Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:20 PM EDT

PDB ID	:	1LGC
Title	:	INTERACTION OF A LEGUME LECTIN WITH THE N2 FRAGMENT OF HUMAN LACTOTRANSFERRIN OR WITH THE ISOLATED BIANTENNARY GLYCOPEPTIDE: ROLE OF THE FUCOSE MOIETY
Authors	:	Bourne, Y.; Cambillau, C.
Deposited on	:	1994-01-07
Resolution	:	2.80 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:

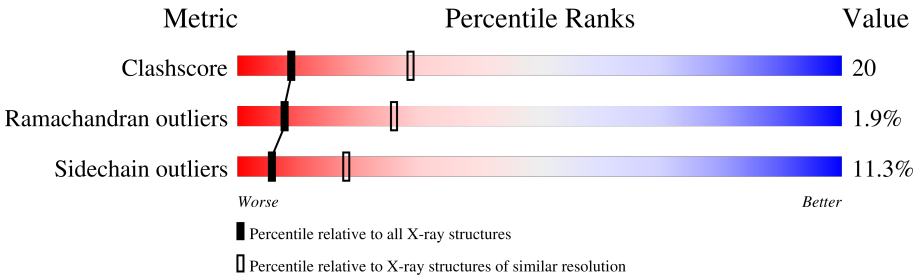
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	57% 35% 7%
1	C	181	61% 33% 6%
1	E	181	48% 48%
2	H	2	50% 50%
2	I	2	50% 50%
2	J	2	50% 50%
3	B	53	55% 36% 6%
3	D	53	58% 28% 9%

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Mol	Chain	Length	Quality of chain
3	F	53	42% 40% 8% 11%
4	G	10	50% 40% 10%
5	K	9	22% 33% 44%
5	L	9	67% 22% 11%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6044 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 LEGUME ISOLECTIN II (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	0	0	0
			1407	896	232	279			
1	C	181	Total	C	N	O	0	0	0
			1407	896	232	279			
1	E	181	Total	C	N	O	0	0	0
			1397	889	231	277			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	PRO	GLN	conflict	UNP P04122
A	168	GLY	ALA	conflict	UNP P04122
C	16	PRO	GLN	conflict	UNP P04122
C	168	GLY	ALA	conflict	UNP P04122
E	16	PRO	GLN	conflict	UNP P04122
E	168	GLY	ALA	conflict	UNP P04122

- Molecule 2 is a protein called DIPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	1	Total	C	N	O	0	0	0
			9	4	2	3			
2	I	1	Total	C	N	O	0	0	0
			9	4	2	3			
2	J	2	Total	C	N	O	0	0	0
			18	9	4	5			

- Molecule 3 is a protein called LEGUME ISOLECTIN II (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	51	Total	C	N	O	0	0	1
			401	261	61	79			

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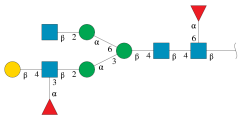
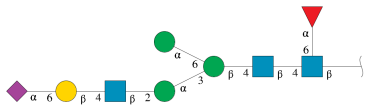
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	48	Total C N O 380 249 58 73	0	0	1
3	F	47	Total C N O 371 244 57 70	0	0	1

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	10	Total C N O 120 68 4 48	0	0	0

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	K	9	Total C N O 116 65 4 47	0	0	0
5	L	9	Total C N O 116 65 4 47	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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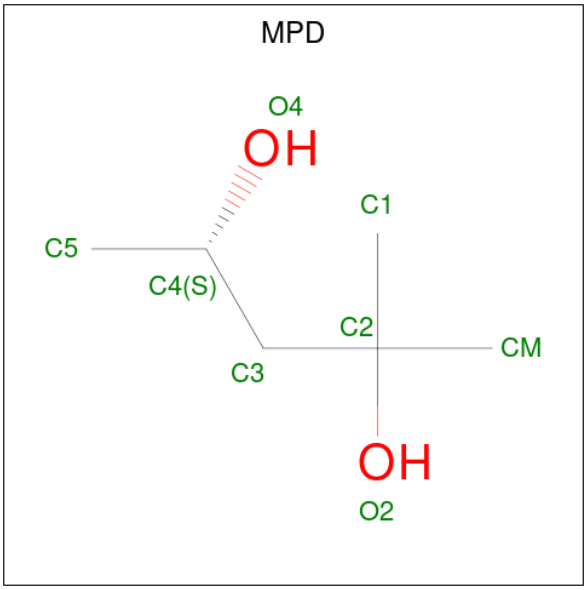
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total Ca 1 1	0	0

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mn 1 1	0	0
7	C	1	Total Mn 1 1	0	0
7	E	1	Total Mn 1 1	0	0

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	74	Total O 74 74	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	15	Total O 15 15	0	0
9	B	22	Total O 22 22	0	0
9	C	74	Total O 74 74	0	0
9	I	8	Total O 8 8	0	0
9	D	21	Total O 21 21	0	0
9	E	48	Total O 48 48	0	0
9	J	6	Total O 6 6	0	0
9	F	11	Total O 11 11	0	0

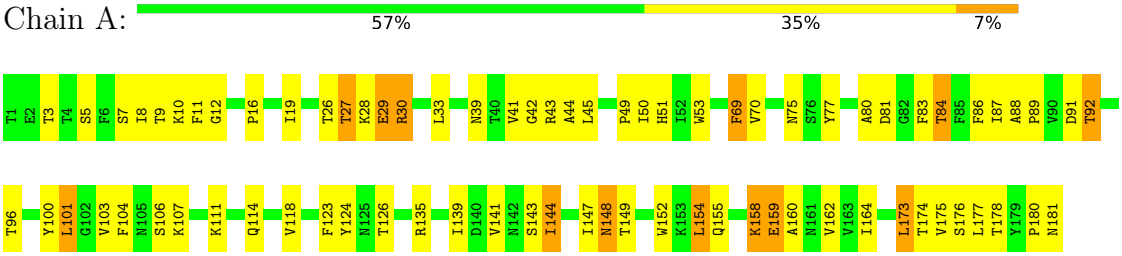
3 Residue-property plots (i)

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. 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.

