



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:29 PM GMT

PDB ID : 4YEF  
Title : beta1 carbohydrate binding module (CBM) of AMP-activated protein kinase (AMPK) in complex with glucosyl-beta-cyclododextrin  
Authors : Mobbs, J.; Gorman, M.A.; Parker, M.W.; Gooley, P.R.; Griffin, M.  
Deposited on : 2015-02-24  
Resolution : 1.72 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

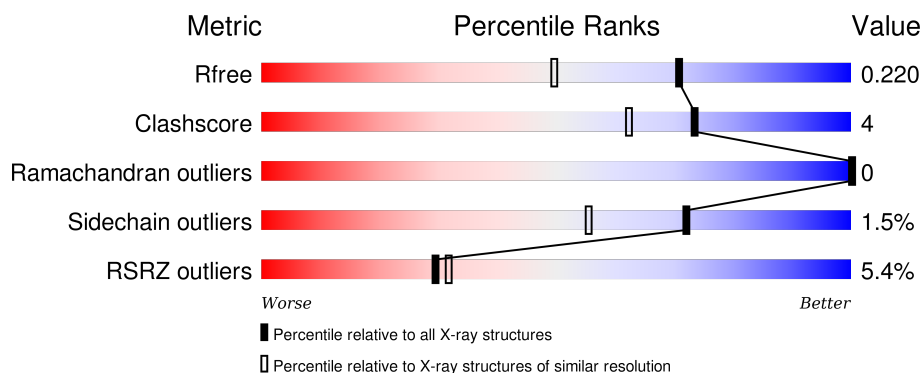
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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))
$R_{free}$	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	89	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	89	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	89	<div> <div></div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	D	89	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>
1	E	89	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>.</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	89	
1	G	89	

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	SO4	D	202	-	-	-	X
4	SO4	F	202	-	-	-	X
5	GLU	G	201[B]	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6310 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 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	0	1	0
			648	416	111	121			
1	B	86	Total	C	N	O	0	0	0
			682	434	118	130			
1	C	79	Total	C	N	O	0	1	0
			637	410	107	120			
1	D	77	Total	C	N	O	0	0	0
			597	386	101	110			
1	E	85	Total	C	N	O	0	1	0
			686	437	118	131			
1	F	77	Total	C	N	O	0	0	0
			596	386	102	108			
1	G	74	Total	C	N	O	0	74	0
			1117	723	185	209			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLY	-	expression tag	UNP P80386
A	69	PRO	-	expression tag	UNP P80386
A	70	LEU	-	expression tag	UNP P80386
A	71	GLY	-	expression tag	UNP P80386
A	72	SER	-	expression tag	UNP P80386
A	73	PRO	-	expression tag	UNP P80386
A	74	ASN	-	expression tag	UNP P80386
A	75	SER	-	expression tag	UNP P80386
B	68	GLY	-	expression tag	UNP P80386
B	69	PRO	-	expression tag	UNP P80386
B	70	LEU	-	expression tag	UNP P80386
B	71	GLY	-	expression tag	UNP P80386
B	72	SER	-	expression tag	UNP P80386
B	73	PRO	-	expression tag	UNP P80386
B	74	ASN	-	expression tag	UNP P80386

