Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2023 – 03:29 pm GMT

PDB ID	:	7R1N
Title	:	Crystal structure of the Tetrameric C-terminal Big_2-CBM56 domains from Paenibacillus illinoisensis (Bacillus circulans IAM1165) beta-1,3-glucanase H
Authors	:	Najmudin, S.; Venditto, I.; Fontes, C.M.G.A.; Bule, P.
Deposited on	:	2022-02-03
Resolution	:	2.07 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:

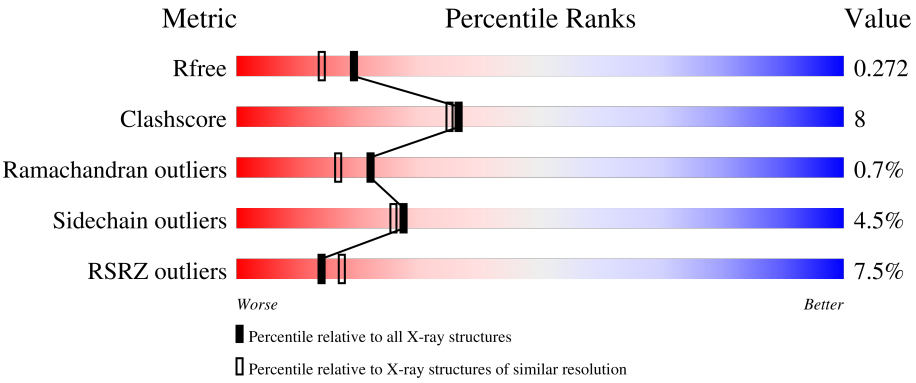
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.07 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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

Mol	Chain	Length	Quality of chain
1	AAA	207	10% 73% 13% • 11%
1	BBB	207	4% 77% 12% 11%
1	CCC	207	3% 76% 12% • 11%
1	DDD	207	10% 71% 15% •• 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11112 atoms, of which 5340 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 Beta-1,3-glucanase bglH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	184	Total	C	H	N	O	S	51	0	0
			2640	837	1303	225	274	1			
1	BBB	184	Total	C	H	N	O	S	51	0	0
			2640	837	1303	225	274	1			
1	CCC	184	Total	C	H	N	O	S	51	0	0
			2640	837	1303	225	274	1			
1	DDD	184	Total	C	H	N	O	S	51	0	0
			2640	837	1303	225	274	1			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP Q45095
AAA	2	GLY	-	expression tag	UNP Q45095
AAA	3	SER	-	expression tag	UNP Q45095
AAA	4	SER	-	expression tag	UNP Q45095
AAA	5	HIS	-	expression tag	UNP Q45095
AAA	6	HIS	-	expression tag	UNP Q45095
AAA	7	HIS	-	expression tag	UNP Q45095
AAA	8	HIS	-	expression tag	UNP Q45095
AAA	9	HIS	-	expression tag	UNP Q45095
AAA	10	HIS	-	expression tag	UNP Q45095
AAA	11	SER	-	expression tag	UNP Q45095
AAA	12	SER	-	expression tag	UNP Q45095
AAA	13	GLY	-	expression tag	UNP Q45095
AAA	14	LEU	-	expression tag	UNP Q45095
AAA	15	VAL	-	expression tag	UNP Q45095
AAA	16	PRO	-	expression tag	UNP Q45095
AAA	17	ARG	-	expression tag	UNP Q45095
AAA	18	GLY	-	expression tag	UNP Q45095
AAA	19	SER	-	expression tag	UNP Q45095
AAA	20	HIS	-	expression tag	UNP Q45095
AAA	21	MET	-	expression tag	UNP Q45095

