



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:10 PM BST

PDB ID : 1G1R
Title : Crystal structure of P-selectin lectin/EGF domains complexed with SLeX
Authors : Somers, W.S.; Camphausen, R.T.
Deposited on : 2000-10-13
Resolution : 3.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

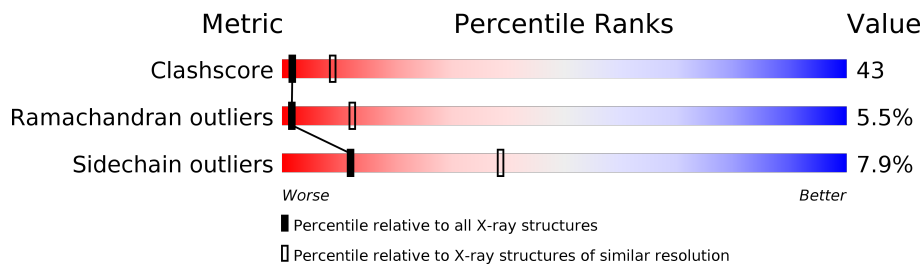
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 on 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	162	41% 54% . ..
1	B	162	39% 49% 10% ..
1	C	162	34% 55% 8% ..
1	D	162	29% 59% 11% .
2	E	4	100%
2	F	4	75% 25%
2	G	4	75% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5451 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.

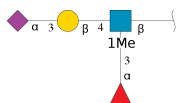
- Molecule 1 is a protein called P-SELECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1315	829	222	253	11	0	0	0
1	B	160	1319	832	223	253	11	0	0	0
1	C	159	1307	825	220	251	11	0	0	0
1	D	160	1319	832	223	253	11	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ASP	GLU	conflict	UNP P16109
A	159	ASP	-	cloning artifact	UNP P16109
A	160	ASP	-	cloning artifact	UNP P16109
A	161	ASP	-	cloning artifact	UNP P16109
A	162	LYS	-	cloning artifact	UNP P16109
B	158	ASP	GLU	conflict	UNP P16109
B	159	ASP	-	cloning artifact	UNP P16109
B	160	ASP	-	cloning artifact	UNP P16109
B	161	ASP	-	cloning artifact	UNP P16109
B	162	LYS	-	cloning artifact	UNP P16109
C	158	ASP	GLU	conflict	UNP P16109
C	159	ASP	-	cloning artifact	UNP P16109
C	160	ASP	-	cloning artifact	UNP P16109
C	161	ASP	-	cloning artifact	UNP P16109
C	162	LYS	-	cloning artifact	UNP P16109
D	158	ASP	GLU	conflict	UNP P16109
D	159	ASP	-	cloning artifact	UNP P16109
D	160	ASP	-	cloning artifact	UNP P16109
D	161	ASP	-	cloning artifact	UNP P16109
D	162	LYS	-	cloning artifact	UNP P16109

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside.

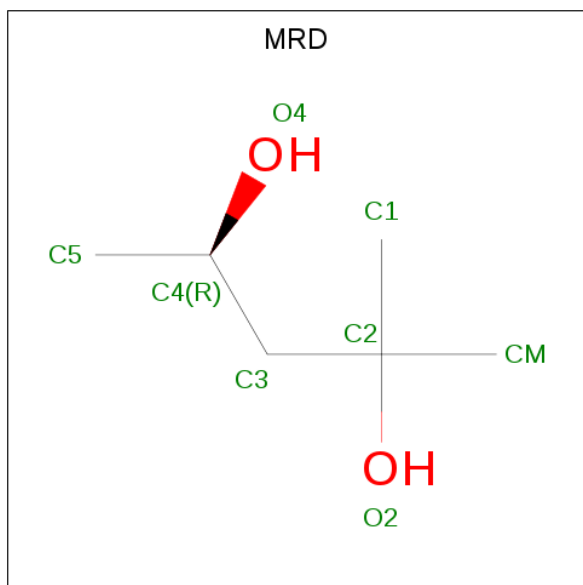


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	57	32	2	23	0	0	0
2	F	4	57	32	2	23	0	0	0
2	G	4	57	32	2	23	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	B	1	1	1	0	0
3	A	1	1	1	0	0
3	D	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		

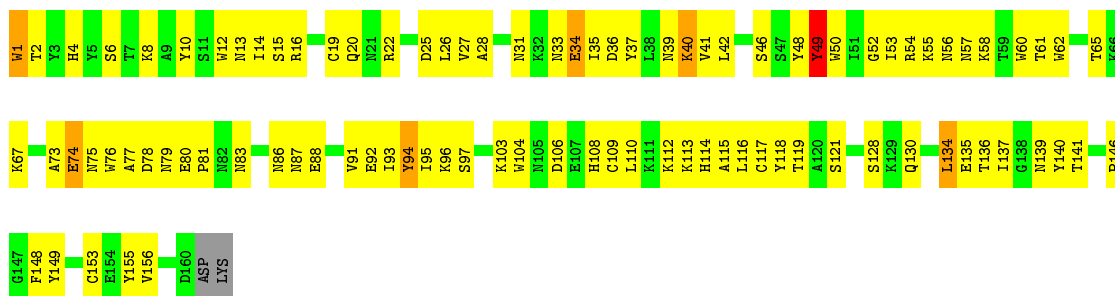
3 Residue-property plots

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.

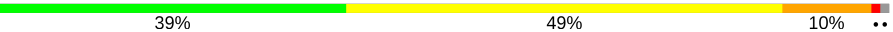
Note EDS was not executed.

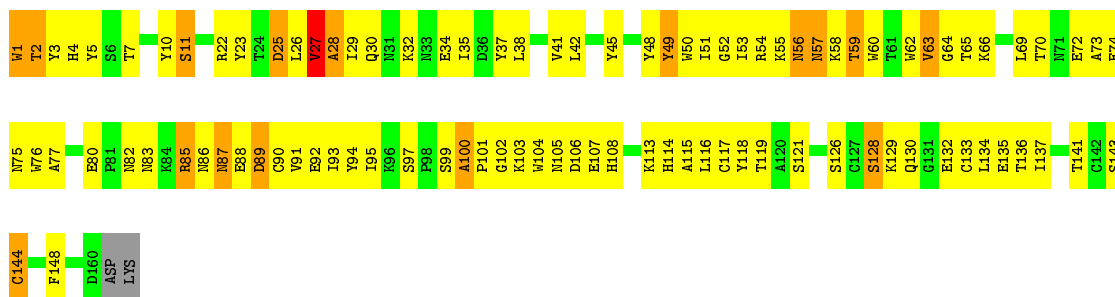
- Molecule 1: P-SELECTIN

Chain A: 

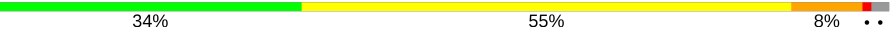


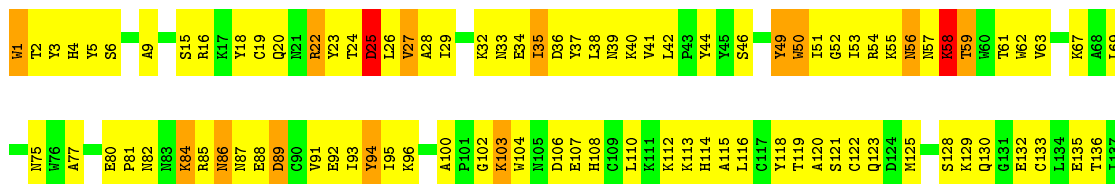
- Molecule 1: P-SELECTIN

Chain B: 



- Molecule 1: P-SELECTIN

Chain C: 





- Molecule 1: P-SELECTIN

Chain D: 29% 59% 11%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside

Chain E: 100%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside

Chain F: 75% 25%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside

Chain G: 75% 25%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.14Å 60.52Å 91.44Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	14.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (14.00-3.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5451	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SIA, GAL, FUC, MAG, MRD

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	0.58	0/1354	0.79	0/1841
1	B	0.47	0/1358	0.68	1/1845 (0.1%)
1	C	0.49	0/1346	0.72	0/1830
1	D	0.42	0/1358	0.67	0/1845
All	All	0.49	0/5416	0.71	1/7361 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ALA	N-CA-C	-5.25	96.83	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1315	0	1208	98	0
1	B	1319	0	1219	108	0
1	C	1307	0	1202	112	0
1	D	1319	0	1219	138	0
2	E	57	0	52	0	0
2	F	57	0	51	4	0
2	G	57	0	51	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	14	0	0
4	C	8	0	14	0	0
All	All	5451	0	5030	450	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 43.

