HD3	2.15	0.47
1:B:1504:ARG:HB3	1:B:1756:GLN:O	2.14	0.47
1:B:1683:TYR:HE2	1:B:1740:LEU:O	1.96	0.47
1:A:961:GLU:O	1:A:962:GLU:HB2	2.14	0.47
1:A:1646:VAL:HG11	1:A:1676:TYR:CE1	2.49	0.47
1:B:1129:LYS:CD	1:B:1201:PRO:HG3	2.44	0.47
1:B:1153:MET:HE3	1:B:1193:MET:HG3	1.96	0.47
1:B:1508:ILE:CD1	1:B:1508:ILE:N	2.78	0.47
1:A:1036:ASN:HA	1:A:1037:PRO:HA	1.59	0.47
1:A:1500:VAL:HG12	1:A:1501:THR:HG23	1.97	0.47
1:A:1704:LEU:O	1:A:1704:LEU:HD12	2.15	0.47
1:B:1498:GLN:OE1	1:B:1504:ARG:HA	2.15	0.47
1:B:1700:LEU:N	1:B:1700:LEU:HD12	2.29	0.47
1:B:1704:LEU:HD12	1:B:1704:LEU:O	2.15	0.47
1:A:1187:LEU:O	1:A:1189:ASN:N	2.44	0.47
1:B:1156:ARG:HG2	1:B:1158:GLN:HB2	1.96	0.47
1:B:1394:TRP:O	1:B:1398:ILE:HG12	2.15	0.47
1:A:1263:TYR:CE1	1:A:1310:MET:HG3	2.49	0.47
1:B:1298:PHE:N	1:B:1299:PRO:HD2	2.29	0.47
1:B:1823:PRO:CB	1:B:1841:ARG:HH21	2.21	0.47
1:A:1329:PRO:O	1:A:1333:ARG:HG3	2.15	0.47
1:B:1059:LYS:HD3	1:B:1060:ASN:N	2.29	0.47
1:B:1083:TYR:CD1	1:B:1083:TYR:C	2.88	0.47
1:A:1798:TYR:HE2	1:A:1839:THR:CG2	2.28	0.46
1:B:1134:PHE:CE1	1:B:1195:VAL:HG11	2.50	0.46
1:B:1260:ALA:HB2	1:B:1301:LEU:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1559:PHE:CD2	1:B:1586:THR:HB	2.50	0.46
1:B:1745:THR:O	1:B:1746:ALA:HB2	2.15	0.46
1:B:1788:ILE:HG22	1:B:1846:HIS:CD2	2.50	0.46
1:B:1136:GLU:HG2	1:B:1166:SER:HB3	1.97	0.46
1:B:1470:LEU:HB3	1:B:1471:PRO:HD2	1.97	0.46
1:B:1784:PHE:HD2	1:B:1785:ASN:N	2.14	0.46
1:A:1442:ASN:C	1:A:1444:PRO:HD3	2.35	0.46
1:A:1614:THR:CG2	1:A:1719:TRP:HB2	2.45	0.46
1:A:1716:ILE:HG22	1:A:1738:ILE:HG12	1.96	0.46
1:B:1145:ASP:HB3	1:B:1149:HIS:CD2	2.50	0.46
1:B:1691:ILE:O	1:B:1698:LYS:NZ	2.49	0.46
1:B:1798:TYR:HE2	1:B:1839:THR:HG23	1.81	0.46
1:A:1104:ILE:O	1:A:1104:ILE:HG13	2.15	0.46
1:A:1694:ARG:NH2	1:A:1743:GLU:HB2	2.30	0.46
1:B:1077:THR:HG23	1:B:1080:GLY:H	1.80	0.46
1:B:1681:ARG:NH1	1:B:1742:ASP:H	1.92	0.46
1:B:1784:PHE:CD2	1:B:1785:ASN:N	2.83	0.46
1:A:1741:ASP:C	1:A:1743:GLU:N	2.64	0.46
1:A:1053:LYS:HA	1:A:1212:LEU:O	2.14	0.46
1:A:1064:VAL:CG1	1:A:1066:VAL:HG13	2.45	0.46
1:A:1153:MET:HE3	1:A:1193:MET:HG3	1.98	0.46
1:A:1575:GLY:C	1:A:1577:PHE:H	2.19	0.46
1:A:1694:ARG:HH22	1:A:1743:GLU:HB2	1.80	0.46
1:B:1733:PHE:HB3	1:B:1797:GLY:HA3	1.98	0.46
1:A:1165:ASN:ND2	1:A:1165:ASN:H	2.14	0.46
1:B:1468:GLN:NE2	1:B:1478:HIS:CD2	2.68	0.46
1:B:1573:GLN:HA	1:B:1608:VAL:HG21	1.97	0.46
1:B:1746:ALA:HB3	1:B:1773:ALA:HB3	1.97	0.46
1:A:1733:PHE:HB3	1:A:1797:GLY:HA3	1.98	0.46
1:A:1746:ALA:HB3	1:A:1773:ALA:HB3	1.97	0.46
1:A:1783:ILE:HD12	1:A:1783:ILE:H	1.81	0.46
1:B:1106:TRP:CZ3	1:B:1108:SER:HB3	2.50	0.46
1:B:1136:GLU:OE1	1:B:1522:HIS:CE1	2.68	0.46
1:B:1791:THR:O	1:B:1793:PRO:HD3	2.15	0.46
1:A:1118:MET:HB2	1:A:1445:PRO:HG2	1.98	0.46
1:A:1346:ASP:O	1:A:1347:GLY:O	2.33	0.46
1:A:1090:ASN:HA	1:A:1091:PRO:HA	1.88	0.46
1:A:1156:ARG:HG2	1:A:1158:GLN:HB2	1.97	0.46
1:B:1283:MET:HA	1:B:1290:THR:O	2.16	0.46
1:B:1443:HIS:O	1:B:1444:PRO:C	2.51	0.46
1:A:1002:LEU:N	1:A:1002:LEU:HD23	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:PRO:HB2	1:A:1613:TYR:CE2	2.51	0.45
1:A:1587:ILE:CG2	1:A:1588:GLY:N	2.79	0.45
1:B:1229:TYR:CE1	1:B:1233:ILE:HD13	2.51	0.45
1:B:1609:LEU:HD13	1:B:1609:LEU:HA	1.81	0.45
1:B:1614:THR:CG2	1:B:1719:TRP:HB2	2.46	0.45
1:B:1638:LEU:HD12	1:B:1638:LEU:C	2.36	0.45
1:A:1240:PRO:HA	1:A:1504:ARG:HH11	1.80	0.45
1:B:1002:LEU:N	1:B:1002:LEU:HD23	2.31	0.45
1:B:1132:TYR:CE1	1:B:1143:ARG:HB2	2.50	0.45
1:B:1165:ASN:ND2	1:B:1165:ASN:H	2.15	0.45
1:B:1513:PHE:O	1:B:1514:PRO:C	2.54	0.45
1:A:1229:TYR:CE1	1:A:1233:ILE:HD13	2.52	0.45
1:B:974:SER:OG	1:B:977:ASN:HB2	2.16	0.45
1:B:1145:ASP:O	1:B:1146:LEU:CB	2.64	0.45
1:B:1221:THR:OG1	1:B:1224:LEU:HD23	2.17	0.45
1:B:1512:THR:HG22	1:B:1516:SER:CB	2.47	0.45
1:A:979:THR:O	1:A:981:ARG:O	2.35	0.45
1:A:1129:LYS:CD	1:A:1201:PRO:HG3	2.45	0.45
1:A:1333:ARG:NH2	1:A:1396:ARG:CD	2.80	0.45
1:A:1508:ILE:CD1	1:A:1508:ILE:N	2.79	0.45
1:A:1513:PHE:CE2	1:A:1514:PRO:HD2	2.51	0.45
1:B:961:GLU:O	1:B:962:GLU:HB2	2.16	0.45
1:B:1218:LEU:C	1:B:1219:GLY:O	2.49	0.45
1:B:1442:ASN:C	1:B:1444:PRO:CD	2.85	0.45
1:B:1606:ARG:HH11	1:B:1606:ARG:CB	2.29	0.45
1:A:1136:GLU:OE1	1:A:1522:HIS:CE1	2.69	0.45
1:B:1333:ARG:NH2	1:B:1396:ARG:CD	2.79	0.45
1:B:1624:HIS:CD2	1:B:1751:PHE:CE2	3.05	0.45
1:A:1157:ASP:HB2	1:A:1425:SER:HB2	1.99	0.45
1:A:1509:THR:O	1:A:1522:HIS:HD2	2.00	0.45
1:A:1513:PHE:CG	1:A:1514:PRO:CD	3.00	0.45
1:B:1443:HIS:O	1:B:1445:PRO:N	2.50	0.45
1:B:1716:ILE:HG22	1:B:1738:ILE:HG12	1.99	0.45
1:A:1542:MET:HE2	1:A:1542:MET:HB3	1.36	0.45
1:A:1807:VAL:O	1:A:1807:VAL:CG2	2.64	0.45
1:B:1672:ASN:HD22	1:B:1673:VAL:N	2.15	0.45
1:A:1045:HIS:CE1	1:A:1051:GLN:HE21	2.35	0.45
1:A:1145:ASP:O	1:A:1146:LEU:CB	2.65	0.45
1:A:1414:PHE:CD1	1:A:1414:PHE:C	2.90	0.45
1:A:1512:THR:HG22	1:A:1516:SER:CB	2.46	0.45
1:A:1788:ILE:HG22	1:A:1846:HIS:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1264:ASP:OD2	1:B:1304:ARG:NH2	2.49	0.45
1:A:1828:ASP:OD1	1:A:1829:PRO:HD2	2.17	0.45
1:B:1118:MET:HB2	1:B:1445:PRO:HG2	1.99	0.45
1:B:1131:LEU:HD13	1:B:1132:TYR:N	2.32	0.44
1:B:1306:LYS:HA	1:B:1310:MET:O	2.18	0.44
1:B:1694:ARG:NH2	1:B:1743:GLU:HB2	2.32	0.44
1:A:1289:PHE:CE1	1:A:1397:GLU:HB3	2.53	0.44
1:B:1601:PHE:O	1:B:1602:VAL:C	2.55	0.44
1:B:1022:LYS:O	1:B:1022:LYS:CG	2.66	0.44
1:B:1040:LEU:HD11	1:B:1042:VAL:CG2	2.47	0.44
1:B:1188:LEU:HD23	1:B:1188:LEU:HA	1.81	0.44
1:B:1751:PHE:HA	1:B:1767:TYR:O	2.16	0.44
1:A:1593:ASP:HB2	1:A:1594:PRO:HD2	1.99	0.44
1:A:1745:THR:O	1:A:1746:ALA:HB2	2.17	0.44
1:B:1355:TRP:N	1:B:1356:PRO:CD	2.80	0.44
1:B:1693:ALA:HB1	1:B:1696:GLU:HB2	2.00	0.44
1:A:998:PHE:CZ	1:A:1112:GLY:HA2	2.52	0.44
1:A:1459:SER:O	1:A:1461:THR:HG22	2.16	0.44
1:B:1090:ASN:HA	1:B:1091:PRO:HA	1.91	0.44
1:A:1026:TYR:O	1:A:1029:ALA:HB3	2.18	0.44
1:A:1355:TRP:HE1	1:A:1421:MET:CE	2.30	0.44
1:A:1022:LYS:O	1:A:1022:LYS:CG	2.65	0.44
1:A:1491:ARG:HG3	1:A:1519:TRP:CE3	2.52	0.44
1:A:1751:PHE:HA	1:A:1767:TYR:O	2.17	0.44
1:B:998:PHE:CZ	1:B:1112:GLY:HA2	2.53	0.44
1:B:1102:GLY:O	1:B:1103:THR:C	2.55	0.44
1:B:1240:PRO:HA	1:B:1504:ARG:HH11	1.81	0.44
1:B:1293:PRO:C	1:B:1295:PHE:H	2.21	0.44
1:B:1452:SER:HB3	1:B:1455:ARG:HG2	1.99	0.44
1:B:1587:ILE:CG2	1:B:1588:GLY:H	2.21	0.44
1:B:1686:TYR:CE2	1:B:1706:HIS:CE1	3.05	0.44
1:A:1803:GLY:HA2	1:A:1832:GLN:CG	2.47	0.44
1:B:962:GLU:CG	1:B:1200:LEU:HD22	2.47	0.44
1:B:1050:LEU:HD12	1:B:1096:ILE:HD13	1.99	0.44
1:B:1353:LYS:HE2	1:B:1377:ARG:O	2.17	0.44
1:B:1565:TYR:O	1:B:1569:VAL:HG23	2.17	0.44
1:A:1169:VAL:HG12	1:A:1171:PRO:HD3	2.00	0.44
1:A:1200:LEU:O	1:A:1202:ALA:N	2.51	0.44
1:A:1319:ALA:HB1	1:A:1380:VAL:HG21	2.00	0.44
1:B:1250:ARG:HG3	1:B:1251:TYR:N	2.30	0.44
1:A:1086:LEU:HD13	1:B:1097:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1355:TRP:HB2	1:A:1356:PRO:HD3	1.99	0.43
1:A:1604:ILE:HG22	1:A:1605:SER:N	2.33	0.43
1:B:1066:VAL:HA	1:B:1067:PRO:HD3	1.84	0.43
1:B:1069:ASN:OD1	1:B:1231:GLU:O	2.35	0.43
1:B:1355:TRP:HE1	1:B:1421:MET:CE	2.31	0.43
1:A:1005:VAL:HG11	1:A:1089:LYS:HA	2.00	0.43
1:A:1798:TYR:HE2	1:A:1839:THR:HG23	1.83	0.43
1:A:1803:GLY:HA2	1:A:1832:GLN:CB	2.48	0.43
1:A:1484:LEU:HD12	1:A:1484:LEU:HA	1.77	0.43
1:B:1272:PRO:O	1:B:1273:TYR:HB3	2.18	0.43
1:B:978:CYS:CB	1:B:985:TRP:HD1	2.32	0.43
1:B:1504:ARG:HH21	1:B:1760:THR:HG23	1.84	0.43
1:B:1725:ASN:OD1	1:B:1727:HIS:HB3	2.19	0.43
1:A:978:CYS:CB	1:A:985:TRP:HD1	2.30	0.43
1:A:1252:GLY:CA	1:A:1587:ILE:HD12	2.48	0.43
1:A:1517:GLY:CA	1:A:1549:ILE:HG12	2.40	0.43
1:A:1681:ARG:HD3	1:A:1741:ASP:CA	2.40	0.43
1:B:1050:LEU:HA	1:B:1050:LEU:HD23	1.70	0.43
1:B:1097:ARG:HG3	1:B:1102:GLY:O	2.18	0.43
1:B:1200:LEU:O	1:B:1202:ALA:N	2.52	0.43
1:B:1217:PHE:HB3	1:B:1228:GLN:HE21	1.84	0.43
1:B:1329:PRO:CB	1:B:1333:ARG:HD2	2.49	0.43
1:B:1508:ILE:N	1:B:1508:ILE:HD12	2.33	0.43
1:B:1650:ILE:CD1	1:B:1653:GLN:HE21	2.31	0.43