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	ALA	-	expression tag	UNP Q45095
AAA	23	SER	-	expression tag	UNP Q45095
BBB	1	MET	-	initiating methionine	UNP Q45095
BBB	2	GLY	-	expression tag	UNP Q45095
BBB	3	SER	-	expression tag	UNP Q45095
BBB	4	SER	-	expression tag	UNP Q45095
BBB	5	HIS	-	expression tag	UNP Q45095
BBB	6	HIS	-	expression tag	UNP Q45095
BBB	7	HIS	-	expression tag	UNP Q45095
BBB	8	HIS	-	expression tag	UNP Q45095
BBB	9	HIS	-	expression tag	UNP Q45095
BBB	10	HIS	-	expression tag	UNP Q45095
BBB	11	SER	-	expression tag	UNP Q45095
BBB	12	SER	-	expression tag	UNP Q45095
BBB	13	GLY	-	expression tag	UNP Q45095
BBB	14	LEU	-	expression tag	UNP Q45095
BBB	15	VAL	-	expression tag	UNP Q45095
BBB	16	PRO	-	expression tag	UNP Q45095
BBB	17	ARG	-	expression tag	UNP Q45095
BBB	18	GLY	-	expression tag	UNP Q45095
BBB	19	SER	-	expression tag	UNP Q45095
BBB	20	HIS	-	expression tag	UNP Q45095
BBB	21	MET	-	expression tag	UNP Q45095
BBB	22	ALA	-	expression tag	UNP Q45095
BBB	23	SER	-	expression tag	UNP Q45095
CCC	1	MET	-	initiating methionine	UNP Q45095
CCC	2	GLY	-	expression tag	UNP Q45095
CCC	3	SER	-	expression tag	UNP Q45095
CCC	4	SER	-	expression tag	UNP Q45095
CCC	5	HIS	-	expression tag	UNP Q45095
CCC	6	HIS	-	expression tag	UNP Q45095
CCC	7	HIS	-	expression tag	UNP Q45095
CCC	8	HIS	-	expression tag	UNP Q45095
CCC	9	HIS	-	expression tag	UNP Q45095
CCC	10	HIS	-	expression tag	UNP Q45095
CCC	11	SER	-	expression tag	UNP Q45095
CCC	12	SER	-	expression tag	UNP Q45095
CCC	13	GLY	-	expression tag	UNP Q45095
CCC	14	LEU	-	expression tag	UNP Q45095
CCC	15	VAL	-	expression tag	UNP Q45095
CCC	16	PRO	-	expression tag	UNP Q45095
CCC	17	ARG	-	expression tag	UNP Q45095

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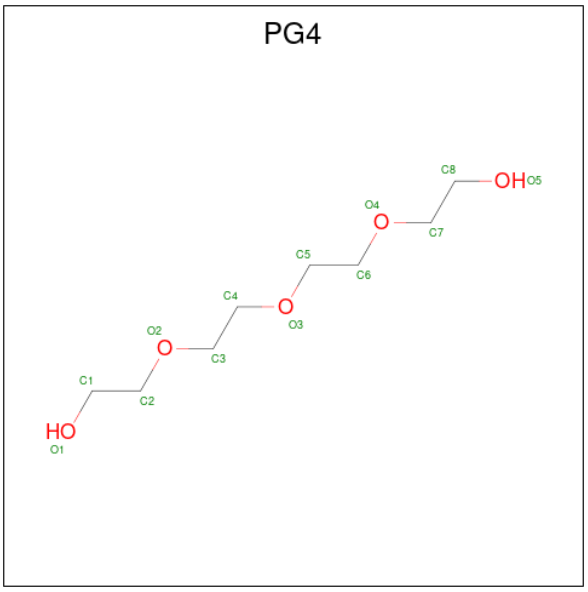
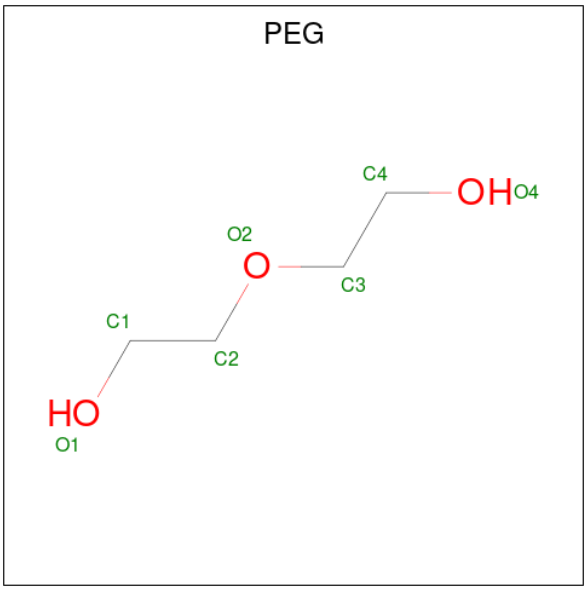
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	18	GLY	-	expression tag	UNP Q45095
CCC	19	SER	-	expression tag	UNP Q45095
CCC	20	HIS	-	expression tag	UNP Q45095
CCC	21	MET	-	expression tag	UNP Q45095
CCC	22	ALA	-	expression tag	UNP Q45095
CCC	23	SER	-	expression tag	UNP Q45095
DDD	1	MET	-	initiating methionine	UNP Q45095
DDD	2	GLY	-	expression tag	UNP Q45095
DDD	3	SER	-	expression tag	UNP Q45095
DDD	4	SER	-	expression tag	UNP Q45095
DDD	5	HIS	-	expression tag	UNP Q45095
DDD	6	HIS	-	expression tag	UNP Q45095
DDD	7	HIS	-	expression tag	UNP Q45095
DDD	8	HIS	-	expression tag	UNP Q45095
DDD	9	HIS	-	expression tag	UNP Q45095
DDD	10	HIS	-	expression tag	UNP Q45095
DDD	11	SER	-	expression tag	UNP Q45095
DDD	12	SER	-	expression tag	UNP Q45095
DDD	13	GLY	-	expression tag	UNP Q45095
DDD	14	LEU	-	expression tag	UNP Q45095
DDD	15	VAL	-	expression tag	UNP Q45095
DDD	16	PRO	-	expression tag	UNP Q45095
DDD	17	ARG	-	expression tag	UNP Q45095
DDD	18	GLY	-	expression tag	UNP Q45095
DDD	19	SER	-	expression tag	UNP Q45095
DDD	20	HIS	-	expression tag	UNP Q45095
DDD	21	MET	-	expression tag	UNP Q45095
DDD	22	ALA	-	expression tag	UNP Q45095
DDD	23	SER	-	expression tag	UNP Q45095

