Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 04:45 PM EST

PDB ID	:	1NMU
Title	:	MBP-L30
Authors	:	Chao, J.A.; Prasad, G.S.; White, S.A.; Stout, C.D.; Williamson, J.R.
Deposited on	:	2003-01-10
Resolution	:	2.31 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:

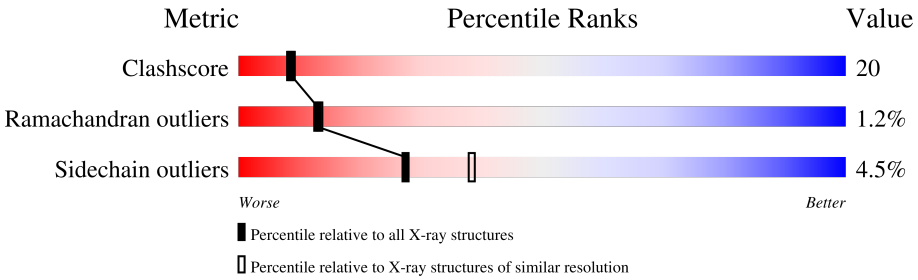
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.31 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	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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	382	73% 22%
1	C	382	71% 24%
2	B	104	62% 35%
2	D	104	31% 56% 12%
3	E	4	25% 75%
3	F	4	25% 75%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7593 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 maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2843	1828	463	546	6			
1	C	368	Total	C	N	O	S	0	0	0
			2843	1828	463	546	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P02928
A	367	ASN	-	cloning artifact	UNP P02928
A	368	SER	-	cloning artifact	UNP P02928
A	369	SER	-	cloning artifact	UNP P02928
A	370	SER	-	cloning artifact	UNP P02928
A	371	VAL	-	cloning artifact	UNP P02928
A	372	PRO	-	cloning artifact	UNP P02928
A	373	GLY	-	cloning artifact	UNP P02928
A	374	ARG	-	cloning artifact	UNP P02928
A	375	GLY	-	cloning artifact	UNP P02928
A	376	SER	-	cloning artifact	UNP P02928
A	377	ILE	-	cloning artifact	UNP P02928
A	378	GLU	-	cloning artifact	UNP P02928
A	379	GLY	-	cloning artifact	UNP P02928
A	380	ARG	-	cloning artifact	UNP P02928
A	381	ALA	-	cloning artifact	UNP P02928
C	0	MET	-	initiating methionine	UNP P02928
C	367	ASN	-	cloning artifact	UNP P02928
C	368	SER	-	cloning artifact	UNP P02928
C	369	SER	-	cloning artifact	UNP P02928
C	370	SER	-	cloning artifact	UNP P02928
C	371	VAL	-	cloning artifact	UNP P02928
C	372	PRO	-	cloning artifact	UNP P02928
C	373	GLY	-	cloning artifact	UNP P02928
C	374	ARG	-	cloning artifact	UNP P02928

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Chain	Residue	Modelled	Actual	Comment	Reference
C	375	GLY	-	cloning artifact	UNP P02928
C	376	SER	-	cloning artifact	UNP P02928
C	377	ILE	-	cloning artifact	UNP P02928
C	378	GLU	-	cloning artifact	UNP P02928
C	379	GLY	-	cloning artifact	UNP P02928
C	380	ARG	-	cloning artifact	UNP P02928
C	381	ALA	-	cloning artifact	UNP P02928

- Molecule 2 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			795	511	133	150	1			
2	D	103	Total	C	N	O	S	0	0	0
			790	508	132	149	1			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	4	Total	C	O	0	0	0
			45	24	21			
3	F	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	26	Total	O	0	0
			26	26		
4	C	75	Total	O	0	0
			75	75		
4	D	1	Total	O	0	0
			1	1		

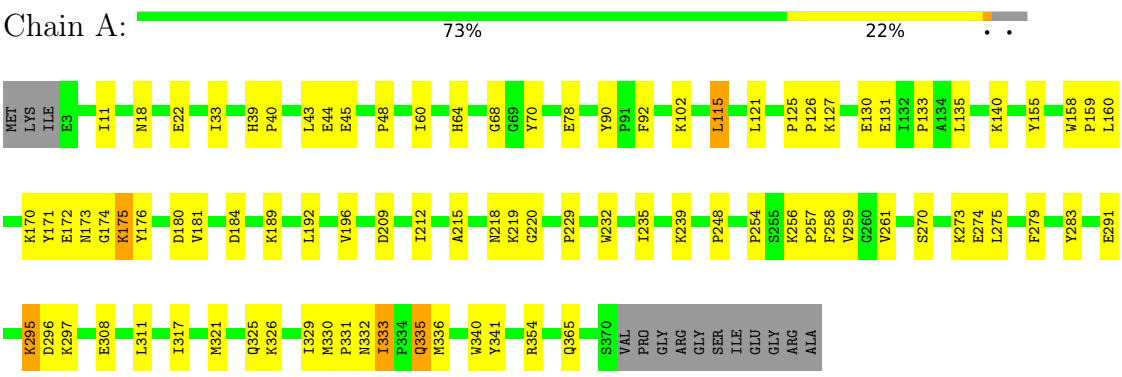
3 Residue-property plots (i)

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.

