



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 AM UTC

PDB ID : 3ZTN / pdb_00003ztn
Title : STRUCTURE OF INFLUENZA A NEUTRALIZING ANTIBODY SELECTED FROM CULTURES OF SINGLE HUMAN PLASMA CELLS IN COMPLEX WITH HUMAN H1 INFLUENZA HAEMAGGLUTININ.
Authors : Hubbard, P.A.; Ritchie, A.J.; Corti, D.; Voss, J.E.; Gamblin, S.J.; Codoni, G.; Macagno, A.; Jarrossay, D.; Pinna, D.; Minola, A.; Vanzetta, F.; Silacci, C.; Fernandez-Rodriguez, B.M.; Agatic, G.; Giacchetto-Sasselli, I.; Vachieri, S.G.; Sallusto, F.; Collins, P.J.; Haire, L.F.; Temperton, N.; Langedijk, J.P.M.; Skehel, J.J.; Lanzavecchia, A.
Deposited on : 2011-07-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12

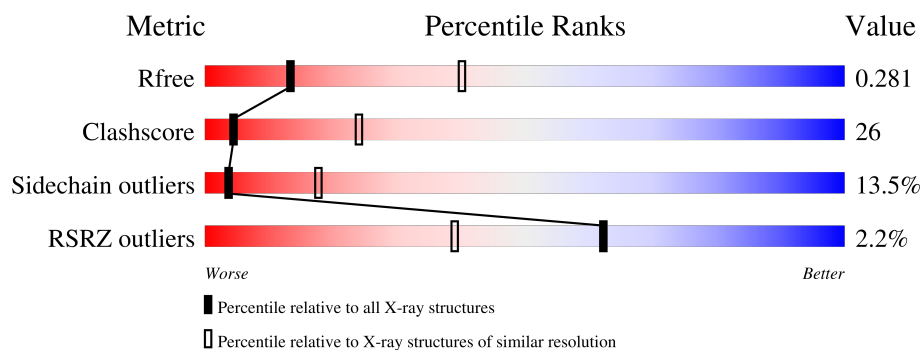
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	327	49% 44% 6%
2	B	176	63% 31% 5%
3	H	226	35% 34% 8% 23%
4	L	218	6% 35% 32% 31%

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	2	 50% 50%
5	E	2	 100%
6	D	3	 33% 67%

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
6	BMA	D	3	X	-	-	-
7	NAG	A	409	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6361 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 HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2469	1567	416	475	11			

- Molecule 2 is a protein called HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1320	833	218	263	6			

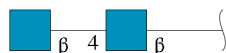
- Molecule 3 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	173	Total	C	N	O	S	0	0	0
			1334	853	220	256	5			

- Molecule 4 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	150	Total	C	N	O	S	0	0	0
			1084	685	177	219	3			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



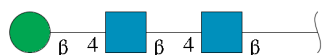
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

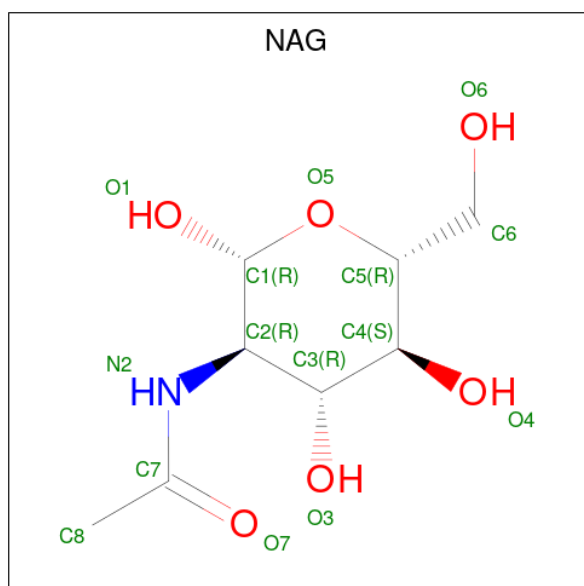
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



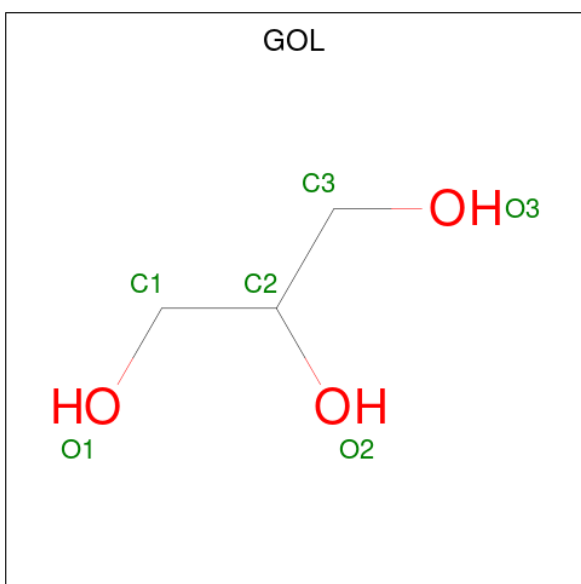
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