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



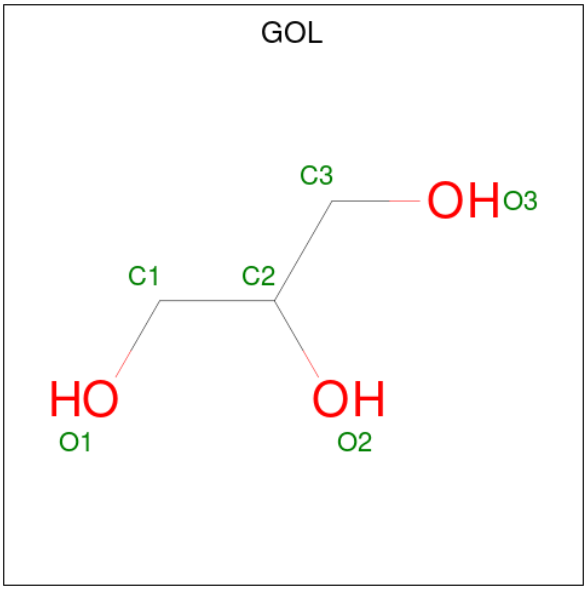
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			31	8	18	5		
2	BBB	1	Total	C	H	O	1	0
			31	8	18	5		
2	CCC	1	Total	C	H	O	1	0
			31	8	18	5		
2	DDD	1	Total	C	H	O	1	0
			31	8	18	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
3	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
3	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
3	BBB	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Cl	0	0
			1	1		
5	BBB	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Mg 1 1	0	0
6	BBB	1	Total Mg 1 1	0	0
6	CCC	1	Total Mg 1 1	0	0
6	DDD	1	Total Mg 1 1	0	0

- Molecule 7 is water.

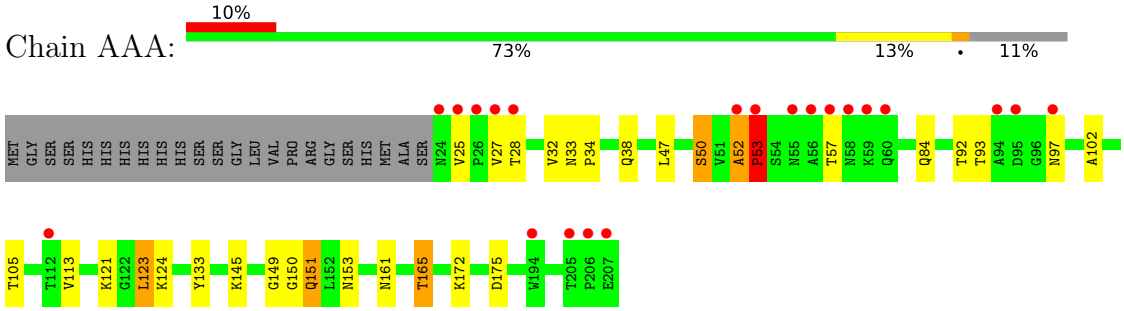
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	87	Total O 87 87	0	0
7	BBB	77	Total O 77 77	0	0
7	CCC	83	Total O 83 83	0	0
7	DDD	79	Total O 79 79	0	0

