Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 01:25 pm GMT

PDB ID	:	4UOQ
Title	:	Nucleophile mutant (E324A) of beta-(1,6)-galactosidase from Bifidobacterium animalis subsp. lactis Bl-04
Authors	:	Viborg, A.H.; Fredslund, F.; Katayama, T.; Nielsen, S.K.; Svensson, B.; Kitaoka, M.; Lo Leggio, L.; Abou Hachem, M.
Deposited on	:	2014-06-09
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

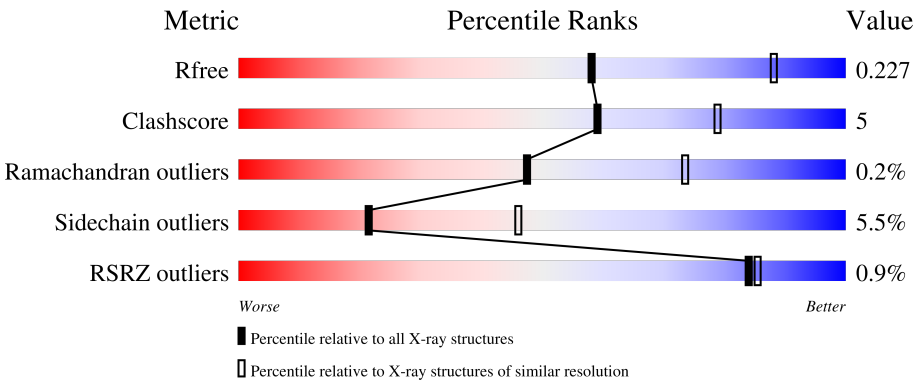
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

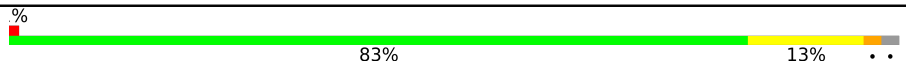
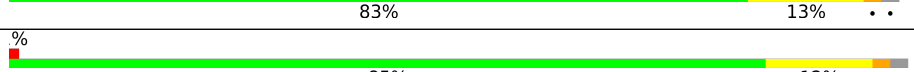
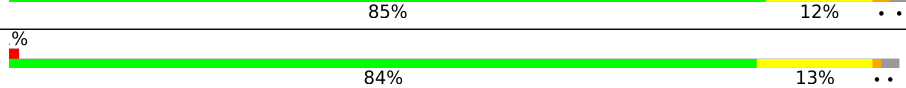
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	695	
1	B	695	
1	C	695	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16764 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.

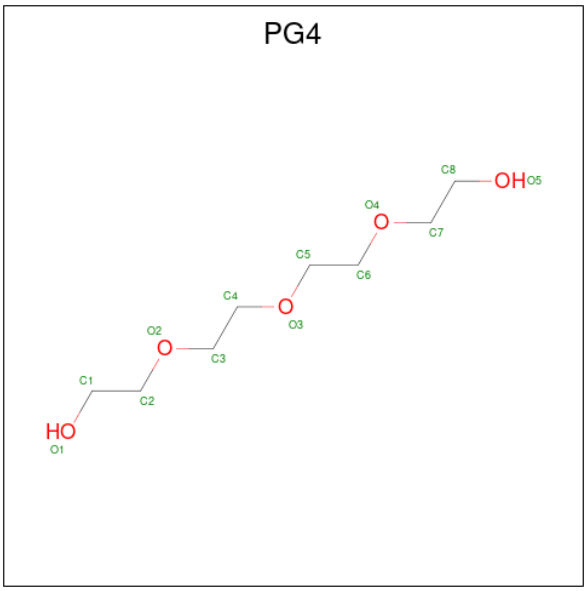
- Molecule 1 is a protein called BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	683	5443	3443	950	1027	23	0	0	0
1	B	684	5452	3448	952	1029	23	0	0	0
1	C	682	5433	3437	947	1026	23	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