All (450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:HB3	1:B:97:SER:HB2	1.35	1.09
1:C:77:ALA:HB2	1:C:103:LYS:HB3	1.41	1.00
1:B:77:ALA:HB3	1:B:80:GLU:HG3	1.43	0.99
1:B:27:VAL:HG21	1:B:116:LEU:HD23	1.47	0.97
1:A:86:ASN:H	1:D:130:GLN:HE21	1.07	0.96
1:D:94:TYR:HB3	1:D:97:SER:HB2	1.49	0.93
1:D:55:LYS:HE3	1:D:58:LYS:HA	1.48	0.93
1:C:108:HIS:HD2	1:C:110:LEU:H	1.14	0.90
1:B:56:ASN:HD22	1:B:56:ASN:H	1.14	0.89
1:A:27:VAL:HG13	1:A:116:LEU:O	1.75	0.87
1:A:128:SER:O	1:A:130:GLN:HG3	1.77	0.83
1:B:54:ARG:HH11	1:B:54:ARG:HG3	1.42	0.82
1:B:37:TYR:O	1:B:41:VAL:HG22	1.78	0.82
1:A:36:ASP:O	1:A:40:LYS:HG2	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ASN:H	1:C:56:ASN:HD22	1.24	0.80
1:A:86:ASN:N	1:D:130:GLN:HE21	1.80	0.80
1:D:54:ARG:HH11	1:D:54:ARG:HG3	1.44	0.80
1:A:86:ASN:H	1:D:130:GLN:NE2	1.79	0.80
1:C:157:ARG:HD2	1:D:36:ASP:OD2	1.80	0.79
1:D:85:ARG:NH2	1:D:85:ARG:HB2	1.97	0.79
1:A:149:TYR:O	1:A:153:CYS:HA	1.83	0.79
1:D:50:TRP:CD1	1:D:113:LYS:HB2	2.17	0.78
1:B:57:ASN:ND2	1:B:58:LYS:H	1.83	0.76
1:D:128:SER:O	1:D:130:GLN:HG3	1.84	0.75
1:D:30:GLN:HA	1:D:73:ALA:HB2	1.67	0.75
1:B:76:TRP:HA	1:B:104:TRP:HB2	1.66	0.75
1:D:5:TYR:HD1	1:D:5:TYR:H	1.32	0.75
1:C:42:LEU:O	1:C:96:LYS:HE2	1.86	0.74
1:C:77:ALA:HB2	1:C:103:LYS:CB	2.16	0.74
1:B:27:VAL:CG1	1:B:116:LEU:HG	2.18	0.73
1:C:39:ASN:HA	1:C:95:ILE:HD12	1.70	0.73
1:D:53:ILE:HD11	1:D:60:TRP:HB3	1.70	0.73
1:B:85:ARG:HB2	1:B:88:GLU:OE1	1.88	0.73
1:C:108:HIS:CD2	1:C:110:LEU:HB2	2.24	0.73
1:A:4:HIS:O	1:A:117:CYS:N	2.17	0.73
1:D:25:ASP:HB3	1:D:118:TYR:HE1	1.54	0.72
1:B:77:ALA:HA	1:B:103:LYS:HG3	1.71	0.72
1:C:19:CYS:SG	1:C:26:LEU:HD23	2.30	0.71
1:D:52:GLY:O	1:D:63:VAL:HG22	1.90	0.71
1:C:6:SER:HB3	1:C:18:TYR:CE1	2.25	0.71
1:C:125:MET:HA	1:C:129:LYS:HE3	1.73	0.71
1:B:27:VAL:HG13	1:B:116:LEU:HG	1.72	0.71
1:B:94:TYR:HB3	1:B:97:SER:CB	2.17	0.71
1:B:50:TRP:CD1	1:B:113:LYS:HB2	2.26	0.70
1:B:1:TRP:CE3	1:B:135:GLU:HG3	2.26	0.70
1:A:31:ASN:OD1	1:A:33:ASN:HB2	1.92	0.69
1:D:27:VAL:HG11	1:D:116:LEU:HG	1.73	0.69
1:D:53:ILE:HG13	1:D:61:THR:O	1.92	0.69
1:A:37:TYR:HA	1:A:40:LYS:HG3	1.75	0.68
1:B:55:LYS:HB2	1:B:60:TRP:CE2	2.29	0.68
1:B:4:HIS:HB2	1:B:117:CYS:HB2	1.75	0.67
1:B:94:TYR:CB	1:B:97:SER:HB2	2.19	0.67
1:B:94:TYR:HD2	1:B:103:LYS:O	1.79	0.66
1:D:55:LYS:CE	1:D:58:LYS:HA	2.24	0.66
1:C:108:HIS:CD2	1:C:110:LEU:H	2.06	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:TYR:OH	1:C:46:SER:HA	1.95	0.66
1:B:77:ALA:HA	1:B:103:LYS:CG	2.26	0.66
1:A:2:THR:OG1	1:A:119:THR:HB	1.95	0.66
1:A:78:ASP:O	1:A:79:ASN:HB2	1.95	0.66
1:D:50:TRP:CE2	1:D:113:LYS:HD2	2.31	0.66
1:B:76:TRP:O	1:B:103:LYS:HG3	1.96	0.65
1:B:56:ASN:HD22	1:B:56:ASN:N	1.88	0.65
1:D:55:LYS:NZ	1:D:58:LYS:HD3	2.10	0.65
1:D:85:ARG:CZ	1:D:85:ARG:HB2	2.26	0.65
1:A:88:GLU:HA	1:A:108:HIS:HA	1.79	0.65
1:B:48:TYR:CD1	1:B:94:TYR:HA	2.31	0.65
1:D:100:ALA:HB1	1:D:103:LYS:HZ2	1.60	0.64
1:A:4:HIS:HB2	1:A:117:CYS:HB2	1.77	0.64
1:D:100:ALA:O	1:D:103:LYS:HD3	1.98	0.64
1:C:28:ALA:HA	1:C:62:TRP:CE3	2.32	0.64
1:A:61:THR:HG23	1:A:67:LYS:O	1.97	0.64
1:A:76:TRP:CD2	1:A:81:PRO:HD3	2.32	0.64
1:B:28:ALA:HA	1:B:62:TRP:CE3	2.34	0.63
1:B:53:ILE:HB	1:B:62:TRP:CE3	2.33	0.63
1:A:27:VAL:HG11	1:A:116:LEU:HG	1.79	0.63
1:A:33:ASN:O	1:A:36:ASP:HB3	1.99	0.63
1:B:77:ALA:HB3	1:B:80:GLU:CG	2.24	0.63
1:D:27:VAL:HG21	1:D:116:LEU:HD23	1.81	0.63
1:D:5:TYR:HE2	1:D:43:PRO:HG3	1.63	0.63
1:A:77:ALA:HA	1:A:103:LYS:CG	2.28	0.62
1:A:93:ILE:O	1:A:93:ILE:HG23	1.98	0.62
1:A:19:CYS:SG	1:A:26:LEU:HD23	2.40	0.62
1:A:22:ARG:HG3	1:A:22:ARG:HH11	1.65	0.62
1:C:95:ILE:HG22	1:C:96:LYS:HG3	1.81	0.62
1:D:50:TRP:NE1	1:D:113:LYS:HB2	2.14	0.62
1:D:78:ASP:O	1:D:79:ASN:HB2	1.99	0.62
1:B:65:THR:O	1:B:66:LYS:HB2	1.99	0.62
1:B:57:ASN:HD22	1:B:58:LYS:H	1.45	0.61
1:D:50:TRP:CZ3	1:D:90:CYS:HB3	2.35	0.61
1:B:62:TRP:HB2	1:B:65:THR:OG1	2.00	0.61
1:B:51:ILE:HD12	1:B:62:TRP:CZ3	2.34	0.61
1:D:47:SER:O	1:D:48:TYR:HB2	1.99	0.61
1:B:69:LEU:HD11	1:B:74:GLU:N	2.15	0.61
1:B:54:ARG:NH1	1:B:54:ARG:HG3	2.06	0.61
1:C:132:GLU:HG3	1:C:133:CYS:H	1.66	0.61
1:D:133:CYS:SG	1:D:140:TYR:CD2	2.94	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:HB2	1:C:88:GLU:OE1	2.01	0.60
1:C:61:THR:HA	1:C:67:LYS:O	2.01	0.60
1:A:42:LEU:HD12	1:A:95:ILE:CD1	2.32	0.60
1:C:107:GLU:HG3	1:C:108:HIS:H	1.67	0.60
1:C:15:SER:HB3	1:C:115:ALA:HB2	1.83	0.60
1:B:107:GLU:HG3	1:B:108:HIS:N	2.17	0.60
1:B:55:LYS:HB2	1:B:60:TRP:CD2	2.37	0.60
1:B:27:VAL:CG2	1:B:116:LEU:HD23	2.26	0.60
1:B:56:ASN:ND2	1:B:56:ASN:H	1.94	0.60
1:B:56:ASN:ND2	1:B:59:THR:O	2.35	0.59
1:D:91:VAL:HG11	1:D:104:TRP:HB3	1.84	0.59
1:D:10:TYR:HB3	1:D:14:ILE:HB	1.84	0.59
1:D:63:VAL:HG23	1:D:64:GLY:H	1.67	0.59
1:B:55:LYS:HE3	1:B:57:ASN:O	2.02	0.59
1:D:38:LEU:HD22	1:D:116:LEU:HD21	1.84	0.59
1:D:61:THR:HG22	1:D:62:TRP:N	2.18	0.59
1:D:54:ARG:HG3	1:D:54:ARG:NH1	2.12	0.59
1:C:37:TYR:O	1:C:40:LYS:HG2	2.02	0.58
1:B:27:VAL:N	1:B:116:LEU:O	2.36	0.58
1:D:43:PRO:HD2	1:D:49:TYR:OH	2.03	0.58
1:A:52:GLY:O	1:A:62:TRP:HA	2.03	0.58
1:B:4:HIS:O	1:B:117:CYS:N	2.35	0.58
1:D:27:VAL:CG1	1:D:116:LEU:HG	2.32	0.58
1:A:27:VAL:CG1	1:A:116:LEU:HG	2.34	0.58
1:C:80:GLU:HA	1:C:81:PRO:O	2.03	0.58
1:C:56:ASN:HD22	1:C:56:ASN:N	1.95	0.58
1:A:77:ALA:HA	1:A:103:LYS:HG2	1.85	0.58
1:A:128:SER:C	1:A:130:GLN:H	2.05	0.58
1:D:102:GLY:C	1:D:103:LYS:HD2	2.23	0.58
1:A:130:GLN:HB3	1:A:148:PHE:CD2	2.39	0.57
1:B:69:LEU:CD1	1:B:73:ALA:HB3	2.34	0.57
1:C:27:VAL:HG21	1:C:116:LEU:HG	1.87	0.57
1:B:133:CYS:O	1:B:134:LEU:HD23	2.05	0.57
1:B:51:ILE:CG2	1:B:93:ILE:HB	2.35	0.57
1:D:125:MET:CE	1:D:128:SER:HA	2.34	0.57
1:A:27:VAL:HG12	1:A:117:CYS:O	2.05	0.57
1:A:49:TYR:HD2	1:A:116:LEU:HB2	1.70	0.57
1:C:130:GLN:HG2	1:C:148:PHE:CE2	2.39	0.57
1:C:80:GLU:HA	1:C:81:PRO:C	2.25	0.57
1:D:24:THR:OG1	1:D:119:THR:HA	2.05	0.57
1:A:55:LYS:HE2	1:A:58:LYS:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:HB	1:A:67:LYS:HG3	1.88	0.56
1:D:75:ASN:ND2	1:D:102:GLY:O	2.38	0.56
1:A:80:GLU:HA	1:A:80:GLU:OE1	2.04	0.56
1:A:8:LYS:HE2	1:A:10:TYR:OH	2.05	0.56
1:B:100:ALA:O	1:B:103:LYS:HB2	2.04	0.56
1:B:51:ILE:HD11	1:B:53:ILE:HG22	1.86	0.56
1:D:139:ASN:O	1:D:140:TYR:HB3	2.05	0.56
1:A:134:LEU:HD23	1:A:134:LEU:O	2.05	0.56
1:B:50:TRP:CE2	1:B:113:LYS:HD2	2.40	0.56
1:A:22:ARG:NH1	1:A:22:ARG:HG3	2.18	0.56
1:D:42:LEU:HD11	1:D:116:LEU:HD11	1.86	0.56
1:A:94:TYR:HB3	1:A:97:SER:HB2	1.88	0.56
1:D:38:LEU:O	1:D:40:LYS:N	2.39	0.56