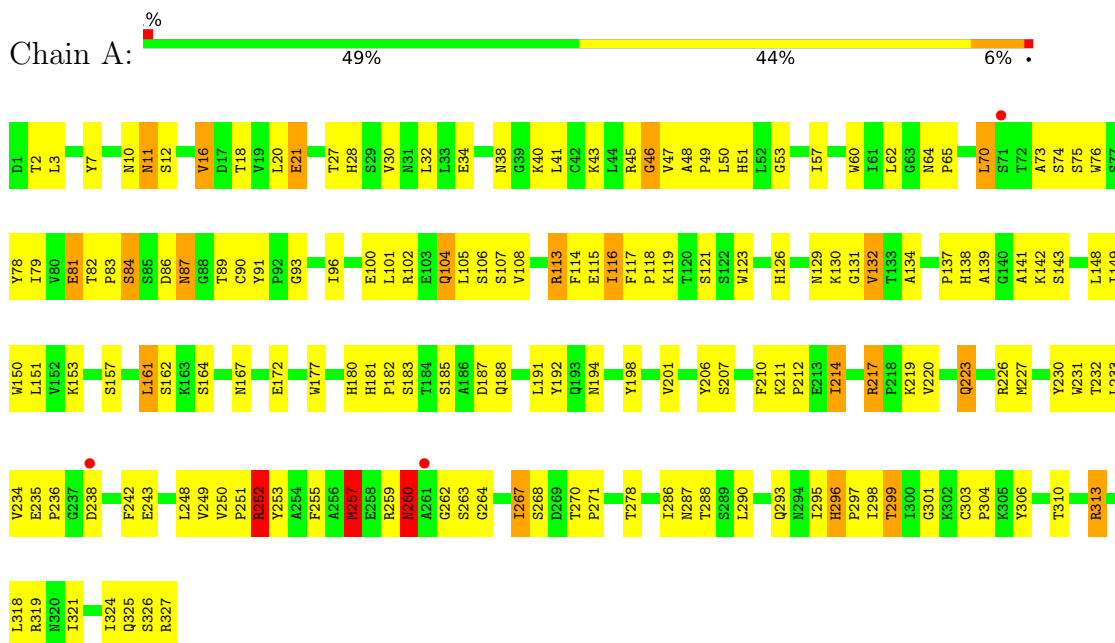


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

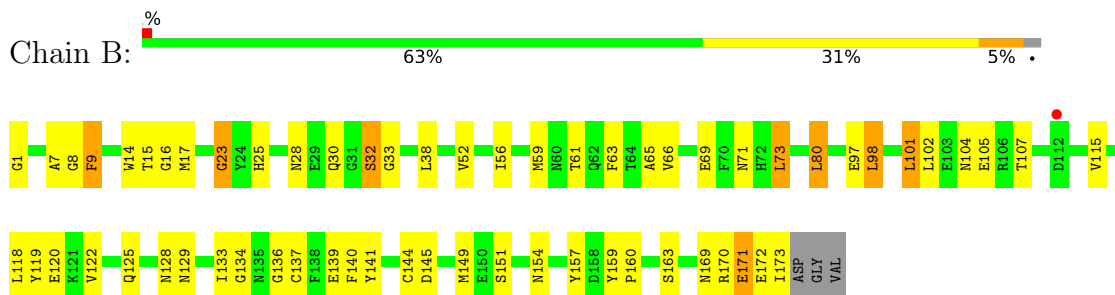
3 Residue-property plots

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

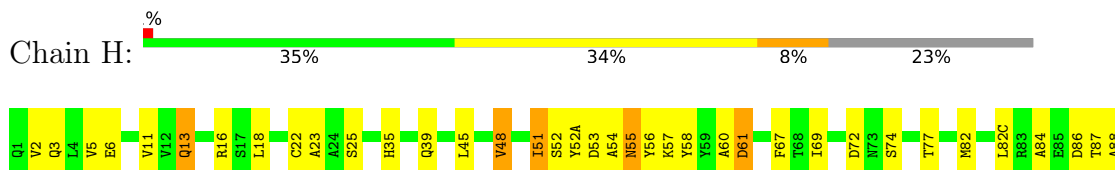
• Molecule 1: HAEMAGGLUTININ

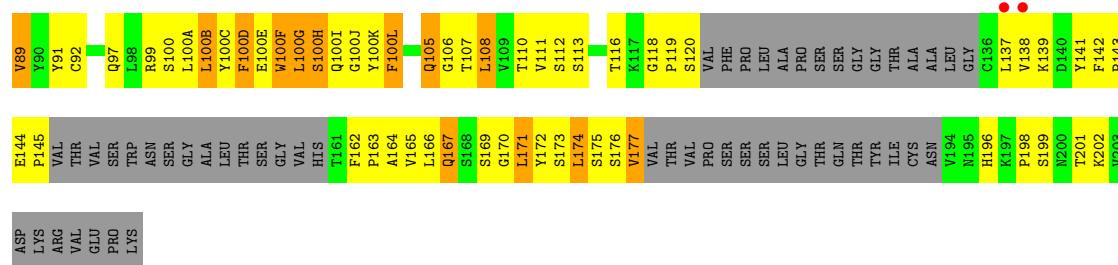


• Molecule 2: HAEMAGGLUTININ

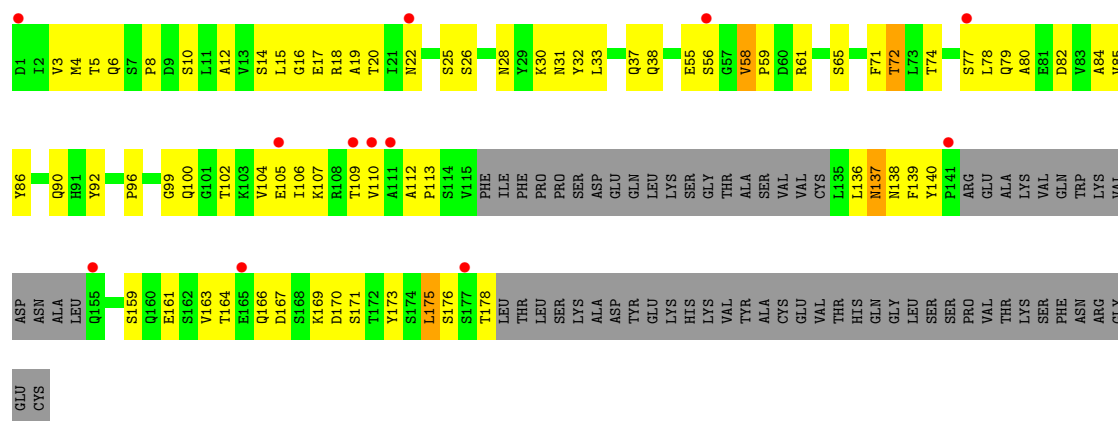


• Molecule 3: FI6V3 ANTIBODY LIGHT CHAIN





• Molecule 4: FI6V3 ANTIBODY LIGHT CHAIN



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	206.10Å 206.10Å 206.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.16 – 3.00 57.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.16-3.00) 97.3 (57.16-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.214 , 0.289 (Not available) , 0.281	Depositor DCC
R_{free} test set	1532 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 94.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, GOL, BMA

