



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 10:12 AM EDT

PDB ID : 3RHF  
Title : Crystal structure of Polyphosphate Kinase 2 from *Arthrobacter aureus* TC1  
Authors : Nocek, B.; Hatzos-Skintges, C.; Feldmann, B.; Babnigg, G.; Joachimiak, A.;  
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Deposited on : 2011-04-11  
Resolution : 2.45 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

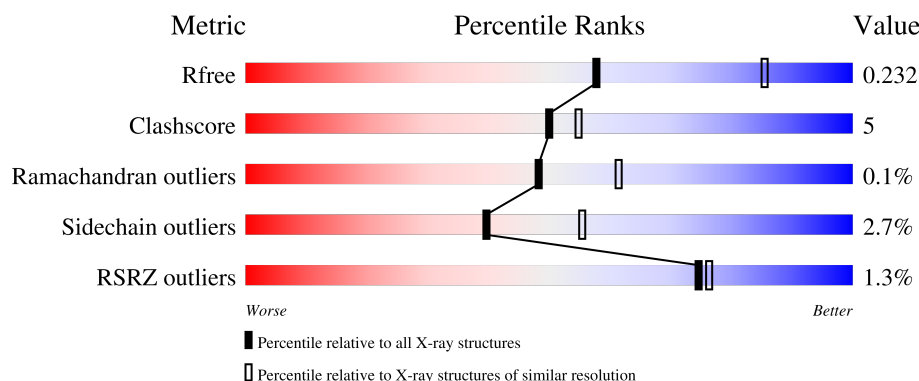
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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  $\geq 3$ , 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	289	<div> <div>2%</div> <div>85% 12% ..</div> </div>
1	B	289	<div> <div>86% 10% ..</div> </div>
1	C	289	<div> <div>2%</div> <div>88% 9% .</div> </div>
1	D	289	<div> <div>2%</div> <div>85% 10% ..</div> </div>

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
3	FLC	B	802	-	X	X	-
3	FLC	D	801	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9424 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 Putative polyphosphate kinase 2 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	Se	0	0	0
			2197	1399	381	412	5			
1	B	281	Total	C	N	O	Se	0	0	0
			2197	1399	381	412	5			
1	C	281	Total	C	N	O	Se	0	0	0
			2195	1397	381	412	5			
1	D	279	Total	C	N	O	Se	0	0	0
			2181	1389	377	410	5			

There are 12 discrepancies between the modelled and reference sequences:

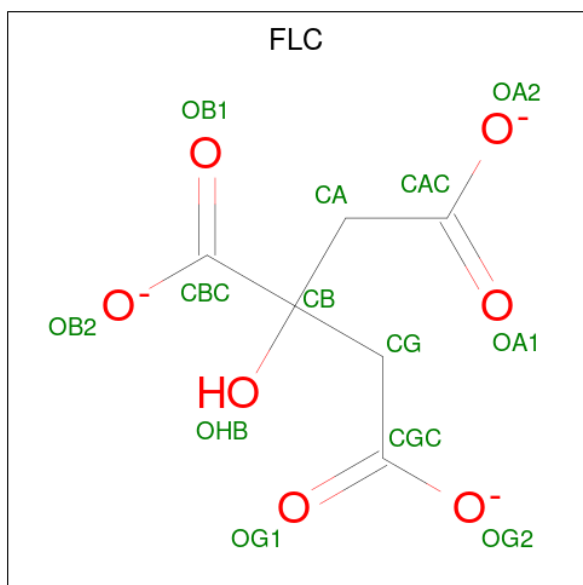
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A1R8G0
A	-1	ASN	-	expression tag	UNP A1R8G0
A	0	ALA	-	expression tag	UNP A1R8G0
B	-2	SER	-	expression tag	UNP A1R8G0
B	-1	ASN	-	expression tag	UNP A1R8G0
B	0	ALA	-	expression tag	UNP A1R8G0
C	-2	SER	-	expression tag	UNP A1R8G0
C	-1	ASN	-	expression tag	UNP A1R8G0
C	0	ALA	-	expression tag	UNP A1R8G0
D	-2	SER	-	expression tag	UNP A1R8G0
D	-1	ASN	-	expression tag	UNP A1R8G0
D	0	ALA	-	expression tag	UNP A1R8G0