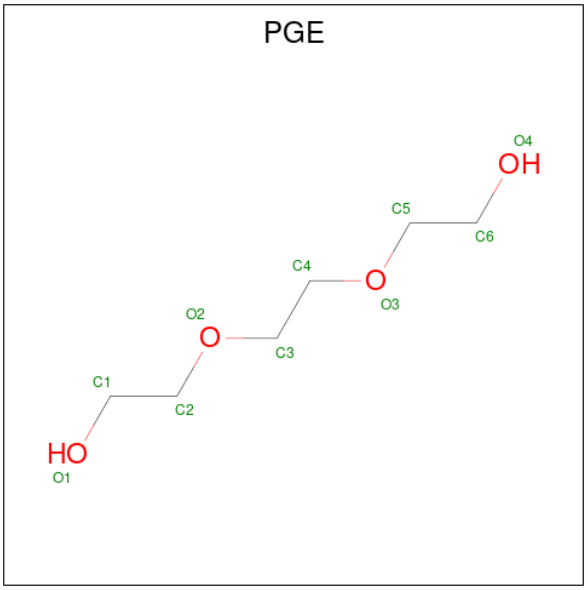
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	GLU	engineered mutation	UNP C6A6W5
B	324	ALA	GLU	engineered mutation	UNP C6A6W5
C	324	ALA	GLU	engineered mutation	UNP C6A6W5

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



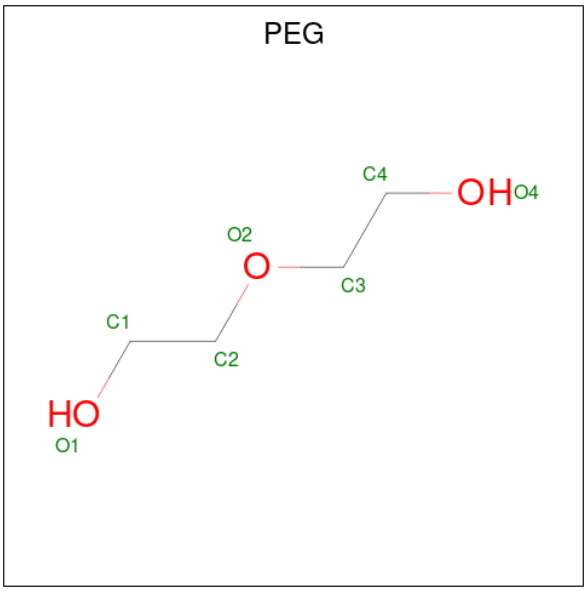
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0
			Total	C	O		
2	C	1	13	8	5	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	10	6	4	0	0
			Total	C	O		
3	B	1	10	6	4	0	0
			Total	C	O		
3	C	1	10	6	4	0	0
			Total	C	O		
3	C	1	10	6	4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
4	A	1	7	4	3	0	0
4	A	1	7	4	3	0	0
4	A	1	7	4	3	0	0
4	B	1	7	4	3	0	0
4	B	1	7	4	3	0	0
4	B	1	7	4	3	0	0
4	B	1	7	4	3	0	0
4	C	1	7	4	3	0	0
4	C	1	7	4	3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0

- Molecule 6 is water.

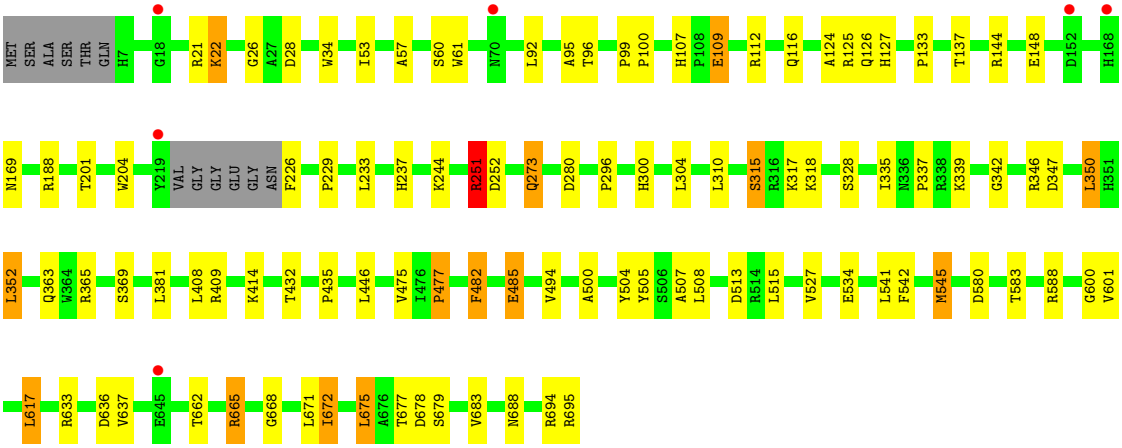
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	114	114	114	0	0
			Total	O		
6	B	101	101	101	0	0
			Total	O		
6	C	84	84	84	0	0

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.