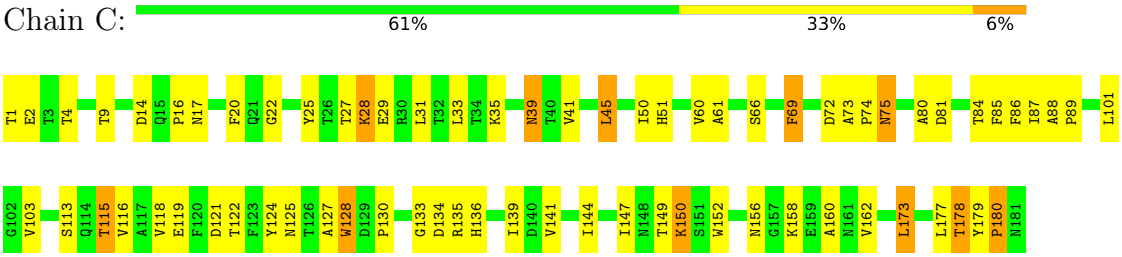
• Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)

Chain A:



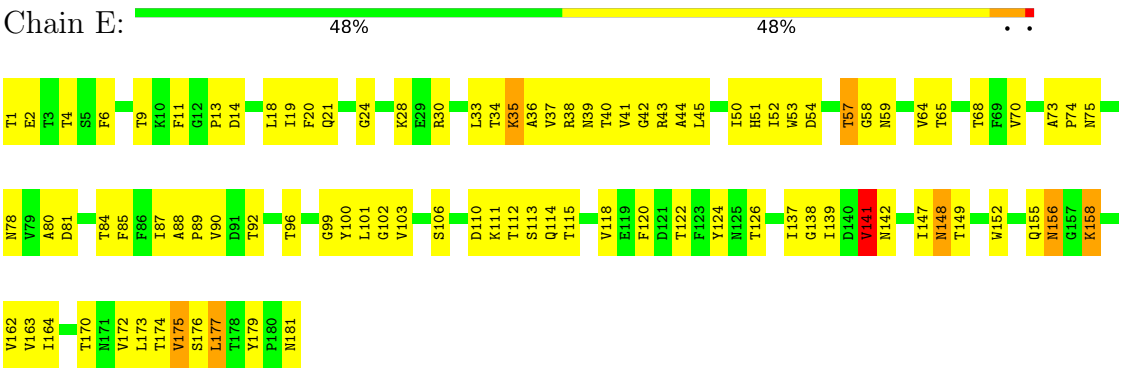
• Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)

Chain C:



• Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)

Chain E:

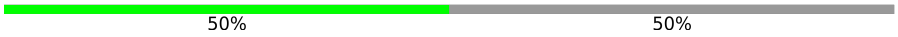


• Molecule 2: DIPEPTIDE

Chain H:

• Molecule 2: DIPEPTIDE

Chain I:



• Molecule 2: DIPEPTIDE

Chain J:

• Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)

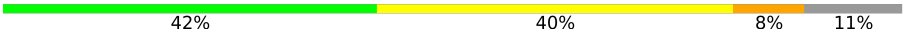
Chain B:

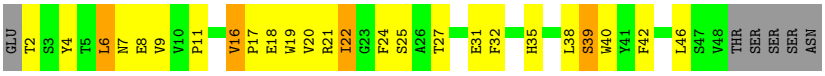
• Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)

Chain D:

• Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)

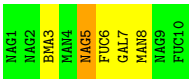
Chain F:





• Molecule 4: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

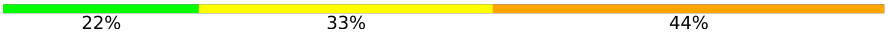
Chain G:



• Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]

beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.00Å 117.00Å 120.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6044	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUC, CA, SIA, BMA, MPD, GAL, NAG, MN

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	0.44	0/1442	0.76	1/1967 (0.1%)
1	C	0.44	0/1442	0.74	0/1967
1	E	0.44	0/1431	0.74	0/1952
2	H	0.93	0/8	0.72	0/8
2	I	0.74	0/8	0.66	0/8
2	J	0.65	0/17	0.56	0/20
3	B	0.47	0/413	0.66	0/566
3	D	0.50	0/392	0.70	0/537
3	F	0.50	0/383	0.65	0/525
All	All	0.45	0/5536	0.73	1/7550 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	LEU	CA-CB-CG	5.12	127.08	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	1407	0	1357	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1407	0	1357	51	0
1	E	1397	0	1346	83	0
2	H	9	0	4	1	0
2	I	9	0	4	0	0
2	J	18	0	11	2	0
3	B	401	0	377	23	0
3	D	380	0	353	18	0
3	F	371	0	344	41	0
4	G	120	0	103	5	0
5	K	116	0	98	5	0
5	L	116	0	98	3	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	E	8	0	14	1	0
9	A	74	0	0	2	0
9	B	22	0	0	1	0
9	C	74	0	0	2	0
9	D	21	0	0	0	0
9	E	48	0	0	4	0
9	F	11	0	0	1	0
9	H	15	0	0	1	0
9	I	8	0	0	0	0
9	J	6	0	0	0	0
All	All	6044	0	5466	228	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 20.