1:A:1355:TRP:N	1:A:1356:PRO:CD	2.81	0.43
1:B:1288:ASP:HB3	1:B:1289:PHE:CD2	2.54	0.43
1:A:1293:PRO:C	1:A:1295:PHE:H	2.20	0.43
1:B:1061:ARG:NH1	1:B:1061:ARG:HG2	2.33	0.43
1:B:1289:PHE:CE1	1:B:1397:GLU:HB3	2.52	0.43
1:B:1346:ASP:O	1:B:1347:GLY:O	2.37	0.43
1:B:1384:ASP:C	1:B:1384:ASP:OD1	2.56	0.43
1:B:1500:VAL:HG12	1:B:1501:THR:HG23	2.00	0.43
1:B:1686:TYR:CD2	1:B:1706:HIS:HE1	2.36	0.43
1:A:1131:LEU:HD13	1:A:1132:TYR:N	2.34	0.43
1:B:1414:PHE:CD1	1:B:1414:PHE:C	2.92	0.43
1:B:1575:GLY:C	1:B:1577:PHE:H	2.21	0.43
1:B:1592:GLN:HE21	1:B:1592:GLN:HB3	1.68	0.43
1:A:1069:ASN:OD1	1:A:1231:GLU:O	2.36	0.43
1:A:1693:ALA:HB1	1:A:1696:GLU:HB2	2.01	0.43
1:B:1234:GLY:HA3	1:B:1518:ARG:HD3	2.00	0.43
1:B:1503:GLN:C	1:B:1758:ILE:HD11	2.40	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1757:SER:HB2	1:B:1760:THR:HG22	1.99	0.43
1:A:1730:ARG:HE	1:A:1752:TRP:HZ3	1.67	0.43
1:A:1838:VAL:C	1:A:1840:ASP:H	2.23	0.43
1:B:1240:PRO:HG2	1:B:1243:SER:HB3	2.01	0.43
1:A:1251:TYR:CE1	1:A:1587:ILE:HB	2.53	0.42
1:A:1311:ARG:NH2	1:A:1756:GLN:OE1	2.52	0.42
1:A:1836:ILE:HG22	1:A:1836:ILE:O	2.18	0.42
1:B:1196:THR:OG1	1:B:1206:ARG:NH2	2.52	0.42
1:B:1407:ASN:HB3	1:B:1409:GLU:OE2	2.19	0.42
1:B:1442:ASN:C	1:B:1444:PRO:HD3	2.39	0.42
1:B:1679:ARG:HD3	1:B:1695:GLY:HA3	2.01	0.42
1:B:1838:VAL:C	1:B:1840:ASP:H	2.21	0.42
1:A:974:SER:OG	1:A:977:ASN:HB2	2.19	0.42
1:A:981:ARG:HG2	1:A:982:GLY:N	2.33	0.42
1:A:1218:LEU:C	1:A:1219:GLY:O	2.53	0.42
1:A:1304:ARG:O	1:A:1307:ALA:HB3	2.18	0.42
1:A:1650:ILE:CD1	1:A:1653:GLN:HE21	2.32	0.42
1:A:1791:THR:O	1:A:1793:PRO:HD3	2.19	0.42
1:B:1045:HIS:CE1	1:B:1051:GLN:HE21	2.36	0.42
1:A:1125:ARG:HA	1:A:1202:ALA:HB2	2.01	0.42
1:A:1329:PRO:CB	1:A:1333:ARG:HD2	2.49	0.42
1:A:1478:HIS:HE1	1:A:1482:HIS:ND1	2.15	0.42
1:A:1573:GLN:HA	1:A:1608:VAL:HG21	2.00	0.42
1:A:1006:SER:OG	1:A:1007:ASP:N	2.52	0.42
1:A:1196:THR:OG1	1:A:1206:ARG:NH2	2.53	0.42
1:A:1221:THR:OG1	1:A:1224:LEU:HB2	2.20	0.42
1:B:1083:TYR:HA	1:B:1097:ARG:O	2.19	0.42
1:B:1304:ARG:O	1:B:1307:ALA:HB3	2.20	0.42
1:A:1404:ASN:OD1	1:A:1405:PRO:HD2	2.19	0.42
1:A:1490:THR:HG22	1:A:1519:TRP:HB2	2.02	0.42
1:A:1775:GLN:O	1:A:1777:THR:HG23	2.19	0.42
1:B:1531:TRP:CZ2	1:B:1567:MET:HA	2.54	0.42
1:A:1102:GLY:O	1:A:1103:THR:C	2.58	0.42
1:A:1272:PRO:O	1:A:1273:TYR:HB3	2.20	0.42
1:A:1443:HIS:O	1:A:1445:PRO:N	2.52	0.42
1:B:981:ARG:O	1:B:983:CYS:N	2.51	0.42
1:B:1036:ASN:HA	1:B:1037:PRO:HA	1.58	0.42
1:B:1803:GLY:HA2	1:B:1832:GLN:CG	2.49	0.42
1:A:1234:GLY:HA3	1:A:1518:ARG:HD3	2.01	0.42
1:B:1050:LEU:HD21	1:B:1083:TYR:CZ	2.54	0.42
1:B:1064:VAL:CG1	1:B:1066:VAL:HG13	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1604:ILE:HG22	1:B:1605:SER:N	2.34	0.42
1:A:1409:GLU:H	1:A:1409:GLU:HG3	1.48	0.42
1:A:1672:ASN:HD22	1:A:1673:VAL:N	2.18	0.42
1:A:1730:ARG:HH21	1:A:1752:TRP:HZ3	1.67	0.42
1:B:1019:ILE:HB	1:B:1038:LEU:HB2	2.01	0.42
1:B:1436:CYS:O	1:B:1437:ARG:CD	2.67	0.42
1:B:1694:ARG:HH22	1:B:1743:GLU:HB2	1.83	0.42
1:B:1809:VAL:O	1:B:1809:VAL:HG13	2.20	0.42
1:B:1836:ILE:O	1:B:1836:ILE:HG22	2.20	0.42
1:A:1097:ARG:HG3	1:A:1102:GLY:O	2.19	0.42
1:A:1224:LEU:HD13	1:A:1224:LEU:HA	1.87	0.42
1:B:981:ARG:HG2	1:B:982:GLY:N	2.35	0.42
1:B:1459:SER:O	1:B:1461:THR:HG22	2.20	0.42
1:A:1188:LEU:HD23	1:A:1188:LEU:HA	1.88	0.42
1:A:1421:MET:HE3	2:C:3:AC1:HC7	2.01	0.42
1:A:1730:ARG:NE	1:A:1752:TRP:CZ3	2.87	0.42
1:B:1139:HIS:HD2	1:B:1151:TRP:CH2	2.38	0.42
1:B:1513:PHE:CG	1:B:1514:PRO:CD	3.03	0.42
1:B:1542:MET:HB3	1:B:1542:MET:HE2	1.43	0.42
1:A:981:ARG:HB2	1:A:1030:PHE:HE1	1.84	0.41
1:A:1298:PHE:HB3	1:A:1299:PRO:HD3	2.01	0.41
1:A:1513:PHE:O	1:A:1514:PRO:C	2.54	0.41
1:A:1679:ARG:HD3	1:A:1695:GLY:HA3	2.01	0.41
1:A:1686:TYR:CE2	1:A:1706:HIS:CE1	3.07	0.41
1:A:1244:LEU:HA	1:A:1244:LEU:HD23	1.79	0.41
1:B:1251:TYR:CE1	1:B:1587:ILE:HB	2.54	0.41
1:B:1593:ASP:HB2	1:B:1594:PRO:HD2	2.02	0.41
1:B:1730:ARG:HH21	1:B:1752:TRP:HZ3	1.68	0.41
1:B:1750:LEU:HD21	1:B:1752:TRP:CD1	2.53	0.41
1:A:1030:PHE:CD2	1:A:1031:PRO:CD	2.84	0.41
1:A:1438:ASP:OD1	1:A:1439:ALA:N	2.52	0.41
1:A:1508:ILE:N	1:A:1508:ILE:HD12	2.34	0.41
1:B:1355:TRP:HB2	1:B:1356:PRO:HD3	2.01	0.41
1:A:1355:TRP:N	1:A:1356:PRO:HD2	2.36	0.41
1:A:1452:SER:HB3	1:A:1455:ARG:HG2	2.02	0.41
1:A:1825:PHE:C	1:A:1825:PHE:CD1	2.94	0.41
1:B:1061:ARG:HD3	1:B:1211:VAL:HG12	2.02	0.41
1:B:1298:PHE:HB3	1:B:1299:PRO:HD3	2.02	0.41
1:B:1355:TRP:N	1:B:1356:PRO:HD2	2.35	0.41
1:A:1088:LYS:HD3	1:A:1095:GLU:OE1	2.21	0.41
1:A:1128:SER:O	1:A:1201:PRO:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1498:GLN:OE1	1:A:1504:ARG:HA	2.20	0.41
1:A:1504:ARG:HH21	1:A:1760:THR:HG23	1.86	0.41
1:B:1008:VAL:HG12	1:B:1010:TYR:CE1	2.55	0.41
1:B:1372:GLN:HE22	1:B:1377:ARG:HH22	1.68	0.41
1:B:1730:ARG:NE	1:B:1752:TRP:CZ3	2.88	0.41
1:A:1062:TYR:CE2	1:A:1480:ASN:HB3	2.55	0.41
1:A:1131:LEU:CD2	1:A:1173:TYR:CD1	3.03	0.41
1:A:1239:VAL:HB	1:A:1240:PRO:HD2	2.02	0.41
1:A:1288:ASP:O	1:A:1289:PHE:HB2	2.20	0.41
1:A:1288:ASP:HB3	1:A:1289:PHE:CD2	2.56	0.41
1:A:1385:PHE:HB2	1:A:1488:SER:OG	2.20	0.41
1:A:1421:MET:HE2	1:A:1421:MET:HB2	1.93	0.41
1:A:1682:TRP:HB2	1:A:1691:ILE:HG22	2.03	0.41
1:B:979:THR:O	1:B:981:ARG:O	2.38	0.41
1:B:981:ARG:HB2	1:B:1030:PHE:HE1	1.84	0.41
1:B:1447:MET:O	1:B:1453:ARG:NH1	2.43	0.41
1:B:1736:PHE:CZ	1:B:1771:PHE:CE1	3.09	0.41
1:A:1468:GLN:NE2	1:A:1478:HIS:CD2	2.71	0.41
1:A:1614:THR:HG23	1:A:1719:TRP:HB2	2.03	0.41
1:A:1644:ASP:OD2	1:A:1676:TYR:OH	2.36	0.41
1:A:1660:PHE:HZ	1:A:1709:LEU:HD13	1.85	0.41
1:B:1140:ARG:HG3	1:B:1144:ARG:NH2	2.35	0.41
1:A:962:GLU:CG	1:A:1200:LEU:HD22	2.44	0.41
1:A:1153:MET:HE1	1:A:1195:VAL:HG13	2.03	0.41
1:A:1736:PHE:HD2	1:A:1736:PHE:HA	1.80	0.41
1:B:1513:PHE:CE2	1:B:1514:PRO:HD2	2.55	0.41
1:A:1187:LEU:HG	1:A:1214:PHE:CZ	2.56	0.41
1:A:1436:CYS:O	1:A:1437:ARG:CD	2.69	0.41
1:A:1470:LEU:HB3	1:A:1471:PRO:HD2	2.03	0.41
1:A:1575:GLY:C	1:A:1577:PHE:N	2.74	0.41
1:A:1726:THR:HA	1:A:1729:SER:HB3	2.03	0.41
1:B:1006:SER:OG	1:B:1007:ASP:N	2.53	0.41
1:B:1098:ARG:HH12	1:B:1181:SER:HB3	1.79	0.41
1:B:1447:MET:O	1:B:1453:ARG:HD3	2.21	0.41
1:B:1491:ARG:O	1:B:1494:TYR:HB3	2.21	0.41
1:B:1552:THR:O	1:B:1579:PRO:HD2	2.21	0.41
1:B:1150:THR:OG1	1:B:1196:THR:HG23	2.21	0.41
1:B:1726:THR:HA	1:B:1729:SER:HB3	2.03	0.41
1:B:1803:GLY:HA2	1:B:1832:GLN:CB	2.51	0.41
1:A:1050:LEU:CD2	1:A:1083:TYR:CZ	3.05	0.40
1:A:1140:ARG:H	1:A:1140:ARG:HG3	1.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:ASN:OD1	1:A:1727:HIS:HB3	2.21	0.40
1:B:1655:LEU:HD23	1:B:1661:LEU:HA	2.03	0.40
1:B:1813:SER:OG	1:B:1825:PHE:HE2	2.04	0.40
1:A:998:PHE:CE1	1:A:1112:GLY:HA2	2.55	0.40
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.86	0.40
1:A:981:ARG:HB2	1:A:1030:PHE:CD1	2.57	0.40
1:A:1040:LEU:HD12	1:A:1040:LEU:C	2.42	0.40
1:A:1073:MET:HB3	1:A:1074:PRO:HD2	2.03	0.40
1:A:1441:LEU:CD1	1:A:1464:MET:HB2	2.33	0.40
1:A:1538:ILE:HG23	1:A:1654:PHE:CD2	2.55	0.40
1:B:994:PRO:HB2	1:B:996:CYS:O	2.22	0.40
1:B:1239:VAL:HB	1:B:1240:PRO:HD2	2.03	0.40
1:B:1443:HIS:N	1:B:1444:PRO:CD	2.85	0.40
1:A:1008:VAL:HG12	1:A:1010:TYR:CE1	2.57	0.40
1:A:1050:LEU:HD12	1:A:1096:ILE:HD13	2.03	0.40
1:A:1363:VAL:HG23	1:A:1376:TYR:CE1	2.56	0.40
1:B:1329:PRO:O	1:B:1330:ALA:C	2.60	0.40
1:B:1432:VAL:CG1	1:B:1433:SER:N	2.83	0.40
1:B:1625:LYS:O	1:B:1629:GLU:HB2	2.22	0.40
1:A:1139:HIS:HD2	1:A:1151:TRP:CH2	2.40	0.40
1:A:1194:ASP:OD1	1:A:1206:ARG:HB2	2.21	0.40
1:A:1228:GLN:HE21	1:A:1228:GLN:HB2	1.61	0.40
1:A:1271:ILE:HA	1:A:1272:PRO:HD3	1.92	0.40
1:A:1809:VAL:HG13	1:A:1809:VAL:O	2.22	0.40
1:A:1844:SER:OG	1:A:1846:HIS:HD2	2.05	0.40
1:B:1844:SER:OG	1:B:1846:HIS:HD2	2.04	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	888/908 (98%)	750 (84%)	109 (12%)	29 (3%)	4 14
1	B	888/908 (98%)	745 (84%)	111 (12%)	32 (4%)	3 12
All	All	1776/1816 (98%)	1495 (84%)	220 (12%)	61 (3%)	3 13

