



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:56 PM EDT

PDB ID : 5C97 / pdb_00005c97
Title : Insulin regulated aminopeptidase
Authors : Mpakali, A.; Saridakis, E.; Harlos, K.; Zhao, Y.; Stratikos, E.
Deposited on : 2015-06-26
Resolution : 3.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

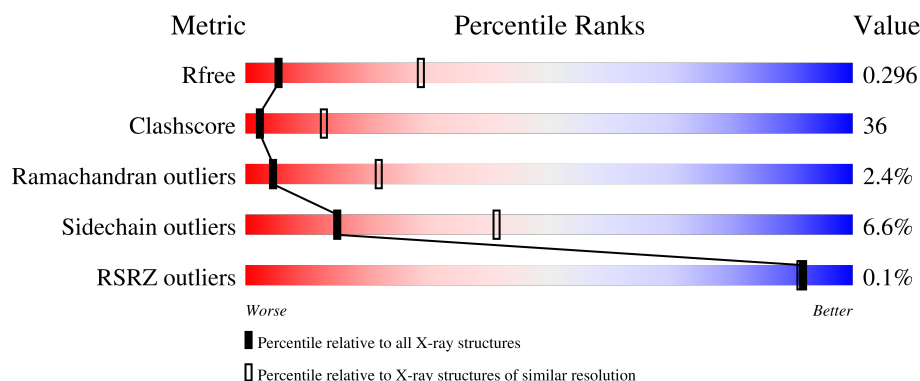
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	912	
1	B	912	
2	C	2	
2	D	2	
2	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 50%50%

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
4	NAG	A	1113	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14098 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 Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	2	0
			6937	4487	1125	1298	27			
1	B	851	Total	C	N	O	S	0	1	0
			6808	4410	1097	1276	25			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	ASN	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	ASN	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

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

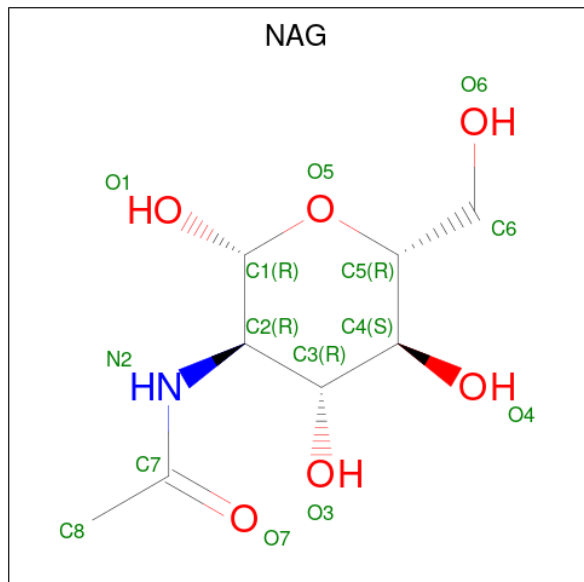


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

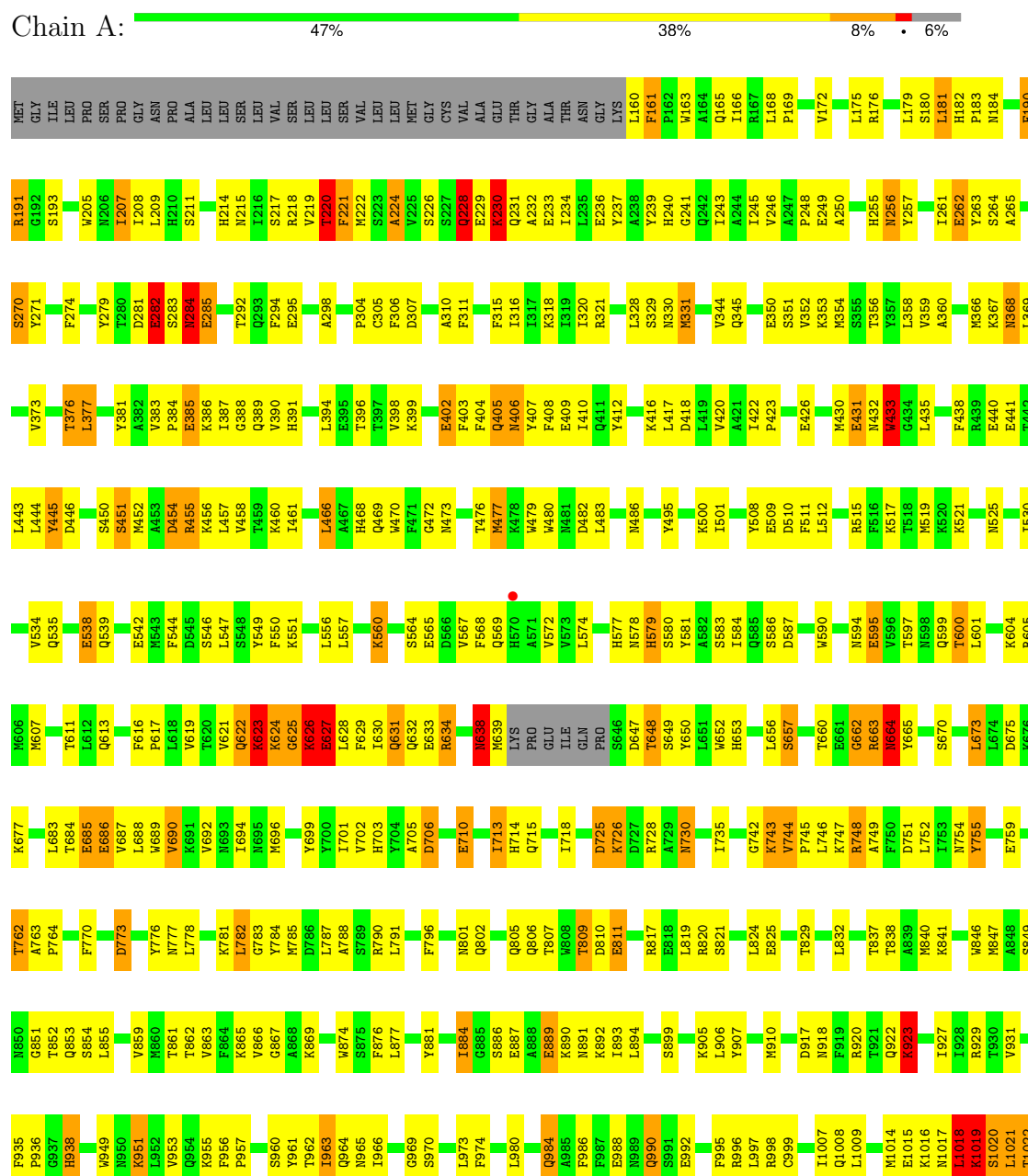
- Molecule 5 is water.

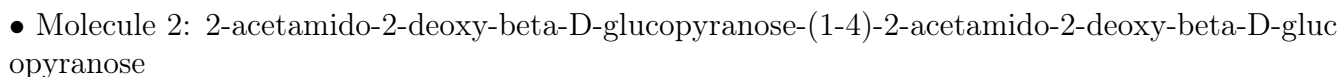
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

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

- Molecule 1: Leucyl-cystinyl aminopeptidase





Chain C:  50% 50%



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

Chain D:  50% 50%



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

Chain E:  50% 50%



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

Chain F:  50% 50%



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

Chain G:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.00Å 260.15Å 73.36Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	68.20 – 3.37 68.20 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.20-3.37) 99.8 (68.20-3.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.285 0.235 , 0.296	Depositor DCC
R_{free} test set	1620 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14098	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.84	4/7115 (0.1%)	1.32	79/9660 (0.8%)
1	B	0.87	12/6979 (0.2%)	1.47	119/9486 (1.3%)
All	All	0.85	16/14094 (0.1%)	1.40	198/19146 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	16
All	All	0	27

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	750	PHE	CA-C	10.21	1.66	1.52
1	B	609	THR	CA-CB	7.53	1.65	1.53
1	B	751	ASP	N-CA	7.48	1.56	1.46
1	A	181	LEU	CA-C	7.36	1.61	1.52
1	B	451	SER	C-O	-7.19	1.15	1.24
1	B	596	VAL	CA-CB	6.66	1.63	1.54
1	A	190	PHE	CA-C	6.25	1.60	1.52
1	B	518	THR	C-O	-6.10	1.17	1.24
1	A	600	THR	CA-CB	6.07	1.60	1.53
1	B	804	GLN	CA-C	5.88	1.60	1.52
1	B	451	SER	CA-C	-5.84	1.45	1.52
1	B	884	ILE	CA-CB	5.59	1.59	1.54
1	B	697	ASN	CG-ND2	5.26	1.44	1.33
1	B	264	SER	CA-C	5.18	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	626	LYS	N-CA	5.12	1.52	1.46
1	B	190	PHE	CA-C	-5.06	1.46	1.52

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	TYR	N-CA-C	14.34	131.14	111.92
1	B	567	VAL	N-CA-C	13.04	122.94	110.42
1	B	451	SER	CA-C-N	-11.84	102.02	123.34
1	B	451	SER	C-N-CA	-11.84	102.02	123.34
1	A	627	GLU	N-CA-C	11.04	134.32	110.80
1	A	623	LYS	N-CA-C	10.72	127.67	108.69
1	B	752	LEU	N-CA-C	-10.66	99.74	111.36
1	B	518	THR	N-CA-C	-10.37	99.53	111.03
1	B	861	THR	N-CA-C	9.53	131.09	110.80
1	A	406	ASN	N-CA-C	-9.38	101.61	113.43
1	B	623	LYS	N-CA-C	9.31	123.72	108.26
1	A	161	PHE	CA-C-N	9.06	131.16	119.84
1	A	161	PHE	C-N-CA	9.06	131.16	119.84
1	B	522	ASP	N-CA-C	-9.01	101.59	114.12
1	B	609	THR	N-CA-C	-8.98	102.45	113.50
1	A	230	LYS	N-CA-C	8.86	122.84	108.32
1	A	191	ARG	CA-CB-CG	8.78	131.65	114.10
1	B	750	PHE	CA-CB-CG	8.71	122.51	113.80
1	B	1012	GLN	CA-CB-CG	8.68	131.45	114.10
1	B	871	ASP	N-CA-C	8.65	121.66	111.71
1	A	538	GLU	N-CA-C	-8.63	102.00	112.54
1	A	782	LEU	N-CA-C	-8.60	99.83	110.41
1	A	190	PHE	N-CA-C	8.54	123.35	108.75
1	B	412	TYR	CA-C-N	8.52	128.25	119.56
1	B	412	TYR	C-N-CA	8.52	128.25	119.56
1	B	665	TYR	CB-CA-C	-8.48	100.10	111.63
1	A	377	LEU	CA-C-N	8.30	133.42	121.80
1	A	377	LEU	C-N-CA	8.30	133.42	121.80
1	B	191	ARG	N-CA-C	8.27	121.73	109.24
1	B	696	MET	CA-C-N	8.19	132.08	120.28
1	B	696	MET	C-N-CA	8.19	132.08	120.28
1	B	567	VAL	CA-C-N	8.08	131.77	120.29
1	B	567	VAL	C-N-CA	8.08	131.77	120.29
1	B	835	CYS	N-CA-C	8.00	120.78	111.02
1	B	577	HIS	CB-CA-C	-7.98	97.28	110.85
1	B	519	MET	N-CA-C	7.92	120.92	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1012	GLN	N-CA-C	-7.69	94.42	110.80
1	B	748	ARG	CG-CD-NE	7.68	128.90	112.00
1	B	600	THR	N-CA-C	7.60	126.98	110.80
1	B	873	GLY	N-CA-C	-7.57	103.72	112.50
1	B	1015	GLU	CB-CG-CD	-7.56	99.75	112.60
1	B	1015	GLU	CA-CB-CG	7.48	129.07	114.10
1	A	377	LEU	CA-CB-CG	7.33	141.94	116.30
1	B	605	ARG	N-CA-C	-7.29	103.85	112.89
1	B	805	GLN	CB-CA-C	-7.29	100.02	111.17
1	A	706	ASP	N-CA-C	7.29	119.22	111.28
1	B	1015	GLU	CB-CA-C	-7.18	96.14	110.42
1	B	681	ILE	CA-C-N	-7.16	111.13	122.73
1	B	681	ILE	C-N-CA	-7.16	111.13	122.73
1	A	638	ASN	N-CA-C	7.15	126.03	110.80
1	B	533	SER	N-CA-C	7.08	120.76	110.42
1	A	649	SER	N-CA-C	-7.06	104.67	112.72
1	A	605	ARG	N-CA-C	-7.04	104.50	113.23
1	B	611	THR	N-CA-C	6.91	120.19	111.69
1	B	751	ASP	N-CA-C	-6.90	104.67	113.23
1	A	431	GLU	N-CA-C	6.85	121.47	113.18
1	B	746	LEU	CA-C-N	6.84	133.28	122.60
1	B	746	LEU	C-N-CA	6.84	133.28	122.60
1	A	1021	LEU	N-CA-C	-6.84	103.00	111.75
1	B	214	HIS	N-CA-C	6.81	120.04	109.07
1	B	454	ASP	N-CA-C	6.78	120.81	112.54
1	B	1000	VAL	N-CA-C	6.70	117.32	110.82
1	A	963	ILE	N-CA-C	-6.69	104.30	113.00
1	B	401	LEU	N-CA-C	-6.69	103.91	111.07
1	A	632	GLN	N-CA-C	6.68	120.39	109.24
1	A	263	TYR	N-CA-C	6.66	118.97	108.79
1	B	812	GLY	N-CA-C	6.63	119.25	111.63
1	A	963	ILE	CA-C-N	6.57	129.93	120.79
1	A	963	ILE	C-N-CA	6.57	129.93	120.79
1	A	221	PHE	N-CA-C	6.37	119.32	109.07
1	B	610	TRP	N-CA-C	6.36	119.51	111.69
1	A	405	GLN	CA-C-N	6.35	135.73	122.58
1	A	405	GLN	C-N-CA	6.35	135.73	122.58
1	B	667	LYS	N-CA-C	6.33	119.53	110.10
1	B	871	ASP	CA-C-N	-6.30	111.36	122.26
1	B	871	ASP	C-N-CA	-6.30	111.36	122.26
1	A	181	LEU	N-CA-C	6.29	119.76	109.06
1	A	664	ASN	CB-CA-C	-6.29	97.90	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	PHE	N-CA-C	-6.27	101.88	109.72
1	B	568	PHE	N-CA-C	-6.26	104.54	111.36
1	A	751	ASP	N-CA-C	-6.26	105.65	113.28
1	B	564	SER	N-CA-C	6.24	117.92	110.19
1	A	405	GLN	N-CA-C	6.23	124.07	110.80
1	A	220	THR	CA-C-N	6.22	131.58	123.00
1	A	220	THR	C-N-CA	6.22	131.58	123.00
1	A	525	ASN	N-CA-C	-6.22	105.73	113.38
1	B	546	SER	N-CA-C	-6.21	105.75	113.15
1	B	992	GLU	N-CA-C	-6.19	105.72	113.28
1	B	283	SER	N-CA-C	-6.19	105.31	112.92
1	B	1012	GLN	CB-CA-C	6.19	122.74	110.42
1	B	455	ARG	CB-CG-CD	6.17	125.50	111.30
1	B	201	LEU	N-CA-C	-6.14	106.38	114.31
1	B	796	PHE	CA-C-N	-6.13	112.89	123.25
1	B	796	PHE	C-N-CA	-6.13	112.89	123.25
1	B	859	VAL	N-CA-C	-6.03	106.62	112.29
1	B	743	LYS	N-CA-C	6.02	123.62	110.80
1	A	664	ASN	N-CA-C	6.01	123.61	110.80
1	B	791	LEU	N-CA-C	-5.98	104.67	111.07
1	B	737	GLU	N-CA-C	-5.98	104.84	111.36
1	A	249	GLU	N-CA-C	5.96	118.14	109.07
1	B	336	SER	N-CA-C	5.95	118.34	108.99
1	A	648	THR	N-CA-C	5.95	118.05	110.61
1	B	264	SER	N-CA-C	5.92	118.86	109.50
1	A	176	ARG	N-CA-C	5.90	118.09	108.76
1	A	918	ASN	N-CA-C	-5.90	105.92	114.12
1	B	455	ARG	CB-CA-C	-5.88	99.79	110.56
1	B	369	LEU	CA-CB-CG	5.87	136.84	116.30
1	B	751	ASP	N-CA-CB	5.86	119.59	110.44
1	A	183	PRO	CA-C-N	-5.86	114.92	123.00
1	A	183	PRO	C-N-CA	-5.86	114.92	123.00
1	B	797	LYS	CA-CB-CG	-5.84	102.42	114.10
1	B	367	LYS	N-CA-C	-5.83	100.91	109.18
1	A	624	LYS	N-CA-C	5.82	117.51	109.54
1	A	622	GLN	CA-C-N	-5.81	112.56	122.33
1	A	622	GLN	C-N-CA	-5.81	112.56	122.33
1	B	567	VAL	N-CA-CB	-5.81	103.75	110.55
1	B	671	VAL	N-CA-C	5.80	118.19	109.20
1	B	628	LEU	CA-CB-CG	5.79	136.55	116.30
1	B	266	ASN	N-CA-C	5.77	118.82	110.28
1	A	684	THR	N-CA-C	5.77	117.37	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	GLU	N-CA-C	5.76	118.06	109.59
1	A	625	GLY	N-CA-C	5.75	124.12	113.76
1	A	433	TRP	CA-CB-CG	-5.73	102.72	113.60
1	B	805	GLN	CA-C-N	-5.72	113.24	121.42
1	B	805	GLN	C-N-CA	-5.72	113.24	121.42
1	A	688	LEU	N-CA-C	-5.71	106.45	113.41
1	A	685	GLU	CA-C-N	-5.69	114.71	123.14
1	A	685	GLU	C-N-CA	-5.69	114.71	123.14
1	B	399	LYS	CA-CB-CG	5.69	125.48	114.10
1	A	917	ASP	N-CA-C	5.68	118.57	111.24
1	B	613	GLN	CA-CB-CG	5.66	125.42	114.10
1	A	998	ARG	N-CA-C	-5.66	105.19	111.36
1	B	451	SER	CA-C-O	-5.65	112.43	120.51
1	B	398	VAL	N-CA-C	5.62	115.75	110.30
1	A	1018	LEU	N-CA-C	-5.59	105.18	111.28
1	B	268	SER	N-CA-C	5.56	117.47	110.24
1	A	670	SER	N-CA-C	5.54	117.49	109.07
1	B	512	LEU	N-CA-C	-5.53	105.25	111.28
1	A	282	GLU	N-CA-C	-5.52	106.38	113.23
1	B	577	HIS	N-CA-CB	5.52	118.33	110.16
1	A	595	GLU	N-CA-C	-5.51	103.87	111.81
1	A	376	THR	CA-C-N	-5.51	115.40	123.00
1	A	376	THR	C-N-CA	-5.51	115.40	123.00
1	B	862	THR	N-CA-C	5.49	117.69	111.11
1	A	445	TYR	N-CA-C	5.46	118.37	109.24
1	B	1015	GLU	N-CA-C	5.43	122.37	110.80
1	B	523	SER	N-CA-C	-5.43	105.92	112.54
1	A	754	ASN	N-CA-C	-5.40	106.65	113.18
1	A	714	HIS	N-CA-C	-5.39	105.48	111.36
1	B	666	SER	N-CA-C	5.37	117.25	108.55
1	B	400	LEU	N-CA-C	-5.36	105.61	111.82
1	A	331	MET	CA-C-N	-5.34	114.21	119.92
1	A	331	MET	C-N-CA	-5.34	114.21	119.92
1	A	451	SER	N-CA-C	5.33	117.76	109.60
1	A	938	HIS	N-CA-C	5.33	117.51	111.11
1	B	751	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	623	LYS	CA-CB-CG	-5.29	103.51	114.10
1	A	191	ARG	CB-CA-C	-5.29	102.36	109.71
1	A	725	ASP	N-CA-C	-5.29	106.78	113.18
1	B	609	THR	N-CA-CB	5.28	118.29	110.53
1	B	774	LEU	N-CA-C	-5.27	105.43	111.07
1	A	1007	ILE	N-CA-C	5.27	115.48	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	960	SER	N-CA-C	-5.26	102.60	110.23
1	B	452	MET	CG-SD-CE	5.26	112.47	100.90
1	B	654	ILE	N-CA-C	5.25	116.01	107.71
1	B	719	ASN	CA-C-N	5.24	125.32	119.87
1	B	719	ASN	C-N-CA	5.24	125.32	119.87
1	B	962	THR	N-CA-C	-5.23	105.66	111.36
1	A	726	LYS	N-CA-C	-5.23	105.25	111.69
1	B	518	THR	CA-C-O	-5.22	115.52	120.90
1	A	923	LYS	N-CA-C	5.22	119.36	112.89
1	A	686	GLU	N-CA-C	5.22	117.90	107.62
1	B	165	GLN	CA-CB-CG	-5.21	103.67	114.10
1	B	625	GLY	N-CA-C	5.21	125.52	113.18
1	B	861	THR	CA-C-N	5.21	127.57	120.54
1	B	861	THR	C-N-CA	5.21	127.57	120.54
1	B	430	MET	N-CA-C	5.21	116.72	108.96
1	B	190	PHE	CA-C-N	-5.20	113.79	122.21
1	B	190	PHE	C-N-CA	-5.20	113.79	122.21
1	A	951	LYS	N-CA-C	-5.19	106.95	113.28
1	B	525	ASN	N-CA-C	-5.17	107.14	113.50
1	B	870	THR	N-CA-C	-5.17	100.03	108.76
1	A	402	GLU	CA-CB-CG	5.17	124.43	114.10
1	A	1022	THR	N-CA-C	5.13	117.61	111.71
1	B	1012	GLN	CB-CG-CD	5.13	121.31	112.60
1	A	285	GLU	N-CA-C	5.12	118.10	109.95
1	B	319	ILE	N-CA-C	5.12	115.34	107.77
1	A	228	GLN	N-CA-C	5.11	117.23	108.90
1	A	627	GLU	CB-CA-C	-5.09	100.28	110.42
1	B	805	GLN	N-CA-C	5.08	118.35	112.97
1	B	612	LEU	CA-CB-CG	5.07	134.03	116.30
1	B	265	ALA	N-CA-C	5.06	121.58	110.80
1	B	892	LYS	N-CA-C	-5.04	107.14	113.28
1	B	521	LYS	CB-CA-C	-5.04	100.40	110.42
1	B	697	ASN	N-CA-CB	-5.03	102.47	110.22
1	B	683	LEU	N-CA-C	5.03	117.92	110.48
1	B	426	GLU	N-CA-C	-5.01	107.44	113.21
1	B	660	THR	N-CA-C	5.00	114.90	108.34