1:A:16:ARG:O	1:A:20:GLN:HG3	2.06	0.55
1:A:6:SER:O	1:A:114:HIS:HD2	1.89	0.55
1:C:33:ASN:HB3	1:D:149:TYR:CD2	2.41	0.55
1:B:69:LEU:HD12	1:B:73:ALA:HB3	1.88	0.55
1:D:34:GLU:O	1:D:37:TYR:HB3	2.06	0.55
1:B:1:TRP:HA	1:B:121:SER:OG	2.07	0.55
1:B:2:THR:O	1:B:118:TYR:HA	2.07	0.55
1:B:53:ILE:HD12	1:B:62:TRP:CE2	2.41	0.55
1:C:27:VAL:HG22	1:C:116:LEU:O	2.06	0.54
1:D:100:ALA:HB1	1:D:103:LYS:NZ	2.21	0.54
1:D:16:ARG:O	1:D:20:GLN:HG3	2.08	0.54
1:B:99:SER:O	1:B:100:ALA:HB2	2.07	0.54
1:D:53:ILE:HG12	1:D:60:TRP:CE3	2.42	0.54
1:B:80:GLU:OE1	1:B:82:ASN:ND2	2.40	0.54
1:A:149:TYR:CE1	1:A:155:TYR:HB3	2.43	0.54
1:B:45:TYR:HB3	1:B:114:HIS:CE1	2.43	0.54
1:A:1:TRP:HA	1:A:121:SER:OG	2.07	0.54
1:A:112:LYS:O	1:A:113:LYS:HG3	2.08	0.53
1:B:3:TYR:CG	1:B:38:LEU:HD21	2.43	0.53
1:D:53:ILE:CG1	1:D:61:THR:O	2.56	0.53
1:B:42:LEU:HD11	1:B:116:LEU:HD11	1.89	0.53
1:C:136:THR:CG2	1:C:141:THR:HG23	2.39	0.53
1:C:81:PRO:HB2	1:C:106:ASP:OD2	2.07	0.53
1:B:10:TYR:O	1:B:11:SER:O	2.26	0.53
1:B:69:LEU:HD12	1:B:70:THR:H	1.73	0.53
1:C:86:ASN:C	1:C:88:GLU:H	2.11	0.53
1:D:152:GLU:HB2	1:D:154:GLU:OE1	2.09	0.53
1:C:18:TYR:O	1:C:22:ARG:HG3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:TRP:HA	1:C:121:SER:OG	2.10	0.52
1:C:86:ASN:O	1:C:88:GLU:HG3	2.10	0.52
1:D:134:LEU:O	1:D:140:TYR:HB2	2.09	0.52
1:B:128:SER:O	1:B:129:LYS:HB2	2.10	0.52
1:B:97:SER:HB3	1:B:101:PRO:HA	1.91	0.52
1:B:87:ASN:O	1:B:108:HIS:HA	2.09	0.52
1:B:89:ASP:OD1	1:B:89:ASP:N	2.42	0.52
1:D:1:TRP:HB3	1:D:135:GLU:OE1	2.08	0.52
1:D:63:VAL:HG23	1:D:64:GLY:N	2.25	0.52
1:D:32:LYS:HE3	1:D:75:ASN:OD1	2.09	0.52
1:C:1:TRP:HB3	1:C:120:ALA:HA	1.91	0.52
1:A:27:VAL:HA	1:A:118:TYR:CD1	2.45	0.52
1:D:5:TYR:CE2	1:D:43:PRO:HG3	2.42	0.52
1:D:6:SER:C	1:D:8:LYS:H	2.13	0.52
1:C:140:TYR:C	1:C:140:TYR:CD2	2.82	0.52
1:C:94:TYR:CD1	1:C:94:TYR:N	2.78	0.52
1:D:134:LEU:H	1:D:134:LEU:HD12	1.75	0.52
1:D:53:ILE:HG12	1:D:60:TRP:HE3	1.75	0.52
1:C:123:GLN:NE2	1:C:123:GLN:HA	2.25	0.52
1:D:156:VAL:HG13	1:D:157:ARG:O	2.09	0.52
1:C:156:VAL:HG13	1:C:156:VAL:O	2.08	0.52
2:F:2:GAL:O5	2:F:4:FUC:H5	2.10	0.52
1:B:69:LEU:HD12	1:B:70:THR:N	2.25	0.51
1:D:83:ASN:HB2	1:D:106:ASP:OD2	2.10	0.51
1:D:42:LEU:HD22	1:D:49:TYR:CE2	2.45	0.51
1:D:19:CYS:SG	1:D:26:LEU:HD23	2.50	0.51
1:D:51:ILE:HG13	1:D:53:ILE:HG22	1.93	0.51
1:B:75:ASN:ND2	1:B:102:GLY:O	2.42	0.51
1:B:48:TYR:HD1	1:B:95:ILE:H	1.58	0.51
1:B:91:VAL:HG22	1:B:106:ASP:HA	1.92	0.51
1:C:50:TRP:HA	1:C:50:TRP:CE3	2.46	0.51
1:B:27:VAL:HG11	1:B:116:LEU:HG	1.89	0.51
1:C:50:TRP:CZ3	1:C:113:LYS:HD2	2.46	0.51
1:A:53:ILE:HD11	1:A:60:TRP:HB3	1.93	0.51
1:D:148:PHE:N	1:D:148:PHE:CD1	2.79	0.51
1:C:130:GLN:HG2	1:C:148:PHE:CD2	2.45	0.51
1:C:52:GLY:O	1:C:63:VAL:HG22	2.10	0.51
1:C:51:ILE:HG21	1:C:93:ILE:HB	1.93	0.51
1:D:60:TRP:O	1:D:61:THR:OG1	2.27	0.51
1:C:36:ASP:OD1	1:C:40:LYS:HD2	2.12	0.50
1:C:49:TYR:CD1	1:C:49:TYR:N	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:HIS:HD2	1:C:23:TYR:CG	2.29	0.50
1:A:73:ALA:O	1:A:74:GLU:C	2.49	0.50
1:B:54:ARG:NE	1:B:90:CYS:SG	2.85	0.50
1:C:122:CYS:HB2	1:C:135:GLU:OE2	2.12	0.50
1:C:140:TYR:O	1:C:140:TYR:CD2	2.65	0.50
1:D:94:TYR:HE2	1:D:105:ASN:CB	2.25	0.50
1:D:6:SER:HB3	1:D:18:TYR:CE1	2.46	0.50
1:B:32:LYS:NZ	1:B:72:GLU:O	2.32	0.50
1:D:55:LYS:HZ1	1:D:58:LYS:C	2.14	0.50
1:D:87:ASN:O	1:D:109:CYS:SG	2.70	0.49
1:B:92:GLU:CD	1:B:113:LYS:HE3	2.32	0.49
1:C:85:ARG:HB2	1:C:88:GLU:CD	2.32	0.49
1:C:95:ILE:CG2	1:C:96:LYS:HG3	2.42	0.49
1:C:29:ILE:HD13	1:C:35:ILE:HG12	1.94	0.49
1:D:87:ASN:ND2	1:D:109:CYS:HB2	2.27	0.49
1:D:76:TRP:O	1:D:103:LYS:HB3	2.12	0.49
1:A:121:SER:N	1:A:135:GLU:OE2	2.45	0.49
1:D:132:GLU:N	1:D:143:SER:O	2.44	0.49
1:A:42:LEU:HD12	1:A:95:ILE:HD11	1.92	0.49
1:B:51:ILE:CD1	1:B:53:ILE:HG22	2.42	0.49
1:D:29:ILE:HD13	1:D:35:ILE:HG12	1.93	0.49
1:D:94:TYR:HE2	1:D:105:ASN:HB2	1.78	0.49
1:D:55:LYS:CE	1:D:58:LYS:HD3	2.43	0.49
1:A:76:TRP:CE2	1:A:81:PRO:HD3	2.48	0.49
1:A:83:ASN:ND2	1:A:106:ASP:O	2.45	0.49
1:B:27:VAL:CG2	1:B:51:ILE:HA	2.43	0.49
1:D:125:MET:HE1	1:D:128:SER:HA	1.94	0.49
1:C:51:ILE:HG13	1:C:53:ILE:HG22	1.95	0.49
1:C:6:SER:O	1:C:114:HIS:HD2	1.95	0.49
1:B:94:TYR:CD2	1:B:103:LYS:O	2.62	0.48
1:C:56:ASN:ND2	1:C:56:ASN:H	2.02	0.48
1:C:92:GLU:HB3	1:C:113:LYS:HE3	1.94	0.48
1:A:128:SER:C	1:A:130:GLN:N	2.67	0.48
1:D:35:ILE:O	1:D:36:ASP:C	2.51	0.48
1:D:125:MET:HE2	1:D:125:MET:HA	1.94	0.48
1:D:124:ASP:C	1:D:126:SER:H	2.17	0.48
1:D:54:ARG:NE	1:D:90:CYS:SG	2.86	0.48
1:B:51:ILE:HG21	1:B:93:ILE:HB	1.94	0.48
1:D:55:LYS:HZ1	1:D:58:LYS:HD3	1.77	0.48
1:C:86:ASN:C	1:C:88:GLU:N	2.67	0.48
1:B:97:SER:O	1:B:101:PRO:HD3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ARG:O	1:C:20:GLN:HG3	2.14	0.48
1:A:16:ARG:HG3	1:A:26:LEU:HG	1.95	0.48
1:D:39:ASN:HA	1:D:95:ILE:HG23	1.96	0.48
1:C:56:ASN:ND2	1:C:59:THR:O	2.46	0.48
1:D:104:TRP:CD1	1:D:104:TRP:N	2.80	0.48
1:B:23:TYR:HB3	1:B:119:THR:OG1	2.14	0.47
1:B:5:TYR:HA	1:B:115:ALA:O	2.14	0.47
1:C:108:HIS:HD2	1:C:110:LEU:N	1.96	0.47
1:D:105:ASN:ND2	1:D:107:GLU:OE2	2.46	0.47
1:B:50:TRP:CD2	1:B:113:LYS:HD2	2.49	0.47
1:D:44:TYR:HB2	1:D:96:LYS:HD3	1.96	0.47
1:C:54:ARG:NE	1:C:89:ASP:OD1	2.48	0.47
1:A:13:ASN:C	1:A:15:SER:N	2.67	0.47
1:D:84:LYS:O	1:D:84:LYS:HG3	2.14	0.47
1:D:83:ASN:HB3	1:D:88:GLU:OE1	2.15	0.47
1:D:99:SER:HB3	2:G:3:SIA:O4	2.14	0.47
1:A:92:GLU:O	1:A:92:GLU:HG3	2.15	0.47
1:C:93:ILE:HG13	1:C:102:GLY:O	2.15	0.47
1:D:97:SER:HB3	1:D:101:PRO:HA	1.94	0.47
1:D:5:TYR:HB2	1:D:49:TYR:HE2	1.79	0.47
1:A:62:TRP:HB2	1:A:65:THR:OG1	2.14	0.47
1:C:54:ARG:NH2	1:C:89:ASP:OD1	2.48	0.47
1:C:50:TRP:HA	1:C:50:TRP:HE3	1.80	0.47
1:A:48:TYR:CD1	1:A:94:TYR:HA	2.49	0.47
1:B:51:ILE:HD11	1:B:53:ILE:CG2	2.45	0.47
1:D:55:LYS:HA	1:D:60:TRP:HA	1.97	0.47
1:C:53:ILE:HG23	1:C:53:ILE:O	2.15	0.47
1:B:82:ASN:ND2	2:F:4:FUC:O4	2.42	0.47
1:A:36:ASP:CG	1:A:40:LYS:HD3	2.35	0.47
1:B:56:ASN:O	1:B:57:ASN:CG	2.54	0.47
1:D:134:LEU:N	1:D:134:LEU:HD12	2.29	0.47
1:B:49:TYR:CD1	1:B:49:TYR:N	2.82	0.47
1:A:54:ARG:HD2	1:A:54:ARG:HA	1.67	0.46
1:D:61:THR:HG23	1:D:67:LYS:O	2.15	0.46
1:A:74:GLU:OE2	1:A:75:ASN:N	2.48	0.46
1:A:108:HIS:O	1:A:110:LEU:N	2.48	0.46
1:C:132:GLU:HG3	1:C:133:CYS:N	2.31	0.46
1:D:134:LEU:HD12	1:D:141:THR:O	2.15	0.46
1:D:85:ARG:HH21	1:D:85:ARG:HB2	1.78	0.46
1:C:149:TYR:CD1	1:D:33:ASN:OD1	2.68	0.46
1:D:78:ASP:O	1:D:79:ASN:CB	2.62	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLN:C	1:C:145:TYR:CD2	2.89	0.46
1:D:61:THR:CG2	1:D:62:TRP:N	2.78	0.46
