Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 12:31 am GMT

PDB ID	:	1H15
Title	:	X-ray crystal structure of HLA-DRA1*0101/DRB5*0101 complexed with a peptide from Epstein Barr Virus DNA polymerase
Authors	:	Lang, H.; Jacobsen, H.; Ikemizu, S.; Andersson, C.; Harlos, K.; Madsen, L.; Hjorth, P.; Sondergaard, L.; Svejgaard, A.; Wucherpfennig, K.; Stuart, D.I.; Bell, J.I.; Jones, E.Y.; Fugger, L.
Deposited on	:	2002-07-02
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

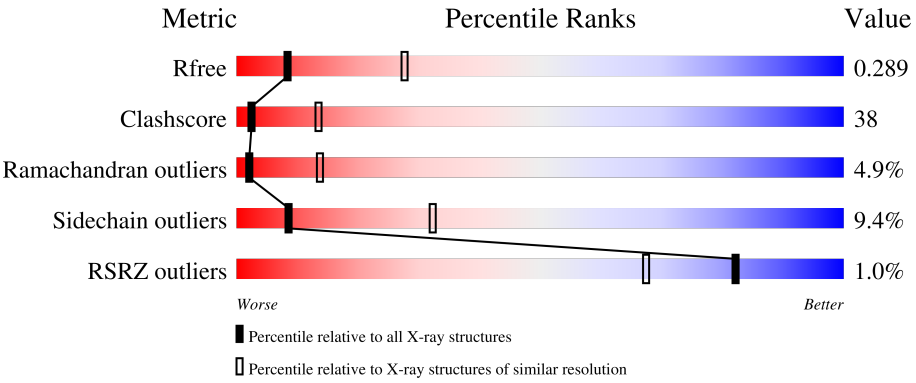
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	182	52% 40% 8%
1	D	182	35% 57% 7%
2	B	190	41% 50% 7%
2	E	190	38% 47% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	14	93% 7%
3	F	14	21% 57% 43%
4	G	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	NAG	G	2	X	-	-	-
5	NAG	D	1184	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6420 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 HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1479	957	240	277	5			
1	D	180	Total	C	N	O	S	0	0	0
			1479	957	240	277	5			

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR BETA 1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1565	979	282	299	5			
2	E	189	Total	C	N	O	S	0	0	0
			1565	979	282	299	5			

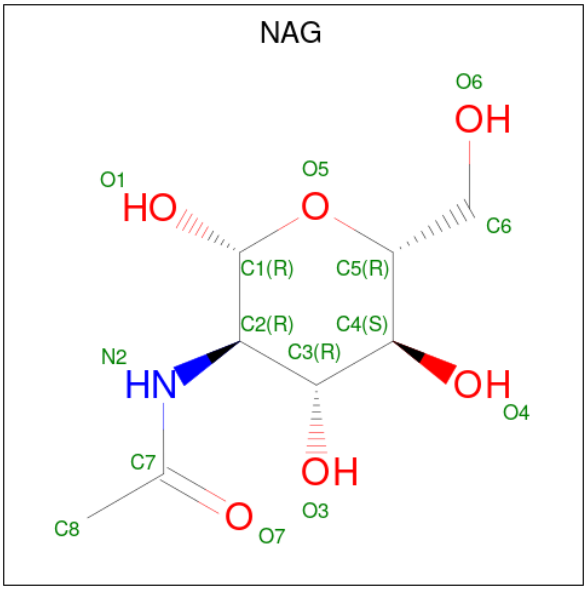
- Molecule 3 is a protein called DNA POLYMERASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	0	0	0
			116	75	22	19			
3	F	14	Total	C	N	O	0	0	0
			116	75	22	19			

- Molecule 4 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
4	G	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

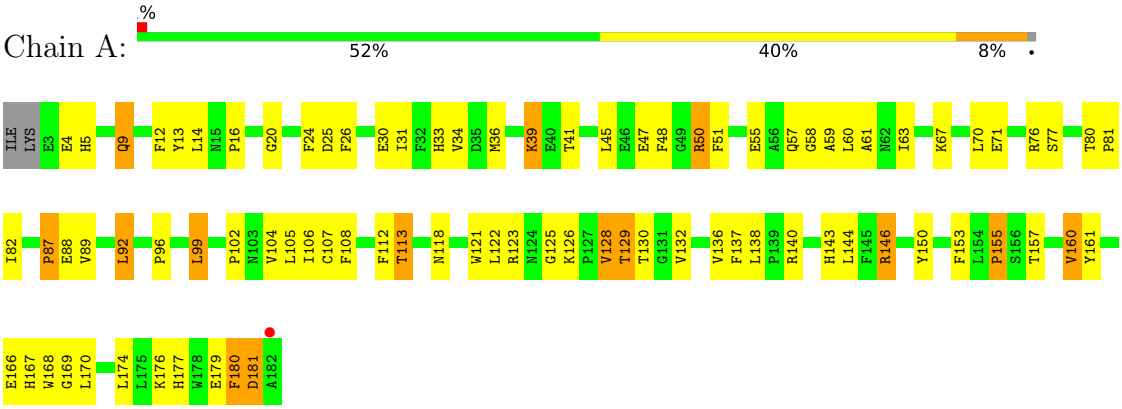
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	8	Total O 8 8	0	0
6	D	2	Total O 2 2	0	0
6	E	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

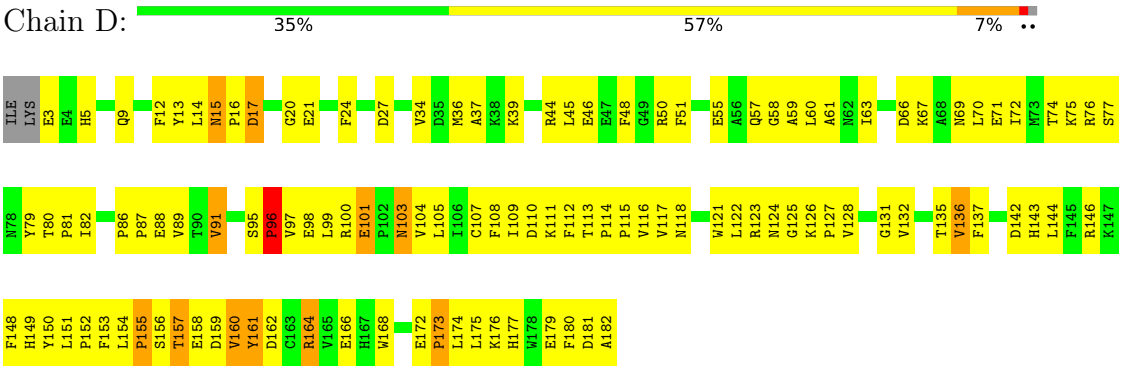
• Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN

Chain A:



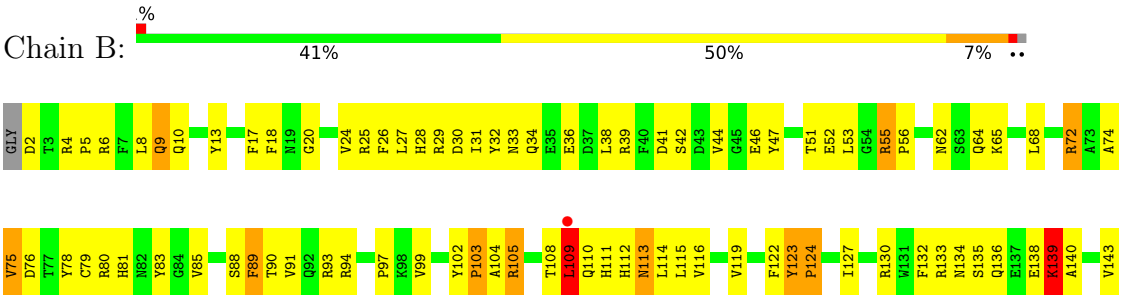
• Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN

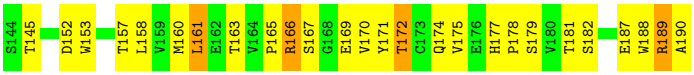
Chain D:



• Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR BETA 1 CHAIN

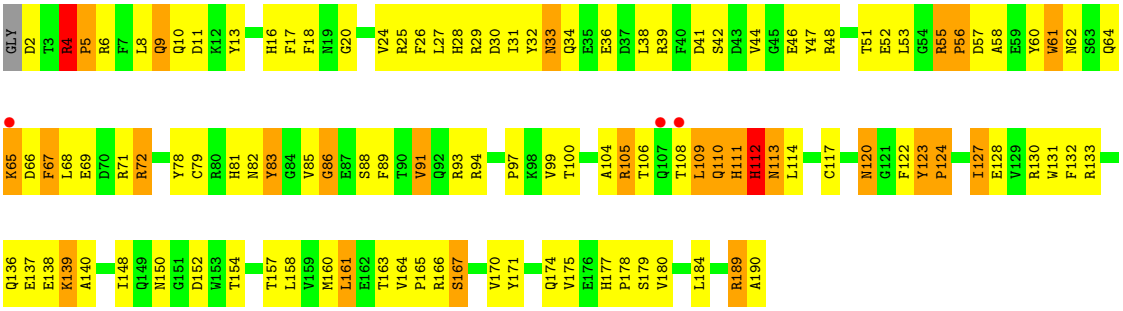
Chain B:





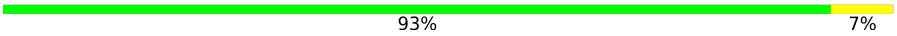
• Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR BETA 1 CHAIN

Chain E:



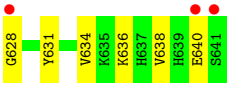
• Molecule 3: DNA POLYMERASE

Chain C:



• Molecule 3: DNA POLYMERASE

Chain F:



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

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	179.24Å 179.24Å 92.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.10 19.88 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.88-3.10) 85.1 (19.88-2.99)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.256 , 0.310 0.240 , 0.289	Depositor DCC
R_{free} test set	1415 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6420	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/1524	0.73	2/2077 (0.1%)
1	D	0.40	0/1524	0.67	0/2077
2	B	0.42	0/1605	0.69	1/2179 (0.0%)
2	E	0.42	0/1605	0.70	0/2179
3	C	0.53	0/120	0.57	0/158
3	F	0.45	0/120	0.51	0/158
All	All	0.43	0/6498	0.69	3/8828 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	GLU	N-CA-C	-6.16	94.37	111.00
1	A	9	GLN	N-CA-C	-5.28	96.73	111.00
2	B	109	LEU	CA-CB-CG	5.12	127.07	115.30

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	1479	0	1410	74	0
1	D	1479	0	1408	128	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1565	0	1469	139	0
2	E	1565	0	1469	158	0
3	C	116	0	108	1	0
3	F	116	0	108	6	0
4	G	28	0	25	7	0
5	A	14	0	13	0	0
5	D	28	0	26	1	0
6	A	12	0	0	0	0
6	B	8	0	0	0	0
6	D	2	0	0	0	0
6	E	8	0	0	1	0
All	All	6420	0	6036	466	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 38.