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



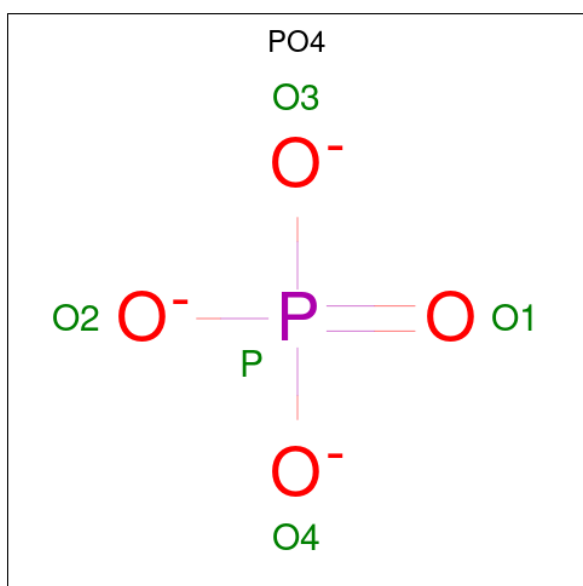
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



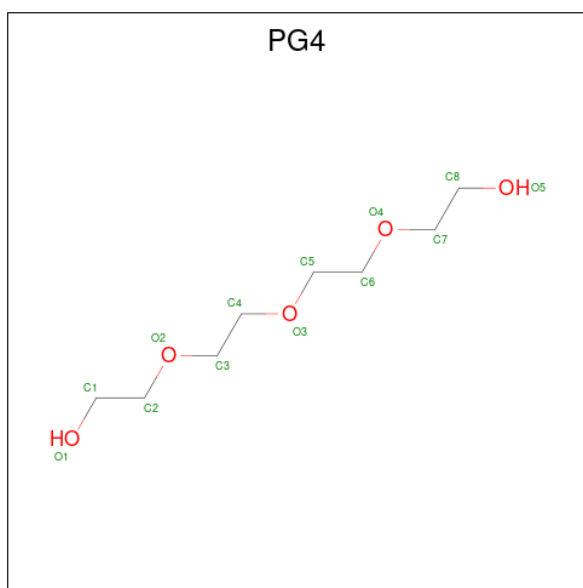
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		
5	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

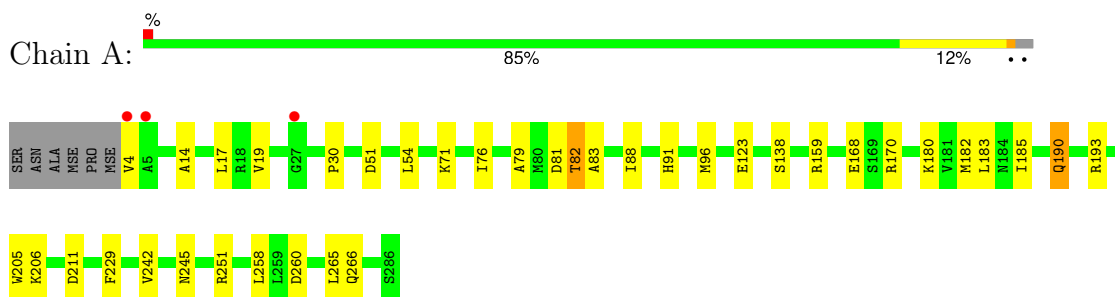
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	98	Total	O	0	0
			98	98		
8	B	113	Total	O	0	0
			113	113		
8	C	131	Total	O	0	0
			131	131		
8	D	119	Total	O	0	0
			119	119		



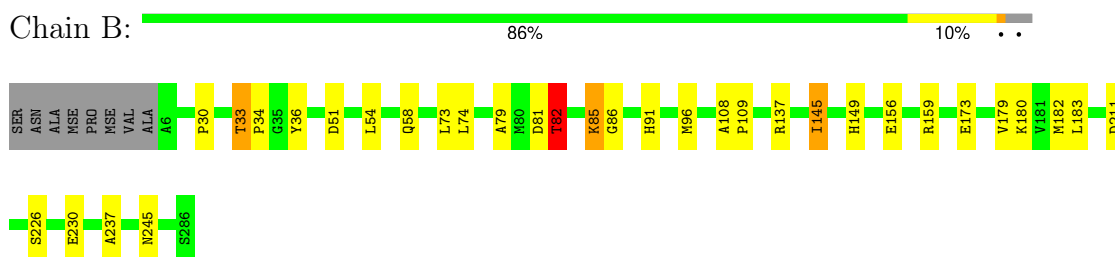
### 3 Residue-property plots [i](#)

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.