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	PRO
1	A	1136	GLU
1	A	1347	GLY
1	A	1443	HIS
1	A	1445	PRO
1	A	1631	VAL
1	A	1668	ARG
1	B	1031	PRO
1	B	1136	GLU
1	B	1347	GLY
1	B	1443	HIS
1	B	1445	PRO
1	B	1631	VAL
1	A	1102	GLY
1	A	1559	PHE
1	A	1832	GLN
1	B	1102	GLY
1	B	1188	LEU
1	B	1559	PHE
1	B	1668	ARG
1	B	1832	GLN
1	A	1188	LEU
1	A	1354	VAL
1	B	1338	ASP
1	B	1354	VAL
1	B	1587	ILE
1	B	1732	LYS
1	A	1338	ASP
1	A	1587	ILE
1	A	1745	THR
1	A	1756	GLN
1	B	1515	SER
1	B	1745	THR
1	A	1515	SER
1	A	1678	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	961	GLU
1	B	1209	GLY
1	B	1294	LYS
1	B	1678	PRO
1	B	1786	ASN
1	B	1797	GLY
1	A	961	GLU
1	A	1160	PRO
1	A	1209	GLY
1	A	1797	GLY
1	B	1160	PRO
1	B	1756	GLN
1	A	1448	PRO
1	A	1602	VAL
1	B	1201	PRO
1	A	1201	PRO
1	B	1133	GLY
1	B	1448	PRO
1	A	1433	SER
1	A	1836	ILE
1	A	1133	GLY
1	A	1812	VAL
1	B	1812	VAL
1	B	1836	ILE
1	B	1595	VAL
1	B	1602	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	773/800 (97%)	696 (90%)	77 (10%)	7 21
1	B	773/800 (97%)	690 (89%)	83 (11%)	6 18
All	All	1546/1600 (97%)	1386 (90%)	160 (10%)	7 20