1:A:1:TRP:N	1:A:135:GLU:OE1	2.46	0.46
1:A:93:ILE:O	1:A:93:ILE:CG2	2.63	0.46
1:B:106:ASP:O	1:B:107:GLU:HB2	2.16	0.46
1:D:108:HIS:O	1:D:110:LEU:N	2.49	0.46
1:D:133:CYS:SG	1:D:140:TYR:HD2	2.36	0.46
1:A:50:TRP:CD1	1:A:113:LYS:HB2	2.51	0.46
1:D:48:TYR:CD1	1:D:94:TYR:HA	2.51	0.46
1:B:55:LYS:NZ	1:B:58:LYS:HA	2.31	0.45
1:B:63:VAL:CG2	1:B:64:GLY:N	2.79	0.45
1:C:23:TYR:HB3	1:C:119:THR:OG1	2.16	0.45
1:C:89:ASP:O	1:C:89:ASP:CG	2.54	0.45
1:B:77:ALA:HB2	1:B:104:TRP:O	2.16	0.45
1:B:136:THR:HG21	1:B:141:THR:HG23	1.97	0.45
1:C:9:ALA:HB1	1:C:112:LYS:HB3	1.97	0.45
1:B:26:LEU:O	1:B:27:VAL:O	2.35	0.45
1:A:27:VAL:HG13	1:A:116:LEU:C	2.35	0.45
1:A:94:TYR:HB3	1:A:97:SER:CB	2.46	0.45
1:B:97:SER:HB3	1:B:101:PRO:CA	2.47	0.45
1:C:2:THR:O	1:C:118:TYR:HA	2.15	0.45
1:A:56:ASN:O	1:A:57:ASN:HB2	2.16	0.45
1:B:1:TRP:CZ2	1:B:30:GLN:HG3	2.51	0.45
1:D:94:TYR:HB3	1:D:97:SER:CB	2.34	0.45
1:B:82:ASN:O	1:B:83:ASN:OD1	2.34	0.45
1:B:92:GLU:OE2	1:B:113:LYS:HE3	2.17	0.45
1:C:81:PRO:CB	1:C:106:ASP:OD2	2.65	0.45
1:C:145:TYR:O	1:C:146:PRO:C	2.54	0.45
1:D:76:TRP:HB3	1:D:77:ALA:H	1.45	0.45
1:B:83:ASN:ND2	1:B:106:ASP:OD2	2.49	0.45
1:A:108:HIS:C	1:A:108:HIS:CD2	2.89	0.45
1:D:112:LYS:C	1:D:113:LYS:HG3	2.36	0.45
1:D:73:ALA:O	1:D:104:TRP:CH2	2.70	0.45
1:C:100:ALA:HB1	1:C:103:LYS:HG3	1.99	0.44
1:C:55:LYS:HB3	1:C:89:ASP:OD2	2.16	0.44
1:C:93:ILE:HG23	1:C:93:ILE:O	2.17	0.44
1:C:132:GLU:CG	1:C:133:CYS:N	2.81	0.44
1:C:32:LYS:O	1:C:35:ILE:N	2.51	0.44
1:D:10:TYR:CD1	1:D:14:ILE:HG21	2.52	0.44
1:D:27:VAL:HG22	1:D:116:LEU:HB3	1.98	0.44
1:C:94:TYR:HD1	1:C:94:TYR:N	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HB3	1:A:106:ASP:HB3	1.99	0.44
1:B:143:SER:O	1:B:144:CYS:C	2.56	0.44
1:B:82:ASN:OD1	2:F:4:FUC:H2	2.18	0.44
1:D:131:GLY:HA2	1:D:145:TYR:CD1	2.52	0.44
1:D:27:VAL:HG11	1:D:116:LEU:CG	2.44	0.44
1:B:132:GLU:OE1	1:B:134:LEU:HD21	2.17	0.44
1:A:27:VAL:HG23	1:A:27:VAL:O	2.17	0.44
1:D:48:TYR:CE1	1:D:94:TYR:HA	2.53	0.44
1:B:59:THR:HG22	1:B:59:THR:O	2.18	0.44
1:C:18:TYR:CE2	1:C:22:ARG:HD2	2.53	0.44
1:D:50:TRP:CZ2	1:D:113:LYS:HD2	2.52	0.44
1:B:27:VAL:HG23	1:B:52:GLY:H	1.83	0.44
1:D:42:LEU:HD11	1:D:116:LEU:CD1	2.48	0.44
1:A:136:THR:HG23	1:A:140:TYR:HA	2.00	0.43
1:C:148:PHE:CD1	1:C:148:PHE:N	2.85	0.43
1:D:86:ASN:O	1:D:87:ASN:HB2	2.18	0.43
1:A:41:VAL:HG23	1:A:42:LEU:N	2.32	0.43
1:D:83:ASN:HD22	1:D:106:ASP:CG	2.20	0.43
1:A:148:PHE:N	1:A:148:PHE:CD1	2.86	0.43
1:B:91:VAL:HG13	1:B:105:ASN:H	1.82	0.43
1:C:136:THR:HG21	1:C:141:THR:HG23	1.99	0.43
1:D:22:ARG:H	1:D:22:ARG:HG3	1.39	0.43
1:A:12:TRP:CZ3	1:A:54:ARG:NH1	2.87	0.43
1:A:61:THR:CG2	1:A:67:LYS:O	2.66	0.43
1:C:50:TRP:CE3	1:C:113:LYS:HD2	2.54	0.43
1:C:128:SER:C	1:C:130:GLN:N	2.71	0.43
1:C:3:TYR:CG	1:C:38:LEU:HD21	2.54	0.43
1:C:54:ARG:HA	1:C:54:ARG:HD2	1.86	0.43
1:D:124:ASP:CG	1:D:125:MET:N	2.71	0.43
1:D:5:TYR:CE2	1:D:43:PRO:CG	3.01	0.43
1:A:36:ASP:O	1:A:37:TYR:C	2.56	0.43
1:A:37:TYR:CA	1:A:40:LYS:HG3	2.47	0.43
1:A:13:ASN:O	1:A:14:ILE:C	2.55	0.43
1:D:83:ASN:ND2	1:D:106:ASP:O	2.52	0.43
1:D:86:ASN:O	1:D:87:ASN:CB	2.66	0.43
1:C:24:THR:O	1:C:25:ASP:HB2	2.19	0.43
1:B:130:GLN:HG2	1:B:148:PHE:CZ	2.54	0.43
1:B:53:ILE:HA	1:B:62:TRP:HA	2.01	0.43
1:C:49:TYR:N	1:C:49:TYR:HD1	2.16	0.42
1:D:124:ASP:C	1:D:126:SER:N	2.72	0.42
1:D:128:SER:O	1:D:130:GLN:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HH21	1:B:22:ARG:CG	2.32	0.42
1:B:53:ILE:HD11	1:B:60:TRP:HB3	2.02	0.42
1:B:82:ASN:HD21	2:F:4:FUC:HO4	1.64	0.42
1:C:29:ILE:HD13	1:C:35:ILE:CG1	2.50	0.42
1:C:53:ILE:HD11	1:C:69:LEU:HD13	2.01	0.42
1:D:38:LEU:C	1:D:40:LYS:H	2.22	0.42
1:A:15:SER:HB3	1:A:115:ALA:HB2	2.01	0.42
1:A:36:ASP:OD1	1:A:40:LYS:HD3	2.19	0.42
1:A:86:ASN:O	1:A:87:ASN:HB3	2.19	0.42
1:D:99:SER:OG	1:D:100:ALA:N	2.53	0.42
1:C:91:VAL:CG1	1:C:104:TRP:HB3	2.50	0.42
1:D:103:LYS:N	1:D:103:LYS:HD2	2.34	0.42
1:C:5:TYR:HA	1:C:115:ALA:O	2.19	0.42
1:C:1:TRP:CD1	1:C:1:TRP:C	2.92	0.42
1:C:1:TRP:O	1:C:138:GLY:N	2.53	0.42
1:C:86:ASN:O	1:C:88:GLU:N	2.52	0.42
1:D:1:TRP:HA	1:D:121:SER:OG	2.20	0.42
1:A:27:VAL:CG2	1:A:27:VAL:O	2.67	0.42
1:A:1:TRP:CH2	1:A:28:ALA:O	2.73	0.42
1:C:18:TYR:CZ	1:C:22:ARG:HD2	2.55	0.42
1:D:65:THR:O	1:D:66:LYS:CB	2.68	0.42
1:A:34:GLU:O	1:A:35:ILE:C	2.58	0.42
1:D:42:LEU:HD21	1:D:116:LEU:HD11	2.02	0.42
1:A:91:VAL:CG1	1:A:104:TRP:HB3	2.50	0.41
1:A:130:GLN:CD	1:A:148:PHE:CE2	2.93	0.41
1:A:39:ASN:O	1:A:96:LYS:NZ	2.53	0.41
1:C:9:ALA:CB	1:C:112:LYS:HB3	2.50	0.41
1:D:29:ILE:HG21	1:D:35:ILE:HD11	2.02	0.41
1:A:27:VAL:HG12	1:A:117:CYS:C	2.41	0.41
1:A:112:LYS:O	1:A:113:LYS:CG	2.67	0.41
1:A:49:TYR:CD2	1:A:116:LEU:HB2	2.54	0.41
1:A:42:LEU:HD12	1:A:95:ILE:HD12	2.01	0.41
1:A:50:TRP:CE2	1:A:113:LYS:HD2	2.55	0.41
1:B:50:TRP:CZ3	1:B:90:CYS:O	2.73	0.41
1:A:2:THR:O	1:A:118:TYR:HA	2.19	0.41
1:C:2:THR:O	1:C:119:THR:N	2.49	0.41
1:C:51:ILE:CG2	1:C:93:ILE:HB	2.50	0.41
1:A:53:ILE:CD1	1:A:60:TRP:HB3	2.50	0.41
1:C:58:LYS:HB2	1:C:58:LYS:NZ	2.35	0.41
1:A:146:PRO:O	1:A:148:PHE:CD1	2.74	0.41
1:C:37:TYR:O	1:C:38:LEU:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:TYR:CZ	1:C:46:SER:HA	2.56	0.41
1:A:149:TYR:O	1:A:153:CYS:CA	2.61	0.41
1:A:76:TRP:HH2	1:A:91:VAL:HG22	1.86	0.41
1:D:30:GLN:O	1:D:31:ASN:HB3	2.20	0.41
1:B:143:SER:O	1:B:144:CYS:O	2.38	0.41
1:A:16:ARG:HE	1:A:25:ASP:CG	2.24	0.41
1:C:35:ILE:HD13	1:C:75:ASN:HD22	1.86	0.41
1:A:134:LEU:O	1:A:140:TYR:HA	2.21	0.41
1:B:32:LYS:HA	1:B:32:LYS:HD3	1.93	0.41
1:C:84:LYS:HB3	1:C:84:LYS:NZ	2.36	0.41
1:D:6:SER:O	1:D:114:HIS:CD2	2.74	0.41
1:D:82:ASN:OD1	1:D:82:ASN:N	2.53	0.41
1:C:1:TRP:O	1:C:138:GLY:CA	2.69	0.40
1:D:5:TYR:HB3	1:D:42:LEU:CD2	2.51	0.40
1:B:30:GLN:HB2	1:B:34:GLU:OE2	2.21	0.40
1:D:127:CYS:O	1:D:128:SER:C	2.60	0.40
1:D:93:ILE:HG23	1:D:93:ILE:O	2.21	0.40
1:B:29:ILE:HD13	1:B:35:ILE:HG12	2.03	0.40
1:C:84:LYS:HZ1	1:C:84:LYS:HB3	1.85	0.40
1:C:125:MET:HG2	1:C:129:LYS:NZ	2.37	0.40
1:C:4:HIS:CD2	1:C:23:TYR:CD1	3.09	0.40
1:D:93:ILE:HA	1:D:103:LYS:O	2.21	0.40
1:C:149:TYR:HB3	1:D:33:ASN:ND2	2.37	0.40
1:A:22:ARG:CG	1:A:22:ARG:HH11	2.33	0.40
1:C:3:TYR:CD2	1:C:38:LEU:HD21	2.57	0.40
1:C:37:TYR:CE2	1:C:41:VAL:HG11	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/162 (98%)	128 (81%)	26 (16%)	4 (2%)	5	26
1	B	158/162 (98%)	128 (81%)	20 (13%)	10 (6%)	1	9
1	C	157/162 (97%)	124 (79%)	24 (15%)	9 (6%)	1	12
1	D	158/162 (98%)	114 (72%)	32 (20%)	12 (8%)	1	6
All	All	631/648 (97%)	494 (78%)	102 (16%)	35 (6%)	2	12