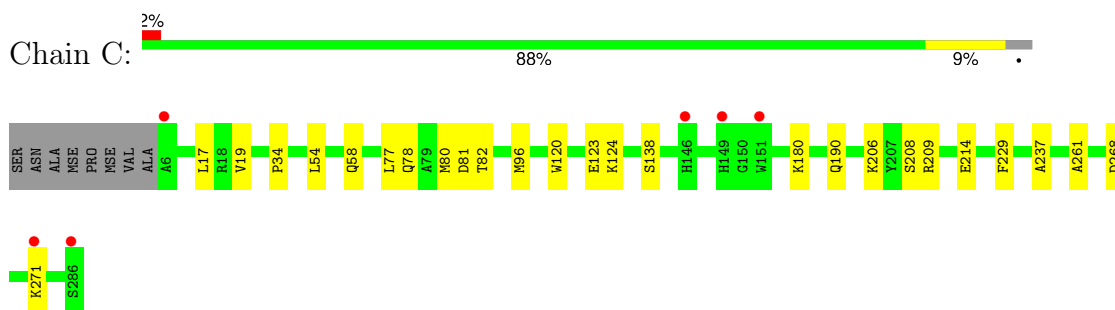
- Molecule 1: Putative polyphosphate kinase 2 family protein



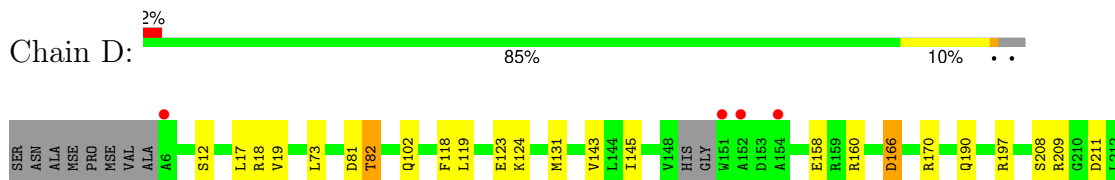
- Molecule 1: Putative polyphosphate kinase 2 family protein

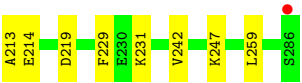


- Molecule 1: Putative polyphosphate kinase 2 family protein



- Molecule 1: Putative polyphosphate kinase 2 family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.35Å 126.35Å 199.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.45 40.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.45) 99.5 (40.00-2.45)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.184 , 0.235 0.183 , 0.232	Depositor DCC
$R_{free}$ test set	3024 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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 43.05 % 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 1.8662e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PG4, PGE, FLC, EDO, PO4