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	0.61	0/2533	1.01	14/3465 (0.4%)
2	B	0.60	0/1348	0.92	4/1830 (0.2%)
3	H	0.55	0/1367	0.86	2/1860 (0.1%)
4	L	0.53	0/1109	1.01	5/1518 (0.3%)
All	All	0.58	0/6357	0.96	25/8673 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	HIS	CA-C-N	7.45	129.16	119.84
1	A	296	HIS	C-N-CA	7.45	129.16	119.84
1	A	260	ASN	N-CA-C	-7.28	104.42	112.72
1	A	117	PHE	CA-C-N	6.67	127.03	119.83
1	A	117	PHE	C-N-CA	6.67	127.03	119.83
4	L	112	ALA	CA-C-N	6.24	127.64	119.84
4	L	112	ALA	C-N-CA	6.24	127.64	119.84
2	B	23	GLY	N-CA-C	6.11	118.82	110.69
3	H	48	VAL	N-CA-C	5.88	117.06	112.12
1	A	278	THR	N-CA-C	-5.87	105.96	114.12
1	A	121	SER	N-CA-C	5.87	118.15	111.11
1	A	252	ARG	N-CA-C	-5.78	103.81	111.96
1	A	214	ILE	N-CA-C	5.55	115.64	107.15
3	H	2	VAL	N-CA-C	5.54	117.43	109.51
4	L	137	ASN	N-CA-C	5.51	117.44	108.63
2	B	134	GLY	N-CA-C	5.50	117.17	111.95
4	L	58	VAL	CA-C-N	5.38	125.39	119.90
4	L	58	VAL	C-N-CA	5.38	125.39	119.90
2	B	15	THR	N-CA-C	-5.35	106.45	112.87
1	A	130	LYS	N-CA-C	-5.32	105.09	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	SER	N-CA-C	5.30	117.12	109.07
1	A	257	MET	N-CA-C	5.26	117.06	108.55
1	A	30	VAL	CB-CA-C	-5.08	102.97	111.29
1	A	46	GLY	N-CA-C	-5.07	109.09	114.67
2	B	122	VAL	N-CA-C	5.04	115.16	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2469	0	2297	152	0
2	B	1320	0	1159	56	0
3	H	1334	0	1255	71	0
4	L	1084	0	950	57	0
5	C	28	0	25	5	0
5	E	28	0	25	0	0
6	D	39	0	34	6	0
7	A	28	0	26	1	0
8	A	20	0	0	0	0
8	L	5	0	0	0	0
9	A	6	0	8	0	0
All	All	6361	0	5779	320	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 26.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.08	1.18
4:L:12:ALA:HB1	4:L:107:LYS:HB2	1.31	1.07
1:A:116:ILE:O	1:A:118:PRO:HD3	1.63	0.98
4:L:163:VAL:HG12	4:L:164:THR:H	1.31	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PRO:HD2	1:A:214:ILE:HD13	1.51	0.93
3:H:87:THR:HG23	3:H:110:THR:HA	1.53	0.90
1:A:16:VAL:HG23	1:A:313:ARG:HB3	1.57	0.87
1:A:287:ASN:ND2	6:D:1:NAG:C1	2.40	0.85
3:H:196:HIS:CD2	3:H:198:PRO:HD2	2.11	0.85
1:A:87:ASN:CG	5:C:1:NAG:C1	2.55	0.80
1:A:43:LYS:HD3	1:A:46:GLY:O	1.82	0.80
1:A:313:ARG:HG2	1:A:313:ARG:NH1	1.81	0.79
1:A:287:ASN:HD21	6:D:1:NAG:C1	1.97	0.78
3:H:170:GLY:C	3:H:171:LEU:HD23	2.07	0.78
1:A:87:ASN:OD1	5:C:1:NAG:C1	2.31	0.78
3:H:18:LEU:HB3	3:H:82:MET:HE3	1.67	0.76
1:A:119:LYS:HG3	1:A:149:ILE:HD11	1.68	0.74
2:B:133:ILE:HG12	2:B:137:CYS:O	1.87	0.74
1:A:287:ASN:CG	6:D:1:NAG:C1	2.61	0.73
1:A:87:ASN:ND2	5:C:1:NAG:C1	2.52	0.72
4:L:159:SER:HA	4:L:178:THR:O	1.89	0.72
1:A:327:ARG:C	2:B:1:GLY:N	2.48	0.72
1:A:235:GLU:HB2	1:A:236:PRO:HD2	1.70	0.72
4:L:175:LEU:HG	4:L:176:SER:H	1.54	0.71
1:A:126:HIS:HB2	1:A:151:LEU:HD22	1.71	0.71
3:H:82:MET:HB3	3:H:82(C):LEU:HD21	1.73	0.71
1:A:324:ILE:O	1:A:324:ILE:HG22	1.90	0.71
1:A:260:ASN:O	1:A:262:GLY:N	2.26	0.69
2:B:128:ASN:HB2	2:B:159:TYR:OH	1.93	0.69
2:B:133:ILE:HD13	2:B:139:GLU:HG3	1.73	0.69
3:H:72:ASP:OD1	3:H:74:SER:HB3	1.92	0.68
4:L:163:VAL:HG12	4:L:164:THR:N	2.07	0.68
1:A:287:ASN:OD1	6:D:1:NAG:C1	2.42	0.68
4:L:37:GLN:HG3	4:L:86:TYR:CE1	2.29	0.67
1:A:327:ARG:O	2:B:1:GLY:HA3	1.94	0.67
3:H:89:VAL:HA	3:H:108:LEU:HA	1.76	0.67
1:A:299:THR:HG23	1:A:303:CYS:SG	2.35	0.67
1:A:82:THR:HG22	1:A:84:SER:H	1.59	0.67
2:B:9:PHE:HD1	2:B:9:PHE:H	1.40	0.67
1:A:50:LEU:HD12	1:A:76:TRP:CE3	2.29	0.67
1:A:50:LEU:HD12	1:A:76:TRP:CD2	2.30	0.67
3:H:201:THR:HG22	3:H:202:LYS:H	1.59	0.67
4:L:18:ARG:HG2	4:L:19:ALA:H	1.59	0.66
4:L:113:PRO:HD3	4:L:139:PHE:HB3	1.77	0.66
1:A:161:LEU:C	1:A:161:LEU:HD12	2.21	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:175:LEU:HG	4:L:176:SER:N	2.12	0.65
1:A:115:GLU:HB2	1:A:253:TYR:CE1	2.33	0.64
1:A:10:ASN:OD1	1:A:12:SER:HB3	1.98	0.63
1:A:49:PRO:HB3	1:A:78:TYR:CZ	2.33	0.63
3:H:171:LEU:HD23	3:H:171:LEU:N	2.12	0.63
1:A:131:GLY:HA3	1:A:150:TRP:HB3	1.79	0.63
2:B:30:GLN:OE1	2:B:145:ASP:HB2	1.99	0.63
3:H:137:LEU:HD12	3:H:138:VAL:H	1.63	0.63
1:A:234:VAL:HG12	1:A:238:ASP:HB3	1.80	0.62
1:A:327:ARG:O	2:B:1:GLY:CA	2.48	0.62
1:A:182:PRO:HD2	1:A:214:ILE:CD1	2.28	0.62
3:H:5:VAL:O	3:H:22:CYS:HA	2.00	0.62
4:L:163:VAL:HA	4:L:175:LEU:HA	1.80	0.62
1:A:20:LEU:C	1:A:21:GLU:HG3	2.25	0.61
1:A:64:ASN:HD21	1:A:90:CYS:HB3	1.64	0.61
4:L:163:VAL:HG22	4:L:175:LEU:HD12	1.82	0.61
1:A:177:TRP:CE2	1:A:201:VAL:HG21	2.35	0.61
1:A:206:TYR:O	1:A:207:SER:HB2	2.00	0.61
1:A:287:ASN:HD21	6:D:1:NAG:C2	2.13	0.61
1:A:248:LEU:HD12	1:A:249:VAL:N	2.16	0.61
3:H:23:ALA:HA	3:H:77:THR:HG22	1.81	0.61
3:H:35:HIS:CD2	3:H:100(L):PHE:HE1	2.18	0.61
1:A:248:LEU:HD12	1:A:249:VAL:H	1.65	0.61
4:L:79:GLN:HG2	4:L:80:ALA:H	1.65	0.61
4:L:107:LYS:HA	4:L:140:TYR:OH	2.00	0.61
1:A:234:VAL:CG1	1:A:238:ASP:HB3	2.29	0.61
1:A:250:VAL:CG1	1:A:251:PRO:HD2	2.31	0.61
1:A:211:LYS:HG3	1:A:212:PRO:HD2	1.82	0.60
3:H:112:SER:HB3	3:H:142:PHE:HZ	1.66	0.60
1:A:149:ILE:HG23	1:A:149:ILE:O	2.01	0.60
2:B:80:LEU:HD12	2:B:80:LEU:O	2.02	0.59
3:H:105:GLN:O	3:H:105:GLN:HG3	2.01	0.59
2:B:71:ASN:O	2:B:73:LEU:N	2.35	0.59
2:B:71:ASN:C	2:B:73:LEU:H	2.11	0.58
1:A:18:THR:HG23	2:B:105:GLU:HA	1.86	0.58
1:A:250:VAL:HG13	1:A:251:PRO:HD2	1.85	0.57
2:B:9:PHE:CD1	2:B:9:PHE:N	2.71	0.57
4:L:80:ALA:C	4:L:82:ASP:H	2.11	0.57
4:L:6:GLN:H	4:L:100:GLN:HE22	1.51	0.57
1:A:3:LEU:HD12	2:B:25:HIS:O	2.05	0.56
1:A:132:VAL:HG22	1:A:143:SER:HA	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:MET:SD	2:B:23:GLY:HA3	2.46	0.56
1:A:41:LEU:HG	1:A:270:THR:HG22	1.88	0.56
3:H:13:GLN:HB2	3:H:16:ARG:NH1	2.20	0.56
1:A:123:TRP:CZ2	1:A:250:VAL:HG11	2.41	0.55
1:A:286:ILE:CD1	1:A:293:GLN:HG3	2.35	0.55
1:A:288:THR:HG22	1:A:304:PRO:HD3	1.87	0.55
4:L:85:VAL:HA	4:L:102:THR:O	2.06	0.55
4:L:79:GLN:HG2	4:L:80:ALA:N	2.21	0.55
1:A:177:TRP:CZ2	1:A:201:VAL:HG21	2.42	0.55
3:H:35:HIS:CD2	3:H:100(L):PHE:CE1	2.95	0.55
3:H:97:GLN:HG2	3:H:100(J):GLY:HA3	1.89	0.54
1:A:11:ASN:HD22	1:A:11:ASN:N	2.06	0.54
4:L:71:PHE:O	4:L:72:THR:HG23	2.08	0.54
1:A:60:TRP:CD1	1:A:70:LEU:HD23	2.43	0.54
3:H:100(H):SER:HB3	4:L:92:TYR:O	2.07	0.54
2:B:9:PHE:HD1	2:B:9:PHE:N	2.05	0.54
1:A:313:ARG:NH1	1:A:313:ARG:CG	2.60	0.54
3:H:139:LYS:HG3	3:H:173:SER:HB3	1.90	0.54
3:H:167:GLN:HG2	3:H:171:LEU:O	2.07	0.53
1:A:96:ILE:HG13	1:A:230:TYR:CE2	2.43	0.53
4:L:175:LEU:CG	4:L:176:SER:N	2.72	0.53
3:H:137:LEU:HD12	3:H:138:VAL:N	2.23	0.53
1:A:167:ASN:ND2	1:A:236:PRO:HA	2.24	0.53
3:H:53:ASP:O	3:H:54:ALA:HB3	2.09	0.53
1:A:296:HIS:CE1	1:A:298:ILE:HB	2.44	0.53
1:A:327:ARG:C	2:B:1:GLY:H1	2.15	0.53
3:H:112:SER:HB3	3:H:142:PHE:CZ	2.44	0.53
1:A:48:ALA:HB1	1:A:49:PRO:HD2	1.91	0.53
1:A:161:LEU:O	1:A:243:GLU:HA	2.08	0.52
1:A:286:ILE:HG21	1:A:295:ILE:HG13	1.91	0.52
1:A:242:PHE:HD2	1:A:248:LEU:HD21	1.75	0.52
1:A:50:LEU:HD23	1:A:50:LEU:C	2.35	0.52
1:A:260:ASN:H	1:A:260:ASN:ND2	2.06	0.52
3:H:118:GLY:HA2	3:H:199:SER:OG	2.09	0.52
2:B:63:PHE:CD1	2:B:63:PHE:C	2.87	0.52
3:H:3:GLN:HB3	3:H:25:SER:HB3	1.92	0.52
2:B:140:PHE:HE2	2:B:149:MET:HE1	1.74	0.52
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.92	0.51
2:B:159:TYR:N	2:B:160:PRO:HD2	2.25	0.51
4:L:3:VAL:H	4:L:26:SER:CB	2.24	0.51
1:A:327:ARG:HB3	2:B:1:GLY:H3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:OD1	7:A:403:NAG:O5	2.28	0.51
1:A:82:THR:HG22	1:A:83:PRO:HD2	1.92	0.51
3:H:57:LYS:HD3	3:H:69:ILE:O	2.11	0.51
4:L:4:MET:O	4:L:99:GLY:HA2	2.11	0.51
4:L:32:TYR:HB2	4:L:92:TYR:HB2	1.93	0.51
1:A:84:SER:O	1:A:86:ASP:N	2.44	0.51
1:A:299:THR:HG21	1:A:303:CYS:HB2	1.92	0.51
1:A:60:TRP:HD1	1:A:70:LEU:HD23	1.74	0.50
1:A:198:TYR:CD1	1:A:198:TYR:C	2.89	0.50
3:H:100(D):PHE:HB2	3:H:100(G):LEU:HG	1.93	0.50
4:L:28:ASN:C	4:L:30:LYS:H	2.20	0.50
1:A:93:GLY:HA3	1:A:227:MET:O	2.10	0.50
1:A:102:ARG:C	1:A:104:GLN:H	2.20	0.50
1:A:87:ASN:HD21	5:C:1:NAG:C1	2.23	0.50
1:A:172:GLU:OE2	1:A:233:LEU:HD13	2.11	0.50
2:B:159:TYR:O	2:B:163:SER:HB3	2.11	0.50