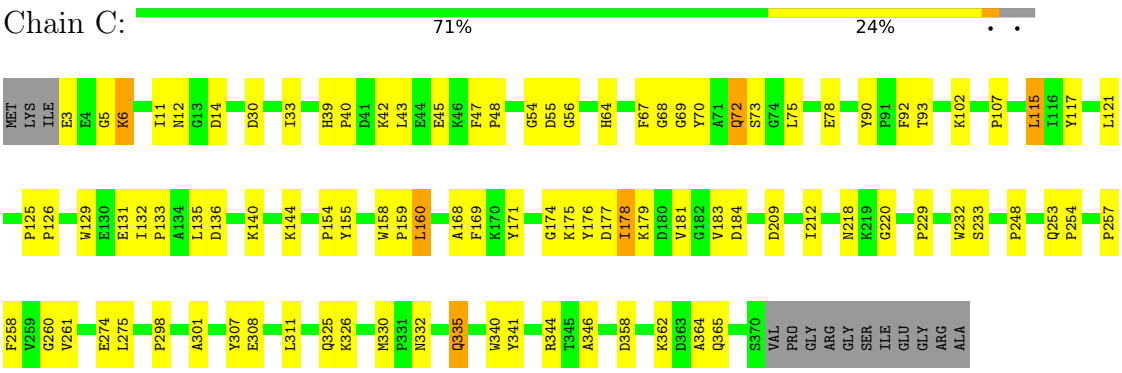
• Molecule 1: maltose-binding periplasmic protein

Chain A:



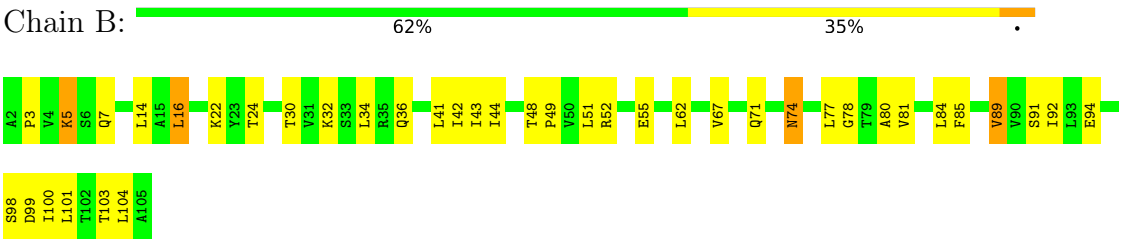
• Molecule 1: maltose-binding periplasmic protein

Chain C:



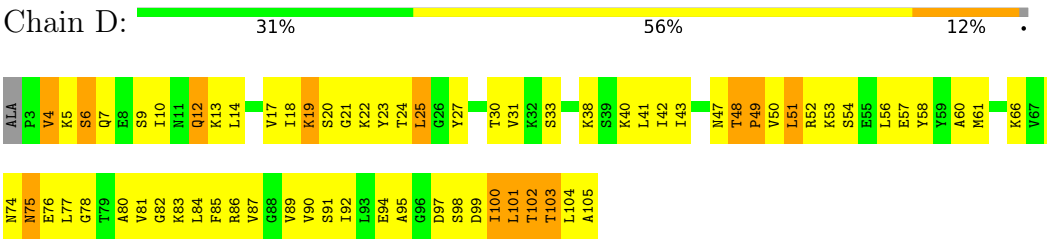
• Molecule 2: 60S ribosomal protein L30

Chain B:



• Molecule 2: 60S ribosomal protein L30

Chain D:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.65Å 118.39Å 153.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.31	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-2.31)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7593	wwPDB-VP
Average B, all atoms (Å^2)	50.0	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: GLC

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	0.36	0/2912	0.59	0/3955
1	C	0.34	0/2912	0.57	0/3955
2	B	0.36	0/804	0.66	0/1080
2	D	0.31	0/799	0.54	0/1072
All	All	0.35	0/7427	0.59	0/10062

There are no bond length outliers.

There are no bond angle outliers.