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	0.91	0/2240	0.84	2/3030 (0.1%)
1	B	0.99	1/2240 (0.0%)	0.85	1/3026 (0.0%)
1	C	1.00	2/2238 (0.1%)	0.87	0/3023
1	D	0.93	1/2222 (0.0%)	0.85	1/3000 (0.0%)
All	All	0.96	4/8940 (0.0%)	0.85	4/12079 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	GLU	CD-OE2	5.25	1.31	1.25
1	D	197	ARG	CB-CG	-5.23	1.38	1.52
1	C	120	TRP	CB-CG	-5.18	1.41	1.50
1	B	230	GLU	CG-CD	5.08	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	251	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	D	219	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	260	ASP	CB-CG-OD1	5.09	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2197	0	2162	25	0
1	B	2197	0	2174	23	0
1	C	2195	0	2167	17	0
1	D	2181	0	2156	22	0
2	A	20	0	28	3	0
2	D	20	0	28	2	0
3	A	13	0	5	1	0
3	B	13	0	5	5	0
3	C	13	0	5	0	0
3	D	13	0	5	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	1	0
4	D	5	0	0	0	0
5	B	26	0	36	1	0
5	C	13	0	18	1	0
5	D	13	0	18	2	0
6	B	1	0	0	0	0
7	C	4	0	6	0	0
7	D	4	0	6	0	0
8	A	98	0	0	1	0
8	B	113	0	0	1	0
8	C	131	0	0	0	0
8	D	119	0	0	3	0
All	All	9424	0	8819	92	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 (92) 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:B:81:ASP:O	1:B:82:THR:HB	1.58	1.00
1:B:33:THR:O	1:B:33:THR:HG22	1.70	0.91
1:C:81:ASP:O	1:C:82:THR:HG22	1.68	0.91
1:A:81:ASP:O	1:A:82:THR:HB	1.72	0.88
1:B:33:THR:O	1:B:33:THR:CG2	2.29	0.81
1:C:58:GLN:HB2	1:C:96:MSE:HE2	1.67	0.76
1:C:82:THR:HG21	1:C:190:GLN:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ASP:O	1:C:82:THR:CG2	2.40	0.70
1:C:80:MSE:HE3	1:C:214:GLU:OE2	1.93	0.68
1:A:17:LEU:HD13	1:A:242:VAL:HG22	1.76	0.68
1:C:124:LYS:HG2	1:D:124:LYS:HG2	1.78	0.65
1:A:82:THR:HG23	1:A:193:ARG:HD2	1.78	0.65
1:A:71:LYS:HD3	1:A:265:LEU:HD22	1.78	0.64
1:C:54:LEU:HD11	1:C:96:MSE:HE3	1.79	0.64
1:C:261:ALA:HB2	5:C:1001:PG4:H51	1.80	0.63
1:D:102:GLN:HG3	1:D:131:MSE:HE2	1.80	0.63
1:A:81:ASP:O	1:A:82:THR:CB	2.47	0.63
1:B:33:THR:HG21	8:B:339:HOH:O	1.98	0.62
1:A:51:ASP:OD1	1:A:91:HIS:HE1	1.84	0.60
1:D:208:SER:HA	5:D:1002:PG4:H82	1.84	0.59
2:A:901:PGE:H5	1:C:208:SER:HA	1.85	0.58
1:B:85:LYS:HE2	3:B:802:FLC:HG1	1.85	0.58
1:A:82:THR:HG21	1:A:190:GLN:HA	1.85	0.58
1:B:54:LEU:HD11	1:B:96:MSE:HE3	1.85	0.57
1:C:54:LEU:CD1	1:C:96:MSE:HE3	2.34	0.57
1:A:54:LEU:HD11	1:A:96:MSE:HE3	1.87	0.57
1:A:54:LEU:HD11	1:A:96:MSE:CE	2.35	0.56
2:A:901:PGE:H52	1:C:209:ARG:H	1.70	0.56
1:D:82:THR:HG21	1:D:190:GLN:HG2	1.88	0.55
1:C:81:ASP:O	1:C:82:THR:CB	2.54	0.55
3:B:802:FLC:CB	3:B:802:FLC:OA2	2.53	0.55
3:B:802:FLC:OG2	3:B:802:FLC:CA	2.55	0.55
1:D:81:ASP:O	1:D:82:THR:HB	2.07	0.55
1:B:33:THR:N	1:B:34:PRO:HD3	2.22	0.54
1:D:81:ASP:O	1:D:82:THR:CB	2.56	0.54
3:D:801:FLC:CB	3:D:801:FLC:OG2	2.56	0.53