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1018	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	1019	LYS	Peptide
1	A	220	THR	Peptide
1	A	230	LYS	Peptide
1	A	284	ASN	Peptide
1	A	404	PHE	Peptide
1	A	626	LYS	Peptide
1	A	627	GLU	Peptide
1	A	638	ASN	Peptide
1	A	662	GLY	Peptide
1	A	730	ASN	Sidechain
1	B	191	ARG	Peptide
1	B	265	ALA	Peptide
1	B	399	LYS	Peptide
1	B	452	MET	Peptide
1	B	486	ASN	Sidechain
1	B	521	LYS	Peptide
1	B	608	LYS	Peptide
1	B	669	GLN	Peptide
1	B	697	ASN	Sidechain
1	B	743	LYS	Peptide
1	B	746	LEU	Peptide
1	B	747	LYS	Peptide
1	B	748	ARG	Peptide
1	B	797	LYS	Peptide
1	B	860	MET	Peptide
1	B	861	THR	Peptide

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	6937	0	6760	426	1
1	B	6808	0	6593	556	0
2	C	28	0	25	3	0
2	D	28	0	25	2	0
2	E	28	0	25	1	0
2	F	28	0	25	1	1
2	G	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	126	0	116	15	0
4	B	84	0	78	6	0
5	A	1	0	0	0	0
All	All	14098	0	13672	988	1

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 36.