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	2843	0	2801	78	0
1	C	2843	0	2801	91	0
2	B	795	0	850	36	0
2	D	790	0	846	105	0
3	E	45	0	38	7	0
3	F	45	0	39	7	0
4	A	130	0	0	4	0
4	B	26	0	0	0	0
4	C	75	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	7593	0	7375	302	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 (302) 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:155:TYR:HB2	3:E:3:GLC:H62	1.28	1.14
2:D:20:SER:HB2	2:D:97:ASP:H	1.20	1.06
1:C:335:GLN:H	1:C:335:GLN:NE2	1.60	0.99
1:A:64:HIS:HD2	1:A:261:VAL:H	1.12	0.97
1:C:155:TYR:HB2	3:F:3:GLC:H62	1.47	0.96
1:C:335:GLN:H	1:C:335:GLN:HE21	1.16	0.92
1:A:335:GLN:NE2	1:A:335:GLN:H	1.68	0.91
2:D:101:LEU:HD22	2:D:101:LEU:H	1.35	0.91
2:B:22:LYS:HD2	2:B:94:GLU:HG3	1.53	0.91
1:A:181:VAL:HB	1:A:365:GLN:HE22	1.40	0.86
1:A:90:TYR:HE1	1:A:308:GLU:HG2	1.40	0.86
2:D:5:LYS:HB2	2:D:71:GLN:HE21	1.41	0.85
1:C:209:ASP:OD1	1:C:212:ILE:HG12	1.78	0.83
2:D:20:SER:HB2	2:D:97:ASP:N	1.93	0.82
2:D:75:ASN:HD22	2:D:76:GLU:H	1.29	0.81
1:C:68:GLY:HA3	1:C:332:ASN:O	1.81	0.81
1:A:155:TYR:CB	3:E:3:GLC:H62	2.11	0.80
2:D:33:SER:HA	2:D:38:LYS:HE2	1.63	0.80
2:D:13:LYS:HG3	2:D:100:ILE:HG22	1.63	0.79
1:C:64:HIS:HD2	1:C:261:VAL:H	1.29	0.79
2:D:104:LEU:HD12	2:D:104:LEU:H	1.48	0.78
2:D:95:ALA:HB3	2:D:101:LEU:HD21	1.65	0.78
1:A:335:GLN:H	1:A:335:GLN:HE21	1.29	0.78
2:D:102:THR:HG22	2:D:103:THR:H	1.49	0.76
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.20	0.76
1:A:181:VAL:HB	1:A:365:GLN:NE2	2.00	0.76
1:A:155:TYR:HB2	3:E:3:GLC:C6	2.13	0.76
1:A:90:TYR:CE1	1:A:308:GLU:HG2	2.21	0.75
1:C:33:ILE:HD13	1:C:275:LEU:HD13	1.67	0.75
2:B:103:THR:HG23	2:B:104:LEU:HD13	1.68	0.74
1:A:175:LYS:HE2	1:A:175:LYS:HA	1.68	0.74
1:C:184:ASP:HB2	1:C:365:GLN:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:LEU:HD23	2:D:42:ILE:N	2.03	0.74
2:D:41:LEU:HD23	2:D:42:ILE:H	1.54	0.72
2:D:74:ASN:ND2	2:D:86:ARG:HD3	2.05	0.71
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.72	0.71
1:C:181:VAL:HB	1:C:365:GLN:HE22	1.57	0.70
2:D:74:ASN:HD22	2:D:86:ARG:HB3	1.56	0.69
2:B:48:THR:HG23	2:B:51:LEU:HB2	1.75	0.69
2:D:75:ASN:ND2	2:D:76:GLU:H	1.90	0.69
1:C:181:VAL:HB	1:C:365:GLN:NE2	2.08	0.68
2:D:95:ALA:CB	2:D:101:LEU:HD21	2.23	0.68
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.29	0.67
2:D:6:SER:O	2:D:7:GLN:HG3	1.93	0.67
2:D:51:LEU:HA	2:D:54:SER:OG	1.94	0.67
2:D:9:SER:O	2:D:12:GLN:HG3	1.96	0.66
2:D:54:SER:HA	2:D:57:GLU:OE2	1.94	0.66
2:B:32:LYS:HE2	2:B:36:GLN:HE22	1.59	0.66
2:B:41:LEU:HD12	2:B:92:ILE:HD13	1.78	0.66
1:C:178:ILE:HD13	1:C:178:ILE:H	1.60	0.65
1:C:42:LYS:HE2	3:F:1:GLC:O2	1.96	0.65
2:D:43:ILE:HB	2:D:90:VAL:CG1	2.26	0.65
2:D:24:THR:HG23	2:D:91:SER:HB3	1.77	0.65
1:A:43:LEU:CD1	1:A:60:ILE:HD11	2.26	0.65
2:B:7:GLN:NE2	2:B:77:LEU:HD23	2.11	0.65
1:C:3:GLU:CB	1:C:6:LYS:HE3	2.26	0.64
2:D:77:LEU:O	2:D:81:VAL:HG23	1.97	0.64
2:D:99:ASP:OD2	2:D:104:LEU:HD21	1.98	0.64
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.63	0.64
1:C:178:ILE:HD13	1:C:178:ILE:N	2.13	0.64
1:A:45:GLU:O	1:A:48:PRO:HD2	1.98	0.63
1:A:335:GLN:NE2	1:A:335:GLN:N	2.45	0.63
1:A:209:ASP:OD1	1:A:212:ILE:HG12	1.97	0.63
2:D:83:LYS:HG2	2:D:85:PHE:CZ	2.34	0.63
1:A:64:HIS:CD2	1:A:261:VAL:H	2.04	0.63
1:C:340:TRP:HB3	3:F:2:GLC:H62	1.81	0.62
1:A:64:HIS:HE1	1:A:330:MET:O	1.82	0.62
2:D:75:ASN:HD22	2:D:75:ASN:N	1.96	0.62
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.64	0.62
2:D:50:VAL:C	2:D:52:ARG:H	2.02	0.61
1:A:68:GLY:HA3	1:A:332:ASN:O	2.01	0.61