1:B:81:ASP:OD2	1:B:211:ASP:OD1	2.27	0.53
1:B:81:ASP:O	1:B:82:THR:CB	2.40	0.53
1:C:19:VAL:HG11	1:C:229:PHE:HB3	1.91	0.53
1:D:118:PHE:CE2	1:D:160:ARG:HG2	2.44	0.52
4:C:288:PO4:O3	4:C:289:PO4:O4	2.27	0.52
1:D:213:ALA:O	1:D:214:GLU:C	2.48	0.52
1:D:123:GLU:HB3	8:D:332:HOH:O	2.10	0.51
1:B:73:LEU:HD23	1:B:74:LEU:N	2.26	0.51
1:B:145:ILE:HG22	1:B:149:HIS:HD2	1.75	0.51
2:D:903:PGE:H42	2:D:903:PGE:O4	2.10	0.50
1:D:158:GLU:OE2	1:D:231:LYS:NZ	2.41	0.50
1:B:179:VAL:HG22	5:B:287:PG4:H62	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ARG:NH1	8:D:529:HOH:O	2.29	0.49
1:A:82:THR:HG22	1:A:185:ILE:CD1	2.42	0.49
1:B:58:GLN:HB2	1:B:96:MSE:HE2	1.95	0.48
3:A:801:FLC:OA2	3:A:801:FLC:CBC	2.61	0.48
1:D:81:ASP:O	1:D:82:THR:HG22	2.13	0.48
1:A:54:LEU:HD21	1:A:96:MSE:HE3	1.95	0.48
1:A:54:LEU:CG	1:A:96:MSE:HE3	2.44	0.48
1:A:81:ASP:OD2	1:A:211:ASP:OD1	2.31	0.48
1:A:30:PRO:O	1:A:245:ASN:HB2	2.13	0.48
1:D:17:LEU:HD13	1:D:242:VAL:HG22	1.96	0.47
1:A:14:ALA:HB2	2:A:902:PGE:H22	1.96	0.47
1:A:123:GLU:OE2	1:A:170:ARG:NH2	2.48	0.47
1:A:170:ARG:NH1	8:A:317:HOH:O	2.38	0.47
1:A:82:THR:HG21	1:A:190:GLN:HG2	1.96	0.46
1:B:33:THR:HG23	1:B:36:TYR:HB3	1.96	0.46
1:C:180:LYS:HE2	1:C:237:ALA:O	2.15	0.46
1:B:86:GLY:N	3:B:802:FLC:HG2	2.31	0.46
1:A:19:VAL:HG11	1:A:229:PHE:HB3	1.99	0.45
1:D:19:VAL:HG11	1:D:229:PHE:HB3	1.99	0.45
1:C:54:LEU:CG	1:C:96:MSE:HE3	2.46	0.45
1:D:247:LYS:HB2	2:D:903:PGE:H3	1.98	0.44
1:D:102:GLN:HG3	1:D:131:MSE:CE	2.46	0.44
1:B:156:GLU:OE2	1:B:159:ARG:NH2	2.50	0.44
1:B:30:PRO:O	1:B:245:ASN:HB2	2.18	0.44
1:A:205:TRP:CE2	1:A:206:LYS:HG3	2.53	0.43
1:B:51:ASP:OD1	1:B:91:HIS:HE1	2.01	0.43
1:A:54:LEU:CD1	1:A:96:MSE:HE3	2.49	0.43
1:B:73:LEU:HD23	1:B:73:LEU:C	2.39	0.43
1:B:86:GLY:H	3:B:802:FLC:HG2	1.84	0.42
1:A:76:ILE:HG23	1:A:138:SER:HB3	2.02	0.42
1:B:108:ALA:HA	1:B:109:PRO:HD3	1.82	0.42
1:D:209:ARG:H	5:D:1002:PG4:H82	1.84	0.42
1:C:78:GLN:NE2	1:C:138:SER:OG	2.50	0.42
1:A:83:ALA:HA	1:A:185:ILE:HD13	2.02	0.42
1:D:145:ILE:HD12	8:D:481:HOH:O	2.20	0.42
1:D:166:ASP:OD2	1:D:170:ARG:NH1	2.49	0.41
1:D:81:ASP:OD2	1:D:211:ASP:OD1	2.38	0.41
1:A:168:GLU:OE1	1:A:180:LYS:NZ	2.50	0.41
1:C:17:LEU:HD21	1:C:34:PRO:HB2	2.03	0.41
1:D:119:LEU:O	1:D:123:GLU:HG3	2.21	0.41
1:A:79:ALA:HB2	1:A:183:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HE2	1:B:237:ALA:HB1	2.03	0.40
1:B:79:ALA:HB2	1:B:183:LEU:HB2	2.03	0.40
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.89	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	281/289 (97%)	269 (96%)	12 (4%)	0	100	100
1	B	279/289 (96%)	270 (97%)	8 (3%)	1 (0%)	30	38
1	C	279/289 (96%)	269 (96%)	10 (4%)	0	100	100
1	D	275/289 (95%)	265 (96%)	10 (4%)	0	100	100
All	All	1114/1156 (96%)	1073 (96%)	40 (4%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	THR