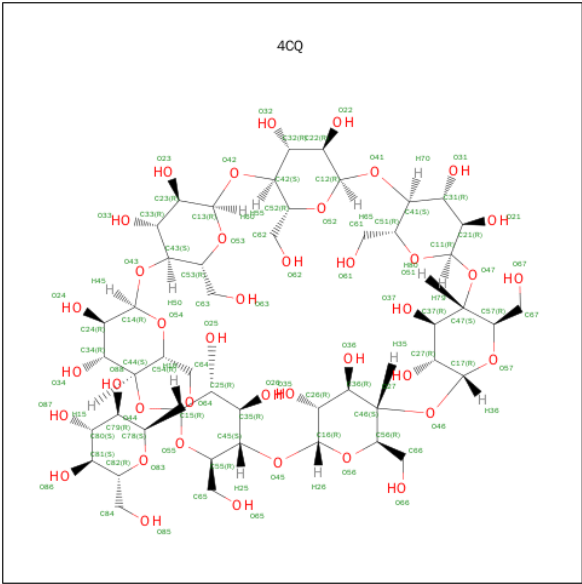
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Chain	Residue	Modelled	Actual	Comment	Reference
B	75	SER	-	expression tag	UNP P80386
C	68	GLY	-	expression tag	UNP P80386
C	69	PRO	-	expression tag	UNP P80386
C	70	LEU	-	expression tag	UNP P80386
C	71	GLY	-	expression tag	UNP P80386
C	72	SER	-	expression tag	UNP P80386
C	73	PRO	-	expression tag	UNP P80386
C	74	ASN	-	expression tag	UNP P80386
C	75	SER	-	expression tag	UNP P80386
D	68	GLY	-	expression tag	UNP P80386
D	69	PRO	-	expression tag	UNP P80386
D	70	LEU	-	expression tag	UNP P80386
D	71	GLY	-	expression tag	UNP P80386
D	72	SER	-	expression tag	UNP P80386
D	73	PRO	-	expression tag	UNP P80386
D	74	ASN	-	expression tag	UNP P80386
D	75	SER	-	expression tag	UNP P80386
E	68	GLY	-	expression tag	UNP P80386
E	69	PRO	-	expression tag	UNP P80386
E	70	LEU	-	expression tag	UNP P80386
E	71	GLY	-	expression tag	UNP P80386
E	72	SER	-	expression tag	UNP P80386
E	73	PRO	-	expression tag	UNP P80386
E	74	ASN	-	expression tag	UNP P80386
E	75	SER	-	expression tag	UNP P80386
F	68	GLY	-	expression tag	UNP P80386
F	69	PRO	-	expression tag	UNP P80386
F	70	LEU	-	expression tag	UNP P80386
F	71	GLY	-	expression tag	UNP P80386
F	72	SER	-	expression tag	UNP P80386
F	73	PRO	-	expression tag	UNP P80386
F	74	ASN	-	expression tag	UNP P80386
F	75	SER	-	expression tag	UNP P80386
G	68	GLY	-	expression tag	UNP P80386
G	69	PRO	-	expression tag	UNP P80386
G	70	LEU	-	expression tag	UNP P80386
G	71	GLY	-	expression tag	UNP P80386
G	72	SER	-	expression tag	UNP P80386
G	73	PRO	-	expression tag	UNP P80386
G	74	ASN	-	expression tag	UNP P80386
G	75	SER	-	expression tag	UNP P80386

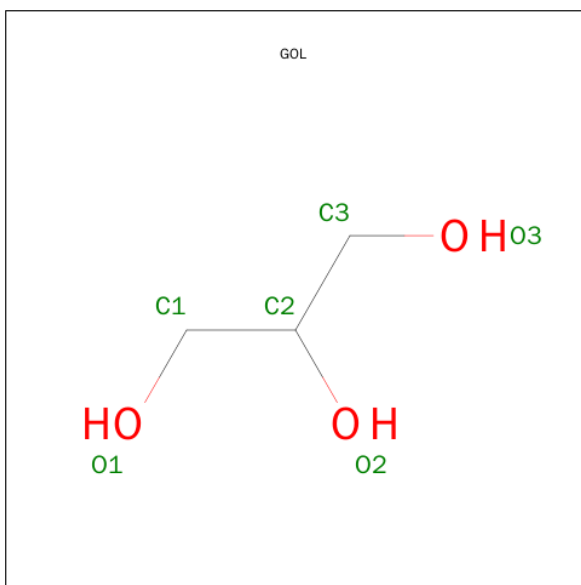
- Molecule 2 is 6-O-alpha-D-Glucosyl-beta-cyclodextrin (three-letter code: 4CQ) (formula:

C<sub>48</sub>H<sub>80</sub>O<sub>40</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			77	42	35		
2	B	1	Total	C	O	0	0
			77	42	35		
2	C	1	Total	C	O	0	0
			77	42	35		
2	D	1	Total	C	O	0	0
			77	42	35		
2	E	1	Total	C	O	0	0
			77	42	35		
2	F	1	Total	C	O	0	0
			77	42	35		
2	G	1	Total	C	O	0	1
			154	84	70		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