All (988) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:CD1	4:A:1113:NAG:H81	1.57	1.33
1:A:574:LEU:HD11	4:A:1113:NAG:C8	1.65	1.26
1:A:367:LYS:HD2	1:A:368:ASN:H	1.02	1.17
1:B:518:THR:O	1:B:521:LYS:HB2	1.49	1.12
1:B:695:ASN:HB3	1:B:726:LYS:HD2	1.31	1.10
1:A:405:GLN:HB2	1:A:406:ASN:HD22	1.16	1.10
1:B:627:GLU:HA	1:B:682:ASN:HB2	1.25	1.08
1:A:191:ARG:HH22	1:A:320:ILE:HB	1.12	1.08
1:A:405:GLN:HG3	1:A:406:ASN:H	0.99	1.07
1:A:574:LEU:HD12	4:A:1113:NAG:H81	1.34	1.07
1:B:1021:LEU:HA	1:B:1024:TRP:HE1	1.16	1.07
1:B:521:LYS:HG3	1:B:547:LEU:HD11	1.37	1.06
1:B:521:LYS:NZ	1:B:699:TYR:OH	1.89	1.06
1:B:518:THR:HG22	1:B:521:LYS:HE2	1.38	1.05
1:A:405:GLN:CG	1:A:406:ASN:H	1.68	1.05
1:B:660:THR:HB	1:B:687:VAL:HG11	1.38	1.05
1:B:452:MET:HE3	1:B:455:ARG:HG2	1.38	1.05
1:B:735:ILE:HG12	1:B:749:ALA:HA	1.33	1.05
1:A:430:MET:HG2	1:A:431:GLU:H	1.23	1.04
1:B:748:ARG:CD	1:B:750:PHE:HB2	1.87	1.03
1:A:574:LEU:HD11	4:A:1113:NAG:H81	1.23	1.02
4:A:1113:NAG:H62	4:A:1114:NAG:C7	1.91	1.01
1:B:563:LEU:HG	1:B:567:VAL:HG21	1.43	1.00
1:B:920:ARG:HH21	1:B:923:LYS:HE2	1.24	0.99
1:B:452:MET:SD	1:B:455:ARG:N	2.36	0.96
1:B:451:SER:O	1:B:452:MET:HE2	1.65	0.96
1:A:405:GLN:HG3	1:A:407:TYR:H	1.31	0.95
1:A:191:ARG:NH2	1:A:320:ILE:HB	1.80	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:LYS:HE2	1:B:612:LEU:HB3	1.49	0.95
1:A:182:HIS:H	1:A:191:ARG:HB2	1.32	0.94
1:B:622:GLN:HE21	1:B:705:ALA:HB2	1.30	0.94
1:A:574:LEU:HD11	4:A:1113:NAG:H83	1.50	0.94
1:B:748:ARG:HE	1:B:1024:TRP:HZ3	1.13	0.93
1:B:748:ARG:HB3	1:B:751:ASP:H	1.31	0.93
1:A:265:ALA:HA	4:A:1106:NAG:H82	1.49	0.92
1:A:574:LEU:CD1	4:A:1113:NAG:C8	2.35	0.92
1:A:405:GLN:HG3	1:A:406:ASN:N	1.83	0.92
1:B:452:MET:CE	1:B:455:ARG:HG2	2.00	0.91
1:A:182:HIS:N	1:A:191:ARG:HB2	1.85	0.91
1:B:455:ARG:HA	1:B:458:VAL:HG12	1.52	0.91
1:A:560:LYS:HD2	1:A:560:LYS:O	1.72	0.89
1:B:190:PHE:O	1:B:191:ARG:NH1	2.05	0.89
1:B:191:ARG:HG3	1:B:264:SER:HA	1.54	0.89
1:B:709:TRP:O	1:B:713:ILE:N	2.05	0.89
1:B:797:LYS:HG2	1:B:800:GLN:HA	1.55	0.88
1:B:637:LEU:HD22	1:B:1009:LEU:HD22	1.53	0.88
1:A:367:LYS:HD2	1:A:368:ASN:N	1.88	0.88
1:A:891:ASN:OD1	1:A:923:LYS:NZ	2.07	0.87
1:B:1021:LEU:HA	1:B:1024:TRP:NE1	1.89	0.87
1:A:184:ASN:HB2	2:C:1:NAG:N2	1.90	0.87
1:B:861:THR:HG21	1:B:864:PHE:HB2	1.55	0.86
1:A:367:LYS:CD	1:A:368:ASN:H	1.87	0.86
1:B:560:LYS:HE3	1:B:568:PHE:HB3	1.58	0.85
1:A:403:PHE:O	1:A:405:GLN:HG2	1.77	0.85
1:B:748:ARG:HD2	1:B:750:PHE:HB2	1.58	0.85
1:A:388:GLY:O	1:A:391:HIS:ND1	2.11	0.84
1:B:653:HIS:CD2	1:B:675:ASP:HB2	2.12	0.84
1:B:857:THR:HA	1:B:860:MET:HB2	1.57	0.83
1:A:477:MET:SD	1:A:486:ASN:ND2	2.50	0.83
1:B:191:ARG:NH1	1:B:265:ALA:O	2.12	0.83
1:A:747:LYS:HE3	1:A:1019:LYS:HE3	1.59	0.82
1:A:521:LYS:HD2	1:A:521:LYS:O	1.79	0.82
1:B:637:LEU:HD13	1:B:1009:LEU:HD13	1.61	0.82
1:B:692:VAL:HB	1:B:702:VAL:HG11	1.61	0.82
1:B:762:THR:HG22	1:B:819:LEU:HB2	1.61	0.82
1:B:433:TRP:HE1	1:B:469:GLN:HA	1.45	0.82
1:B:430:MET:HG3	1:B:432:ASN:H	1.45	0.81
1:B:521:LYS:CG	1:B:547:LEU:HD11	2.10	0.81
1:B:602:ASP:OD1	1:B:603:VAL:N	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLN:HB2	1:A:406:ASN:ND2	1.94	0.80
1:A:433:TRP:HE1	1:A:469:GLN:HA	1.44	0.80
1:B:985:ALA:O	1:B:989:ASN:ND2	2.15	0.80
1:B:632:GLN:NE2	1:B:652:TRP:O	2.14	0.80
1:B:748:ARG:HD2	1:B:750:PHE:CB	2.12	0.80
1:B:745:PRO:C	1:B:747:LYS:H	1.90	0.80
1:B:748:ARG:NE	1:B:1024:TRP:HZ3	1.80	0.79
1:A:626:LYS:C	1:A:627:GLU:HG2	2.06	0.79
1:B:748:ARG:HB3	1:B:751:ASP:N	1.98	0.79
1:B:977:LYS:HG2	1:B:1011:ILE:HD13	1.64	0.78
1:B:623:LYS:HE2	1:B:627:GLU:C	2.09	0.78
1:B:191:ARG:CG	1:B:264:SER:HA	2.13	0.78
1:B:281:ASP:HB3	1:B:285:GLU:H	1.49	0.78
1:B:430:MET:HB3	1:B:437:THR:OG1	1.83	0.78
1:B:369:LEU:HG	1:B:387:ILE:HG21	1.66	0.77
1:B:1015:GLU:HB3	1:B:1016:LYS:HG3	1.66	0.77
1:B:486:ASN:N	1:B:486:ASN:HD22	1.81	0.77
1:B:367:LYS:NZ	1:B:384:PRO:O	2.18	0.77
1:B:627:GLU:HA	1:B:682:ASN:CB	2.13	0.77
1:A:1017:ASN:O	1:A:1019:LYS:HB2	1.84	0.77
1:B:623:LYS:HG3	1:B:628:LEU:HD23	1.67	0.77
1:B:795:VAL:HA	1:B:798:LEU:HD12	1.65	0.76
1:A:184:ASN:HB2	2:C:1:NAG:HN2	1.50	0.76
1:A:634:ARG:HG2	1:A:652:TRP:HH2	1.50	0.76
1:A:270:SER:OG	1:A:271:TYR:N	2.14	0.76
1:A:451:SER:OG	1:A:454:ASP:OD1	2.02	0.76
4:A:1113:NAG:O6	4:A:1114:NAG:O7	2.02	0.76
1:B:385:GLU:H	1:B:385:GLU:CD	1.93	0.76
1:A:861:THR:O	1:A:865:LYS:HD2	1.86	0.76
1:A:966:ILE:O	1:A:970:SER:OG	2.02	0.76
1:A:220:THR:HG21	1:A:231:GLN:HA	1.67	0.76
1:B:336:SER:OG	1:B:346:ASP:HA	1.85	0.76
1:B:653:HIS:HD2	1:B:675:ASP:HB2	1.49	0.75
1:B:891:ASN:OD1	1:B:923:LYS:NZ	2.20	0.75
1:B:1014:MET:HE3	1:B:1018:LEU:HB2	1.68	0.75
1:B:563:LEU:HG	1:B:567:VAL:CG2	2.15	0.75
1:A:625:GLY:N	1:A:627:GLU:OE1	2.19	0.75
1:A:1016:LYS:HE3	1:A:1016:LYS:HA	1.68	0.75
1:B:399:LYS:HB2	1:B:402:GLU:HB2	1.66	0.75
1:B:595:GLU:HA	1:B:599:GLN:HA	1.67	0.75
1:B:920:ARG:NH2	1:B:923:LYS:HE2	2.00	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PHE:HA	1:A:298:ALA:HB3	1.67	0.74
1:B:401:LEU:HG	1:B:405:GLN:HE21	1.50	0.74
4:A:1113:NAG:C6	4:A:1114:NAG:O7	2.35	0.74
4:A:1113:NAG:C6	4:A:1114:NAG:C7	2.65	0.74
1:B:796:PHE:CE2	1:B:797:LYS:HD2	2.21	0.74
1:A:172:VAL:HG21	1:A:207:ILE:HD13	1.69	0.74
1:A:207:ILE:HG13	1:A:245:ILE:HD11	1.68	0.74
1:B:623:LYS:HD3	1:B:624:LYS:N	2.03	0.74
1:A:433:TRP:CD1	1:A:473:ASN:HD22	2.06	0.74
1:A:747:LYS:HZ2	1:A:1024:TRP:HB3	1.52	0.74
1:A:220:THR:HG23	1:A:221:PHE:H	1.53	0.74
1:A:511:PHE:HE2	1:A:557:LEU:HD22	1.53	0.74
1:A:1020:SER:HB2	1:A:1023:TRP:CD1	2.23	0.73
1:A:660:THR:HB	1:A:687:VAL:HG11	1.69	0.73
1:B:691:LYS:HD3	1:B:731:LEU:HD21	1.69	0.73
1:B:684:THR:OG1	1:B:685:GLU:OE1	2.06	0.73
1:B:710:GLU:HA	1:B:713:ILE:HB	1.70	0.73
1:A:218:ARG:N	1:A:262:GLU:OE1	2.20	0.72
1:A:389:GLN:OE1	1:A:446:ASP:HB2	1.89	0.72
1:A:623:LYS:HD3	1:A:628:LEU:HA	1.72	0.72
1:B:183:PRO:HA	1:B:190:PHE:HA	1.71	0.72
1:A:626:LYS:H	1:A:627:GLU:CD	1.97	0.72
1:A:1024:TRP:CG	1:A:1025:LEU:H	2.07	0.72
1:B:977:LYS:HZ1	1:B:980:LEU:HD22	1.55	0.72
1:B:521:LYS:HB3	1:B:522:ASP:HB2	1.72	0.71
1:A:482:ASP:OD1	1:A:586:SER:HB2	1.88	0.71
1:B:178:GLU:OE1	1:B:195:THR:OG1	2.07	0.71
1:A:215:ASN:HB3	1:A:264:SER:HB2	1.70	0.71
1:B:861:THR:HG21	1:B:864:PHE:CB	2.21	0.71
1:B:367:LYS:HG2	1:B:387:ILE:HD11	1.71	0.71
1:B:427:ALA:O	1:B:439:ARG:NH1	2.24	0.71
1:A:307:ASP:HA	1:A:356:THR:HG21	1.73	0.70
1:B:977:LYS:NZ	1:B:980:LEU:HD22	2.06	0.70
1:A:1017:ASN:C	1:A:1019:LYS:HB2	2.16	0.70
1:B:604:LYS:HD2	1:B:607:MET:HG2	1.72	0.70
1:B:966:ILE:O	1:B:970:SER:OG	2.09	0.70
1:A:597:THR:CB	1:A:601:LEU:HG	2.21	0.70
1:A:403:PHE:C	1:A:405:GLN:HG2	2.16	0.70
1:A:521:LYS:HG3	1:A:547:LEU:CD1	2.22	0.70
1:A:630:ILE:HG21	1:A:656:LEU:HD11	1.73	0.70
1:B:748:ARG:HD2	1:B:750:PHE:C	2.17	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:LEU:HB3	1:A:1019:LYS:HE2	1.74	0.70
1:A:406:ASN:O	1:A:409:GLU:HG3	1.91	0.69
1:A:634:ARG:HG2	1:A:652:TRP:CH2	2.26	0.69
1:A:728:ARG:HD2	1:A:755:TYR:OH	1.93	0.69
1:B:486:ASN:N	1:B:486:ASN:ND2	2.40	0.69
1:B:256:ASN:C	1:B:257:TYR:HD1	2.00	0.69
1:A:560:LYS:HD2	1:A:560:LYS:C	2.16	0.69
1:B:746:LEU:HD22	1:B:1020:SER:OG	1.93	0.69
1:B:748:ARG:HD3	1:B:750:PHE:HB2	1.73	0.69
1:A:622:GLN:O	1:A:623:LYS:NZ	2.25	0.68
1:B:214:HIS:NE2	1:B:301:SER:O	2.25	0.68
4:A:1113:NAG:H62	4:A:1114:NAG:O7	1.91	0.68
1:B:768:ALA:O	1:B:772:THR:OG1	2.11	0.68
1:B:626:LYS:O	1:B:683:LEU:N	2.23	0.68
1:B:856:PRO:HB2	1:B:859:VAL:HG22	1.75	0.68
1:A:964:GLN:OE1	1:A:965:ASN:HB2	1.93	0.68
1:B:861:THR:OG1	1:B:863:VAL:N	2.26	0.68
1:A:396:THR:HA	1:A:399:LYS:NZ	2.09	0.68
1:A:622:GLN:HG3	1:A:705:ALA:HB2	1.75	0.68
1:A:1015:GLU:C	1:A:1016:LYS:HD2	2.18	0.68
1:B:797:LYS:HG2	1:B:800:GLN:CA	2.22	0.68
1:B:212:THR:O	1:B:214:HIS:N	2.23	0.68
1:A:595:GLU:OE2	4:A:1114:NAG:O6	2.13	0.67
1:B:369:LEU:HG	1:B:387:ILE:CG2	2.24	0.67
1:A:696:MET:CG	1:A:730:ASN:HD22	2.06	0.67
1:B:567:VAL:HG23	1:B:568:PHE:N	2.08	0.67
1:B:452:MET:SD	1:B:455:ARG:HG2	2.34	0.67
1:B:748:ARG:CZ	1:B:750:PHE:HB3	2.24	0.67
1:B:954:GLN:HG2	1:B:955:LYS:HD2	1.75	0.67
1:A:405:GLN:HG3	1:A:407:TYR:N	2.06	0.67
1:A:713:ILE:HD13	1:A:752:LEU:HA	1.77	0.67
1:A:402:GLU:C	1:A:405:GLN:HB3	2.20	0.67
1:A:624:LYS:C	1:A:627:GLU:OE1	2.38	0.67
1:B:399:LYS:HA	1:B:402:GLU:H	1.58	0.67
1:B:484:TRP:HB3	1:B:548:SER:HB3	1.76	0.66
1:A:623:LYS:CD	1:A:628:LEU:HD12	2.26	0.66
1:A:853:GLN:NE2	1:A:854:SER:O	2.27	0.66
1:B:167:ARG:HH21	1:B:479:TRP:NE1	1.93	0.66
1:A:748:ARG:HG2	1:A:748:ARG:HH11	1.60	0.66
1:A:706:ASP:O	1:A:710:GLU:HG3	1.95	0.66
1:A:560:LYS:HB2	1:A:568:PHE:CG	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:ILE:HD12	1:B:719:ASN:HB3	1.78	0.66
1:A:920:ARG:HH22	1:A:922:GLN:CD	2.04	0.66
1:A:166:ILE:HG22	1:A:240:HIS:NE2	2.10	0.66
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.59	0.66
1:B:689:TRP:CD1	1:B:715:GLN:HG3	2.30	0.66
1:A:629:PHE:HB3	1:A:631:GLN:HE22	1.59	0.66
1:B:750:PHE:O	1:B:753:ILE:HG22	1.95	0.66
1:B:343:LEU:HD23	1:B:344:VAL:N	2.12	0.65
1:A:710:GLU:HA	1:A:713:ILE:HG22	1.78	0.65
1:A:696:MET:HG3	1:A:730:ASN:ND2	2.11	0.65
1:B:623:LYS:HD3	1:B:623:LYS:C	2.21	0.65
1:A:626:LYS:N	1:A:627:GLU:OE1	2.29	0.65
1:B:510:ASP:OD1	1:B:511:PHE:N	2.29	0.65
1:B:623:LYS:HE2	1:B:627:GLU:CA	2.26	0.65
1:A:182:HIS:HB2	1:A:191:ARG:CZ	2.26	0.65
1:B:322:ASP:OD2	2:E:2:NAG:O6	2.14	0.65
1:B:608:LYS:CE	1:B:612:LEU:HB3	2.25	0.65
1:B:525:ASN:OD1	1:B:614:LYS:NZ	2.29	0.65
1:B:608:LYS:HD3	1:B:612:LEU:H	1.62	0.65
1:B:695:ASN:HB3	1:B:726:LYS:CD	2.20	0.65
1:B:282:GLU:HG2	1:B:385:GLU:HG2	1.78	0.65
1:A:663:ARG:HG2	1:A:664:ASN:OD1	1.97	0.64
1:B:161:PHE:HE1	1:B:163:TRP:O	1.79	0.64
1:A:747:LYS:NZ	1:A:1024:TRP:HB3	2.12	0.64
1:B:541:GLU:HA	1:B:544:PHE:HD1	1.60	0.64
1:B:748:ARG:NE	1:B:1024:TRP:CZ3	2.52	0.64
1:B:796:PHE:CZ	1:B:832:LEU:HB3	2.33	0.64
1:B:977:LYS:NZ	1:B:1008:GLN:HA	2.13	0.64
1:A:224:ALA:O	1:A:226:SER:N	2.30	0.64
1:B:596:VAL:HG12	1:B:598:ASN:H	1.61	0.64
1:A:182:HIS:HB2	1:A:191:ARG:CG	2.27	0.64
1:A:166:ILE:HG22	1:A:240:HIS:CD2	2.33	0.64
1:A:331:MET:HE3	1:A:352:VAL:H	1.62	0.64
1:B:478:LYS:HD2	1:B:585:GLN:HG3	1.78	0.64
1:B:510:ASP:O	1:B:513:ASP:HB3	1.97	0.64
1:A:445:TYR:OH	1:A:455:ARG:HD2	1.97	0.64
1:A:623:LYS:HG2	1:A:627:GLU:CD	2.22	0.64
1:B:329:SER:OG	1:B:330:ASN:N	2.29	0.64
1:A:182:HIS:HB2	1:A:191:ARG:HG3	1.78	0.64
1:A:755:TYR:OH	1:A:759:GLU:OE1	2.15	0.64
1:A:445:TYR:CZ	1:A:455:ARG:HD2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ALA:HB3	4:B:1107:NAG:H82	1.80	0.64
1:A:315:PHE:N	1:A:351:SER:OG	2.30	0.63
1:B:459:THR:HG22	1:B:498:LEU:HD11	1.79	0.63
1:B:174:PRO:HA	1:B:198:VAL:HG12	1.79	0.63
1:B:735:ILE:CG1	1:B:749:ALA:HA	2.19	0.63
1:B:738:LEU:HB3	1:B:743:LYS:CB	2.28	0.63
1:B:748:ARG:NE	1:B:750:PHE:HB2	2.13	0.63
1:B:1012:GLN:O	1:B:1014:MET:N	2.31	0.63
1:A:220:THR:OG1	1:A:232:ALA:N	2.29	0.63
1:A:725:ASP:OD1	1:A:726:LYS:NZ	2.18	0.63
1:B:187:SER:OG	1:B:188:MET:N	2.28	0.63
1:B:411:GLN:HG3	4:B:1112:NAG:H82	1.81	0.63
1:B:477:MET:SD	1:B:478:LYS:N	2.71	0.63
1:B:861:THR:HG22	1:B:892:LYS:HD3	1.81	0.63
1:A:949:TRP:O	1:A:953:VAL:HG23	1.98	0.63
1:B:578:ASN:HD22	4:B:1113:NAG:C7	2.09	0.63
1:A:433:TRP:HE1	1:A:469:GLN:CA	2.12	0.63
1:A:560:LYS:HB2	1:A:568:PHE:CD1	2.33	0.63
1:B:541:GLU:HA	1:B:544:PHE:CD1	2.33	0.63
1:B:215:ASN:ND2	1:B:264:SER:HB3	2.14	0.63
1:A:762:THR:HB	1:A:819:LEU:HB2	1.81	0.62
1:B:590:TRP:HB3	1:B:604:LYS:CB	2.29	0.62
1:B:872:LYS:HD2	1:B:875:SER:HB2	1.81	0.62
1:A:426:GLU:N	1:A:426:GLU:OE1	2.33	0.62
1:B:788:ALA:O	1:B:791:LEU:HB3	1.99	0.62
1:A:663:ARG:HD3	1:A:664:ASN:HD21	1.65	0.62
1:B:745:PRO:O	1:B:747:LYS:N	2.32	0.62
1:B:762:THR:CG2	1:B:819:LEU:HB2	2.28	0.62
1:B:373:VAL:HG22	1:B:374:ASN:H	1.65	0.62
1:A:726:LYS:HD3	1:A:726:LYS:N	2.14	0.62
1:B:623:LYS:HG2	1:B:628:LEU:HA	1.82	0.62
1:B:797:LYS:HZ2	1:B:800:GLN:HG3	1.64	0.62
1:A:430:MET:HG2	1:A:431:GLU:N	2.04	0.62
1:B:696:MET:SD	1:B:730:ASN:ND2	2.72	0.62
1:B:1023:TRP:CE3	1:B:1024:TRP:HB3	2.35	0.61
1:A:184:ASN:CB	2:C:1:NAG:N2	2.62	0.61
1:A:1020:SER:HB2	1:A:1023:TRP:HD1	1.66	0.61
1:B:560:LYS:HE3	1:B:568:PHE:CD1	2.36	0.61
1:A:809:THR:HG22	1:A:810:ASP:H	1.65	0.61
1:B:256:ASN:O	1:B:257:TYR:HD1	1.82	0.61
1:B:627:GLU:CA	1:B:682:ASN:HB2	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:THR:HG21	1:B:653:HIS:ND1	2.15	0.61
1:A:367:LYS:HG3	1:A:387:ILE:HG12	1.82	0.61
1:A:211:SER:HB2	1:A:304:PRO:HB3	1.83	0.61
1:B:457:LEU:HA	1:B:460:LYS:HB3	1.82	0.61
1:B:880:LYS:O	1:B:884:ILE:HG22	2.01	0.61
1:B:321:ARG:N	1:B:343:LEU:HD21	2.16	0.61
1:B:559:LEU:HD23	1:B:568:PHE:HE2	1.66	0.61
1:B:560:LYS:HE3	1:B:568:PHE:CB	2.29	0.61
1:B:282:GLU:HG2	1:B:385:GLU:CG	2.31	0.61
1:B:621:VAL:HG21	1:B:692:VAL:HG21	1.83	0.61
1:B:811:GLU:O	1:B:820:ARG:NH2	2.31	0.61
1:A:368:ASN:C	1:A:368:ASN:HD22	2.10	0.60
1:B:560:LYS:CE	1:B:568:PHE:HB3	2.29	0.60
1:A:161:PHE:CE1	1:A:163:TRP:HB3	2.35	0.60
1:B:294:PHE:HA	1:B:298:ALA:HB3	1.83	0.60
1:B:748:ARG:CD	1:B:750:PHE:CB	2.67	0.60
1:B:1012:GLN:C	1:B:1015:GLU:HG3	2.25	0.60
1:A:984:GLN:O	1:A:988:GLU:HG2	2.01	0.60
1:B:536:SER:OG	1:B:537:SER:N	2.33	0.60
1:B:562:TYR:CG	1:B:655:PRO:HB3	2.36	0.60
1:B:853:GLN:OE1	1:B:854:SER:N	2.34	0.60
1:B:433:TRP:NE1	1:B:469:GLN:HA	2.16	0.60
1:B:562:TYR:CD1	1:B:655:PRO:HB3	2.35	0.60
1:A:368:ASN:C	1:A:368:ASN:ND2	2.60	0.60
1:B:178:GLU:HA	1:B:316:ILE:O	2.01	0.60
1:B:373:VAL:HG22	1:B:374:ASN:N	2.17	0.60
1:B:861:THR:N	1:B:892:LYS:HD3	2.17	0.60
1:A:180:SER:OG	1:A:193:SER:HB3	2.02	0.60
1:A:781:LYS:HD2	1:A:938:HIS:CG	2.37	0.60
1:A:861:THR:HG22	1:A:865:LYS:HE3	1.83	0.60
1:B:695:ASN:HB2	1:B:697:ASN:OD1	2.02	0.60
1:B:942:TRP:NE1	1:B:946:LYS:HE2	2.17	0.60
1:A:220:THR:CG2	1:A:231:GLN:HA	2.32	0.59
1:B:455:ARG:O	1:B:459:THR:N	2.22	0.59
1:A:405:GLN:CG	1:A:406:ASN:N	2.48	0.59
1:B:980:LEU:HG	1:B:984:GLN:NE2	2.17	0.59
1:B:445:TYR:CE1	1:B:450:SER:HB2	2.37	0.59
1:B:521:LYS:CD	1:B:522:ASP:HB2	2.32	0.59
1:B:860:MET:O	1:B:861:THR:HB	1.94	0.59
1:A:283:SER:O	1:A:284:ASN:HB2	2.01	0.59
1:A:438:PHE:HE2	1:A:461:ILE:HG22	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PHE:HZ	1:B:423:PRO:HD2	1.66	0.59
1:B:564:SER:O	1:B:567:VAL:HG22	2.03	0.59
1:A:432:ASN:HB2	1:A:435:LEU:O	2.02	0.59
1:B:296:PRO:HB2	1:B:297:LEU:HD12	1.84	0.59
1:B:746:LEU:HG	1:B:747:LYS:N	2.17	0.59
1:A:182:HIS:HB2	1:A:191:ARG:NE	2.17	0.59
1:B:748:ARG:NH1	1:B:750:PHE:HB3	2.16	0.59
1:B:746:LEU:HD22	1:B:1020:SER:CB	2.33	0.59
1:A:284:ASN:HB3	1:A:285:GLU:HB2	1.84	0.59
1:B:281:ASP:OD1	1:B:282:GLU:N	2.36	0.59
1:B:499:GLU:OE1	1:B:508:TYR:HB3	2.03	0.59
1:B:180:SER:HB3	1:B:193:SER:HB3	1.84	0.58
1:B:608:LYS:NZ	1:B:613:GLN:HG3	2.18	0.58
1:B:843:PHE:HB2	1:B:863:VAL:HG13	1.85	0.58
1:A:165:GLN:OE1	1:A:165:GLN:N	2.36	0.58
1:A:587:ASP:HA	1:A:590:TRP:CD1	2.38	0.58
1:A:696:MET:CG	1:A:730:ASN:ND2	2.66	0.58
1:B:954:GLN:HG2	1:B:955:LYS:CD	2.33	0.58
1:A:787:LEU:HD22	1:A:1025:LEU:HD23	1.85	0.58
1:A:623:LYS:NZ	1:A:629:PHE:H	2.02	0.58
1:A:689:TRP:CD1	1:A:715:GLN:HE21	2.21	0.58
1:A:368:ASN:OD1	2:D:1:NAG:C2	2.47	0.58
1:B:862:THR:O	1:B:865:LYS:HB2	2.04	0.58
1:B:540:ILE:O	1:B:543:MET:HB2	2.04	0.57
1:B:784:TYR:CE2	1:B:1018:LEU:HD11	2.39	0.57
1:B:991:SER:HB2	1:B:994:THR:H	1.69	0.57
1:A:237:TYR:HE2	1:A:240:HIS:HD1	1.52	0.57
1:A:182:HIS:H	1:A:191:ARG:CB	2.12	0.57
1:B:430:MET:SD	1:B:431:GLU:N	2.77	0.57
1:A:935:PHE:HB3	1:A:936:PRO:HD3	1.86	0.57
1:A:623:LYS:HG2	1:A:627:GLU:CG	2.34	0.57
1:A:773:ASP:OD1	1:A:777:ASN:ND2	2.38	0.57
1:B:196:ILE:N	1:B:259:LEU:O	2.30	0.57
1:B:861:THR:HG1	1:B:863:VAL:HB	1.70	0.57
1:A:452:MET:HE3	1:A:817:ARG:NH2	2.19	0.57
1:B:545:ASP:C	1:B:547:LEU:H	2.12	0.57
1:A:234:ILE:HD12	1:A:234:ILE:O	2.05	0.57
1:A:255:HIS:HB2	1:A:257:TYR:CE1	2.40	0.57
1:A:664:ASN:O	1:A:665:TYR:HB2	2.04	0.57
1:A:783:GLY:O	1:A:785:MET:N	2.34	0.57
1:A:735:ILE:HG12	1:A:749:ALA:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:TYR:CZ	1:B:414:LEU:HB2	2.40	0.57
1:A:886:SER:O	1:A:890:LYS:HG3	2.04	0.56
1:B:320:ILE:HG23	1:B:343:LEU:HD22	1.86	0.56
1:B:451:SER:O	1:B:452:MET:CE	2.48	0.56
1:A:521:LYS:HG3	1:A:547:LEU:HD11	1.86	0.56
1:B:331:MET:HE3	1:B:332:PRO:HD2	1.87	0.56
1:A:281:ASP:HB3	1:A:285:GLU:H	1.70	0.56
1:A:781:LYS:HE2	1:A:973:LEU:HD13	1.87	0.56
1:B:176:ARG:O	1:B:197:SER:OG	2.22	0.56
1:B:1005:GLU:O	1:B:1009:LEU:HG	2.04	0.56
1:A:508:TYR:CE1	1:A:509:GLU:HG3	2.41	0.56
1:B:789:SER:O	1:B:793:THR:HG23	2.05	0.56
1:B:555:LEU:HD21	1:B:610:TRP:HB3	1.88	0.56
1:B:977:LYS:HZ3	1:B:1008:GLN:HA	1.69	0.56
1:B:312:LYS:NZ	1:B:476:THR:OG1	2.38	0.56
1:A:182:HIS:CB	1:A:191:ARG:HB2	2.35	0.56
1:A:219:VAL:HG22	1:A:261:ILE:HA	1.87	0.56
1:B:704:TYR:HB3	1:B:708:ASP:CB	2.36	0.56
1:A:182:HIS:O	1:A:190:PHE:HA	2.06	0.56
1:A:456:LYS:O	1:A:460:LYS:HG2	2.06	0.56
1:B:452:MET:SD	1:B:452:MET:C	2.87	0.56
1:B:992:GLU:N	1:B:992:GLU:OE1	2.38	0.56
1:A:479:TRP:HZ3	1:A:534:VAL:O	1.89	0.55
1:A:747:LYS:NZ	1:A:1021:LEU:HA	2.21	0.55
1:B:204:THR:OG1	1:B:206:ASN:OD1	2.18	0.55
1:A:515:ARG:NH2	1:A:696:MET:O	2.35	0.55
1:B:592:SER:OG	4:B:1113:NAG:H81	2.07	0.55
2:F:1:NAG:O6	2:F:2:NAG:C7	2.54	0.55
1:A:992:GLU:N	1:A:992:GLU:OE1	2.38	0.55
1:B:651:LEU:HD21	1:B:676:LYS:HA	1.89	0.55
1:B:332:PRO:HG3	1:B:416:LYS:HB3	1.88	0.55
1:B:748:ARG:HG3	1:B:751:ASP:CG	2.32	0.55
1:B:1005:GLU:HA	1:B:1008:GLN:OE1	2.07	0.55
1:A:623:LYS:HZ2	1:A:629:PHE:N	2.04	0.55
1:A:784:TYR:CZ	1:A:1018:LEU:HD21	2.41	0.55
1:B:455:ARG:CA	1:B:458:VAL:HG12	2.33	0.55
1:B:792:VAL:O	1:B:796:PHE:N	2.38	0.55
1:A:469:GLN:HB2	1:A:470:TRP:CE3	2.42	0.55
1:B:442:THR:O	1:B:458:VAL:HG23	2.06	0.55
1:B:951:LYS:HE3	1:B:955:LYS:HD3	1.89	0.55
1:A:262:GLU:C	1:A:262:GLU:CD	2.75	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:HIS:HA	1:B:573:VAL:HB	1.88	0.55
1:A:386:LYS:C	1:A:388:GLY:H	2.14	0.54
1:A:713:ILE:HD12	1:A:713:ILE:O	2.07	0.54
1:B:704:TYR:O	1:B:709:TRP:HZ3	1.90	0.54
1:B:861:THR:HG21	1:B:864:PHE:CG	2.41	0.54
1:B:884:ILE:HD12	1:B:885:GLY:H	1.71	0.54
1:A:228:GLN:OE1	1:A:229:GLU:N	2.33	0.54
1:A:433:TRP:NE1	1:A:469:GLN:HA	2.20	0.54
1:A:405:GLN:CG	1:A:407:TYR:H	2.15	0.54
1:B:468:HIS:O	1:B:473:ASN:ND2	2.40	0.54
1:B:661:GLU:C	1:B:687:VAL:HG22	2.31	0.54
1:B:881:TYR:O	1:B:890:LYS:HE2	2.06	0.54
1:A:281:ASP:OD1	1:A:282:GLU:N	2.38	0.54
1:B:281:ASP:CG	1:B:283:SER:H	2.15	0.54
1:B:411:GLN:CG	4:B:1112:NAG:H82	2.37	0.54
1:B:797:LYS:NZ	1:B:800:GLN:HG3	2.22	0.54
1:B:216:ILE:HA	1:B:263:TYR:HA	1.89	0.54
1:B:680:VAL:O	1:B:681:ILE:HD12	2.08	0.54
1:B:1009:LEU:O	1:B:1013:TRP:N	2.31	0.54
1:A:454:ASP:OD1	1:A:454:ASP:N	2.33	0.54
1:A:849:SER:O	1:A:852:THR:N	2.24	0.54
1:B:521:LYS:NZ	1:B:699:TYR:HH	1.99	0.54
1:B:214:HIS:HE1	1:B:300:ARG:O	1.91	0.54
1:B:564:SER:OG	1:B:565:GLU:N	2.40	0.54
1:B:797:LYS:NZ	1:B:800:GLN:O	2.40	0.54
1:B:859:VAL:O	1:B:861:THR:HA	2.08	0.54
1:A:446:ASP:C	1:A:446:ASP:OD1	2.51	0.54
1:A:564:SER:HB3	1:A:567:VAL:HG23	1.90	0.54
1:A:747:LYS:HE2	1:A:1021:LEU:HD23	1.89	0.54
1:A:992:GLU:HA	1:A:995:PHE:HB3	1.90	0.54
1:B:380:ILE:HG21	1:B:390:VAL:HB	1.89	0.54
1:B:503:LYS:HG3	1:B:503:LYS:O	2.08	0.54
1:B:1021:LEU:HD23	1:B:1024:TRP:HE1	1.73	0.54
1:B:189:THR:HG23	1:B:265:ALA:HA	1.90	0.54
1:B:255:HIS:HB2	1:B:257:TYR:CE1	2.43	0.54
1:B:401:LEU:O	1:B:405:GLN:HG3	2.08	0.54
1:B:521:LYS:HG3	1:B:547:LEU:CD1	2.24	0.54
1:B:825:GLU:CD	1:B:862:THR:HA	2.33	0.54
1:A:232:ALA:HB2	1:A:248:PRO:HD3	1.89	0.53
1:B:256:ASN:C	1:B:257:TYR:CD1	2.86	0.53
1:B:389:GLN:HG2	1:B:446:ASP:HB2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLY:HA3	1:A:685:GLU:CD	2.33	0.53
1:A:747:LYS:HZ1	1:A:1021:LEU:HA	1.73	0.53
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.89	0.53
1:B:720:PRO:HB2	1:B:728:ARG:HD3	1.91	0.53
1:A:191:ARG:CZ	1:A:320:ILE:HD13	2.39	0.53
1:B:495:TYR:O	1:B:499:GLU:HG3	2.07	0.53
1:B:516:PHE:HE2	1:B:767:GLU:HG3	1.74	0.53
1:A:182:HIS:CB	1:A:191:ARG:HG3	2.39	0.53
1:B:164:ALA:C	1:B:165:GLN:HG2	2.34	0.53
1:A:220:THR:HG23	1:A:221:PHE:N	2.20	0.53
1:B:183:PRO:HB3	1:B:190:PHE:HB3	1.90	0.53
1:B:651:LEU:HD11	1:B:677:LYS:N	2.24	0.53
1:B:825:GLU:HG2	1:B:862:THR:OG1	2.08	0.53
1:A:179:LEU:HD21	1:A:181:LEU:HD11	1.91	0.53
1:A:366:MET:SD	1:A:381:TYR:HB3	2.49	0.53
1:A:534:VAL:O	1:A:535:GLN:HG3	2.09	0.53
1:A:802:GLN:O	1:A:806:GLN:HG2	2.08	0.53
1:B:886:SER:O	1:B:890:LYS:HB2	2.09	0.53
1:A:331:MET:HG3	1:A:351:SER:HA	1.90	0.53
1:B:521:LYS:HD2	1:B:522:ASP:HB2	1.90	0.53
1:B:955:LYS:HD2	1:B:955:LYS:N	2.24	0.53
1:A:358:LEU:HD11	1:A:473:ASN:HA	1.91	0.53
1:B:195:THR:HA	1:B:260:LYS:HA	1.89	0.52
1:B:518:THR:O	1:B:521:LYS:HE3	2.09	0.52
1:B:984:GLN:HG3	1:B:1004:LEU:HD22	1.91	0.52
1:A:396:THR:HA	1:A:399:LYS:HZ2	1.73	0.52
1:A:881:TYR:CE1	1:A:890:LYS:HB3	2.44	0.52
1:A:657:SER:HB2	1:A:694:ILE:HG13	1.90	0.52
1:B:234:ILE:O	1:B:235:LEU:HD23	2.08	0.52
1:B:538:GLU:O	1:B:541:GLU:HG2	2.09	0.52
1:A:217:SER:HB2	1:A:262:GLU:CD	2.33	0.52
1:B:796:PHE:CD1	1:B:832:LEU:HD13	2.44	0.52
1:B:976:THR:C	1:B:1011:ILE:HD11	2.35	0.52
1:A:320:ILE:HG23	1:A:344:VAL:O	2.09	0.52
1:B:401:LEU:HG	1:B:405:GLN:NE2	2.19	0.52
1:B:762:THR:HG21	1:B:815:SER:O	2.09	0.52
1:B:714:HIS:O	1:B:718:ILE:HG23	2.09	0.52
1:B:748:ARG:NH1	1:B:750:PHE:O	2.42	0.52
1:A:782:LEU:HD11	1:A:1014:MET:HG3	1.91	0.52
1:B:295:GLU:OE2	1:B:544:PHE:CZ	2.63	0.52
1:A:801:ASN:O	1:A:805:GLN:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HD11	1:B:329:SER:HB2	1.91	0.52
1:B:1012:GLN:O	1:B:1015:GLU:HG3	2.10	0.52
1:B:443:LEU:HA	1:B:458:VAL:HG23	1.91	0.52
1:A:859:VAL:O	1:A:863:VAL:HG23	2.11	0.51
1:B:630:ILE:HG21	1:B:656:LEU:HD11	1.92	0.51
1:A:168:LEU:HD13	1:A:306:PHE:HD1	1.76	0.51
1:A:394:LEU:O	1:A:398:VAL:HG23	2.09	0.51
1:A:796:PHE:HB2	1:A:832:LEU:HD13	1.93	0.51
1:B:626:LYS:HE2	1:B:684:THR:O	2.10	0.51
1:B:747:LYS:O	1:B:748:ARG:HB2	2.09	0.51
1:A:628:LEU:HD11	1:A:690:VAL:HG21	1.92	0.51
1:B:322:ASP:OD1	1:B:323:GLU:N	2.42	0.51
1:B:376:THR:HA	1:B:415:LYS:O	2.10	0.51
1:A:521:LYS:HG3	1:A:547:LEU:HD12	1.92	0.51
1:A:840:MET:HE1	1:A:867:GLY:HA2	1.93	0.51