All (466) 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:D:16:PRO:HG2	2:E:6:ARG:HA	1.20	1.14
2:E:109:LEU:HD22	2:E:110:GLN:HG3	1.38	1.02
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.43	0.96
2:B:47:TYR:H	2:B:62:ASN:HD21	1.06	0.93
2:E:112:HIS:HA	2:E:164:VAL:HG12	1.49	0.93
1:D:89:VAL:HG12	1:D:176:LYS:HG3	1.55	0.86
2:B:167:SER:HA	2:B:190:ALA:HB2	1.54	0.86
1:D:160:VAL:HG13	1:D:177:HIS:HE1	1.43	0.83
2:B:130:ARG:HD2	2:B:174:GLN:OE1	1.78	0.82
2:E:47:TYR:H	2:E:62:ASN:HD21	1.29	0.81
2:E:93:ARG:O	2:E:94:ARG:HG3	1.80	0.81
2:E:62:ASN:HA	2:E:68:LEU:HD22	1.64	0.80
2:E:46:GLU:HB2	2:E:62:ASN:OD1	1.82	0.79
2:E:106:THR:HG23	2:E:113:ASN:OD1	1.82	0.79
2:E:139:LYS:HD2	2:E:140:ALA:N	1.97	0.79
2:B:55:ARG:HB3	2:B:56:PRO:HD3	1.66	0.78
2:E:97:PRO:HG3	2:E:122:PHE:HB3	1.64	0.78
1:A:160:VAL:HG22	1:A:179:GLU:HB3	1.65	0.78
2:E:139:LYS:HE3	2:E:139:LYS:H	1.48	0.78
1:D:108:PHE:CZ	1:D:146:ARG:HD2	2.20	0.77
1:D:123:ARG:HG2	1:D:124:ASN:ND2	1.99	0.77
2:B:29:ARG:HG2	2:B:36:GLU:OE2	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:ASN:HD22	2:E:114:LEU:H	1.34	0.76
2:E:55:ARG:HB3	2:E:56:PRO:HD3	1.68	0.76
2:E:139:LYS:HD2	2:E:140:ALA:H	1.52	0.75
1:D:109:ILE:HG22	1:D:112:PHE:CE1	2.21	0.75
2:B:65:LYS:NZ	2:B:65:LYS:HB3	2.02	0.75
1:D:89:VAL:O	1:D:176:LYS:HE3	1.87	0.75
2:E:114:LEU:HD11	2:E:160:MET:HE3	1.68	0.75
1:D:132:VAL:HG23	1:D:150:TYR:O	1.88	0.74
2:E:139:LYS:H	2:E:139:LYS:CE	2.00	0.74
2:B:139:LYS:N	2:B:139:LYS:HE3	2.03	0.74
2:B:89:PHE:HD2	2:B:90:THR:HG23	1.52	0.74
2:E:17:PHE:HD1	2:E:24:VAL:HG22	1.53	0.73
2:E:157:THR:C	2:E:158:LEU:HD12	2.08	0.73
2:B:81:HIS:O	2:B:85:VAL:HG23	1.89	0.73
2:E:123:TYR:O	2:E:124:PRO:C	2.27	0.73
1:D:81:PRO:HG3	2:E:5:PRO:HB3	1.71	0.72
1:A:14:LEU:HD13	2:B:8:LEU:HD13	1.70	0.72
1:D:91:VAL:HG23	1:D:107:CYS:HA	1.70	0.72
1:D:108:PHE:HZ	1:D:146:ARG:HD2	1.56	0.71
1:D:160:VAL:HG13	1:D:177:HIS:CE1	2.24	0.71
2:E:123:TYR:HB3	2:E:124:PRO:HD3	1.73	0.71
2:E:106:THR:HG22	2:E:106:THR:O	1.91	0.71
2:B:123:TYR:O	2:B:124:PRO:C	2.27	0.70
2:B:123:TYR:HB3	2:B:124:PRO:HD3	1.73	0.70
2:B:17:PHE:HD1	2:B:24:VAL:HG22	1.56	0.70
1:D:96:PRO:HD3	2:E:120:ASN:HD21	1.57	0.69
1:D:39:LYS:HD3	1:D:60:LEU:HD13	1.74	0.69
2:E:94:ARG:HG3	2:E:94:ARG:HH11	1.55	0.69
2:E:47:TYR:HB2	2:E:62:ASN:HD21	1.57	0.69
1:D:74:THR:HG22	1:D:79:TYR:CD2	2.28	0.69
1:D:96:PRO:HD3	2:E:120:ASN:ND2	2.08	0.68
2:B:134:ASN:HD21	2:B:169:GLU:HA	1.59	0.68
1:D:16:PRO:CG	2:E:6:ARG:HA	2.12	0.67
2:E:105:ARG:O	2:E:105:ARG:HD3	1.94	0.67
1:D:39:LYS:HD3	1:D:60:LEU:CD1	2.24	0.67
2:E:67:PHE:HE2	2:E:71:ARG:HE	1.42	0.67
1:A:180:PHE:O	1:A:181:ASP:HB2	1.93	0.67
2:B:62:ASN:HA	2:B:68:LEU:HD13	1.76	0.67
1:A:77:SER:HB3	2:B:53:LEU:HD11	1.76	0.67
2:B:72:ARG:O	2:B:75:VAL:HG22	1.94	0.67
2:E:17:PHE:CD1	2:E:24:VAL:HG22	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:TYR:H	2:B:62:ASN:ND2	1.89	0.66
2:B:89:PHE:CD2	2:B:90:THR:HG23	2.30	0.66
1:D:14:LEU:HD13	2:E:8:LEU:HD13	1.76	0.66
4:G:1:NAG:H4	4:G:2:NAG:HN2	1.60	0.66
1:D:21:GLU:OE1	1:D:137:PHE:HB2	1.95	0.66
1:D:74:THR:HG22	1:D:79:TYR:HD2	1.61	0.65
2:E:139:LYS:H	2:E:139:LYS:CD	2.10	0.65
1:D:99:LEU:HD22	1:D:157:THR:HG22	1.79	0.65
2:E:161:LEU:HD22	2:E:163:THR:HG23	1.78	0.65
2:E:124:PRO:HD2	2:E:177:HIS:CE1	2.33	0.64
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.62	0.64
2:E:109:LEU:O	2:E:110:GLN:HB2	1.98	0.64
1:D:5:HIS:HD2	1:D:27:ASP:OD2	1.79	0.64
1:D:111:LYS:C	1:D:144:LEU:HD13	2.18	0.64
2:B:113:ASN:ND2	2:B:114:LEU:H	1.95	0.64
2:B:170:VAL:HA	2:B:189:ARG:HB3	1.80	0.64
2:E:113:ASN:ND2	2:E:114:LEU:H	1.94	0.64
2:E:47:TYR:H	2:E:62:ASN:ND2	1.95	0.64
1:D:50:ARG:NH1	1:D:50:ARG:HB3	2.14	0.63
1:D:98:GLU:O	1:D:101:GLU:HB2	1.98	0.63
2:E:68:LEU:HG	2:E:72:ARG:NH1	2.13	0.63
2:E:89:PHE:O	2:E:93:ARG:HB2	1.98	0.63
1:A:181:ASP:HB2	2:E:105:ARG:HH21	1.62	0.63
2:B:138:GLU:C	2:B:139:LYS:HE3	2.19	0.63
1:D:39:LYS:CD	1:D:60:LEU:HD13	2.28	0.63
1:A:118:ASN:HB2	1:A:166:GLU:HG3	1.81	0.63
2:E:46:GLU:HA	2:E:68:LEU:HD11	1.81	0.62
2:E:111:HIS:O	2:E:112:HIS:O	2.16	0.62
2:E:170:VAL:HG12	2:E:189:ARG:HB3	1.81	0.62
2:E:124:PRO:HD2	2:E:177:HIS:HE1	1.65	0.62
1:D:50:ARG:HB3	1:D:50:ARG:HH11	1.64	0.62
2:E:38:LEU:HD13	2:E:58:ALA:HB2	1.82	0.62
1:A:81:PRO:CG	2:B:5:PRO:HB3	2.30	0.61
2:E:138:GLU:HG2	2:E:161:LEU:HD21	1.81	0.61
2:E:30:ASP:HB3	2:E:38:LEU:HB3	1.82	0.61
1:A:108:PHE:CE1	1:A:146:ARG:HD2	2.35	0.61
2:B:2:ASP:OD2	2:B:4:ARG:HG2	2.00	0.61
2:E:127:ILE:HG12	2:E:128:GLU:N	2.16	0.61
2:B:27:LEU:HD13	2:B:41:ASP:HA	1.82	0.61
2:B:99:VAL:HG21	2:B:175:VAL:HG21	1.83	0.61
2:B:65:LYS:HB3	2:B:65:LYS:HZ2	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:THR:HG22	2:B:187:GLU:HG2	1.82	0.60
1:D:123:ARG:C	1:D:125:GLY:H	2.04	0.60
1:D:180:PHE:CD1	1:D:181:ASP:HB2	2.36	0.60
1:D:77:SER:O	1:D:80:THR:HG23	2.00	0.60
1:D:77:SER:HB3	2:E:53:LEU:HD11	1.83	0.60
1:D:110:ASP:OD1	1:D:111:LYS:N	2.35	0.60
2:B:145:THR:HG21	2:B:158:LEU:HB2	1.84	0.60
2:B:167:SER:HA	2:B:190:ALA:CB	2.29	0.59
2:E:41:ASP:HB3	2:E:44:VAL:HG23	1.84	0.59
1:A:77:SER:O	1:A:80:THR:HG23	2.02	0.59
2:E:139:LYS:HE3	2:E:139:LYS:N	2.16	0.59
1:D:97:VAL:HG23	1:D:103:ASN:HD22	1.67	0.59
2:B:17:PHE:CD1	2:B:24:VAL:HG22	2.37	0.59
2:E:47:TYR:HB2	2:E:62:ASN:ND2	2.17	0.59
1:D:75:LYS:C	1:D:77:SER:H	2.06	0.59
2:B:123:TYR:CD1	2:B:124:PRO:N	2.70	0.59
2:E:86:GLY:C	2:E:88:SER:H	2.06	0.59
2:E:123:TYR:CD1	2:E:124:PRO:N	2.71	0.59
2:B:62:ASN:HD22	2:B:68:LEU:CD1	2.16	0.59
2:E:170:VAL:HG23	2:E:170:VAL:O	2.02	0.58
2:B:93:ARG:O	2:B:94:ARG:NH1	2.37	0.58
1:A:67:LYS:O	1:A:71:GLU:HG3	2.04	0.58
1:A:123:ARG:HG3	1:A:161:TYR:CE2	2.38	0.58
2:E:81:HIS:O	2:E:85:VAL:HG23	2.04	0.57
1:A:87:PRO:HD3	1:A:167:HIS:CD2	2.39	0.57
2:B:116:VAL:HG22	2:B:160:MET:CG	2.27	0.57
2:B:127:ILE:HG13	2:B:177:HIS:HB2	1.87	0.57
1:D:13:TYR:CE1	1:D:67:LYS:HG3	2.40	0.57
2:E:27:LEU:HD13	2:E:41:ASP:HA	1.86	0.57
2:E:38:LEU:CD1	2:E:58:ALA:HB2	2.35	0.57
1:D:45:LEU:HD12	1:D:48:PHE:CE1	2.40	0.57
1:D:180:PHE:CE1	1:D:181:ASP:HB2	2.40	0.57
2:B:85:VAL:HG12	2:B:85:VAL:O	2.05	0.56
2:B:52:GLU:HA	2:B:52:GLU:OE1	2.05	0.56
1:A:13:TYR:CE1	1:A:67:LYS:HG3	2.40	0.56
1:D:36:MET:CE	1:D:63:ILE:HG21	2.35	0.56
2:E:109:LEU:O	2:E:110:GLN:CB	2.53	0.56
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.38	0.56
1:D:162:ASP:OD1	1:D:177:HIS:HA	2.06	0.56
4:G:1:NAG:O6	4:G:1:NAG:H2	2.06	0.56
2:B:17:PHE:HB3	2:B:20:GLY:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:GLU:HG2	2:B:161:LEU:HD21	1.87	0.56
1:D:100:ARG:O	1:D:154:LEU:HD11	2.06	0.56
1:A:4:GLU:C	1:A:5:HIS:ND1	2.60	0.56
1:A:108:PHE:HE1	1:A:146:ARG:HD2	1.70	0.56
1:A:34:VAL:HG21	1:A:59:ALA:CB	2.35	0.56
2:B:41:ASP:HB3	2:B:44:VAL:HG23	1.87	0.55
2:E:94:ARG:HG3	2:E:94:ARG:NH1	2.21	0.55
1:A:82:ILE:HG22	2:B:6:ARG:O	2.07	0.55
2:B:163:THR:O	2:B:165:PRO:HD3	2.06	0.55
2:E:26:PHE:HB3	2:E:42:SER:HB3	1.88	0.55
1:A:130:THR:C	1:A:132:VAL:H	2.09	0.55
1:D:117:VAL:HG22	1:D:118:ASN:N	2.22	0.55
2:E:114:LEU:HD21	2:E:160:MET:CE	2.36	0.55
2:E:10:GLN:HB3	2:E:31:ILE:HB	1.88	0.55
2:B:51:THR:HG22	2:E:51:THR:HG22	1.88	0.55
1:D:34:VAL:HG21	1:D:59:ALA:CB	2.36	0.55
1:D:113:THR:OG1	1:D:114:PRO:HA	2.06	0.55
1:A:168:TRP:HE1	4:G:1:NAG:H82	1.72	0.55
1:A:89:VAL:O	1:A:176:LYS:HE3	2.07	0.54
2:E:85:VAL:HG12	2:E:85:VAL:O	2.07	0.54
1:D:9:GLN:HG3	1:D:24:PHE:CE1	2.42	0.54
1:D:115:PRO:HB2	1:D:137:PHE:CE1	2.42	0.54
1:A:34:VAL:HG21	1:A:59:ALA:HB3	1.90	0.54
1:A:136:VAL:HG23	1:A:137:PHE:N	2.23	0.54
2:B:132:PHE:HB2	2:B:172:THR:OG1	2.08	0.54
2:B:134:ASN:OD1	2:B:170:VAL:HG22	2.07	0.54
2:B:29:ARG:NH1	2:B:36:GLU:OE2	2.41	0.54
2:B:30:ASP:HB3	2:B:38:LEU:HB3	1.88	0.54
2:B:93:ARG:HD3	2:B:123:TYR:CD2	2.42	0.54
2:B:145:THR:CG2	2:B:158:LEU:HB2	2.37	0.54
2:B:170:VAL:HG23	2:B:170:VAL:O	2.08	0.54
2:B:97:PRO:HA	2:B:122:PHE:HB3	1.90	0.54
1:D:179:GLU:HG3	1:D:182:ALA:HB3	1.90	0.54
2:E:47:TYR:N	2:E:62:ASN:HD21	2.03	0.54
2:E:161:LEU:HD22	2:E:163:THR:CG2	2.38	0.54
2:B:138:GLU:O	2:B:140:ALA:N	2.41	0.54
1:A:5:HIS:HD2	1:A:26:PHE:CZ	2.26	0.53
1:A:57:GLN:HA	1:A:60:LEU:HD12	1.90	0.53
1:D:44:ARG:O	1:D:45:LEU:HD23	2.09	0.53
1:D:67:LYS:O	1:D:71:GLU:HG3	2.09	0.53
2:E:52:GLU:OE1	2:E:52:GLU:HA	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD23	1:A:92:LEU:N	2.24	0.52
2:E:60:TYR:HB2	6:E:2002:HOH:O	2.09	0.52
2:B:74:ALA:O	2:B:76:ASP:N	2.42	0.52
2:B:138:GLU:HG2	2:B:161:LEU:HD11	1.91	0.52
1:D:159:ASP:O	1:D:160:VAL:HG23	2.10	0.52
2:E:68:LEU:HG	2:E:72:ARG:HH11	1.74	0.52
1:A:140:ARG:HD3	1:A:144:LEU:HB2	1.91	0.52
2:B:115:LEU:HD21	2:B:188:TRP:CE3	2.44	0.52
1:D:121:TRP:O	1:D:122:LEU:HD23	2.09	0.52
2:E:17:PHE:HB3	2:E:20:GLY:O	2.09	0.52
2:B:133:ARG:HG3	2:B:171:TYR:CE2	2.45	0.52
1:D:34:VAL:HG21	1:D:59:ALA:HB3	1.91	0.52
1:D:57:GLN:HA	1:D:60:LEU:HD12	1.92	0.52
2:B:102:TYR:CE2	2:B:116:VAL:HB	2.45	0.51
2:B:104:ALA:O	2:B:105:ARG:HG3	2.10	0.51
2:E:127:ILE:HG12	2:E:128:GLU:H	1.75	0.51
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.92	0.51
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.46	0.51
2:B:102:TYR:C	2:B:102:TYR:CD2	2.84	0.51
2:B:94:ARG:HG3	2:B:94:ARG:HH11	1.75	0.51
1:D:36:MET:HE2	1:D:63:ILE:HG21	1.90	0.51
1:D:109:ILE:N	1:D:109:ILE:HD12	2.25	0.51
1:A:36:MET:CE	1:A:63:ILE:HG21	2.41	0.51
1:D:99:LEU:C	1:D:100:ARG:HG2	2.31	0.51
1:D:161:TYR:CD1	1:D:161:TYR:N	2.79	0.51
2:E:28:HIS:O	2:E:39:ARG:HA	2.10	0.51
1:A:39:LYS:HD2	1:A:60:LEU:HD13	1.93	0.51
2:B:94:ARG:NH1	2:B:94:ARG:HG3	2.25	0.51
2:B:170:VAL:HG12	2:B:189:ARG:HB3	1.92	0.51
2:E:177:HIS:CG	2:E:178:PRO:HD2	2.46	0.51
2:B:189:ARG:HH11	2:B:189:ARG:CG	2.23	0.51
2:B:26:PHE:HB3	2:B:42:SER:HB3	1.92	0.50
2:E:106:THR:C	2:E:108:THR:H	2.13	0.50
2:E:167:SER:HA	2:E:190:ALA:CB	2.41	0.50
1:A:4:GLU:O	1:A:5:HIS:ND1	2.43	0.50
2:B:52:GLU:OE2	2:E:55:ARG:NH1	2.45	0.50
2:B:133:ARG:HG2	2:B:133:ARG:HH11	1.76	0.50
1:A:129:THR:O	1:A:130:THR:HG23	2.12	0.50
2:E:114:LEU:HD21	2:E:160:MET:HE3	1.93	0.50
2:B:108:THR:HG21	2:B:112:HIS:O	2.12	0.50
1:D:105:LEU:HG	1:D:153:PHE:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:ARG:HG2	2:E:36:GLU:OE2	2.12	0.50
2:B:134:ASN:ND2	2:B:169:GLU:HA	2.27	0.50
1:D:9:GLN:HB2	2:E:78:TYR:OH	2.11	0.50
2:E:62:ASN:N	2:E:62:ASN:HD22	2.10	0.50
2:B:32:TYR:O	2:B:34:GLN:N	2.45	0.49
2:B:133:ARG:HD2	2:B:169:GLU:OE2	2.12	0.49
1:D:117:VAL:HG22	1:D:118:ASN:H	1.76	0.49
2:B:74:ALA:C	2:B:76:ASP:N	2.64	0.49
2:E:64:GLN:C	2:E:66:ASP:H	2.15	0.49