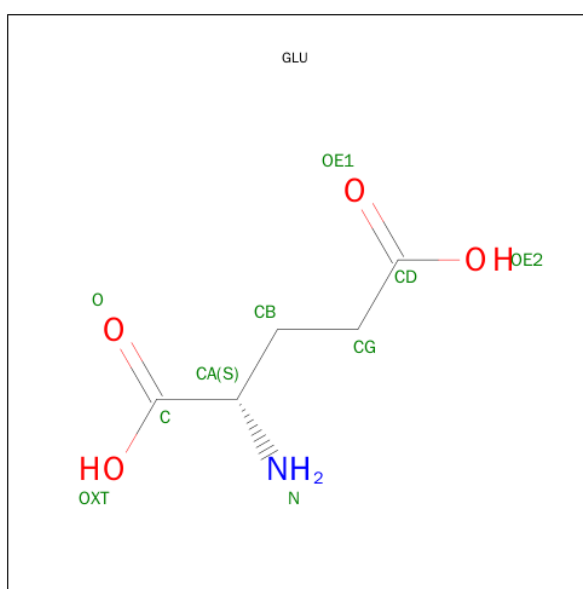
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	119	Total	O	0	0
			119	119		
6	B	156	Total	O	0	0
			156	156		
6	C	120	Total	O	0	0
			120	120		
6	D	57	Total	O	0	0
			57	57		

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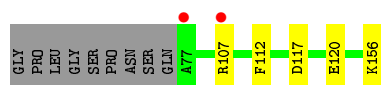
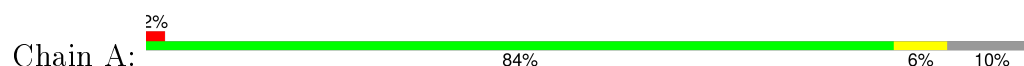
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	149	Total 149	O 149	0	0
6	F	59	Total 59	O 59	0	0
6	G	24	Total 24	O 24	0	0

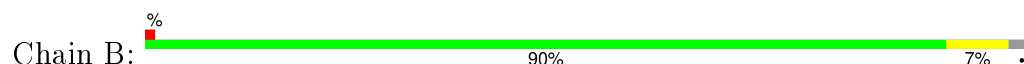
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

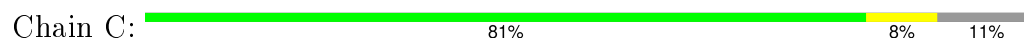
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



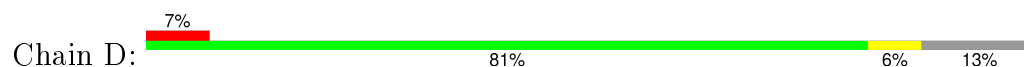
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



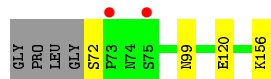
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1

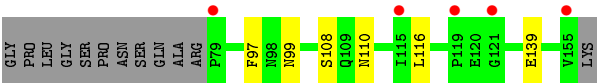


- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1

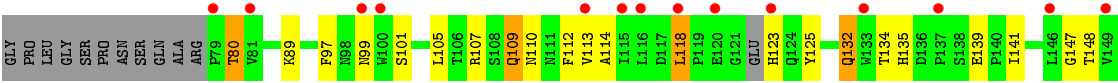


- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1





● Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.72Å 68.39Å 92.21Å 111.72° 95.56° 90.06°	Depositor
Resolution (Å)	43.71 – 1.72 43.71 – 1.72	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.71-1.72) 84.6 (43.71-1.72)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.178 , 0.213 0.186 , 0.220	Depositor DCC
$R_{free}$ test set	4764 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 32.7	EDS
Estimated twinning fraction	0.479 for -h,k,-k-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 95125 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, SO4, 4CQ