1:B:1012:GLN:O	1:B:1013:TRP:C	2.53	0.51
1:A:320:ILE:HG13	1:A:345:GLN:CB	2.40	0.51
1:B:630:ILE:HG22	1:B:674:LEU:HD22	1.92	0.51
1:A:376:THR:HG21	1:A:412:TYR:CD2	2.45	0.51
1:A:452:MET:HE1	1:A:455:ARG:NH1	2.26	0.51
1:A:521:LYS:HE3	1:A:547:LEU:HD13	1.92	0.51
1:B:748:ARG:CB	1:B:751:ASP:H	2.15	0.51
1:B:761:HIS:O	1:B:764:PRO:HD2	2.10	0.51
1:B:861:THR:HG22	1:B:892:LYS:CD	2.40	0.51
1:A:403:PHE:CB	1:A:501:ILE:HD11	2.40	0.51
1:B:205:TRP:CZ3	1:B:249:GLU:HA	2.45	0.51
1:A:747:LYS:HE3	1:A:1019:LYS:CE	2.36	0.51
1:A:747:LYS:HZ3	1:A:1024:TRP:HE3	1.59	0.51
1:A:1017:ASN:HA	1:A:1019:LYS:HG3	1.92	0.51
1:B:472:GLY:HA2	1:B:486:ASN:OD1	2.10	0.51
1:A:457:LEU:O	1:A:461:ILE:HG13	2.11	0.51
1:A:634:ARG:CG	1:A:652:TRP:HH2	2.21	0.51
1:B:192:GLY:O	1:B:193:SER:HB2	2.10	0.51
1:B:596:VAL:HG21	1:B:601:LEU:HB2	1.92	0.51
1:B:321:ARG:HD2	1:B:322:ASP:O	2.11	0.51
1:B:561:THR:HG21	1:B:697:ASN:ND2	2.26	0.51
1:B:748:ARG:HD2	1:B:750:PHE:CA	2.41	0.51
1:A:207:ILE:HB	1:A:245:ILE:HG12	1.93	0.50
1:A:519:MET:HG2	1:A:699:TYR:CE1	2.46	0.50
1:B:469:GLN:HB2	1:B:470:TRP:CE3	2.46	0.50
1:B:596:VAL:CG1	1:B:597:THR:N	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:O	1:A:220:THR:OG1	2.26	0.50
1:A:220:THR:CG2	1:A:221:PHE:N	2.74	0.50
1:A:951:LYS:O	1:A:955:LYS:HD2	2.11	0.50
1:B:181:LEU:HB2	1:B:319:ILE:HG22	1.93	0.50
1:B:808:TRP:CZ2	1:B:824:LEU:HD22	2.46	0.50
1:B:925:SER:HB3	1:B:962:THR:HG23	1.93	0.50
1:A:980:LEU:HD22	1:A:1008:GLN:HG3	1.92	0.50
1:A:1024:TRP:CG	1:A:1025:LEU:N	2.76	0.50
1:B:748:ARG:NE	1:B:750:PHE:CB	2.74	0.50
1:B:786:ASP:N	1:B:786:ASP:OD1	2.45	0.50
1:A:245:ILE:HG13	1:A:245:ILE:O	2.11	0.50
1:A:445:TYR:CE1	1:A:450:SER:HB2	2.46	0.50
1:A:997:LEU:HB3	1:A:999:CYS:SG	2.52	0.50
1:B:1012:GLN:HA	1:B:1015:GLU:HG3	1.94	0.50
1:A:180:SER:HB3	1:A:318:LYS:HE3	1.93	0.50
1:B:160:LEU:HD12	1:B:161:PHE:H	1.76	0.50
1:B:773:ASP:HA	1:B:776:TYR:HB3	1.93	0.50
1:A:673:LEU:O	1:A:673:LEU:HD23	2.11	0.50
1:A:696:MET:SD	1:A:730:ASN:ND2	2.85	0.50
1:A:874:TRP:CD2	1:A:905:LYS:HD3	2.47	0.50
1:B:617:PRO:HB3	1:B:652:TRP:CE3	2.47	0.50
1:B:1007:ILE:HG22	1:B:1011:ILE:HD12	1.93	0.50
1:A:623:LYS:HG2	1:A:627:GLU:HG3	1.93	0.50
1:A:887:GLU:HA	1:A:890:LYS:HD2	1.92	0.50
1:B:281:ASP:CG	1:B:282:GLU:N	2.69	0.50
1:A:745:PRO:HG2	1:A:748:ARG:HG3	1.94	0.50
1:B:191:ARG:HG3	1:B:263:TYR:O	2.12	0.50
1:B:560:LYS:HE3	1:B:568:PHE:CG	2.46	0.50
1:A:809:THR:HB	1:A:811:GLU:HG2	1.94	0.49
1:A:1024:TRP:CZ3	1:A:1025:LEU:HD13	2.47	0.49
1:A:218:ARG:O	1:A:262:GLU:HB3	2.12	0.49
1:A:438:PHE:CD1	1:A:443:LEU:HD11	2.48	0.49
1:A:517:LYS:HE3	1:A:770:PHE:CZ	2.47	0.49
1:B:604:LYS:CD	1:B:607:MET:HG2	2.42	0.49
1:A:209:LEU:HG	1:A:305:CYS:C	2.38	0.49
1:A:220:THR:O	1:A:229:GLU:OE2	2.30	0.49
1:A:544:PHE:HA	1:A:549:TYR:OH	2.11	0.49
1:A:889:GLU:HA	1:A:892:LYS:HG3	1.95	0.49
1:B:748:ARG:NH2	1:B:794:ARG:CZ	2.75	0.49
1:B:802:GLN:O	1:B:806:GLN:HG2	2.11	0.49
1:B:1023:TRP:CZ3	1:B:1024:TRP:HB3	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HD11	1:A:381:TYR:CD2	2.47	0.49
1:B:432:ASN:HB2	1:B:435:LEU:O	2.12	0.49
1:B:512:LEU:HD22	1:B:726:LYS:HB2	1.95	0.49
1:B:735:ILE:HD13	1:B:752:LEU:HB2	1.93	0.49
1:A:205:TRP:CZ3	1:A:250:ALA:HB2	2.46	0.49
1:B:352:VAL:HG21	1:B:581:TYR:CE2	2.47	0.49
1:A:403:PHE:O	1:A:403:PHE:CG	2.65	0.49
1:A:549:TYR:N	1:A:549:TYR:CD1	2.80	0.49
1:B:746:LEU:HD22	1:B:1020:SER:HB2	1.94	0.49
1:B:315:PHE:N	1:B:351:SER:OG	2.46	0.49
1:B:385:GLU:N	1:B:385:GLU:OE1	2.43	0.49
1:B:704:TYR:HB3	1:B:708:ASP:HB2	1.94	0.49
1:B:934[B]:HIS:CD2	1:B:936:PRO:HD2	2.48	0.49
1:B:975:SER:C	1:B:1011:ILE:HG13	2.37	0.49
1:B:1012:GLN:CA	1:B:1015:GLU:HG3	2.43	0.49
1:B:367:LYS:HD3	1:B:384:PRO:HA	1.93	0.49
1:B:427:ALA:HB3	1:B:439:ARG:HG2	1.93	0.49
1:A:239:TYR:HD2	1:A:240:HIS:CE1	2.31	0.49
1:A:445:TYR:CE1	1:A:455:ARG:HG2	2.48	0.49
1:B:176:ARG:HB2	1:B:314:THR:OG1	2.12	0.49
1:B:575:TYR:HD2	1:B:576:LEU:HD12	1.77	0.49
1:B:860:MET:O	1:B:860:MET:HG2	2.12	0.49
1:A:331:MET:HE3	1:A:352:VAL:N	2.28	0.49
1:A:621:VAL:HG21	1:A:692:VAL:HG21	1.95	0.49
1:B:389:GLN:HB2	1:B:444:LEU:HB3	1.95	0.49
1:B:567:VAL:HG23	1:B:568:PHE:H	1.78	0.49
1:B:608:LYS:HG3	1:B:608:LYS:O	2.13	0.49
1:B:631:GLN:HG2	1:B:633:GLU:OE2	2.13	0.49
1:A:403:PHE:C	1:A:405:GLN:CG	2.86	0.48
1:A:412:TYR:CE2	1:A:417:LEU:HB2	2.48	0.48
1:A:817:ARG:HG2	1:A:820:ARG:HH21	1.77	0.48
1:B:857:THR:HG22	1:B:860:MET:HE3	1.95	0.48
1:B:578:ASN:ND2	4:B:1113:NAG:O7	2.46	0.48
1:A:279:TYR:HE2	1:A:383:VAL:HG21	1.77	0.48
1:A:613:GLN:OE1	1:A:650:TYR:HA	2.13	0.48
1:B:343:LEU:HD23	1:B:343:LEU:C	2.38	0.48
1:B:399:LYS:HE3	1:B:402:GLU:OE1	2.13	0.48
1:B:402:GLU:HA	1:B:405:GLN:OE1	2.13	0.48
1:A:957:PRO:HG2	1:A:960:SER:HB3	1.94	0.48
1:B:954:GLN:C	1:B:955:LYS:HD2	2.38	0.48
1:A:534:VAL:HG13	1:A:539:GLN:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LYS:HE3	1:A:699:TYR:HE2	1.78	0.48
1:A:742:GLY:O	1:A:744:VAL:N	2.46	0.48
1:B:567:VAL:CG2	1:B:568:PHE:N	2.76	0.48
1:B:708:ASP:O	1:B:711:ALA:HB3	2.14	0.48
1:B:713:ILE:HG22	1:B:717:LYS:NZ	2.28	0.48
1:B:977:LYS:CG	1:B:1011:ILE:HG21	2.44	0.48
1:B:1001:GLN:HA	1:B:1004:LEU:HD12	1.94	0.48
1:A:217:SER:H	1:A:262:GLU:CD	2.19	0.48
1:B:379:SER:OG	1:B:418:ASP:OD1	2.32	0.48
1:A:551:LYS:HE3	1:A:699:TYR:CE2	2.48	0.48
1:B:608:LYS:HZ3	1:B:613:GLN:HG3	1.78	0.48
1:A:256:ASN:OD1	1:A:256:ASN:N	2.44	0.48
1:A:470:TRP:H	1:A:470:TRP:HE3	1.62	0.48
1:A:713:ILE:CD1	1:A:752:LEU:HA	2.43	0.48
1:B:220:THR:O	1:B:259:LEU:HD12	2.13	0.48
1:B:1012:GLN:O	1:B:1015:GLU:N	2.47	0.48
1:A:386:LYS:C	1:A:388:GLY:N	2.72	0.48
1:B:367:LYS:HG2	1:B:387:ILE:CD1	2.41	0.48
1:B:160:LEU:HD12	1:B:161:PHE:N	2.29	0.47
1:B:606:MET:HE3	1:B:607:MET:SD	2.54	0.47
1:B:203:VAL:HG22	1:B:250:ALA:HB1	1.96	0.47
1:B:324:GLN:HG3	1:B:325:TYR:CD1	2.49	0.47
1:B:402:GLU:HA	1:B:405:GLN:CD	2.38	0.47
1:B:510:ASP:O	1:B:514:ALA:N	2.45	0.47
1:B:680:VAL:C	1:B:681:ILE:HD12	2.39	0.47
1:B:748:ARG:HG3	1:B:751:ASP:OD1	2.14	0.47
1:A:951:LYS:N	1:A:951:LYS:CD	2.77	0.47
1:A:964:GLN:CD	1:A:965:ASN:HB2	2.40	0.47
1:B:174:PRO:HD2	1:B:311:PHE:HD2	1.79	0.47
1:B:379:SER:OG	1:B:381:TYR:HE1	1.97	0.47
1:B:400:LEU:HG	1:B:502:PHE:HE1	1.80	0.47
1:B:945:VAL:HG21	1:B:970:SER:OG	2.13	0.47
1:B:324:GLN:HE21	1:B:325:TYR:HE1	1.60	0.47
1:B:408:PHE:O	1:B:410:ILE:N	2.43	0.47
1:B:518:THR:C	1:B:521:LYS:HE3	2.39	0.47
1:B:1009:LEU:O	1:B:1013:TRP:HB2	2.15	0.47
1:A:546:SER:O	1:A:550:PHE:HD2	1.97	0.47
1:A:594:ASN:O	1:A:600:THR:HG22	2.15	0.47
1:B:394:LEU:O	1:B:398:VAL:HG23	2.15	0.47
1:B:403:PHE:CD1	1:B:403:PHE:C	2.92	0.47
1:A:354:MET:HE3	1:A:359:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:MET:HB2	1:A:910:MET:HE3	1.73	0.47
1:B:536:SER:HB3	1:B:539:GLN:OE1	2.14	0.47
1:B:977:LYS:HZ1	1:B:1008:GLN:HG3	1.78	0.47
1:A:617:PRO:HB3	1:A:652:TRP:CE3	2.49	0.47
1:B:172:VAL:HG23	1:B:306:PHE:HE2	1.80	0.47
1:B:558:MET:HE1	1:B:610:TRP:CE2	2.50	0.47
1:B:691:LYS:NZ	1:B:693:ASN:O	2.47	0.47
1:B:861:THR:OG1	1:B:864:PHE:N	2.46	0.47
1:B:994:THR:HA	1:B:997:LEU:HD11	1.97	0.47
1:A:776:TYR:CD1	1:A:776:TYR:C	2.92	0.47
1:B:547:LEU:HA	1:B:547:LEU:HD12	1.62	0.47
1:B:994:THR:O	1:B:997:LEU:HD12	2.15	0.47
1:A:274:PHE:HD1	1:A:292:THR:HG22	1.80	0.47
1:B:572:VAL:HG13	1:B:576:LEU:HD13	1.96	0.47
1:A:222:MET:HG3	1:A:229:GLU:OE1	2.14	0.46
1:A:560:LYS:NZ	1:A:565:GLU:HB3	2.30	0.46
1:A:1016:LYS:HA	1:A:1016:LYS:CE	2.37	0.46
1:B:237:TYR:HE2	1:B:240:HIS:ND1	2.13	0.46
1:B:245:ILE:HD13	1:B:259:LEU:HD21	1.97	0.46
1:B:425:PHE:CD2	1:B:920:ARG:NH1	2.84	0.46
1:B:884:ILE:HG13	1:B:886:SER:H	1.79	0.46
1:A:1021:LEU:HD22	1:A:1025:LEU:HD22	1.97	0.46
1:B:462:ILE:O	1:B:466:LEU:HB2	2.16	0.46
1:B:620:THR:OG1	1:B:622:GLN:OE1	2.27	0.46
1:B:693:ASN:ND2	1:B:696:MET:HA	2.29	0.46
1:B:748:ARG:CZ	1:B:750:PHE:CB	2.92	0.46
1:A:389:GLN:O	1:A:389:GLN:HG3	2.16	0.46
1:A:807:THR:O	1:A:820:ARG:HD3	2.15	0.46
1:B:191:ARG:NE	1:B:263:TYR:CD2	2.83	0.46
1:B:312:LYS:HG2	1:B:353:LYS:HB3	1.97	0.46
1:B:484:TRP:HZ2	1:B:531:SER:HB2	1.80	0.46
1:A:580:SER:O	1:A:581[B]:TYR:CG	2.68	0.46
1:A:660:THR:CB	1:A:687:VAL:HG11	2.41	0.46
1:B:688:LEU:O	1:B:711:ALA:HB1	2.16	0.46
1:B:718:ILE:HG13	1:B:719:ASN:N	2.29	0.46
1:B:718:ILE:HG13	1:B:719:ASN:H	1.80	0.46
1:A:233:GLU:O	1:A:246:VAL:HG22	2.14	0.46
1:A:623:LYS:HG2	1:A:627:GLU:OE2	2.16	0.46
1:A:869:LYS:NZ	1:A:899:SER:O	2.39	0.46
1:B:715:GLN:CD	1:B:718:ILE:HG12	2.39	0.46
1:A:310:ALA:HA	1:A:583:SER:OG	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:THR:O	1:A:584:ILE:HG13	2.16	0.46
1:B:257:TYR:CD1	1:B:257:TYR:N	2.84	0.46
1:B:405:GLN:HA	1:B:470:TRP:CZ2	2.51	0.46
1:A:320:ILE:HD11	1:A:345:GLN:OE1	2.16	0.46
1:A:747:LYS:NZ	1:A:1020:SER:O	2.49	0.46
1:B:460:LYS:HD2	1:B:494:GLU:CB	2.45	0.46
1:A:175:LEU:HD12	1:A:175:LEU:O	2.16	0.46
1:A:623:LYS:CD	1:A:628:LEU:HA	2.42	0.46
1:A:906:LEU:HD22	1:A:931:VAL:HG22	1.97	0.46
1:B:804:GLN:OE1	1:B:805:GLN:HG3	2.16	0.46
1:A:604:LYS:HA	1:A:604:LYS:HD3	1.73	0.46
1:A:951:LYS:HB3	1:A:955:LYS:NZ	2.31	0.46
1:A:331:MET:HE3	1:A:351:SER:HA	1.98	0.45
1:B:194:VAL:O	1:B:260:LYS:HA	2.16	0.45
1:B:233:GLU:OE1	1:B:234:ILE:N	2.49	0.45
1:B:452:MET:HE3	1:B:455:ARG:CG	2.28	0.45
1:B:715:GLN:HA	1:B:718:ILE:HG12	1.98	0.45
1:B:748:ARG:CZ	1:B:1024:TRP:HZ3	2.29	0.45
1:B:960:SER:O	1:B:963:ILE:HG22	2.16	0.45
1:B:977:LYS:HE2	1:B:1011:ILE:HB	1.98	0.45
1:B:994:THR:HA	1:B:997:LEU:CD1	2.46	0.45
1:A:630:ILE:HG21	1:A:656:LEU:CD1	2.46	0.45
1:B:179:LEU:HA	1:B:193:SER:O	2.16	0.45
1:B:423:PRO:HA	1:B:440:GLU:OE1	2.16	0.45
1:B:559:LEU:HD23	1:B:568:PHE:CE2	2.48	0.45
1:B:595:GLU:O	1:B:596:VAL:O	2.33	0.45
1:B:601:LEU:HD12	1:B:601:LEU:HA	1.71	0.45
1:B:861:THR:OG1	1:B:863:VAL:HB	2.16	0.45
1:B:916:GLY:HA2	1:B:919:PHE:O	2.16	0.45
1:A:236:GLU:HA	1:A:243:ILE:HA	1.98	0.45
1:A:387:ILE:O	1:A:390:VAL:HG22	2.16	0.45
1:A:623:LYS:HE3	1:A:628:LEU:HD12	1.97	0.45
1:A:886:SER:OG	1:A:889:GLU:HG3	2.16	0.45
1:B:214:HIS:CE1	1:B:300:ARG:O	2.69	0.45
1:B:341:ASP:OD1	1:B:342:GLY:N	2.49	0.45
1:B:372:ASP:OD1	1:B:372:ASP:N	2.41	0.45
1:B:387:ILE:HG23	1:B:390:VAL:HG21	1.99	0.45
1:B:590:TRP:HB3	1:B:604:LYS:HG3	1.99	0.45
1:A:410:ILE:HD11	1:A:577:HIS:CD2	2.52	0.45
1:B:521:LYS:CE	1:B:522:ASP:HB2	2.45	0.45
1:B:563:LEU:CG	1:B:567:VAL:HG21	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:PHE:CZ	1:A:990:GLN:NE2	2.84	0.45
1:B:271:TYR:OH	1:B:426:GLU:OE1	2.13	0.45
1:B:623:LYS:HE2	1:B:627:GLU:N	2.32	0.45
1:B:725:ASP:O	1:B:764:PRO:HG3	2.16	0.45
1:B:978:THR:OG1	1:B:979:HIS:N	2.48	0.45
1:B:996:ARG:HA	1:B:1001:GLN:OE1	2.16	0.45
1:B:1017:ASN:O	1:B:1021:LEU:HG	2.17	0.45
1:B:172:VAL:HG21	1:B:207:ILE:HG23	1.99	0.45
1:B:545:ASP:OD2	1:B:547:LEU:HB3	2.17	0.45
1:B:745:PRO:C	1:B:747:LYS:N	2.58	0.45
1:B:796:PHE:CE1	1:B:832:LEU:HB3	2.51	0.45
1:A:181:LEU:C	1:A:191:ARG:HE	2.25	0.45
1:A:211:SER:N	1:A:241:GLY:O	2.38	0.45
1:B:190:PHE:HD1	1:B:267:ILE:HG12	1.81	0.45
1:B:445:TYR:OH	1:B:447:SER:HA	2.16	0.45
1:B:466:LEU:O	1:B:469:GLN:HG2	2.17	0.45
1:A:360:ALA:HB2	1:A:432:ASN:OD1	2.17	0.45
1:A:495:TYR:HE1	1:A:510:ASP:HB2	1.82	0.45
1:A:556:LEU:O	1:A:560:LYS:HB3	2.17	0.45
1:A:653:HIS:HD2	1:A:675:ASP:CB	2.30	0.45
1:B:352:VAL:HG21	1:B:581:TYR:HE2	1.82	0.45
1:B:796:PHE:CG	1:B:832:LEU:HD13	2.52	0.45
1:B:949:TRP:O	1:B:953:VAL:HG13	2.16	0.45
1:B:1000:VAL:O	1:B:1004:LEU:HG	2.16	0.45
1:A:295:GLU:HB3	1:A:430:MET:SD	2.57	0.45
1:B:847:MET:HE3	1:B:847:MET:HB2	1.88	0.45
1:A:728:ARG:NH1	1:A:759:GLU:OE2	2.50	0.44
1:B:433:TRP:HE1	1:B:469:GLN:CA	2.22	0.44
1:B:460:LYS:NZ	1:B:491:THR:O	2.50	0.44
1:B:604:LYS:HD3	1:B:604:LYS:HA	1.70	0.44
1:B:606:MET:HG3	1:B:653:HIS:HB2	1.99	0.44
1:B:637:LEU:CD2	1:B:1009:LEU:HD22	2.35	0.44
1:A:368:ASN:HD22	1:A:369:LEU:N	2.15	0.44
1:A:1016:LYS:HD2	1:A:1016:LYS:N	2.30	0.44
1:B:320:ILE:C	1:B:343:LEU:HD21	2.42	0.44
1:B:367:LYS:HZ2	1:B:387:ILE:HG13	1.82	0.44
1:B:368:ASN:O	1:B:369:LEU:HD23	2.17	0.44
1:B:713:ILE:HG22	1:B:717:LYS:HZ2	1.80	0.44
1:A:163:TRP:HB2	1:A:208:ILE:HD13	1.98	0.44
1:A:320:ILE:HG13	1:A:345:GLN:HA	2.00	0.44
1:A:539:GLN:HA	1:A:542:GLU:CD	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:TYR:HA	1:A:910:MET:HE2	2.00	0.44
1:B:176:ARG:NE	1:B:350:GLU:OE1	2.50	0.44
1:B:177:TYR:CD2	1:B:196:ILE:HG12	2.52	0.44
1:B:412:TYR:HA	1:B:413:PRO:HD3	1.62	0.44
1:B:742:GLY:O	1:B:744:VAL:N	2.45	0.44
1:A:329:SER:OG	1:A:330:ASN:N	2.51	0.44
1:A:825:GLU:HB3	1:A:862:THR:OG1	2.18	0.44
1:A:961:TYR:O	1:A:964:GLN:OE1	2.35	0.44
1:B:203:VAL:HA	1:B:251:LEU:O	2.17	0.44
1:B:439:ARG:O	1:B:440:GLU:C	2.61	0.44
1:B:545:ASP:C	1:B:547:LEU:N	2.74	0.44
1:A:182:HIS:CA	1:A:191:ARG:HB2	2.46	0.44
1:A:438:PHE:CE2	1:A:461:ILE:HG22	2.51	0.44
1:B:609:THR:HG21	1:B:653:HIS:CE1	2.53	0.44
1:A:884:ILE:O	1:A:890:LYS:HE2	2.18	0.44
1:B:215:ASN:O	1:B:264:SER:N	2.51	0.44
1:B:486:ASN:ND2	1:B:486:ASN:H	2.14	0.44
1:B:500:LYS:HB2	1:B:500:LYS:HE3	1.70	0.44
1:A:163:TRP:CD2	1:A:169:PRO:HG3	2.52	0.44
1:A:182:HIS:CB	1:A:191:ARG:CZ	2.95	0.44
1:A:403:PHE:CG	1:A:501:ILE:HD11	2.53	0.44
1:A:616:PHE:HE2	1:A:701:ILE:HG13	1.82	0.44
1:B:912:SER:HB3	1:B:917:ASP:HB2	1.99	0.44
1:A:408:PHE:CD2	1:A:470:TRP:CG	3.05	0.44
1:B:913:SER:OG	1:B:924:LEU:HB2	2.18	0.44
1:A:455:ARG:HA	1:A:458:VAL:HG12	1.98	0.43
1:B:445:TYR:CZ	1:B:447:SER:HA	2.53	0.43
1:A:476:THR:HG22	1:A:477:MET:N	2.33	0.43
1:A:623:LYS:HE2	1:A:623:LYS:HB2	1.66	0.43
1:A:1021:LEU:HB3	1:A:1025:LEU:HD23	1.99	0.43
1:B:183:PRO:HA	1:B:190:PHE:CA	2.44	0.43
1:B:512:LEU:HD12	1:B:512:LEU:HA	1.75	0.43
1:B:685:GLU:OE1	1:B:685:GLU:N	2.51	0.43
1:B:861:THR:CG2	1:B:864:PHE:HB2	2.38	0.43
1:B:921:THR:HG22	1:B:956:PHE:HZ	1.84	0.43
1:B:1008:GLN:O	1:B:1012:GLN:HB3	2.18	0.43
1:A:281:ASP:CB	1:A:285:GLU:H	2.32	0.43
1:A:399:LYS:NZ	1:A:399:LYS:HB2	2.31	0.43
1:A:683:LEU:HD13	1:A:685:GLU:O	2.18	0.43
1:A:703:HIS:HE1	1:A:744:VAL:HG23	1.83	0.43
1:A:881:TYR:HE1	1:A:890:LYS:O	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:TRP:CZ2	1:B:744:VAL:HG22	2.53	0.43
1:B:797:LYS:HG2	1:B:800:GLN:CB	2.48	0.43
1:B:861:THR:HG22	1:B:892:LYS:CG	2.48	0.43
1:A:384:PRO:O	1:A:385:GLU:C	2.61	0.43
1:B:190:PHE:O	1:B:191:ARG:HG2	2.19	0.43
1:B:196:ILE:HG22	1:B:198:VAL:HG13	2.00	0.43
1:B:748:ARG:NH2	1:B:794:ARG:NH2	2.66	0.43
1:B:861:THR:O	1:B:861:THR:HG23	2.17	0.43
1:A:161:PHE:HE1	1:A:163:TRP:HB3	1.80	0.43
1:A:405:GLN:CB	1:A:406:ASN:HD22	2.07	0.43
1:A:647:ASP:OD1	1:A:648:THR:N	2.51	0.43
1:A:696:MET:CB	1:A:730:ASN:HD22	2.32	0.43
1:B:538:GLU:C	1:B:540:ILE:H	2.25	0.43
1:B:653:HIS:HB3	1:B:673:LEU:HD11	2.00	0.43
1:B:792:VAL:HG13	1:B:826:PHE:CZ	2.54	0.43
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.82	0.43
1:A:840:MET:HE2	1:A:866:VAL:HG12	2.01	0.43
1:B:501:ILE:HG13	1:B:502:PHE:CD1	2.54	0.43
1:A:163:TRP:CE3	1:A:169:PRO:HG3	2.53	0.43
1:A:963:ILE:HD12	1:A:963:ILE:HA	1.79	0.43
1:B:195:THR:HA	1:B:259:LEU:O	2.19	0.43
1:A:403:PHE:O	1:A:403:PHE:CD2	2.72	0.43
1:A:607:MET:O	1:A:611:THR:HG23	2.19	0.43
1:A:778:LEU:HD23	1:A:778:LEU:HA	1.87	0.43
1:A:1020:SER:C	1:A:1022:THR:N	2.74	0.43
1:B:514:ALA:O	1:B:518:THR:OG1	2.27	0.43
1:B:549:TYR:N	1:B:549:TYR:CD1	2.87	0.43
1:B:951:LYS:HD3	1:B:951:LYS:HA	1.86	0.43
1:A:422:ILE:HA	1:A:423:PRO:HD3	1.65	0.42
1:A:512:LEU:HD12	1:A:512:LEU:HA	1.52	0.42
1:B:468:HIS:HE2	1:B:487:GLU:CD	2.27	0.42
1:B:542:GLU:C	1:B:544:PHE:H	2.26	0.42
1:B:748:ARG:HH22	1:B:794:ARG:NE	2.17	0.42
1:A:315:PHE:O	1:A:350:GLU:HA	2.19	0.42
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.88	0.42
1:B:479:TRP:CG	1:B:480:TRP:N	2.87	0.42
1:B:727:ASP:OD1	1:B:728:ARG:N	2.52	0.42
1:A:511:PHE:CE2	1:A:557:LEU:HD22	2.43	0.42
1:A:626:LYS:N	1:A:686:GLU:OE2	2.52	0.42
1:A:653:HIS:HD2	1:A:675:ASP:HB2	1.85	0.42
1:A:783:GLY:O	1:A:785:MET:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:HB3	1:B:346:ASP:OD2	2.18	0.42
1:B:400:LEU:HD23	1:B:501:ILE:HD11	2.01	0.42
1:B:522:ASP:OD1	1:B:527:SER:OG	2.36	0.42
1:A:209:LEU:HD12	1:A:306:PHE:CE2	2.53	0.42
1:A:433:TRP:HE1	1:A:469:GLN:CB	2.32	0.42
1:A:440:GLU:CG	1:A:444:LEU:HD11	2.50	0.42
1:A:956:PHE:HA	1:A:957:PRO:HD2	1.94	0.42
1:B:367:LYS:NZ	1:B:387:ILE:HG13	2.34	0.42
1:B:425:PHE:C	1:B:427:ALA:H	2.27	0.42
1:A:480:TRP:CE3	1:A:483:LEU:HD12	2.54	0.42
1:A:495:TYR:CD1	1:A:511:PHE:HB2	2.54	0.42
1:A:788:ALA:O	1:A:791:LEU:HB3	2.20	0.42
1:A:965:ASN:O	1:A:969:GLY:N	2.40	0.42
1:B:542:GLU:C	1:B:544:PHE:N	2.78	0.42
1:B:596:VAL:HG13	1:B:597:THR:H	1.84	0.42
1:B:1012:GLN:O	1:B:1015:GLU:CG	2.67	0.42
1:A:376:THR:HG21	1:A:412:TYR:CE2	2.54	0.42
1:A:569:GLN:O	1:A:572:VAL:HB	2.19	0.42
1:B:978:THR:H	1:B:978:THR:HG23	1.59	0.42
1:A:215:ASN:H	4:A:1106:NAG:H81	1.83	0.42
1:A:320:ILE:HG13	1:A:345:GLN:HB2	2.00	0.42
1:A:619:VAL:HB	1:A:702:VAL:HG22	2.00	0.42
1:A:633:GLU:CG	1:A:634:ARG:N	2.83	0.42
1:A:1009:LEU:HD23	1:A:1009:LEU:HA	1.85	0.42
1:B:920:ARG:CZ	1:B:922:GLN:HE21	2.32	0.42
1:A:219:VAL:O	1:A:220:THR:CB	2.66	0.42
1:A:480:TRP:C	1:A:482:ASP:H	2.26	0.42
1:A:710:GLU:HA	1:A:713:ILE:CG2	2.48	0.42
1:A:742:GLY:C	1:A:744:VAL:H	2.28	0.42
1:B:452:MET:SD	1:B:455:ARG:CG	3.06	0.42
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.84	0.42
1:A:306:PHE:HB3	1:A:311:PHE:CD2	2.54	0.42
1:A:653:HIS:CD2	1:A:675:ASP:HB2	2.54	0.42
1:A:837:THR:O	1:A:838:THR:C	2.63	0.42
1:B:747:LYS:O	1:B:748:ARG:CB	2.67	0.42
1:B:980:LEU:O	1:B:984:GLN:NE2	2.52	0.42
1:A:367:LYS:CE	1:A:368:ASN:O	2.68	0.42
1:A:403:PHE:HB2	1:A:501:ILE:HD11	2.02	0.42
1:A:435:LEU:HA	1:A:435:LEU:HD12	1.84	0.42
1:B:419:LEU:HG	1:B:438:PHE:HE1	1.84	0.42
1:B:796:PHE:CZ	1:B:797:LYS:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:HD22	1:B:966:ILE:HD13	2.02	0.42
1:A:538:GLU:O	1:A:542:GLU:HB3	2.20	0.41
1:A:809:THR:HG21	1:A:811:GLU:OE2	2.19	0.41
1:B:977:LYS:NZ	1:B:1011:ILE:HD13	2.35	0.41
1:A:929:ARG:NH2	1:A:965:ASN:ND2	2.68	0.41
1:B:797:LYS:HB3	1:B:800:GLN:HB2	2.02	0.41
1:A:217:SER:OG	4:A:1104:NAG:H81	2.19	0.41
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.79	0.41
1:B:360:ALA:HB2	1:B:432:ASN:CG	2.45	0.41
1:B:383:VAL:CG2	1:B:384:PRO:HD2	2.50	0.41
1:B:628:LEU:O	1:B:630:ILE:HG12	2.21	0.41
1:B:738:LEU:O	1:B:741:LEU:N	2.54	0.41
1:B:1021:LEU:HD23	1:B:1024:TRP:NE1	2.34	0.41
1:A:791:LEU:HA	1:A:1025:LEU:HD11	2.01	0.41
1:B:608:LYS:HZ1	1:B:613:GLN:HG3	1.85	0.41
1:B:631:GLN:HG3	1:B:677:LYS:O	2.21	0.41
1:B:653:HIS:HA	1:B:675:ASP:HA	2.02	0.41
1:B:743:LYS:CB	1:B:744:VAL:HB	2.51	0.41
1:B:816:MET:HE2	1:B:816:MET:HB3	1.86	0.41
1:B:979:HIS:O	1:B:980:LEU:C	2.64	0.41
1:A:389:GLN:CD	1:A:446:ASP:HB2	2.44	0.41
1:A:472:GLY:HA2	1:A:477:MET:HE1	2.02	0.41
1:A:894:LEU:HD21	1:A:927:ILE:HG13	2.02	0.41
1:B:392:TYR:CE1	1:B:455:ARG:CZ	3.04	0.41
1:B:896:ALA:O	1:B:899:SER:N	2.41	0.41
1:A:431:GLU:CD	1:A:468:HIS:CG	2.98	0.41
1:B:485:LEU:HA	1:B:485:LEU:HD12	1.83	0.41
1:B:626:LYS:HG3	1:B:685:GLU:O	2.20	0.41
1:B:779:LEU:CB	1:B:788:ALA:HB2	2.50	0.41
1:B:872:LYS:HD2	1:B:875:SER:CB	2.49	0.41
1:A:578:ASN:ND2	1:A:579:HIS:HE1	2.19	0.41
1:B:399:LYS:HB2	1:B:399:LYS:HE3	1.89	0.41
1:B:452:MET:HG3	1:B:452:MET:O	2.20	0.41
1:B:538:GLU:C	1:B:540:ILE:N	2.78	0.41
1:B:689:TRP:HB3	1:B:715:GLN:HG3	2.03	0.41
1:A:169:PRO:HG2	1:A:208:ILE:HD12	2.03	0.41
1:A:441:GLU:OE2	1:A:887:GLU:HG2	2.20	0.41
1:A:825:GLU:O	1:A:829:THR:OG1	2.21	0.41
1:A:938:HIS:CE1	1:A:974:PHE:CE1	3.08	0.41
1:A:961:TYR:O	1:A:961:TYR:CG	2.73	0.41
1:B:210:HIS:ND1	1:B:307:ASP:HB3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:HG23	1:B:343:LEU:CD2	2.51	0.41
1:B:433:TRP:CE2	1:B:473:ASN:HB2	2.56	0.41
1:B:521:LYS:HB2	1:B:521:LYS:HE3	1.57	0.41
1:A:218:ARG:NH1	1:A:262:GLU:HB2	2.35	0.41
1:A:230:LYS:HE2	1:A:230:LYS:HB2	1.91	0.41
1:A:316:ILE:O	1:A:316:ILE:HG13	2.21	0.41
1:A:381:TYR:OH	2:D:1:NAG:H82	2.20	0.41
1:A:416:LYS:HD2	1:A:418:ASP:OD2	2.20	0.41
1:A:480:TRP:HE3	1:A:483:LEU:HD12	1.86	0.41
1:A:578:ASN:ND2	1:A:579:HIS:CE1	2.89	0.41
1:A:746:LEU:HD23	1:A:1021:LEU:HD21	2.02	0.41
1:B:207:ILE:HD13	1:B:259:LEU:HD22	2.03	0.41
1:B:408:PHE:HZ	1:B:493:MET:HG3	1.86	0.41
1:B:567:VAL:H	1:B:567:VAL:HG13	1.50	0.41
1:B:594:ASN:O	1:B:600:THR:N	2.47	0.41
1:B:609:THR:CG2	1:B:653:HIS:ND1	2.83	0.41
1:B:617:PRO:HA	1:B:633:GLU:O	2.21	0.41
1:B:784:TYR:N	1:B:784:TYR:CD1	2.89	0.41
1:A:226:SER:C	1:A:228:GLN:H	2.30	0.41
1:A:623:LYS:CE	1:A:628:LEU:HD12	2.51	0.41
1:A:696:MET:HB2	1:A:730:ASN:HD22	1.86	0.41
1:A:846:TRP:CD1	1:A:855:LEU:HG	2.56	0.41
1:B:387:ILE:HG21	1:B:387:ILE:HD13	1.67	0.41
1:B:404:PHE:CE1	1:B:497:SER:HB3	2.56	0.41
1:B:456:LYS:HE3	1:B:818:GLU:OE2	2.20	0.41
1:B:623:LYS:HE2	1:B:627:GLU:CB	2.51	0.41
1:B:845:ASP:O	1:B:848:ALA:HB3	2.21	0.41
1:A:270:SER:O	1:A:271:TYR:CG	2.73	0.40
1:A:321:ARG:H	1:A:321:ARG:HG3	1.70	0.40
1:A:405:GLN:HG3	1:A:406:ASN:CA	2.48	0.40
1:A:657:SER:HB2	1:A:694:ILE:CG1	2.51	0.40
1:A:752:LEU:O	1:A:755:TYR:HB3	2.21	0.40
1:A:279:TYR:CE2	1:A:383:VAL:HG21	2.55	0.40
1:A:811:GLU:O	1:A:820:ARG:NH2	2.48	0.40
1:A:992:GLU:O	1:A:996:ARG:HG3	2.21	0.40
1:B:817:ARG:NE	1:B:858:ASP:OD2	2.54	0.40
1:B:980:LEU:HD22	1:B:1008:GLN:HG3	2.03	0.40
1:A:214:HIS:CE1	1:A:304:PRO:HD3	2.55	0.40
1:A:841:LYS:HE3	1:A:841:LYS:HB3	1.63	0.40
1:A:849:SER:C	1:A:851:GLY:N	2.79	0.40
1:B:333:LYS:NZ	1:B:346:ASP:CG	2.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:MET:HG3	1:A:876:PHE:CG	2.57	0.40
1:A:877:LEU:HD22	1:A:893:ILE:HG12	2.04	0.40
1:B:420:VAL:HG13	1:B:437:THR:HG22	2.03	0.40
1:B:482:ASP:OD1	1:B:482:ASP:C	2.65	0.40
1:B:569:GLN:O	1:B:573:VAL:HG23	2.21	0.40
1:B:608:LYS:CD	1:B:612:LEU:H	2.32	0.40
1:B:797:LYS:HB3	1:B:800:GLN:OE1	2.22	0.40
1:A:352:VAL:HG22	1:A:353:LYS:H	1.86	0.40
1:B:191:ARG:HA	1:B:191:ARG:HD3	1.19	0.40
1:B:455:ARG:O	1:B:456:LYS:C	2.64	0.40
1:B:509:GLU:HG2	1:B:763:ALA:HB2	2.02	0.40
1:B:520:LYS:HD2	1:B:737:GLU:OE2	2.22	0.40
1:B:738:LEU:C	1:B:743:LYS:CB	2.94	0.40
1:B:748:ARG:HD2	1:B:751:ASP:N	2.37	0.40
1:B:753:ILE:HA	1:B:753:ILE:HD12	1.83	0.40
1:B:943:ASP:O	1:B:947:GLU:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:CD	2:F:2:NAG:O7[1_554]	1.77	0.43