2:E:86:GLY:C	2:E:88:SER:N	2.64	0.49
2:E:152:ASP:OD1	2:E:152:ASP:O	2.31	0.49
1:D:45:LEU:HB2	1:D:48:PHE:CD1	2.48	0.49
1:A:123:ARG:HG3	1:A:161:TYR:CZ	2.48	0.49
1:A:168:TRP:NE1	4:G:1:NAG:H82	2.28	0.49
1:D:97:VAL:HG23	1:D:103:ASN:ND2	2.27	0.49
2:E:91:VAL:HG12	2:E:91:VAL:O	2.12	0.49
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.48	0.49
2:B:74:ALA:C	2:B:76:ASP:H	2.17	0.48
2:B:143:VAL:HG22	1:D:175:LEU:HB3	1.95	0.48
1:D:58:GLY:O	1:D:61:ALA:HB3	2.13	0.48
1:D:15:ASN:HD22	1:D:70:LEU:HG	1.78	0.48
2:B:111:HIS:ND1	2:B:111:HIS:N	2.61	0.48
2:B:170:VAL:HG12	2:B:189:ARG:CB	2.43	0.48
1:D:75:LYS:O	1:D:77:SER:N	2.47	0.48
2:E:108:THR:HB	2:E:111:HIS:CE1	2.49	0.48
2:E:130:ARG:HD2	2:E:174:GLN:OE1	2.13	0.48
2:B:93:ARG:O	2:B:94:ARG:HG3	2.14	0.48
2:B:172:THR:CG2	2:B:187:GLU:HG2	2.43	0.48
1:D:89:VAL:CG1	1:D:176:LYS:HG3	2.35	0.48
2:B:34:GLN:O	2:B:34:GLN:HG2	2.14	0.48
2:E:86:GLY:HA3	2:E:89:PHE:CE2	2.49	0.48
1:A:160:VAL:HG13	1:A:177:HIS:CE1	2.49	0.48
2:E:93:ARG:HG2	2:E:94:ARG:N	2.27	0.48
1:A:47:GLU:HA	1:A:50:ARG:NH1	2.29	0.48
1:D:116:VAL:HG11	1:D:168:TRP:CH2	2.49	0.48
2:E:180:VAL:HG21	2:E:184:LEU:HD12	1.96	0.48
4:G:2:NAG:H61	4:G:2:NAG:H2	1.95	0.48
1:A:12:PHE:O	1:A:20:GLY:HA2	2.13	0.47
2:E:158:LEU:HD12	2:E:158:LEU:N	2.28	0.47
2:E:29:ARG:NH1	2:E:36:GLU:OE2	2.48	0.47
2:E:177:HIS:C	2:E:179:SER:H	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ASN:ND2	2:B:68:LEU:HD11	2.29	0.47
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.49	0.47
2:B:27:LEU:CD1	2:B:41:ASP:HA	2.43	0.47
1:D:115:PRO:HB2	1:D:137:PHE:CD1	2.50	0.47
2:E:25:ARG:NH2	2:E:41:ASP:OD2	2.48	0.47
2:E:133:ARG:HG2	2:E:133:ARG:HH11	1.79	0.47
4:G:1:NAG:C4	4:G:2:NAG:HN2	2.27	0.47
2:B:109:LEU:HD22	2:B:110:GLN:NE2	2.29	0.47
1:D:3:GLU:HB3	2:E:18:PHE:CZ	2.50	0.47
1:A:81:PRO:HG3	2:B:5:PRO:HB3	1.96	0.47
1:A:122:LEU:HA	1:A:126:LYS:O	2.15	0.47
1:D:50:ARG:NH1	1:D:51:PHE:CE2	2.83	0.47
1:D:81:PRO:CG	2:E:5:PRO:HB3	2.42	0.47
1:D:87:PRO:HG3	1:D:112:PHE:CB	2.45	0.47
2:E:34:GLN:HG2	2:E:34:GLN:O	2.14	0.47
2:E:44:VAL:HG11	2:E:48:ARG:HE	1.77	0.47
2:E:61:TRP:HE3	2:E:61:TRP:HA	1.79	0.47
2:E:61:TRP:HA	2:E:61:TRP:CE3	2.50	0.47
2:E:132:PHE:CD2	2:E:137:GLU:HA	2.49	0.47
2:B:99:VAL:CG2	2:B:175:VAL:HG21	2.43	0.47
2:E:99:VAL:HG21	2:E:175:VAL:HG21	1.96	0.47
1:A:5:HIS:HD2	1:A:26:PHE:HZ	1.61	0.47
2:E:16:HIS:HD2	2:E:27:LEU:HD23	1.79	0.47
2:E:32:TYR:O	2:E:34:GLN:N	2.48	0.47
2:B:2:ASP:HB2	4:G:2:NAG:H83	1.96	0.46
2:B:97:PRO:CA	2:B:122:PHE:HB3	2.45	0.46
1:D:121:TRP:O	1:D:127:PRO:HA	2.15	0.46
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.78	0.46
1:D:12:PHE:CD1	1:D:12:PHE:C	2.89	0.46
2:E:4:ARG:HB3	2:E:4:ARG:HH11	1.79	0.46
2:B:169:GLU:O	2:B:189:ARG:HB2	2.15	0.46
2:E:65:LYS:HD3	2:E:68:LEU:HD23	1.95	0.46
2:E:180:VAL:HG11	2:E:184:LEU:HD11	1.98	0.46
2:B:10:GLN:HB3	2:B:31:ILE:HB	1.97	0.46
2:B:132:PHE:O	2:B:171:TYR:HA	2.16	0.46
1:D:12:PHE:O	1:D:20:GLY:HA2	2.16	0.46
1:D:164:ARG:HA	1:D:174:LEU:O	2.15	0.46
2:E:16:HIS:CD2	2:E:27:LEU:HD23	2.51	0.46
1:A:160:VAL:HG13	1:A:177:HIS:HE1	1.81	0.46
2:B:113:ASN:HD22	2:B:114:LEU:H	1.63	0.46
1:D:126:LYS:HA	1:D:127:PRO:HD3	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:177:HIS:ND1	2:E:178:PRO:HD2	2.31	0.46
1:A:9:GLN:HB2	2:B:78:TYR:OH	2.15	0.46
1:A:160:VAL:CG1	1:A:177:HIS:HE1	2.28	0.46
2:B:62:ASN:HD22	2:B:68:LEU:HD11	1.81	0.46
1:D:179:GLU:HG3	1:D:182:ALA:CB	2.46	0.46
2:E:123:TYR:CG	2:E:124:PRO:N	2.81	0.46
1:D:118:ASN:HB2	1:D:166:GLU:CG	2.45	0.46
2:E:139:LYS:CD	2:E:139:LYS:N	2.74	0.46
1:A:36:MET:HE2	1:A:63:ILE:HG21	1.99	0.45
2:B:177:HIS:O	2:B:179:SER:N	2.44	0.45
1:D:69:ASN:OD1	3:F:638:VAL:HG23	2.16	0.45
1:A:130:THR:C	1:A:132:VAL:N	2.70	0.45
2:B:166:ARG:HB2	2:B:169:GLU:OE1	2.16	0.45
1:A:99:LEU:HG	1:A:180:PHE:HE1	1.80	0.45
2:B:52:GLU:OE1	2:E:52:GLU:OE1	2.34	0.45
1:D:108:PHE:CE1	1:D:146:ARG:HD2	2.50	0.45
2:E:82:ASN:OD1	3:F:631:TYR:HD1	2.00	0.45
2:B:124:PRO:HD2	2:B:177:HIS:CE1	2.52	0.45
2:B:143:VAL:HG22	1:D:175:LEU:CB	2.47	0.45
1:D:109:ILE:HG22	1:D:112:PHE:CD1	2.50	0.45
2:B:152:ASP:O	2:B:153:TRP:HB2	2.16	0.45
1:A:58:GLY:O	1:A:61:ALA:HB3	2.17	0.45
1:D:95:SER:O	1:D:96:PRO:O	2.35	0.45
1:A:33:HIS:CG	1:A:136:VAL:HG11	2.52	0.45
1:D:15:ASN:HB3	1:D:16:PRO:HD3	1.99	0.45
2:B:90:THR:OG1	2:B:91:VAL:N	2.50	0.45
2:B:127:ILE:HD11	2:B:175:VAL:CG1	2.47	0.45
2:E:123:TYR:HB3	2:E:124:PRO:CD	2.45	0.44
1:A:99:LEU:CD1	1:A:180:PHE:HE1	2.30	0.44
2:E:133:ARG:HG3	2:E:171:TYR:CE2	2.53	0.44
1:A:9:GLN:HG3	1:A:24:PHE:CE1	2.52	0.44
1:A:12:PHE:CD1	1:A:12:PHE:C	2.91	0.44
2:B:133:ARG:HG2	2:B:133:ARG:NH1	2.33	0.44
2:B:134:ASN:O	2:B:135:SER:C	2.56	0.44
1:D:70:LEU:HB2	2:E:9:GLN:HG3	2.00	0.44
1:A:45:LEU:HD12	1:A:48:PHE:CZ	2.53	0.44
2:B:109:LEU:CD1	2:B:110:GLN:HE22	2.30	0.44
2:B:189:ARG:CG	2:B:189:ARG:NH1	2.80	0.44
2:B:28:HIS:O	2:B:39:ARG:HA	2.18	0.44
2:B:46:GLU:HB3	2:B:68:LEU:HD21	2.00	0.44
2:E:71:ARG:NH1	3:F:634:VAL:HG11	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:HIS:CE1	2:B:31:ILE:HD11	2.52	0.44
2:B:51:THR:HA	2:E:51:THR:HA	2.00	0.44
2:B:119:VAL:HB	2:B:157:THR:HG22	2.00	0.44
1:D:135:THR:HG1	1:D:148:PHE:H	1.65	0.44
1:D:48:PHE:CD1	1:D:48:PHE:N	2.84	0.44
1:D:66:ASP:OD1	3:F:636:LYS:HG2	2.17	0.44
2:E:32:TYR:CE2	2:E:33:ASN:ND2	2.86	0.44
1:A:77:SER:HB3	2:B:53:LEU:CD1	2.46	0.44
2:B:123:TYR:HB3	2:B:124:PRO:CD	2.44	0.44
1:A:106:ILE:HG23	1:A:150:TYR:CE1	2.52	0.44
1:D:118:ASN:HB2	1:D:166:GLU:HG2	1.99	0.43
2:E:65:LYS:CD	2:E:68:LEU:HD23	2.48	0.43
1:D:114:PRO:HB2	1:D:115:PRO:HD2	2.00	0.43
2:B:18:PHE:CD1	2:B:18:PHE:N	2.86	0.43
1:D:75:LYS:C	1:D:77:SER:N	2.70	0.43
1:D:123:ARG:O	1:D:125:GLY:N	2.52	0.43
2:E:170:VAL:O	2:E:170:VAL:CG2	2.66	0.43
1:A:14:LEU:CD1	2:B:8:LEU:HD13	2.42	0.43
1:D:164:ARG:HB2	1:D:175:LEU:CD2	2.48	0.43
5:D:1184:NAG:O3	5:D:1184:NAG:H83	2.18	0.43
2:E:32:TYR:CZ	2:E:33:ASN:ND2	2.86	0.43
2:B:105:ARG:HD3	2:B:108:THR:CB	2.48	0.43
1:D:82:ILE:HG13	2:E:33:ASN:HB3	2.00	0.43
1:D:132:VAL:HB	1:D:151:LEU:HD12	2.00	0.43
1:A:136:VAL:O	1:A:138:LEU:HD12	2.19	0.43
1:A:167:HIS:CD2	1:A:169:GLY:H	2.37	0.43
2:E:152:ASP:OD1	2:E:152:ASP:C	2.57	0.43
1:D:123:ARG:C	1:D:125:GLY:N	2.71	0.43
2:E:97:PRO:HG3	2:E:122:PHE:CB	2.41	0.43
2:E:104:ALA:C	2:E:105:ARG:HG3	2.39	0.43
1:D:99:LEU:CD2	1:D:157:THR:HG22	2.46	0.43
2:E:39:ARG:HG3	2:E:39:ARG:HH11	1.84	0.43
2:E:164:VAL:HG23	2:E:164:VAL:O	2.18	0.43
1:D:51:PHE:O	3:F:628:GLY:HA3	2.19	0.43
1:D:136:VAL:HG23	1:D:137:PHE:N	2.33	0.43
1:A:70:LEU:HB2	2:B:9:GLN:HG3	2.01	0.42
1:D:86:PRO:HA	1:D:87:PRO:HD3	1.85	0.42
2:B:138:GLU:HA	2:B:138:GLU:OE1	2.18	0.42
2:B:115:LEU:HD11	2:B:188:TRP:CZ3	2.54	0.42
1:D:17:ASP:OD1	1:D:17:ASP:N	2.52	0.42
2:E:2:ASP:OD2	2:E:4:ARG:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:VAL:HG22	1:D:152:PRO:HA	2.02	0.42
2:B:24:VAL:HG21	2:B:80:ARG:HG3	2.02	0.42
2:B:47:TYR:N	2:B:62:ASN:HD21	1.91	0.42
2:B:157:THR:C	2:B:158:LEU:HD12	2.39	0.42
2:B:181:THR:HG23	2:B:182:SER:N	2.34	0.42
1:D:9:GLN:HB3	2:E:13:TYR:HB2	2.01	0.42
1:D:45:LEU:HB2	1:D:48:PHE:CE1	2.54	0.42
1:D:82:ILE:HB	2:E:33:ASN:OD1	2.19	0.42
2:E:138:GLU:HA	2:E:139:LYS:HE3	2.02	0.42
2:E:148:ILE:HG22	2:E:148:ILE:O	2.19	0.42
2:E:167:SER:HA	2:E:190:ALA:HB3	2.00	0.42
2:B:13:TYR:CE2	2:B:28:HIS:CD2	3.08	0.42
1:D:160:VAL:CG1	1:D:177:HIS:HE1	2.22	0.42
2:E:166:ARG:O	2:E:167:SER:C	2.58	0.42
2:B:4:ARG:HG3	2:B:6:ARG:NH1	2.34	0.42
1:D:128:VAL:O	1:D:128:VAL:HG23	2.18	0.42
2:B:112:HIS:CD2	1:D:160:VAL:HG23	2.55	0.42
2:B:105:ARG:HG3	2:B:113:ASN:ND2	2.34	0.42
2:B:109:LEU:HD13	2:B:110:GLN:HE22	1.85	0.42
1:D:72:ILE:HD13	3:F:640:GLU:HB2	2.01	0.41
1:D:123:ARG:HG2	1:D:124:ASN:HD22	1.78	0.41
2:E:83:TYR:CD1	2:E:83:TYR:C	2.93	0.41
1:A:51:PHE:O	3:C:628:GLY:HA3	2.20	0.41
1:A:181:ASP:HB2	2:E:105:ARG:NH2	2.33	0.41
1:D:88:GLU:OE2	1:D:111:LYS:HD3	2.20	0.41
2:B:46:GLU:HA	2:B:68:LEU:HD11	2.01	0.41
1:D:101:GLU:OE1	1:D:101:GLU:HA	2.19	0.41
2:E:65:LYS:O	2:E:69:GLU:HB2	2.20	0.41
1:A:9:GLN:HB3	2:B:13:TYR:HB2	2.02	0.41
2:E:67:PHE:C	2:E:67:PHE:CD2	2.94	0.41
1:A:108:PHE:HE1	1:A:146:ARG:CD	2.32	0.41
1:A:170:LEU:HD13	1:A:174:LEU:HB2	2.02	0.41
2:E:94:ARG:HA	2:E:124:PRO:HD3	2.01	0.41
1:D:142:ASP:O	1:D:143:HIS:HB2	2.20	0.41
1:D:179:GLU:O	1:D:182:ALA:HB3	2.20	0.41
2:E:133:ARG:HG2	2:E:133:ARG:NH1	2.36	0.41
1:D:48:PHE:N	1:D:48:PHE:HD1	2.18	0.41
1:D:70:LEU:HA	2:E:9:GLN:HG3	2.02	0.41
1:D:95:SER:O	1:D:96:PRO:C	2.57	0.41
1:D:172:GLU:O	1:D:173:PRO:C	2.59	0.41
2:E:150:ASN:HB2	2:E:154:THR:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:83:TYR:OH	2:E:91:VAL:HG11	2.20	0.41
2:E:94:ARG:HG2	2:E:124:PRO:HG2	2.03	0.41
2:E:104:ALA:O	2:E:105:ARG:C	2.59	0.41
1:A:4:GLU:HB2	2:B:17:PHE:O	2.21	0.41
1:A:153:PHE:CE2	1:A:155:PRO:HG3	2.55	0.41
2:B:161:LEU:HD22	2:B:163:THR:HG23	2.03	0.41
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.87	0.41
1:D:15:ASN:HB2	1:D:70:LEU:HD21	2.02	0.41
1:D:164:ARG:HA	1:D:175:LEU:HD23	2.02	0.41
2:E:18:PHE:N	2:E:18:PHE:CD1	2.88	0.41
2:E:106:THR:O	2:E:106:THR:CG2	2.63	0.41
1:A:30:GLU:O	2:B:153:TRP:NE1	2.46	0.41
1:A:112:PHE:O	1:A:113:THR:HB	2.21	0.41
1:D:45:LEU:O	1:D:46:GLU:C	2.59	0.41
2:E:177:HIS:ND1	2:E:179:SER:HB2	2.35	0.41
1:A:130:THR:O	1:A:132:VAL:N	2.54	0.40
1:A:138:LEU:HD12	1:A:138:LEU:N	2.35	0.40
2:B:170:VAL:HG12	2:B:189:ARG:HD2	2.02	0.40
1:D:39:LYS:HD2	1:D:60:LEU:HD13	2.01	0.40
2:E:46:GLU:HB2	2:E:62:ASN:CG	2.41	0.40
1:D:103:ASN:O	1:D:104:VAL:HG23	2.22	0.40
1:A:129:THR:O	1:A:130:THR:CG2	2.68	0.40
2:B:4:ARG:HA	2:B:5:PRO:HD3	1.86	0.40
2:B:83:TYR:CE1	2:B:91:VAL:HG21	2.56	0.40
2:B:170:VAL:HG12	2:B:189:ARG:CG	2.51	0.40
1:D:96:PRO:CD	2:E:120:ASN:HD21	2.29	0.40
1:D:156:SER:C	1:D:158:GLU:H	2.24	0.40
2:E:166:ARG:HE	2:E:166:ARG:HB3	1.53	0.40
1:A:121:TRP:HB2	1:A:128:VAL:HG13	2.03	0.40
1:D:161:TYR:N	1:D:161:TYR:HD1	2.20	0.40
2:E:133:ARG:HG3	2:E:171:TYR:CZ	2.57	0.40
2:E:47:TYR:CB	2:E:62:ASN:HD21	2.31	0.40
2:E:97:PRO:CG	2:E:122:PHE:HB3	2.44	0.40
2:E:177:HIS:C	2:E:179:SER:N	2.74	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	178/182 (98%)	148 (83%)	23 (13%)	7 (4%)	3 18
1	D	178/182 (98%)	137 (77%)	34 (19%)	7 (4%)	3 18
2	B	187/190 (98%)	154 (82%)	24 (13%)	9 (5%)	2 14
2	E	187/190 (98%)	141 (75%)	32 (17%)	14 (8%)	1 6
3	C	12/14 (86%)	12 (100%)	0	0	100 100
3	F	12/14 (86%)	12 (100%)	0	0	100 100
All	All	754/772 (98%)	604 (80%)	113 (15%)	37 (5%)	2 14