All (228) 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:C:160:ALA:HB1	1:C:177:LEU:HD11	1.38	1.04
1:E:54:ASP:HB2	3:F:46:LEU:HD21	1.62	0.82
1:C:14:ASP:HA	9:C:306:HOH:O	1.80	0.79
3:F:16:VAL:HG22	3:F:17:PRO:HD2	1.66	0.77
1:A:33:LEU:O	1:A:42:GLY:HA3	1.86	0.76
1:A:45:LEU:HD21	1:A:86:PHE:CZ	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:HB1	1:C:177:LEU:CD1	2.19	0.69
1:E:4:THR:HG21	1:E:50:ILE:HG22	1.74	0.68
1:A:118:VAL:HG11	1:A:164:ILE:HD13	1.75	0.68
1:E:162:VAL:HG22	1:E:177:LEU:HD22	1.76	0.68
3:F:17:PRO:HB2	9:F:163:HOH:O	1.93	0.68
1:E:87:ILE:HG22	3:F:16:VAL:HG21	1.75	0.67
3:D:43:ASN:HD22	3:D:44:SER:N	1.93	0.66
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.79	0.65
1:C:150:LYS:HD2	3:D:5:THR:O	1.96	0.65
1:A:107:LYS:NZ	1:A:107:LYS:HB3	2.13	0.64
1:E:57:THR:HB	1:E:59:ASN:OD1	1.98	0.64
9:E:347:HOH:O	3:F:22:ILE:HD13	1.96	0.64
1:E:68:THR:HG23	3:F:38:LEU:HB2	1.80	0.64
1:C:113:SER:O	1:C:115:THR:HG22	1.97	0.63
1:E:52:ILE:HG22	3:F:18:GLU:O	1.99	0.63
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.80	0.63
1:E:84:THR:HG21	1:E:103:VAL:HG21	1.79	0.63
1:E:158:LYS:HB2	1:E:179:TYR:CE2	2.34	0.62
1:E:33:LEU:O	1:E:42:GLY:HA3	2.00	0.61
1:E:33:LEU:HD11	3:F:24:PHE:HB2	1.82	0.61
3:D:13:LYS:HB2	3:D:13:LYS:NZ	2.15	0.61
1:E:137:ILE:HD11	1:E:177:LEU:HB2	1.82	0.61
1:E:147:ILE:O	1:E:148:ASN:HB2	2.00	0.61
1:C:173:LEU:O	3:D:7:ASN:HA	2.02	0.60
1:A:111:LYS:NZ	1:A:111:LYS:HB3	2.17	0.59
1:E:111:LYS:HD3	9:E:320:HOH:O	2.02	0.59
1:E:155:GLN:HB2	1:E:179:TYR:CE2	2.38	0.59
5:K:3:BMA:H4	5:K:8:MAN:C2	2.31	0.59
1:E:148:ASN:OD1	3:F:6:LEU:HD21	2.03	0.58
1:C:122:THR:HA	1:C:135:ARG:HG2	1.85	0.58
1:E:35:LYS:O	1:E:37:VAL:N	2.37	0.58
1:E:90:VAL:HG13	3:F:21:ARG:NH2	2.18	0.58
1:A:12:GLY:O	1:A:26:THR:HG21	2.04	0.57
1:C:84:THR:HB	3:D:25:SER:HB3	1.87	0.57
1:C:160:ALA:CB	1:C:177:LEU:HD11	2.26	0.57
1:A:49:PRO:HD2	1:C:17:ASN:HA	1.87	0.57
3:B:38:LEU:N	3:B:38:LEU:HD12	2.20	0.57
5:K:3:BMA:H4	5:K:8:MAN:C1	2.35	0.57
1:A:152:TRP:CZ2	1:A:154:LEU:HD23	2.40	0.56
1:A:80:ALA:HB2	1:A:123:PHE:CD2	2.40	0.56
3:B:16:VAL:HG13	3:B:20:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:ALA:HB3	1:E:156:ASN:OD1	2.04	0.56
4:G:5:NAG:N2	4:G:6:FUC:O5	2.39	0.56
1:E:118:VAL:HG21	1:E:164:ILE:HD13	1.86	0.56
1:A:80:ALA:HB2	1:A:123:PHE:HD2	1.71	0.56
3:B:11:PRO:HG2	3:B:15:PHE:HE2	1.71	0.56
1:E:38:ARG:O	1:E:40:THR:HG23	2.06	0.56
1:C:136:HIS:HA	1:C:152:TRP:HB3	1.87	0.55
1:E:173:LEU:O	3:F:7:ASN:HA	2.06	0.55
1:E:120:PHE:CE2	1:E:177:LEU:HD23	2.42	0.55
1:A:148:ASN:HD22	1:A:149:THR:H	1.54	0.55
3:D:22:ILE:HD13	3:D:42:PHE:CE1	2.42	0.55
3:B:48:VAL:HG21	1:C:9:THR:OG1	2.07	0.55
4:G:5:NAG:N2	4:G:6:FUC:C1	2.69	0.55
1:C:87:ILE:HB	1:C:116:VAL:HG22	1.89	0.54
1:E:158:LYS:HB2	1:E:179:TYR:HE2	1.70	0.54
1:E:176:SER:HA	3:F:4:TYR:O	2.07	0.54
1:E:33:LEU:HD11	3:F:24:PHE:CB	2.37	0.54
1:E:152:TRP:HE1	1:E:179:TYR:HE1	1.54	0.54
1:E:84:THR:HB	3:F:25:SER:OG	2.07	0.54
1:E:110:ASP:OD2	1:E:112:THR:HB	2.09	0.53
1:C:80:ALA:CB	3:D:31:GLU:HB2	2.38	0.53
1:E:92:THR:HA	9:E:336:HOH:O	2.09	0.53
1:E:148:ASN:ND2	3:F:8:GLU:HG2	2.24	0.53
1:E:139:ILE:HD12	3:F:8:GLU:HB2	1.90	0.52
1:C:14:ASP:O	1:C:16:PRO:HD3	2.10	0.52
1:C:45:LEU:HD12	3:D:21:ARG:HD3	1.90	0.52
1:E:19:ILE:O	1:E:44:ALA:HA	2.09	0.52
1:E:162:VAL:CG2	1:E:177:LEU:HD22	2.39	0.52
1:A:87:ILE:HG22	3:B:16:VAL:HG21	1.91	0.52
1:A:160:ALA:HB1	1:A:177:LEU:HG	1.92	0.52
1:C:101:LEU:HD23	1:C:144:ILE:HD11	1.92	0.52
1:A:162:VAL:HA	1:A:176:SER:O	2.10	0.52
1:E:51:HIS:HB2	3:F:19:TRP:CZ3	2.45	0.52
1:E:51:HIS:HB2	3:F:19:TRP:CH2	2.45	0.51
1:C:28:LYS:HG2	9:C:362:HOH:O	2.11	0.51
1:E:87:ILE:O	1:E:115:THR:HG23	2.11	0.50
1:A:43:ARG:HH22	1:A:92:THR:CG2	2.23	0.50
1:C:22:GLY:HA3	1:C:41:VAL:O	2.11	0.50
1:C:150:LYS:NZ	1:C:150:LYS:HB2	2.26	0.50
3:F:16:VAL:CG2	3:F:17:PRO:HD2	2.37	0.50
3:B:11:PRO:HG2	3:B:15:PHE:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:HG21	1:C:103:VAL:HG21	1.93	0.50
1:A:164:ILE:HA	1:A:174:THR:O	2.12	0.50
1:C:4:THR:HG21	1:C:50:ILE:CD1	2.41	0.50
1:E:81:ASP:OD1	1:E:99:GLY:HA2	2.11	0.50
1:E:122:THR:HG22	1:E:152:TRP:CZ3	2.47	0.50
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.47	0.49
1:E:70:VAL:HG23	3:F:38:LEU:HD11	1.94	0.49
1:C:80:ALA:HB3	3:D:31:GLU:HB2	1.94	0.49
1:E:30:ARG:HE	3:F:38:LEU:HD21	1.75	0.49
1:A:75:ASN:OD1	1:A:77:TYR:HD2	1.95	0.49
4:G:5:NAG:H61	4:G:7:GAL:O2	2.13	0.49
5:L:2:NAG:C1	5:L:2:NAG:O7	2.60	0.49
1:A:144:ILE:HD13	1:A:144:ILE:O	2.12	0.49
1:C:75:ASN:HD22	1:C:75:ASN:H	1.58	0.49
1:E:1:THR:HA	3:F:46:LEU:O	2.13	0.49
3:F:22:ILE:HD13	3:F:22:ILE:H	1.78	0.49
1:E:149:THR:HG23	8:E:303:MPD:H53	1.95	0.48
1:E:148:ASN:HD22	3:F:8:GLU:HG2	1.78	0.48
1:C:25:TYR:OH	1:C:35:LYS:HD3	2.13	0.48
1:E:37:VAL:HG12	1:E:38:ARG:N	2.29	0.48
1:E:101:LEU:O	1:E:103:VAL:HG23	2.14	0.48
1:E:74:PRO:HG3	3:F:32:PHE:CE2	2.49	0.48
1:A:155:GLN:HB3	1:A:158:LYS:HB2	1.96	0.47
1:E:164:ILE:HG12	1:E:175:VAL:HB	1.96	0.47
1:A:96:THR:HG23	4:G:6:FUC:H63	1.96	0.47
1:A:101:LEU:HA	3:B:27:THR:OG1	2.15	0.47
1:A:70:VAL:HG22	1:A:159:GLU:HB3	1.97	0.47
1:A:100:TYR:CE1	1:A:106:SER:HA	2.49	0.47
1:A:100:TYR:HA	1:A:144:ILE:HG13	1.97	0.47
1:C:141:VAL:O	1:C:141:VAL:HG23	2.14	0.47
1:E:13:PRO:HB3	9:E:328:HOH:O	2.13	0.47