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	0.66	0/670	0.74	0/912
1	B	0.69	0/702	0.76	0/956
1	C	0.67	0/659	0.74	0/898
1	D	0.59	0/616	0.73	0/843
1	E	0.73	0/709	0.76	0/965
1	F	0.57	0/615	0.75	0/841
1	G	152.08	26/1176 (2.2%)	4.95	42/1606 (2.6%)
All	All	72.69	26/5147 (0.5%)	2.46	42/7021 (0.6%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	109[A]	GLN	CD-OE1	2102.00	47.48	1.24
1	G	109[B]	GLN	CD-OE1	2102.00	47.48	1.24
1	G	109[A]	GLN	CD-NE2	1872.02	48.12	1.32
1	G	109[B]	GLN	CD-NE2	1872.02	48.12	1.32
1	G	89[A]	LYS	C-O	1623.10	32.07	1.23
1	G	89[B]	LYS	C-O	1623.10	32.07	1.23
1	G	89[A]	LYS	CG-CD	905.23	32.30	1.52
1	G	89[B]	LYS	CG-CD	905.23	32.30	1.52
1	G	99[A]	ASN	CG-OD1	884.25	20.69	1.24
1	G	99[B]	ASN	CG-OD1	884.25	20.69	1.24
1	G	99[A]	ASN	CG-ND2	857.64	22.77	1.32
1	G	99[B]	ASN	CG-ND2	857.64	22.77	1.32
1	G	80[A]	THR	CB-OG1	511.09	11.65	1.43
1	G	80[B]	THR	CB-OG1	511.09	11.65	1.43
1	G	153[A]	ILE	CB-CG1	374.67	12.03	1.54
1	G	153[B]	ILE	CB-CG1	374.67	12.03	1.54
1	G	80[A]	THR	CB-CG2	328.13	12.35	1.52
1	G	80[B]	THR	CB-CG2	328.13	12.35	1.52
1	G	132[A]	GLN	CB-CG	295.10	9.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	132[B]	GLN	CB-CG	295.10	9.49	1.52
1	G	153[A]	ILE	CB-CG2	266.01	9.77	1.52
1	G	153[B]	ILE	CB-CG2	266.01	9.77	1.52
1	G	123[A]	HIS	CB-CG	143.70	4.08	1.50
1	G	123[B]	HIS	CB-CG	143.70	4.08	1.50
1	G	118[A]	LEU	CB-CG	128.63	5.25	1.52
1	G	118[B]	LEU	CB-CG	128.63	5.25	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	89[A]	LYS	O-C-N	-63.56	21.01	122.70
1	G	89[B]	LYS	O-C-N	-63.56	21.01	122.70
1	G	99[A]	ASN	OD1-CG-ND2	-51.99	2.32	121.90
1	G	99[B]	ASN	OD1-CG-ND2	-51.99	2.32	121.90
1	G	109[A]	GLN	OE1-CD-NE2	-51.88	2.57	121.90
1	G	109[B]	GLN	OE1-CD-NE2	-51.88	2.57	121.90
1	G	153[A]	ILE	CG1-CB-CG2	-48.02	5.77	111.40
1	G	153[B]	ILE	CG1-CB-CG2	-48.02	5.77	111.40
1	G	80[A]	THR	OG1-CB-CG2	-43.02	11.07	110.00
1	G	80[B]	THR	OG1-CB-CG2	-43.02	11.07	110.00
1	G	123[A]	HIS	CA-CB-CG	34.17	171.69	113.60
1	G	123[B]	HIS	CA-CB-CG	34.17	171.69	113.60
1	G	80[A]	THR	CA-CB-CG2	29.68	153.96	112.40
1	G	80[B]	THR	CA-CB-CG2	29.68	153.96	112.40
1	G	132[A]	GLN	CB-CG-CD	-29.65	34.52	111.60
1	G	132[B]	GLN	CB-CG-CD	-29.65	34.52	111.60
1	G	109[A]	GLN	CG-CD-OE1	-22.03	77.54	121.60
1	G	109[B]	GLN	CG-CD-OE1	-22.03	77.54	121.60
1	G	118[A]	LEU	CB-CG-CD1	-20.59	76.00	111.00
1	G	118[B]	LEU	CB-CG-CD1	-20.59	76.00	111.00
1	G	99[A]	ASN	CB-CG-OD1	-18.77	84.07	121.60
1	G	99[B]	ASN	CB-CG-OD1	-18.77	84.07	121.60
1	G	80[A]	THR	CA-CB-OG1	17.79	146.36	109.00
1	G	80[B]	THR	CA-CB-OG1	17.79	146.36	109.00
1	G	109[A]	GLN	CG-CD-NE2	-15.46	79.60	116.70
1	G	109[B]	GLN	CG-CD-NE2	-15.46	79.60	116.70
1	G	89[A]	LYS	CB-CG-CD	-14.98	72.65	111.60
1	G	89[B]	LYS	CB-CG-CD	-14.98	72.65	111.60
1	G	118[A]	LEU	CB-CG-CD2	-14.34	86.62	111.00
1	G	118[B]	LEU	CB-CG-CD2	-14.34	86.62	111.00
1	G	99[A]	ASN	CB-CG-ND2	-13.83	83.51	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	99[B]	ASN	CB-CG-ND2	-13.83	83.51	116.70
1	G	123[A]	HIS	CB-CG-ND1	-11.74	93.85	123.20
1	G	123[B]	HIS	CB-CG-ND1	-11.74	93.85	123.20
1	G	132[A]	GLN	CA-CB-CG	-10.72	89.82	113.40
1	G	132[B]	GLN	CA-CB-CG	-10.72	89.82	113.40
1	G	89[A]	LYS	CA-C-O	-8.72	101.78	120.10
1	G	89[B]	LYS	CA-C-O	-8.72	101.78	120.10
1	G	123[A]	HIS	CB-CG-CD2	-8.15	105.53	130.80
1	G	123[B]	HIS	CB-CG-CD2	-8.15	105.53	130.80
1	G	153[A]	ILE	CB-CG1-CD1	-6.79	94.89	113.90
1	G	153[B]	ILE	CB-CG1-CD1	-6.79	94.89	113.90