4:L:104:VAL:HG12	4:L:104:VAL:O	2.09	0.50
1:A:250:VAL:HG12	1:A:251:PRO:N	2.26	0.50
1:A:270:THR:HG23	1:A:271:PRO:HD2	1.92	0.50
3:H:119:PRO:HA	3:H:141:TYR:HB3	1.93	0.50
2:B:14:TRP:C	2:B:16:GLY:H	2.18	0.50
2:B:14:TRP:C	2:B:16:GLY:N	2.69	0.50
3:H:58:TYR:HE2	3:H:100(B):LEU:HB3	1.77	0.50
1:A:16:VAL:HG22	2:B:104:ASN:HD21	1.76	0.50
1:A:123:TRP:HZ2	1:A:250:VAL:HG11	1.76	0.50
4:L:38:GLN:O	4:L:84:ALA:HB1	2.11	0.50
1:A:11:ASN:HD22	1:A:11:ASN:H	1.58	0.50
1:A:177:TRP:HZ3	1:A:232:THR:HG22	1.77	0.49
1:A:286:ILE:HD12	1:A:293:GLN:HG3	1.93	0.49
4:L:31:ASN:O	4:L:33:LEU:N	2.46	0.49
1:A:100:GLU:O	1:A:104:GLN:HB2	2.13	0.49
1:A:113:ARG:HB2	1:A:255:PHE:CD2	2.48	0.49
2:B:125:GLN:OE1	2:B:157:TYR:HB3	2.13	0.49
2:B:172:GLU:O	2:B:173:ILE:O	2.31	0.49
4:L:12:ALA:CB	4:L:107:LYS:HB2	2.22	0.49
1:A:16:VAL:HG22	2:B:104:ASN:ND2	2.27	0.49
4:L:167:ASP:C	4:L:169:LYS:H	2.20	0.49
1:A:62:LEU:HD12	1:A:89:THR:HG22	1.95	0.48
4:L:3:VAL:H	4:L:26:SER:HB3	1.78	0.48
4:L:14:SER:O	4:L:16:GLY:N	2.46	0.48
1:A:299:THR:CG2	1:A:303:CYS:SG	3.01	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HD2	1:A:226:ARG:CG	2.43	0.48
4:L:32:TYR:HD1	4:L:32:TYR:H	1.61	0.48
1:A:325:GLN:HG3	1:A:326:SER:N	2.28	0.48
1:A:49:PRO:HB3	1:A:78:TYR:CE2	2.48	0.48
4:L:80:ALA:C	4:L:82:ASP:N	2.72	0.48
3:H:53:ASP:CG	3:H:55:ASN:OD1	2.57	0.47
1:A:38:ASN:O	1:A:40:LYS:HG2	2.13	0.47
4:L:12:ALA:HA	4:L:105:GLU:O	2.15	0.47
1:A:138:HIS:O	1:A:139:ALA:HB3	2.14	0.47
2:B:98:LEU:O	2:B:102:LEU:HG	2.15	0.47
3:H:52(A):TYR:CD2	3:H:99:ARG:HA	2.49	0.47
1:A:91:TYR:CE2	1:A:223:GLN:HG2	2.49	0.47
1:A:119:LYS:O	1:A:119:LYS:HG2	2.15	0.47
1:A:248:LEU:HG	1:A:250:VAL:HG22	1.95	0.47
3:H:116:THR:HG22	3:H:116:THR:O	2.13	0.47
4:L:14:SER:O	4:L:17:GLU:HG3	2.15	0.47
1:A:134:ALA:O	1:A:137:PRO:HD3	2.15	0.47
3:H:162:PHE:HB3	3:H:163:PRO:HD2	1.96	0.47
1:A:327:ARG:C	2:B:1:GLY:H3	2.23	0.47
1:A:148:LEU:HB3	1:A:249:VAL:HG12	1.97	0.46
1:A:210:PHE:HE2	1:A:230:TYR:CZ	2.32	0.46
1:A:252:ARG:HD2	1:A:253:TYR:CE2	2.50	0.46
4:L:8:PRO:HG2	4:L:10:SER:O	2.15	0.46
1:A:79:ILE:HD12	1:A:106:SER:HA	1.96	0.46
3:H:201:THR:HG22	3:H:202:LYS:N	2.28	0.46
1:A:11:ASN:H	1:A:11:ASN:ND2	2.14	0.46
1:A:82:THR:CG2	1:A:83:PRO:HD2	2.45	0.46
4:L:90:GLN:NE2	4:L:96:PRO:HA	2.31	0.46
1:A:101:LEU:HD13	1:A:231:TRP:CD2	2.51	0.46
1:A:113:ARG:O	1:A:113:ARG:HG3	2.16	0.46
1:A:182:PRO:HG2	1:A:188:GLN:OE1	2.16	0.46
3:H:53:ASP:OD1	3:H:55:ASN:OD1	2.34	0.46
4:L:15:LEU:HD23	4:L:78:LEU:O	2.16	0.46
4:L:22:ASN:HA	4:L:72:THR:CG2	2.46	0.46
1:A:297:PRO:HG3	1:A:306:TYR:CE2	2.50	0.46
4:L:161:GLU:CD	4:L:161:GLU:H	2.24	0.46
5:C:1:NAG:O4	5:C:2:NAG:H62	2.16	0.46
3:H:97:GLN:HG2	3:H:100(J):GLY:CA	2.46	0.45
1:A:65:PRO:HB3	1:A:138:HIS:HB2	1.99	0.45
1:A:38:ASN:C	1:A:38:ASN:OD1	2.58	0.45
2:B:14:TRP:HE3	2:B:17:MET:HE2	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PHE:CE2	1:A:116:ILE:HG23	2.52	0.45
4:L:4:MET:SD	4:L:25:SER:HB2	2.56	0.45
3:H:167:GLN:HG3	3:H:169:SER:OG	2.17	0.45
4:L:22:ASN:HA	4:L:72:THR:HG22	1.99	0.45
3:H:165:VAL:O	3:H:166:LEU:C	2.60	0.45
2:B:71:ASN:C	2:B:73:LEU:N	2.73	0.45
4:L:166:GLN:CG	4:L:173:TYR:CE1	3.00	0.45
1:A:7:TYR:HB2	1:A:318:LEU:CD2	2.46	0.45
4:L:32:TYR:CD1	4:L:32:TYR:N	2.85	0.45
1:A:217:ARG:HD2	1:A:226:ARG:HG3	1.98	0.45
3:H:51:ILE:HG13	3:H:57:LYS:HG2	1.97	0.45
3:H:60:ALA:O	3:H:61:ASP:C	2.60	0.44
3:H:162:PHE:CE2	4:L:176:SER:HB2	2.52	0.44
3:H:176:SER:O	3:H:177:VAL:HG13	2.17	0.44
1:A:82:THR:HG22	1:A:83:PRO:N	2.32	0.44
1:A:181:HIS:HA	1:A:182:PRO:HD3	1.79	0.44
1:A:250:VAL:HG12	1:A:251:PRO:CD	2.47	0.44
2:B:80:LEU:HD12	2:B:80:LEU:C	2.43	0.44
1:A:7:TYR:HA	2:B:17:MET:HE1	1.99	0.44
1:A:82:THR:HG22	1:A:83:PRO:CD	2.47	0.44
3:H:88:ALA:O	3:H:108:LEU:HD12	2.16	0.44
3:H:105:GLN:HE21	3:H:105:GLN:HB2	1.63	0.44
3:H:162:PHE:N	3:H:162:PHE:CD1	2.84	0.44
1:A:108:VAL:HG11	1:A:257:MET:HE2	2.00	0.44
3:H:141:TYR:O	3:H:142:PHE:HB2	2.18	0.44
4:L:166:GLN:HG3	4:L:173:TYR:CE1	2.53	0.44
2:B:52:VAL:O	2:B:56:ILE:HG13	2.18	0.44
3:H:82:MET:CB	3:H:82(C):LEU:HD21	2.43	0.44
2:B:133:ILE:CD1	2:B:139:GLU:HG3	2.44	0.44
2:B:118:LEU:HD23	2:B:118:LEU:HA	1.75	0.44
1:A:51:HIS:HD2	1:A:53:GLY:H	1.65	0.44
3:H:91:TYR:CE1	3:H:106:GLY:HA3	2.53	0.44
3:H:144:GLU:HA	3:H:145:PRO:C	2.42	0.44
4:L:136:LEU:HD13	4:L:175:LEU:CD2	2.47	0.44
1:A:27:THR:C	1:A:28:HIS:ND1	2.76	0.43
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.53	0.43
2:B:38:LEU:HD22	3:H:100(F):TRP:CZ2	2.52	0.43
2:B:59:MET:HE2	2:B:59:MET:HB2	1.94	0.43
2:B:140:PHE:CE2	2:B:149:MET:HE1	2.53	0.43
3:H:165:VAL:O	3:H:165:VAL:HG23	2.18	0.43
1:A:32:LEU:HA	1:A:290:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:HD21	6:D:1:NAG:C7	2.32	0.43
4:L:163:VAL:O	4:L:164:THR:HG23	2.19	0.43
1:A:263:SER:OG	1:A:264:GLY:N	2.47	0.43
2:B:32:SER:OG	2:B:33:GLY:N	2.51	0.43
3:H:100(F):TRP:O	3:H:100(G):LEU:O	2.35	0.43
1:A:149:ILE:O	1:A:149:ILE:CG2	2.67	0.43
1:A:180:HIS:HB2	1:A:227:MET:HE2	2.01	0.43
2:B:144:CYS:HB3	2:B:149:MET:HE2	2.00	0.43
2:B:169:ASN:C	2:B:171:GLU:H	2.27	0.43
3:H:119:PRO:O	3:H:120:SER:C	2.60	0.43
4:L:170:ASP:O	4:L:171:SER:HB2	2.18	0.43
1:A:131:GLY:CA	1:A:150:TRP:HB3	2.46	0.43
2:B:38:LEU:HB3	3:H:100(F):TRP:CH2	2.54	0.43
3:H:11:VAL:HA	3:H:110:THR:O	2.19	0.43
1:A:73:ALA:C	1:A:75:SER:H	2.27	0.43
1:A:115:GLU:OE2	1:A:118:PRO:HA	2.19	0.43
1:A:116:ILE:C	1:A:118:PRO:HD3	2.41	0.43
1:A:206:TYR:O	1:A:207:SER:CB	2.65	0.43
1:A:319:ARG:O	1:A:321:ILE:HG13	2.19	0.42
4:L:33:LEU:HD13	4:L:71:PHE:CD1	2.54	0.42
1:A:296:HIS:HA	1:A:297:PRO:HD3	1.64	0.42
3:H:82(C):LEU:HB3	3:H:111:VAL:HG21	2.01	0.42
3:H:142:PHE:HA	3:H:143:PRO:HA	1.75	0.42
4:L:170:ASP:OD1	4:L:171:SER:N	2.52	0.42
1:A:191:LEU:HB3	1:A:192:TYR:CE1	2.54	0.42
1:A:206:TYR:CD2	1:A:207:SER:N	2.88	0.42
2:B:98:LEU:HD12	2:B:98:LEU:HA	1.84	0.42
3:H:84:ALA:C	3:H:86:ASP:N	2.77	0.42
4:L:28:ASN:O	4:L:30:LYS:N	2.51	0.42
2:B:129:ASN:HD21	2:B:163:SER:HA	1.84	0.42
3:H:52(A):TYR:CD1	3:H:53:ASP:N	2.88	0.42
3:H:175:SER:O	3:H:176:SER:HB2	2.19	0.42
1:A:49:PRO:HB3	1:A:78:TYR:CE1	2.55	0.42
1:A:220:VAL:O	1:A:223:GLN:HB2	2.19	0.42
1:A:327:ARG:C	2:B:1:GLY:CA	2.92	0.42
1:A:107:SER:C	1:A:260:ASN:HD21	2.28	0.42
1:A:141:ALA:O	1:A:142:LYS:C	2.62	0.42
3:H:119:PRO:HD3	3:H:201:THR:OG1	2.19	0.42
1:A:299:THR:HG21	1:A:303:CYS:CB	2.50	0.42
2:B:141:TYR:CE2	2:B:170:ARG:HG2	2.55	0.41
3:H:18:LEU:HD12	3:H:18:LEU:HA	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:77:SER:O	4:L:79:GLN:N	2.53	0.41
1:A:10:ASN:ND2	1:A:27:THR:HB	2.35	0.41
1:A:45:ARG:C	1:A:47:VAL:H	2.28	0.41
2:B:65:ALA:O	2:B:66:VAL:C	2.62	0.41
2:B:105:GLU:HA	2:B:105:GLU:OE1	2.21	0.41
4:L:55:GLU:O	4:L:56:SER:C	2.63	0.41
3:H:164:ALA:HA	3:H:174:LEU:HB3	2.02	0.41
1:A:60:TRP:HZ3	1:A:105:LEU:HD13	1.84	0.41
1:A:319:ARG:HD2	1:A:321:ILE:HD11	2.03	0.41
3:H:67:PHE:CZ	3:H:82:MET:HG2	2.54	0.41
3:H:52:SER:HB3	3:H:56:TYR:HB2	2.02	0.41
1:A:153:LYS:HB2	1:A:157:SER:O	2.20	0.41
1:A:298:ILE:HD13	1:A:298:ILE:HA	1.71	0.41
2:B:7:ALA:O	2:B:8:GLY:C	2.64	0.41
2:B:28:ASN:C	2:B:30:GLN:H	2.28	0.41
2:B:101:LEU:HD12	2:B:101:LEU:HA	1.57	0.41
3:H:11:VAL:HG21	3:H:142:PHE:HE2	1.86	0.41
1:A:114:PHE:CD1	1:A:114:PHE:N	2.89	0.41
1:A:301:GLY:O	2:B:63:PHE:HA	2.21	0.41
3:H:67:PHE:CE1	3:H:82:MET:HG2	2.56	0.41
4:L:25:SER:O	4:L:26:SER:C	2.63	0.41
4:L:58:VAL:HA	4:L:59:PRO:HD3	1.86	0.41
1:A:250:VAL:CG1	1:A:251:PRO:CD	2.97	0.41
2:B:61:THR:O	2:B:61:THR:HG23	2.21	0.41
3:H:6:GLU:OE2	3:H:91:TYR:HA	2.21	0.41
1:A:150:TRP:HZ2	1:A:180:HIS:CE1	2.40	0.40
4:L:137:ASN:O	4:L:138:ASN:HB2	2.21	0.40
3:H:141:TYR:CE1	3:H:172:TYR:O	2.75	0.40
1:A:81:GLU:O	1:A:267:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/288 (90%)	224 (87%)	34 (13%)	4	18
2	B	126/151 (83%)	112 (89%)	14 (11%)	6	25
3	H	141/191 (74%)	114 (81%)	27 (19%)	1	8
4	L	105/193 (54%)	95 (90%)	10 (10%)	8	31
All	All	630/823 (76%)	545 (86%)	85 (14%)	4	18