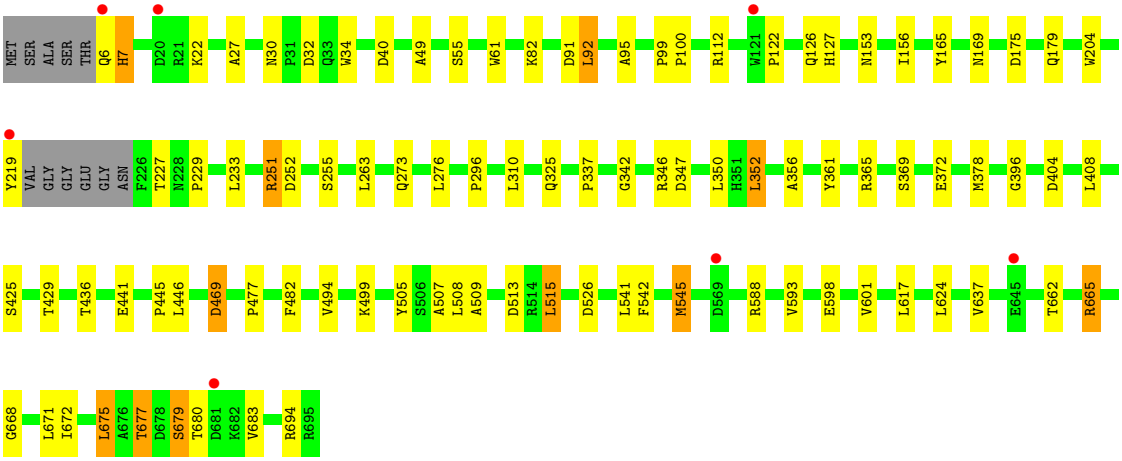
• Molecule 1: BETA-GALACTOSIDASE

Chain A:



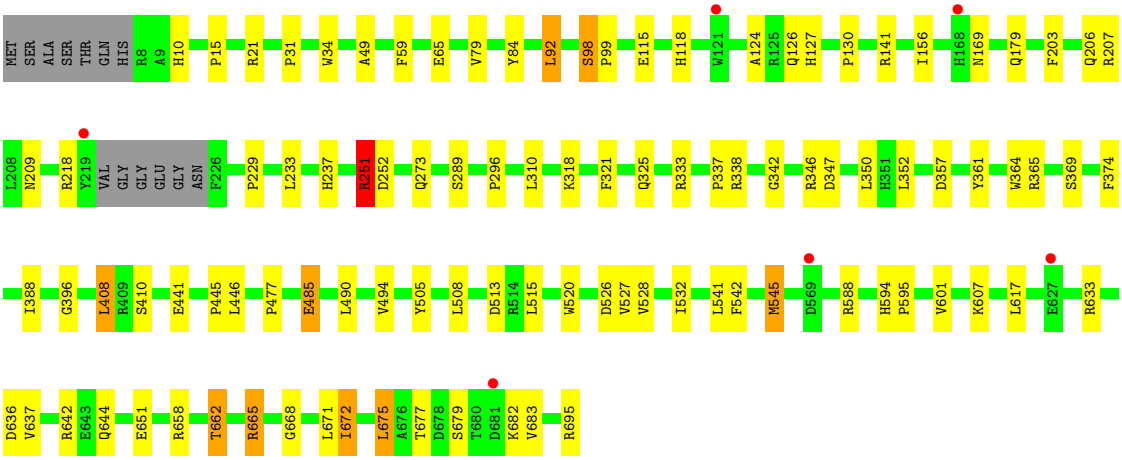
• Molecule 1: BETA-GALACTOSIDASE

Chain B:



• Molecule 1: BETA-GALACTOSIDASE

Chain C:


MET
SER
ALA
SER
THR
GLN
HIS
R8
A9
H10
P15
R21
P31
W34
A49
F59
E65
V79
Y84
L92
S98
P99
E115
H118
W121
A124
R125
Q126
H127
P130
R141
I156
H168
N169
Q179
F203
Q206
R207
L208
N209
R218
Y219
VAL
GLY
GLY
GLU
GLY
ASN
F226
P229
L233
H237
R251
D252
Q273
S289
P296
L310
K318
F321
Q325
R333
P337
R338
G342
R346
D347
L350
H351
L352
D357
Y361
W364
R365
S369
F374
I388
G396
L408
R409
S410
E441
P445
L446
P477
E485
L490
V494
Y505
L508
D513
R514
L515
W520
D526
V527
V528
I532
L541
F542
M545
D569
R588
H594
P595
V601
K607
L617
E627
R633
D636
V637
R642
E643
Q644
E651
R658
T662
R665
G668
L671
I672
L675
A676
T677
D678
S679
T680
D681
K682
V683
R695