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	648	0	621	4	0
1	B	682	0	647	4	0
1	C	637	0	605	5	0
1	D	597	0	554	9	0
1	E	686	0	657	3	0
1	F	596	0	553	5	0
1	G	1117	0	1000	22	0
2	A	77	0	69	0	0
2	B	77	0	69	0	0
2	C	77	0	69	1	0
2	D	77	0	69	0	0
2	E	77	0	69	0	0
2	F	77	0	69	0	0
2	G	154	0	138	3	0
3	A	6	0	8	0	0
3	C	6	0	8	1	0
4	B	10	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	10	0	0	0	0
4	F	5	0	0	0	0
5	G	5	0	1	0	0
6	A	119	0	0	1	1
6	B	156	0	0	1	1
6	C	120	0	0	1	2
6	D	57	0	0	2	0
6	E	149	0	0	1	2
6	F	59	0	0	2	1
6	G	24	0	0	6	1
All	All	6310	0	5206	44	4

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 4.

All (44) 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:D:115:ILE:O	1:G:141[A]:ILE:HG12	1.61	1.00
1:G:147[A]:GLY:O	6:G:301:HOH:O	1.87	0.93
1:G:153[B]:ILE:C	6:G:305:HOH:O	2.09	0.91
1:G:107[B]:ARG:HD3	1:G:112[B]:PHE:CZ	2.11	0.86
2:G:202[B]:4CQ:H70	6:G:321:HOH:O	1.80	0.79
1:G:147[B]:GLY:O	6:G:303:HOH:O	2.02	0.77
1:G:110[A]:ASN:ND2	6:G:304:HOH:O	2.18	0.76
1:D:139:GLU:OE1	6:D:301:HOH:O	2.12	0.67
1:E:120:GLU:OE2	1:E:156:LYS:OXT	2.13	0.65
1:B:120:GLU:OE2	1:B:156:LYS:OXT	2.16	0.64
1:F:97:PHE:CE1	1:F:116:LEU:HD21	2.33	0.63
1:G:134[A]:THR:HG21	6:G:312:HOH:O	1.98	0.63
1:F:139:GLU:OE1	6:F:301:HOH:O	2.16	0.62
1:B:105:LEU:HD22	1:B:114:ALA:HB2	1.83	0.61
1:A:107:ARG:NH2	6:A:301:HOH:O	2.34	0.61
1:B:122:GLU:OE2	6:B:301:HOH:O	2.16	0.59
2:C:201:4CQ:O66	1:F:110:ASN:ND2	2.34	0.58
1:D:115:ILE:CG2	1:G:139[A]:GLU:O	2.54	0.55
1:D:115:ILE:HG21	1:G:139[A]:GLU:O	2.08	0.54
1:D:115:ILE:O	1:G:101[B]:SER:HB2	2.08	0.54
1:C:145[B]:GLN:NE2	6:C:301:HOH:O	2.20	0.52
1:F:99:ASN:HB2	6:F:311:HOH:O	2.11	0.51
1:A:107:ARG:HD2	1:A:112:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:349:HOH:O	1:G:135[A]:HIS:HE1	1.93	0.50
1:G:148[A]:THR:HG21	2:G:202[A]:4CQ:H48	1.93	0.50
1:C:109:GLN:O	1:C:110:ASN:HB2	2.13	0.49
1:C:120:GLU:OE1	1:C:156:LYS:OXT	2.31	0.49
1:G:105[A]:LEU:HD22	1:G:114[A]:ALA:HB2	1.96	0.48
1:D:116:LEU:HD23	1:G:141[A]:ILE:HG13	1.96	0.47
1:G:109[A]:GLN:O	1:G:110[A]:ASN:CB	2.63	0.47
1:G:113[B]:VAL:HG12	1:G:114[B]:ALA:N	2.31	0.45
1:A:120:GLU:OE1	1:A:156:LYS:OXT	2.35	0.44
1:G:109[A]:GLN:O	1:G:110[A]:ASN:HB3	2.18	0.44
1:D:115:ILE:O	1:G:141[A]:ILE:CG1	2.48	0.43
1:B:74:ASN:HB2	1:C:115:ILE:O	2.18	0.43
1:F:97:PHE:CE1	1:F:116:LEU:CD2	3.01	0.42
1:A:117:ASP:OD2	1:E:72:SER:N	2.53	0.42
1:G:97[B]:PHE:HE2	1:G:125[B]:TYR:HB3	1.85	0.42
1:G:148[B]:THR:HG21	2:G:202[B]:4CQ:H48	2.01	0.42
1:D:115:ILE:HG23	1:G:139[A]:GLU:O	2.19	0.41
1:C:97:PHE:HA	3:C:202:GOL:H32	2.01	0.41
1:G:109[B]:GLN:O	1:G:110[B]:ASN:HB3	2.19	0.41
1:D:115:ILE:HG23	1:D:115:ILE:O	2.21	0.41
1:E:99:ASN:ND2	6:E:305:HOH:O	2.53	0.41