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	105	ARG
2	B	139	LYS
1	D	136	VAL
2	E	112	HIS
2	E	123	TYR
2	E	167	SER
1	A	125	GLY
2	B	33	ASN
2	B	123	TYR
1	D	76	ARG
2	E	33	ASN
1	A	87	PRO
1	A	181	ASP
2	B	79	CYS
1	D	155	PRO
1	D	173	PRO
2	E	4	ARG
2	E	65	LYS
2	E	79	CYS
2	E	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	ARG
2	B	103	PRO
2	B	178	PRO
1	D	37	ALA
1	D	131	GLY
2	E	91	VAL
1	D	96	PRO
2	E	5	PRO
1	A	102	PRO
1	A	113	THR
1	A	155	PRO
2	E	124	PRO
2	B	75	VAL
2	B	124	PRO
2	E	86	GLY
2	E	56	PRO
2	E	127	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	164/166 (99%)	148 (90%)	16 (10%)	8 29
1	D	164/166 (99%)	151 (92%)	13 (8%)	12 40
2	B	171/171 (100%)	156 (91%)	15 (9%)	10 36
2	E	171/171 (100%)	150 (88%)	21 (12%)	4 19
3	C	12/12 (100%)	12 (100%)	0	100 100
3	F	12/12 (100%)	12 (100%)	0	100 100
All	All	694/698 (99%)	629 (91%)	65 (9%)	8 32