3 Residue-property plots (i)

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

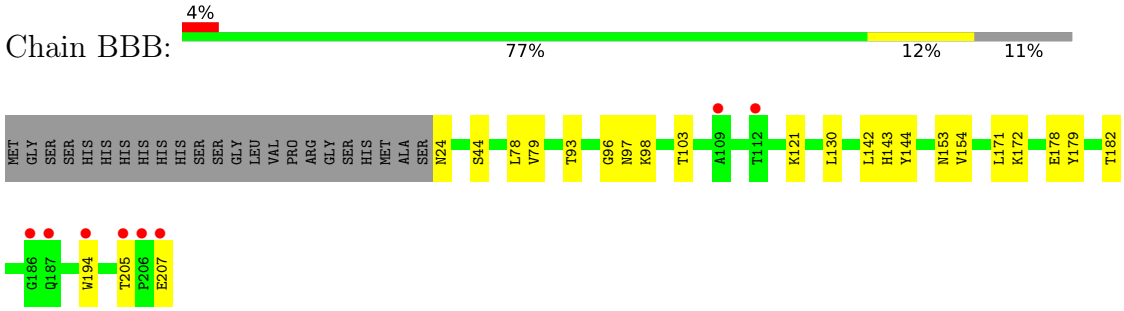
• Molecule 1: Beta-1,3-glucanase bglH

Chain AAA:



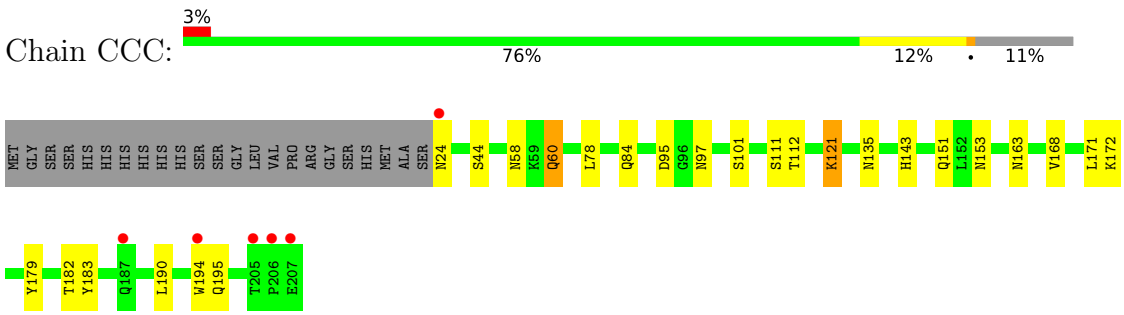
• Molecule 1: Beta-1,3-glucanase bglH

Chain BBB:



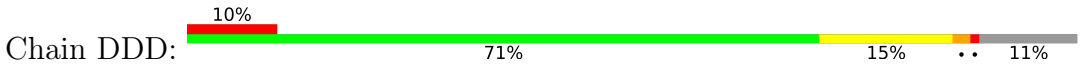
• Molecule 1: Beta-1,3-glucanase bglH

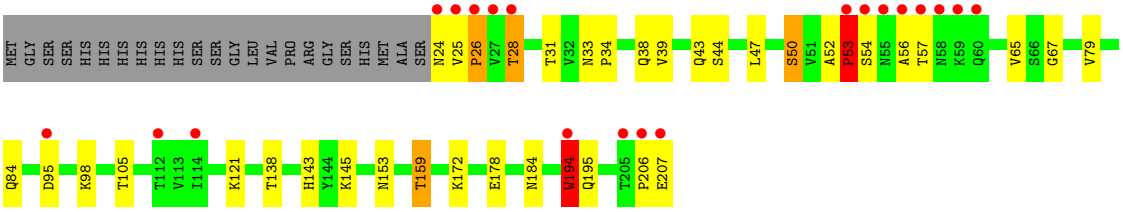
Chain CCC:



• Molecule 1: Beta-1,3-glucanase bglH

Chain DDD:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER N24 V25 P26 V27 T28 T31 V32 N33 P34 Q38 V39 Q43 S44 L47 S50 V51 A52 P53 S54 N55 A56 T57 N58 K59 Q60 V65 S66 G67 V79
Q84 D95 K98 T105 T112 V113 I114 K121 T138 H143 Y144 K145 N153 T159 K172 E178 N184 W194 Q195 T205 P206 E207

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.65Å 101.14Å 107.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.11 – 2.07 53.05 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.5 (53.11-2.07) 96.7 (53.05-2.07)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.271 0.211 , 0.272	Depositor DCC
R_{free} test set	2428 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11112	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1562e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, MG, PEG, PG4

