



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:52 AM JST

PDB ID : 7EE6
Title : Crystal structure of PltC toxin
Authors : Liu, X.Y.; Chen, Z.; Gao, X.
Deposited on : 2021-03-17
Resolution : 2.29 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)
Xtrriage (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

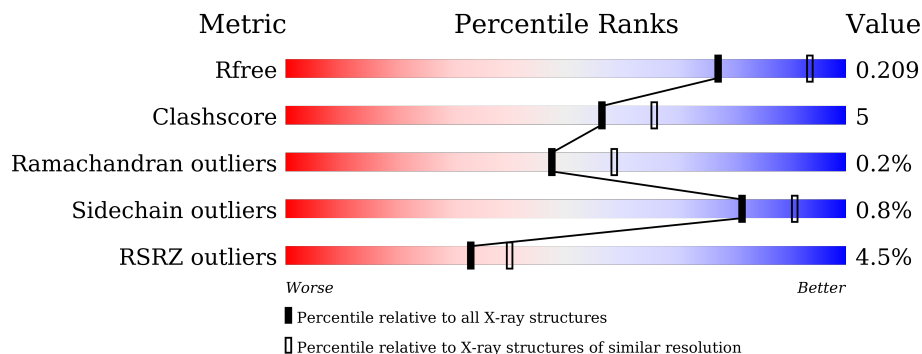
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	120	
1	B	120	
1	C	120	
1	D	120	
1	E	120	
2	F	248	

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Mol	Chain	Length	Quality of chain
3	G	224	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	E	201	-	-	-	X
4	PEG	G	303	-	-	-	X
5	ACN	G	305	-	-	-	X
5	ACN	G	308	-	-	-	X
6	GOL	A	204	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8956 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 Subtilase cytotoxin subunit B-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	Total 932	C 589	N 151	O 184	S 8	0	1	0
1	B	120	Total 939	C 591	N 153	O 187	S 8	0	0	0
1	C	120	Total 939	C 591	N 153	O 187	S 8	0	0	0
1	D	118	Total 924	C 583	N 150	O 183	S 8	0	0	0
1	E	119	Total 931	C 587	N 151	O 185	S 8	0	0	0

- Molecule 2 is a protein called Cytolethal distending toxin subunit B family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	248	Total 1916	C 1207	N 349	O 355	S 5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	270	LEU	-	expression tag	UNP A0A718C6E5

- Molecule 3 is a protein called Pertussis-like toxin subunit ArtA.

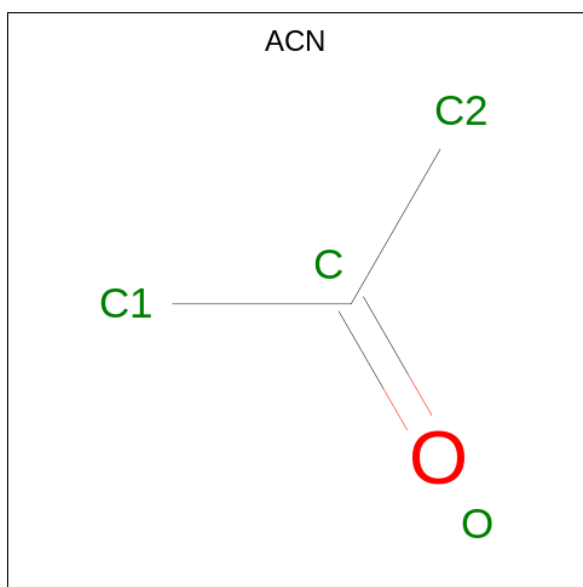
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	217	Total 1711	C 1088	N 286	O 330	S 7	0	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is ACETONE (three-letter code: ACN) (formula: C₃H₆O).