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	967	TYR
1	A	969	ASP
1	A	985	TRP
1	A	990	SER
1	A	993	VAL
1	A	1002	LEU
1	A	1016	THR
1	A	1019	ILE
1	A	1022	LYS
1	A	1040	LEU
1	A	1066	VAL
1	A	1072	SER
1	A	1073	MET
1	A	1103	THR
1	A	1106	TRP
1	A	1121	ARG
1	A	1124	THR
1	A	1126	LEU
1	A	1131	LEU
1	A	1140	ARG
1	A	1141	SER
1	A	1156	ARG
1	A	1165	ASN
1	A	1166	SER
1	A	1187	LEU
1	A	1188	LEU
1	A	1189	ASN
1	A	1198	GLN
1	A	1200	LEU
1	A	1207	THR
1	A	1218	LEU
1	A	1224	LEU
1	A	1250	ARG
1	A	1274	ASP
1	A	1294	LYS
1	A	1301	LEU
1	A	1323	ASN
1	A	1349	ILE
1	A	1363	VAL
1	A	1372	GLN
1	A	1397	GLU
1	A	1406	GLN
1	A	1409	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1420	ASP
1	A	1423	GLU
1	A	1437	ARG
1	A	1453	ARG
1	A	1464	MET
1	A	1484	LEU
1	A	1504	ARG
1	A	1508	ILE
1	A	1512	THR
1	A	1545	SER
1	A	1564	GLU
1	A	1590	ARG
1	A	1609	LEU
1	A	1631	VAL
1	A	1638	LEU
1	A	1642	VAL
1	A	1672	ASN
1	A	1707	ILE
1	A	1716	ILE
1	A	1730	ARG
1	A	1743	GLU
1	A	1745	THR
1	A	1763	LYS
1	A	1765	LEU
1	A	1775	GLN
1	A	1784	PHE
1	A	1792	ASN
1	A	1796	LEU
1	A	1798	TYR
1	A	1810	THR
1	A	1817	SER
1	A	1825	PHE
1	A	1841	ARG
1	A	1842	ASN
1	B	967	TYR
1	B	969	ASP
1	B	985	TRP
1	B	990	SER
1	B	993	VAL
1	B	999	VAL
1	B	1002	LEU
1	B	1016	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1019	ILE
1	B	1022	LYS
1	B	1040	LEU
1	B	1066	VAL
1	B	1068	LEU
1	B	1072	SER
1	B	1073	MET
1	B	1082	LEU
1	B	1100	SER
1	B	1103	THR
1	B	1106	TRP
1	B	1121	ARG
1	B	1124	THR
1	B	1126	LEU
1	B	1131	LEU
1	B	1140	ARG
1	B	1141	SER
1	B	1156	ARG
1	B	1165	ASN
1	B	1166	SER
1	B	1187	LEU
1	B	1188	LEU
1	B	1189	ASN
1	B	1198	GLN
1	B	1200	LEU
1	B	1207	THR
1	B	1218	LEU
1	B	1224	LEU
1	B	1250	ARG
1	B	1274	ASP
1	B	1294	LYS
1	B	1301	LEU
1	B	1323	ASN
1	B	1349	ILE
1	B	1363	VAL
1	B	1372	GLN
1	B	1397	GLU
1	B	1406	GLN
1	B	1409	GLU
1	B	1420	ASP
1	B	1423	GLU
1	B	1437	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1453	ARG
1	B	1464	MET
1	B	1484	LEU
1	B	1498	GLN
1	B	1500	VAL
1	B	1504	ARG
1	B	1508	ILE
1	B	1512	THR
1	B	1564	GLU
1	B	1590	ARG
1	B	1609	LEU
1	B	1631	VAL
1	B	1638	LEU
1	B	1642	VAL
1	B	1672	ASN
1	B	1691	ILE
1	B	1707	ILE
1	B	1716	ILE
1	B	1730	ARG
1	B	1743	GLU
1	B	1745	THR
1	B	1763	LYS
1	B	1765	LEU
1	B	1775	GLN
1	B	1784	PHE
1	B	1792	ASN
1	B	1796	LEU
1	B	1798	TYR
1	B	1810	THR
1	B	1817	SER
1	B	1825	PHE
1	B	1841	ARG
1	B	1842	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1045	HIS
1	A	1047	ASN
1	A	1058	ASN
1	A	1165	ASN
1	A	1183	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1198	GLN
1	A	1228	GLN
1	A	1372	GLN
1	A	1406	GLN
1	A	1467	GLN
1	A	1468	GLN
1	A	1478	HIS
1	A	1503	GLN
1	A	1522	HIS
1	A	1592	GLN
1	A	1610	GLN
1	A	1653	GLN
1	A	1672	ASN
1	A	1706	HIS
1	A	1792	ASN
1	A	1846	HIS
1	B	1045	HIS
1	B	1047	ASN
1	B	1058	ASN
1	B	1165	ASN
1	B	1183	HIS
1	B	1198	GLN
1	B	1228	GLN
1	B	1372	GLN
1	B	1406	GLN
1	B	1467	GLN
1	B	1468	GLN
1	B	1478	HIS
1	B	1503	GLN
1	B	1522	HIS
1	B	1592	GLN
1	B	1610	GLN
1	B	1653	GLN
1	B	1672	ASN
1	B	1706	HIS
1	B	1792	ASN
1	B	1846	HIS