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	11	ASN
1	A	16	VAL
1	A	21	GLU
1	A	34	GLU
1	A	57	ILE
1	A	70	LEU
1	A	74	SER
1	A	81	GLU
1	A	84	SER
1	A	87	ASN
1	A	104	GLN
1	A	113	ARG
1	A	116	ILE
1	A	129	ASN
1	A	132	VAL
1	A	161	LEU
1	A	162	SER
1	A	164	SER
1	A	183	SER
1	A	185	SER
1	A	187	ASP
1	A	194	ASN
1	A	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	LYS
1	A	223	GLN
1	A	252	ARG
1	A	257	MET
1	A	259	ARG
1	A	260	ASN
1	A	267	ILE
1	A	299	THR
1	A	310	THR
1	A	313	ARG
2	B	9	PHE
2	B	32	SER
2	B	69	GLU
2	B	73	LEU
2	B	80	LEU
2	B	97	GLU
2	B	98	LEU
2	B	101	LEU
2	B	107	THR
2	B	115	VAL
2	B	120	GLU
2	B	151	SER
2	B	154	ASN
2	B	171	GLU
3	H	13	GLN
3	H	48	VAL
3	H	51	ILE
3	H	55	ASN
3	H	61	ASP
3	H	89	VAL
3	H	92	CYS
3	H	100	SER
3	H	100(A)	LEU
3	H	100(B)	LEU
3	H	100(C)	TYR
3	H	100(D)	PHE
3	H	100(E)	GLU
3	H	100(F)	TRP
3	H	100(G)	LEU
3	H	100(H)	SER
3	H	100(I)	GLN
3	H	100(K)	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	100(L)	PHE
3	H	105	GLN
3	H	107	THR
3	H	108	LEU
3	H	113	SER
3	H	167	GLN
3	H	171	LEU
3	H	174	LEU
3	H	177	VAL
4	L	5	THR
4	L	20	THR
4	L	61	ARG
4	L	65	SER
4	L	72	THR
4	L	74	THR
4	L	106	ILE
4	L	109	THR
4	L	110	VAL
4	L	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	31	ASN
1	A	64	ASN
1	A	87	ASN
1	A	104	GLN
1	A	138	HIS
1	A	147	ASN
1	A	156	ASN
1	A	167	ASN
1	A	223	GLN
1	A	260	ASN
1	A	287	ASN
1	A	325	GLN
2	B	62	GLN
2	B	72	HIS
2	B	114	ASN
2	B	129	ASN
3	H	13	GLN
3	H	76	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	81	GLN
3	H	82(A)	ASN
3	H	105	GLN
3	H	195	ASN
4	L	42	GLN
4	L	100	GLN
4	L	158	ASN
4	L	160	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](#)