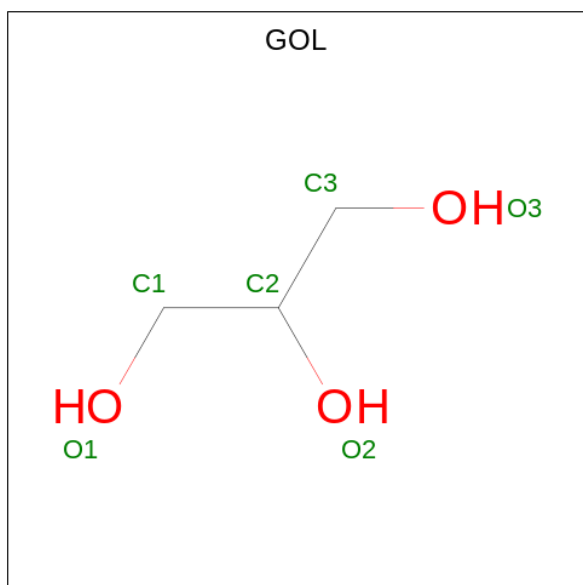
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 3 1	0	0
5	A	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	E	1	Total C O 4 3 1	0	0
5	G	1	Total C O 4 3 1	0	0
5	G	1	Total C O 4 3 1	0	0
5	G	1	Total C O 4 3 1	0	0
5	G	1	Total C O 4 3 1	0	0

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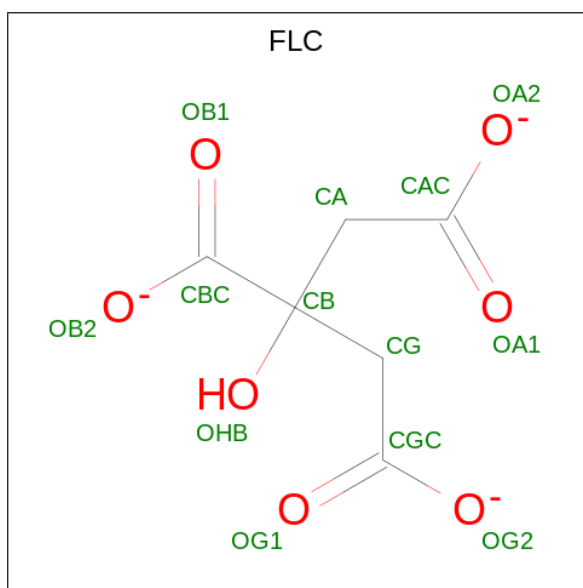
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			4	3	1		
5	G	1	Total	C	O	0	0
			4	3	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	C O	0	0
			13	6 7		
7	G	1	Total	C O	0	0
			13	6 7		

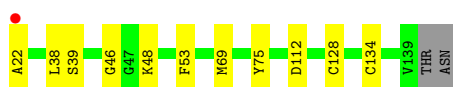
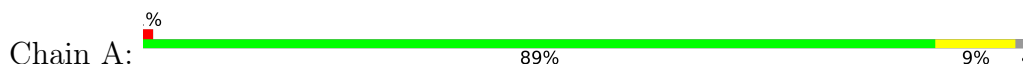
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	68	Total	O	0	0
			68	68		
8	B	58	Total	O	0	0
			58	58		
8	C	53	Total	O	0	0
			53	53		
8	D	59	Total	O	0	0
			59	59		
8	E	63	Total	O	0	0
			63	63		
8	F	56	Total	O	0	0
			56	56		
8	G	93	Total	O	0	0
			93	93		

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.

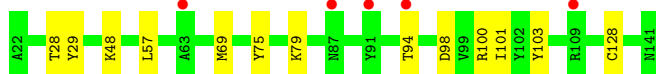
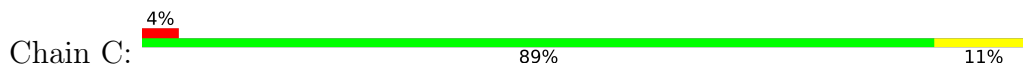
- Molecule 1: Subtilase cytotoxin subunit B-like protein



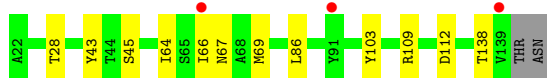
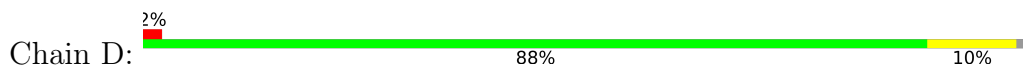
- Molecule 1: Subtilase cytotoxin subunit B-like protein



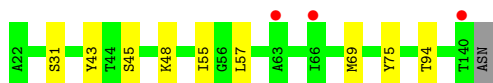
- Molecule 1: Subtilase cytotoxin subunit B-like protein