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	858/912 (94%)	760 (89%)	84 (10%)	14 (2%)	7	29
1	B	844/912 (92%)	743 (88%)	74 (9%)	27 (3%)	3	17
All	All	1702/1824 (93%)	1503 (88%)	158 (9%)	41 (2%)	4	22

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ALA
1	A	270	SER
1	A	284	ASN
1	A	626	LYS
1	A	627	GLU
1	A	638	ASN
1	A	664	ASN
1	A	718	ILE
1	A	743	LYS
1	A	1020	SER
1	B	265	ALA
1	B	409	GLU
1	B	536	SER
1	B	596	VAL
1	B	670	SER
1	B	743	LYS
1	B	744	VAL
1	B	746	LEU
1	B	748	ARG
1	B	861	THR
1	B	1015	GLU
1	A	385	GLU
1	B	193	SER
1	B	213	GLY
1	B	373	VAL
1	B	521	LYS
1	B	1013	TRP
1	A	599	GLN
1	A	1019	LYS
1	B	223	SER
1	B	599	GLN
1	A	663	ARG
1	B	600	THR
1	B	535	GLN
1	B	627	GLU
1	B	628	LEU
1	B	1012	GLN
1	B	507	SER
1	B	719	ASN
1	B	1022	THR
1	B	296	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	756/813 (93%)	710 (94%)	46 (6%)	17	43
1	B	736/813 (90%)	683 (93%)	53 (7%)	13	39
All	All	1492/1626 (92%)	1393 (93%)	99 (7%)	15	41

