



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:31 PM UTC

PDB ID : 1JV2 / pdb_00001jv2
Title : CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF IN-TEGRIN ALPHAVBETA3
Authors : Xiong, J.P.; Stehle, T.; Diefenbach, B.; Zhang, R.; Dunker, R.; Scott, D.; Joachimiak, A.; Goodman, S.L.; Arnaout, M.A.
Deposited on : 2001-08-28
Resolution : 3.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

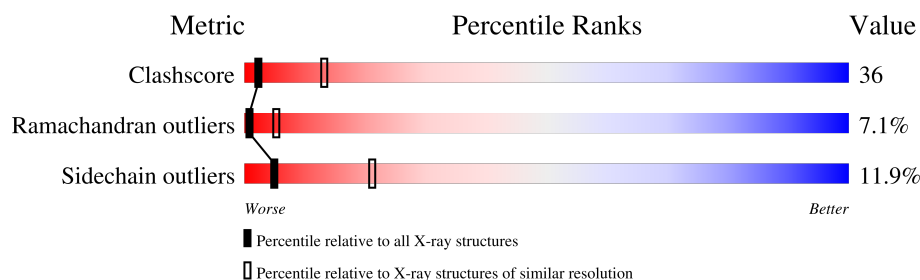
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

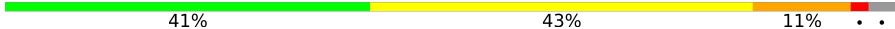
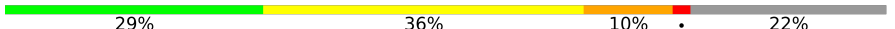
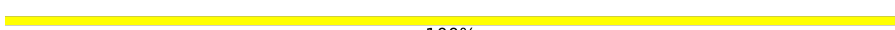
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	
2	B	692	
3	C	2	
3	D	2	
3	E	2	
3	G	2	
4	F	2	
4	H	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	I	2	 100%

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	NDG	I	2	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called INTEGRIN, ALPHA V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	927	Total	C	N	O	S	0	0	0
			7216	4568	1224	1389	35			

- Molecule 2 is a protein called PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	539	Total	C	N	O	S	0	0	0
			4182	2594	700	842	46			

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



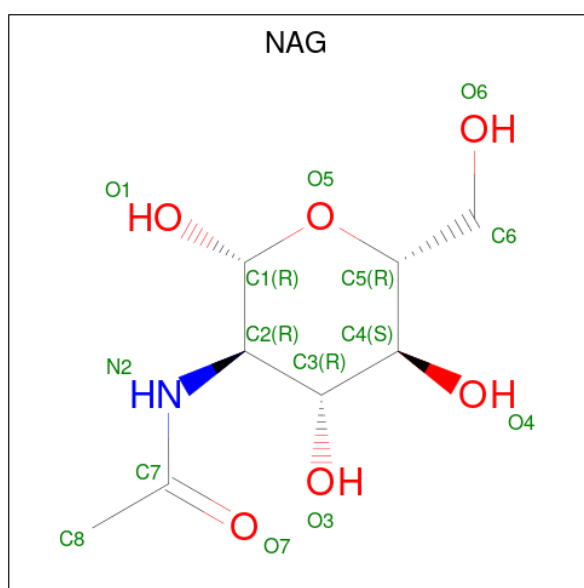
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

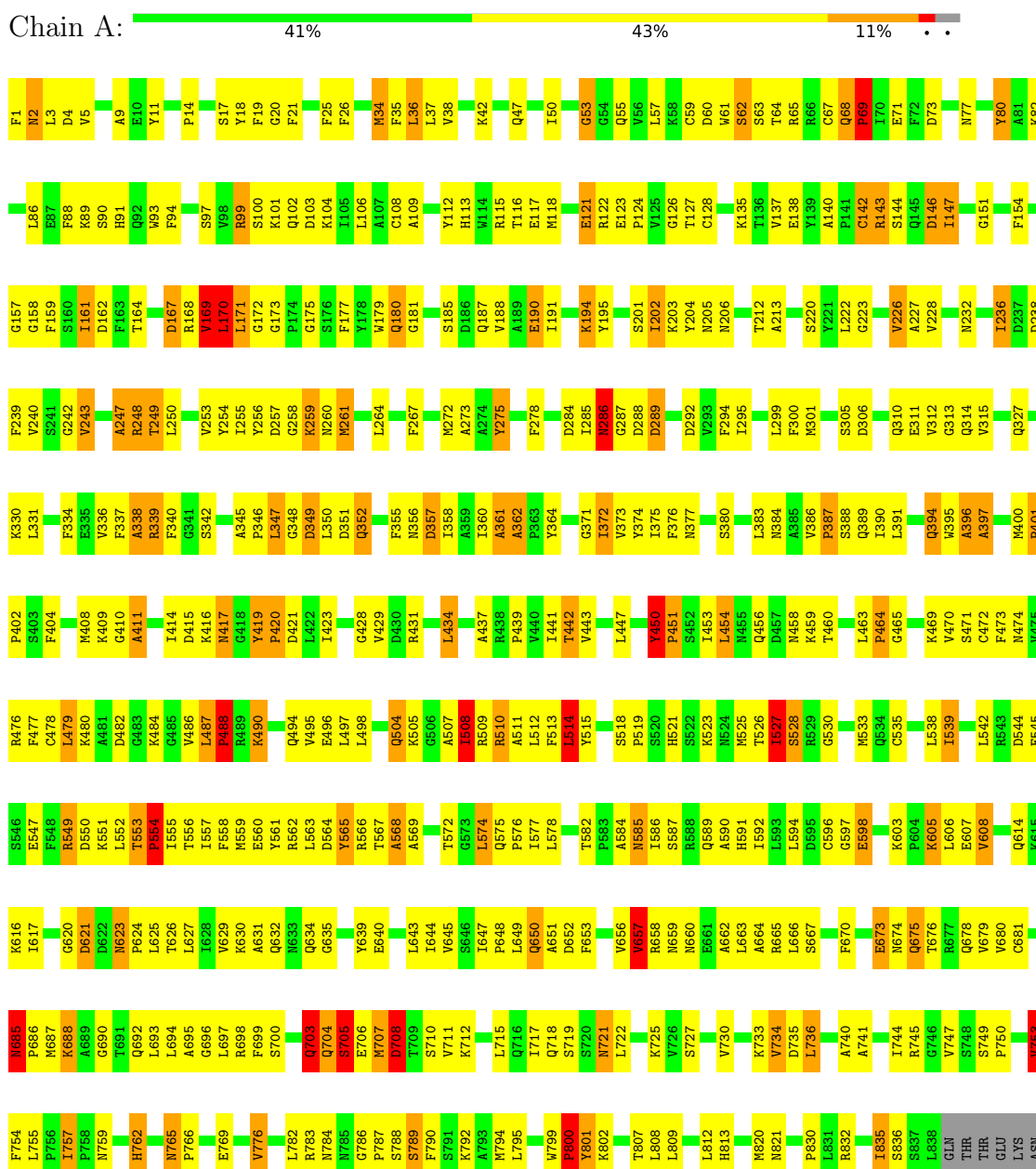
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total 5	Ca 5	0	0
6	B	1	Total 1	Ca 1	0	0

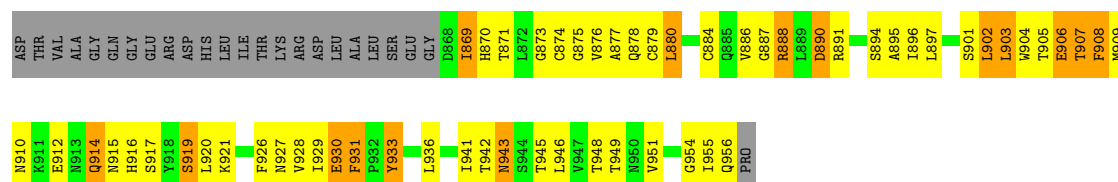
3 Residue-property plots

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

Note EDS was not executed.

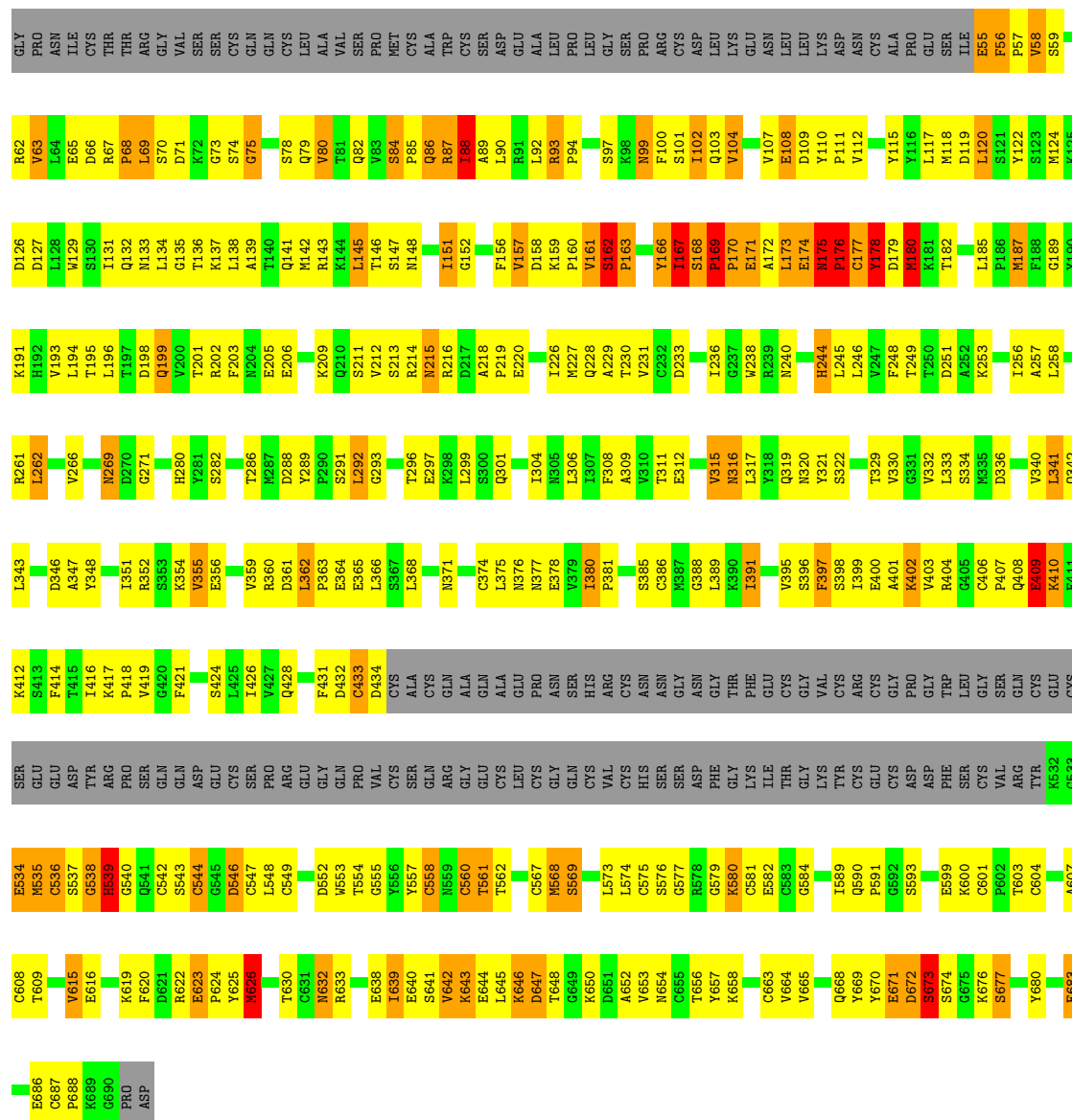
• Molecule 1: INTEGRIN, ALPHA V





• Molecule 2: PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT

Chain B: 29% 36% 10% 22%



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

Chain C: 100%

MAG1
MAG2

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

Chain D:  100%MAG1
MAG2

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

Chain E:  50% 50%MAG1
MAG2

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

Chain G:  100%MAG1
MAG2

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

Chain F:  50% 50%MAG1
NDG2

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

Chain H:  50% 50%MAG1
NDG2

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

Chain I:  100%MAG1
NDG2

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.00Å 130.00Å 307.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11656	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NDG, 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	0.60	0/7372	1.20	80/9994 (0.8%)
2	B	0.57	0/4256	1.19	40/5754 (0.7%)
All	All	0.59	0/11628	1.20	120/15748 (0.8%)