### 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	221/223 (99%)	213 (96%)	8 (4%)	30	44
1	B	223/223 (100%)	216 (97%)	7 (3%)	35	50
1	C	222/223 (100%)	218 (98%)	4 (2%)	54	68
1	D	221/223 (99%)	216 (98%)	5 (2%)	45	61
All	All	887/892 (99%)	863 (97%)	24 (3%)	40	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	82	THR
1	A	88	ILE
1	A	159	ARG
1	A	182	MSE
1	A	190	GLN
1	A	258	LEU
1	A	266	GLN
1	B	33	THR
1	B	82	THR
1	B	85	LYS
1	B	145	ILE
1	B	173	GLU
1	B	182	MSE
1	B	226	SER
1	C	77	LEU
1	C	206	LYS
1	C	268	ASP
1	C	271	LYS
1	D	12	SER
1	D	73	LEU
1	D	82	THR
1	D	143	VAL
1	D	166	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	B	149	HIS
1	B	184	ASN
1	C	78	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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$
2	PGE	D	903	-	9,9,9	0.73	0	8,8,8	0.42	0
2	PGE	A	902	-	9,9,9	0.68	0	8,8,8	0.60	0
4	PO4	A	287	-	4,4,4	0.89	0	6,6,6	1.25	1 (16%)
3	FLC	D	801	-	12,12,12	1.54	3 (25%)	17,17,17	4.99	9 (52%)
3	FLC	A	801	-	12,12,12	1.70	2 (16%)	17,17,17	1.45	2 (11%)
2	PGE	A	901	-	9,9,9	0.95	0	8,8,8	1.23	0
5	PG4	B	287	-	12,12,12	0.78	0	11,11,11	0.48	0
4	PO4	B	289	-	4,4,4	0.73	0	6,6,6	1.23	0
7	EDO	C	901	-	3,3,3	0.95	0	2,2,2	0.19	0
5	PG4	D	1002	-	12,12,12	0.61	0	11,11,11	0.52	0
5	PG4	B	1001	-	12,12,12	0.70	0	11,11,11	0.46	0
4	PO4	B	288	-	4,4,4	0.55	0	6,6,6	0.99	0
3	FLC	B	802	-	12,12,12	2.12	4 (33%)	17,17,17	5.34	7 (41%)
4	PO4	C	289	-	4,4,4	2.31	3 (75%)	6,6,6	1.00	0
4	PO4	C	288	-	4,4,4	0.70	0	6,6,6	1.01	1 (16%)
5	PG4	C	1001	-	12,12,12	0.65	0	11,11,11	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	D	288	-	4,4,4	0.52	0	6,6,6	0.80	0
3	FLC	C	801	-	12,12,12	1.33	1 (8%)	17,17,17	1.35	2 (11%)
4	PO4	C	287	-	4,4,4	0.85	0	6,6,6	0.80	0
4	PO4	A	288	-	4,4,4	1.83	2 (50%)	6,6,6	1.08	0
2	PGE	D	901	-	9,9,9	0.65	0	8,8,8	0.38	0
7	EDO	D	287	-	3,3,3	0.73	0	2,2,2	0.33	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
5	PG4	C	1001	-	-	5/10/10/10	-
2	PGE	A	901	-	-	4/7/7/7	-
5	PG4	B	287	-	-	6/10/10/10	-
2	PGE	D	903	-	-	2/7/7/7	-
3	FLC	C	801	-	-	0/16/16/16	-
2	PGE	A	902	-	-	5/7/7/7	-
7	EDO	C	901	-	-	0/1/1/1	-
5	PG4	D	1002	-	-	7/10/10/10	-
3	FLC	D	801	-	-	8/16/16/16	-
2	PGE	D	901	-	-	3/7/7/7	-
5	PG4	B	1001	-	-	4/10/10/10	-
3	FLC	A	801	-	-	13/16/16/16	-
3	FLC	B	802	-	-	10/16/16/16	-
7	EDO	D	287	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	FLC	CA-CB	4.13	1.59	1.54
3	B	802	FLC	CB-CBC	3.36	1.56	1.53
3	A	801	FLC	CG-CB	3.30	1.58	1.54
4	C	289	PO4	P-O2	-2.86	1.46	1.54
4	A	288	PO4	P-O1	2.84	1.57	1.50
3	D	801	FLC	CB-CBC	2.83	1.56	1.53
4	C	289	PO4	P-O4	-2.77	1.46	1.54
3	D	801	FLC	OHB-CB	2.59	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FLC	CA-CB	2.58	1.57	1.54
3	B	802	FLC	OB1-CBC	2.39	1.29	1.22
3	C	801	FLC	CA-CB	2.27	1.56	1.54
4	C	289	PO4	P-O3	-2.19	1.48	1.54
3	B	802	FLC	OHB-CB	2.10	1.47	1.43
4	A	288	PO4	P-O2	2.08	1.60	1.54
3	D	801	FLC	OA2-CAC	-2.03	1.24	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	FLC	OHB-CB-CBC	-13.59	89.69	108.96
3	B	802	FLC	OHB-CB-CG	-12.80	80.18	109.38
3	D	801	FLC	OHB-CB-CG	-10.89	84.53	109.38
3	D	801	FLC	OHB-CB-CBC	-10.01	94.76	108.96
3	D	801	FLC	OHB-CB-CA	-8.21	90.66	109.38
3	B	802	FLC	OHB-CB-CA	-7.85	91.48	109.38
3	D	801	FLC	OB2-CBC-CB	6.29	125.22	113.14
3	D	801	FLC	CA-CB-CBC	5.69	122.62	110.03
3	D	801	FLC	CG-CB-CBC	4.72	120.47	110.03
3	B	802	FLC	CA-CB-CBC	4.57	120.14	110.03
3	B	802	FLC	CG-CB-CBC	4.52	120.03	110.03
3	D	801	FLC	OB1-CBC-CB	-4.36	113.65	122.09
3	A	801	FLC	OB2-CBC-CB	3.97	120.75	113.14
3	B	802	FLC	CG-CB-CA	3.81	119.08	109.31
3	C	801	FLC	OB2-CBC-CB	3.54	119.93	113.14
3	D	801	FLC	CG-CB-CA	2.96	116.91	109.31
3	A	801	FLC	OHB-CB-CBC	-2.94	104.78	108.96
3	B	802	FLC	OB2-CBC-CB	2.86	118.63	113.14
3	D	801	FLC	OG1-CGC-CG	-2.54	115.77	122.95
4	A	287	PO4	O4-P-O2	2.37	115.28	107.91
4	C	288	PO4	O3-P-O1	-2.08	103.60	110.95
3	C	801	FLC	OHB-CB-CA	-2.05	104.69	109.38