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.56Å 150.56Å 237.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.70 19.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-2.70) 99.8 (19.93-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 2.71Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.227 0.181 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16764	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE, PG4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/5597	0.62	2/7630 (0.0%)
1	B	0.44	0/5606	0.58	0/7642
1	C	0.45	0/5586	0.60	1/7615 (0.0%)
All	All	0.45	0/16789	0.60	3/22887 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	251	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	352	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5443	0	5151	62	0
1	B	5452	0	5159	46	0
1	C	5433	0	5144	52	0
2	A	13	0	18	0	0
2	C	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	14	3	0
3	B	10	0	14	1	0
3	C	20	0	28	1	0
4	A	28	0	40	2	0
4	B	28	0	40	0	0
4	C	14	0	20	0	0
5	A	1	0	0	0	0
6	A	114	0	0	3	0
6	B	101	0	0	2	0
6	C	84	0	0	5	0
All	All	16764	0	15646	152	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 5.

All (152) 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:251:ARG:HH11	1:A:251:ARG:HG2	1.40	0.86
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.40	0.85
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.43	0.83
1:A:346:ARG:NH1	1:A:347:ASP:OD1	2.13	0.82
1:C:346:ARG:NH1	1:C:347:ASP:OD1	2.13	0.81
1:B:542:PHE:HD1	1:B:545:MET:HE3	1.51	0.75
1:A:201:THR:O	6:A:2021:HOH:O	2.06	0.74
1:A:665:ARG:NH2	1:A:668:GLY:O	2.23	0.72
1:C:115:GLU:O	1:C:218:ARG:NH1	2.25	0.69
1:C:665:ARG:NH2	1:C:668:GLY:O	2.28	0.67
1:B:665:ARG:NH2	1:B:668:GLY:O	2.28	0.66
1:B:40:ASP:OD1	1:B:82:LYS:NZ	2.29	0.66
1:A:633:ARG:NH1	1:A:636:ASP:OD1	2.29	0.66
1:B:671:LEU:HD11	1:B:694:ARG:HB2	1.78	0.65
1:B:346:ARG:NH1	1:B:347:ASP:OD1	2.31	0.64
1:C:333:ARG:NH1	6:C:2035:HOH:O	2.30	0.63
1:A:527:VAL:HG12	1:A:601:VAL:HG21	1.81	0.63
1:A:414:LYS:HE3	3:A:1697:PGE:H4	1.81	0.63
1:C:251:ARG:HG2	1:C:251:ARG:NH1	2.13	0.62
1:B:6:GLN:N	6:B:2001:HOH:O	2.33	0.60
1:B:296:PRO:HB3	1:B:337:PRO:HG2	1.83	0.60
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.10	0.60
1:A:125:ARG:HB3	1:B:204:TRP:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:N	1:A:485:GLU:OE1	2.34	0.59
1:C:542:PHE:HD1	1:C:545:MET:HE3	1.65	0.59
1:C:207:ARG:NH1	1:C:209:ASN:OD1	2.36	0.58
1:C:485:GLU:OE1	1:C:485:GLU:N	2.35	0.58
1:C:126:GLN:O	1:C:169:ASN:HB3	2.05	0.57
1:A:342:GLY:HA3	1:A:675:LEU:HD22	1.87	0.56
1:C:296:PRO:HB3	1:C:337:PRO:HG2	1.88	0.56
1:A:144:ARG:O	1:A:148:GLU:HG2	2.05	0.56
1:B:92:LEU:HB2	1:B:156:ILE:HG23	1.89	0.55
1:A:251:ARG:NH1	1:A:252:ASP:OD1	2.40	0.55