7 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	$\# Z > 2$
5	NAG	C	1	5	14,14,15	0.55	0	17,19,21	1.06	1 (5%)
5	NAG	C	2	5	14,14,15	0.54	0	17,19,21	0.87	0
6	NAG	D	1	6	14,14,15	0.51	0	17,19,21	1.79	3 (17%)
6	NAG	D	2	6	14,14,15	0.64	0	17,19,21	0.93	0
6	BMA	D	3	6	11,11,12	0.45	0	15,15,17	1.19	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.44	0	17,19,21	1.72	3 (17%)
5	NAG	E	2	5	14,14,15	0.45	0	17,19,21	1.47	3 (17%)

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	C	1	5	-	3/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	0/1/1/1
6	NAG	D	1	6	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	BMA	D	3	6	3/3/4/5	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1	NAG	C1-O5-C5	5.60	119.69	112.19
5	E	1	NAG	C1-O5-C5	4.44	118.13	112.19
6	D	3	BMA	C1-O5-C5	3.82	117.31	112.19
5	E	1	NAG	O5-C1-C2	-3.77	105.46	111.29
5	E	2	NAG	C1-O5-C5	2.86	116.02	112.19
6	D	1	NAG	C2-N2-C7	-2.66	119.33	122.90
5	E	2	NAG	C1-C2-N2	2.48	114.34	110.43
5	E	2	NAG	C4-C3-C2	-2.17	107.83	111.02
5	C	1	NAG	C2-N2-C7	-2.13	120.05	122.90
6	D	1	NAG	C3-C4-C5	2.02	113.90	110.23
5	E	1	NAG	C3-C4-C5	2.02	113.90	110.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	3	BMA	C2
6	D	3	BMA	C5
6	D	3	BMA	C3

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

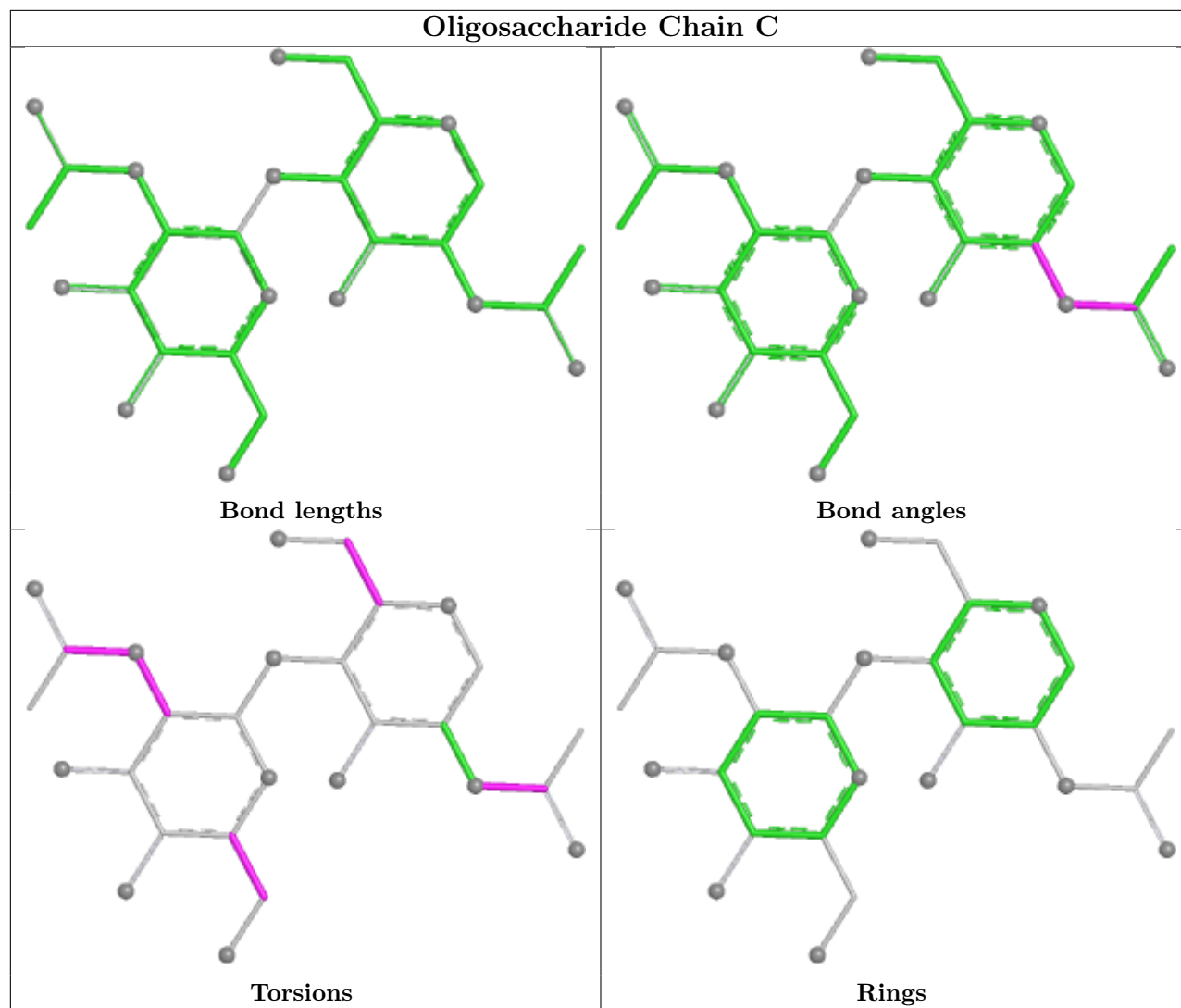
Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O7-C7-N2-C2
6	D	3	BMA	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
5	C	1	NAG	C8-C7-N2-C2
6	D	3	BMA	O5-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O7-C7-N2-C2
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
6	D	2	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	C	2	NAG	C3-C2-N2-C7
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
6	D	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O7-C7-N2-C2