1:C:335:GLN:NE2	1:C:335:GLN:N	2.40	0.61
1:A:40:PRO:HB3	1:C:253:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:PRO:HB2	2:D:52:ARG:HB2	1.83	0.60
2:B:99:ASP:O	2:B:103:THR:HG22	2.02	0.60
1:A:140:LYS:HE2	4:A:506:HOH:O	2.00	0.60
1:A:295:LYS:HA	1:A:295:LYS:HE3	1.84	0.60
2:D:100:ILE:HA	2:D:104:LEU:HD22	1.83	0.60
2:B:100:ILE:HG13	2:B:104:LEU:HD22	1.84	0.60
2:D:27:TYR:O	2:D:31:VAL:HG23	2.02	0.59
2:B:52:ARG:HD2	2:B:55:GLU:OE1	2.01	0.59
2:D:5:LYS:HD2	2:D:68:TYR:CE1	2.38	0.59
2:D:101:LEU:H	2:D:101:LEU:CD2	2.14	0.58
2:B:5:LYS:HB2	2:B:5:LYS:NZ	2.17	0.58
1:C:64:HIS:CD2	1:C:261:VAL:H	2.18	0.58
2:D:19:LYS:HB2	2:D:19:LYS:NZ	2.19	0.58
1:A:296:ASP:O	1:A:297:LYS:HD3	2.04	0.58
1:C:358:ASP:O	1:C:362:LYS:HG3	2.04	0.58
1:C:115:LEU:HG	1:C:248:PRO:HD3	1.86	0.57
1:C:64:HIS:HE1	1:C:330:MET:O	1.87	0.57
1:A:43:LEU:HD13	1:A:60:ILE:HD11	1.85	0.57
2:D:102:THR:HB	2:D:104:LEU:CD1	2.35	0.57
1:C:40:PRO:HG2	1:C:43:LEU:HB3	1.85	0.57
2:D:50:VAL:HG12	2:D:51:LEU:HD13	1.85	0.57
1:A:333:ILE:HG12	1:A:335:GLN:HE21	1.69	0.57
1:A:48:PRO:HG3	1:A:70:TYR:HE1	1.68	0.57
2:B:32:LYS:CE	2:B:36:GLN:HE22	2.18	0.57
2:D:75:ASN:ND2	2:D:75:ASN:N	2.53	0.57
1:A:295:LYS:HE3	1:A:295:LYS:CA	2.35	0.56
1:C:171:TYR:OH	1:C:174:GLY:HA2	2.05	0.56
1:C:346:ALA:HB2	1:C:364:ALA:HB2	1.87	0.56
1:A:126:PRO:HB3	1:A:131:GLU:HG3	1.86	0.56
1:A:130:GLU:O	1:A:133:PRO:HD2	2.04	0.56
2:D:43:ILE:HB	2:D:90:VAL:HG13	1.87	0.56
1:C:218:ASN:N	1:C:218:ASN:HD22	2.02	0.56
1:C:54:GLY:HA3	2:D:53:LYS:NZ	2.21	0.55
2:D:14:LEU:HD12	2:D:14:LEU:C	2.26	0.55
2:D:25:LEU:HD11	2:D:81:VAL:HG11	1.88	0.55
2:D:100:ILE:HD13	2:D:101:LEU:HD22	1.88	0.55
2:D:25:LEU:N	2:D:25:LEU:HD22	2.21	0.55
2:D:13:LYS:CG	2:D:100:ILE:HG22	2.36	0.55
1:C:155:TYR:CB	3:F:3:GLC:H62	2.29	0.55
1:C:335:GLN:HE21	1:C:335:GLN:N	1.96	0.55
2:D:84:LEU:N	2:D:84:LEU:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HD13	1:C:275:LEU:CD1	2.37	0.54
1:A:78:GLU:OE1	1:A:102:LYS:HD2	2.07	0.54
1:C:155:TYR:HB2	3:F:3:GLC:C6	2.30	0.54
2:D:24:THR:CG2	2:D:91:SER:HB3	2.37	0.54
2:D:104:LEU:H	2:D:104:LEU:CD1	2.19	0.54
2:D:5:LYS:HB2	2:D:71:GLN:NE2	2.15	0.54
2:D:75:ASN:HD22	2:D:76:GLU:N	2.00	0.54
2:B:14:LEU:HB3	2:B:80:ALA:HB1	1.88	0.54
1:C:311:LEU:N	1:C:311:LEU:HD12	2.22	0.54
2:D:43:ILE:O	2:D:89:VAL:HA	2.08	0.54
1:A:170:LYS:HD3	1:A:180:ASP:OD1	2.08	0.54
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.08	0.54
1:C:47:PHE:HB3	1:C:48:PRO:HD3	1.91	0.53
1:C:75:LEU:HD11	2:D:4:VAL:HG13	1.90	0.53
1:A:184:ASP:O	1:A:189:LYS:HE3	2.08	0.53
1:C:178:ILE:H	1:C:178:ILE:CD1	2.20	0.53
2:D:102:THR:HB	2:D:104:LEU:HD13	1.89	0.53
1:C:171:TYR:HB2	1:C:176:TYR:CE1	2.44	0.53
1:A:175:LYS:HE2	1:A:176:TYR:H	1.74	0.53
1:A:192:LEU:O	1:A:196:VAL:HG23	2.08	0.53
2:B:74:ASN:HB2	2:B:85:PHE:CE2	2.44	0.53
1:C:136:ASP:OD1	1:C:140:LYS:HE2	2.09	0.53
2:D:100:ILE:HD13	2:D:100:ILE:N	2.24	0.53
1:A:239:LYS:HA	1:A:239:LYS:HZ3	1.73	0.52
2:B:74:ASN:HD22	2:B:77:LEU:HD12	1.75	0.52
2:D:74:ASN:HD21	2:D:86:ARG:HD3	1.75	0.52
1:A:64:HIS:HD2	1:A:261:VAL:N	1.93	0.52
2:B:77:LEU:HB3	2:B:81:VAL:HG13	1.89	0.52
1:C:90:TYR:HE1	1:C:308:GLU:HG2	1.73	0.52
1:C:45:GLU:O	1:C:48:PRO:HD2	2.10	0.52
2:D:13:LYS:HG3	2:D:100:ILE:CG2	2.36	0.52
1:C:307:TYR:CE1	1:C:311:LEU:HD11	2.45	0.51
2:B:48:THR:HG22	2:B:51:LEU:HD22	1.93	0.51
2:D:86:ARG:HG3	2:D:86:ARG:HH11	1.76	0.51
2:D:43:ILE:HD12	2:D:43:ILE:N	2.26	0.51
1:A:354:ARG:HD3	1:A:354:ARG:O	2.11	0.50
1:C:232:TRP:HB2	1:C:298:PRO:HG2	1.93	0.50
1:C:307:TYR:O	1:C:311:LEU:HD13	2.11	0.50