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	PRO	CA-C-N	-12.68	107.89	120.31
2	B	169	PRO	C-N-CA	-12.68	107.89	120.31
1	A	68	GLN	CA-C-N	11.50	134.22	119.84
1	A	68	GLN	C-N-CA	11.50	134.22	119.84
1	A	190	GLU	N-CA-C	-11.23	98.25	113.18
1	A	875	GLY	N-CA-C	-11.22	101.57	113.58
1	A	912	GLU	N-CA-C	11.02	134.26	110.80
2	B	340	VAL	N-CA-C	10.89	123.04	110.62
1	A	685	ASN	CA-C-N	-10.61	106.58	119.84
1	A	685	ASN	C-N-CA	-10.61	106.58	119.84
1	A	687	MET	N-CA-C	-9.86	95.10	109.59
2	B	66	ASP	N-CA-C	-9.85	97.52	110.43
2	B	626	MET	N-CA-C	-9.73	99.97	112.23
1	A	657	VAL	N-CA-C	9.60	120.98	108.12
1	A	703	GLN	N-CA-C	9.23	130.47	110.80
2	B	378	GLU	N-CA-C	-9.19	94.52	109.96
2	B	180	MET	N-CA-C	-9.13	96.77	110.28
2	B	591	PRO	N-CA-C	-9.11	104.08	114.92
2	B	409	GLU	N-CA-C	9.08	122.51	110.53
1	A	450	TYR	CA-C-N	-8.97	110.48	119.90
1	A	450	TYR	C-N-CA	-8.97	110.48	119.90
1	A	954	GLY	N-CA-C	8.81	127.08	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	ASN	CA-C-N	8.58	129.10	119.92
1	A	765	ASN	C-N-CA	8.58	129.10	119.92
1	A	931	PHE	CA-C-N	8.43	128.03	118.85
1	A	931	PHE	C-N-CA	8.43	128.03	118.85
1	A	568	ALA	N-CA-C	8.00	120.14	108.86
2	B	63	VAL	N-CA-C	7.92	117.88	111.62
1	A	907	THR	N-CA-C	-7.87	104.16	113.21
1	A	338	ALA	N-CA-C	-7.84	96.50	108.96
1	A	800	PRO	N-CA-C	-7.16	97.72	112.47
1	A	876	VAL	N-CA-C	-7.16	105.65	111.81
1	A	109	ALA	CA-C-N	7.12	126.80	119.82
1	A	109	ALA	C-N-CA	7.12	126.80	119.82
2	B	664	VAL	N-CA-C	7.05	118.02	107.51
1	A	755	LEU	N-CA-C	6.99	125.26	109.81
1	A	621	ASP	N-CA-C	6.96	120.67	110.59
1	A	180	GLN	N-CA-C	-6.95	103.79	111.36
1	A	582	THR	CA-C-N	6.84	127.38	119.99
1	A	582	THR	C-N-CA	6.84	127.38	119.99
2	B	282	SER	N-CA-C	6.80	118.35	111.07
2	B	590	GLN	N-CA-C	6.79	124.81	109.81
2	B	175	ASN	CA-C-N	-6.78	111.37	119.84
2	B	175	ASN	C-N-CA	-6.78	111.37	119.84
1	A	362	ALA	CA-C-N	6.59	126.28	119.82
1	A	362	ALA	C-N-CA	6.59	126.28	119.82
1	A	776	VAL	N-CA-C	-6.51	98.08	107.78
2	B	604	CYS	CA-C-N	6.50	126.88	119.93
2	B	604	CYS	C-N-CA	6.50	126.88	119.93
1	A	896	ILE	N-CA-C	6.38	117.97	108.46
2	B	178	TYR	N-CA-C	6.35	121.79	111.37
2	B	558	CYS	CA-C-N	6.33	129.24	120.63
2	B	558	CYS	C-N-CA	6.33	129.24	120.63
1	A	226	VAL	N-CA-C	6.29	116.65	108.35
1	A	690	GLY	N-CA-C	-6.27	106.43	115.27
2	B	672	ASP	N-CA-C	6.27	124.15	110.80
1	A	585	ASN	CB-CA-C	-6.26	102.09	110.79
1	A	705	SER	N-CA-C	6.14	123.89	110.80
2	B	171	GLU	N-CA-C	-6.13	104.89	112.38
2	B	321	TYR	N-CA-C	-6.09	104.75	111.82
2	B	163	PRO	N-CA-C	6.09	121.83	113.98
1	A	261	MET	N-CA-C	-6.09	105.81	113.23
1	A	454	LEU	N-CA-C	6.05	118.81	109.07
2	B	560	CYS	N-CA-C	6.00	118.30	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	PRO	CA-C-N	6.00	126.44	119.47
1	A	401	PRO	C-N-CA	6.00	126.44	119.47
1	A	53	GLY	N-CA-C	-5.98	107.49	115.32
2	B	203	PHE	N-CA-C	-5.96	104.70	111.14
1	A	80	TYR	N-CA-C	-5.95	106.35	113.97
1	A	879	CYS	N-CA-C	5.95	119.78	110.32
1	A	451	PRO	N-CA-C	-5.88	101.92	110.80
1	A	117	GLU	N-CA-C	-5.85	105.03	111.82
2	B	93	ARG	N-CA-C	-5.84	103.41	110.13
1	A	158	GLY	N-CA-C	-5.83	107.28	115.32
1	A	419	TYR	CA-C-N	5.81	127.10	119.84
1	A	419	TYR	C-N-CA	5.81	127.10	119.84
2	B	538	GLY	N-CA-C	-5.80	99.44	113.18
2	B	136	THR	N-CA-C	-5.80	104.33	111.40
1	A	553	THR	CA-C-N	5.79	127.08	119.84
1	A	553	THR	C-N-CA	5.79	127.08	119.84
1	A	2	ASN	N-CA-C	5.79	117.81	107.80
1	A	735	ASP	N-CA-C	5.74	118.88	109.76
2	B	653	VAL	N-CA-C	5.72	117.58	108.89
1	A	442	THR	N-CA-C	-5.68	100.44	109.76
1	A	880	LEU	N-CA-C	-5.66	96.31	107.69
1	A	115	ARG	N-CA-C	-5.57	100.61	109.96
1	A	361	ALA	N-CA-C	5.55	118.51	108.69
1	A	744	ILE	N-CA-C	5.46	114.66	106.42
1	A	170	LEU	N-CA-C	-5.46	101.65	110.32
1	A	930	GLU	N-CA-C	5.40	117.98	108.75
1	A	673	GLU	N-CA-C	-5.35	105.87	112.72
2	B	162	SER	CA-C-N	-5.34	114.58	119.82
2	B	162	SER	C-N-CA	-5.34	114.58	119.82
2	B	589	ILE	N-CA-C	-5.32	98.27	109.34
1	A	753	VAL	N-CA-CB	5.30	118.14	111.46
2	B	170	PRO	N-CA-C	-5.30	103.52	111.57
2	B	177	CYS	N-CA-C	-5.29	99.53	110.80
1	A	68	GLN	CB-CA-C	5.29	116.83	108.84
1	A	757	ILE	CA-C-N	5.29	126.11	119.98
1	A	757	ILE	C-N-CA	5.29	126.11	119.98
1	A	339	ARG	N-CA-C	-5.25	103.21	110.35
1	A	708	ASP	N-CA-C	-5.24	99.64	110.80
1	A	553	THR	N-CA-C	-5.24	98.13	108.71
1	A	605	LYS	N-CA-C	-5.23	99.99	108.52
1	A	757	ILE	N-CA-C	5.21	120.13	108.88
1	A	159	PHE	N-CA-C	-5.20	105.73	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	GLU	N-CA-C	5.15	116.58	111.07
1	A	247	ALA	CB-CA-C	-5.15	110.66	116.63
2	B	397	PHE	N-CA-C	5.15	119.31	112.72
1	A	169	VAL	N-CA-C	5.13	120.00	109.34
1	A	535	CYS	N-CA-C	5.12	118.06	109.96
2	B	380	ILE	CA-C-N	5.12	125.41	119.93
2	B	380	ILE	C-N-CA	5.12	125.41	119.93
1	A	47	GLN	N-CA-C	-5.12	102.19	109.62
1	A	286	ASN	N-CA-C	5.11	117.42	110.88
1	A	488	PRO	N-CA-C	5.08	122.94	112.47
2	B	673	SER	N-CA-C	5.05	121.56	110.80
1	A	135	LYS	N-CA-C	5.05	117.01	109.59
1	A	933	TYR	N-CA-C	-5.01	103.44	110.50
1	A	566	ARG	N-CA-C	-5.00	104.99	111.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7216	0	7036	506	0
2	B	4182	0	4030	319	0
3	C	28	0	25	3	0
3	D	28	0	25	3	0
3	E	28	0	25	3	0
3	G	28	0	25	1	0
4	F	28	0	24	7	0
4	H	28	0	24	3	0
4	I	28	0	24	10	0
5	A	28	0	26	8	0
5	B	28	0	26	5	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
All	All	11656	0	11290	825	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 36.