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)

6 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	C	1	2	12,12,12	1.59	3 (25%)	17,17,17	2.72	4 (23%)
2	GLC	C	2	2	11,11,12	1.82	5 (45%)	15,15,17	2.71	5 (33%)
2	AC1	C	3	2	21,22,23	1.96	8 (38%)	22,32,34	1.19	3 (13%)
2	GLC	D	1	2	12,12,12	1.63	2 (16%)	17,17,17	2.41	3 (17%)
2	GLC	D	2	2	11,11,12	1.94	5 (45%)	15,15,17	0.92	1 (6%)
2	AC1	D	3	2	21,22,23	1.87	8 (38%)	22,32,34	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	AC1	C	3	2	-	3/6/43/46	0/2/2/2
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	AC1	D	3	2	-	4/6/43/46	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	O5-C1	-4.19	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C7B-C5B	4.09	1.38	1.32
2	C	3	AC1	C3B-C4A	-3.58	1.47	1.53
2	D	3	AC1	C4A-C5B	-3.57	1.48	1.51
2	D	1	GLC	O2-C2	3.53	1.51	1.43
2	C	3	AC1	C7B-C5B	3.43	1.37	1.32
2	C	3	AC1	C4A-C5B	-3.18	1.48	1.51
2	C	2	GLC	O5-C1	-3.09	1.38	1.43
2	C	3	AC1	O2-C2	-3.06	1.36	1.43
2	C	1	GLC	O2-C2	2.98	1.50	1.43
2	C	2	GLC	O5-C5	-2.81	1.37	1.43
2	C	3	AC1	C3-C4	-2.68	1.48	1.53
2	D	3	AC1	C3-C4	-2.46	1.48	1.53
2	D	3	AC1	O2-C2	-2.43	1.38	1.43
2	C	2	GLC	O3-C3	-2.43	1.37	1.43
2	D	2	GLC	O5-C5	-2.38	1.38	1.43
2	D	2	GLC	O3-C3	-2.35	1.37	1.43
2	C	1	GLC	C6-C5	2.35	1.59	1.51
2	C	1	GLC	C4-C3	-2.29	1.46	1.52
2	D	3	AC1	O2B-C2B	-2.28	1.37	1.43
2	C	2	GLC	O2-C2	-2.28	1.38	1.43
2	C	3	AC1	O4-C4A	-2.27	1.37	1.42
2	D	1	GLC	C6-C5	2.24	1.59	1.51
2	C	3	AC1	O3B-C3B	-2.18	1.37	1.43
2	D	2	GLC	O2-C2	-2.16	1.38	1.43
2	C	3	AC1	O3-C3	2.12	1.48	1.43
2	D	3	AC1	O5-C1	-2.08	1.40	1.43
2	D	3	AC1	O3-C3	2.07	1.47	1.43
2	C	2	GLC	C4-C5	-2.06	1.48	1.53
2	D	3	AC1	O3B-C3B	-2.03	1.38	1.43
2	D	2	GLC	C4-C5	-2.03	1.48	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GLC	O5-C5-C4	7.67	123.62	109.69
2	D	1	GLC	O5-C5-C4	7.15	122.68	109.69
2	C	2	GLC	C1-C2-C3	6.53	117.69	109.67
2	C	1	GLC	C1-C2-C3	6.51	123.83	110.31
2	D	1	GLC	C1-C2-C3	5.56	121.85	110.31
2	C	2	GLC	O5-C1-C2	5.23	118.84	110.77
2	C	2	GLC	C1-O5-C5	3.97	117.57	112.19
2	C	3	AC1	C2-C3-C4	-2.98	108.00	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C2-C3-C4	2.57	115.34	110.89
2	C	1	GLC	C3-C4-C5	-2.46	105.85	110.24
2	C	3	AC1	O3-C3-C4	2.40	114.51	109.66
2	D	1	GLC	C6-C5-C4	-2.36	107.47	113.00
2	C	1	GLC	O5-C1-C2	2.31	114.41	110.28
2	C	3	AC1	O4-C4A-C3B	-2.29	105.81	110.53
2	C	2	GLC	O3-C3-C2	-2.08	106.01	109.99
2	D	2	GLC	O6-C6-C5	-2.03	104.34	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