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	FLC	OHB-CB-CBC-OB2
3	B	802	FLC	OHB-CB-CBC-OB1
3	B	802	FLC	OHB-CB-CBC-OB2
3	B	802	FLC	CA-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
2	A	902	PGE	O2-C3-C4-O3
5	C	1001	PG4	O1-C1-C2-O2
3	A	801	FLC	CAC-CA-CB-CBC
3	A	801	FLC	CAC-CA-CB-OHB
3	A	801	FLC	CBC-CB-CG-CGC
3	B	802	FLC	CAC-CA-CB-CBC
3	D	801	FLC	CBC-CB-CG-CGC
3	D	801	FLC	OHB-CB-CG-CGC
5	C	1001	PG4	O3-C5-C6-O4
5	B	287	PG4	O3-C5-C6-O4
5	B	1001	PG4	O3-C5-C6-O4
2	A	902	PGE	C1-C2-O2-C3
2	A	901	PGE	O2-C3-C4-O3
2	D	903	PGE	O3-C5-C6-O4
5	D	1002	PG4	O3-C5-C6-O4
3	A	801	FLC	CAC-CA-CB-CG
3	B	802	FLC	CAC-CA-CB-OHB
2	A	901	PGE	O3-C5-C6-O4
3	A	801	FLC	CG-CB-CBC-OB2
3	D	801	FLC	CAC-CA-CB-CG
2	A	902	PGE	O1-C1-C2-O2
5	B	1001	PG4	O4-C7-C8-O5
5	B	287	PG4	O4-C7-C8-O5
5	D	1002	PG4	O1-C1-C2-O2
2	A	901	PGE	C4-C3-O2-C2
5	D	1002	PG4	O4-C7-C8-O5
5	B	1001	PG4	O1-C1-C2-O2
5	D	1002	PG4	C6-C5-O3-C4
3	A	801	FLC	CA-CB-CG-CGC
2	D	903	PGE	O1-C1-C2-O2
5	B	287	PG4	O2-C3-C4-O3
2	A	902	PGE	C4-C3-O2-C2
2	D	901	PGE	O3-C5-C6-O4
5	D	1002	PG4	C8-C7-O4-C6
2	A	901	PGE	C6-C5-O3-C4
2	D	901	PGE	C6-C5-O3-C4
3	A	801	FLC	CA-CB-CBC-OB1
3	A	801	FLC	CG-CB-CBC-OB1
5	B	287	PG4	C5-C6-O4-C7
2	A	902	PGE	O3-C5-C6-O4
2	D	901	PGE	O1-C1-C2-O2
5	B	287	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	B	802	FLC	CB-CG-CGC-OG2
5	C	1001	PG4	O2-C3-C4-O3
3	A	801	FLC	OHB-CB-CBC-OB1
3	A	801	FLC	CA-CB-CBC-OB2
3	D	801	FLC	CA-CB-CBC-OB1
3	D	801	FLC	CA-CB-CBC-OB2
3	B	802	FLC	CB-CG-CGC-OG1
3	B	802	FLC	OHB-CB-CG-CGC
5	C	1001	PG4	C1-C2-O2-C3
5	D	1002	PG4	C1-C2-O2-C3
5	D	1002	PG4	O2-C3-C4-O3
5	C	1001	PG4	O4-C7-C8-O5
3	A	801	FLC	CB-CG-CGC-OG2
3	A	801	FLC	CB-CG-CGC-OG1
5	B	287	PG4	C4-C3-O2-C2
3	B	802	FLC	CB-CA-CAC-OA1
3	B	802	FLC	CB-CA-CAC-OA2
3	D	801	FLC	CB-CG-CGC-OG1
5	B	1001	PG4	O2-C3-C4-O3
3	D	801	FLC	CB-CA-CAC-OA2
3	D	801	FLC	CB-CG-CGC-OG2