1:C:527:VAL:HG12	1:C:601:VAL:HG21	1.89	0.54
1:C:441:GLU:O	1:C:445:PRO:HD2	2.08	0.54
1:C:124:ALA:O	1:C:127:HIS:ND1	2.38	0.54
1:B:229:PRO:HB2	1:B:513:ASP:OD2	2.08	0.53
1:C:237:HIS:HE1	6:C:2027:HOH:O	1.91	0.53
1:A:296:PRO:HB3	1:A:337:PRO:HG2	1.91	0.53
1:A:335:ILE:O	1:A:337:PRO:HD3	2.08	0.53
1:A:542:PHE:HD2	1:A:545:MET:HE3	1.75	0.52
1:C:229:PRO:HB2	1:C:513:ASP:OD2	2.09	0.52
1:C:662:THR:HG23	1:C:682:LYS:HD2	1.91	0.52
1:B:251:ARG:NH1	1:B:252:ASP:OD1	2.43	0.52
1:B:126:GLN:O	1:B:169:ASN:HB3	2.10	0.52
1:A:112:ARG:HD3	1:A:169:ASN:HB2	1.90	0.52
1:C:251:ARG:NH1	1:C:252:ASP:OD1	2.44	0.51
1:A:126:GLN:O	1:A:169:ASN:HB3	2.10	0.51
1:A:229:PRO:HB2	1:A:513:ASP:OD2	2.10	0.51
1:A:116:GLN:OE1	1:C:118:HIS:ND1	2.44	0.51
1:A:409:ARG:HH21	4:A:1700:PEG:H31	1.75	0.51
1:C:633:ARG:NH1	1:C:636:ASP:OD1	2.44	0.50
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.15	0.50
1:A:317:LYS:HD2	3:A:1697:PGE:H22	1.93	0.50
1:B:255:SER:HB3	1:B:263:LEU:HD11	1.92	0.50
1:B:342:GLY:HA3	1:B:675:LEU:HD22	1.94	0.50
1:A:315:SER:OG	1:A:318:LYS:O	2.30	0.50
1:A:296:PRO:HG2	1:B:542:PHE:CD1	2.47	0.50
1:A:542:PHE:O	1:A:545:MET:HB2	2.13	0.49
1:A:409:ARG:HE	4:A:1700:PEG:H31	1.78	0.49
1:C:520:TRP:O	1:C:532:ILE:N	2.43	0.49
1:B:6:GLN:O	1:B:7:HIS:HB2	2.12	0.48
1:C:15:PRO:HG3	1:C:21:ARG:HA	1.94	0.48
1:B:165:TYR:O	1:B:276:LEU:HD21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HD22	1:B:356:ALA:O	2.14	0.48
1:B:441:GLU:O	1:B:445:PRO:HD2	2.14	0.48
1:C:494:VAL:HG11	1:C:601:VAL:HG23	1.97	0.47
1:A:226:PHE:HD1	1:A:432:THR:HG1	1.58	0.47
1:A:109:GLU:H	1:A:109:GLU:HG3	1.37	0.47
1:C:130:PRO:HG2	6:C:2008:HOH:O	2.13	0.47
1:C:357:ASP:OD1	1:C:642:ARG:NH2	2.30	0.47
1:B:509:ALA:HB2	1:B:515:LEU:HD12	1.96	0.47
1:A:244:LYS:NZ	1:A:280:ASP:OD2	2.39	0.47
1:A:204:TRP:HA	1:C:59:PHE:CG	2.50	0.47
1:B:32:ASP:OD1	1:B:32:ASP:N	2.47	0.47
1:A:671:LEU:HD11	1:A:694:ARG:HB2	1.97	0.46
1:A:485:GLU:H	1:A:485:GLU:CD	2.18	0.46
1:A:304:LEU:HD22	1:A:350:LEU:HB3	1.98	0.46
1:C:84:TYR:CD2	3:C:1700:PGE:H1	2.50	0.46
1:C:651:GLU:OE1	1:C:695:ARG:NH1	2.27	0.46
1:A:26:GLY:HA3	1:A:53:ILE:O	2.16	0.46
1:A:665:ARG:NH1	1:A:678:ASP:OD2	2.49	0.46
1:B:677:THR:HG22	6:B:2101:HOH:O	2.14	0.46
1:A:124:ALA:O	1:A:127:HIS:ND1	2.48	0.46
1:A:475:VAL:O	1:A:477:PRO:HD3	2.16	0.46
1:C:410:SER:HB3	1:C:644:GLN:HG2	1.97	0.46
1:B:153:ASN:ND2	3:B:1697:PGE:O2	2.49	0.45
1:A:617:LEU:HD12	1:A:617:LEU:HA	1.82	0.45
1:A:188:ARG:HB2	6:A:2017:HOH:O	2.17	0.45
1:A:328:SER:HA	1:A:339:LYS:HG3	1.99	0.45
1:C:31:PRO:HG3	1:C:79:VAL:HG21	1.98	0.45
1:A:346:ARG:NH2	1:A:688:ASN:OD1	2.49	0.45
1:B:49:ALA:O	1:B:396:GLY:HA3	2.17	0.45
1:B:499:LYS:HE2	1:B:624:LEU:O	2.16	0.45
1:A:21:ARG:O	1:A:22:LYS:HD2	2.17	0.45
1:A:671:LEU:O	1:A:672:ILE:HD12	2.17	0.45
1:C:49:ALA:O	1:C:396:GLY:HA3	2.17	0.44