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	AAA	0.81	0/1366	1.06	1/1879 (0.1%)
1	BBB	0.81	0/1366	1.00	1/1879 (0.1%)
1	CCC	0.82	0/1366	1.07	1/1879 (0.1%)
1	DDD	0.84	0/1366	1.03	3/1879 (0.2%)
All	All	0.82	0/5464	1.04	6/7516 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1
1	DDD	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	194	TRP	N-CA-CB	6.99	123.19	110.60
1	AAA	53	PRO	N-CA-CB	-6.23	95.75	102.60
1	DDD	33	ASN	CB-CA-C	5.92	122.25	110.40
1	CCC	112	THR	CA-CB-OG1	-5.44	97.58	109.00
1	DDD	53	PRO	N-CA-CB	-5.43	96.63	102.60
1	BBB	103	THR	CA-CB-OG1	-5.38	97.71	109.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	52	ALA	Peptide
1	DDD	52	ALA	Peptide

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	AAA	1337	1303	1298	26	0
1	BBB	1337	1303	1298	15	0
1	CCC	1337	1303	1298	20	1
1	DDD	1337	1303	1298	25	1
2	AAA	13	18	18	4	0
2	BBB	13	18	18	0	0
2	CCC	13	18	18	0	0
2	DDD	13	18	18	2	0
3	AAA	21	30	30	3	0
3	BBB	7	10	10	0	0
4	AAA	6	8	8	1	0
4	DDD	6	8	8	2	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
7	AAA	87	0	0	5	1
7	BBB	77	0	0	2	0
7	CCC	83	0	0	2	1
7	DDD	79	0	0	1	0
All	All	5772	5340	5320	85	2

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 8.