1:E:114:GLN:O	3:F:16:VAL:HG23	2.14	0.47
1:C:119:GLU:OE2	1:C:121:ASP:HB2	2.14	0.47
1:A:9:THR:O	1:A:10:LYS:HG3	2.15	0.47
1:A:26:THR:HG22	9:A:336:HOH:O	2.14	0.47
1:A:173:LEU:O	3:B:7:ASN:HB2	2.15	0.47
9:H:265:HOH:O	4:G:8:MAN:O4	2.20	0.47
1:C:149:THR:CG2	1:C:150:LYS:N	2.77	0.47
1:E:80:ALA:HB3	3:F:31:GLU:HB2	1.97	0.47
1:A:11:PHE:O	1:A:29:GLU:HA	2.15	0.46
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:VAL:O	1:E:142:ASN:HB2	2.15	0.46
1:A:180:PRO:O	1:A:181:ASN:HB2	2.16	0.46
1:A:26:THR:O	1:A:26:THR:HG23	2.16	0.46
1:A:43:ARG:HH22	1:A:92:THR:HG22	1.80	0.46
1:E:89:PRO:O	1:E:92:THR:HG22	2.16	0.46
1:E:80:ALA:CB	3:F:31:GLU:HB2	2.46	0.46
1:A:69:PHE:CE1	1:A:160:ALA:HB3	2.51	0.45
1:C:25:TYR:CE2	1:C:27:THR:OG1	2.69	0.45
1:C:69:PHE:HA	3:D:37:VAL:HA	1.98	0.45
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.98	0.45
1:E:137:ILE:HG22	1:E:138:GLY:N	2.31	0.45
3:B:14:GLU:HB2	9:B:75:HOH:O	2.16	0.45
1:A:139:ILE:O	1:A:147:ILE:HG12	2.16	0.45
1:A:111:LYS:HB3	1:A:111:LYS:HZ2	1.81	0.45
1:A:80:ALA:O	3:B:32:PHE:HA	2.17	0.45
1:E:96:THR:O	1:E:102:GLY:HA2	2.17	0.45
5:K:7:SIA:O6	5:K:7:SIA:C9	2.64	0.45
1:C:51:HIS:CD2	3:D:46:LEU:HD23	2.51	0.45
1:E:78:ASN:HD21	2:J:512:ASN:ND2	2.14	0.45
1:C:152:TRP:HA	3:D:4:TYR:CE2	2.52	0.45
3:D:13:LYS:HB2	3:D:13:LYS:HZ3	1.82	0.44
1:A:83:PHE:CZ	3:B:24:PHE:CD1	3.05	0.44
1:C:60:VAL:HG12	1:C:61:ALA:N	2.33	0.44
1:E:20:PHE:HB3	1:E:24:GLY:O	2.18	0.44
1:E:122:THR:HG22	1:E:152:TRP:HZ3	1.83	0.44
1:A:159:GLU:H	1:A:159:GLU:HG2	1.70	0.44
1:E:102:GLY:N	3:F:27:THR:HG21	2.33	0.44
1:A:5:SER:OG	3:B:43:ASN:ND2	2.50	0.44
1:A:148:ASN:HD22	1:A:149:THR:N	2.14	0.44
1:E:100:TYR:HE2	1:E:106:SER:HA	1.83	0.44
1:A:41:VAL:HA	3:B:27:THR:HG22	2.00	0.44
1:A:70:VAL:CG2	1:A:159:GLU:HB3	2.48	0.44
1:C:69:PHE:HD1	1:C:69:PHE:H	1.66	0.44
1:C:84:THR:CG2	1:C:85:PHE:N	2.80	0.44
1:C:45:LEU:HD22	1:C:86:PHE:CZ	2.53	0.44
1:E:52:ILE:HG23	1:E:53:TRP:HD1	1.83	0.44
1:A:27:THR:O	1:A:30:ARG:HG2	2.17	0.44
1:C:125:ASN:HB2	1:C:128:TRP:NE1	2.33	0.43
1:C:130:PRO:HG2	1:C:149:THR:HG21	1.99	0.43
1:E:11:PHE:HE1	3:F:39:SER:HA	1.84	0.43
1:A:114:GLN:HA	3:B:15:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:HD12	1:C:178:THR:N	2.32	0.43
1:E:41:VAL:HG13	3:F:27:THR:HG22	1.99	0.43
1:E:162:VAL:HG12	1:E:163:VAL:N	2.33	0.43
1:E:174:THR:HA	3:F:6:LEU:O	2.18	0.43
1:E:84:THR:CG2	1:E:85:PHE:N	2.82	0.43
1:A:51:HIS:HB3	9:A:305:HOH:O	2.19	0.43
3:B:6:LEU:HD12	3:B:7:ASN:H	1.84	0.43
1:E:9:THR:HG22	1:E:9:THR:O	2.18	0.43
1:A:19:ILE:O	1:A:44:ALA:HA	2.19	0.43
1:E:65:THR:HB	3:F:42:PHE:HD2	1.83	0.43
1:A:9:THR:O	1:A:9:THR:HG22	2.19	0.42
1:A:53:TRP:O	3:B:18:GLU:HG2	2.19	0.42
1:A:107:LYS:HB3	1:A:107:LYS:HZ3	1.81	0.42
1:E:34:THR:HG23	1:E:40:THR:OG1	2.19	0.42
1:A:178:THR:O	1:A:180:PRO:HD3	2.19	0.42
3:F:17:PRO:HG2	3:F:20:VAL:HG12	2.00	0.42
1:C:124:TYR:CD1	1:C:133:GLY:HA2	2.53	0.42
1:E:30:ARG:HE	3:F:38:LEU:CD2	2.33	0.42
1:A:3:THR:HG23	3:B:44:SER:O	2.19	0.42
3:D:5:THR:CG2	3:D:6:LEU:N	2.83	0.42
2:H:512:ASN:OD1	2:H:512:ASN:N	2.52	0.42
1:C:139:ILE:O	1:C:147:ILE:HG22	2.19	0.42
2:J:512:ASN:ND2	5:L:1:NAG:O7	2.52	0.42
1:A:80:ALA:HA	1:A:81:ASP:HA	1.64	0.42
1:C:179:TYR:HA	1:C:180:PRO:HD2	1.83	0.42
3:D:5:THR:HG22	3:D:6:LEU:N	2.34	0.42
1:E:90:VAL:HG13	3:F:21:ARG:HH21	1.83	0.42
1:A:7:SER:HB2	1:C:1:THR:O	2.20	0.42
5:K:1:NAG:H61	5:K:2:NAG:O7	2.20	0.42
3:F:6:LEU:HD23	3:F:6:LEU:HA	1.82	0.42
1:C:20:PHE:HE1	1:C:31:LEU:CD1	2.33	0.41
1:A:8:ILE:HG21	1:A:11:PHE:CE2	2.55	0.41
1:E:78:ASN:HD21	5:L:1:NAG:H2	1.84	0.41
1:E:148:ASN:HD22	3:F:8:GLU:CG	2.33	0.41
1:A:16:PRO:HD2	3:D:19:TRP:CE2	2.55	0.41
1:E:33:LEU:HD23	1:E:33:LEU:HA	1.84	0.41
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.56	0.41
1:E:124:TYR:CE2	1:E:126:THR:HG22	2.56	0.41
1:E:172:VAL:O	1:E:172:VAL:HG13	2.21	0.41
1:E:28:LYS:HD3	1:E:30:ARG:HH11	1.86	0.41
5:K:4:MAN:H2	5:K:5:NAG:H2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:THR:HB	3:F:35:HIS:HD2	1.84	0.41
1:A:5:SER:HA	3:B:42:PHE:O	2.21	0.41
3:B:16:VAL:HG13	3:B:20:VAL:CG1	2.50	0.41
3:B:41:TYR:OH	3:B:43:ASN:HB2	2.21	0.41
1:A:181:ASN:O	3:B:1:GLU:N	2.53	0.41
1:C:45:LEU:HA	3:D:23:GLY:HA3	2.03	0.40
1:C:136:HIS:HB2	1:C:149:THR:HG23	2.04	0.40
1:A:84:THR:HG22	3:B:25:SER:HB3	2.04	0.40
1:C:4:THR:HG21	1:C:50:ILE:HD13	2.03	0.40
3:D:43:ASN:HD22	3:D:43:ASN:C	2.23	0.40
1:E:6:PHE:HZ	3:F:40:TRP:CZ2	2.39	0.40
1:E:88:ALA:HB2	1:E:115:THR:HG23	2.04	0.40
1:A:152:TRP:HA	3:B:4:TYR:CE2	2.57	0.40
1:C:14:ASP:C	1:C:16:PRO:HD3	2.42	0.40
1:C:73:ALA:HB3	1:C:156:ASN:ND2	2.36	0.40
3:F:9:VAL:O	3:F:11:PRO:HD3	2.21	0.40
1:C:73:ALA:HA	1:C:74:PRO:HD3	1.92	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	179/181 (99%)	164 (92%)	14 (8%)	1 (1%)	25 56
1	C	179/181 (99%)	145 (81%)	29 (16%)	5 (3%)	5 17
1	E	179/181 (99%)	147 (82%)	25 (14%)	7 (4%)	3 10
3	B	49/53 (92%)	44 (90%)	5 (10%)	0	100 100
3	D	46/53 (87%)	41 (89%)	5 (11%)	0	100 100
3	F	45/53 (85%)	39 (87%)	6 (13%)	0	100 100
All	All	677/702 (96%)	580 (86%)	84 (12%)	13 (2%)	8 26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	39	ASN
1	C	134	ASP
1	E	36	ALA
1	E	39	ASN
1	A	101	LEU
1	E	148	ASN
1	C	127	ALA
1	E	75	ASN
1	E	156	ASN
1	C	128	TRP
1	E	58	GLY
1	E	141	VAL
1	C	180	PRO