1:A:239:LYS:HA	1:A:239:LYS:NZ	2.26	0.50
1:C:55:ASP:CG	1:C:56:GLY:H	2.14	0.50
2:B:43:ILE:HD12	2:B:92:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:HD2	1:A:326:LYS:O	2.12	0.50
1:A:43:LEU:HD13	1:A:60:ILE:CD1	2.42	0.49
1:A:220:GLY:HA2	4:A:383:HOH:O	2.11	0.49
2:D:78:GLY:N	2:D:87:VAL:HG22	2.27	0.49
1:C:177:ASP:OD1	1:C:179:LYS:HB2	2.12	0.49
1:C:274:GLU:OE1	1:C:274:GLU:HA	2.11	0.49
2:D:66:LYS:HD3	2:D:105:ALA:O	2.12	0.49
2:B:41:LEU:HD13	2:B:42:ILE:N	2.27	0.49
2:D:17:VAL:HG22	2:D:98:SER:CB	2.41	0.49
2:D:27:TYR:HB2	2:D:52:ARG:HH22	1.77	0.49
1:C:75:LEU:HD11	2:D:4:VAL:CG1	2.43	0.49
1:C:78:GLU:OE1	1:C:102:LYS:HD2	2.12	0.49
1:A:259:VAL:HB	1:A:329:ILE:HA	1.94	0.49
2:B:92:ILE:N	2:B:92:ILE:HD12	2.27	0.49
1:C:126:PRO:HB3	1:C:131:GLU:CG	2.42	0.49
2:D:18:ILE:HD11	2:D:81:VAL:HA	1.95	0.49
2:D:75:ASN:ND2	2:D:76:GLU:N	2.60	0.49
2:D:30:THR:HG23	2:D:42:ILE:HD12	1.95	0.49
2:D:77:LEU:HD22	2:D:87:VAL:CG2	2.43	0.49
1:C:220:GLY:HA2	4:C:425:HOH:O	2.13	0.48
2:D:14:LEU:HD11	2:D:80:ALA:O	2.13	0.48
2:D:41:LEU:HD22	2:D:43:ILE:CD1	2.43	0.48
1:A:18:ASN:O	1:A:22:GLU:HG2	2.13	0.48
1:A:341:TYR:HE2	3:E:1:GLC:H61	1.78	0.48
2:D:21:GLY:HA3	2:D:94:GLU:O	2.13	0.48
2:D:101:LEU:HD22	2:D:101:LEU:N	2.16	0.48
2:B:41:LEU:CD1	2:B:43:ILE:HG13	2.44	0.48
1:C:307:TYR:CZ	1:C:311:LEU:HD11	2.48	0.48
2:D:82:GLY:C	2:D:83:LYS:HD2	2.33	0.48
1:A:33:ILE:HD13	1:A:275:LEU:CD1	2.41	0.48
2:D:102:THR:HG22	2:D:103:THR:N	2.23	0.48
1:A:274:GLU:HB2	4:A:416:HOH:O	2.15	0.47
1:A:44:GLU:OE2	3:E:2:GLC:H2	2.13	0.47
2:D:49:PRO:HB2	2:D:52:ARG:CB	2.44	0.47
1:A:92:PHE:CZ	1:A:329:ILE:HD12	2.50	0.47
1:A:333:ILE:HD13	1:A:336:MET:HG2	1.97	0.47
1:C:6:LYS:HA	1:C:33:ILE:HG23	1.96	0.47
1:C:93:THR:HB	1:C:107:PRO:HB3	1.97	0.47
1:C:126:PRO:HG3	1:C:135:LEU:HD22	1.97	0.47
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.49	0.47
2:D:77:LEU:HD22	2:D:87:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:CD1	1:A:275:LEU:HD22	2.45	0.47
1:A:127:LYS:NZ	1:A:127:LYS:HB3	2.30	0.46
1:A:170:LYS:HD2	1:A:172:GLU:OE1	2.15	0.46
1:C:159:PRO:HG3	1:C:257:PRO:HA	1.97	0.46
2:D:33:SER:HA	2:D:38:LYS:CE	2.42	0.46
2:B:41:LEU:HD11	2:B:43:ILE:HG13	1.97	0.46
2:D:50:VAL:C	2:D:52:ARG:N	2.68	0.46
1:A:127:LYS:HG3	4:A:471:HOH:O	2.16	0.46
1:A:126:PRO:HG3	1:A:135:LEU:HD22	1.98	0.46
1:A:11:ILE:O	1:A:39:HIS:HA	2.16	0.46
1:C:40:PRO:HG2	1:C:43:LEU:CB	2.47	0.45
2:B:74:ASN:HA	2:B:77:LEU:HD11	1.97	0.45
2:B:78:GLY:H	2:B:81:VAL:CG1	2.29	0.45
2:D:41:LEU:HD22	2:D:43:ILE:HD12	1.98	0.45
2:D:41:LEU:HD11	2:D:105:ALA:HB3	1.97	0.45
2:D:50:VAL:O	2:D:52:ARG:N	2.49	0.45
2:D:47:ASN:O	2:D:48:THR:O	2.35	0.45
2:D:27:TYR:CE1	2:D:31:VAL:HG21	2.51	0.45
1:C:154:PRO:HD3	1:C:344:ARG:HG3	1.99	0.45
2:B:48:THR:CG2	2:B:51:LEU:HB2	2.44	0.45
2:D:75:ASN:ND2	2:D:75:ASN:H	2.15	0.45
1:A:279:PHE:O	1:A:283:TYR:HB2	2.18	0.44
1:C:69:GLY:O	1:C:72:GLN:HB3	2.16	0.44
1:C:340:TRP:HB3	3:F:2:GLC:C6	2.47	0.44
2:D:27:TYR:HB2	2:D:52:ARG:NH2	2.32	0.44
2:D:56:LEU:O	2:D:60:ALA:HB2	2.16	0.44
1:A:175:LYS:HE2	1:A:175:LYS:CA	2.45	0.44
2:D:19:LYS:HB2	2:D:19:LYS:HZ3	1.79	0.44
2:D:95:ALA:HB1	2:D:98:SER:OG	2.18	0.44
1:C:67:PHE:CD1	1:C:67:PHE:N	2.85	0.44
1:C:73:SER:HB3	2:D:4:VAL:HG12	1.99	0.44
1:C:129:TRP:CE2	1:C:160:LEU:HG	2.53	0.44
1:C:132:ILE:N	1:C:133:PRO:CD	2.81	0.44
2:D:81:VAL:HG12	2:D:81:VAL:O	2.17	0.44
1:C:260:GLY:HA2	1:C:330:MET:HE2	2.00	0.44
1:A:175:LYS:CE	1:A:176:TYR:H	2.31	0.44
1:C:12:ASN:HD22	1:C:14:ASP:CG	2.21	0.44
2:D:17:VAL:HA	2:D:20:SER:OG	2.18	0.44