1:A:414:LYS:CE	3:A:1697:PGE:H4	2.48	0.44
1:C:594:HIS:HA	1:C:595:PRO:HD2	1.89	0.44
1:A:237:HIS:HD2	6:A:2026:HOH:O	1.99	0.44
1:B:296:PRO:CB	1:B:337:PRO:HG2	2.46	0.44
1:C:671:LEU:O	1:C:672:ILE:HD12	2.18	0.44
1:A:57:ALA:HA	1:A:60:SER:OG	2.18	0.44
1:B:325:GLN:HG3	1:B:361:TYR:CD1	2.52	0.44
1:C:289:SER:HA	1:C:321:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:NZ	1:B:404:ASP:OD1	2.51	0.43
1:B:679:SER:OG	1:B:680:THR:N	2.50	0.43
1:C:10:HIS:HB2	1:C:318:LYS:HD3	2.00	0.43
1:B:372:GLU:HB3	1:C:203:PHE:HD2	1.83	0.43
1:C:65:GLU:OE2	1:C:141:ARG:NH2	2.49	0.43
1:C:92:LEU:HB2	1:C:156:ILE:HG23	2.00	0.43
1:A:534:GLU:OE2	1:C:338:ARG:HD2	2.18	0.43
1:B:494:VAL:HG11	1:B:601:VAL:HG23	2.01	0.42
1:C:607:LYS:HE3	6:C:2063:HOH:O	2.18	0.42
1:B:27:ALA:HB2	1:B:378:MET:SD	2.60	0.42
1:C:325:GLN:HG3	1:C:361:TYR:CD1	2.55	0.42
1:A:34:TRP:CZ2	1:A:365:ARG:HD3	2.54	0.42
1:B:526:ASP:OD1	1:B:526:ASP:N	2.52	0.42
1:A:500:ALA:N	1:A:600:GLY:O	2.40	0.42
1:C:388:ILE:HA	6:C:2054:HOH:O	2.19	0.42
1:A:482:PHE:HB2	1:A:507:ALA:HA	2.02	0.42
1:B:425:SER:O	1:B:429:THR:HG23	2.20	0.42
1:C:490:LEU:O	1:C:494:VAL:HG23	2.20	0.42
1:A:107:HIS:ND1	1:A:109:GLU:OE2	2.52	0.42
1:A:381:LEU:HD13	1:B:515:LEU:HB3	2.02	0.42
1:B:99:PRO:HA	1:B:100:PRO:HD3	1.85	0.42
1:B:482:PHE:HB2	1:B:507:ALA:HA	2.02	0.42
1:A:61:TRP:CE3	1:A:96:THR:HA	2.55	0.41
1:C:98:SER:HA	1:C:99:PRO:HD2	1.77	0.41
1:C:528:VAL:HA	1:C:601:VAL:HG11	2.02	0.41
1:B:542:PHE:O	1:B:545:MET:HB2	2.20	0.41
1:C:342:GLY:HA3	1:C:675:LEU:HD22	2.03	0.41
1:A:363:GLN:H	1:A:363:GLN:HG2	1.79	0.41
1:A:435:PRO:HD3	1:C:374:PHE:CG	2.56	0.41
1:A:494:VAL:HG11	1:A:601:VAL:HG23	2.02	0.41
1:A:580:ASP:HB3	1:A:583:THR:HG23	2.01	0.41
1:A:300:HIS:HE1	1:A:347:ASP:OD2	2.03	0.41
1:B:175:ASP:O	1:B:179:GLN:HG3	2.20	0.41
1:A:133:PRO:O	1:A:137:THR:HG23	2.21	0.41
1:A:273:GLN:HE21	1:A:273:GLN:HB2	1.59	0.41
1:B:55:SER:HA	1:B:91:ASP:O	2.21	0.41
1:B:469:ASP:OD1	1:B:469:ASP:N	2.42	0.41
1:C:34:TRP:CZ2	1:C:365:ARG:HD3	2.56	0.41
1:B:122:PRO:HA	1:B:127:HIS:ND1	2.36	0.41
1:C:364:TRP:CD1	1:C:365:ARG:HB2	2.56	0.41
1:C:658:ARG:HA	1:C:658:ARG:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:ASP:OD1	1:C:526:ASP:N	2.53	0.40
1:A:99:PRO:HA	1:A:100:PRO:HD3	1.87	0.40
1:B:34:TRP:CZ2	1:B:365:ARG:HD3	2.56	0.40
1:B:61:TRP:HB2	1:B:95:ALA:O	2.22	0.40
1:C:408:LEU:O	1:C:644:GLN:NE2	2.55	0.40
1:A:61:TRP:HB2	1:A:95:ALA:O	2.20	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	679/695 (98%)	660 (97%)	17 (2%)	2 (0%)	41	66
1	B	680/695 (98%)	663 (98%)	15 (2%)	2 (0%)	41	66
1	C	678/695 (98%)	660 (97%)	17 (2%)	1 (0%)	51	78
All	All	2037/2085 (98%)	1983 (97%)	49 (2%)	5 (0%)	47	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	HIS
1	A	477	PRO
1	B	477	PRO
1	C	477	PRO
1	A	504	TYR