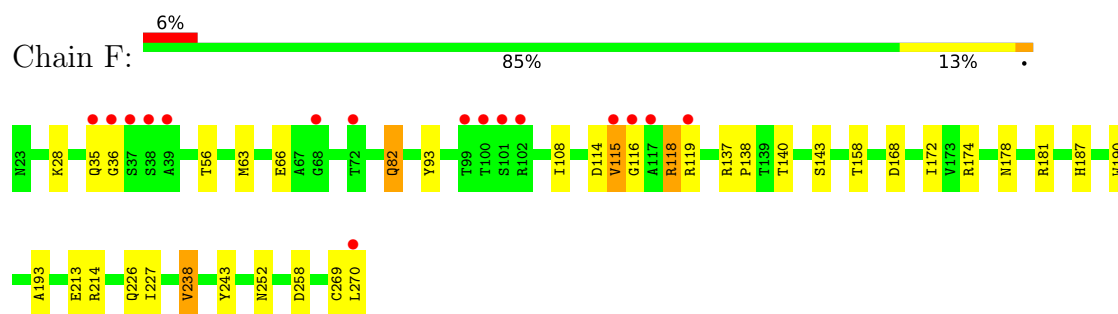
- Molecule 1: Subtilase cytotoxin subunit B-like protein



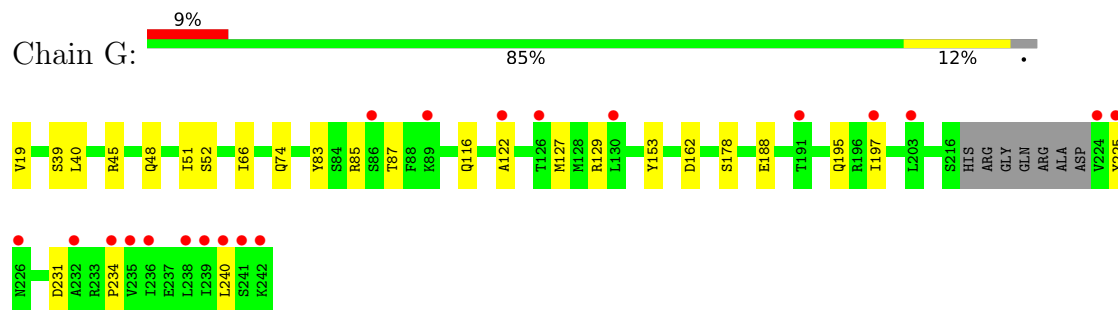
- Molecule 1: Subtilase cytotoxin subunit B-like protein



- Molecule 2: Cytolethal distending toxin subunit B family protein



- Molecule 3: Pertussis-like toxin subunit ArtA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.00Å 184.17Å 68.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.29 49.08 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.08-2.29) 99.5 (49.08-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.170 , 0.209 0.170 , 0.209	Depositor DCC
R_{free} test set	3391 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8956	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FLC, ACN, PEG

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	0.46	0/953	0.62	0/1289
1	B	0.46	0/960	0.61	0/1299
1	C	0.49	0/960	0.67	0/1299
1	D	0.43	0/945	0.57	0/1278
1	E	0.41	0/952	0.60	0/1288
2	F	0.48	1/1958 (0.1%)	0.65	0/2673
3	G	0.44	0/1750	0.58	0/2375
All	All	0.46	1/8478 (0.0%)	0.62	0/11501

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	82	GLN	C-N	8.13	1.49	1.34

There are no bond angle outliers.