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	156/156 (100%)	137 (88%)	19 (12%)	5 15
1	C	156/156 (100%)	138 (88%)	18 (12%)	5 17
1	E	154/156 (99%)	140 (91%)	14 (9%)	9 27
2	H	1/2 (50%)	0	1 (100%)	0 0
2	I	1/2 (50%)	1 (100%)	0	100 100
2	J	2/2 (100%)	0	2 (100%)	0 0
3	B	44/47 (94%)	39 (89%)	5 (11%)	5 18
3	D	40/47 (85%)	37 (92%)	3 (8%)	13 37
3	F	39/47 (83%)	34 (87%)	5 (13%)	4 13
All	All	593/615 (96%)	526 (89%)	67 (11%)	6 18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	LYS
1	A	29	GLU
1	A	30	ARG
1	A	39	ASN
1	A	50	ILE
1	A	69	PHE
1	A	84	THR
1	A	91	ASP
1	A	92	THR
1	A	135	ARG
1	A	141	VAL
1	A	143	SER
1	A	144	ILE
1	A	148	ASN
1	A	158	LYS
1	A	159	GLU
1	A	173	LEU
1	A	175	VAL
2	H	512	ASN
3	B	2	THR
3	B	16	VAL
3	B	36	GLU
3	B	43	ASN
3	B	48	VAL
1	C	2	GLU
1	C	28	LYS
1	C	29	GLU
1	C	33	LEU
1	C	39	ASN
1	C	45	LEU
1	C	66	SER
1	C	69	PHE
1	C	72	ASP
1	C	75	ASN
1	C	81	ASP
1	C	115	THR
1	C	118	VAL
1	C	150	LYS
1	C	158	LYS
1	C	162	VAL
1	C	173	LEU
1	C	178	THR