All (4) 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)
6:B:339:HOH:O	6:C:358:HOH:O[1_655]	1.86	0.34
6:A:328:HOH:O	6:E:331:HOH:O[1_655]	1.98	0.22
6:F:307:HOH:O	6:G:318:HOH:O[1_644]	1.99	0.21
6:C:419:HOH:O	6:E:447:HOH:O[1_545]	2.11	0.09

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	79/89 (89%)	78 (99%)	1 (1%)	0	100	100
1	B	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
1	C	78/89 (88%)	77 (99%)	1 (1%)	0	100	100
1	D	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
1	E	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
1	F	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
1	G	140/89 (157%)	138 (99%)	2 (1%)	0	100	100
All	All	615/623 (99%)	605 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	71/78 (91%)	71 (100%)	0	100	100
1	B	75/78 (96%)	75 (100%)	0	100	100
1	C	70/78 (90%)	70 (100%)	0	100	100
1	D	63/78 (81%)	61 (97%)	2 (3%)	46	23
1	E	77/78 (99%)	77 (100%)	0	100	100
1	F	62/78 (80%)	61 (98%)	1 (2%)	70	53
1	G	118/78 (151%)	110 (93%)	8 (7%)	20	4
All	All	536/546 (98%)	525 (98%)	11 (2%)	72	40

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	107	ARG
1	D	108	SER
1	F	108	SER

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Mol	Chain	Res	Type
1	G	80[A]	THR
1	G	80[B]	THR
1	G	118[A]	LEU
1	G	118[B]	LEU
1	G	132[A]	GLN
1	G	132[B]	GLN
1	G	153[A]	ILE
1	G	153[B]	ILE