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	932	0	878	11	0
1	B	939	0	881	5	0
1	C	939	0	881	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	924	0	868	9	0
1	E	931	0	875	5	0
2	F	1916	0	1903	29	0
3	G	1711	0	1661	20	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
4	D	21	0	30	4	0
4	E	14	0	20	1	0
4	F	7	0	10	1	0
4	G	14	0	20	1	0
5	A	8	0	12	2	0
5	B	16	0	24	2	0
5	C	4	0	6	0	0
5	D	8	0	12	1	0
5	E	4	0	6	0	0
5	G	24	0	36	0	0
6	A	6	0	8	3	0
6	B	12	0	16	0	0
6	C	12	0	16	0	0
6	E	12	0	16	0	0
6	F	12	0	16	1	0
7	F	13	0	5	0	0
7	G	13	0	5	0	0
8	A	68	0	0	1	0
8	B	58	0	0	0	0
8	C	53	0	0	1	0
8	D	59	0	0	0	0
8	E	63	0	0	0	0
8	F	56	0	0	2	0
8	G	93	0	0	1	0
All	All	8956	0	8225	84	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 (84) 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:38:LEU:HG	5:A:202:ACN:H23	1.70	0.74
3:G:48:GLN:HE22	3:G:195:GLN:HE22	1.34	0.73
1:A:46:GLY:H	6:A:204:GOL:H32	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:48:GLN:HE22	3:G:195:GLN:NE2	1.94	0.65
2:F:190:TRP:CE2	2:F:238:VAL:HG13	2.32	0.64
2:F:115:VAL:HG12	2:F:118:ARG:HG3	1.83	0.61
1:B:59:HIS:O	1:B:62:GLU:HG2	2.01	0.60
3:G:51:ILE:HG13	3:G:52:SER:N	2.17	0.59
3:G:19:VAL:N	3:G:178:SER:HG	2.01	0.59
1:D:109:ARG:NH1	4:D:201:PEG:H11	2.18	0.58
2:F:115:VAL:HG13	2:F:116:GLY:N	2.19	0.57
2:F:187:HIS:HB2	8:F:453:HOH:O	2.03	0.57
1:C:48:LYS:HD3	1:C:75:TYR:OH	2.06	0.56
1:E:31:SER:H	4:E:201:PEG:H22	1.71	0.56
1:C:69:MET:HE1	1:C:101:ILE:HG21	1.87	0.55
1:D:109:ARG:HH12	4:D:201:PEG:H11	1.72	0.55
1:D:86:LEU:HD12	5:D:204:ACN:H23	1.88	0.55
1:A:46:GLY:N	6:A:204:GOL:H11	2.22	0.55
3:G:116:GLN:NE2	3:G:188:GLU:OE2	2.27	0.54
1:A:48:LYS:NZ	8:A:304:HOH:O	2.39	0.54
2:F:63:MET:HG2	2:F:158:THR:HB	1.90	0.54
1:E:94:THR:HG23	3:G:122:ALA:HB3	1.90	0.53
2:F:63:MET:CE	2:F:193:ALA:HB3	2.38	0.53
2:F:114:ASP:OD2	2:F:137:ARG:NH1	2.41	0.53
3:G:40:LEU:HD23	3:G:66:ILE:HG13	1.90	0.53
3:G:85:ARG:HD3	3:G:225:TYR:OH	2.08	0.53
1:A:46:GLY:H	6:A:204:GOL:C3	2.21	0.53
3:G:162:ASP:HB3	4:G:303:PEG:H32	1.91	0.52
2:F:138:PRO:CG	2:F:172:ILE:HD13	2.40	0.52
3:G:127:MET:HG3	3:G:197:ILE:HG21	1.92	0.51
1:E:48:LYS:HD3	1:E:75:TYR:OH	2.11	0.50
2:F:28:LYS:NZ	6:F:303:GOL:H12	2.26	0.50
2:F:226:GLN:HG3	2:F:227:ILE:N	2.26	0.50
2:F:63:MET:HE1	2:F:193:ALA:HB3	1.92	0.50
1:C:29:TYR:CD1	1:C:100:ARG:HD3	2.47	0.49
1:C:57:LEU:HD11	1:C:69:MET:HE1	1.93	0.49
1:A:22:ALA:HB1	1:D:112:ASP:OD1	2.12	0.49
1:C:48:LYS:HD3	1:C:75:TYR:CZ	2.48	0.49
1:C:98:ASP:HB3	1:C:128:CYS:HB2	1.95	0.48