2:B:30:THR:HG23	2:B:91:SER:HB2	1.99	0.43
2:B:103:THR:HG23	2:B:104:LEU:CD1	2.43	0.43
2:B:16:LEU:HD13	2:B:98:SER:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:THR:OG1	2:B:91:SER:HB3	2.18	0.43
1:C:169:PHE:CD1	1:C:178:ILE:HA	2.53	0.43
1:A:270:SER:O	1:A:273:LYS:NZ	2.51	0.43
1:A:331:PRO:HD2	1:A:336:MET:SD	2.58	0.43
2:D:87:VAL:HG23	2:D:87:VAL:O	2.18	0.43
1:A:43:LEU:C	1:A:43:LEU:HD12	2.38	0.43
2:B:62:LEU:HA	1:C:92:PHE:HB3	2.00	0.43
1:C:218:ASN:N	1:C:218:ASN:ND2	2.67	0.43
1:C:274:GLU:HB2	4:C:457:HOH:O	2.18	0.43
2:D:41:LEU:HD11	2:D:105:ALA:CB	2.48	0.43
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.53	0.43
1:A:158:TRP:N	1:A:159:PRO:CD	2.82	0.43
2:D:17:VAL:CG2	2:D:100:ILE:HD12	2.49	0.43
2:D:40:LYS:HB2	2:D:92:ILE:O	2.19	0.43
2:D:74:ASN:HD22	2:D:86:ARG:CB	2.30	0.43
1:A:33:ILE:HD13	1:A:275:LEU:HD22	2.00	0.43
1:A:254:PRO:HB3	1:A:326:LYS:HD3	2.00	0.43
2:D:58:TYR:O	2:D:61:MET:HB3	2.18	0.43
1:A:125:PRO:HA	1:A:126:PRO:HD3	1.81	0.42
1:C:181:VAL:HG12	1:C:183:VAL:HG13	2.01	0.42
1:C:254:PRO:HB3	1:C:326:LYS:HD3	2.01	0.42
1:C:311:LEU:N	1:C:311:LEU:CD1	2.82	0.42
2:B:44:ILE:HG12	2:B:89:VAL:HG13	2.01	0.42
1:C:140:LYS:HD3	1:C:144:LYS:O	2.18	0.42
1:A:317:ILE:O	1:A:321:MET:HG2	2.19	0.42
2:B:3:PRO:HB3	2:B:71:GLN:HE22	1.84	0.42
1:C:11:ILE:O	1:C:39:HIS:HA	2.18	0.42
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.91	0.42
1:C:54:GLY:HA3	2:D:53:LYS:HZ2	1.83	0.42
1:C:301:ALA:HA	4:C:402:HOH:O	2.18	0.42
2:D:18:ILE:HG23	2:D:23:TYR:CZ	2.54	0.42
1:A:340:TRP:HB3	3:E:2:GLC:C6	2.48	0.42
2:B:3:PRO:CB	2:B:71:GLN:HE22	2.32	0.42
1:C:117:TYR:CE2	1:C:125:PRO:HD3	2.54	0.42
1:C:33:ILE:CD1	1:C:275:LEU:HD22	2.50	0.42
1:C:178:ILE:N	1:C:178:ILE:CD1	2.79	0.42
2:D:47:ASN:OD1	2:D:48:THR:N	2.52	0.42
2:D:82:GLY:O	2:D:83:LYS:HD2	2.19	0.42
2:D:99:ASP:CG	2:D:104:LEU:HD21	2.40	0.42
2:D:104:LEU:HD12	2:D:104:LEU:N	2.27	0.42
1:A:115:LEU:HG	1:A:248:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ASN:O	2:D:48:THR:C	2.57	0.42
1:A:159:PRO:HG3	1:A:257:PRO:HA	2.00	0.41
1:C:125:PRO:HA	1:C:126:PRO:HD3	1.83	0.41
1:A:215:ALA:O	1:A:219:LYS:HG3	2.19	0.41
1:A:291:GLU:HG3	1:A:295:LYS:HD2	2.01	0.41
1:A:340:TRP:HB3	3:E:2:GLC:H62	2.02	0.41
1:C:126:PRO:HB3	1:C:131:GLU:HG3	2.02	0.41
1:C:168:ALA:O	1:C:181:VAL:HA	2.20	0.41
1:C:177:ASP:C	1:C:179:LYS:H	2.24	0.41
2:B:16:LEU:HD23	2:B:16:LEU:HA	1.90	0.41
2:B:62:LEU:HA	1:C:92:PHE:CB	2.51	0.41
2:D:74:ASN:ND2	2:D:86:ARG:HB3	2.30	0.41
1:A:39:HIS:ND1	1:A:39:HIS:O	2.54	0.41
1:C:6:LYS:HA	1:C:33:ILE:CG2	2.50	0.41
1:C:158:TRP:N	1:C:159:PRO:CD	2.84	0.41
1:C:341:TYR:HE2	3:F:1:GLC:H62	1.85	0.41
2:D:99:ASP:O	2:D:104:LEU:HD13	2.20	0.41
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.86	0.41
1:C:171:TYR:CE1	1:C:175:LYS:N	2.89	0.40
1:A:295:LYS:HE3	1:A:295:LYS:N	2.36	0.40
2:B:32:LYS:CE	2:B:36:GLN:NE2	2.84	0.40
2:B:103:THR:O	2:B:104:LEU:HD12	2.20	0.40
2:D:22:LYS:N	2:D:94:GLU:O	2.54	0.40
2:D:17:VAL:HG22	2:D:98:SER:OG	2.21	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	366/382 (96%)	355 (97%)	10 (3%)	1 (0%)	41 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	366/382 (96%)	346 (94%)	19 (5%)	1 (0%)	41 50
2	B	102/104 (98%)	96 (94%)	5 (5%)	1 (1%)	15 17
2	D	101/104 (97%)	80 (79%)	13 (13%)	8 (8%)	1 0
All	All	935/972 (96%)	877 (94%)	47 (5%)	11 (1%)	13 13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	49	PRO
2	D	4	VAL
2	D	48	THR
2	D	102	THR
1	A	173	ASN
1	C	5	GLY
2	D	49	PRO
2	D	51	LEU
2	D	103	THR
2	D	10	ILE
2	D	6	SER