All (85) 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)
2:DDD:301:PG4:H71	4:DDD:302:GOL:O2	1.49	1.10
1:CCC:60:GLN:HA	1:CCC:60:GLN:OE1	1.65	0.94
1:AAA:175:ASP:OD2	1:DDD:172:LYS:NZ	2.16	0.78
1:AAA:150:GLY:HA3	3:AAA:305:PEG:H22	1.66	0.78
1:AAA:84:GLN:HG3	7:AAA:462:HOH:O	1.85	0.77
1:AAA:33:ASN:HB2	7:AAA:470:HOH:O	1.87	0.73
1:CCC:121:LYS:N	1:CCC:121:LYS:HD2	2.02	0.73
1:BBB:143:HIS:HD2	1:BBB:153:ASN:OD1	1.71	0.72
1:DDD:143:HIS:HD2	1:DDD:153:ASN:OD1	1.74	0.71
1:AAA:52:ALA:HB2	4:AAA:304:GOL:H2	1.72	0.70
1:DDD:25:VAL:HA	1:DDD:57:THR:OG1	1.94	0.68
2:DDD:301:PG4:H71	4:DDD:302:GOL:HO2	1.60	0.67
1:CCC:95:ASP:OD2	7:CCC:401:HOH:O	2.13	0.66
1:CCC:151:GLN:NE2	1:CCC:153:ASN:OD1	2.28	0.66
1:DDD:28:THR:CG2	1:DDD:53:PRO:HD2	2.27	0.65
1:BBB:143:HIS:HE1	1:BBB:182:THR:OG1	1.81	0.64
1:CCC:60:GLN:OE1	1:CCC:60:GLN:CA	2.44	0.64
1:BBB:93:THR:HG22	1:BBB:98:LYS:N	2.13	0.63
1:BBB:96:GLY:O	7:BBB:401:HOH:O	2.15	0.63
1:BBB:93:THR:CG2	1:BBB:98:LYS:H	2.13	0.61
1:AAA:150:GLY:CA	3:AAA:305:PEG:H22	2.33	0.59
1:DDD:25:VAL:HB	1:DDD:26:PRO:CD	2.32	0.58
1:CCC:84:GLN:OE1	7:CCC:402:HOH:O	2.17	0.57
1:DDD:28:THR:HG22	1:DDD:53:PRO:HD2	1.86	0.56
1:AAA:151:GLN:OE1	1:AAA:153:ASN:ND2	2.36	0.56
1:AAA:92:THR:HG23	7:AAA:422:HOH:O	2.06	0.56
1:AAA:50:SER:HB2	7:AAA:470:HOH:O	2.05	0.55
1:AAA:28:THR:OG1	1:AAA:53:PRO:HD2	2.06	0.55
1:AAA:124:LYS:HZ3	2:AAA:301:PG4:H71	1.72	0.55
1:CCC:121:LYS:HD2	1:CCC:121:LYS:H	1.70	0.54
1:BBB:44:SER:HB3	1:BBB:78:LEU:HD11	1.90	0.54
1:DDD:28:THR:HB	1:DDD:53:PRO:HD2	1.89	0.54
1:DDD:38:GLN:HA	1:DDD:105:THR:O	2.08	0.53
1:CCC:58:ASN:OD1	1:CCC:60:GLN:HB2	2.08	0.53
1:DDD:31:THR:HG23	1:DDD:50:SER:HB2	1.90	0.52
1:BBB:143:HIS:O	1:BBB:179:TYR:HA	2.10	0.52
1:DDD:53:PRO:HB2	1:DDD:56:ALA:HB2	1.92	0.51
1:BBB:130:LEU:HG	1:BBB:171:LEU:HD12	1.93	0.50
1:DDD:65:VAL:HG22	1:DDD:67:GLY:H	1.78	0.49
1:CCC:143:HIS:HD2	1:CCC:153:ASN:OD1	1.95	0.49
1:AAA:113:VAL:HG11	2:AAA:301:PG4:H72	1.96	0.48
1:DDD:143:HIS:CD2	1:DDD:153:ASN:OD1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:25:VAL:HB	1:DDD:26:PRO:HD3	1.96	0.48
1:AAA:123:LEU:HD22	1:AAA:123:LEU:C	2.34	0.47
1:CCC:172:LYS:HD2	1:CCC:172:LYS:N	2.30	0.47
1:AAA:150:GLY:H	3:AAA:305:PEG:H42	1.80	0.47
1:AAA:38:GLN:HA	1:AAA:105:THR:O	2.15	0.47
1:AAA:93:THR:O	1:AAA:97:ASN:HA	2.15	0.47
1:CCC:143:HIS:CD2	1:CCC:153:ASN:OD1	2.68	0.47
1:CCC:190:LEU:C	1:CCC:190:LEU:HD12	2.36	0.46
1:DDD:138:THR:OG1	1:DDD:184:ASN:HB3	2.15	0.46
1:AAA:165:THR:HG22	7:BBB:406:HOH:O	2.15	0.46
1:BBB:93:THR:HG23	1:BBB:97:ASN:N	2.31	0.46
1:DDD:145:LYS:HB3	1:DDD:145:LYS:HE3	1.85	0.45
1:CCC:194:TRP:CD1	1:CCC:194:TRP:N	2.81	0.45
1:AAA:161:ASN:ND2	7:AAA:401:HOH:O	2.33	0.45
1:DDD:84:GLN:HG3	7:DDD:442:HOH:O	2.16	0.45
1:CCC:44:SER:HB3	1:CCC:78:LEU:HD11	1.98	0.45
1:AAA:124:LYS:NZ	2:AAA:301:PG4:H52	2.32	0.45
1:BBB:143:HIS:CE1	1:BBB:182:THR:OG1	2.68	0.45
1:BBB:143:HIS:CD2	1:BBB:153:ASN:OD1	2.61	0.44
1:CCC:168:VAL:HG12	1:CCC:171:LEU:HD11	1.98	0.44
1:BBB:142:LEU:HB3	1:BBB:154:VAL:CG2	2.47	0.44
1:AAA:123:LEU:C	1:AAA:123:LEU:CD2	2.86	0.44
1:CCC:179:TYR:CZ	1:CCC:195:GLN:HB2	2.52	0.43
1:DDD:34:PRO:HD2	1:DDD:47:LEU:HD23	2.00	0.43
1:AAA:145:LYS:NZ	1:AAA:149:GLY:O	2.50	0.43
1:BBB:44:SER:HA	1:BBB:79:VAL:O	2.19	0.43
1:AAA:172:LYS:HE3	1:DDD:172:LYS:HE2	2.00	0.43
1:DDD:24:ASN:OD1	1:DDD:26:PRO:HD2	2.19	0.43
1:BBB:130:LEU:HG	1:BBB:171:LEU:CD1	2.50	0.42
1:DDD:39:VAL:HB	1:DDD:43:GLN:HB2	2.01	0.42
1:DDD:28:THR:CB	1:DDD:53:PRO:HD2	2.49	0.42
1:CCC:143:HIS:CE1	1:CCC:182:THR:OG1	2.72	0.42
1:DDD:44:SER:HA	1:DDD:79:VAL:O	2.20	0.42
1:AAA:34:PRO:HD2	1:AAA:47:LEU:HD22	2.02	0.42
1:CCC:135:ASN:HA	1:CCC:163:ASN:OD1	2.20	0.42
1:CCC:183:TYR:CE1	1:CCC:190:LEU:HD11	2.55	0.42
1:DDD:178:GLU:HA	1:DDD:195:GLN:O	2.19	0.42
1:CCC:101:SER:OG	1:DDD:159:THR:HA	2.20	0.41
1:BBB:144:TYR:HA	1:BBB:178:GLU:O	2.21	0.41
1:DDD:26:PRO:HA	1:DDD:95:ASP:OD2	2.20	0.41
1:AAA:32:VAL:CG1	1:AAA:102:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:133:TYR:CG	2:AAA:301:PG4:H12	2.56	0.41
1:AAA:27:VAL:HG11	1:AAA:93:THR:HG21	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AAA:478:HOH:O	7:CCC:476:HOH:O[4_446]	2.04	0.16
1:CCC:151:GLN:OE1	1:DDD:194:TRP:H[3_545]	1.60	0.00