1:C:79:LYS:NZ	8:C:301:HOH:O	2.46	0.48
2:F:269:CYS:O	2:F:270:LEU:HB2	2.13	0.48
3:G:83:TYR:CD2	3:G:153:TYR:HB2	2.49	0.48
3:G:74:GLN:HG2	8:G:434:HOH:O	2.13	0.48
3:G:87:THR:HG23	3:G:225:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:ASP:HB3	2:F:118:ARG:HB2	1.96	0.47
1:B:98:ASP:H	5:B:205:ACN:H13	1.78	0.47
2:F:138:PRO:HG3	2:F:172:ILE:HD13	1.96	0.47
2:F:168:ASP:O	2:F:172:ILE:HG12	2.14	0.47
1:E:43:TYR:CE2	1:E:45:SER:HB2	2.49	0.47
1:D:64:ILE:O	1:D:67:ASN:HB3	2.15	0.47
2:F:56:THR:O	3:G:45:ARG:NH1	2.47	0.47
2:F:190:TRP:CZ2	2:F:238:VAL:HG13	2.50	0.46
3:G:87:THR:HG23	3:G:225:TYR:CE1	2.50	0.46
1:A:38:LEU:HG	5:A:202:ACN:C2	2.44	0.46
1:A:112:ASP:OD1	1:B:22:ALA:N	2.48	0.46
2:F:174:ARG:NH2	8:F:403:HOH:O	2.44	0.46
3:G:85:ARG:CD	3:G:225:TYR:OH	2.63	0.46
1:C:94:THR:HG21	3:G:240:LEU:HD21	1.98	0.46
2:F:243:TYR:CE2	3:G:39:SER:HB2	2.51	0.46
1:E:55:ILE:HD12	1:E:57:LEU:HD21	1.98	0.45
1:C:69:MET:CE	1:C:101:ILE:HG21	2.44	0.45
1:D:66:ILE:HG21	1:D:103:TYR:CZ	2.52	0.45
1:C:94:THR:O	3:G:129:ARG:HD3	2.16	0.45
2:F:140:THR:HB	2:F:143:SER:HB2	1.99	0.44
3:G:231:ASP:O	3:G:234:PRO:HD2	2.17	0.44
1:C:28:THR:HG22	1:C:103:TYR:CZ	2.53	0.44
1:B:61:SER:H	5:B:204:ACN:H23	1.83	0.43
1:D:138:THR:H	4:D:203:PEG:H12	1.83	0.43
2:F:35:GLN:HB2	2:F:66:GLU:OE1	2.18	0.43
4:D:202:PEG:H42	4:D:202:PEG:H22	1.52	0.43
1:B:91:TYR:O	1:B:94:THR:HB	2.19	0.43
2:F:213:GLU:OE1	2:F:214:ARG:NH1	2.51	0.43
1:D:28:THR:OG1	1:D:103:TYR:O	2.37	0.42
2:F:178:ASN:HA	2:F:181:ARG:HG2	2.02	0.42
1:A:48:LYS:HD3	1:A:75:TYR:OH	2.20	0.42
1:D:43:TYR:CE2	1:D:45:SER:HB2	2.55	0.41
1:A:39:SER:O	1:A:53:PHE:HA	2.20	0.41
2:F:36:GLY:HA2	2:F:258:ASP:H	1.86	0.41
2:F:138:PRO:HG2	2:F:172:ILE:HD13	2.01	0.41
2:F:252:ASN:HD22	4:F:302:PEG:H22	1.86	0.41
2:F:270:LEU:HD12	2:F:270:LEU:HA	1.96	0.40
1:A:128:CYS:HA	1:A:134:CYS:HA	2.03	0.40
2:F:93:TYR:HB2	2:F:108:ILE:HB	2.02	0.40
2:F:115:VAL:HG22	2:F:116:GLY:H	1.87	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	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
1	B	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
1	C	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
1	D	116/120 (97%)	112 (97%)	4 (3%)	0	100	100
1	E	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
2	F	246/248 (99%)	234 (95%)	10 (4%)	2 (1%)	19	23
3	G	213/224 (95%)	208 (98%)	5 (2%)	0	100	100
All	All	1045/1072 (98%)	1014 (97%)	29 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	115	VAL
2	F	118	ARG