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	CYS
1	B	11	SER
1	B	27	VAL
1	B	126	SER
1	B	144	CYS
1	C	144	CYS
1	D	58	LYS
1	D	76	TRP
1	D	109	CYS
1	B	85	ARG
1	C	27	VAL
1	C	58	LYS
1	D	7	THR
1	D	32	LYS
1	D	39	ASN
1	D	129	LYS
1	D	139	ASN
1	B	128	SER
1	B	137	ILE
1	C	25	ASP
1	D	25	ASP
1	D	48	TYR
1	D	111	LYS
1	B	25	ASP
1	B	57	ASN
1	C	82	ASN
1	D	140	TYR
1	A	94	TYR
1	A	139	ASN
1	C	57	ASN
1	C	87	ASN
1	C	94	TYR
1	A	137	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	100	ALA
1	C	103	LYS

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	142/147 (97%)	133 (94%)	9 (6%)	18	47
1	B	143/147 (97%)	131 (92%)	12 (8%)	11	36
1	C	141/147 (96%)	127 (90%)	14 (10%)	8	27
1	D	143/147 (97%)	133 (93%)	10 (7%)	15	44
All	All	569/588 (97%)	524 (92%)	45 (8%)	12	39

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	TRP
1	A	34	GLU
1	A	40	LYS
1	A	46	SER
1	A	49	TYR
1	A	74	GLU
1	A	134	LEU
1	A	141	THR
1	A	156	VAL
1	B	1	TRP
1	B	2	THR
1	B	7	THR
1	B	25	ASP
1	B	27	VAL
1	B	49	TYR
1	B	56	ASN
1	B	59	THR
1	B	63	VAL
1	B	86	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	87	ASN
1	B	89	ASP
1	C	1	TRP
1	C	22	ARG
1	C	25	ASP
1	C	34	GLU
1	C	35	ILE
1	C	49	TYR
1	C	50	TRP
1	C	56	ASN
1	C	58	LYS
1	C	59	THR
1	C	84	LYS
1	C	86	ASN
1	C	89	ASP
1	C	154	GLU
1	D	1	TRP
1	D	5	TYR
1	D	22	ARG
1	D	41	VAL
1	D	53	ILE
1	D	85	ARG
1	D	103	LYS
1	D	124	ASP
1	D	125	MET
1	D	134	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	30	GLN
1	A	79	ASN
1	A	83	ASN
1	A	87	ASN
1	A	114	HIS
1	B	21	ASN
1	B	56	ASN
1	B	57	ASN
1	B	83	ASN
1	B	105	ASN
1	C	56	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	75	ASN
1	C	79	ASN
1	C	108	HIS
1	C	114	HIS
1	C	123	GLN
1	D	21	ASN
1	D	79	ASN
1	D	83	ASN
1	D	87	ASN
1	D	123	GLN
1	D	130	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 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	MAG	E	1	2	16,16,16	1.67	3 (18%)	22,22,22	1.80	4 (18%)
2	GAL	E	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.22	2 (13%)
2	SIA	E	3	2	17,20,21	1.72	4 (23%)	21,28,31	1.41	2 (9%)
2	FUC	E	4	3,2	10,10,11	1.35	1 (10%)	14,14,16	1.12	1 (7%)
2	MAG	F	1	2	16,16,16	1.47	2 (12%)	22,22,22	1.62	6 (27%)
2	GAL	F	2	2	11,11,12	1.12	1 (9%)	15,15,17	1.17	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	F	3	2	17,20,21	1.58	4 (23%)	21,28,31	1.35	2 (9%)
2	FUC	F	4	3,2	10,10,11	0.97	0	14,14,16	0.86	0
2	MAG	G	1	2	16,16,16	1.62	4 (25%)	22,22,22	1.39	3 (13%)
2	GAL	G	2	2	11,11,12	1.52	3 (27%)	15,15,17	1.30	3 (20%)
2	SIA	G	3	2	17,20,21	1.81	4 (23%)	21,28,31	1.42	4 (19%)
2	FUC	G	4	3,2	10,10,11	1.54	2 (20%)	14,14,16	0.93	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	MAG	E	1	2	-	3/8/28/28	0/1/1/1
2	GAL	E	2	2	-	1/2/19/22	0/1/1/1
2	SIA	E	3	2	-	2/14/34/38	0/1/1/1
2	FUC	E	4	3,2	-	-	0/1/1/1
2	MAG	F	1	2	-	3/8/28/28	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	SIA	F	3	2	-	2/14/34/38	0/1/1/1
2	FUC	F	4	3,2	-	-	0/1/1/1
2	MAG	G	1	2	-	1/8/28/28	0/1/1/1
2	GAL	G	2	2	-	1/2/19/22	0/1/1/1
2	SIA	G	3	2	-	4/14/34/38	0/1/1/1
2	FUC	G	4	3,2	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	SIA	C4-C5	3.73	1.56	1.53
2	E	3	SIA	C7-C6	3.55	1.57	1.53
2	E	1	MAG	O1-C1	3.38	1.46	1.40
2	G	1	MAG	C4-C5	3.33	1.60	1.53
2	F	1	MAG	O1-C1	3.22	1.45	1.40
2	E	1	MAG	C4-C5	3.13	1.59	1.53
2	G	3	SIA	C3-C2	3.11	1.57	1.52
2	E	3	SIA	C3-C2	3.09	1.57	1.52
2	F	3	SIA	C4-C5	3.08	1.55	1.53
2	G	4	FUC	C2-C3	2.89	1.56	1.52
2	E	1	MAG	C4-C3	2.79	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	MAG	O1-C1	2.79	1.45	1.40
2	G	2	GAL	C1-C2	2.67	1.58	1.52
2	F	3	SIA	C3-C2	2.61	1.56	1.52
2	G	3	SIA	C6-C5	2.55	1.57	1.53
2	F	3	SIA	C8-C7	2.42	1.58	1.53
2	E	3	SIA	O6-C6	2.33	1.47	1.44
2	F	3	SIA	C11-C10	2.33	1.55	1.50
2	G	2	GAL	C2-C3	2.29	1.55	1.52
2	G	3	SIA	C8-C7	2.29	1.57	1.53
2	F	1	MAG	C4-C5	2.28	1.57	1.53
2	E	4	FUC	C2-C3	2.26	1.55	1.52
2	E	2	GAL	C1-C2	2.19	1.57	1.52
2	G	1	MAG	C3-C2	2.18	1.57	1.53
2	G	4	FUC	C1-C2	2.14	1.57	1.52
2	E	3	SIA	C6-C5	2.13	1.56	1.53
2	G	2	GAL	C4-C5	2.11	1.57	1.53
2	G	1	MAG	C4-C3	2.04	1.57	1.52
2	F	2	GAL	C2-C3	2.01	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	MAG	O1-C1-C2	6.52	118.14	108.14
2	F	1	MAG	O1-C1-C2	5.17	116.06	108.14
2	G	1	MAG	O1-C1-C2	3.93	114.16	108.14
2	E	3	SIA	C6-O6-C2	3.67	119.19	111.34
2	E	3	SIA	C3-C4-C5	-3.30	107.47	111.46
2	F	2	GAL	C1-O5-C5	3.29	116.65	112.19
2	G	3	SIA	C6-O6-C2	3.17	118.12	111.34
2	E	2	GAL	C1-O5-C5	2.87	116.08	112.19
2	F	3	SIA	C6-O6-C2	2.77	117.26	111.34
2	F	1	MAG	C1-C2-N2	-2.68	106.38	111.00
2	G	1	MAG	C8-C7-N2	-2.60	111.70	116.10
2	G	3	SIA	C5-N5-C10	2.58	129.44	123.18
2	F	1	MAG	C8-C7-N2	-2.57	111.74	116.10
2	G	2	GAL	C1-O5-C5	2.55	115.65	112.19
2	G	1	MAG	O7-C7-N2	2.47	126.50	121.95
2	G	3	SIA	C8-C7-C6	-2.44	108.41	113.03
2	F	1	MAG	O7-C7-N2	2.44	126.44	121.95
2	F	3	SIA	C5-N5-C10	2.43	129.09	123.18
2	G	2	GAL	O4-C4-C3	-2.31	105.00	110.35
2	E	1	MAG	C6-C5-C4	2.26	118.31	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	FUC	C1-O5-C5	2.24	117.85	112.78
2	E	1	MAG	CM-O1-C1	2.23	116.72	113.27
2	G	3	SIA	C11-C10-N5	2.18	119.79	116.10
2	F	2	GAL	O4-C4-C3	-2.18	105.32	110.35
2	F	1	MAG	CM-O1-C1	2.11	116.53	113.27
2	E	1	MAG	C8-C7-N2	-2.11	112.53	116.10
2	G	2	GAL	C1-C2-C3	-2.05	107.14	109.67
2	F	1	MAG	C6-C5-C4	2.04	117.78	113.00
2	E	2	GAL	O4-C4-C3	-2.04	105.64	110.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