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

Mol	Chain	Res	Type
1	F	110	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

17 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
2	4CQ	A	201	-	84,84,96	0.55	0	126,126,144	1.01	7 (5%)
3	GOL	A	202	-	5,5,5	0.65	0	5,5,5	1.35	1 (20%)
2	4CQ	B	201	-	84,84,96	0.53	0	126,126,144	0.97	5 (3%)
4	SO4	B	202	-	4,4,4	0.74	0	6,6,6	0.58	0
4	SO4	B	203	-	4,4,4	0.42	0	6,6,6	0.81	0
2	4CQ	C	201	-	84,84,96	0.51	0	126,126,144	1.02	8 (6%)
3	GOL	C	202	-	5,5,5	0.59	0	5,5,5	0.65	0
2	4CQ	D	201	-	84,84,96	0.39	0	126,126,144	0.85	4 (3%)
4	SO4	D	202	-	4,4,4	0.76	0	6,6,6	0.27	0
2	4CQ	E	201	-	84,84,96	0.53	0	126,126,144	0.92	5 (3%)
4	SO4	E	202	-	4,4,4	0.86	0	6,6,6	0.92	0
4	SO4	E	203	-	4,4,4	0.47	0	6,6,6	0.34	0
2	4CQ	F	201	-	84,84,96	0.42	0	126,126,144	0.83	3 (2%)
4	SO4	F	202	-	4,4,4	0.77	0	6,6,6	0.16	0
5	GLU	G	201[B]	-	1,4,9	0.84	0	1,4,11	0.39	0
2	4CQ	G	202[A]	-	84,84,96	0.35	0	126,126,144	1.03	7 (5%)
2	4CQ	G	202[B]	-	84,84,96	0.35	0	126,126,144	0.95	7 (5%)

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
2	4CQ	A	201	-	-	0/42/182/207	0/0/8/9
3	GOL	A	202	-	-	0/4/4/4	0/0/0/0
2	4CQ	B	201	-	-	0/42/182/207	0/0/8/9
4	SO4	B	202	-	-	0/0/0/0	0/0/0/0
4	SO4	B	203	-	-	0/0/0/0	0/0/0/0
2	4CQ	C	201	-	-	0/42/182/207	0/0/8/9
3	GOL	C	202	-	-	0/4/4/4	0/0/0/0
2	4CQ	D	201	-	-	0/42/182/207	0/0/8/9
4	SO4	D	202	-	-	0/0/0/0	0/0/0/0
2	4CQ	E	201	-	-	0/42/182/207	0/0/8/9
4	SO4	E	202	-	-	0/0/0/0	0/0/0/0
4	SO4	E	203	-	-	0/0/0/0	0/0/0/0
2	4CQ	F	201	-	-	0/42/182/207	0/0/8/9
4	SO4	F	202	-	-	0/0/0/0	0/0/0/0
5	GLU	G	201[B]	-	-	0/0/2/9	0/0/0/0
2	4CQ	G	202[A]	-	-	0/42/182/207	0/0/8/9
2	4CQ	G	202[B]	-	-	0/42/182/207	0/0/8/9