All (825) 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)
4:F:2:NDG:H2	4:F:2:NDG:H6C2	1.19	1.12
1:A:585:ASN:HD22	3:E:1:NAG:H62	1.13	1.10
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.34	1.08
1:A:127:THR:HG22	1:A:140:ALA:HB2	1.39	1.03
2:B:648:THR:HA	4:I:2:NDG:C1	1.89	1.02
2:B:646:LYS:O	4:I:2:NDG:H8C3	1.63	0.98
1:A:808:LEU:HD13	1:A:920:LEU:HD22	1.46	0.98
2:B:94:PRO:HD3	2:B:433:CYS:HB3	1.44	0.98
1:A:749:SER:HB3	1:A:750:PRO:HD3	1.47	0.97
2:B:167:ILE:HD11	2:B:216:ARG:HE	1.29	0.97
2:B:371:ASN:ND2	5:B:3371:NAG:H62	1.78	0.96
4:F:1:NAG:H61	4:F:1:NAG:H2	1.47	0.96
1:A:458:ASN:HD22	5:A:2458:NAG:H4	1.31	0.95
1:A:585:ASN:ND2	3:E:1:NAG:H62	1.80	0.95
1:A:753:VAL:HG22	1:A:951:VAL:HG12	1.44	0.95
1:A:463:LEU:HG	1:A:464:PRO:HD2	1.46	0.94
1:A:59:CYS:HA	1:A:67:CYS:HB2	1.49	0.94
2:B:138:LEU:HD23	2:B:151:ILE:HD11	1.49	0.94
2:B:648:THR:HG22	4:I:2:NDG:H2	1.48	0.93
2:B:371:ASN:HD22	5:B:3371:NAG:H62	1.35	0.92
2:B:672:ASP:H	2:B:676:LYS:HB3	1.35	0.91
1:A:685:ASN:HB3	1:A:686:PRO:HD3	1.51	0.91
2:B:403:VAL:HG11	2:B:431:PHE:HE2	1.36	0.91
1:A:286:ASN:H	1:A:286:ASN:HD22	1.18	0.90
2:B:639:ILE:H	2:B:639:ILE:HD12	1.34	0.90
1:A:259:LYS:HE3	1:A:259:LYS:HA	1.50	0.90
1:A:585:ASN:HD22	3:E:1:NAG:C6	1.82	0.90
1:A:835:ILE:HG12	1:A:836:SER:H	1.35	0.89
1:A:439:PRO:HB3	1:A:487:LEU:HD22	1.55	0.88
2:B:169:PRO:HB2	2:B:170:PRO:CD	2.04	0.88
2:B:110:TYR:HD1	2:B:111:PRO:HD2	1.36	0.87
2:B:403:VAL:HG11	2:B:431:PHE:CE2	2.09	0.87
1:A:869:ILE:HG23	1:A:870:HIS:H	1.38	0.87
4:F:2:NDG:H6C2	4:F:2:NDG:C2	2.02	0.86
1:A:556:THR:HG22	1:A:589:GLN:HG2	1.58	0.86
1:A:260:ASN:HD22	5:A:2260:NAG:H61	1.40	0.86
1:A:339:ARG:O	1:A:362:ALA:HA	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:SER:OG	2:B:85:PRO:HD3	1.75	0.85
2:B:57:PRO:HA	2:B:93:ARG:NH2	1.91	0.85
1:A:236:ILE:HD12	1:A:236:ILE:H	1.42	0.84
1:A:707:MET:HE3	1:A:707:MET:HA	1.58	0.84
2:B:642:VAL:HG11	2:B:646:LYS:HA	1.59	0.84
1:A:745:ARG:HB3	2:B:603:THR:HG21	1.58	0.83
1:A:921:LYS:HD2	1:A:946:LEU:HD12	1.59	0.83
2:B:110:TYR:CD1	2:B:111:PRO:HD2	2.14	0.83
1:A:550:ASP:H	1:A:551:LYS:HZ1	1.26	0.82
2:B:366:LEU:HB3	2:B:403:VAL:HG12	1.61	0.82
2:B:212:VAL:HG12	2:B:213:SER:H	1.44	0.81
1:A:667:SER:HA	2:B:535:MET:SD	2.20	0.81
1:A:508:ILE:HD12	1:A:508:ILE:H	1.47	0.80
1:A:106:LEU:HD11	1:A:128:CYS:HB3	1.62	0.80
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.62	0.80
1:A:515:TYR:HE1	1:A:539:ILE:HD13	1.46	0.80
2:B:88:ILE:HD13	2:B:89:ALA:N	1.97	0.80
1:A:487:LEU:HG	1:A:488:PRO:HD3	1.62	0.79
1:A:620:GLY:H	1:A:703:GLN:HB2	1.45	0.79
2:B:168:SER:H	2:B:169:PRO:HD3	1.45	0.79
1:A:3:LEU:HD21	1:A:350:LEU:HD13	1.65	0.78
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.65	0.78
1:A:59:CYS:HA	1:A:67:CYS:CB	2.14	0.78
1:A:550:ASP:H	1:A:551:LYS:NZ	1.81	0.78
1:A:605:LYS:HD2	1:A:634:GLN:HB3	1.66	0.78
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.63	0.78
1:A:474:ASN:HD21	1:A:539:ILE:HG13	1.46	0.78
1:A:711:VAL:HG23	1:A:736:LEU:HD11	1.65	0.78
2:B:173:LEU:HA	2:B:176:PRO:HD2	1.63	0.78
2:B:652:ALA:HB1	2:B:669:TYR:O	1.84	0.77
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.49	0.77
1:A:469:LYS:H	1:A:469:LYS:HD3	1.49	0.77
1:A:80:TYR:HB2	1:A:86:LEU:HD23	1.66	0.77
1:A:710:SER:HA	1:A:736:LEU:HD13	1.65	0.77
2:B:391:ILE:HD12	2:B:391:ILE:H	1.48	0.77
1:A:2:ASN:HD22	1:A:577:ILE:HD13	1.49	0.76
1:A:608:VAL:HG13	1:A:717:ILE:HD11	1.66	0.76
1:A:77:ASN:HD21	1:A:89:LYS:N	1.83	0.76
2:B:417:LYS:HB3	2:B:424:SER:HB3	1.68	0.76
4:F:1:NAG:H2	4:F:1:NAG:C6	2.15	0.76
1:A:338:ALA:HA	1:A:364:TYR:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:VAL:HG13	1:A:698:ARG:HE	1.51	0.76
1:A:712:LYS:HA	1:A:733:LYS:HA	1.66	0.75
1:A:112:TYR:HB3	1:A:126:GLY:HA2	1.66	0.75
1:A:300:PHE:HB3	1:A:313:GLY:HA2	1.68	0.75
1:A:789:SER:HB3	1:A:890:ASP:HA	1.68	0.75
2:B:71:ASP:HB3	2:B:108:GLU:HB2	1.67	0.75
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.69	0.74
1:A:248:ARG:NH1	1:A:248:ARG:HB2	2.03	0.74
1:A:820:MET:HG3	1:A:886:VAL:HG22	1.68	0.74
1:A:620:GLY:C	1:A:891:ARG:HH12	1.96	0.74
1:A:286:ASN:HD22	1:A:286:ASN:N	1.82	0.74
2:B:639:ILE:HG22	2:B:640:GLU:H	1.51	0.74
1:A:334:PHE:HE1	1:A:387:PRO:HG2	1.52	0.73
2:B:643:LYS:HD3	2:B:643:LYS:H	1.53	0.73
1:A:450:TYR:HD1	1:A:474:ASN:HB2	1.53	0.73
2:B:167:ILE:HD11	2:B:216:ARG:NE	2.04	0.73
1:A:946:LEU:H	1:A:946:LEU:HD23	1.54	0.72
2:B:194:LEU:HB2	2:B:206:GLU:HG3	1.70	0.72
2:B:160:PRO:HA	2:B:187:MET:HG2	1.71	0.72
2:B:567:CYS:SG	2:B:584:GLY:O	2.48	0.72
1:A:706:GLU:C	1:A:708:ASP:H	1.98	0.72
1:A:349:ASP:H	1:A:420:PRO:HG2	1.55	0.71
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.26	0.71
1:A:260:ASN:HD22	5:A:2260:NAG:C6	2.02	0.71
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.19	0.71
2:B:87:ARG:HH12	2:B:428:GLN:CD	1.98	0.71
2:B:93:ARG:HA	2:B:432:ASP:O	1.89	0.71
2:B:399:ILE:HD13	2:B:416:ILE:HD13	1.71	0.71
1:A:402:PRO:HA	1:A:428:GLY:HA3	1.72	0.71
2:B:119:ASP:O	2:B:124:MET:HG3	1.90	0.71
2:B:230:THR:HG23	2:B:304:ILE:HG13	1.71	0.71
2:B:359:VAL:HG12	2:B:360:ARG:H	1.55	0.71
2:B:73:GLY:HA3	2:B:109:ASP:O	1.91	0.71
2:B:166:TYR:CZ	2:B:216:ARG:HG3	2.26	0.71
1:A:77:ASN:HD21	1:A:89:LYS:H	1.39	0.70
1:A:927:ASN:HD22	1:A:928:VAL:N	1.89	0.70
2:B:56:PHE:CD2	2:B:56:PHE:N	2.58	0.70
1:A:180:GLN:HE22	1:A:213:ALA:HB3	1.56	0.70
1:A:740:ALA:HA	1:A:786:GLY:HA3	1.74	0.69
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.73	0.69
2:B:56:PHE:N	2:B:56:PHE:HD2	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.75	0.69
2:B:212:VAL:HG12	2:B:213:SER:N	2.06	0.69
1:A:59:CYS:CA	1:A:67:CYS:HB2	2.23	0.69
1:A:906:GLU:C	1:A:908:PHE:H	2.01	0.69
2:B:361:ASP:O	2:B:362:LEU:HB3	1.91	0.69
2:B:639:ILE:HD12	2:B:639:ILE:N	2.08	0.69
2:B:309:ALA:HB1	2:B:333:LEU:HD13	1.73	0.68
1:A:458:ASN:HD22	5:A:2458:NAG:C4	2.06	0.68
2:B:157:VAL:HG13	2:B:158:ASP:H	1.59	0.68
2:B:58:VAL:CG1	2:B:93:ARG:H	2.07	0.67
2:B:58:VAL:HG12	2:B:93:ARG:H	1.59	0.67
2:B:650:LYS:HG2	4:I:1:NAG:H62	1.76	0.67
1:A:260:ASN:ND2	5:A:2260:NAG:C6	2.57	0.67
2:B:99:ASN:HD22	2:B:99:ASN:H	1.42	0.67
2:B:88:ILE:HD13	2:B:89:ALA:H	1.60	0.67
2:B:371:ASN:HD22	5:B:3371:NAG:C6	2.05	0.67
1:A:417:ASN:HA	1:A:486:VAL:HG23	1.77	0.66
2:B:122:TYR:HA	2:B:212:VAL:HG11	1.76	0.66
2:B:185:LEU:CD1	2:B:211:SER:HB3	2.25	0.66
2:B:187:MET:HE2	2:B:187:MET:HA	1.77	0.66
1:A:395:TRP:HB3	1:A:429:VAL:HG11	1.77	0.66
2:B:168:SER:N	2:B:169:PRO:HD3	2.09	0.66
2:B:187:MET:HA	2:B:187:MET:CE	2.25	0.66
4:H:1:NAG:O6	4:H:2:NDG:C1	2.44	0.66
1:A:423:ILE:HG12	1:A:434:LEU:CD2	2.25	0.66
2:B:111:PRO:HA	2:B:146:THR:HG21	1.77	0.66
2:B:375:LEU:HD13	2:B:630:THR:HG22	1.76	0.66
1:A:377:ASN:O	1:A:383:LEU:HD12	1.96	0.66
1:A:552:LEU:HD11	1:A:592:ILE:H	1.59	0.66
1:A:487:LEU:HG	1:A:488:PRO:CD	2.26	0.66
1:A:664:ALA:HB3	1:A:695:ALA:HB2	1.77	0.66
2:B:399:ILE:HG22	2:B:400:GLU:H	1.59	0.66
1:A:375:ILE:HG12	1:A:389:GLN:HB3	1.78	0.66
1:A:624:PRO:HG2	4:H:2:NDG:H3	1.77	0.65
1:A:68:GLN:HB3	1:A:69:PRO:HD2	1.77	0.65
2:B:354:LYS:HA	2:B:386:CYS:O	1.95	0.65
1:A:605:LYS:H	1:A:635:GLY:H	1.44	0.65
1:A:25:PHE:HE1	1:A:410:GLY:HA2	1.61	0.65
1:A:474:ASN:ND2	1:A:539:ILE:HG13	2.10	0.65
2:B:347:ALA:O	2:B:351:ILE:HG12	1.96	0.65
1:A:164:THR:HG22	1:A:228:VAL:HG21	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.77	0.65
3:G:1:NAG:H61	3:G:2:NAG:O5	1.97	0.65
1:A:515:TYR:CE1	1:A:539:ILE:HD13	2.30	0.65
1:A:835:ILE:HG12	1:A:836:SER:N	2.11	0.65
2:B:657:TYR:CE2	2:B:665:VAL:HB	2.31	0.65
4:F:1:NAG:C6	4:F:1:NAG:C2	2.72	0.65
1:A:510:ARG:NH1	1:A:555:ILE:HG12	2.11	0.64
1:A:544:ASP:O	1:A:547:GLU:HG2	1.97	0.64
2:B:639:ILE:H	2:B:639:ILE:CD1	2.09	0.64
2:B:670:TYR:HD1	2:B:671:GLU:H	1.43	0.64
1:A:458:ASN:ND2	5:A:2458:NAG:C4	2.61	0.64
2:B:58:VAL:HG22	2:B:93:ARG:HH21	1.63	0.64
1:A:539:ILE:N	1:A:539:ILE:HD12	2.11	0.64
2:B:417:LYS:HB3	2:B:424:SER:CB	2.27	0.64
1:A:1:PHE:HB2	1:A:388:SER:HB3	1.79	0.64
1:A:562:ARG:HB3	1:A:562:ARG:NH1	2.12	0.64
1:A:450:TYR:CD1	1:A:474:ASN:HB2	2.32	0.63
1:A:914:GLN:HB3	1:A:916:HIS:ND1	2.12	0.63
2:B:623:GLU:HB3	2:B:624:PRO:HD2	1.78	0.63
1:A:374:TYR:HD1	1:A:390:ILE:HG22	1.63	0.63
1:A:463:LEU:CG	1:A:464:PRO:HD2	2.25	0.63
1:A:783:ARG:HB2	1:A:894:SER:HB3	1.80	0.63
1:A:248:ARG:HB2	1:A:248:ARG:HH11	1.63	0.63
4:F:2:NDG:H2	4:F:2:NDG:C6	2.03	0.63
1:A:707:MET:HG3	1:A:707:MET:O	1.98	0.62
2:B:168:SER:H	2:B:169:PRO:CD	2.10	0.62
2:B:534:GLU:HG2	2:B:544:CYS:SG	2.38	0.62
1:A:42:LYS:NZ	1:A:93:TRP:HE1	1.98	0.62
2:B:672:ASP:N	2:B:676:LYS:HB3	2.12	0.62
1:A:349:ASP:C	1:A:351:ASP:H	2.06	0.62
1:A:802:LYS:O	1:A:877:ALA:HB1	2.00	0.62
1:A:222:LEU:HD12	1:A:223:GLY:N	2.14	0.62
1:A:254:TYR:OH	3:D:1:NAG:H62	2.00	0.62
1:A:539:ILE:HD12	1:A:539:ILE:H	1.64	0.61
1:A:741:ALA:H	1:A:786:GLY:HA3	1.63	0.61
2:B:308:PHE:HB2	2:B:330:VAL:HG12	1.81	0.61
2:B:312:GLU:HA	2:B:315:VAL:CG2	2.30	0.61
2:B:537:SER:HB2	2:B:539:HIS:H	1.64	0.61
1:A:645:VAL:HB	1:A:679:VAL:HB	1.82	0.61
2:B:639:ILE:HG22	2:B:640:GLU:N	2.14	0.61
2:B:111:PRO:HA	2:B:146:THR:CG2	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:SER:HB3	2:B:402:LYS:HG3	1.82	0.61
2:B:167:ILE:CD1	2:B:216:ARG:HE	2.10	0.61
2:B:151:ILE:O	2:B:196:LEU:HA	2.00	0.61
2:B:171:GLU:C	2:B:173:LEU:H	2.09	0.61
2:B:228:GLN:C	2:B:230:THR:H	2.09	0.61
1:A:704:GLN:HG2	1:A:707:MET:SD	2.41	0.61
2:B:129:TRP:O	2:B:132:GLN:HG2	2.00	0.61
2:B:87:ARG:HH12	2:B:428:GLN:NE2	1.99	0.60
1:A:647:ILE:HD11	1:A:670:PHE:HE2	1.66	0.60
1:A:753:VAL:CG2	1:A:951:VAL:HG12	2.25	0.60
2:B:375:LEU:HD11	2:B:633:ARG:HB3	1.83	0.60
2:B:214:ARG:HG3	2:B:214:ARG:HH11	1.65	0.60
1:A:626:THR:HG22	1:A:698:ARG:HB3	1.84	0.60
2:B:134:LEU:HG	2:B:135:GLY:H	1.66	0.60
2:B:170:PRO:HD2	2:B:173:LEU:HD12	1.83	0.60
1:A:232:ASN:HB2	1:A:264:LEU:HD21	1.83	0.60
2:B:249:THR:HA	2:B:309:ALA:O	2.01	0.60
1:A:549:ARG:HG3	1:A:551:LYS:NZ	2.16	0.60
1:A:562:ARG:HB3	1:A:562:ARG:HH11	1.66	0.60
1:A:314:GLN:NE2	1:A:330:LYS:HG2	2.17	0.59
1:A:247:ALA:HB3	1:A:250:LEU:HB2	1.84	0.59
1:A:787:PRO:HA	1:A:891:ARG:HH11	1.67	0.59
2:B:87:ARG:O	2:B:88:ILE:HB	2.01	0.59
1:A:625:LEU:HD21	1:A:734:VAL:HG21	1.83	0.59
2:B:399:ILE:HG22	2:B:400:GLU:N	2.17	0.59
1:A:222:LEU:HD12	1:A:223:GLY:H	1.66	0.59
2:B:269:ASN:HD22	2:B:271:GLY:H	1.49	0.59
2:B:668:GLN:HE21	2:B:670:TYR:HD2	1.50	0.59
1:A:203:LYS:HD2	1:A:203:LYS:H	1.66	0.59
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.15	0.59
1:A:458:ASN:ND2	5:A:2458:NAG:H4	2.06	0.59
1:A:608:VAL:O	1:A:730:VAL:HG21	2.03	0.59
1:A:674:ASN:C	1:A:676:THR:H	2.11	0.59
1:A:563:LEU:HG	1:A:564:ASP:H	1.68	0.59
1:A:809:LEU:HG	1:A:920:LEU:HD13	1.85	0.59
2:B:406:CYS:HB2	2:B:431:PHE:HB3	1.85	0.59
1:A:629:VAL:O	1:A:694:LEU:HD12	2.03	0.59
1:A:869:ILE:HG23	1:A:870:HIS:N	2.15	0.59
1:A:902:LEU:HD23	1:A:902:LEU:O	2.02	0.59
1:A:170:LEU:HD13	1:A:226:VAL:CG2	2.32	0.58
1:A:170:LEU:HG	1:A:239:PHE:CD2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:CZ	1:A:258:GLY:HA2	2.38	0.58
1:A:903:LEU:HD22	1:A:905:THR:H	1.68	0.58
1:A:127:THR:HG22	1:A:140:ALA:CB	2.24	0.58
2:B:670:TYR:HB3	2:B:676:LYS:HE2	1.85	0.58
1:A:248:ARG:HD3	1:A:248:ARG:N	2.17	0.58
1:A:608:VAL:HA	1:A:630:LYS:O	2.03	0.58
1:A:749:SER:HB3	1:A:750:PRO:CD	2.29	0.58
2:B:104:VAL:HG21	2:B:418:PRO:HG2	1.84	0.58
2:B:119:ASP:HB3	2:B:124:MET:HE2	1.84	0.58
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.85	0.58
1:A:349:ASP:HB3	1:A:352:GLN:H	1.67	0.58
1:A:621:ASP:N	1:A:891:ARG:HH12	2.02	0.58
1:A:629:VAL:O	1:A:694:LEU:HA	2.03	0.58
1:A:644:ILE:HD13	1:A:680:VAL:HG22	1.85	0.58
1:A:97:SER:HB2	1:A:161:ILE:HG12	1.84	0.58
2:B:616:GLU:HG2	2:B:657:TYR:OH	2.04	0.58
1:A:456:GLN:NE2	1:A:545:GLU:HG3	2.19	0.58
1:A:789:SER:CB	1:A:890:ASP:HA	2.32	0.58
1:A:951:VAL:O	1:A:951:VAL:HG23	2.04	0.58
2:B:341:LEU:C	2:B:343:LEU:H	2.12	0.58
2:B:624:PRO:C	2:B:626:MET:H	2.12	0.58
2:B:426:ILE:HD12	2:B:426:ILE:N	2.19	0.57
2:B:668:GLN:NE2	2:B:670:TYR:HD2	2.02	0.57
1:A:180:GLN:NE2	1:A:213:ALA:HB3	2.19	0.57
1:A:187:GLN:O	1:A:191:ILE:HG13	2.04	0.57
1:A:478:CYS:SG	1:A:533:MET:HB2	2.45	0.57
1:A:549:ARG:HE	1:A:549:ARG:HA	1.68	0.57
1:A:653:PHE:HA	1:A:699:PHE:HD1	1.68	0.57
2:B:359:VAL:HG12	2:B:360:ARG:N	2.19	0.57
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.87	0.57
1:A:666:LEU:O	2:B:535:MET:SD	2.63	0.57
1:A:443:VAL:HG23	1:A:480:LYS:O	2.05	0.57
1:A:177:PHE:CD1	1:A:212:THR:HA	2.40	0.57
2:B:397:PHE:O	2:B:398:SER:HB3	2.03	0.57
1:A:2:ASN:HD22	1:A:577:ILE:CD1	2.16	0.57
2:B:231:VAL:HG11	2:B:271:GLY:O	2.05	0.57
1:A:334:PHE:CE1	1:A:387:PRO:HG2	2.38	0.57
1:A:873:GLY:HA3	1:A:921:LYS:HB3	1.86	0.57
2:B:97:SER:HB3	2:B:402:LYS:CG	2.34	0.57
1:A:88:PHE:CE1	1:A:122:ARG:HG2	2.40	0.56
1:A:621:ASP:OD1	1:A:787:PRO:HB3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:VAL:CG1	1:A:698:ARG:HE	2.18	0.56
2:B:539:HIS:O	2:B:542:CYS:HB3	2.06	0.56
1:A:53:GLY:O	1:A:94:PHE:HB3	2.05	0.56
1:A:914:GLN:HB3	1:A:916:HIS:CE1	2.40	0.56
2:B:180:MET:HE1	2:B:214:ARG:NE	2.21	0.56
2:B:205:GLU:HG3	2:B:209:LYS:NZ	2.21	0.56
1:A:346:PRO:HA	1:A:358:ILE:HG13	1.87	0.56
1:A:703:GLN:O	1:A:705:SER:N	2.37	0.56
1:A:955:ILE:HD11	2:B:686:GLU:O	2.06	0.56
1:A:605:LYS:HD2	1:A:634:GLN:CB	2.33	0.56
1:A:617:ILE:HG13	1:A:617:ILE:O	2.06	0.56
1:A:942:THR:O	1:A:943:ASN:HB2	2.06	0.56
2:B:159:LYS:NZ	2:B:288:ASP:HA	2.21	0.56
2:B:168:SER:HA	2:B:174:GLU:OE2	2.05	0.56
1:A:464:PRO:HG2	1:A:465:GLY:H	1.70	0.55
2:B:647:ASP:HB3	2:B:668:GLN:HE22	1.71	0.55
1:A:142:CYS:C	1:A:144:SER:H	2.14	0.55
2:B:84:SER:CB	2:B:85:PRO:HD3	2.35	0.55
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.87	0.55
2:B:574:LEU:HD11	2:B:581:CYS:HB2	1.88	0.55
1:A:286:ASN:N	1:A:286:ASN:ND2	2.52	0.55
1:A:350:LEU:HG	1:A:357:ASP:OD1	2.06	0.55
1:A:550:ASP:N	1:A:551:LYS:HZ1	2.00	0.55
1:A:782:LEU:HD11	1:A:926:PHE:CD1	2.41	0.55
2:B:355:VAL:HG21	2:B:395:VAL:HG21	1.88	0.55
1:A:9:ALA:HB3	1:A:434:LEU:CB	2.36	0.55
1:A:57:LEU:N	1:A:57:LEU:HD12	2.22	0.55
1:A:417:ASN:HA	1:A:486:VAL:CG2	2.36	0.55
2:B:341:LEU:HD23	2:B:342:GLN:H	1.72	0.55
1:A:62:SER:O	1:A:64:THR:N	2.40	0.55
1:A:175:GLY:HA2	1:A:179:TRP:HA	1.89	0.55
2:B:244:HIS:O	2:B:245:LEU:HD12	2.06	0.55
1:A:137:VAL:HG12	1:A:195:TYR:CD1	2.42	0.55
1:A:498:LEU:HD12	1:A:558:PHE:CD2	2.42	0.55
1:A:799:TRP:C	1:A:800:PRO:O	2.45	0.55
1:A:514:LEU:HB2	1:A:539:ILE:HB	1.88	0.55
1:A:299:LEU:HD11	1:A:339:ARG:NH1	2.21	0.54
2:B:341:LEU:HD23	2:B:342:GLN:N	2.22	0.54
1:A:180:GLN:HE22	1:A:213:ALA:H	1.53	0.54
1:A:736:LEU:O	1:A:936:LEU:HD23	2.07	0.54
2:B:156:PHE:HB2	2:B:189:GLY:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ALA:CB	3:D:2:NAG:H83	2.36	0.54
1:A:605:LYS:HB3	1:A:634:GLN:HB3	1.88	0.54
2:B:319:GLN:HG2	2:B:330:VAL:HG21	1.90	0.54
2:B:623:GLU:CB	2:B:624:PRO:HD2	2.37	0.54
1:A:557:ILE:N	1:A:557:ILE:HD12	2.23	0.54
1:A:927:ASN:HD22	1:A:927:ASN:C	2.14	0.54
1:A:450:TYR:CB	1:A:451:PRO:HD3	2.38	0.54
1:A:511:ALA:HB2	1:A:555:ILE:HG21	1.89	0.54
1:A:345:ALA:HB2	1:A:408:MET:HG3	1.89	0.54
1:A:871:THR:HA	1:A:919:SER:HB2	1.89	0.54
2:B:141:GLN:HG3	2:B:341:LEU:HD11	1.89	0.54
1:A:124:PRO:HD2	1:A:154:PHE:CD2	2.42	0.54
2:B:568:MET:O	2:B:569:SER:HB3	2.06	0.54
1:A:647:ILE:HD12	1:A:651:ALA:HB3	1.90	0.54
1:A:61:TRP:HB2	1:A:414:ILE:HD11	1.90	0.54
2:B:348:TYR:CZ	2:B:352:ARG:HD2	2.42	0.53
2:B:388:GLY:O	2:B:633:ARG:HD3	2.06	0.53
2:B:535:MET:C	2:B:537:SER:H	2.16	0.53
1:A:157:GLY:HA2	1:A:172:GLY:O	2.08	0.53
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.91	0.53
1:A:660:ASN:HB3	1:A:663:LEU:HD12	1.90	0.53
2:B:62:ARG:HD2	2:B:85:PRO:HB3	1.90	0.53
1:A:627:LEU:HD12	1:A:699:PHE:HE2	1.74	0.53
1:A:914:GLN:C	1:A:916:HIS:H	2.16	0.53
1:A:451:PRO:HD2	1:A:473:PHE:HA	1.90	0.53
1:A:42:LYS:NZ	1:A:93:TRP:NE1	2.57	0.53
1:A:284:ASP:HA	1:A:292:ASP:OD1	2.09	0.53
1:A:800:PRO:HB3	1:A:808:LEU:HD11	1.90	0.53
2:B:151:ILE:C	2:B:196:LEU:HD23	2.33	0.53
5:B:3371:NAG:O7	5:B:3371:NAG:H3	2.08	0.53
1:A:239:PHE:N	1:A:256:TYR:O	2.40	0.53
1:A:477:PHE:CD2	1:A:477:PHE:N	2.77	0.53
2:B:624:PRO:O	2:B:625:TYR:HB2	2.09	0.53
2:B:645:LEU:HD23	2:B:645:LEU:H	1.74	0.53
1:A:255:ILE:O	1:A:264:LEU:HB2	2.09	0.53
1:A:375:ILE:O	1:A:375:ILE:HG13	2.09	0.53
2:B:173:LEU:C	2:B:175:ASN:H	2.16	0.53
2:B:534:GLU:C	2:B:536:CYS:H	2.16	0.52
1:A:3:LEU:CD2	1:A:350:LEU:HD22	2.39	0.52
1:A:138:GLU:CD	1:A:143:ARG:HH22	2.17	0.52
1:A:169:VAL:O	1:A:185:SER:HA	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:GLY:N	2:B:196:LEU:HD23	2.25	0.52
1:A:220:SER:O	1:A:243:VAL:HG12	2.08	0.52
1:A:373:VAL:HG23	1:A:404:PHE:HE2	1.74	0.52
1:A:384:ASN:ND2	1:A:386:VAL:HG22	2.24	0.52
1:A:34:MET:HG3	1:A:414:ILE:HA	1.92	0.52
1:A:340:PHE:C	1:A:342:SER:H	2.17	0.52
1:A:549:ARG:HG3	1:A:551:LYS:HZ1	1.74	0.52
2:B:368:LEU:HG	2:B:399:ILE:CG2	2.39	0.52
1:A:19:PHE:CD1	1:A:431:ARG:HA	2.44	0.52
1:A:657:VAL:HG12	1:A:659:ASN:HD21	1.73	0.52
2:B:185:LEU:HD11	2:B:211:SER:HB3	1.91	0.52
2:B:557:TYR:O	2:B:558:CYS:HB2	2.10	0.52
1:A:99:ARG:HG3	1:A:162:ASP:HA	1.91	0.52
2:B:59:SER:O	2:B:90:LEU:HA	2.10	0.52
2:B:599:GLU:HG2	2:B:600:LYS:N	2.23	0.52
2:B:670:TYR:O	2:B:677:SER:HA	2.09	0.52
2:B:226:ILE:HD11	2:B:248:PHE:CD1	2.45	0.52
1:A:238:ASP:HB3	1:A:256:TYR:O	2.09	0.52
1:A:542:LEU:HD11	1:A:555:ILE:CD1	2.40	0.52
2:B:157:VAL:HG13	2:B:158:ASP:N	2.24	0.52
2:B:561:THR:HG22	2:B:562:THR:H	1.75	0.52
1:A:77:ASN:ND2	1:A:89:LYS:H	2.07	0.51
1:A:487:LEU:CG	1:A:488:PRO:HD3	2.35	0.51
1:A:542:LEU:HD11	1:A:555:ILE:HD13	1.91	0.51
1:A:511:ALA:O	1:A:512:LEU:HD23	2.10	0.51
1:A:312:VAL:HG12	1:A:336:VAL:HA	1.92	0.51
1:A:347:LEU:HD12	1:A:358:ILE:N	2.25	0.51
1:A:915:ASN:ND2	1:A:915:ASN:H	2.08	0.51
2:B:90:LEU:HD11	2:B:401:ALA:HB3	1.91	0.51
2:B:134:LEU:HG	2:B:135:GLY:N	2.26	0.51
1:A:509:ARG:HD3	1:A:519:PRO:HG3	1.91	0.51
1:A:794:MET:O	1:A:926:PHE:HA	2.10	0.51
1:A:21:PHE:HE1	2:B:266:VAL:HG11	1.76	0.51
1:A:102:GLN:C	1:A:104:LYS:H	2.17	0.51
1:A:526:THR:HG22	1:A:527:ILE:N	2.26	0.51
2:B:269:ASN:ND2	2:B:271:GLY:H	2.09	0.51
2:B:159:LYS:HD2	2:B:289:TYR:CZ	2.45	0.51
1:A:561:TYR:CZ	1:A:584:ALA:HA	2.45	0.51
1:A:820:MET:HE2	1:A:895:ALA:HB1	1.93	0.51
1:A:928:VAL:CG2	1:A:941:ILE:HB	2.41	0.51
2:B:642:VAL:CG2	2:B:680:TYR:HB3	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LEU:HB3	1:A:681:CYS:HB2	1.93	0.51
2:B:118:MET:HE2	2:B:124:MET:HE3	1.93	0.51
1:A:375:ILE:CG1	1:A:389:GLN:HB3	2.41	0.50
1:A:171:LEU:C	1:A:171:LEU:HD23	2.37	0.50