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ILE
1	A	220	THR
1	A	228	GLN
1	A	256	ASN
1	A	262	GLU
1	A	282	GLU
1	A	368	ASN
1	A	373	VAL
1	A	377	LEU
1	A	420	VAL
1	A	433	TRP
1	A	454	ASP
1	A	455	ARG
1	A	466	LEU
1	A	477	MET
1	A	500	LYS
1	A	530	ILE
1	A	560	LYS
1	A	579	HIS
1	A	623	LYS
1	A	631	GLN
1	A	634	ARG
1	A	639	MET
1	A	657	SER
1	A	664	ASN
1	A	673	LEU
1	A	677	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	690	VAL
1	A	710	GLU
1	A	713	ILE
1	A	743	LYS
1	A	744	VAL
1	A	748	ARG
1	A	755	TYR
1	A	762	THR
1	A	773	ASP
1	A	790	ARG
1	A	809	THR
1	A	821	SER
1	A	884	ILE
1	A	889	GLU
1	A	923	LYS
1	A	962	THR
1	A	984	GLN
1	A	990	GLN
1	A	1019	LYS
1	B	176	ARG
1	B	191	ARG
1	B	195	THR
1	B	219	VAL
1	B	233	GLU
1	B	252	LEU
1	B	262	GLU
1	B	295	GLU
1	B	312	LYS
1	B	316	ILE
1	B	323	GLU
1	B	333	LYS
1	B	334	LYS
1	B	338	VAL
1	B	387	ILE
1	B	405	GLN
1	B	420	VAL
1	B	426	GLU
1	B	431	GLU
1	B	433	TRP
1	B	457	LEU
1	B	486	ASN
1	B	500	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	503	LYS
1	B	504	GLU
1	B	521	LYS
1	B	530	ILE
1	B	535	GLN
1	B	549	TYR
1	B	567	VAL
1	B	596	VAL
1	B	614	LYS
1	B	622	GLN
1	B	623	LYS
1	B	666	SER
1	B	673	LEU
1	B	682	ASN
1	B	687	VAL
1	B	690	VAL
1	B	744	VAL
1	B	746	LEU
1	B	753	ILE
1	B	758	ASN
1	B	773	ASP
1	B	794	ARG
1	B	861	THR
1	B	872	LYS
1	B	923	LYS
1	B	929	ARG
1	B	951	LYS
1	B	953	VAL
1	B	984	GLN
1	B	992	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	405	GLN
1	A	406	ASN
1	A	525	ASN
1	A	577	HIS
1	A	579	HIS
1	A	632	GLN
1	A	664	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	730	ASN
1	A	733	ASN
1	A	734	ASN
1	A	761	HIS
1	A	831	ASN
1	A	853	GLN
1	B	165	GLN
1	B	255	HIS
1	B	324	GLN
1	B	406	ASN
1	B	411	GLN
1	B	432	ASN
1	B	528	HIS
1	B	715	GLN
1	B	733	ASN
1	B	761	HIS
1	B	918	ASN
1	B	922	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	1.12	1 (7%)	17,19,21	1.31	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.57	0
2	NAG	D	1	2,1	14,14,15	1.18	2 (14%)	17,19,21	1.05	1 (5%)
2	NAG	D	2	2	14,14,15	0.57	0	17,19,21	0.63	0
2	NAG	E	1	2,1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.51	0
2	NAG	F	1	2,1	14,14,15	1.92	4 (28%)	17,19,21	2.13	5 (29%)
2	NAG	F	2	2	14,14,15	0.35	0	17,19,21	0.56	0
2	NAG	G	1	2,1	14,14,15	0.95	2 (14%)	17,19,21	0.74	1 (5%)
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	5.39	1.59	1.52
2	D	1	NAG	O5-C1	-3.62	1.37	1.43
2	F	1	NAG	O5-C1	-2.81	1.39	1.43
2	G	1	NAG	C1-C2	2.67	1.56	1.52
2	C	1	NAG	C1-C2	2.63	1.55	1.52
2	F	1	NAG	C3-C2	2.32	1.57	1.52
2	F	1	NAG	C2-N2	2.29	1.50	1.46
2	G	1	NAG	O5-C1	2.27	1.47	1.43
2	D	1	NAG	C2-N2	-2.00	1.42	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	-5.68	104.58	112.19
2	F	1	NAG	C1-C2-N2	-4.44	103.44	110.43
2	D	1	NAG	C1-O5-C5	-3.38	107.65	112.19
2	C	1	NAG	O3-C3-C4	2.72	116.78	110.38
2	F	1	NAG	O5-C1-C2	-2.61	107.25	111.29
2	C	1	NAG	O5-C1-C2	-2.34	107.67	111.29
2	C	1	NAG	O5-C5-C6	-2.31	103.17	107.66
2	G	1	NAG	C1-O5-C5	2.29	115.25	112.19
2	F	1	NAG	O5-C5-C4	-2.11	105.70	110.83
2	F	1	NAG	C4-C3-C2	2.04	114.00	111.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