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	293/305 (96%)	283 (97%)	10 (3%)	37 51
1	C	293/305 (96%)	283 (97%)	10 (3%)	37 51
2	B	87/87 (100%)	79 (91%)	8 (9%)	9 10
2	D	87/87 (100%)	81 (93%)	6 (7%)	15 20
All	All	760/784 (97%)	726 (96%)	34 (4%)	27 38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	121	LEU
1	A	160	LEU
1	A	175	LYS
1	A	258	PHE
1	A	295	LYS
1	A	311	LEU
1	A	325	GLN
1	A	333	ILE
1	A	335	GLN
2	B	5	LYS
2	B	16	LEU
2	B	34	LEU
2	B	67	VAL
2	B	74	ASN
2	B	84	LEU
2	B	89	VAL
2	B	101	LEU
1	C	6	LYS
1	C	30	ASP
1	C	72	GLN
1	C	115	LEU
1	C	160	LEU
1	C	178	ILE
1	C	233	SER
1	C	258	PHE
1	C	325	GLN
1	C	335	GLN
2	D	12	GLN
2	D	19	LYS
2	D	25	LEU
2	D	75	ASN
2	D	100	ILE
2	D	101	LEU

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

Mol	Chain	Res	Type
1	A	64	HIS
1	A	100	ASN
1	A	173	ASN
1	A	201	ASN
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	325	GLN
1	A	335	GLN
1	A	367	ASN
2	B	36	GLN
2	B	71	GLN
2	B	74	ASN
1	C	64	HIS
1	C	72	GLN
1	C	100	ASN
1	C	173	ASN
1	C	201	ASN
1	C	218	ASN
1	C	325	GLN
1	C	335	GLN
1	C	367	ASN
2	D	12	GLN
2	D	71	GLN
2	D	75	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	E	1	3	12,12,12	0.97	1 (8%)	17,17,17	2.11	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	E	2	3	11,11,12	1.20	1 (9%)	15,15,17	3.41	8 (53%)
3	GLC	E	3	3	11,11,12	1.15	1 (9%)	15,15,17	3.38	9 (60%)
3	GLC	E	4	3	11,11,12	1.33	1 (9%)	15,15,17	2.53	5 (33%)
3	GLC	F	1	3	12,12,12	0.97	1 (8%)	17,17,17	2.10	5 (29%)
3	GLC	F	2	3	11,11,12	1.30	1 (9%)	15,15,17	3.41	8 (53%)
3	GLC	F	3	3	11,11,12	1.18	1 (9%)	15,15,17	3.29	8 (53%)
3	GLC	F	4	3	11,11,12	1.23	2 (18%)	15,15,17	2.30	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	E	1	3	-	2/2/22/22	0/1/1/1
3	GLC	E	2	3	-	2/2/19/22	0/1/1/1
3	GLC	E	3	3	-	0/2/19/22	0/1/1/1
3	GLC	E	4	3	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1
3	GLC	F	3	3	-	0/2/19/22	0/1/1/1
3	GLC	F	4	3	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	GLC	O4-C4	-2.98	1.36	1.43
3	F	4	GLC	O4-C4	-2.58	1.36	1.43
3	E	2	GLC	C4-C3	2.47	1.58	1.52
3	F	2	GLC	C4-C3	2.40	1.58	1.52
3	E	1	GLC	O3-C3	2.32	1.48	1.43
3	F	1	GLC	O3-C3	2.25	1.48	1.43
3	F	4	GLC	C2-C3	-2.25	1.49	1.52
3	F	3	GLC	C4-C5	2.21	1.57	1.53
3	E	3	GLC	C4-C5	2.20	1.57	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	GLC	C1-O5-C5	8.64	123.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	GLC	C1-O5-C5	8.54	123.77	112.19
3	E	3	GLC	C1-O5-C5	7.43	122.26	112.19
3	F	3	GLC	C1-O5-C5	7.04	121.73	112.19
3	E	3	GLC	O2-C2-C3	5.64	121.44	110.14
3	E	1	GLC	C1-O5-C5	5.64	124.31	113.66
3	F	1	GLC	C1-O5-C5	5.63	124.29	113.66
3	F	3	GLC	O2-C2-C3	5.61	121.37	110.14
3	E	4	GLC	C1-C2-C3	5.18	116.04	109.67
3	E	2	GLC	O5-C1-C2	5.14	118.70	110.77
3	E	4	GLC	C1-O5-C5	5.12	119.13	112.19
3	F	4	GLC	C1-O5-C5	5.02	119.00	112.19
3	F	3	GLC	C1-C2-C3	4.97	115.77	109.67
3	E	3	GLC	C1-C2-C3	4.82	115.59	109.67
3	F	2	GLC	O5-C1-C2	4.76	118.12	110.77
3	F	4	GLC	C1-C2-C3	4.72	115.46	109.67
3	F	2	GLC	O4-C4-C5	4.31	120.00	109.30
3	E	2	GLC	O4-C4-C5	4.27	119.90	109.30
3	E	3	GLC	O3-C3-C4	4.18	120.02	110.35
3	E	4	GLC	O2-C2-C3	4.14	118.43	110.14
3	F	3	GLC	O3-C3-C4	3.99	119.58	110.35
3	F	4	GLC	O2-C2-C3	3.96	118.07	110.14
3	E	2	GLC	C6-C5-C4	3.89	122.12	113.00
3	F	2	GLC	O5-C5-C4	-3.81	101.56	110.83
3	F	3	GLC	O5-C1-C2	3.70	116.49	110.77
3	F	2	GLC	C6-C5-C4	3.70	121.68	113.00
3	F	1	GLC	C1-C2-C3	3.69	117.98	110.31
3	E	3	GLC	O5-C1-C2	3.67	116.44	110.77
3	E	1	GLC	C1-C2-C3	3.67	117.93	110.31
3	E	2	GLC	O5-C5-C4	-3.47	102.38	110.83
3	F	2	GLC	C3-C4-C5	-2.77	105.31	110.24
3	E	3	GLC	C6-C5-C4	2.76	119.46	113.00
3	E	2	GLC	C3-C4-C5	-2.71	105.41	110.24
3	F	1	GLC	C4-C3-C2	2.70	115.54	110.82
3	F	2	GLC	O5-C5-C6	-2.70	102.97	107.20
3	E	1	GLC	C4-C3-C2	2.66	115.47	110.82
3	F	3	GLC	C6-C5-C4	2.61	119.12	113.00
3	E	4	GLC	O5-C1-C2	2.58	114.76	110.77
3	E	2	GLC	O5-C5-C6	-2.53	103.24	107.20
3	E	3	GLC	O5-C5-C6	-2.48	103.32	107.20
3	E	2	GLC	C2-C3-C4	2.47	115.16	110.89
3	F	2	GLC	C2-C3-C4	2.41	115.06	110.89
3	E	1	GLC	O1-C1-C2	2.34	115.61	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	GLC	C2-C3-C4	-2.29	106.92	110.89
3	F	1	GLC	O5-C1-C2	2.27	114.34	110.28
3	E	1	GLC	O5-C1-C2	2.23	114.27	110.28
3	E	3	GLC	C2-C3-C4	-2.16	107.15	110.89
3	E	3	GLC	O4-C4-C5	2.15	114.63	109.30
3	F	3	GLC	O5-C5-C6	-2.15	103.84	107.20
3	F	1	GLC	O1-C1-C2	2.13	115.04	109.03
3	E	4	GLC	O5-C5-C6	-2.04	104.01	107.20
3	F	4	GLC	O5-C1-C2	2.04	113.92	110.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
3	E	2	GLC	C4-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6
3	E	1	GLC	C4-C5-C6-O6