2:B:656:THR:HA	2:B:665:VAL:O	2.11	0.50
1:A:558:PHE:CZ	1:A:585:ASN:OD1	2.64	0.50
1:A:558:PHE:CE2	1:A:560:GLU:HG3	2.46	0.50
1:A:794:MET:HG2	1:A:929:ILE:HD13	1.93	0.50
1:A:394:GLN:N	1:A:394:GLN:HE21	2.09	0.50
2:B:257:ALA:O	2:B:258:LEU:HB2	2.11	0.50
2:B:319:GLN:O	2:B:322:SER:HB3	2.12	0.50
1:A:498:LEU:O	1:A:558:PHE:N	2.44	0.50
1:A:597:GLY:O	1:A:598:GLU:HB3	2.12	0.50
1:A:873:GLY:CA	1:A:921:LYS:HB3	2.41	0.50
1:A:914:GLN:OE1	1:A:914:GLN:HA	2.11	0.50
2:B:62:ARG:HA	2:B:88:ILE:HG12	1.94	0.50
1:A:61:TRP:CZ2	1:A:415:ASP:HB3	2.46	0.50
1:A:146:ASP:OD1	1:A:151:GLY:HA3	2.11	0.49
1:A:301:MET:HA	1:A:310:GLN:O	2.12	0.49
1:A:340:PHE:CZ	1:A:360:ILE:HG21	2.47	0.49
1:A:305:SER:HB3	2:B:552:ASP:HB2	1.93	0.49
1:A:526:THR:C	1:A:527:ILE:HG12	2.36	0.49
1:A:550:ASP:CG	1:A:551:LYS:H	2.20	0.49
1:A:808:LEU:O	1:A:809:LEU:HB2	2.11	0.49
2:B:580:LYS:HZ3	2:B:580:LYS:HB2	1.77	0.49
2:B:623:GLU:HB3	2:B:624:PRO:CD	2.42	0.49
1:A:477:PHE:CE1	1:A:495:VAL:HG11	2.47	0.49
1:A:594:LEU:C	1:A:596:CYS:H	2.19	0.49
1:A:624:PRO:CG	4:H:2:NDG:H3	2.41	0.49
2:B:157:VAL:HG12	2:B:189:GLY:H	1.76	0.49
2:B:297:GLU:O	2:B:301:GLN:HG3	2.12	0.49
1:A:5:VAL:HG12	1:A:5:VAL:O	2.12	0.49
1:A:11:TYR:CD1	1:A:36:LEU:HD22	2.47	0.49
2:B:104:VAL:CG2	2:B:421:PHE:HE2	2.25	0.49
1:A:236:ILE:H	1:A:236:ILE:CD1	2.11	0.49
1:A:526:THR:HG22	1:A:527:ILE:H	1.76	0.49
1:A:887:GLY:O	1:A:888:ARG:HB3	2.12	0.49
2:B:607:ALA:C	2:B:609:THR:H	2.20	0.49
1:A:188:VAL:C	1:A:190:GLU:H	2.20	0.49
2:B:366:LEU:HB3	2:B:403:VAL:CG1	2.37	0.49
2:B:647:ASP:HB3	2:B:668:GLN:NE2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASP:HB2	1:A:530:GLY:HA2	1.93	0.49
2:B:341:LEU:C	2:B:343:LEU:N	2.67	0.49
1:A:18:TYR:CE1	1:A:42:LYS:HD2	2.48	0.49
1:A:273:ALA:HB3	2:B:292:LEU:HD22	1.95	0.49
1:A:300:PHE:HB3	1:A:313:GLY:CA	2.41	0.49
2:B:180:MET:HE1	2:B:214:ARG:CZ	2.43	0.49
1:A:450:TYR:HB3	1:A:451:PRO:HD3	1.94	0.49
2:B:262:LEU:N	2:B:262:LEU:HD23	2.28	0.49
1:A:121:GLU:HG2	1:A:123:GLU:HG3	1.95	0.48
1:A:248:ARG:HH11	1:A:248:ARG:CB	2.26	0.48
1:A:632:GLN:HG2	1:A:692:GLN:HG3	1.95	0.48
1:A:747:VAL:HG13	1:A:747:VAL:O	2.12	0.48
2:B:646:LYS:HD2	2:B:646:LYS:H	1.77	0.48
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.94	0.48
1:A:242:GLY:HA2	1:A:253:VAL:HG22	1.95	0.48
1:A:248:ARG:HH11	1:A:248:ARG:H	1.60	0.48
1:A:300:PHE:CB	1:A:313:GLY:HA2	2.41	0.48
1:A:9:ALA:HB3	1:A:434:LEU:HB2	1.94	0.48
1:A:232:ASN:HB2	1:A:264:LEU:CD2	2.44	0.48
1:A:554:PRO:HG3	1:A:591:HIS:CD2	2.48	0.48
2:B:233:ASP:HA	2:B:238:TRP:HD1	1.78	0.48
4:F:1:NAG:H61	4:F:1:NAG:C2	2.20	0.48
1:A:674:ASN:HB3	1:A:676:THR:HG22	1.96	0.48
2:B:69:LEU:HD21	2:B:78:SER:HB2	1.95	0.48
2:B:161:VAL:HG22	2:B:162:SER:H	1.78	0.48
2:B:687:CYS:HB3	2:B:688:PRO:HD2	1.95	0.48
1:A:168:ARG:CG	1:A:168:ARG:NH1	2.74	0.48
1:A:249:THR:CG2	2:B:256:ILE:HD13	2.43	0.48
2:B:356:GLU:HA	2:B:385:SER:HB3	1.95	0.48
2:B:641:SER:OG	2:B:683:GLU:HB3	2.13	0.48
1:A:394:GLN:HE21	1:A:394:GLN:H	1.60	0.48
2:B:56:PHE:CZ	2:B:93:ARG:HD3	2.48	0.48
2:B:133:ASN:HD22	2:B:137:LYS:HD3	1.78	0.48
2:B:360:ARG:O	2:B:361:ASP:HB2	2.13	0.48
1:A:285:ILE:HB	1:A:294:PHE:HZ	1.78	0.48
2:B:58:VAL:HG12	2:B:93:ARG:N	2.28	0.48
2:B:101:SER:HA	2:B:398:SER:HA	1.95	0.48
2:B:535:MET:O	2:B:537:SER:N	2.45	0.48
1:A:177:PHE:HB2	1:A:180:GLN:HG3	1.96	0.48
1:A:88:PHE:CZ	1:A:122:ARG:HG2	2.49	0.48
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:SER:OG	1:A:519:PRO:HD2	2.14	0.47
1:A:639:TYR:O	1:A:719:SER:HB2	2.14	0.47
1:A:657:VAL:CG1	1:A:698:ARG:HH21	2.27	0.47
1:A:801:TYR:HB3	1:A:878:GLN:O	2.13	0.47
2:B:193:VAL:O	2:B:194:LEU:HB3	2.14	0.47
2:B:212:VAL:CG1	2:B:213:SER:H	2.22	0.47
1:A:239:PHE:O	1:A:255:ILE:HA	2.13	0.47
1:A:249:THR:HG22	1:A:273:ALA:HA	1.96	0.47
1:A:441:ILE:HD11	1:A:576:PRO:HB2	1.95	0.47
1:A:707:MET:HA	1:A:707:MET:CE	2.37	0.47
1:A:936:LEU:N	1:A:936:LEU:HD12	2.28	0.47
2:B:143:ARG:C	2:B:145:LEU:H	2.20	0.47
2:B:82:GLN:HG2	2:B:107:VAL:HG12	1.96	0.47
2:B:215:ASN:H	2:B:215:ASN:HD22	1.63	0.47
1:A:170:LEU:HD13	1:A:226:VAL:HG21	1.97	0.47
1:A:227:ALA:O	1:A:240:VAL:HB	2.13	0.47
1:A:470:VAL:HG22	1:A:471:SER:N	2.29	0.47
1:A:606:LEU:CB	1:A:727:SER:HB3	2.45	0.47
1:A:906:GLU:C	1:A:908:PHE:N	2.71	0.47
1:A:3:LEU:HA	1:A:437:ALA:HA	1.96	0.47
1:A:441:ILE:O	1:A:578:LEU:HA	2.14	0.47
1:A:754:PHE:HE2	2:B:658:LYS:HE2	1.79	0.47
2:B:90:LEU:HD11	2:B:401:ALA:CB	2.45	0.47
1:A:201:SER:OG	1:A:202:ILE:N	2.48	0.47
1:A:753:VAL:O	1:A:951:VAL:HA	2.14	0.47
2:B:58:VAL:HG12	2:B:92:LEU:HA	1.96	0.47
1:A:228:VAL:HG23	1:A:238:ASP:O	2.14	0.47
1:A:510:ARG:O	1:A:542:LEU:HD12	2.14	0.47
1:A:706:GLU:C	1:A:708:ASP:N	2.67	0.47
2:B:57:PRO:HA	2:B:93:ARG:HH22	1.74	0.47
2:B:115:TYR:HB3	2:B:246:LEU:HD12	1.96	0.47
2:B:100:PHE:CZ	2:B:399:ILE:HB	2.49	0.47
2:B:648:THR:CA	4:I:2:NDG:C1	2.79	0.47
1:A:14:PRO:HG2	1:A:17:SER:CB	2.45	0.47
1:A:487:LEU:H	1:A:488:PRO:CD	2.28	0.47
1:A:523:LYS:HA	1:A:523:LYS:HD2	1.78	0.47
2:B:102:ILE:CG2	2:B:397:PHE:HB2	2.44	0.47
2:B:124:MET:HA	2:B:127:ASP:OD1	2.15	0.47
2:B:333:LEU:HG	2:B:334:SER:H	1.79	0.47
1:A:36:LEU:HG	1:A:423:ILE:HD13	1.96	0.46
1:A:170:LEU:HD13	1:A:226:VAL:HG22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD22	1:A:525:MET:HE1	1.98	0.46
1:A:497:LEU:HA	1:A:558:PHE:O	2.14	0.46
1:A:608:VAL:HG13	1:A:717:ILE:CD1	2.42	0.46
1:A:762:HIS:ND1	1:A:762:HIS:C	2.73	0.46
2:B:158:ASP:OD1	2:B:159:LYS:N	2.47	0.46
2:B:575:CYS:C	2:B:577:GLY:H	2.23	0.46
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.95	0.46
1:A:17:SER:HA	1:A:42:LYS:O	2.15	0.46
1:A:416:LYS:H	1:A:416:LYS:HD2	1.80	0.46
1:A:420:PRO:O	1:A:421:ASP:CG	2.57	0.46
1:A:510:ARG:H	1:A:510:ARG:HD3	1.79	0.46
2:B:647:ASP:CG	2:B:648:THR:N	2.73	0.46
1:A:260:ASN:O	1:A:261:MET:HB3	2.15	0.46
1:A:349:ASP:HB3	1:A:352:GLN:HA	1.96	0.46
1:A:740:ALA:HB2	1:A:788:SER:O	2.15	0.46
1:A:792:LYS:HB2	1:A:930:GLU:HB3	1.95	0.46
1:A:36:LEU:HD11	1:A:434:LEU:HD23	1.98	0.46
1:A:61:TRP:CZ2	1:A:415:ASP:CB	2.99	0.46
1:A:705:SER:HB2	1:A:933:TYR:HE2	1.81	0.46
1:A:802:LYS:HG2	1:A:807:THR:HA	1.97	0.46
2:B:366:LEU:HA	2:B:402:LYS:O	2.15	0.46
1:A:495:VAL:HG23	1:A:561:TYR:HB3	1.98	0.46
3:C:1:NAG:C6	3:C:2:NAG:C1	2.94	0.46
1:A:620:GLY:CA	1:A:891:ARG:HH12	2.27	0.46
1:A:765:ASN:HA	1:A:766:PRO:HD2	1.71	0.46
1:A:927:ASN:HA	1:A:942:THR:HG22	1.97	0.46
2:B:168:SER:O	2:B:169:PRO:O	2.33	0.46
1:A:61:TRP:CG	1:A:414:ILE:HG12	2.50	0.46
1:A:253:VAL:HG21	1:A:295:ILE:CG2	2.46	0.46
1:A:498:LEU:HD12	1:A:558:PHE:HD2	1.78	0.46
1:A:91:HIS:NE2	3:C:2:NAG:H82	2.31	0.46
1:A:338:ALA:HB1	1:A:362:ALA:HB1	1.97	0.46
1:A:404:PHE:C	1:A:404:PHE:CD2	2.92	0.46
1:A:657:VAL:CG2	1:A:663:LEU:HD13	2.46	0.46
2:B:104:VAL:HG21	2:B:421:PHE:HE2	1.81	0.46
2:B:426:ILE:HD12	2:B:426:ILE:H	1.80	0.46
1:A:349:ASP:HB3	1:A:352:GLN:N	2.31	0.46
1:A:434:LEU:HA	1:A:434:LEU:HD22	1.74	0.46
1:A:578:LEU:N	1:A:578:LEU:HD22	2.31	0.46
1:A:886:VAL:HG12	1:A:887:GLY:N	2.30	0.46
1:A:180:GLN:HE22	1:A:213:ALA:CB	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:HB3	1:A:342:SER:HB2	1.97	0.46
1:A:514:LEU:HB3	1:A:515:TYR:CD1	2.51	0.46
2:B:115:TYR:CD1	2:B:236:ILE:HG23	2.51	0.46
2:B:199:GLN:HB2	2:B:202:ARG:HB3	1.98	0.46
1:A:301:MET:HG2	1:A:311:GLU:HA	1.97	0.45
1:A:525:MET:HB3	1:A:526:THR:H	1.59	0.45
2:B:92:LEU:O	2:B:431:PHE:HA	2.15	0.45
2:B:404:ARG:HG3	2:B:548:LEU:HD13	1.99	0.45
2:B:549:CYS:SG	2:B:555:GLY:O	2.73	0.45
1:A:299:LEU:HD21	2:B:257:ALA:HB3	1.97	0.45
1:A:658:ARG:HB3	1:A:665:ARG:HH21	1.81	0.45
1:A:830:PRO:C	1:A:832:ARG:H	2.24	0.45
2:B:315:VAL:HG12	2:B:316:ASN:N	2.30	0.45
2:B:642:VAL:HG21	2:B:680:TYR:HB3	1.97	0.45
2:B:647:ASP:CB	2:B:668:GLN:HE22	2.28	0.45
1:A:239:PHE:CE1	1:A:258:GLY:HA2	2.52	0.45
1:A:497:LEU:O	1:A:498:LEU:HD23	2.17	0.45
1:A:784:ASN:HD21	1:A:789:SER:HA	1.81	0.45
1:A:410:GLY:O	1:A:411:ALA:HB2	2.17	0.45
1:A:469:LYS:HD3	1:A:469:LYS:N	2.23	0.45
1:A:820:MET:CE	1:A:895:ALA:HB1	2.46	0.45
2:B:102:ILE:HG23	2:B:397:PHE:HB2	1.99	0.45
1:A:647:ILE:HB	1:A:651:ALA:CB	2.46	0.45
1:A:710:SER:CA	1:A:736:LEU:HD13	2.42	0.45
2:B:55:GLU:C	2:B:56:PHE:HD2	2.25	0.45
1:A:278:PHE:HE2	1:A:342:SER:O	1.99	0.45
2:B:67:ARG:O	2:B:68:PRO:C	2.59	0.45
1:A:565:TYR:HB3	1:A:575:GLN:HE21	1.81	0.45
1:A:721:ASN:O	1:A:725:LYS:HB3	2.17	0.45
2:B:554:THR:HG23	2:B:560:CYS:HB3	1.99	0.45
1:A:19:PHE:HD1	1:A:431:ARG:HA	1.82	0.45
2:B:622:ARG:HG2	2:B:623:GLU:N	2.31	0.45
1:A:336:VAL:O	1:A:337:PHE:HB2	2.16	0.45
2:B:162:SER:CB	2:B:163:PRO:CD	2.95	0.45
2:B:632:ASN:H	2:B:632:ASN:ND2	2.14	0.45
2:B:646:LYS:HD2	4:I:2:NDG:H8C1	1.98	0.45
1:A:55:GLN:OE1	1:A:69:PRO:HG3	2.16	0.45
1:A:648:PRO:HG3	1:A:711:VAL:CG1	2.47	0.45
2:B:173:LEU:CA	2:B:176:PRO:HD2	2.40	0.45
1:A:247:ALA:C	1:A:248:ARG:HD3	2.43	0.44
1:A:1:PHE:HB3	1:A:377:ASN:OD1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TYR:CE1	1:A:36:LEU:HD22	2.51	0.44
1:A:314:GLN:HE22	1:A:330:LYS:HG2	1.81	0.44
1:A:617:ILE:HD11	1:A:736:LEU:HD12	1.99	0.44
1:A:799:TRP:CD1	1:A:800:PRO:O	2.71	0.44
1:A:927:ASN:C	1:A:927:ASN:ND2	2.75	0.44
1:A:946:LEU:H	1:A:946:LEU:CD2	2.25	0.44
2:B:332:VAL:HG12	2:B:674:SER:OG	2.17	0.44
2:B:593:SER:HB3	2:B:601:CYS:SG	2.57	0.44
1:A:64:THR:O	1:A:65:ARG:HB2	2.17	0.44
1:A:565:TYR:HB3	1:A:575:GLN:NE2	2.31	0.44
2:B:156:PHE:HA	2:B:189:GLY:O	2.17	0.44
1:A:68:GLN:CB	1:A:69:PRO:HD2	2.43	0.44
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.99	0.44
1:A:248:ARG:HH11	1:A:248:ARG:N	2.15	0.44
1:A:645:VAL:HG22	1:A:715:LEU:CD2	2.47	0.44
1:A:650:GLN:CD	1:A:650:GLN:H	2.25	0.44
1:A:784:ASN:ND2	1:A:789:SER:HA	2.32	0.44
2:B:159:LYS:HZ1	2:B:288:ASP:HA	1.81	0.44
2:B:173:LEU:C	2:B:175:ASN:N	2.73	0.44
1:A:478:CYS:O	1:A:479:LEU:HB3	2.16	0.44
1:A:741:ALA:N	1:A:786:GLY:HA3	2.30	0.44
1:A:800:PRO:O	1:A:801:TYR:HB2	2.17	0.44
1:A:869:ILE:HG13	1:A:870:HIS:ND1	2.33	0.44
1:A:21:PHE:CE1	2:B:266:VAL:HG11	2.53	0.44
1:A:108:CYS:SG	1:A:161:ILE:HD13	2.58	0.44
1:A:469:LYS:H	1:A:469:LYS:CD	2.26	0.44
1:A:527:ILE:O	1:A:528:SER:HB2	2.16	0.44
1:A:812:LEU:O	1:A:813:HIS:HB3	2.18	0.44
2:B:79:GLN:O	2:B:80:VAL:O	2.36	0.44
2:B:652:ALA:HB2	2:B:670:TYR:HA	1.99	0.44
1:A:36:LEU:HD11	1:A:434:LEU:CD2	2.47	0.44
2:B:115:TYR:CE1	2:B:236:ILE:HG23	2.52	0.44
2:B:540:GLY:C	2:B:542:CYS:H	2.26	0.44
1:A:549:ARG:HA	1:A:549:ARG:NE	2.33	0.44
1:A:555:ILE:N	1:A:590:ALA:O	2.46	0.44
1:A:821:ASN:HD22	1:A:821:ASN:HA	1.70	0.44
2:B:84:SER:HG	2:B:103:GLN:H	1.66	0.44
2:B:112:VAL:HG21	2:B:142:MET:CE	2.47	0.44
2:B:168:SER:N	2:B:169:PRO:CD	2.74	0.44
2:B:227:MET:O	2:B:231:VAL:HG22	2.18	0.44
2:B:333:LEU:HG	2:B:334:SER:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:VAL:O	2:B:385:SER:HA	2.18	0.44
2:B:646:LYS:H	2:B:646:LYS:CD	2.31	0.44
1:A:259:LYS:HA	1:A:259:LYS:CE	2.33	0.44
1:A:97:SER:OG	1:A:108:CYS:HB2	2.18	0.43
1:A:170:LEU:HD11	1:A:239:PHE:HB3	2.00	0.43
1:A:790:PHE:C	1:A:790:PHE:CD1	2.95	0.43
1:A:264:LEU:O	3:D:1:NAG:H81	2.18	0.43
1:A:348:GLY:O	1:A:356:ASN:HA	2.18	0.43
1:A:450:TYR:CB	1:A:451:PRO:CD	2.96	0.43
1:A:513:PHE:CD1	1:A:521:HIS:HB2	2.53	0.43
1:A:946:LEU:HD23	1:A:946:LEU:N	2.29	0.43
2:B:356:GLU:HA	2:B:385:SER:CB	2.47	0.43
2:B:363:PRO:HB2	2:B:366:LEU:CD2	2.48	0.43
2:B:652:ALA:CB	2:B:670:TYR:HA	2.47	0.43
1:A:25:PHE:CE1	1:A:410:GLY:HA2	2.49	0.43
1:A:390:ILE:O	1:A:390:ILE:HG13	2.18	0.43
2:B:82:GLN:O	2:B:104:VAL:HA	2.18	0.43
1:A:521:HIS:CE1	1:A:538:LEU:HD11	2.52	0.43
2:B:62:ARG:HG3	2:B:63:VAL:N	2.32	0.43
2:B:573:LEU:HD23	2:B:574:LEU:N	2.32	0.43
1:A:340:PHE:O	1:A:361:ALA:O	2.36	0.43
1:A:607:GLU:CD	1:A:632:GLN:HB2	2.43	0.43
1:A:674:ASN:C	1:A:676:THR:N	2.76	0.43
2:B:650:LYS:HG2	4:I:1:NAG:C6	2.46	0.43
1:A:275:TYR:CE1	2:B:256:ILE:HD11	2.54	0.43
1:A:456:GLN:CD	1:A:545:GLU:HG3	2.44	0.43
2:B:74:SER:O	2:B:75:GLY:C	2.62	0.43
2:B:228:GLN:C	2:B:230:THR:N	2.75	0.43
2:B:240:ASN:HD22	2:B:240:ASN:N	2.17	0.43
2:B:646:LYS:O	4:I:2:NDG:C8	2.51	0.43
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.84	0.43
1:A:187:GLN:NE2	1:A:206:ASN:HB2	2.34	0.43
1:A:429:VAL:HB	1:A:431:ARG:HH11	1.83	0.43
1:A:808:LEU:O	1:A:808:LEU:HD12	2.18	0.43
2:B:62:ARG:NH1	2:B:85:PRO:HB2	2.34	0.43
1:A:787:PRO:HA	1:A:891:ARG:HD3	2.00	0.43
2:B:146:THR:HG22	2:B:147:SER:N	2.33	0.43
2:B:244:HIS:ND1	2:B:244:HIS:N	2.66	0.43
2:B:366:LEU:HD11	2:B:414:PHE:CE2	2.54	0.43
2:B:418:PRO:HB2	2:B:421:PHE:CD2	2.53	0.43
2:B:599:GLU:HG2	2:B:600:LYS:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:O	1:A:103:ASP:HB2	2.19	0.43
1:A:272:MET:HE1	5:B:3320:NAG:O7	2.18	0.43
2:B:139:ALA:O	2:B:143:ARG:N	2.52	0.43
2:B:676:LYS:HG2	2:B:677:SER:N	2.32	0.43
1:A:102:GLN:O	1:A:102:GLN:HG2	2.19	0.43
1:A:372:ILE:HA	1:A:391:LEU:O	2.18	0.43
1:A:339:ARG:HD3	1:A:364:TYR:CD1	2.54	0.42
1:A:376:PHE:CD1	1:A:376:PHE:N	2.84	0.42
1:A:605:LYS:H	1:A:635:GLY:N	2.14	0.42
2:B:71:ASP:CB	2:B:108:GLU:HB2	2.42	0.42
2:B:126:ASP:N	2:B:126:ASP:OD2	2.51	0.42
2:B:173:LEU:HD11	2:B:178:TYR:CE1	2.54	0.42
2:B:356:GLU:HB3	2:B:419:VAL:CG2	2.49	0.42
2:B:363:PRO:HB2	2:B:366:LEU:HD23	2.00	0.42
1:A:26:PHE:HB2	1:A:37:LEU:HD21	2.01	0.42
1:A:550:ASP:CG	1:A:551:LYS:N	2.77	0.42
1:A:800:PRO:HG3	1:A:921:LYS:O	2.19	0.42
2:B:138:LEU:HA	2:B:341:LEU:HD12	2.00	0.42
1:A:113:HIS:NE2	1:A:124:PRO:HB3	2.34	0.42
1:A:173:GLY:O	1:A:181:GLY:HA2	2.19	0.42
1:A:349:ASP:C	1:A:351:ASP:N	2.74	0.42
1:A:42:LYS:HZ3	1:A:93:TRP:NE1	2.17	0.42
1:A:384:ASN:HD21	1:A:386:VAL:HG22	1.84	0.42
1:A:454:LEU:HG	1:A:591:HIS:O	2.19	0.42
1:A:454:LEU:HA	5:A:2458:NAG:H61	2.00	0.42
1:A:474:ASN:ND2	1:A:539:ILE:HA	2.34	0.42
1:A:476:ARG:HG3	1:A:476:ARG:O	2.18	0.42
1:A:721:ASN:HD22	1:A:722:LEU:H	1.67	0.42
1:A:776:VAL:HG11	1:A:949:THR:HG21	2.00	0.42
2:B:87:ARG:HG3	2:B:88:ILE:H	1.84	0.42
2:B:567:CYS:O	2:B:568:MET:O	2.37	0.42
1:A:253:VAL:HG21	1:A:295:ILE:HG21	2.00	0.42
1:A:416:LYS:HD2	1:A:416:LYS:N	2.34	0.42
1:A:901:SER:O	1:A:902:LEU:HB3	2.19	0.42
1:A:2:ASN:HA	1:A:389:GLN:OE1	2.19	0.42
1:A:113:HIS:HD2	1:A:122:ARG:O	2.02	0.42
1:A:409:LYS:HD2	1:A:410:GLY:H	1.84	0.42
1:A:717:ILE:HG22	1:A:718:GLN:N	2.34	0.42
1:A:769:GLU:OE1	1:A:835:ILE:HA	2.20	0.42
1:A:20:GLY:HA2	1:A:38:VAL:HG13	2.02	0.42
1:A:116:THR:HG22	1:A:147:ILE:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:NE2	1:A:213:ALA:H	2.17	0.42
1:A:557:ILE:O	1:A:587:SER:HB2	2.20	0.42
1:A:741:ALA:H	1:A:786:GLY:CA	2.32	0.42
2:B:68:PRO:HD3	2:B:84:SER:HA	2.02	0.42
2:B:226:ILE:HD11	2:B:248:PHE:CG	2.54	0.42
2:B:374:CYS:SG	2:B:395:VAL:HB	2.60	0.42
2:B:409:GLU:O	2:B:410:LYS:HB2	2.18	0.42
2:B:553:TRP:HE3	2:B:560:CYS:O	2.01	0.42
2:B:246:LEU:HD23	2:B:306:LEU:HD13	2.02	0.42
1:A:441:ILE:HB	1:A:578:LEU:HD13	2.02	0.42
1:A:792:LYS:HA	1:A:887:GLY:HA2	2.01	0.42
1:A:871:THR:HG23	1:A:871:THR:O	2.20	0.42
2:B:191:LYS:HG3	2:B:280:HIS:CD2	2.55	0.42
2:B:406:CYS:O	2:B:406:CYS:SG	2.77	0.42
1:A:487:LEU:N	1:A:488:PRO:CD	2.82	0.42
1:A:603:LYS:HB2	1:A:603:LYS:HE3	1.79	0.42
1:A:749:SER:CB	1:A:750:PRO:HD3	2.34	0.42
1:A:578:LEU:HD22	1:A:578:LEU:H	1.85	0.41
1:A:586:ILE:HD12	1:A:586:ILE:HA	1.78	0.41
1:A:809:LEU:HD22	1:A:901:SER:OG	2.20	0.41
2:B:111:PRO:HB2	2:B:148:ASN:HD22	1.85	0.41
1:A:674:ASN:ND2	1:A:675:GLN:H	2.18	0.41
1:A:194:LYS:HE2	1:A:194:LYS:HB2	1.82	0.41
1:A:639:TYR:O	1:A:640:GLU:C	2.64	0.41
1:A:712:LYS:CA	1:A:733:LYS:HA	2.42	0.41
2:B:575:CYS:HB2	2:B:579:GLY:O	2.19	0.41
2:B:624:PRO:C	2:B:626:MET:N	2.77	0.41
1:A:395:TRP:CB	1:A:429:VAL:HG21	2.50	0.41
1:A:453:ILE:C	1:A:454:LEU:HD23	2.45	0.41
1:A:504:GLN:HB3	1:A:505:LYS:H	1.55	0.41
1:A:647:ILE:HD12	1:A:651:ALA:CB	2.51	0.41
2:B:215:ASN:HD22	2:B:215:ASN:N	2.18	0.41
2:B:534:GLU:C	2:B:536:CYS:N	2.78	0.41
2:B:622:ARG:CG	2:B:623:GLU:H	2.34	0.41
2:B:622:ARG:CG	2:B:623:GLU:N	2.83	0.41
2:B:658:LYS:HA	2:B:663:CYS:O	2.19	0.41
1:A:568:ALA:HB1	1:A:574:LEU:H	1.85	0.41
2:B:214:ARG:HG3	2:B:214:ARG:NH1	2.31	0.41
3:C:1:NAG:H61	3:C:2:NAG:O5	2.20	0.41
2:B:58:VAL:H	2:B:93:ARG:HH21	1.68	0.41
2:B:650:LYS:HA	4:I:1:NAG:O6	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PHE:O	1:A:2:ASN:OD1	2.38	0.41
1:A:396:ALA:O	1:A:397:ALA:HB2	2.21	0.41
1:A:487:LEU:O	1:A:488:PRO:O	2.39	0.41
1:A:627:LEU:O	1:A:696:GLY:HA2	2.21	0.41
2:B:103:GLN:HG3	2:B:396:SER:HB2	2.01	0.41
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.91	0.41
1:A:50:ILE:HD12	1:A:89:LYS:HB2	2.02	0.41
2:B:568:MET:O	2:B:569:SER:CB	2.68	0.41
2:B:580:LYS:NZ	2:B:582:GLU:HB2	2.36	0.41
2:B:615:VAL:O	2:B:620:PHE:HD1	2.03	0.41
1:A:347:LEU:CD1	1:A:357:ASP:HB2	2.51	0.41
1:A:355:PHE:CZ	1:A:380:SER:HB3	2.56	0.41
1:A:375:ILE:CD1	1:A:389:GLN:HB3	2.51	0.41
1:A:614:GLN:NE2	1:A:616:LYS:HD2	2.36	0.41
2:B:199:GLN:C	2:B:201:THR:H	2.29	0.41
2:B:251:ASP:HA	2:B:311:THR:OG1	2.21	0.41
2:B:293:GLY:O	2:B:296:THR:HB	2.21	0.41
2:B:375:LEU:HA	2:B:375:LEU:HD23	1.74	0.41
2:B:646:LYS:HD2	4:I:2:NDG:C8	2.51	0.41
1:A:623:ASN:O	1:A:700:SER:HA	2.21	0.41
1:A:784:ASN:O	1:A:891:ARG:O	2.39	0.41
2:B:534:GLU:CG	2:B:544:CYS:SG	3.06	0.41
1:A:429:VAL:HG23	1:A:431:ARG:HG3	2.03	0.40
1:A:631:ALA:HA	1:A:717:ILE:HD11	2.03	0.40
2:B:65:GLU:O	2:B:65:GLU:HG3	2.19	0.40
2:B:102:ILE:C	2:B:102:ILE:HD13	2.46	0.40
2:B:120:LEU:HA	2:B:120:LEU:HD12	1.83	0.40
2:B:380:ILE:HA	2:B:381:PRO:HD2	1.88	0.40
1:A:507:ALA:C	1:A:509:ARG:H	2.29	0.40
1:A:674:ASN:O	1:A:676:THR:N	2.47	0.40
1:A:693:LEU:HA	1:A:693:LEU:HD13	1.81	0.40
2:B:111:PRO:HB3	2:B:148:ASN:HB3	2.02	0.40
2:B:177:CYS:SG	2:B:214:ARG:HB3	2.62	0.40
2:B:638:GLU:O	2:B:638:GLU:HG3	2.21	0.40
1:A:55:GLN:HG3	1:A:57:LEU:HD11	2.04	0.40
1:A:142:CYS:C	1:A:144:SER:N	2.79	0.40
1:A:496:GLU:O	1:A:559:MET:HA	2.21	0.40
1:A:653:PHE:HA	1:A:699:PHE:CD1	2.52	0.40
2:B:315:VAL:O	2:B:317:LEU:N	2.55	0.40
2:B:421:PHE:N	2:B:421:PHE:CD1	2.86	0.40
2:B:575:CYS:O	2:B:577:GLY:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:625:TYR:HD1	2:B:625:TYR:HA	1.76	0.40
1:A:104:LYS:HE3	1:A:167:ASP:OD1	2.22	0.40
1:A:490:LYS:HG3	1:A:567:THR:HG23	2.04	0.40
1:A:645:VAL:HG21	1:A:697:LEU:CD1	2.51	0.40
1:A:651:ALA:O	1:A:652:ASP:HB2	2.22	0.40
1:A:908:PHE:HB3	1:A:909:MET:H	1.51	0.40
2:B:178:TYR:CG	2:B:179:ASP:N	2.89	0.40
2:B:185:LEU:HD12	2:B:211:SER:HB3	2.01	0.40
2:B:534:GLU:OE1	2:B:544:CYS:SG	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	923/957 (96%)	708 (77%)	157 (17%)	58 (6%)	1	6
2	B	535/692 (77%)	388 (72%)	102 (19%)	45 (8%)	0	4
All	All	1458/1649 (88%)	1096 (75%)	259 (18%)	103 (7%)	1	5