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	25	ASP
1	A	39	LYS
1	A	41	THR
1	A	50	ARG
1	A	55	GLU
1	A	92	LEU
1	A	96	PRO
1	A	99	LEU
1	A	104	VAL
1	A	128	VAL
1	A	129	THR
1	A	146	ARG
1	A	157	THR
1	A	160	VAL
1	A	180	PHE
2	B	9	GLN
2	B	55	ARG
2	B	64	GLN
2	B	72	ARG
2	B	88	SER
2	B	89	PHE
2	B	103	PRO
2	B	109	LEU
2	B	113	ASN
2	B	136	GLN
2	B	139	LYS
2	B	161	LEU
2	B	166	ARG
2	B	172	THR
2	B	189	ARG
1	D	15	ASN
1	D	17	ASP
1	D	55	GLU
1	D	91	VAL
1	D	96	PRO
1	D	101	GLU
1	D	103	ASN
1	D	149	HIS
1	D	155	PRO
1	D	157	THR
1	D	160	VAL
1	D	161	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	164	ARG
2	E	4	ARG
2	E	9	GLN
2	E	11	ASP
2	E	55	ARG
2	E	57	ASP
2	E	61	TRP
2	E	67	PHE
2	E	72	ARG
2	E	83	TYR
2	E	100	THR
2	E	105	ARG
2	E	109	LEU
2	E	111	HIS
2	E	112	HIS
2	E	113	ASN
2	E	120	ASN
2	E	136	GLN
2	E	139	LYS
2	E	161	LEU
2	E	165	PRO
2	E	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
2	B	10	GLN
2	B	62	ASN
2	B	110	GLN
2	B	112	HIS
2	B	113	ASN
2	B	149	GLN
1	D	5	HIS
1	D	15	ASN
1	D	103	ASN
1	D	124	ASN
1	D	149	HIS
2	E	10	GLN
2	E	34	GLN
2	E	62	ASN
2	E	64	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	112	HIS
2	E	113	ASN
2	E	120	ASN
2	E	149	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)