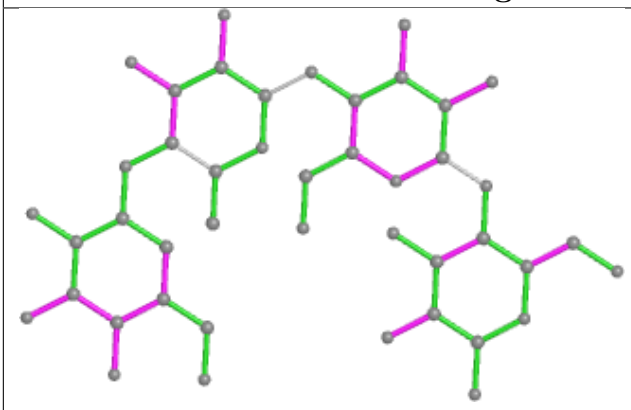
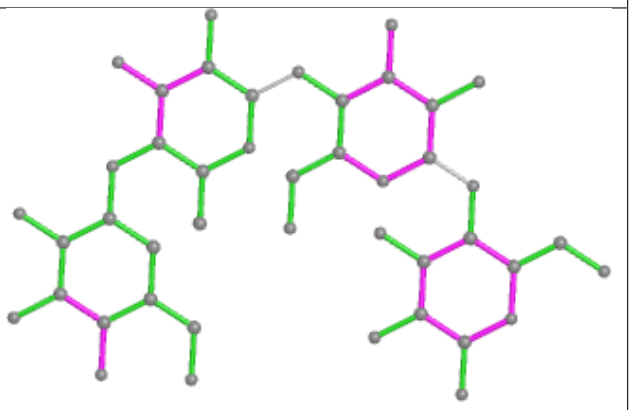
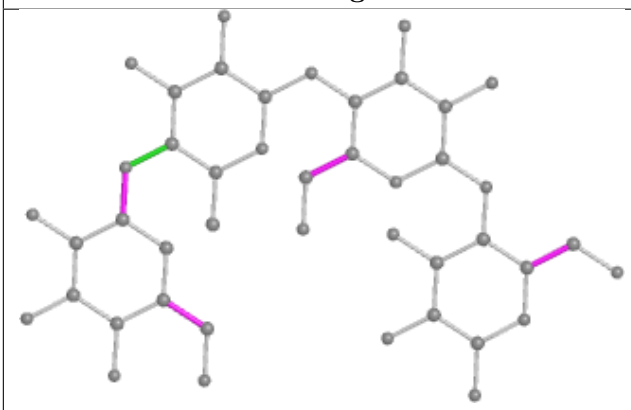
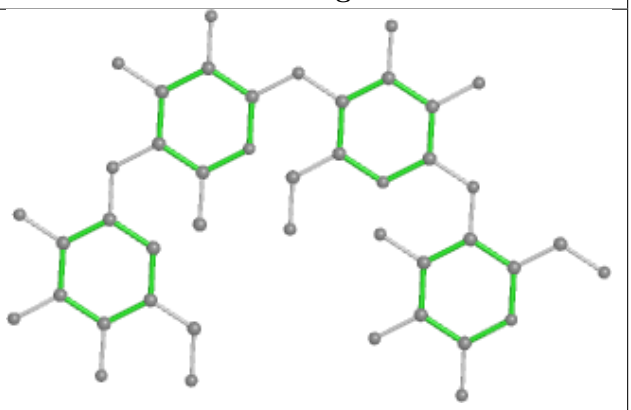
Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C7B-C1B-N4A-C4
2	C	3	AC1	C7B-C5B-C6B-O6B
2	D	3	AC1	C7B-C1B-N4A-C4
2	D	3	AC1	C4A-C5B-C6B-O6B
2	D	2	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	3	AC1	C3-C4-N4A-C1B
2	C	3	AC1	C4A-C5B-C6B-O6B
2	D	3	AC1	C7B-C5B-C6B-O6B