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	69	PRO
1	A	118	MET
1	A	169	VAL
1	A	205	ASN
1	A	396	ALA
1	A	411	ALA
1	A	417	ASN
1	A	420	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	450	TYR
1	A	484	LYS
1	A	487	LEU
1	A	488	PRO
1	A	504	GLN
1	A	514	LEU
1	A	527	ILE
1	A	572	THR
1	A	685	ASN
1	A	688	LYS
1	A	703	GLN
1	A	704	GLN
1	A	705	SER
1	A	757	ILE
1	A	869	ILE
1	A	874	CYS
1	A	888	ARG
2	B	70	SER
2	B	80	VAL
2	B	88	ILE
2	B	162	SER
2	B	167	ILE
2	B	168	SER
2	B	169	PRO
2	B	176	PRO
2	B	199	GLN
2	B	377	ASN
2	B	536	CYS
2	B	546	ASP
2	B	568	MET
2	B	569	SER
1	A	71	GLU
1	A	82	LYS
1	A	101	LYS
1	A	167	ASP
1	A	287	GLY
1	A	289	ASP
1	A	397	ALA
1	A	464	PRO
1	A	528	SER
1	A	554	PRO
1	A	707	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	708	ASP
1	A	759	ASN
1	A	801	TYR
1	A	835	ILE
1	A	917	SER
2	B	75	GLY
2	B	84	SER
2	B	86	GLN
2	B	157	VAL
2	B	182	THR
2	B	253	LYS
2	B	316	ASN
2	B	346	ASP
2	B	433	CYS
2	B	576	SER
2	B	673	SER
2	B	677	SER
1	A	569	ALA
1	A	675	GLN
1	A	908	PHE
1	A	943	ASN
2	B	172	ALA
2	B	407	PRO
2	B	410	LYS
2	B	412	LYS
2	B	547	CYS
2	B	608	CYS
1	A	62	SER
1	A	194	LYS
1	A	598	GLU
1	A	662	ALA
2	B	362	LEU
2	B	535	MET
2	B	538	GLY
2	B	539	HIS
2	B	671	GLU
1	A	288	ASP
1	A	371	GLY
1	A	800	PRO
1	A	890	ASP
1	A	910	ASN
2	B	315	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	402	LYS
2	B	623	GLU
2	B	643	LYS
2	B	647	ASP
1	A	202	ILE
1	A	387	PRO
2	B	175	ASN
2	B	229	ALA
2	B	543	SER
1	A	508	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	787/812 (97%)	703 (89%)	84 (11%)	6	25
2	B	484/616 (79%)	417 (86%)	67 (14%)	3	15
All	All	1271/1428 (89%)	1120 (88%)	151 (12%)	5	21