2 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	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	0.65	0	17,19,21	1.04	2 (11%)
4	NAG	G	2	4	14,14,15	0.87	1 (7%)	17,19,21	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	1/1/5/7	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	NAG	C1-C2	2.13	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C2-N2-C7	-2.71	119.05	122.90
4	G	2	NAG	C1-O5-C5	2.54	115.64	112.19
4	G	1	NAG	C1-O5-C5	2.11	115.05	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	2	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7

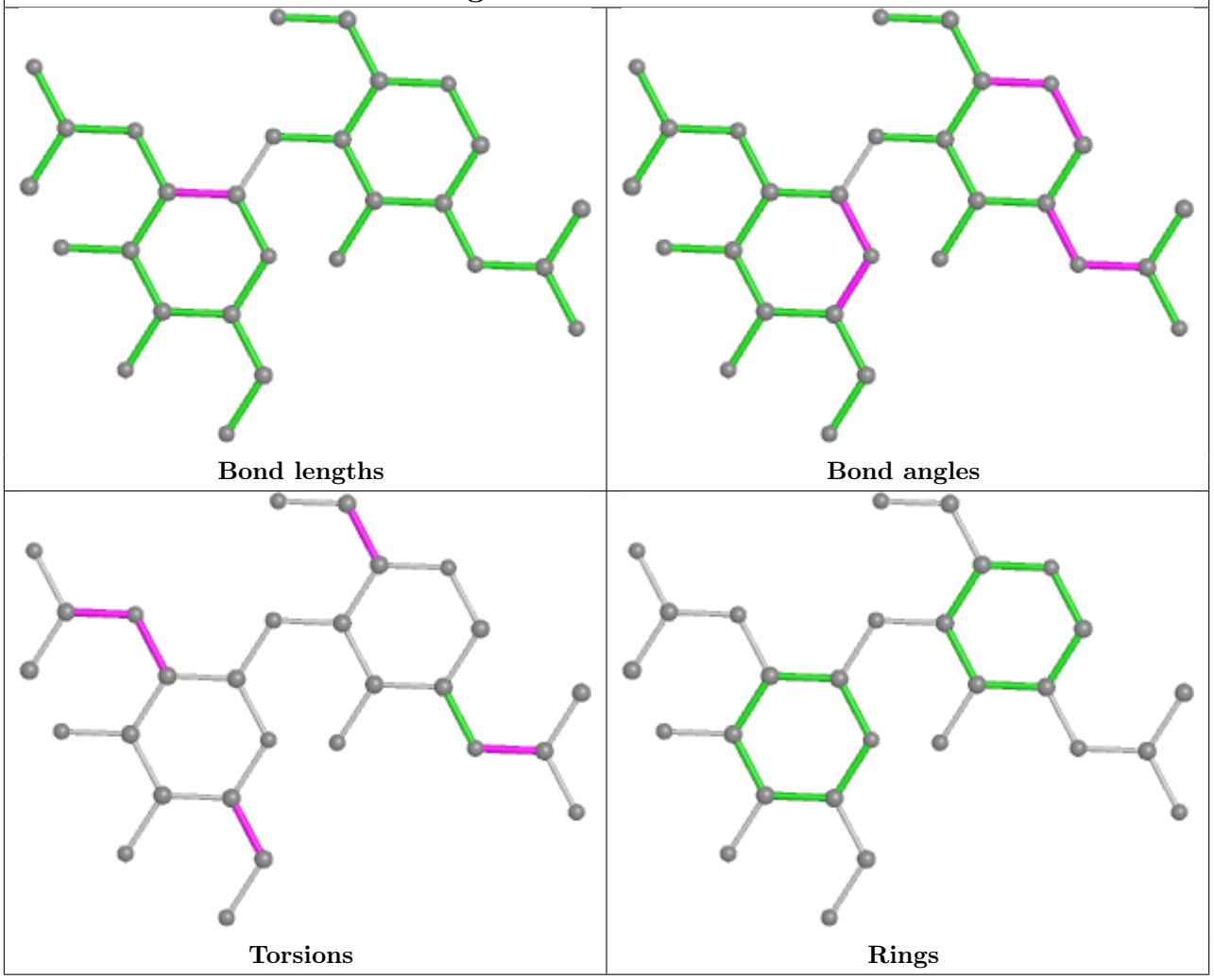
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	4	0
4	G	1	NAG	5	0