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	102/103 (99%)	101 (99%)	1 (1%)	76	87
1	B	103/103 (100%)	102 (99%)	1 (1%)	76	87
1	C	103/103 (100%)	103 (100%)	0	100	100
1	D	101/103 (98%)	100 (99%)	1 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	102/103 (99%)	101 (99%)	1 (1%)	76	87
2	F	205/205 (100%)	202 (98%)	3 (2%)	65	79
3	G	191/196 (97%)	191 (100%)	0	100	100
All	All	907/916 (99%)	900 (99%)	7 (1%)	81	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	MET
1	B	69	MET
1	D	69	MET
1	E	69	MET
2	F	82	GLN
2	F	119	ARG
2	F	238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	195	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	E	202	-	6,6,6	0.18	0	5,5,5	0.15	0
4	PEG	G	303	-	6,6,6	0.49	0	5,5,5	0.40	0
5	ACN	D	205	-	3,3,3	0.76	0	3,3,3	0.23	0
5	ACN	B	205	-	3,3,3	0.77	0	3,3,3	0.27	0
4	PEG	D	202	-	6,6,6	0.52	0	5,5,5	0.45	0
5	ACN	B	204	-	3,3,3	0.79	0	3,3,3	0.24	0
4	PEG	D	203	-	6,6,6	0.48	0	5,5,5	0.23	0
5	ACN	A	203	-	3,3,3	0.77	0	3,3,3	0.23	0
4	PEG	D	201	-	6,6,6	0.50	0	5,5,5	0.66	0
5	ACN	E	203	-	3,3,3	0.80	0	3,3,3	0.30	0
5	ACN	D	204	-	3,3,3	0.69	0	3,3,3	0.08	0
4	PEG	A	201	-	6,6,6	0.51	0	5,5,5	0.94	0
5	ACN	C	201	-	3,3,3	0.76	0	3,3,3	0.42	0
6	GOL	E	205	-	5,5,5	0.61	0	5,5,5	0.75	0
5	ACN	G	308	-	3,3,3	0.74	0	3,3,3	0.26	0
6	GOL	F	303	-	5,5,5	0.53	0	5,5,5	0.38	0
6	GOL	E	204	-	5,5,5	0.49	0	5,5,5	0.29	0
6	GOL	B	207	-	5,5,5	0.66	0	5,5,5	0.59	0
6	GOL	C	202	-	5,5,5	0.49	0	5,5,5	0.36	0
4	PEG	F	302	-	6,6,6	0.47	0	5,5,5	0.32	0
4	PEG	E	201	-	6,6,6	0.50	0	5,5,5	0.25	0
4	PEG	G	302	-	6,6,6	0.49	0	5,5,5	0.29	0
5	ACN	G	304	-	3,3,3	0.72	0	3,3,3	0.17	0
6	GOL	B	206	-	5,5,5	0.52	0	5,5,5	0.21	0
6	GOL	C	203	-	5,5,5	0.55	0	5,5,5	0.64	0
6	GOL	F	304	-	5,5,5	0.56	0	5,5,5	0.29	0
5	ACN	A	202	-	3,3,3	0.71	0	3,3,3	0.18	0
5	ACN	B	202	-	3,3,3	0.70	0	3,3,3	0.30	0
6	GOL	A	204	-	5,5,5	0.57	0	5,5,5	0.75	0
5	ACN	G	307	-	3,3,3	0.76	0	3,3,3	0.13	0
5	ACN	G	306	-	3,3,3	0.76	0	3,3,3	0.22	0
5	ACN	G	309	-	3,3,3	0.77	0	3,3,3	0.17	0
5	ACN	G	305	-	3,3,3	0.81	0	3,3,3	0.33	0
7	FLC	G	301	-	12,12,12	1.04	0	17,17,17	1.81	4 (23%)
5	ACN	B	203	-	3,3,3	0.67	0	3,3,3	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FLC	F	301	-	12,12,12	1.00	0	17,17,17	1.54	2 (11%)
4	PEG	B	201	-	6,6,6	0.50	0	5,5,5	0.20	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	PEG	E	202	-	-	2/4/4/4	-
4	PEG	G	303	-	-	4/4/4/4	-
4	PEG	D	202	-	-	3/4/4/4	-
4	PEG	D	203	-	-	1/4/4/4	-
4	PEG	D	201	-	-	3/4/4/4	-
4	PEG	A	201	-	-	3/4/4/4	-
6	GOL	E	205	-	-	2/4/4/4	-
6	GOL	F	303	-	-	4/4/4/4	-
6	GOL	E	204	-	-	2/4/4/4	-
6	GOL	B	207	-	-	0/4/4/4	-
6	GOL	C	202	-	-	4/4/4/4	-
4	PEG	F	302	-	-	1/4/4/4	-
4	PEG	E	201	-	-	3/4/4/4	-
4	PEG	G	302	-	-	3/4/4/4	-
6	GOL	C	203	-	-	2/4/4/4	-
6	GOL	B	206	-	-	0/4/4/4	-
6	GOL	F	304	-	-	4/4/4/4	-
6	GOL	A	204	-	-	2/4/4/4	-
7	FLC	G	301	-	-	2/16/16/16	-
7	FLC	F	301	-	-	7/16/16/16	-
4	PEG	B	201	-	-	2/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	301	FLC	OB2-CBC-CB	4.27	120.46	113.05
7	F	301	FLC	OB2-CBC-CB	3.72	119.51	113.05
7	G	301	FLC	OB1-CBC-CB	-2.48	118.74	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	301	FLC	OA2-CAC-CA	2.29	121.71	114.35
7	G	301	FLC	CB-CA-CAC	-2.17	108.57	113.81
7	G	301	FLC	OG2-CGC-CG	2.13	121.19	114.35