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	34	MET
1	A	36	LEU
1	A	60	ASP
1	A	69	PRO
1	A	73	ASP
1	A	90	SER
1	A	99	ARG
1	A	100	SER
1	A	121	GLU
1	A	142	CYS
1	A	143	ARG
1	A	146	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	147	ILE
1	A	161	ILE
1	A	170	LEU
1	A	171	LEU
1	A	236	ILE
1	A	243	VAL
1	A	248	ARG
1	A	249	THR
1	A	257	ASP
1	A	259	LYS
1	A	275	TYR
1	A	286	ASN
1	A	289	ASP
1	A	306	ASP
1	A	327	GLN
1	A	331	LEU
1	A	347	LEU
1	A	349	ASP
1	A	352	GLN
1	A	357	ASP
1	A	372	ILE
1	A	394	GLN
1	A	434	LEU
1	A	442	THR
1	A	447	LEU
1	A	459	LYS
1	A	460	THR
1	A	472	CYS
1	A	479	LEU
1	A	490	LYS
1	A	494	GLN
1	A	508	ILE
1	A	510	ARG
1	A	514	LEU
1	A	527	ILE
1	A	539	ILE
1	A	549	ARG
1	A	553	THR
1	A	554	PRO
1	A	565	TYR
1	A	574	LEU
1	A	608	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	623	ASN
1	A	649	LEU
1	A	650	GLN
1	A	656	VAL
1	A	657	VAL
1	A	673	GLU
1	A	678	GLN
1	A	685	ASN
1	A	688	LYS
1	A	703	GLN
1	A	721	ASN
1	A	734	VAL
1	A	736	LEU
1	A	753	VAL
1	A	762	HIS
1	A	789	SER
1	A	880	LEU
1	A	897	LEU
1	A	902	LEU
1	A	903	LEU
1	A	904	TRP
1	A	906	GLU
1	A	907	THR
1	A	914	GLN
1	A	919	SER
1	A	931	PHE
1	A	945	THR
1	A	948	THR
1	A	956	GLN
2	B	55	GLU
2	B	56	PHE
2	B	58	VAL
2	B	68	PRO
2	B	69	LEU
2	B	86	GLN
2	B	87	ARG
2	B	88	ILE
2	B	99	ASN
2	B	102	ILE
2	B	104	VAL
2	B	108	GLU
2	B	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	120	LEU
2	B	131	ILE
2	B	145	LEU
2	B	151	ILE
2	B	161	VAL
2	B	166	TYR
2	B	167	ILE
2	B	173	LEU
2	B	174	GLU
2	B	176	PRO
2	B	178	TYR
2	B	180	MET
2	B	187	MET
2	B	195	THR
2	B	198	ASP
2	B	215	ASN
2	B	220	GLU
2	B	244	HIS
2	B	261	ARG
2	B	262	LEU
2	B	269	ASN
2	B	286	THR
2	B	291	SER
2	B	292	LEU
2	B	299	LEU
2	B	320	ASN
2	B	329	THR
2	B	336	ASP
2	B	341	LEU
2	B	355	VAL
2	B	364	GLU
2	B	376	ASN
2	B	389	LEU
2	B	391	ILE
2	B	408	GLN
2	B	409	GLU
2	B	434	ASP
2	B	534	GLU
2	B	539	HIS
2	B	544	CYS
2	B	546	ASP
2	B	561	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	580	LYS
2	B	615	VAL
2	B	619	LYS
2	B	626	MET
2	B	632	ASN
2	B	639	ILE
2	B	642	VAL
2	B	644	GLU
2	B	646	LYS
2	B	654	ASN
2	B	673	SER
2	B	683	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	77	ASN
1	A	92	GLN
1	A	156	GLN
1	A	180	GLN
1	A	205	ASN
1	A	271	GLN
1	A	310	GLN
1	A	314	GLN
1	A	327	GLN
1	A	384	ASN
1	A	394	GLN
1	A	455	ASN
1	A	456	GLN
1	A	474	ASN
1	A	521	HIS
1	A	575	GLN
1	A	580	GLN
1	A	614	GLN
1	A	633	ASN
1	A	659	ASN
1	A	660	ASN
1	A	674	ASN
1	A	685	ASN
1	A	692	GLN
1	A	702	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	703	GLN
1	A	721	ASN
1	A	732	HIS
1	A	759	ASN
1	A	778	HIS
1	A	821	ASN
1	A	927	ASN
1	A	935	ASN
2	B	99	ASN
2	B	133	ASN
2	B	215	ASN
2	B	240	ASN
2	B	255	HIS
2	B	269	ASN
2	B	279	ASN
2	B	316	ASN
2	B	319	GLN
2	B	376	ASN
2	B	428	GLN
2	B	629	ASN
2	B	632	ASN
2	B	668	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 ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	1,3	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
3	NAG	C	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.72	0
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	1.35	2 (11%)
3	NAG	D	2	3	14,14,15	0.79	1 (7%)	17,19,21	0.71	0
3	NAG	E	1	1,3	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.64	0
4	NAG	F	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	0.92	1 (5%)
4	NDG	F	2	4	14,14,15	0.59	0	17,19,21	0.71	0
3	NAG	G	1	1,3	14,14,15	0.49	0	17,19,21	0.84	0
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.64	0
4	NAG	H	1	4,2	14,14,15	0.44	0	17,19,21	1.15	1 (5%)
4	NDG	H	2	4	14,14,15	0.47	0	17,19,21	0.70	0
4	NAG	I	1	4,2	14,14,15	0.55	0	17,19,21	1.31	2 (11%)
4	NDG	I	2	4	14,14,15	0.79	0	17,19,21	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	3/6/23/26	0/1/1/1
4	NDG	F	2	4	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	1/6/23/26	0/1/1/1
4	NDG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	0/6/23/26	0/1/1/1
4	NDG	I	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.38	1.55	1.52
4	F	1	NAG	C1-C2	2.31	1.55	1.52
3	D	2	NAG	C1-C2	2.11	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C4-C3-C2	-3.92	105.28	111.02
4	H	1	NAG	C2-N2-C7	-3.53	118.17	122.90
3	D	1	NAG	O5-C1-C2	-2.83	106.91	111.29
4	F	1	NAG	C2-N2-C7	-2.81	119.14	122.90
4	I	1	NAG	C1-O5-C5	2.41	115.42	112.19
3	E	1	NAG	C2-N2-C7	-2.22	119.93	122.90
4	I	2	NDG	O5-C1-C2	-2.16	107.96	111.29
4	I	1	NAG	C2-N2-C7	-2.10	120.09	122.90
3	C	1	NAG	C2-N2-C7	-2.02	120.20	122.90