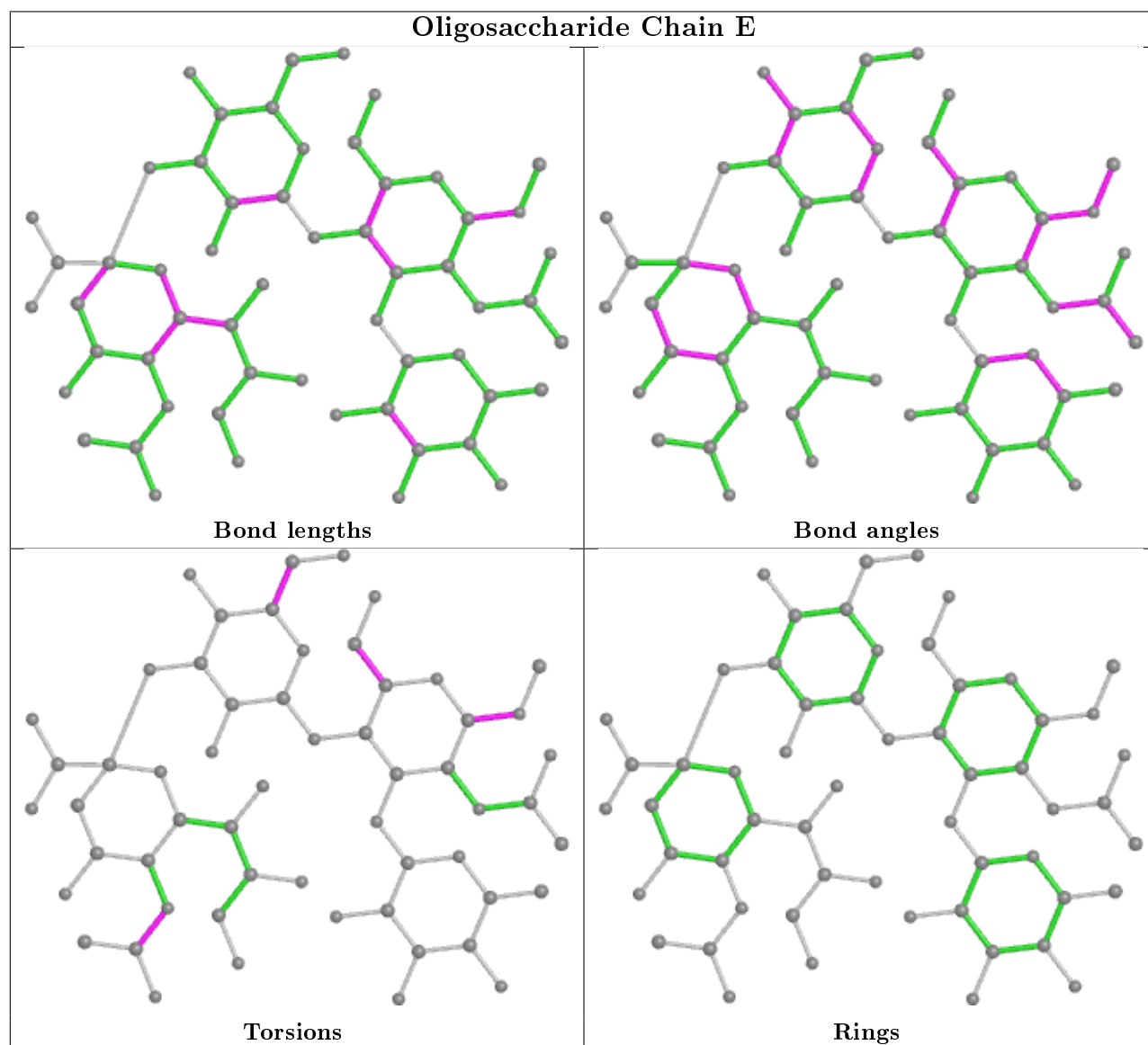
Mol	Chain	Res	Type	Atoms
2	F	1	MAG	C2-C1-O1-CM
2	E	1	MAG	C2-C1-O1-CM
2	E	1	MAG	C4-C5-C6-O6
2	E	1	MAG	O5-C5-C6-O6
2	E	3	SIA	C11-C10-N5-C5
2	E	3	SIA	O10-C10-N5-C5
2	F	3	SIA	C11-C10-N5-C5
2	F	3	SIA	O10-C10-N5-C5
2	G	3	SIA	C11-C10-N5-C5
2	G	3	SIA	O10-C10-N5-C5
2	G	1	MAG	O5-C1-O1-CM
2	G	2	GAL	O5-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6
2	G	3	SIA	C7-C8-C9-O9
2	G	3	SIA	O8-C8-C9-O9
2	F	1	MAG	C4-C5-C6-O6
2	F	1	MAG	O5-C5-C6-O6