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	202	GOL	O1-C1-C2-O2
6	C	202	GOL	O1-C1-C2-C3
6	C	203	GOL	C1-C2-C3-O3
6	E	204	GOL	O1-C1-C2-C3
6	E	205	GOL	C1-C2-C3-O3
6	F	304	GOL	O1-C1-C2-C3
6	F	304	GOL	C1-C2-C3-O3
6	F	304	GOL	O2-C2-C3-O3
7	F	301	FLC	CA-CB-CBC-OB1
7	F	301	FLC	CA-CB-CBC-OB2
7	F	301	FLC	OHB-CB-CBC-OB1
7	F	301	FLC	OHB-CB-CBC-OB2
6	C	203	GOL	O2-C2-C3-O3
4	A	201	PEG	O2-C3-C4-O4
4	B	201	PEG	O1-C1-C2-O2
4	D	202	PEG	O1-C1-C2-O2
4	D	201	PEG	O1-C1-C2-O2
4	G	303	PEG	O1-C1-C2-O2
4	D	202	PEG	C4-C3-O2-C2
6	A	204	GOL	C1-C2-C3-O3
6	F	303	GOL	O1-C1-C2-C3
6	F	303	GOL	C1-C2-C3-O3
6	A	204	GOL	O2-C2-C3-O3
6	E	205	GOL	O2-C2-C3-O3
6	F	304	GOL	O1-C1-C2-O2
4	G	302	PEG	O1-C1-C2-O2
4	G	303	PEG	C1-C2-O2-C3
4	G	302	PEG	O2-C3-C4-O4
6	E	204	GOL	O1-C1-C2-O2
6	F	303	GOL	O2-C2-C3-O3
4	B	201	PEG	C1-C2-O2-C3
4	D	203	PEG	C4-C3-O2-C2
4	E	202	PEG	C1-C2-O2-C3
4	G	302	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	D	201	PEG	C4-C3-O2-C2
6	C	202	GOL	O2-C2-C3-O3
4	E	201	PEG	O1-C1-C2-O2
4	F	302	PEG	C1-C2-O2-C3
4	A	201	PEG	C1-C2-O2-C3
4	G	303	PEG	C4-C3-O2-C2
4	E	201	PEG	C1-C2-O2-C3
7	G	301	FLC	CA-CB-CBC-OB1
4	E	202	PEG	C4-C3-O2-C2
4	G	303	PEG	O2-C3-C4-O4
6	F	303	GOL	O1-C1-C2-O2
4	D	202	PEG	C1-C2-O2-C3
4	A	201	PEG	C4-C3-O2-C2
7	F	301	FLC	CB-CA-CAC-OA2
7	F	301	FLC	CB-CA-CAC-OA1
6	C	202	GOL	C1-C2-C3-O3
4	E	201	PEG	C4-C3-O2-C2
7	F	301	FLC	CA-CB-CG-CGC
4	D	201	PEG	C1-C2-O2-C3
7	G	301	FLC	OHB-CB-CG-CGC