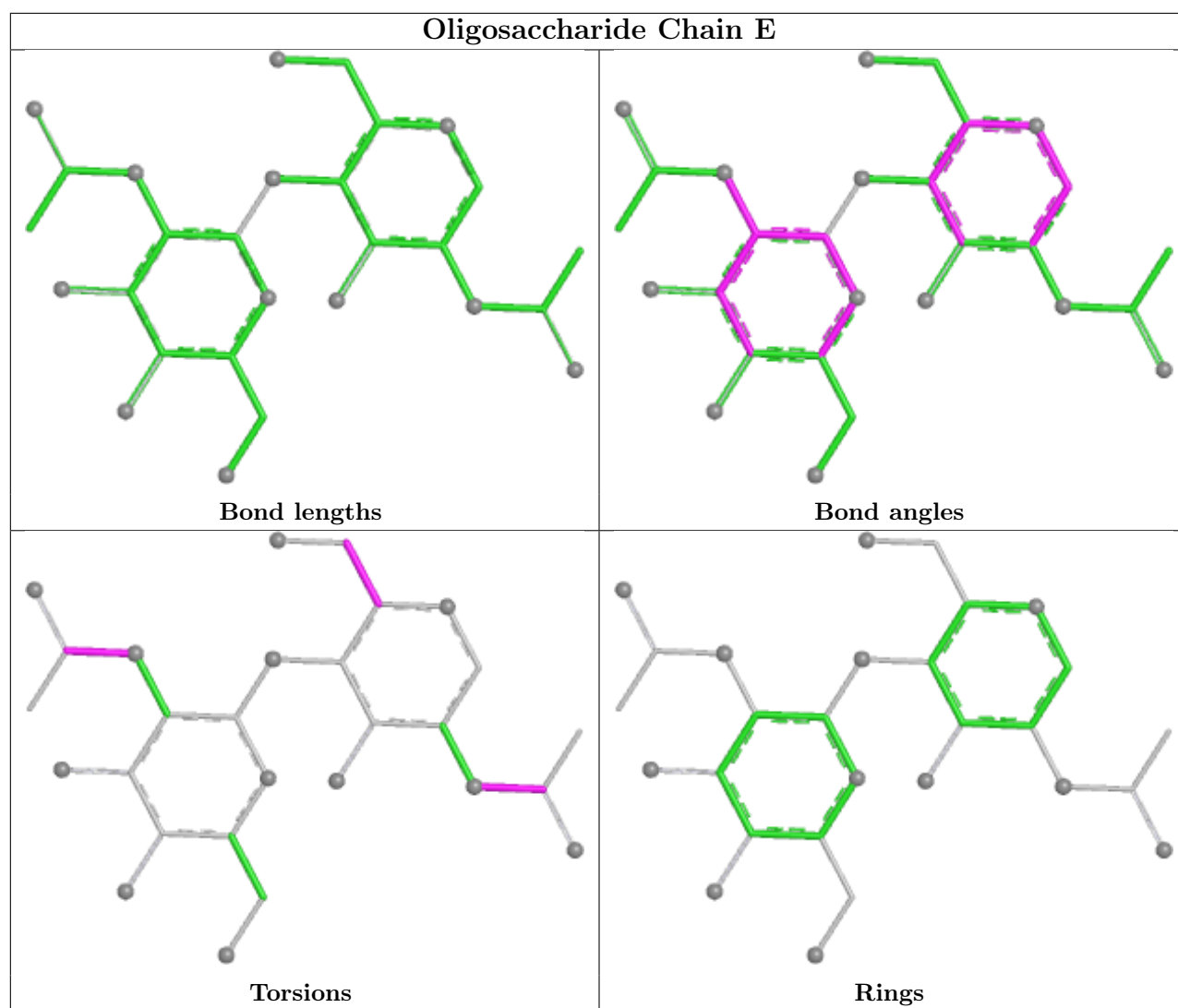
There are no ring outliers.

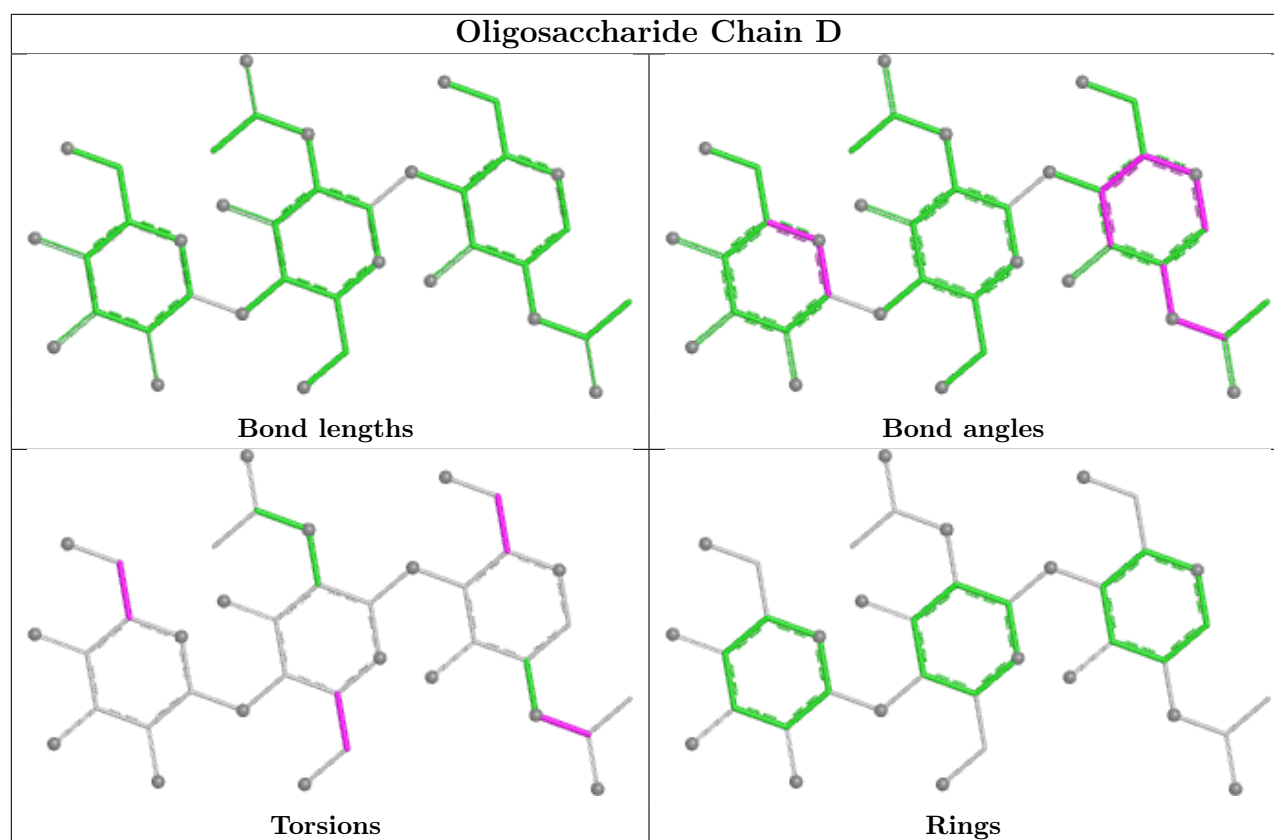
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	1	0
6	D	1	NAG	6	0
5	C	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.







5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
8	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.07	0
7	NAG	A	403	-	14,14,15	0.73	1 (7%)	17,19,21	1.49	1 (5%)
8	SO4	A	412	-	4,4,4	0.26	0	6,6,6	0.18	0
7	NAG	A	409	1	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
8	SO4	A	410	-	4,4,4	0.22	0	6,6,6	0.07	0
8	SO4	A	411	-	4,4,4	0.24	0	6,6,6	0.13	0
9	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.82	0
8	SO4	A	413	-	4,4,4	0.26	0	6,6,6	0.10	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
7	NAG	A	409	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	A	403	-	-	4/6/23/26	0/1/1/1
9	GOL	A	414	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	403	NAG	C1-C2	2.33	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	403	NAG	C1-O5-C5	4.60	118.35	112.19
7	A	409	NAG	C1-O5-C5	2.06	114.95	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	409	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	414	GOL	C1-C2-C3-O3
9	A	414	GOL	O2-C2-C3-O3
7	A	403	NAG	C8-C7-N2-C2
7	A	403	NAG	O7-C7-N2-C2
7	A	403	NAG	O5-C5-C6-O6
7	A	403	NAG	C4-C5-C6-O6
7	A	409	NAG	C8-C7-N2-C2
7	A	409	NAG	O7-C7-N2-C2
9	A	414	GOL	O1-C1-C2-C3
9	A	414	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	403	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/327 (100%)	-0.21	3 (0%) 81 61	43, 69, 107, 130	0
2	B	173/176 (98%)	-0.19	1 (0%) 85 69	40, 74, 125, 146	0
3	H	173/226 (76%)	-0.13	2 (1%) 76 55	43, 71, 152, 191	0
4	L	150/218 (68%)	0.36	12 (8%) 18 9	58, 99, 150, 168	0
All	All	823/947 (86%)	-0.09	18 (2%) 62 39	40, 74, 137, 191	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	ALA	3.6
4	L	141	PRO	3.2
4	L	105	GLU	2.7
3	H	138	VAL	2.6
4	L	56	SER	2.5
4	L	109	THR	2.4
1	A	238	ASP	2.3
4	L	177	SER	2.3
4	L	165	GLU	2.2
2	B	112	ASP	2.2
4	L	22	ASN	2.1
4	L	1	ASP	2.1
4	L	77	SER	2.1
4	L	155	GLN	2.1
3	H	137	LEU	2.0
4	L	110	VAL	2.0
1	A	71	SER	2.0
4	L	111	ALA	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 ⓘ