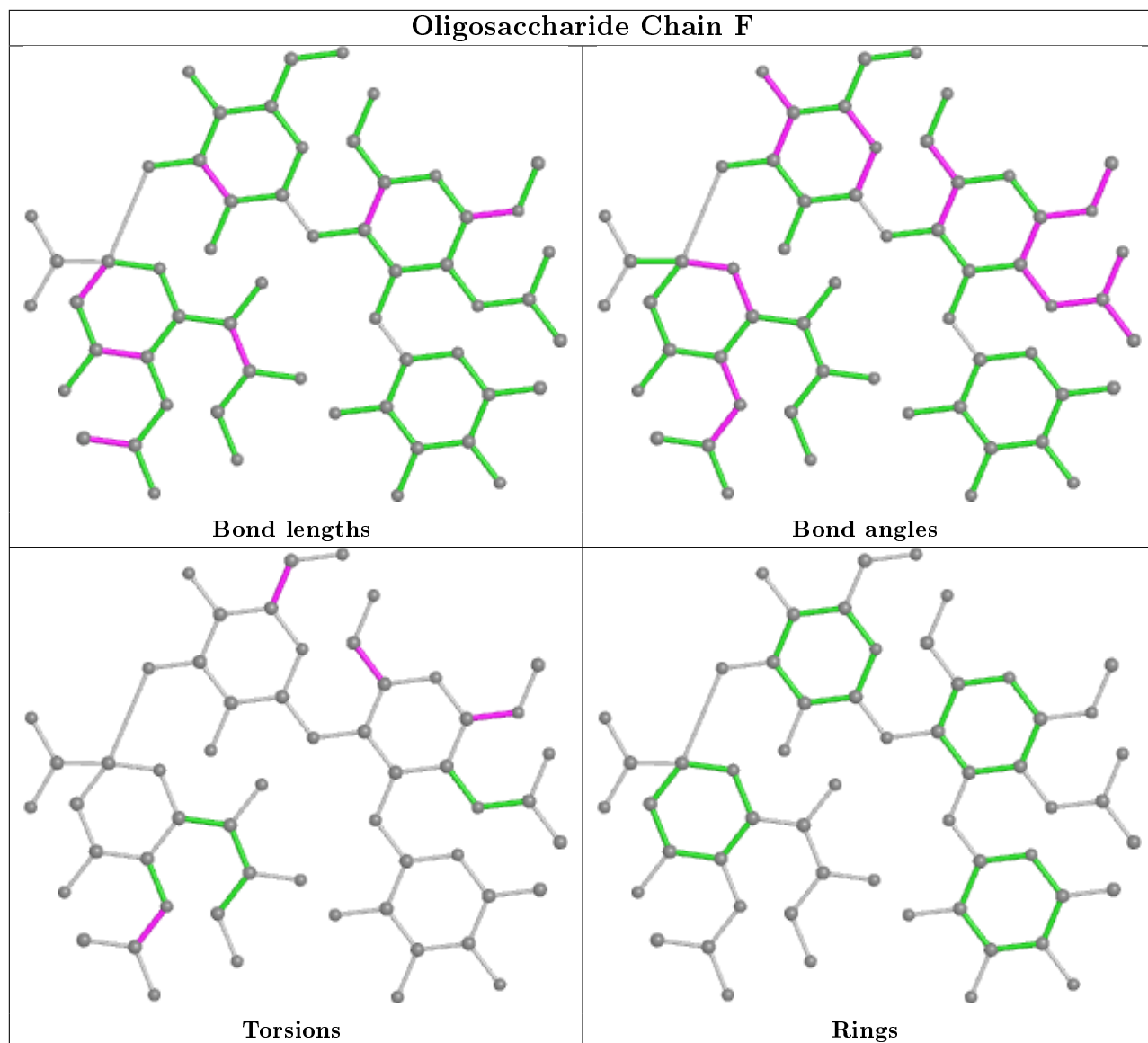
There are no ring outliers.