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Mol	Chain	Res	Type
3	D	21	ARG
3	D	38	LEU
3	D	43	ASN
1	E	2	GLU
1	E	14	ASP
1	E	18	LEU
1	E	35	LYS
1	E	45	LEU
1	E	57	THR
1	E	64	VAL
1	E	113	SER
1	E	141	VAL
1	E	158	LYS
1	E	170	THR
1	E	175	VAL
1	E	177	LEU
1	E	181	ASN
2	J	512	ASN
2	J	513	GLN
3	F	2	THR
3	F	6	LEU
3	F	16	VAL
3	F	22	ILE
3	F	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	148	ASN
1	A	155	GLN
3	B	35	HIS
3	B	43	ASN
1	C	21	GLN
1	C	51	HIS
1	C	59	ASN
1	C	75	ASN
1	C	114	GLN
3	D	43	ASN
1	E	21	GLN
1	E	78	ASN
1	E	181	ASN

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Mol	Chain	Res	Type
3	F	35	HIS
3	F	43	ASN

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)

28 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	2,4	14,14,15	0.58	0	17,19,21	0.60	0
4	FUC	G	10	4	10,10,11	0.47	0	14,14,16	0.56	0
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.77	0
4	BMA	G	3	4	11,11,12	0.45	0	15,15,17	1.11	2 (13%)
4	MAN	G	4	4	11,11,12	0.62	0	15,15,17	0.79	0
4	NAG	G	5	4	14,14,15	1.03	0	17,19,21	0.91	1 (5%)
4	FUC	G	6	4	10,10,11	0.68	0	14,14,16	1.00	0
4	GAL	G	7	4	11,11,12	0.51	0	15,15,17	0.80	0
4	MAN	G	8	4	11,11,12	0.68	0	15,15,17	0.70	0
4	NAG	G	9	4	14,14,15	0.56	0	17,19,21	0.56	0
5	NAG	K	1	5,2	14,14,15	0.58	0	17,19,21	0.76	1 (5%)
5	NAG	K	2	5	14,14,15	0.53	0	17,19,21	1.20	2 (11%)
5	BMA	K	3	5	11,11,12	0.69	0	15,15,17	0.60	0
5	MAN	K	4	5	11,11,12	0.39	0	15,15,17	0.82	0
5	NAG	K	5	5	14,14,15	0.56	0	17,19,21	0.56	0
5	GAL	K	6	5	11,11,12	0.44	0	15,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SIA	K	7	5	20,20,21	0.93	1 (5%)	24,28,31	0.91	1 (4%)
5	MAN	K	8	5	11,11,12	0.59	0	15,15,17	1.06	1 (6%)
5	FUC	K	9	5	10,10,11	0.36	0	14,14,16	0.57	0
5	NAG	L	1	5,2	14,14,15	0.56	0	17,19,21	0.88	0
5	NAG	L	2	5	14,14,15	0.64	0	17,19,21	1.04	3 (17%)
5	BMA	L	3	5	11,11,12	0.61	0	15,15,17	0.51	0
5	MAN	L	4	5	11,11,12	0.56	0	15,15,17	0.79	0
5	NAG	L	5	5	14,14,15	0.45	0	17,19,21	0.54	0
5	GAL	L	6	5	11,11,12	0.38	0	15,15,17	0.77	0
5	SIA	L	7	5	20,20,21	0.90	1 (5%)	24,28,31	0.91	2 (8%)
5	MAN	L	8	5	11,11,12	0.54	0	15,15,17	0.53	0
5	FUC	L	9	5	10,10,11	0.30	0	14,14,16	0.39	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	NAG	G	1	2,4	-	0/6/23/26	0/1/1/1
4	FUC	G	10	4	-	-	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	NAG	G	5	4	-	0/6/23/26	0/1/1/1
4	FUC	G	6	4	-	-	0/1/1/1
4	GAL	G	7	4	-	2/2/19/22	0/1/1/1
4	MAN	G	8	4	-	0/2/19/22	0/1/1/1
4	NAG	G	9	4	-	3/6/23/26	0/1/1/1
5	NAG	K	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1
5	NAG	K	5	5	-	0/6/23/26	0/1/1/1
5	GAL	K	6	5	-	1/2/19/22	0/1/1/1
5	SIA	K	7	5	-	3/18/34/38	0/1/1/1
5	MAN	K	8	5	-	0/2/19/22	0/1/1/1
5	FUC	K	9	5	-	-	0/1/1/1
5	NAG	L	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	0/1/1/1
5	NAG	L	5	5	-	1/6/23/26	0/1/1/1
5	GAL	L	6	5	-	2/2/19/22	0/1/1/1
5	SIA	L	7	5	-	8/18/34/38	0/1/1/1
5	MAN	L	8	5	-	0/2/19/22	0/1/1/1
5	FUC	L	9	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	7	SIA	C2-C1	2.32	1.54	1.52
5	K	7	SIA	C2-C1	2.10	1.54	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	2	NAG	C4-C3-C2	-3.69	105.61	111.02
4	G	3	BMA	C6-C5-C4	-3.07	105.81	113.00
5	K	8	MAN	C1-O5-C5	2.95	116.19	112.19
5	L	2	NAG	C4-C3-C2	-2.40	107.50	111.02
4	G	5	NAG	C6-C5-C4	2.37	118.55	113.00
5	L	2	NAG	O5-C1-C2	-2.36	107.56	111.29
5	L	2	NAG	C1-C2-N2	2.31	114.44	110.49
5	L	7	SIA	C4-C3-C2	2.24	113.83	109.81
5	L	7	SIA	O1B-C1-C2	2.23	119.40	113.03
4	G	3	BMA	C3-C4-C5	2.12	114.02	110.24
5	K	2	NAG	O5-C1-C2	-2.11	107.96	111.29
5	K	7	SIA	O1B-C1-C2	2.09	119.00	113.03
5	K	1	NAG	C3-C4-C5	-2.05	106.59	110.24