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	572/580 (99%)	540 (94%)	32 (6%)	21	45
1	B	573/580 (99%)	540 (94%)	33 (6%)	20	43
1	C	571/580 (98%)	542 (95%)	29 (5%)	24	50
All	All	1716/1740 (99%)	1622 (94%)	94 (6%)	21	46

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	28	ASP
1	A	92	LEU
1	A	109	GLU
1	A	233	LEU
1	A	251	ARG
1	A	273	GLN
1	A	310	LEU
1	A	315	SER
1	A	350	LEU
1	A	352	LEU
1	A	369	SER
1	A	408	LEU
1	A	446	LEU
1	A	482	PHE
1	A	485	GLU
1	A	505	TYR
1	A	508	LEU
1	A	515	LEU
1	A	541	LEU
1	A	545	MET
1	A	588	ARG
1	A	617	LEU
1	A	637	VAL
1	A	662	THR
1	A	665	ARG
1	A	672	ILE
1	A	675	LEU
1	A	677	THR
1	A	679	SER

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Mol	Chain	Res	Type
1	A	683	VAL
1	A	695	ARG
1	B	30	ASN
1	B	92	LEU
1	B	112	ARG
1	B	219	TYR
1	B	227	THR
1	B	233	LEU
1	B	251	ARG
1	B	273	GLN
1	B	310	LEU
1	B	350	LEU
1	B	352	LEU
1	B	369	SER
1	B	408	LEU
1	B	436	THR
1	B	446	LEU
1	B	469	ASP
1	B	505	TYR
1	B	508	LEU
1	B	515	LEU
1	B	541	LEU
1	B	545	MET
1	B	588	ARG
1	B	593	VAL
1	B	598	GLU
1	B	617	LEU
1	B	637	VAL
1	B	662	THR
1	B	665	ARG
1	B	672	ILE
1	B	675	LEU
1	B	677	THR
1	B	679	SER
1	B	683	VAL
1	C	92	LEU
1	C	98	SER
1	C	179	GLN
1	C	206	GLN
1	C	233	LEU
1	C	251	ARG
1	C	273	GLN

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Mol	Chain	Res	Type
1	C	310	LEU
1	C	350	LEU
1	C	352	LEU
1	C	369	SER
1	C	408	LEU
1	C	446	LEU
1	C	485	GLU
1	C	505	TYR
1	C	508	LEU
1	C	515	LEU
1	C	541	LEU
1	C	545	MET
1	C	588	ARG
1	C	617	LEU
1	C	637	VAL
1	C	662	THR
1	C	665	ARG
1	C	672	ILE
1	C	675	LEU
1	C	677	THR
1	C	679	SER
1	C	683	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	C	237	HIS