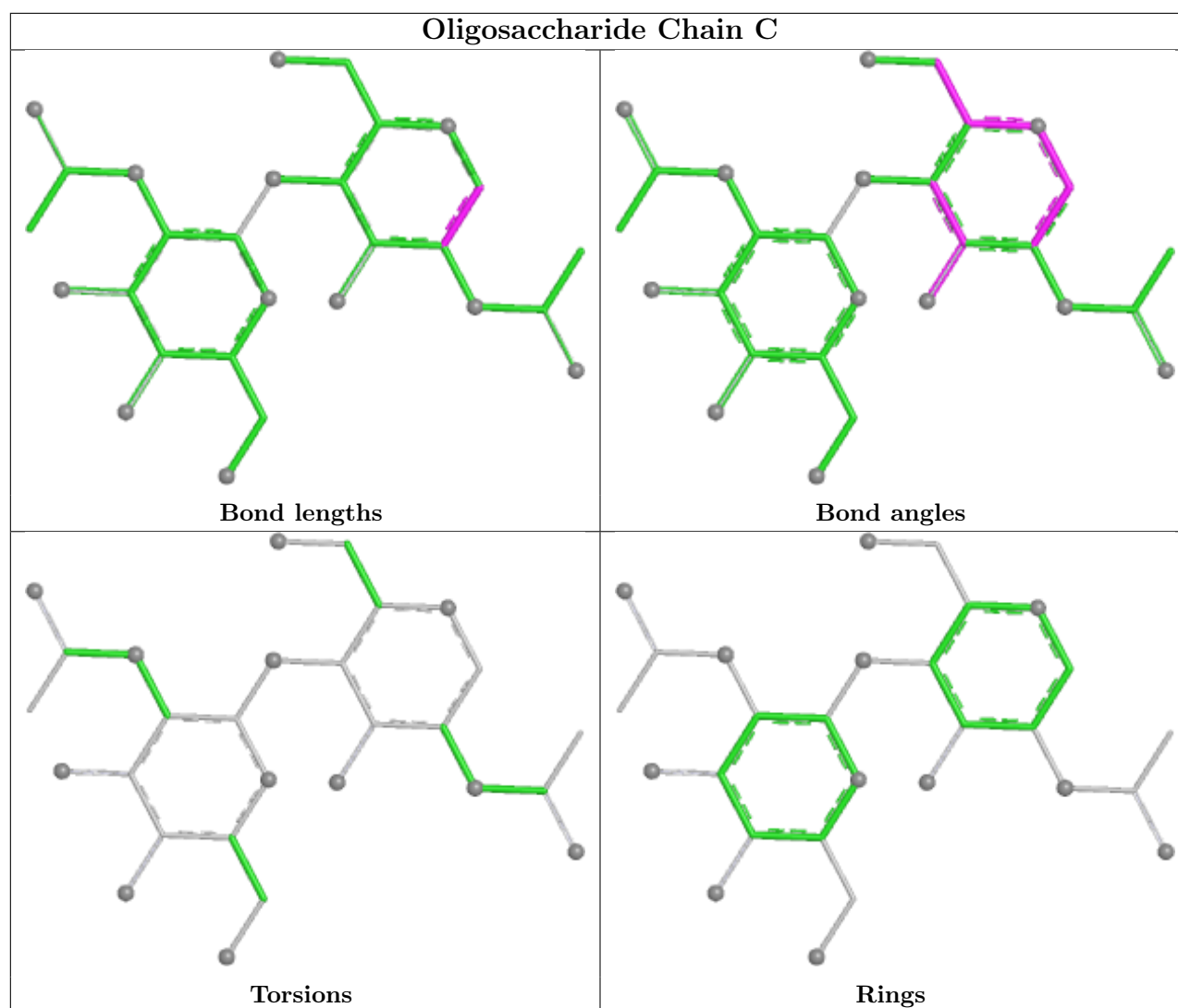
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7

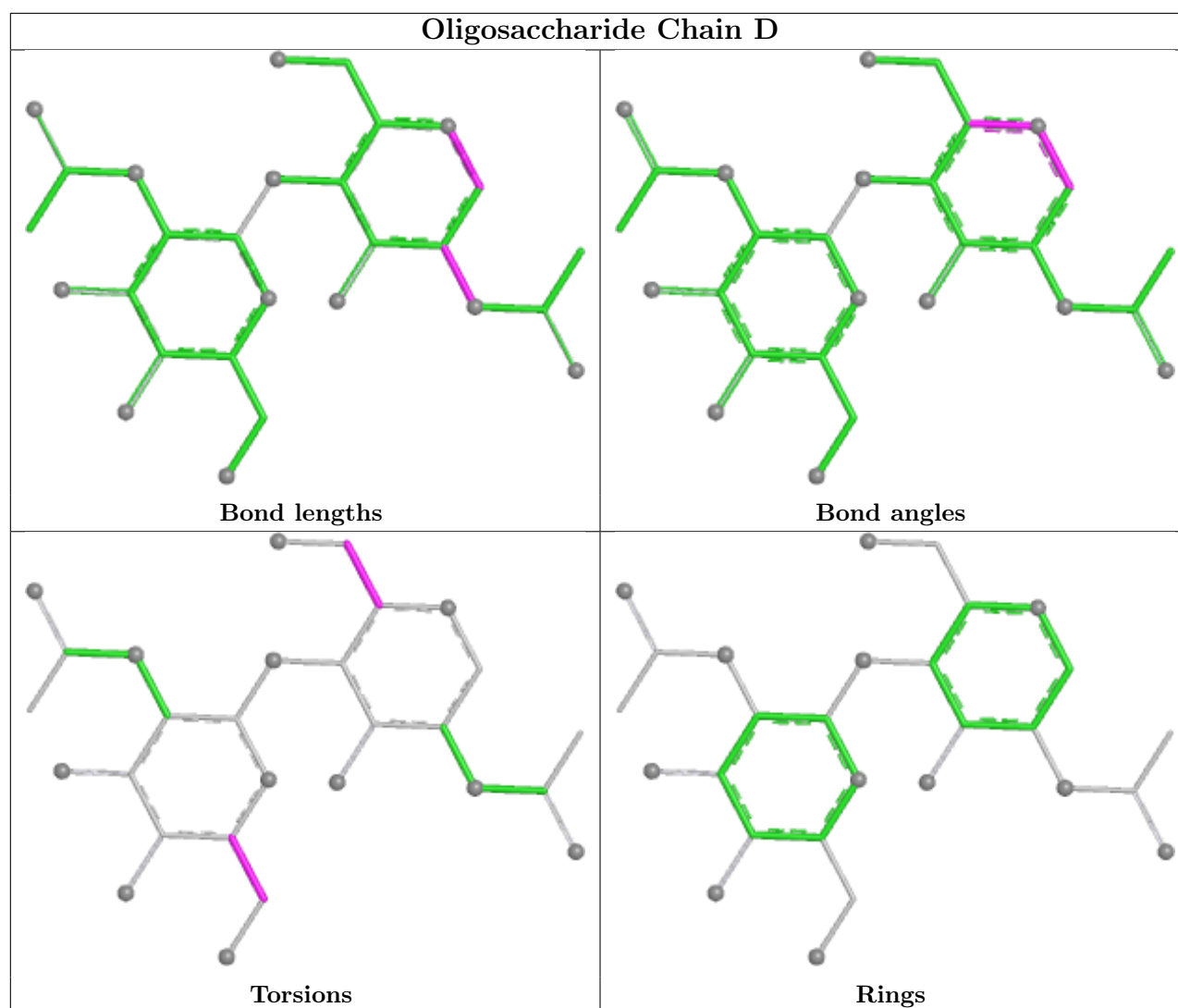
There are no ring outliers.

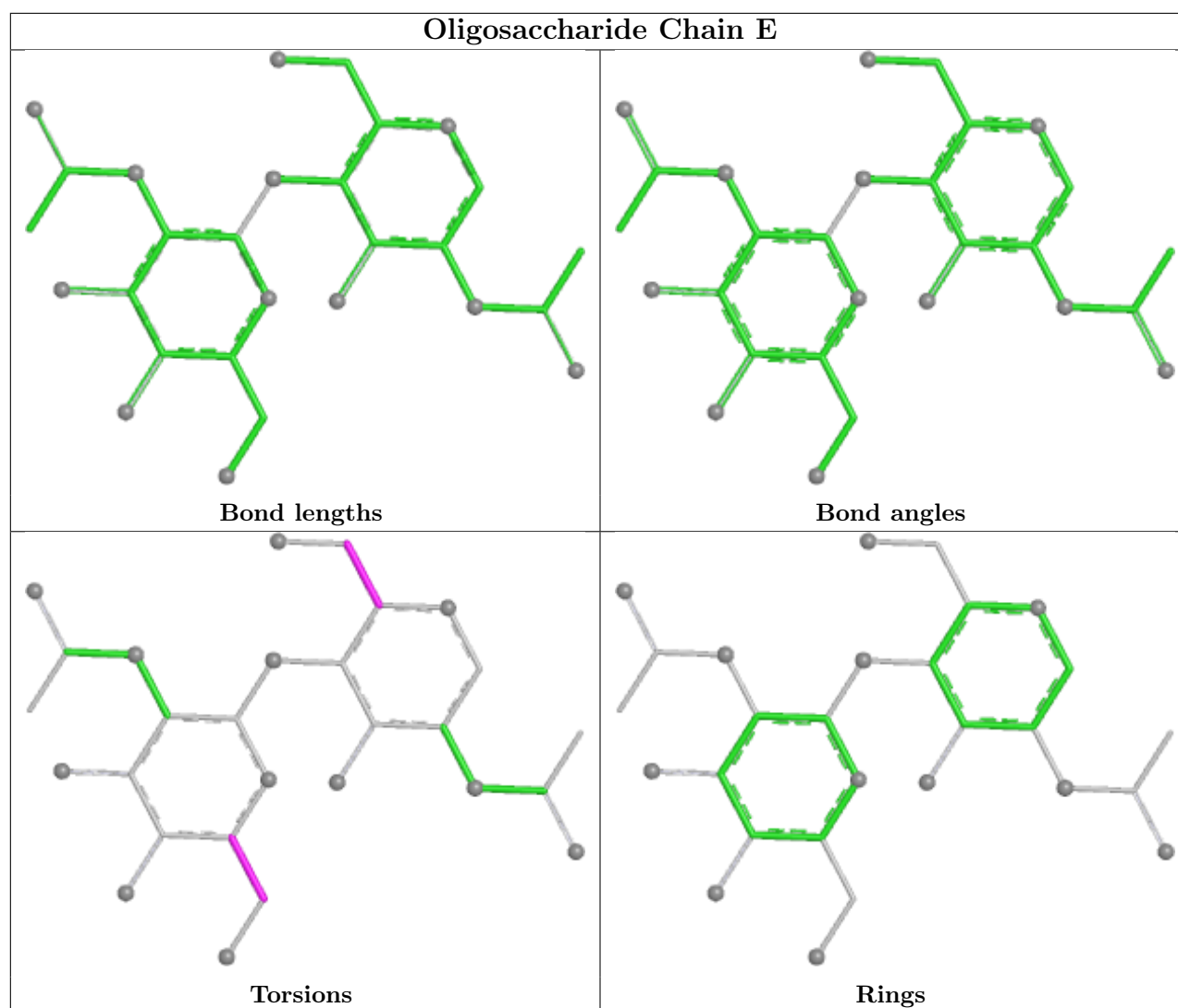
5 monomers are involved in 8 short contacts:

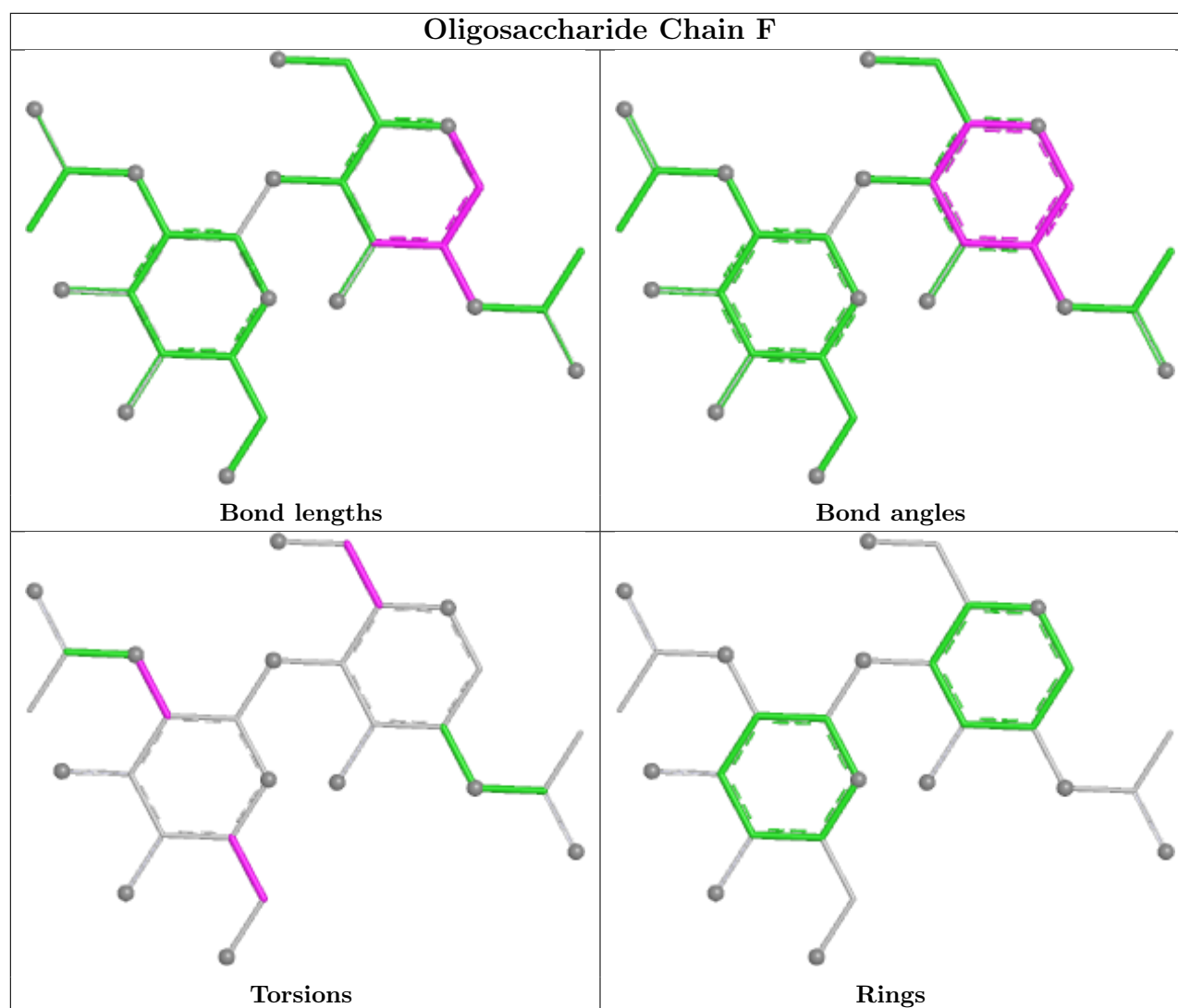
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	F	2	NAG	1	1
2	D	1	NAG	2	0
2	E	2	NAG	1	0
2	C	1	NAG	3	0