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	7	SIA	C7-C8-C9-O9
5	K	7	SIA	O8-C8-C9-O9
5	L	7	SIA	C5-C6-C7-O7
5	L	7	SIA	O6-C6-C7-O7
5	L	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	G	7	GAL	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
4	G	7	GAL	C4-C5-C6-O6
5	L	6	GAL	C4-C5-C6-O6
5	K	2	NAG	C1-C2-N2-C7
5	L	6	GAL	O5-C5-C6-O6
5	K	6	GAL	O5-C5-C6-O6
5	L	7	SIA	O1A-C1-C2-O6
4	G	2	NAG	C3-C2-N2-C7
4	G	9	NAG	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
4	G	9	NAG	O5-C5-C6-O6
5	L	7	SIA	C6-C7-C8-O8
5	L	7	SIA	O1A-C1-C2-C3
5	L	7	SIA	O1B-C1-C2-C3
5	K	4	MAN	O5-C5-C6-O6
5	L	7	SIA	C5-C6-C7-C8
5	K	7	SIA	O1A-C1-C2-O6
5	L	4	MAN	O5-C5-C6-O6
5	L	7	SIA	O7-C7-C8-O8
5	K	3	BMA	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
4	G	9	NAG	C1-C2-N2-C7
4	G	2	NAG	C4-C5-C6-O6
5	L	5	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	7	SIA	1	0
5	K	1	NAG	1	0
4	G	6	FUC	3	0
5	K	4	MAN	1	0
5	K	8	MAN	2	0
4	G	5	NAG	3	0
5	K	2	NAG	1	0
5	K	3	BMA	2	0
4	G	8	MAN	1	0
4	G	7	GAL	1	0

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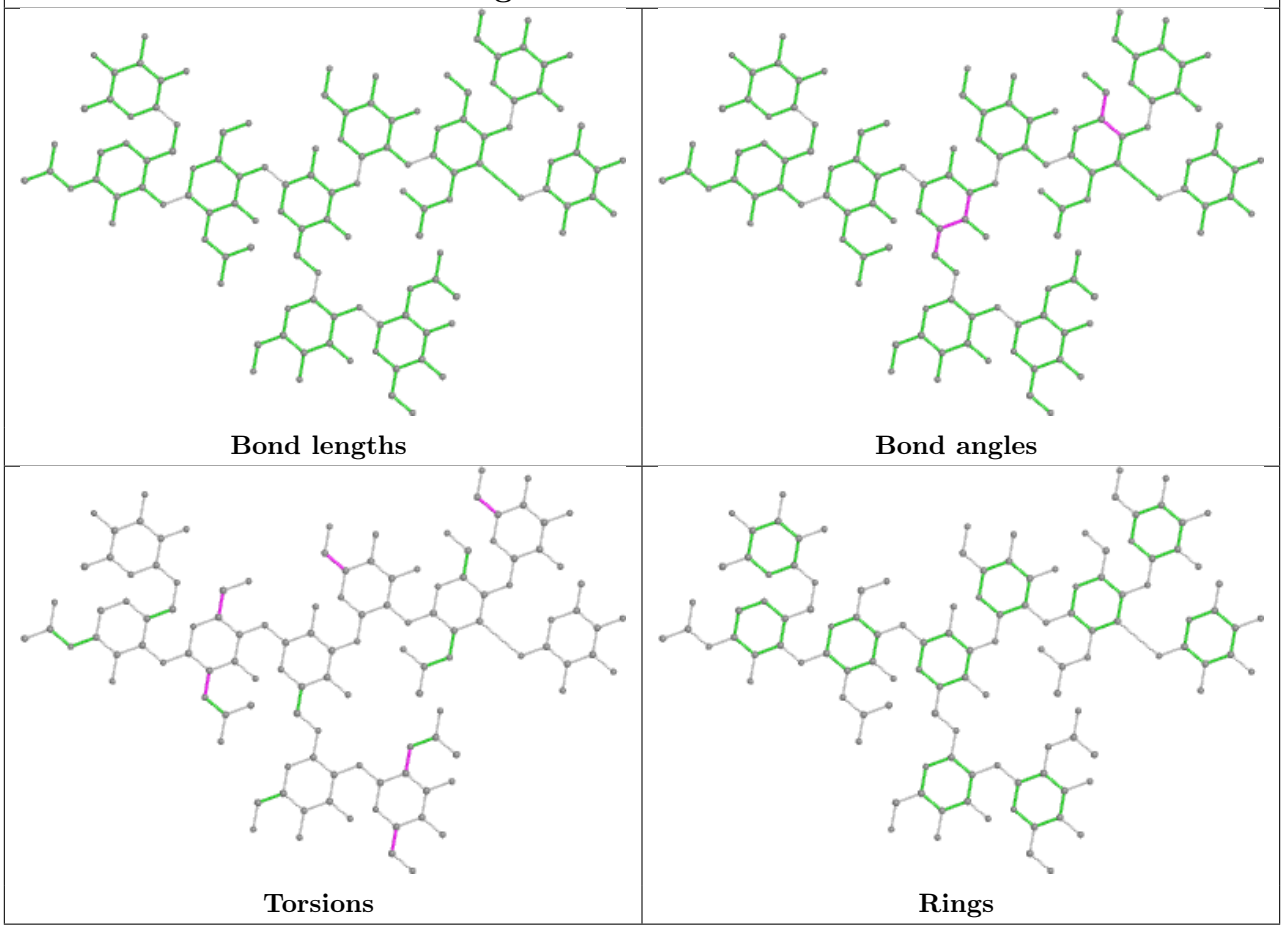
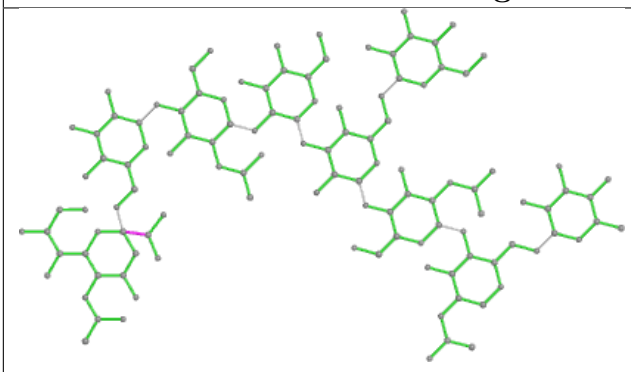
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	5	NAG	1	0
5	L	1	NAG	2	0
5	L	2	NAG	1	0