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	PGE	B	1697	-	9,9,9	0.67	0	8,8,8	0.44	0
2	PG4	A	1696	-	12,12,12	0.73	0	11,11,11	0.58	0
2	PG4	C	1696	-	12,12,12	0.64	0	11,11,11	0.47	0
4	PEG	A	1699	-	6,6,6	0.50	0	5,5,5	0.32	0
4	PEG	C	1699	-	6,6,6	0.54	0	5,5,5	0.36	0
4	PEG	A	1701	-	6,6,6	0.52	0	5,5,5	0.20	0
4	PEG	B	1698	-	6,6,6	0.56	0	5,5,5	0.23	0
3	PGE	C	1698	-	9,9,9	0.67	0	8,8,8	1.15	1 (12%)
4	PEG	A	1700	-	6,6,6	0.49	0	5,5,5	0.43	0
4	PEG	C	1697	-	6,6,6	0.56	0	5,5,5	0.11	0
4	PEG	A	1698	-	6,6,6	0.70	0	5,5,5	0.74	0
4	PEG	B	1699	-	6,6,6	0.59	0	5,5,5	0.18	0
4	PEG	B	1696	-	6,6,6	0.64	0	5,5,5	0.58	0
4	PEG	B	1700	-	6,6,6	0.60	0	5,5,5	0.26	0
3	PGE	A	1697	-	9,9,9	0.64	0	8,8,8	0.47	0
3	PGE	C	1700	-	9,9,9	0.60	0	8,8,8	0.21	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
3	PGE	B	1697	-	-	0/7/7/7	-
2	PG4	A	1696	-	-	2/10/10/10	-
2	PG4	C	1696	-	-	1/10/10/10	-
4	PEG	A	1699	-	-	2/4/4/4	-
4	PEG	C	1699	-	-	1/4/4/4	-
4	PEG	A	1701	-	-	2/4/4/4	-
4	PEG	B	1698	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	C	1698	-	-	3/7/7/7	-
4	PEG	A	1700	-	-	3/4/4/4	-
4	PEG	C	1697	-	-	0/4/4/4	-
4	PEG	A	1698	-	-	0/4/4/4	-
4	PEG	B	1699	-	-	0/4/4/4	-
4	PEG	B	1696	-	-	0/4/4/4	-
4	PEG	B	1700	-	-	1/4/4/4	-
3	PGE	A	1697	-	-	3/7/7/7	-
3	PGE	C	1700	-	-	2/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1698	PGE	C3-O2-C2	2.00	121.97	113.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1698	PEG	O1-C1-C2-O2
3	A	1697	PGE	O3-C5-C6-O4
3	C	1700	PGE	O3-C5-C6-O4
4	B	1700	PEG	O2-C3-C4-O4
2	A	1696	PG4	O3-C5-C6-O4
4	A	1700	PEG	O2-C3-C4-O4
4	A	1701	PEG	O1-C1-C2-O2
3	C	1698	PGE	O2-C3-C4-O3
4	A	1699	PEG	O1-C1-C2-O2
3	A	1697	PGE	C4-C3-O2-C2
4	A	1699	PEG	C1-C2-O2-C3
3	C	1700	PGE	O2-C3-C4-O3
2	A	1696	PG4	O2-C3-C4-O3
4	A	1700	PEG	O1-C1-C2-O2
4	C	1699	PEG	O2-C3-C4-O4
3	A	1697	PGE	C1-C2-O2-C3
2	C	1696	PG4	O4-C7-C8-O5
3	C	1698	PGE	O1-C1-C2-O2
3	C	1698	PGE	O3-C5-C6-O4
4	A	1700	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1701	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1697	PGE	1	0
4	A	1700	PEG	2	0
3	A	1697	PGE	3	0
3	C	1700	PGE	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	683/695 (98%)	-0.51	6 (0%)	84	85	22, 35, 56, 95	0
1	B	684/695 (98%)	-0.50	7 (1%)	82	83	20, 36, 58, 86	0
1	C	682/695 (98%)	-0.48	6 (0%)	84	85	24, 38, 57, 93	0
All	All	2049/2085 (98%)	-0.50	19 (0%)	84	85	20, 36, 57, 95	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	TYR	5.5
1	A	152	ASP	3.7
1	B	6	GLN	3.6
1	B	219	TYR	3.2
1	C	219	TYR	3.1
1	C	168	HIS	3.0
1	C	681	ASP	3.0
1	A	168	HIS	2.9
1	C	569	ASP	2.8
1	B	20	ASP	2.5
1	A	70	ASN	2.4
1	B	569	ASP	2.4
1	B	681	ASP	2.3
1	A	18	GLY	2.2
1	A	645	GLU	2.1
1	B	121	TRP	2.1
1	B	645	GLU	2.1
1	C	121	TRP	2.1
1	C	627	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	A	1701	7/7	0.77	0.32	58,61,63,63	0
3	PGE	C	1698	10/10	0.83	0.19	35,40,53,57	0
3	PGE	C	1700	10/10	0.85	0.25	50,56,62,62	0
3	PGE	B	1697	10/10	0.85	0.24	48,57,61,64	0
4	PEG	B	1700	7/7	0.85	0.42	32,46,52,54	0
4	PEG	C	1699	7/7	0.85	0.35	54,58,66,70	0
4	PEG	A	1698	7/7	0.86	0.17	30,33,39,40	0
4	PEG	C	1697	7/7	0.88	0.20	37,45,55,55	0
2	PG4	A	1696	13/13	0.88	0.20	25,37,48,49	0
4	PEG	A	1699	7/7	0.89	0.17	33,40,44,46	0
3	PGE	A	1697	10/10	0.90	0.28	31,41,48,48	0
4	PEG	A	1700	7/7	0.91	0.29	39,50,60,61	0
2	PG4	C	1696	13/13	0.91	0.21	26,42,49,50	0
4	PEG	B	1696	7/7	0.91	0.14	27,29,37,39	0
4	PEG	B	1699	7/7	0.92	0.32	46,48,52,54	0
4	PEG	B	1698	7/7	0.94	0.14	28,33,44,45	0
5	ZN	A	1702	1/1	0.98	0.08	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.