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

Oligosaccharide Chain G



5.6 Ligand geometry (i)

3 ligands 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	$\#\|Z\| > 2$
5	NAG	A	1185	1	14,14,15	0.78	0	17,19,21	1.06	2 (11%)
5	NAG	D	1183	1	14,14,15	0.55	0	17,19,21	0.61	0
5	NAG	D	1184	1	14,14,15	0.79	1 (7%)	17,19,21	0.64	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	D	1184	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	D	1183	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1185	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1184	NAG	C1-C2	2.17	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1185	NAG	C4-C3-C2	-2.34	107.59	111.02
5	A	1185	NAG	C2-N2-C7	-2.19	119.78	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	1184	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1185	NAG	C8-C7-N2-C2
5	A	1185	NAG	O7-C7-N2-C2
5	D	1183	NAG	C8-C7-N2-C2
5	D	1183	NAG	O7-C7-N2-C2
5	D	1184	NAG	C8-C7-N2-C2
5	D	1184	NAG	O7-C7-N2-C2
5	A	1185	NAG	O5-C5-C6-O6
5	D	1183	NAG	O5-C5-C6-O6
5	A	1185	NAG	C4-C5-C6-O6
5	D	1183	NAG	C4-C5-C6-O6
5	D	1184	NAG	O5-C5-C6-O6
5	D	1184	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1184	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	180/182 (98%)	-0.92	1 (0%) 89 78	12, 34, 67, 95	0
1	D	180/182 (98%)	-0.59	0 100 100	40, 69, 101, 116	0
2	B	189/190 (99%)	-0.61	1 (0%) 91 81	21, 53, 113, 142	0
2	E	189/190 (99%)	-0.45	3 (1%) 72 51	23, 67, 109, 144	0
3	C	14/14 (100%)	-0.70	0 100 100	33, 51, 74, 82	0
3	F	14/14 (100%)	0.90	3 (21%) 0 0	90, 104, 138, 142	0
All	All	766/772 (99%)	-0.61	8 (1%) 82 67	12, 58, 104, 144	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	641	SER	4.2
2	B	109	LEU	3.8
3	F	628	GLY	2.9
1	A	182	ALA	2.6
3	F	640	GLU	2.6
2	E	108	THR	2.1
2	E	65	LYS	2.1
2	E	107	GLN	2.0

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

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

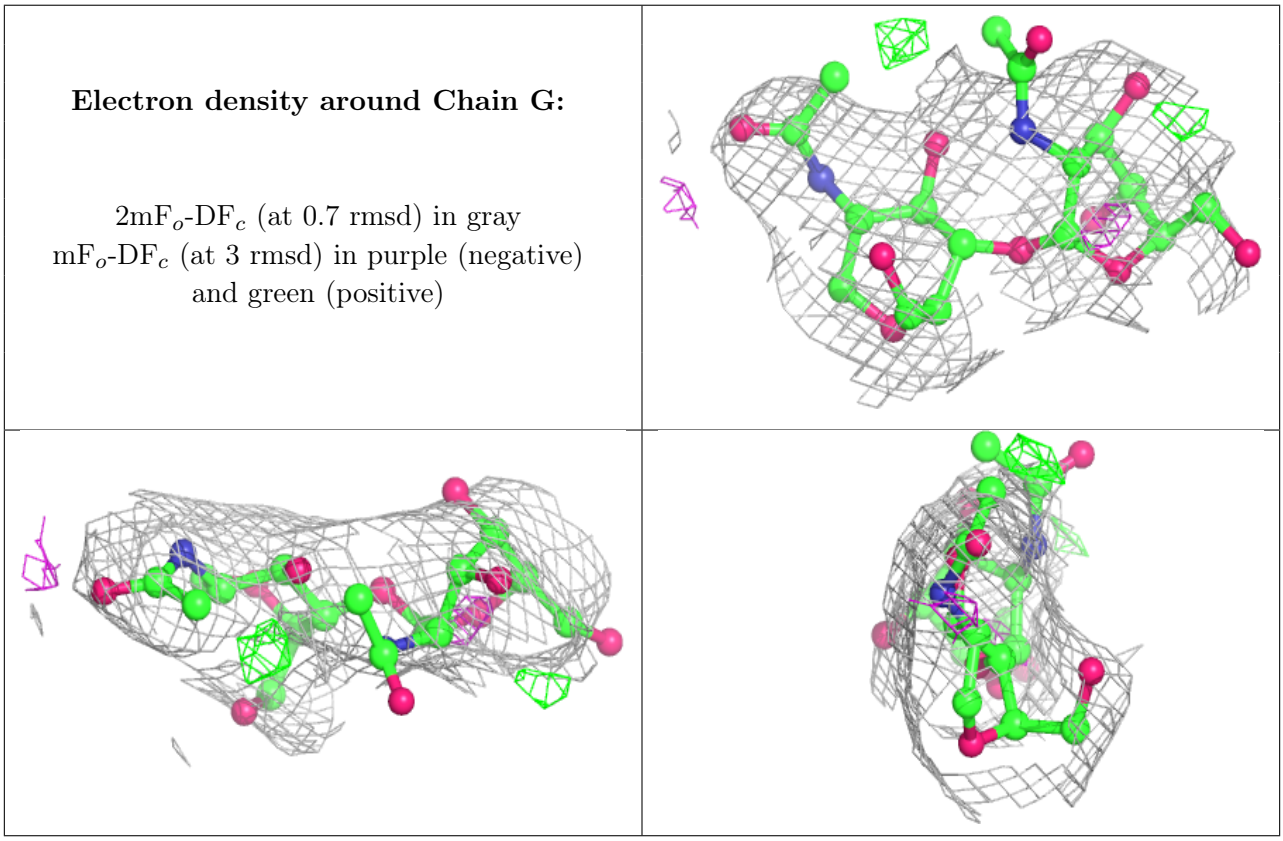
6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	2	14/15	0.88	0.35	118,125,133,135	0
4	NAG	G	1	14/15	0.94	0.13	69,80,94,104	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	1184	14/15	0.62	0.39	151,158,160,161	0
5	NAG	A	1185	14/15	0.76	0.28	102,112,115,116	0
5	NAG	D	1183	14/15	0.78	0.28	122,130,136,138	0

6.5 Other polymers (i)

There are no such residues in this entry.