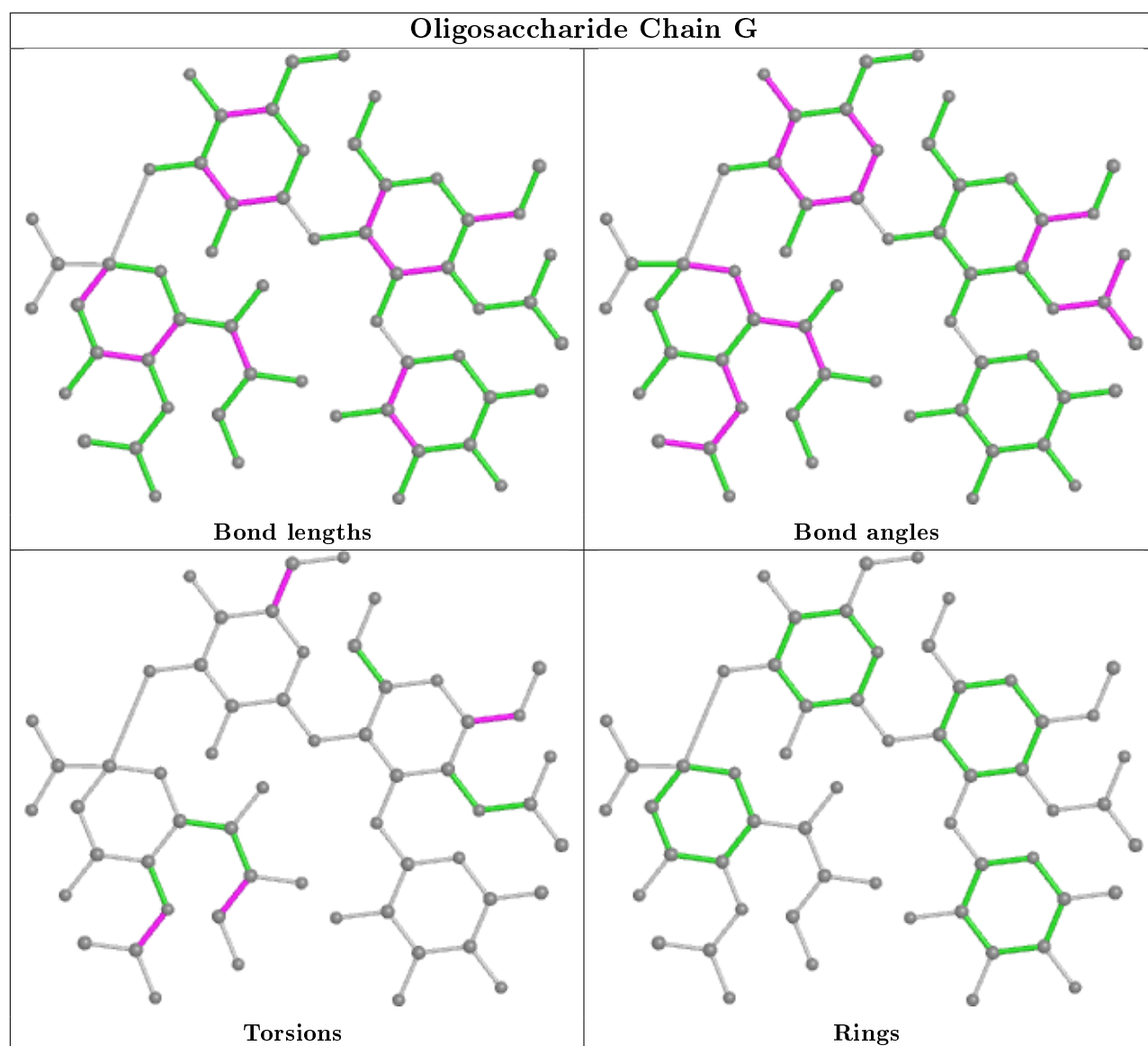
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	FUC	4	0
2	G	3	SIA	1	0
2	F	2	GAL	1	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	MRD	A	806	-	7,7,7	0.69	0	9,10,10	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MRD	C	805	-	7,7,7	0.81	0	9,10,10	0.44	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
4	MRD	A	806	-	-	1/5/5/5	-
4	MRD	C	805	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	MRD	O2-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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.