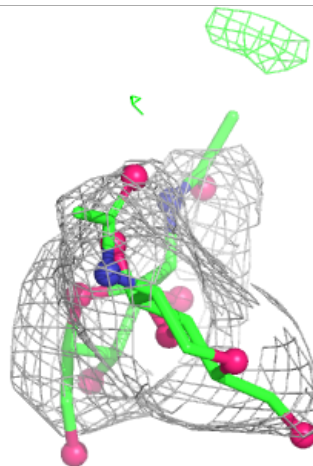
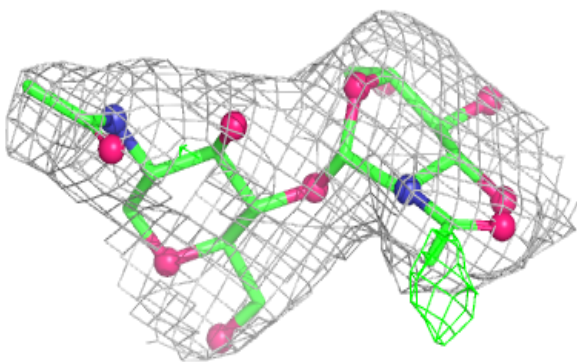
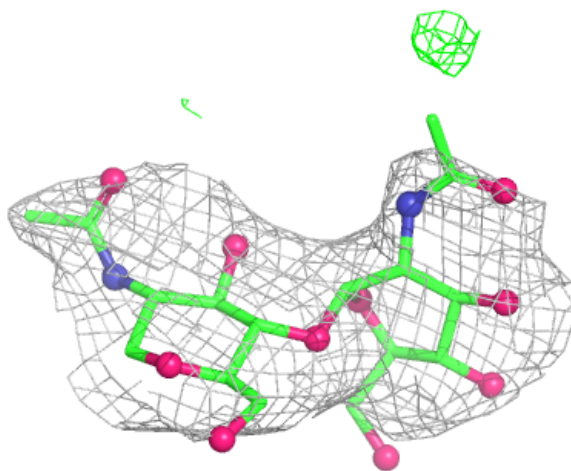
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	1	14/15	-	-	72,94,106,109	0
5	NAG	C	2	14/15	-	-	118,126,131,134	0
5	NAG	E	2	14/15	0.69	0.13	138,145,155,160	0
5	NAG	E	1	14/15	0.89	0.11	82,101,119,135	0
6	NAG	D	1	14/15	-	-	46,63,81,85	0
6	NAG	D	2	14/15	-	-	64,73,81,83	0
6	BMA	D	3	11/12	-	-	91,99,108,119	0

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

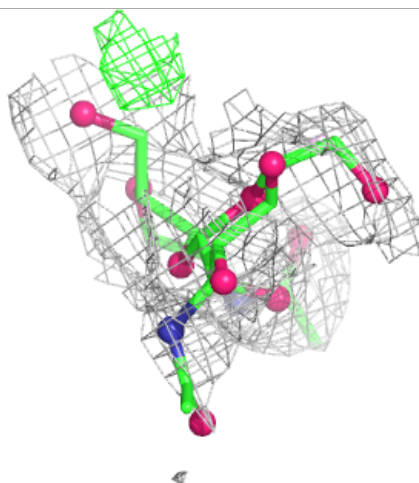
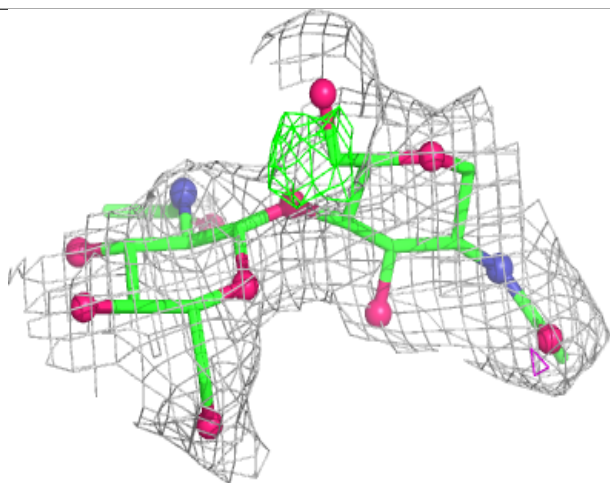
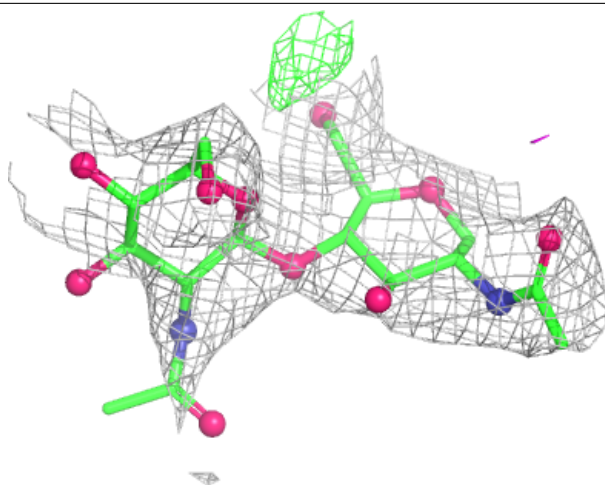
Electron density around Chain C:

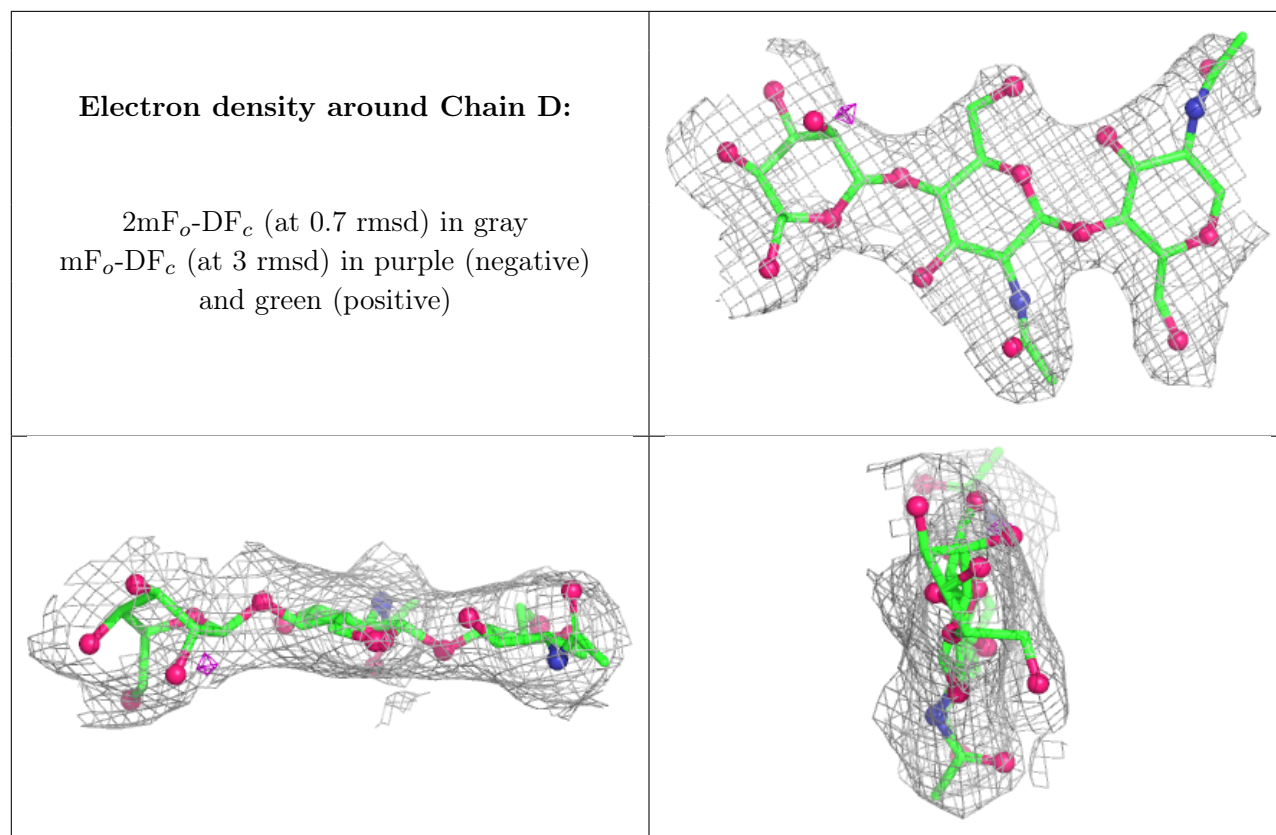
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	A	411	5/5	0.63	0.14	151,152,155,156	0
7	NAG	A	409	14/15	0.68	0.13	90,107,117,121	0
8	SO4	A	413	5/5	0.77	0.09	153,153,154,154	0
8	SO4	A	412	5/5	0.79	0.10	138,140,144,149	0
8	SO4	A	410	5/5	0.79	0.08	154,155,156,160	0
7	NAG	A	403	14/15	0.82	0.14	110,128,136,138	0
8	SO4	L	301	5/5	0.84	0.09	139,146,149,151	0
9	GOL	A	414	6/6	0.92	0.13	61,68,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.