There are no ring outliers.

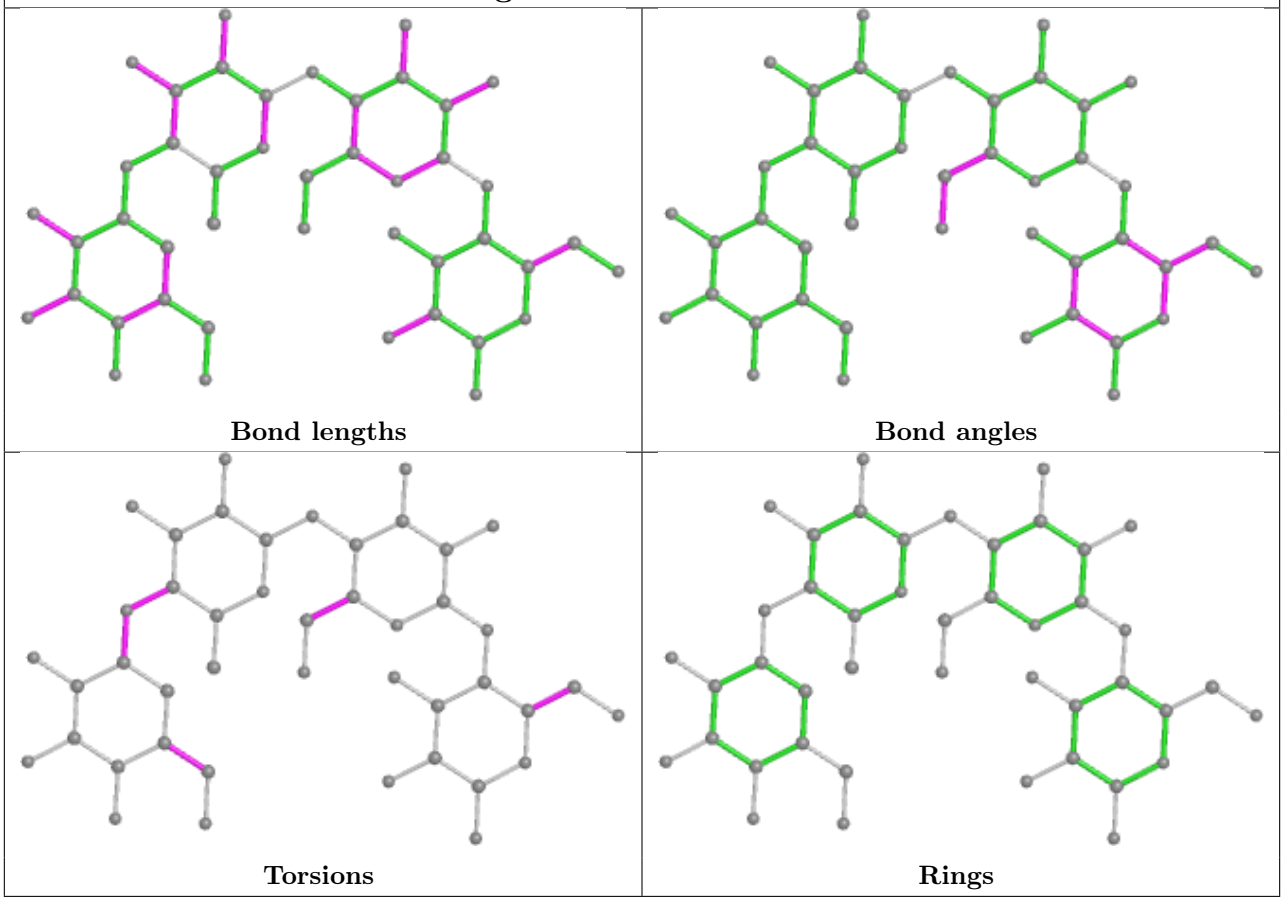
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	AC1	2	0
2	C	2	GLC	5	0
2	C	1	GLC	5	0

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

Oligosaccharide Chain C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain D