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	903	PGE	2	0
2	A	902	PGE	1	0
3	D	801	FLC	1	0
3	A	801	FLC	1	0
2	A	901	PGE	2	0
5	B	287	PG4	1	0
5	D	1002	PG4	2	0
3	B	802	FLC	5	0
4	C	289	PO4	1	0
4	C	288	PO4	1	0
5	C	1001	PG4	1	0

## 5.7 Other polymers

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/289 (96%)	-0.50	3 (1%) 77 79	21, 33, 55, 68	0
1	B	276/289 (95%)	-0.57	0 100 100	20, 30, 50, 61	0
1	C	276/289 (95%)	-0.53	6 (2%) 62 65	19, 28, 55, 68	0
1	D	274/289 (94%)	-0.49	5 (1%) 67 69	20, 31, 58, 73	0
All	All	1104/1156 (95%)	-0.52	14 (1%) 74 76	19, 31, 55, 73	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ALA	4.3
1	D	6	ALA	3.8
1	C	6	ALA	3.5
1	D	151	TRP	3.2
1	D	286	SER	3.2
1	C	271	LYS	3.1
1	C	286	SER	2.9
1	A	4	VAL	2.9
1	D	154	ALA	2.7
1	D	152	ALA	2.6
1	C	149	HIS	2.4
1	A	27	GLY	2.4
1	C	146	HIS	2.3
1	C	151	TRP	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	FLC	A	801	13/13	0.76	0.14	43,58,61,63	0
7	EDO	C	901	4/4	0.79	0.21	43,45,46,46	0
4	PO4	C	289	5/5	0.80	0.18	55,59,62,64	0
5	PG4	B	287	13/13	0.84	0.15	43,45,65,67	0
7	EDO	D	287	4/4	0.84	0.23	52,52,53,53	0
5	PG4	B	1001	13/13	0.87	0.13	59,62,68,68	0
3	FLC	B	802	13/13	0.87	0.11	33,44,48,50	0
4	PO4	A	288	5/5	0.89	0.18	33,36,40,44	0
5	PG4	C	1001	13/13	0.89	0.13	41,49,57,58	0
4	PO4	B	288	5/5	0.90	0.10	62,63,63,64	0
4	PO4	C	288	5/5	0.90	0.12	51,52,53,56	0
2	PGE	D	903	10/10	0.90	0.13	43,46,50,51	0
2	PGE	A	902	10/10	0.90	0.11	49,49,53,53	0
2	PGE	D	901	10/10	0.92	0.09	40,41,46,47	0
4	PO4	A	287	5/5	0.93	0.10	56,57,59,59	0
2	PGE	A	901	10/10	0.93	0.09	22,26,30,31	0
5	PG4	D	1002	13/13	0.94	0.09	25,30,52,54	0
4	PO4	C	287	5/5	0.94	0.10	51,52,54,55	0
3	FLC	D	801	13/13	0.94	0.08	31,37,38,40	0
4	PO4	B	289	5/5	0.95	0.15	41,42,46,48	0
6	CL	B	290	1/1	0.96	0.11	60,60,60,60	0
3	FLC	C	801	13/13	0.96	0.07	30,34,37,41	0
4	PO4	D	288	5/5	0.96	0.08	52,52,53,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.