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	AAA	182/207 (88%)	171 (94%)	10 (6%)	1 (0%)	29 25
1	BBB	182/207 (88%)	169 (93%)	13 (7%)	0	100 100
1	CCC	182/207 (88%)	169 (93%)	13 (7%)	0	100 100
1	DDD	182/207 (88%)	165 (91%)	13 (7%)	4 (2%)	6 2
All	All	728/828 (88%)	674 (93%)	49 (7%)	5 (1%)	22 17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	53	PRO
1	DDD	53	PRO
1	DDD	54	SER
1	DDD	26	PRO
1	DDD	206	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	AAA	146/165 (88%)	138 (94%)	8 (6%)	21	18
1	BBB	146/165 (88%)	140 (96%)	6 (4%)	30	30
1	CCC	146/165 (88%)	141 (97%)	5 (3%)	37	37
1	DDD	146/165 (88%)	139 (95%)	7 (5%)	25	23
All	All	584/660 (88%)	558 (96%)	26 (4%)	27	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	25	VAL
1	AAA	50	SER
1	AAA	53	PRO
1	AAA	57	THR
1	AAA	121	LYS
1	AAA	123	LEU
1	AAA	151	GLN
1	AAA	165	THR
1	BBB	24	ASN
1	BBB	121	LYS
1	BBB	172	LYS
1	BBB	194	TRP
1	BBB	205	THR
1	BBB	207	GLU
1	CCC	24	ASN
1	CCC	60	GLN
1	CCC	97	ASN
1	CCC	111	SER
1	CCC	121	LYS
1	DDD	28	THR
1	DDD	50	SER
1	DDD	98	LYS
1	DDD	121	LYS
1	DDD	159	THR