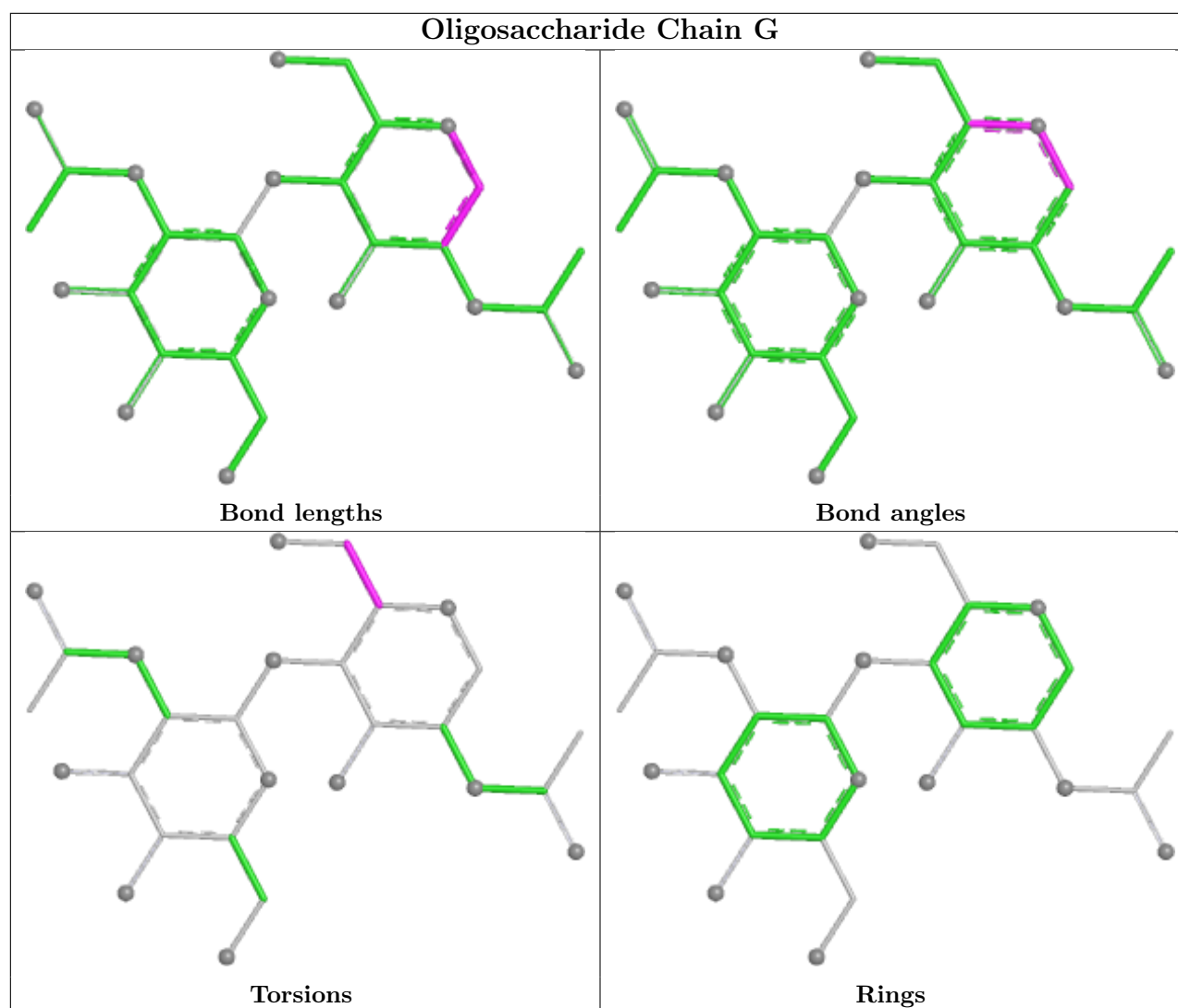
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	NAG	A	1109	1	14,14,15	0.48	0	17,19,21	1.09	1 (5%)
4	NAG	A	1106	1	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	A	1113	1	14,14,15	0.59	0	17,19,21	0.91	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1111	1	14,14,15	0.50	0	17,19,21	0.58	0
4	NAG	A	1112	1	14,14,15	1.23	1 (7%)	17,19,21	1.42	1 (5%)
4	NAG	B	1113	1	14,14,15	0.87	1 (7%)	17,19,21	0.60	0
4	NAG	A	1111	1	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
4	NAG	B	1104	1	14,14,15	0.98	1 (7%)	17,19,21	0.63	1 (5%)
4	NAG	B	1110	1	14,14,15	0.66	1 (7%)	17,19,21	0.65	0
4	NAG	B	1107	1	14,14,15	0.51	0	17,19,21	0.50	0
4	NAG	B	1112	1	14,14,15	0.34	0	17,19,21	0.61	0
4	NAG	A	1105	1	14,14,15	0.50	0	17,19,21	0.83	1 (5%)
4	NAG	A	1114	-	14,14,15	0.71	0	17,19,21	0.62	0
4	NAG	A	1110	1	14,14,15	0.75	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	A	1104	1	14,14,15	0.78	1 (7%)	17,19,21	0.87	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1109	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1106	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1113	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1111	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1112	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1113	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1111	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1104	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1110	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1107	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1112	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1105	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1114	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1110	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1104	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1112	NAG	O5-C1	4.45	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	NAG	C1-C2	2.62	1.55	1.52
4	A	1110	NAG	O5-C1	2.60	1.48	1.43
4	A	1104	NAG	O5-C1	2.58	1.48	1.43
4	B	1113	NAG	O5-C1	2.55	1.48	1.43
4	B	1110	NAG	O5-C1	2.08	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1112	NAG	C1-O5-C5	5.63	119.73	112.19
4	A	1109	NAG	C1-O5-C5	3.86	117.36	112.19
4	A	1110	NAG	C1-O5-C5	3.60	117.01	112.19
4	A	1104	NAG	C1-O5-C5	3.30	116.61	112.19
4	A	1113	NAG	C1-C2-N2	2.50	114.37	110.43
4	A	1105	NAG	C1-O5-C5	2.38	115.38	112.19
4	A	1111	NAG	C1-O5-C5	2.34	115.33	112.19
4	A	1113	NAG	C1-O5-C5	-2.26	109.16	112.19
4	B	1104	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1113	NAG	O5-C5-C6-O6
4	A	1112	NAG	O5-C5-C6-O6
4	B	1112	NAG	O5-C5-C6-O6
4	B	1111	NAG	C4-C5-C6-O6
4	B	1104	NAG	O5-C5-C6-O6
4	B	1111	NAG	O5-C5-C6-O6
4	A	1112	NAG	C4-C5-C6-O6
4	B	1113	NAG	C4-C5-C6-O6
4	A	1113	NAG	C4-C5-C6-O6
4	A	1113	NAG	O5-C5-C6-O6
4	B	1112	NAG	C4-C5-C6-O6
4	B	1104	NAG	C4-C5-C6-O6
4	A	1105	NAG	O5-C5-C6-O6
4	B	1110	NAG	O5-C5-C6-O6
4	A	1110	NAG	C4-C5-C6-O6
4	A	1105	NAG	C4-C5-C6-O6
4	A	1112	NAG	C1-C2-N2-C7
4	A	1105	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1106	NAG	2	0
4	A	1113	NAG	11	0
4	B	1113	NAG	3	0
4	B	1107	NAG	1	0
4	B	1112	NAG	2	0
4	A	1114	NAG	6	0
4	A	1104	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	860/912 (94%)	-0.66	1 (0%) 92 91	68, 116, 159, 184	2 (0%)
1	B	851/912 (93%)	-0.59	0 100 100	71, 141, 167, 189	1 (0%)
All	All	1711/1824 (93%)	-0.63	1 (0%) 92 91	68, 131, 162, 189	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	570[A]	HIS	2.7

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.

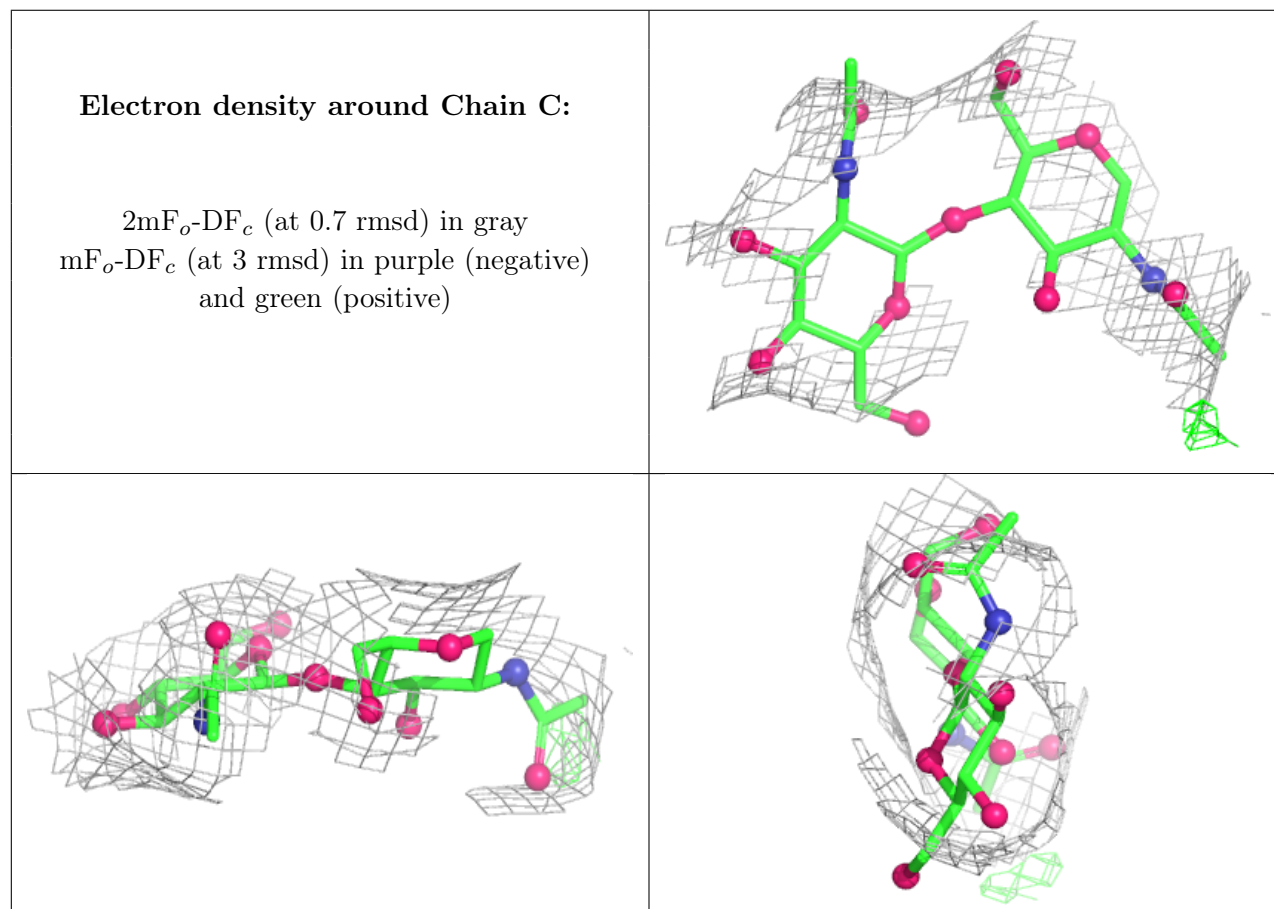
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.53	0.06	169,174,178,178	0
2	NAG	D	2	14/15	0.62	0.07	166,182,196,202	0
2	NAG	G	2	14/15	0.72	0.07	155,181,185,185	0
2	NAG	F	2	14/15	0.73	0.10	158,165,174,176	0
2	NAG	E	1	14/15	0.75	0.07	157,163,171,173	0
2	NAG	G	1	14/15	0.76	0.07	145,160,172,173	0
2	NAG	C	1	14/15	0.78	0.08	135,147,158,159	0
2	NAG	C	2	14/15	0.79	0.06	160,168,175,176	0

Continued on next page...

Continued from previous page...

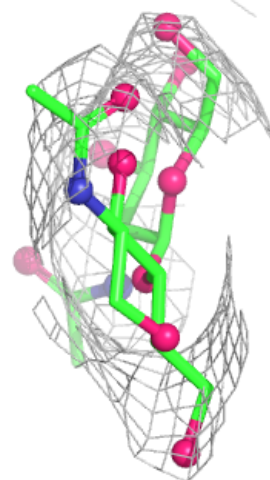
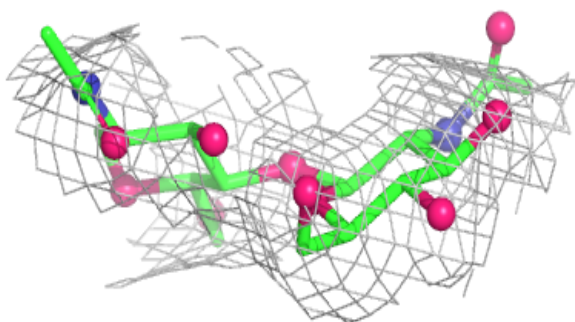
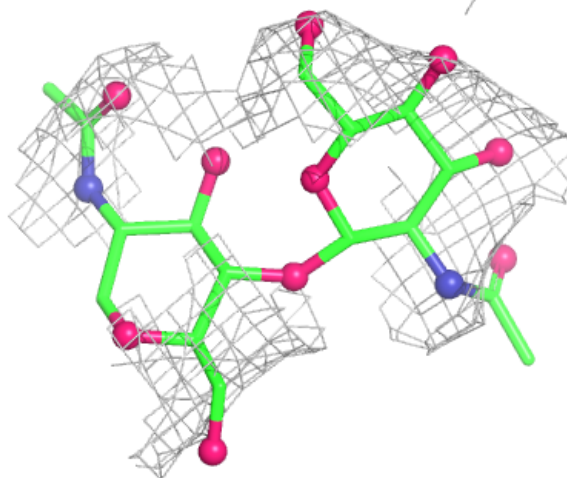
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	1	14/15	0.81	0.07	151,163,175,181	0
2	NAG	D	1	14/15	0.83	0.07	146,153,162,173	0

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.



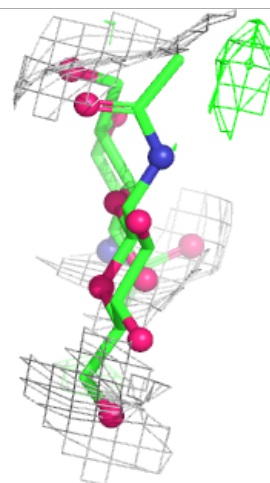
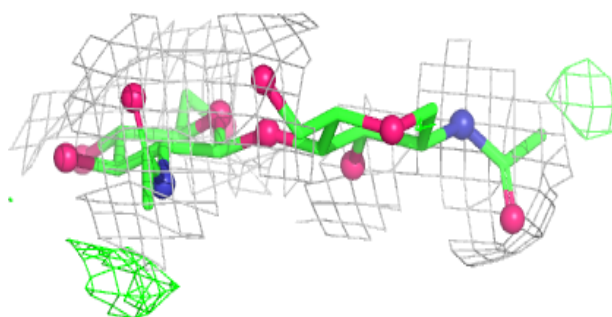
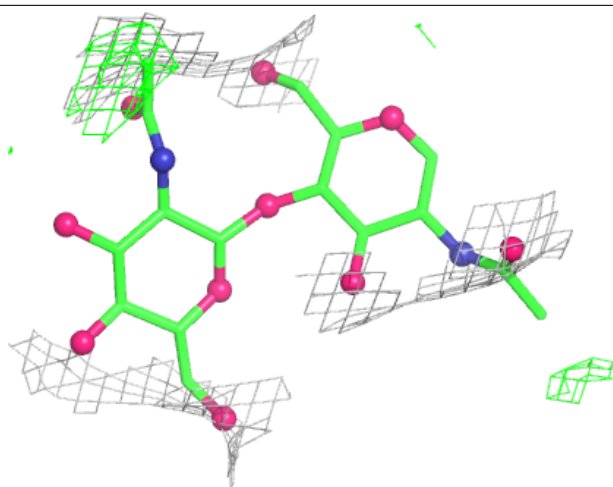
Electron density around Chain D:

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



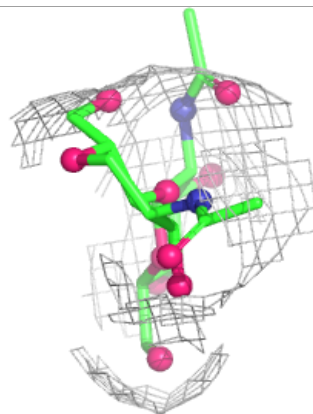
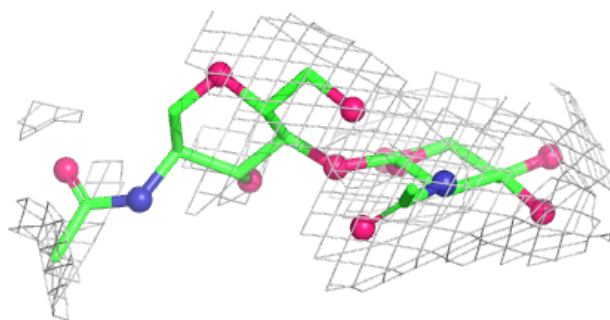
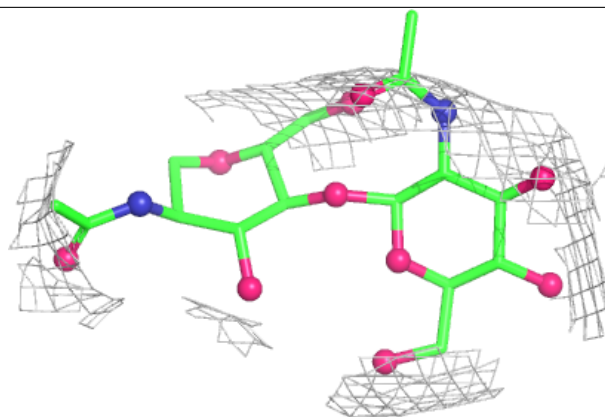
Electron density around Chain E:

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

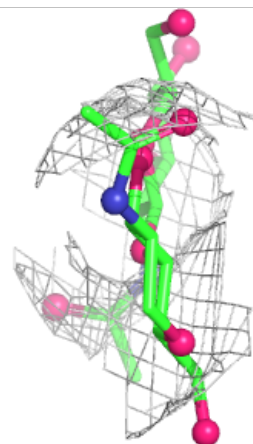
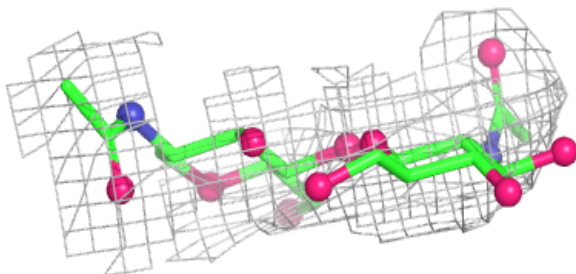
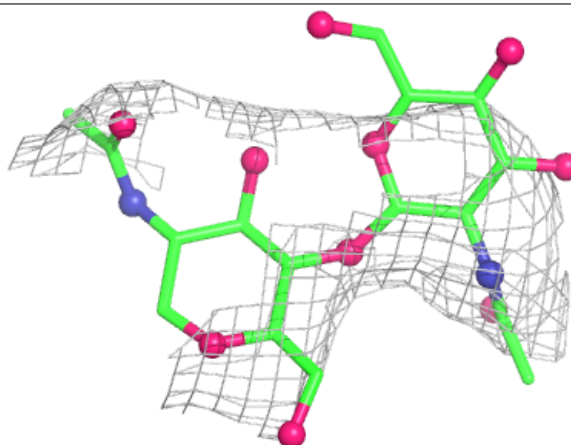


Electron density around Chain F:

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

**Electron density around Chain G:**

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1106	14/15	-0.11	0.14	146,164,179,183	0
4	NAG	A	1109	14/15	0.36	0.10	144,166,176,184	0
4	NAG	A	1112	14/15	0.37	0.08	157,172,178,180	0
4	NAG	B	1113	14/15	0.58	0.07	143,153,171,182	0
4	NAG	A	1104	14/15	0.61	0.07	160,165,175,176	0
4	NAG	B	1104	14/15	0.65	0.07	162,180,186,189	0
4	NAG	B	1111	14/15	0.66	0.13	150,163,166,167	0
4	NAG	B	1110	14/15	0.67	0.07	166,174,187,189	0
4	NAG	A	1114	14/15	0.69	0.08	123,136,144,170	0
4	NAG	A	1113	14/15	0.71	0.10	121,136,145,146	0
4	NAG	B	1112	14/15	0.71	0.07	166,184,188,195	0
4	NAG	A	1110	14/15	0.71	0.08	127,139,149,152	0
4	NAG	B	1107	14/15	0.72	0.07	144,155,160,163	0
4	NAG	A	1105	14/15	0.78	0.07	147,162,165,170	0
4	NAG	A	1111	14/15	0.85	0.07	114,132,145,145	0
3	ZN	A	1101	1/1	0.95	0.10	83,83,83,83	1
3	ZN	B	1101	1/1	0.98	0.04	143,143,143,143	0

6.5 Other polymers

There are no such residues in this entry.