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	303	PEG	1	0
5	B	205	ACN	1	0
4	D	202	PEG	1	0
5	B	204	ACN	1	0
4	D	203	PEG	1	0
4	D	201	PEG	2	0
5	D	204	ACN	1	0
6	F	303	GOL	1	0
4	F	302	PEG	1	0
4	E	201	PEG	1	0
5	A	202	ACN	2	0
6	A	204	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	118/120 (98%)	-0.21	1 (0%) 86 89	31, 38, 56, 74	0
1	B	120/120 (100%)	-0.26	0 100 100	31, 41, 56, 103	0
1	C	120/120 (100%)	-0.08	5 (4%) 36 43	34, 44, 64, 85	0
1	D	118/120 (98%)	-0.11	3 (2%) 57 64	31, 42, 56, 63	0
1	E	119/120 (99%)	-0.04	3 (2%) 57 64	34, 45, 61, 111	0
2	F	248/248 (100%)	0.15	16 (6%) 18 24	37, 53, 91, 133	0
3	G	217/224 (96%)	0.15	20 (9%) 9 12	33, 43, 68, 100	0
All	All	1060/1072 (98%)	-0.01	48 (4%) 33 40	31, 44, 70, 133	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	38	SER	5.8
3	G	242	LYS	5.0
3	G	241	SER	4.7
1	E	140	THR	4.1
3	G	236	ILE	4.1
2	F	37	SER	4.1
1	D	139	VAL	3.9
2	F	102	ARG	3.7
3	G	240	LEU	3.5
2	F	100	THR	3.4
3	G	224	VAL	3.3
3	G	239	ILE	3.3
2	F	117	ALA	3.3
1	C	94	THR	3.3
1	A	22	ALA	3.2
2	F	35	GLN	3.1
1	D	66	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	116	GLY	3.1
1	E	66	ILE	3.1
3	G	130	LEU	3.0
3	G	238	LEU	3.0
2	F	36	GLY	2.8
3	G	86	SER	2.7
3	G	191	THR	2.7
1	C	109	ARG	2.7
3	G	235	VAL	2.7
2	F	101	SER	2.7
3	G	126	THR	2.7
3	G	197	ILE	2.6
2	F	119	ARG	2.6
2	F	39	ALA	2.6
2	F	72	THR	2.5
3	G	234	PRO	2.5
3	G	225	TYR	2.5
3	G	203	LEU	2.4
1	D	91	TYR	2.4
2	F	270	LEU	2.4
1	E	63	ALA	2.4
3	G	89	LYS	2.4
3	G	232	ALA	2.3
1	C	63	ALA	2.3
3	G	122	ALA	2.3
2	F	115	VAL	2.2
2	F	99	THR	2.2
1	C	87	ASN	2.1
1	C	91	TYR	2.1
2	F	68	GLY	2.0
3	G	226	ASN	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	E	201	7/7	0.45	0.43	82,97,104,115	0
4	PEG	E	202	7/7	0.68	0.37	77,84,92,97	0
5	ACN	G	305	4/4	0.69	0.40	51,58,66,78	0
6	GOL	A	204	6/6	0.69	0.41	64,71,76,85	0
6	GOL	C	202	6/6	0.71	0.16	66,74,78,81	0
4	PEG	D	201	7/7	0.77	0.25	60,63,67,68	0
5	ACN	G	308	4/4	0.77	0.41	67,71,84,92	0
6	GOL	F	303	6/6	0.78	0.31	67,70,80,89	0
5	ACN	B	202	4/4	0.79	0.34	54,58,66,77	0
4	PEG	G	302	7/7	0.79	0.34	68,74,80,86	0
7	FLC	G	301	13/13	0.79	0.15	58,77,85,87	0
4	PEG	G	303	7/7	0.80	0.51	64,68,90,94	0
4	PEG	F	302	7/7	0.80	0.26	74,83,90,97	0
5	ACN	B	204	4/4	0.80	0.21	65,69,71,76	0
4	PEG	D	203	7/7	0.83	0.39	73,77,83,84	0
5	ACN	B	203	4/4	0.83	0.29	54,64,64,68	0
6	GOL	B	207	6/6	0.83	0.18	68,71,74,76	0
5	ACN	E	203	4/4	0.84	0.19	72,79,82,86	0
6	GOL	E	204	6/6	0.84	0.16	65,72,81,84	0
5	ACN	G	309	4/4	0.86	0.20	73,79,80,85	0
5	ACN	A	203	4/4	0.87	0.26	65,66,70,70	0
5	ACN	A	202	4/4	0.88	0.23	33,42,46,48	0
5	ACN	C	201	4/4	0.88	0.33	48,54,58,63	0
5	ACN	D	205	4/4	0.89	0.15	62,63,71,72	0
5	ACN	B	205	4/4	0.91	0.20	70,72,74,77	0
4	PEG	A	201	7/7	0.92	0.23	39,50,52,61	0
5	ACN	G	306	4/4	0.92	0.28	61,61,62,67	0
5	ACN	G	307	4/4	0.93	0.14	58,58,60,64	0
6	GOL	E	205	6/6	0.93	0.15	43,53,61,66	0
4	PEG	B	201	7/7	0.93	0.15	64,69,73,79	0
5	ACN	G	304	4/4	0.93	0.23	50,53,59,66	0
5	ACN	D	204	4/4	0.94	0.17	34,38,39,39	0
4	PEG	D	202	7/7	0.94	0.20	38,49,52,56	0
6	GOL	B	206	6/6	0.95	0.20	39,45,51,55	0
7	FLC	F	301	13/13	0.95	0.12	51,58,66,68	0
6	GOL	C	203	6/6	0.95	0.13	46,58,61,69	0
6	GOL	F	304	6/6	0.96	0.16	69,70,75,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.