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Mol	Chain	Res	Type
1	DDD	194	TRP
1	DDD	207	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	DDD	302	-	5,5,5	0.19	0	5,5,5	0.66	0
3	PEG	AAA	303	-	6,6,6	0.32	0	5,5,5	0.23	0
2	PG4	CCC	301	-	12,12,12	0.21	0	11,11,11	0.29	0
2	PG4	DDD	301	-	12,12,12	0.26	0	11,11,11	0.23	0
3	PEG	BBB	302	-	6,6,6	0.31	0	5,5,5	0.31	0
3	PEG	AAA	305	-	6,6,6	0.36	0	5,5,5	0.33	0
2	PG4	BBB	301	-	12,12,12	0.24	0	11,11,11	0.33	0
4	GOL	AAA	304	-	5,5,5	0.16	0	5,5,5	0.42	0
3	PEG	AAA	302	-	6,6,6	0.16	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PG4	AAA	301	-	12,12,12	0.59	0	11,11,11	0.60	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	GOL	DDD	302	-	-	1/4/4/4	-
3	PEG	AAA	303	-	-	1/4/4/4	-
2	PG4	CCC	301	-	-	4/10/10/10	-
2	PG4	DDD	301	-	-	4/10/10/10	-
3	PEG	BBB	302	-	-	1/4/4/4	-
3	PEG	AAA	305	-	-	2/4/4/4	-
2	PG4	BBB	301	-	-	2/10/10/10	-
4	GOL	AAA	304	-	-	2/4/4/4	-
3	PEG	AAA	302	-	-	2/4/4/4	-
2	PG4	AAA	301	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	PG4	C5-C6-O4-C7
2	BBB	301	PG4	O4-C7-C8-O5
2	AAA	301	PG4	O2-C3-C4-O3
2	CCC	301	PG4	O3-C5-C6-O4
2	CCC	301	PG4	O4-C7-C8-O5
2	DDD	301	PG4	O1-C1-C2-O2
3	AAA	302	PEG	O1-C1-C2-O2
4	AAA	304	GOL	O1-C1-C2-C3
3	AAA	303	PEG	O2-C3-C4-O4
2	DDD	301	PG4	O2-C3-C4-O3
3	AAA	305	PEG	O1-C1-C2-O2
3	BBB	302	PEG	O1-C1-C2-O2
3	AAA	305	PEG	C4-C3-O2-C2
2	BBB	301	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	AAA	302	PEG	C4-C3-O2-C2
2	CCC	301	PG4	C8-C7-O4-C6
2	AAA	301	PG4	O3-C5-C6-O4
2	DDD	301	PG4	C8-C7-O4-C6
2	AAA	301	PG4	C1-C2-O2-C3
2	CCC	301	PG4	O1-C1-C2-O2
2	AAA	301	PG4	O1-C1-C2-O2
4	AAA	304	GOL	O1-C1-C2-O2
4	DDD	302	GOL	C1-C2-C3-O3
2	DDD	301	PG4	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	302	GOL	2	0
2	DDD	301	PG4	2	0
3	AAA	305	PEG	3	0
4	AAA	304	GOL	1	0
2	AAA	301	PG4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	184/207 (88%)	0.24	21 (11%) 5 6	18, 26, 54, 78	0
1	BBB	184/207 (88%)	-0.01	8 (4%) 35 40	18, 27, 49, 77	0
1	CCC	184/207 (88%)	-0.03	6 (3%) 46 52	17, 25, 46, 88	0
1	DDD	184/207 (88%)	0.38	20 (10%) 5 7	17, 27, 66, 86	0
All	All	736/828 (88%)	0.14	55 (7%) 14 17	17, 26, 54, 88	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	25	VAL	8.4
1	DDD	24	ASN	7.5
1	DDD	56	ALA	7.0
1	DDD	26	PRO	6.2
1	AAA	24	ASN	6.0
1	AAA	57	THR	5.9
1	DDD	57	THR	5.9
1	CCC	206	PRO	5.6
1	AAA	207	GLU	5.6
1	DDD	207	GLU	5.5
1	DDD	54	SER	5.3
1	AAA	25	VAL	5.3
1	DDD	206	PRO	4.8
1	CCC	205	THR	4.6
1	DDD	27	VAL	4.0
1	BBB	187	GLN	3.9
1	AAA	26	PRO	3.8
1	DDD	194	TRP	3.7
1	CCC	187	GLN	3.6
1	DDD	53	PRO	3.3
1	DDD	55	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	24	ASN	3.1
1	BBB	112	THR	3.1
1	AAA	27	VAL	3.1
1	DDD	58	ASN	3.0
1	CCC	207	GLU	3.0
1	AAA	58	ASN	3.0
1	AAA	53	PRO	3.0
1	DDD	59	LYS	2.9
1	AAA	56	ALA	2.8
1	BBB	206	PRO	2.8
1	BBB	205	THR	2.7
1	AAA	95	ASP	2.7
1	AAA	206	PRO	2.7
1	DDD	28	THR	2.7
1	DDD	205	THR	2.7
1	AAA	55	ASN	2.6
1	AAA	28	THR	2.6
1	BBB	186	GLY	2.6
1	DDD	60	GLN	2.6
1	BBB	207	GLU	2.6
1	DDD	95	ASP	2.5
1	AAA	52	ALA	2.5
1	CCC	194	TRP	2.4
1	AAA	59	LYS	2.3
1	BBB	194	TRP	2.3
1	DDD	112	THR	2.3
1	BBB	109	ALA	2.2
1	AAA	94	ALA	2.2
1	AAA	194	TRP	2.2
1	AAA	112	THR	2.2
1	AAA	60	GLN	2.1
1	AAA	205	THR	2.1
1	AAA	97	ASN	2.0
1	DDD	114	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	DDD	302	6/6	0.54	0.30	20,54,57,61	2
3	PEG	AAA	305	7/7	0.74	0.22	43,43,46,47	1
3	PEG	AAA	303	7/7	0.83	0.14	40,42,45,45	1
4	GOL	AAA	304	6/6	0.85	0.18	40,48,49,53	2
3	PEG	AAA	302	7/7	0.85	0.13	41,42,43,44	1
2	PG4	BBB	301	13/13	0.87	0.13	38,42,47,48	1
2	PG4	AAA	301	13/13	0.88	0.13	31,37,41,43	1
3	PEG	BBB	302	7/7	0.88	0.22	39,40,42,43	1
2	PG4	DDD	301	13/13	0.89	0.12	35,41,47,47	1
2	PG4	CCC	301	13/13	0.95	0.12	27,33,38,43	1
5	CL	AAA	306	1/1	0.99	0.11	23,23,23,23	0
5	CL	BBB	303	1/1	0.99	0.12	18,18,18,18	0
6	MG	AAA	307	1/1	0.99	0.11	15,15,15,15	0
6	MG	BBB	304	1/1	0.99	0.12	16,16,16,16	0
6	MG	CCC	302	1/1	0.99	0.17	16,16,16,16	0
6	MG	DDD	303	1/1	0.99	0.19	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.