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	I	2	NDG	O5-C5-C6-O6
4	I	2	NDG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
4	H	2	NDG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

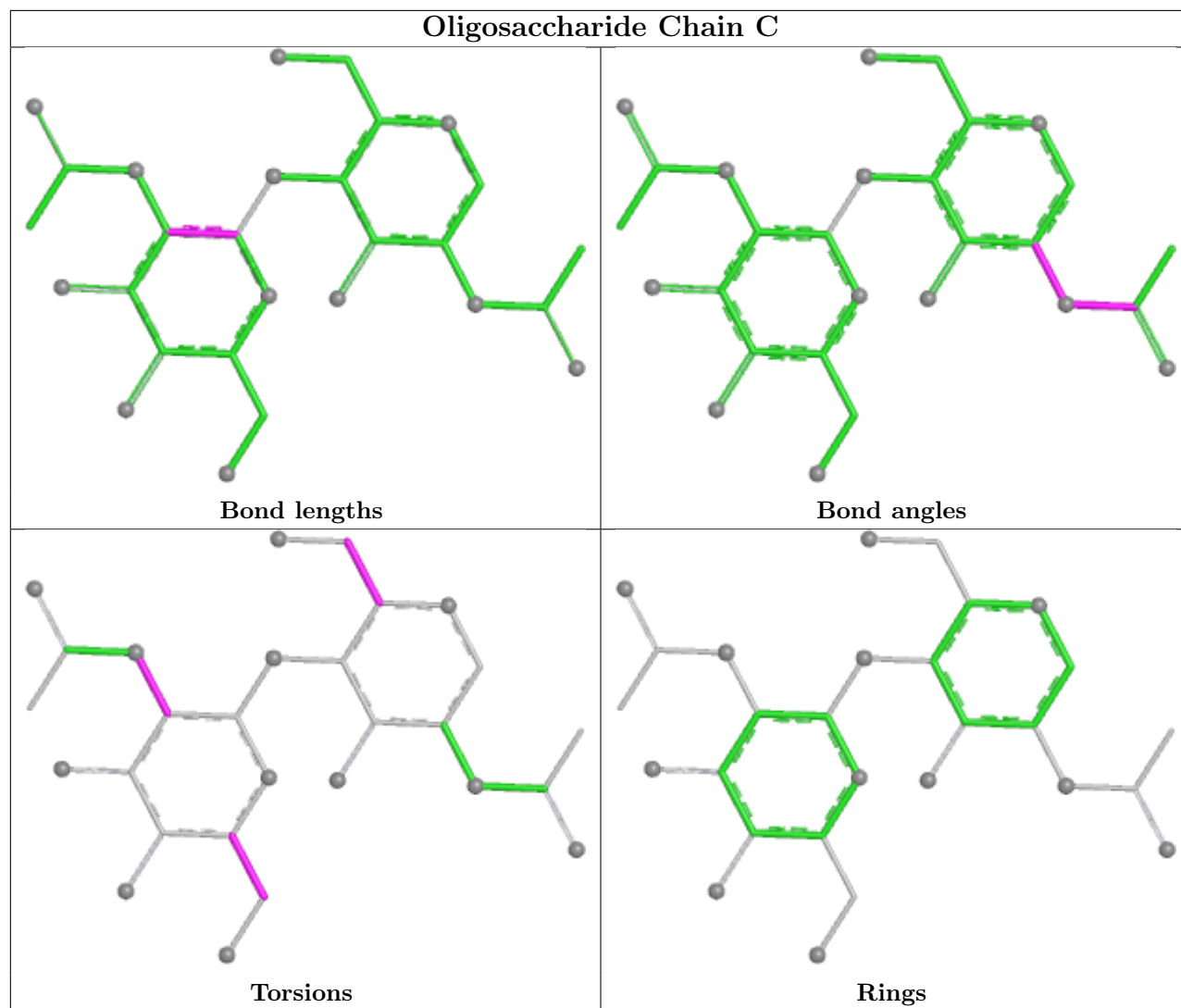
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C1-C2-N2-C7
4	F	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

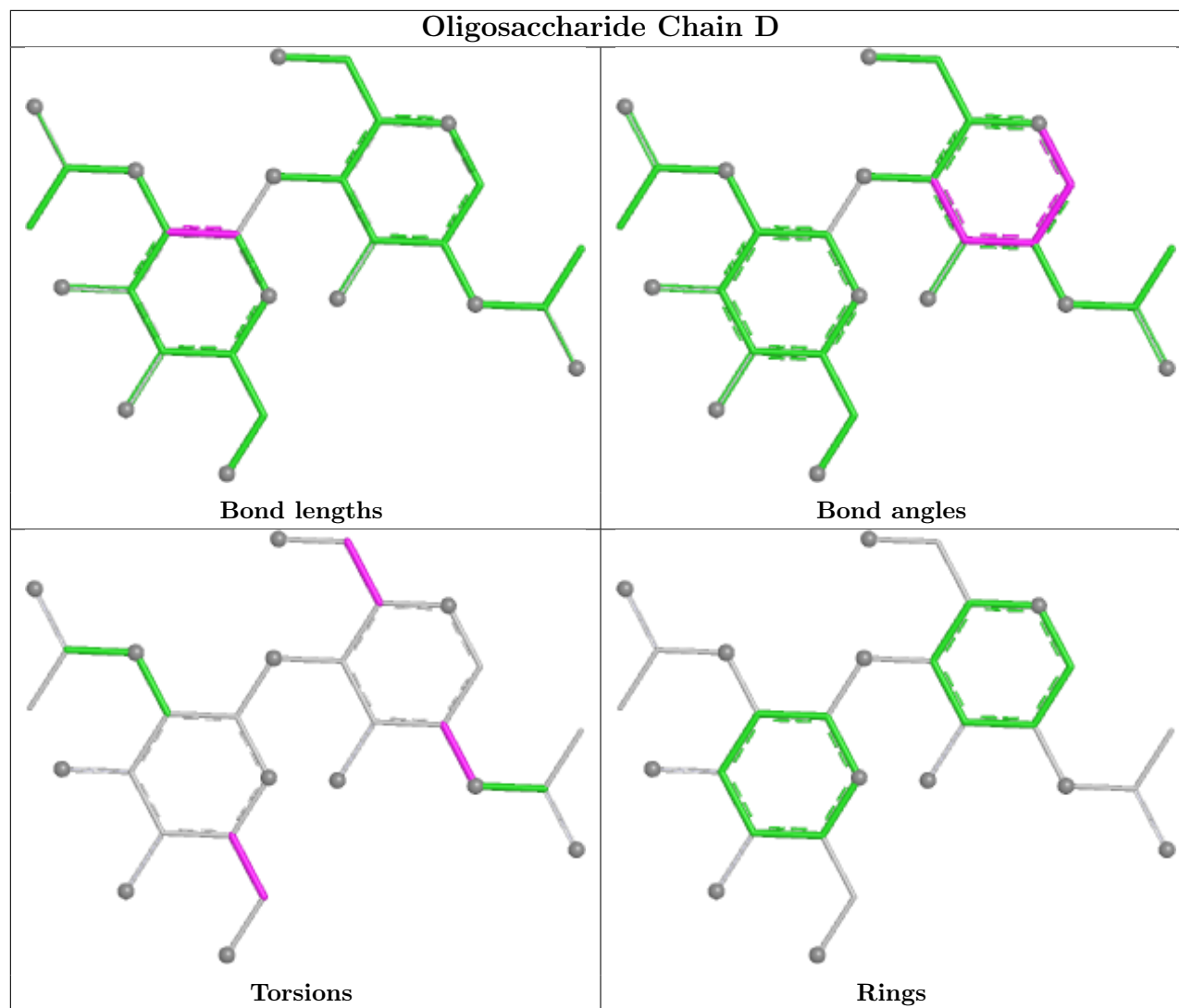
There are no ring outliers.

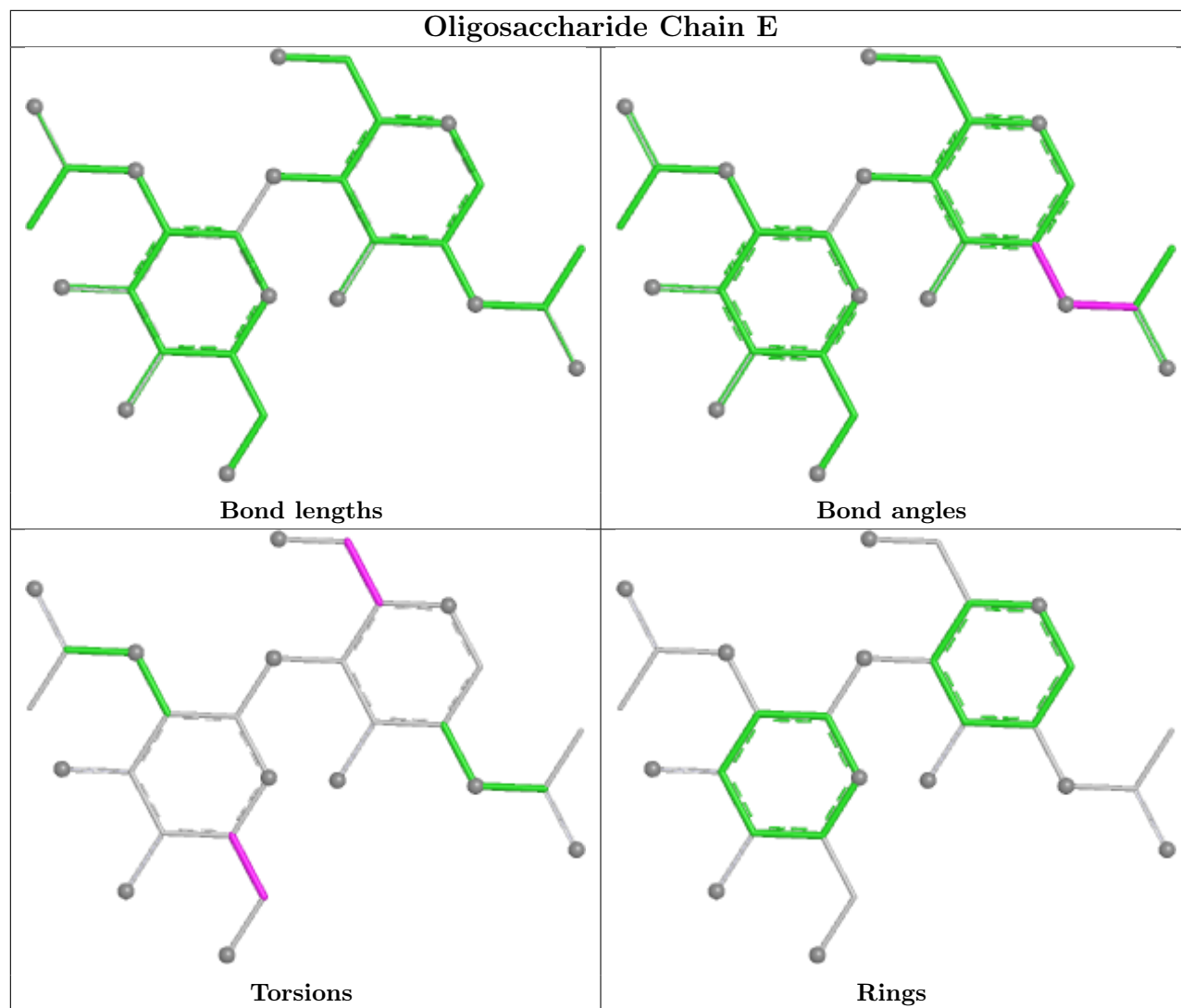
13 monomers are involved in 30 short contacts:

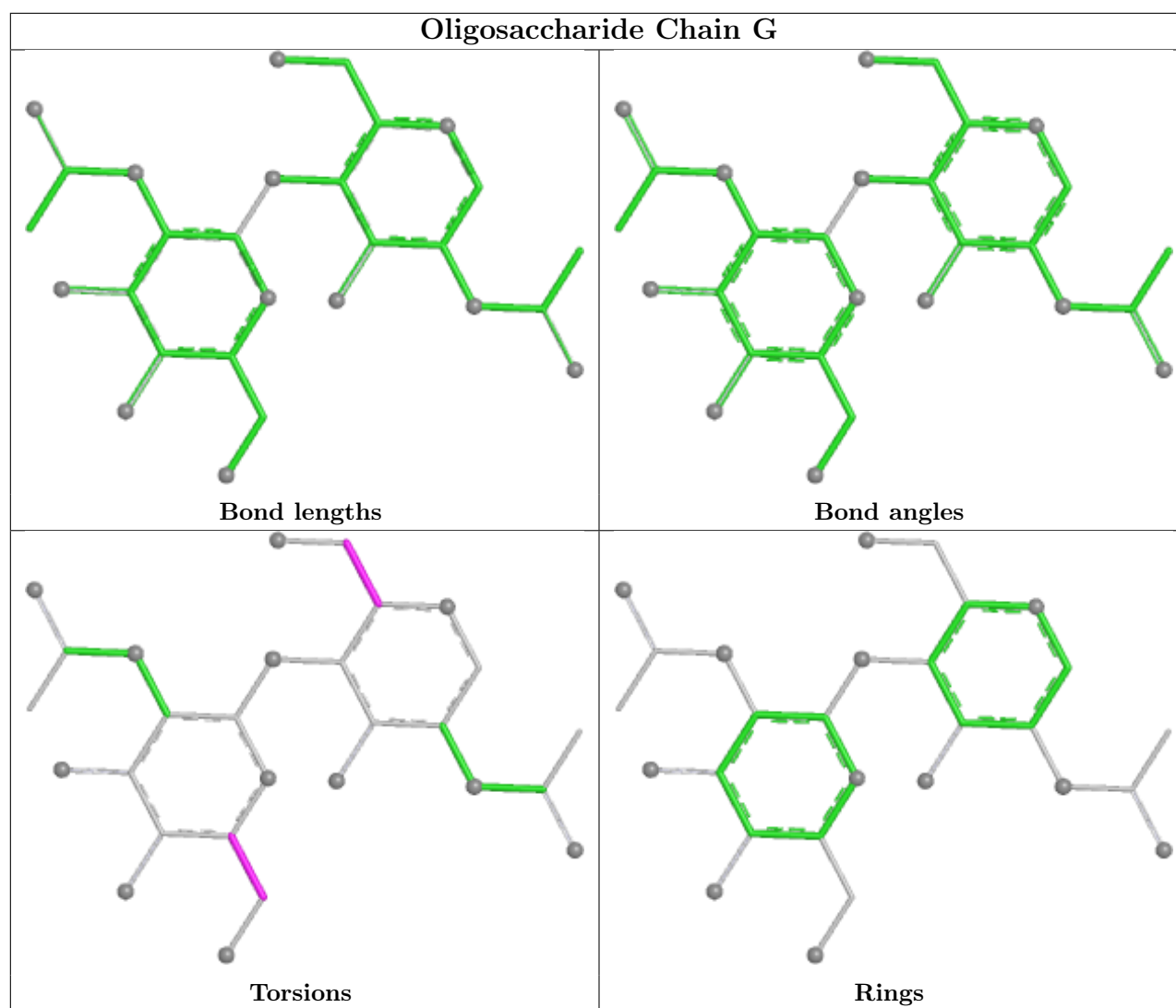
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	3	0
4	H	2	NDG	3	0
3	C	1	NAG	2	0
3	C	2	NAG	3	0
3	G	2	NAG	1	0
4	F	2	NDG	3	0
4	F	1	NAG	4	0
3	G	1	NAG	1	0
4	I	2	NDG	7	0
3	D	2	NAG	1	0
4	H	1	NAG	1	0
3	D	1	NAG	2	0
3	E	1	NAG	3	0

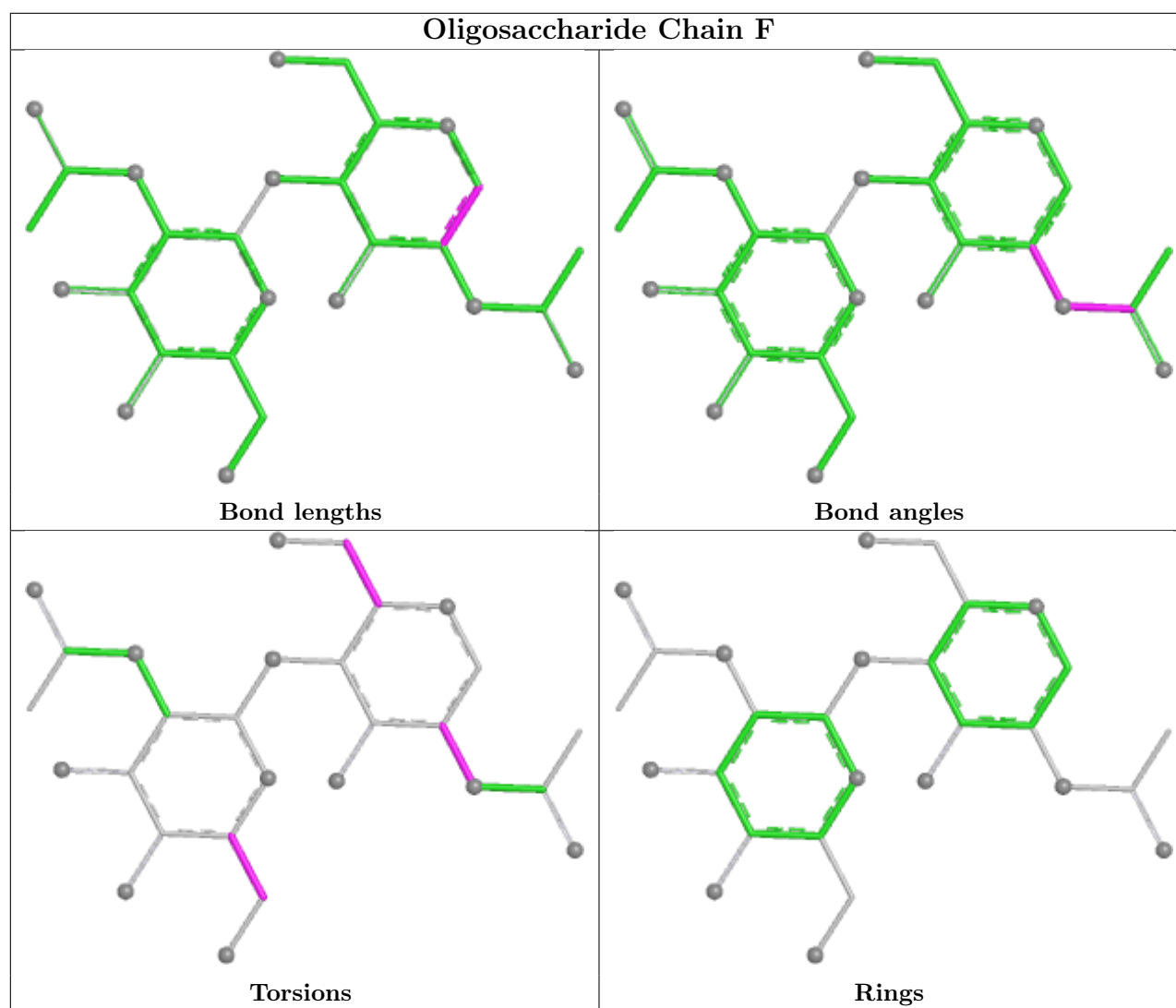
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

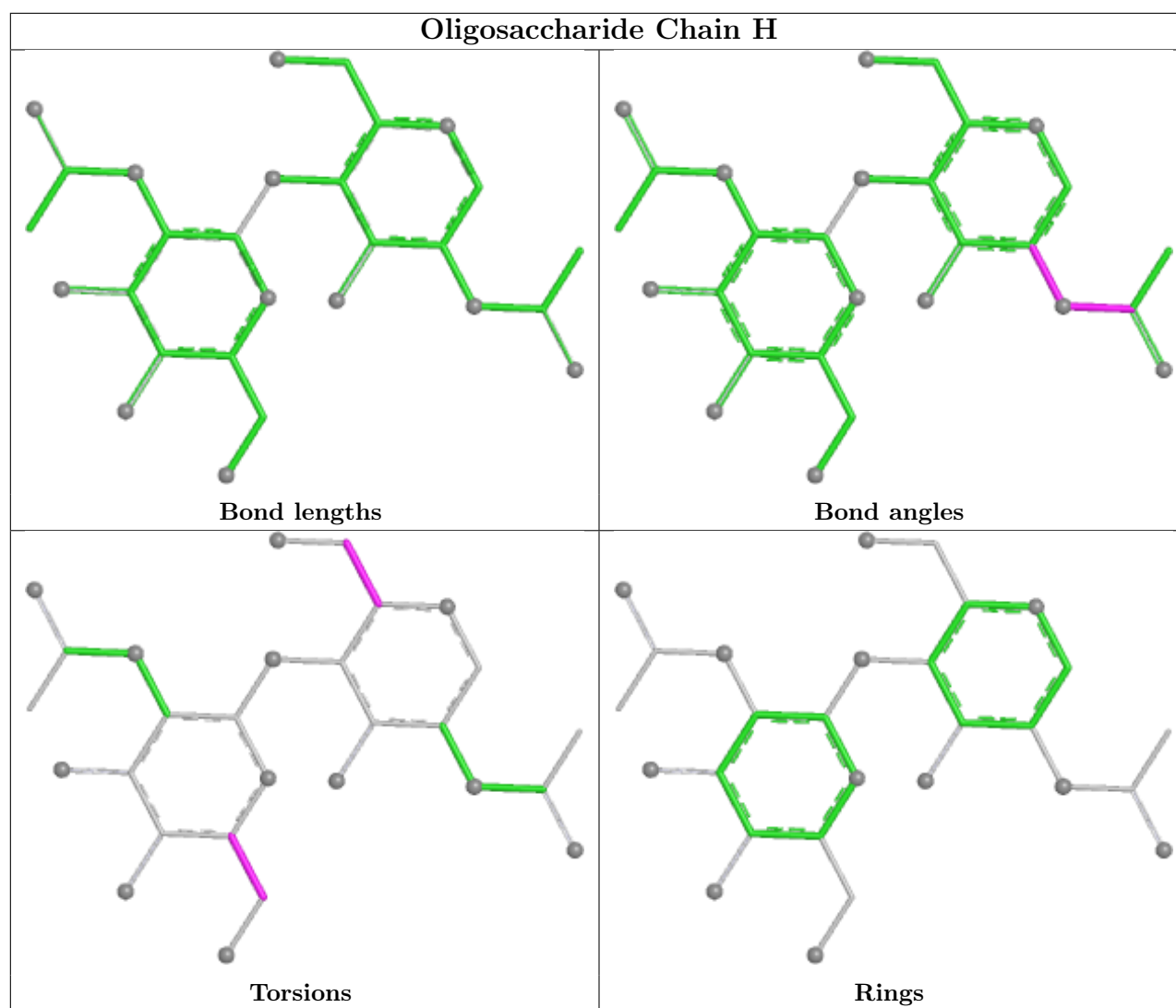


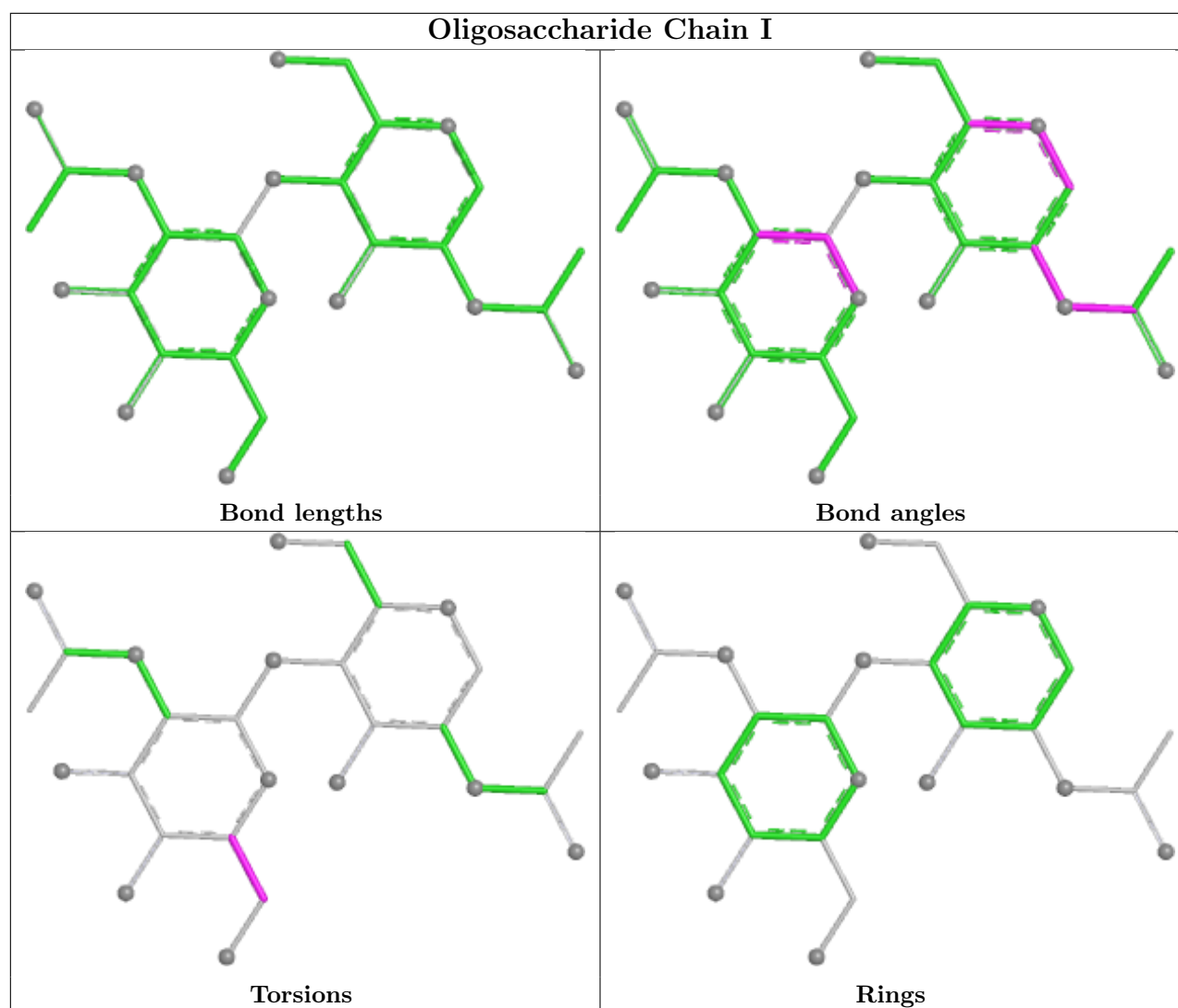












5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
5	NAG	B	3371	2	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
5	NAG	A	2458	1	14,14,15	0.74	0	17,19,21	0.85	1 (5%)
5	NAG	B	3320	2	14,14,15	0.45	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	2260	1	14,14,15	0.50	0	17,19,21	0.74	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
5	NAG	B	3371	2	-	4/6/23/26	0/1/1/1
5	NAG	A	2458	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3320	2	-	1/6/23/26	0/1/1/1
5	NAG	A	2260	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3371	NAG	C2-N2-C7	-3.10	118.75	122.90
5	A	2458	NAG	C2-N2-C7	-2.27	119.86	122.90
5	B	3320	NAG	C2-N2-C7	-2.15	120.02	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3371	NAG	O5-C5-C6-O6
5	B	3371	NAG	C4-C5-C6-O6
5	B	3320	NAG	O5-C5-C6-O6
5	A	2260	NAG	O5-C5-C6-O6
5	A	2260	NAG	C1-C2-N2-C7
5	B	3371	NAG	C1-C2-N2-C7
5	A	2260	NAG	C3-C2-N2-C7
5	A	2458	NAG	C3-C2-N2-C7
5	B	3371	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3371	NAG	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2458	NAG	5	0
5	B	3320	NAG	1	0
5	A	2260	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.