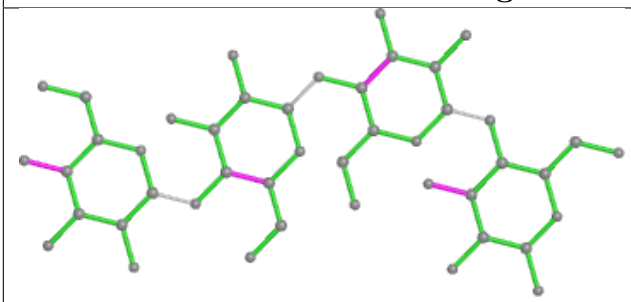
There are no ring outliers.

6 monomers are involved in 14 short contacts:

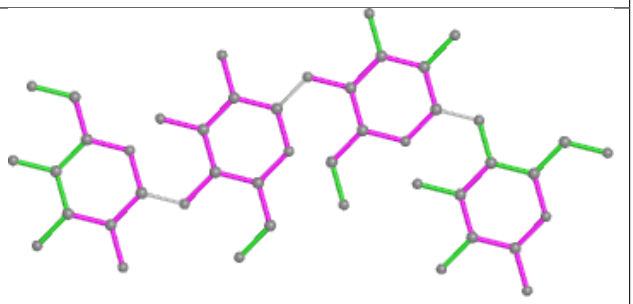
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	GLC	3	0
3	E	1	GLC	1	0
3	E	2	GLC	3	0
3	F	2	GLC	2	0
3	F	1	GLC	2	0
3	E	3	GLC	3	0

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

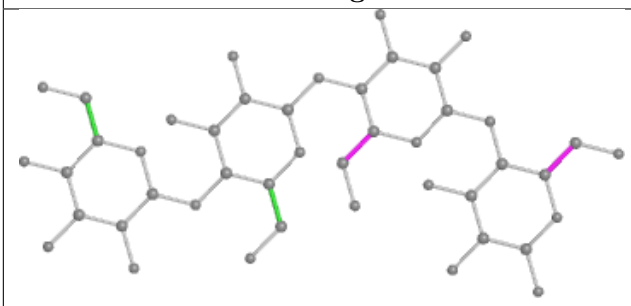
Oligosaccharide Chain E



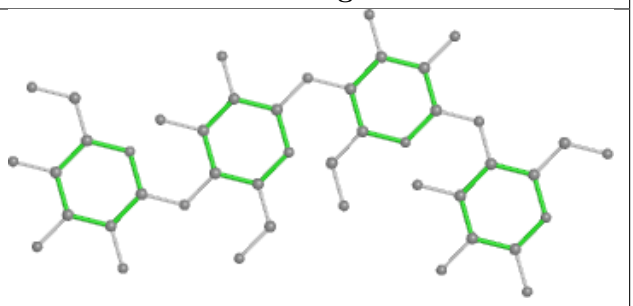
Bond lengths



Bond angles

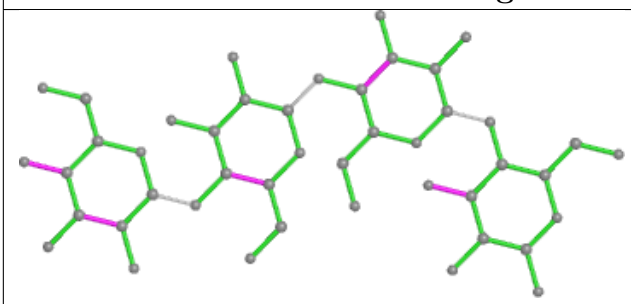


Torsions

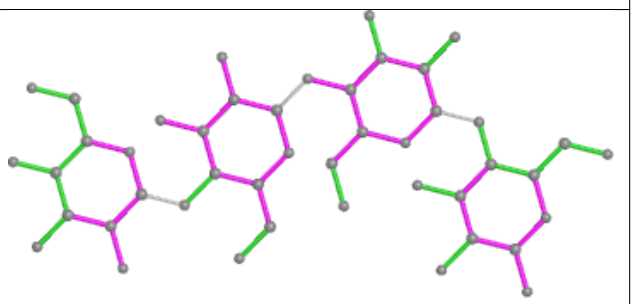


Rings

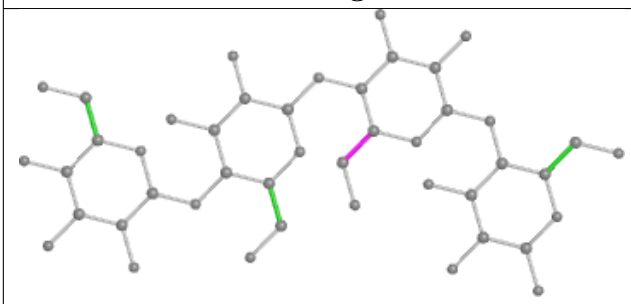
Oligosaccharide Chain F



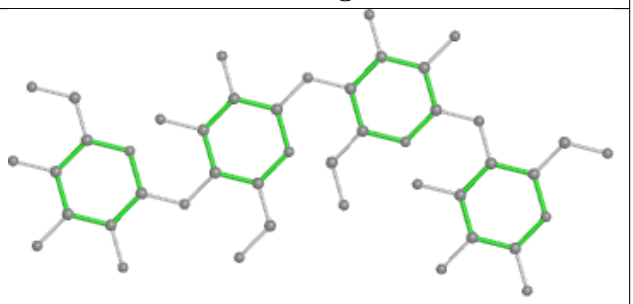
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

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.