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

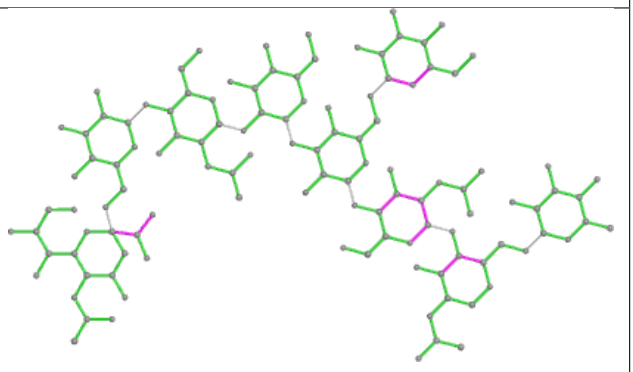
Oligosaccharide Chain G



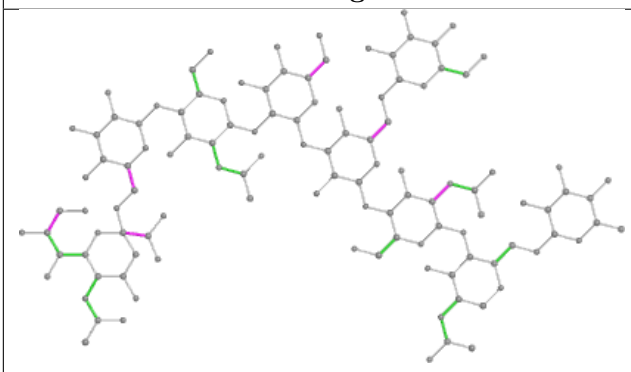
Oligosaccharide Chain K



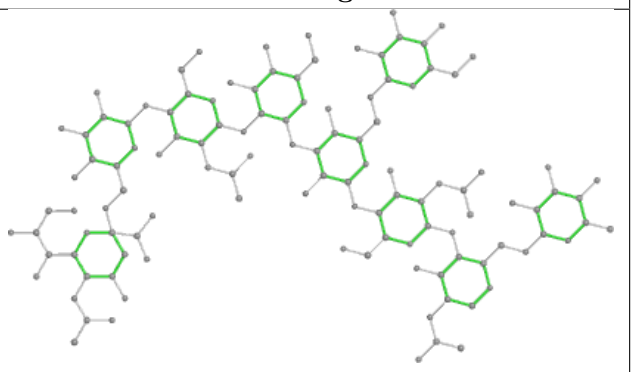
Bond lengths



Bond angles

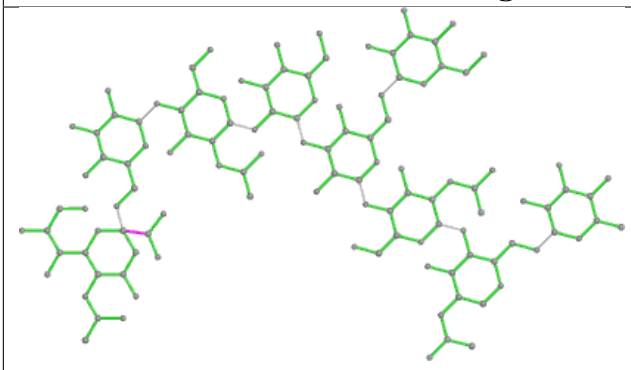


Torsions

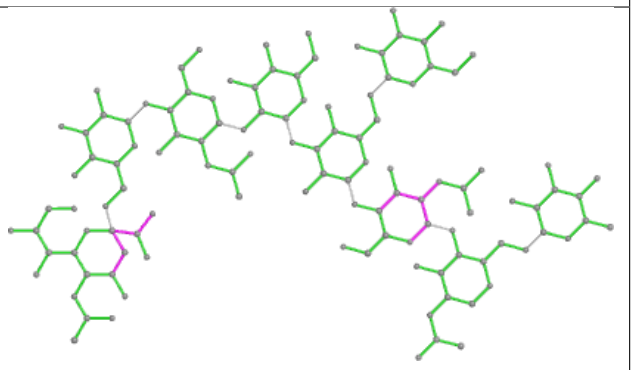


Rings

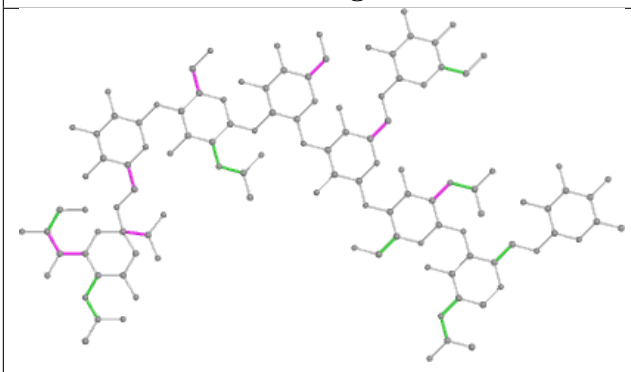
Oligosaccharide Chain L



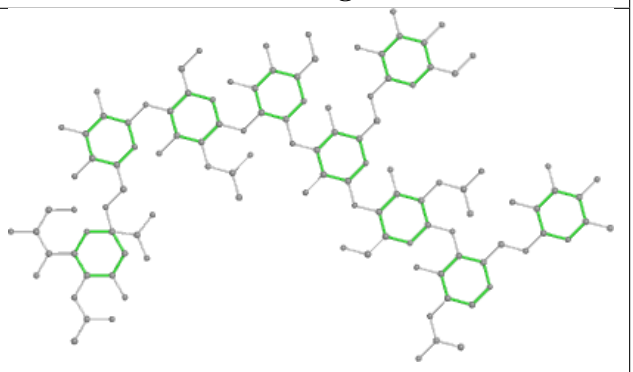
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
8	MPD	E	303	-	7,7,7	0.52	0	9,10,10	0.38	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
8	MPD	E	303	-	-	1/5/5/5	-

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
8	E	303	MPD	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	303	MPD	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

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.