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	890/908 (98%)	0.19	31 (3%)	44	39	45, 81, 135, 207	0
1	B	890/908 (98%)	0.30	64 (7%)	15	11	50, 85, 141, 211	0
All	All	1780/1816 (98%)	0.25	95 (5%)	26	22	45, 83, 137, 211	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1443	HIS	7.3
1	B	1733	PHE	5.8
1	B	991	SER	5.7
1	B	1821	ILE	5.7
1	B	1815	SER	5.2
1	B	1823	PRO	5.1
1	B	1819	MET	4.9
1	B	1843	ILE	4.7
1	B	1764	GLY	4.6
1	B	1806	SER	4.5
1	B	1840	ASP	4.5
1	B	1820	VAL	4.4
1	B	1836	ILE	4.4
1	B	1825	PHE	4.3
1	A	989	ASN	4.0
1	B	1839	THR	4.0
1	B	1829	PRO	3.9
1	B	1765	LEU	3.8
1	B	1807	VAL	3.7
1	A	1812	VAL	3.7
1	A	1809	VAL	3.6
1	B	1434	PRO	3.6
1	A	1345	ASN	3.4
1	A	1645	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1512	THR	3.2
1	B	1668	ARG	3.1
1	A	1437	ARG	3.1
1	B	1824	SER	3.0
1	A	1511	SER	2.9
1	A	1367	LEU	2.9
1	A	1009	GLN	2.9
1	A	1565	TYR	2.8
1	B	1796	LEU	2.8
1	B	1841	ARG	2.8
1	A	1512	THR	2.8
1	B	1814	ILE	2.8
1	B	1697	TRP	2.8
1	B	1822	THR	2.8
1	B	1845	LEU	2.8
1	B	1826	ASN	2.7
1	A	1509	THR	2.7
1	B	1795	LYS	2.6
1	A	1550	SER	2.6
1	B	1406	GLN	2.6
1	A	1486	GLY	2.6
1	A	1545	SER	2.6
1	A	1364	ASN	2.6
1	A	1815	SER	2.5
1	B	1834	LEU	2.5
1	B	1606	ARG	2.5
1	A	988	SER	2.5
1	A	1774	SER	2.5
1	B	1695	GLY	2.5
1	B	1740	LEU	2.5
1	B	1168	GLY	2.5
1	B	1024	SER	2.5
1	B	1178	GLU	2.5
1	A	1840	ASP	2.4
1	B	989	ASN	2.4
1	B	1761	TYR	2.4
1	A	1168	GLY	2.4
1	A	1189	ASN	2.4
1	B	1704	LEU	2.4
1	B	1812	VAL	2.3
1	B	1791	THR	2.3
1	B	1023	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	971	ASN	2.3
1	A	973	ALA	2.3
1	B	1245	GLY	2.3
1	B	1565	TYR	2.3
1	B	1762	GLY	2.3
1	B	1511	SER	2.3
1	B	1827	ASN	2.3
1	B	995	PHE	2.2
1	B	1189	ASN	2.2
1	B	1022	LYS	2.2
1	A	1524	LEU	2.2
1	B	1550	SER	2.2
1	A	1361	VAL	2.2
1	B	1581	SER	2.2
1	B	1835	SER	2.2
1	B	1782	ILE	2.2
1	B	1846	HIS	2.2
1	B	1597	TRP	2.2
1	A	1581	SER	2.2
1	B	990	SER	2.1
1	B	1785	ASN	2.1
1	A	1742	ASP	2.1
1	A	1348	ASP	2.1
1	B	1646	VAL	2.1
1	A	1443	HIS	2.0
1	B	1705	ASP	2.0
1	A	1540	GLY	2.0
1	B	1731	GLN	2.0
1	B	1818	GLY	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)

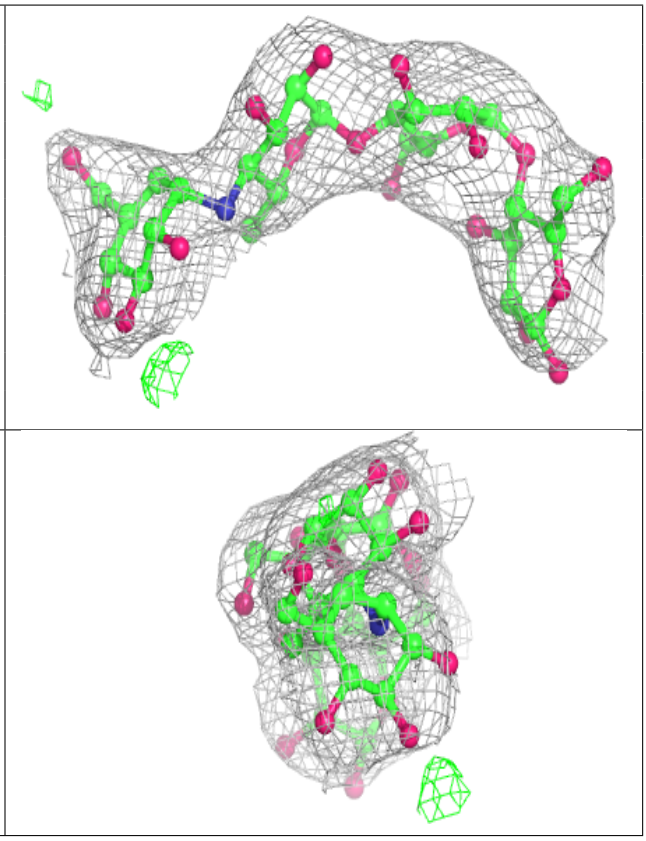
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1	12/12	0.93	0.18	85,104,117,124	0
2	AC1	C	3	21/22	0.94	0.21	53,73,89,115	0
2	GLC	D	1	12/12	0.95	0.18	78,88,120,121	0
2	AC1	D	3	21/22	0.96	0.18	56,81,104,109	0
2	GLC	D	2	11/12	0.97	0.13	54,84,95,102	0
2	GLC	C	2	11/12	0.98	0.11	77,83,115,123	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.

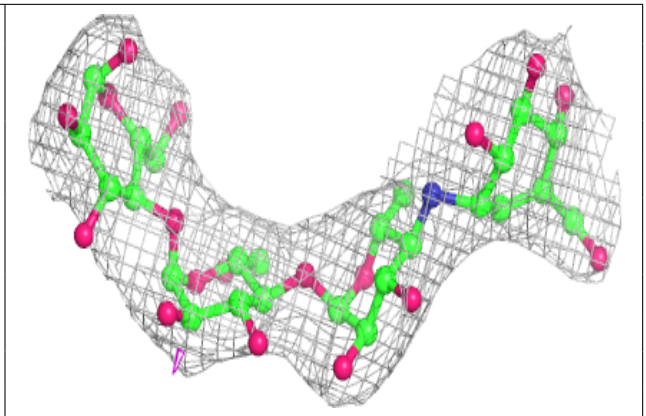
Electron density around Chain C:

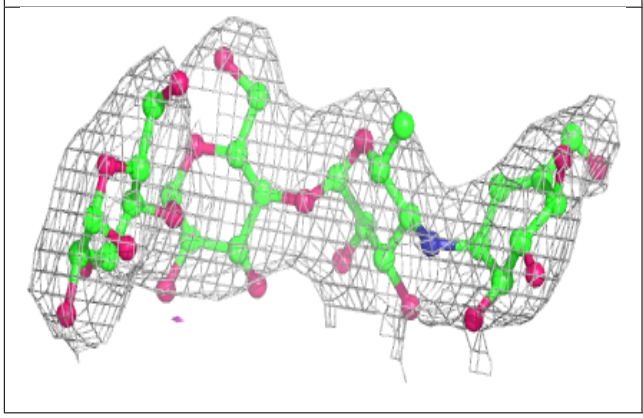
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

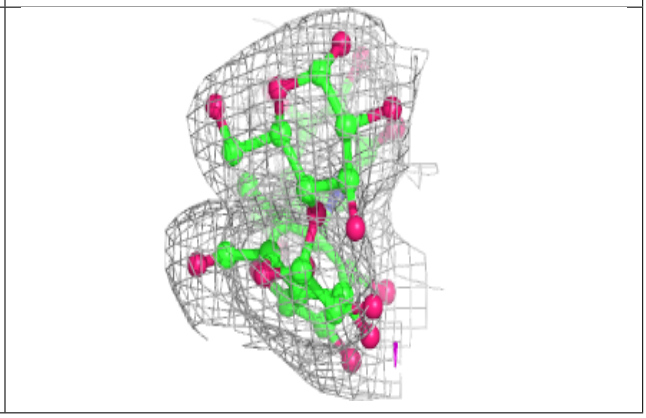


Electron density around Chain D:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.