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	4CQ	O63-C63-C53	-3.03	101.18	111.30
2	C	201	4CQ	O63-C63-C53	-3.02	101.21	111.30
2	G	202[A]	4CQ	C14-O43-C43	-3.00	110.02	118.00
2	B	201	4CQ	O63-C63-C53	-2.85	101.78	111.30
2	E	201	4CQ	O22-C22-C12	-2.77	103.86	110.01
2	A	201	4CQ	O63-C63-C53	-2.71	102.26	111.30
2	G	202[B]	4CQ	C13-O42-C42	-2.70	110.82	118.00
2	D	201	4CQ	O33-C33-C43	-2.57	103.80	109.89
2	G	202[A]	4CQ	O26-C26-C16	-2.50	104.45	110.01
2	G	202[B]	4CQ	C15-O44-C44	-2.47	111.42	118.00
2	D	201	4CQ	O63-C63-C53	-2.44	103.16	111.30
2	G	202[A]	4CQ	C16-O45-C45	-2.40	111.62	118.00
2	A	201	4CQ	C14-O43-C43	-2.35	111.76	118.00
2	G	202[A]	4CQ	C13-O42-C42	-2.35	111.76	118.00
2	C	201	4CQ	C14-O43-C43	-2.26	112.00	118.00
2	B	201	4CQ	O22-C22-C12	-2.22	105.09	110.01
2	C	201	4CQ	O62-C62-C52	-2.19	103.98	111.30
2	F	201	4CQ	O37-C37-C27	-2.19	105.42	110.36
2	C	201	4CQ	O56-C56-C46	-2.16	105.16	109.78
2	G	202[B]	4CQ	O26-C26-C16	-2.15	105.23	110.01
2	F	201	4CQ	O63-C63-C53	-2.15	104.11	111.30
2	G	202[B]	4CQ	C16-O45-C45	-2.11	112.38	118.00
2	C	201	4CQ	O67-C67-C57	-2.11	104.26	111.30
2	A	201	4CQ	C16-O56-C56	-2.05	109.71	113.74
2	G	202[A]	4CQ	C17-O57-C57	-2.02	109.77	113.74
2	C	201	4CQ	O21-C21-C31	-2.00	105.84	110.36
3	A	202	GOL	O2-C2-C3	2.00	118.08	108.47
2	D	201	4CQ	O53-C53-C43	2.01	114.06	109.78
2	A	201	4CQ	C33-C43-C53	2.01	115.45	110.85
2	A	201	4CQ	C14-O54-C54	2.10	117.86	113.74
2	G	202[B]	4CQ	O53-C53-C63	2.11	111.85	106.38
2	D	201	4CQ	C13-O53-C53	2.21	118.08	113.74
2	F	201	4CQ	O57-C57-C67	2.30	112.35	106.38
2	E	201	4CQ	O51-C51-C61	2.41	112.62	106.38
2	E	201	4CQ	C13-O53-C53	2.54	118.72	113.74
2	B	201	4CQ	O53-C53-C43	2.70	115.53	109.78
2	G	202[B]	4CQ	C13-O53-C53	3.01	119.65	113.74
2	B	201	4CQ	O51-C51-C61	3.04	114.26	106.38
2	E	201	4CQ	O53-C53-C43	3.05	116.28	109.78
2	A	201	4CQ	C13-O53-C53	3.17	119.97	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	4CQ	C13-O53-C53	3.25	120.12	113.74
2	A	201	4CQ	O53-C53-C43	3.28	116.78	109.78
2	B	201	4CQ	C13-O53-C53	3.52	120.65	113.74
2	G	202[B]	4CQ	O53-C53-C43	3.95	118.20	109.78
2	C	201	4CQ	O53-C53-C43	4.11	118.54	109.78
2	G	202[A]	4CQ	C13-O53-C53	4.32	122.22	113.74
2	G	202[A]	4CQ	O53-C53-C43	4.61	119.62	109.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	4CQ	1	0
3	C	202	GOL	1	0
2	G	202[A]	4CQ	1	0
2	G	202[B]	4CQ	2	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<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	80/89 (89%)	-0.13	2 (2%) 61 65	12, 19, 48, 60	0
1	B	86/89 (96%)	-0.15	1 (1%) 81 85	12, 18, 42, 70	0
1	C	79/89 (88%)	-0.21	0 100 100	12, 19, 40, 59	0
1	D	77/89 (86%)	0.26	6 (7%) 16 18	14, 31, 57, 72	0
1	E	85/89 (95%)	-0.07	2 (2%) 62 67	11, 18, 42, 54	0
1	F	77/89 (86%)	0.20	5 (6%) 22 24	14, 32, 57, 67	0
1	G	74/89 (83%)	1.15	14 (18%) 2 2	18, 26, 45, 54	8 (10%)
All	All	558/623 (89%)	0.13	30 (5%) 29 32	11, 21, 51, 72	8 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	73	PRO	5.6
1	G	81[A]	VAL	4.6
1	B	73	PRO	4.3
1	G	79[A]	PRO	4.0
1	F	155	VAL	3.9
1	G	115[A]	ILE	3.4
1	D	118	LEU	3.3
1	G	100[A]	TRP	3.2
1	F	121	GLY	3.1
1	G	123[A]	HIS	3.0
1	A	77	ALA	3.0
1	G	146[A]	LEU	3.0
1	D	121	GLY	2.9
1	G	120[A]	GLU	2.8
1	F	115	ILE	2.8
1	G	116[A]	LEU	2.8
1	G	137[A]	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	118[A]	LEU	2.7
1	D	119	PRO	2.7
1	G	113[A]	VAL	2.6
1	E	75	SER	2.5
1	A	107	ARG	2.4
1	F	79	PRO	2.3
1	G	149[A]	VAL	2.2
1	F	119	PRO	2.2
1	G	133[A]	TRP	2.2
1	D	153	ILE	2.1
1	D	79	PRO	2.1
1	D	80	THR	2.0
1	G	99[A]	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	F	202	5/5	0.95	0.27	7.83	45,46,49,49	0
5	GLU	G	201[B]	5/10	0.75	0.34	2.80	38,38,41,44	5
4	SO4	D	202	5/5	0.96	0.14	2.73	43,43,46,47	0
2	4CQ	G	202[B]	77/88	0.89	0.16	0.50	26,36,41,41	77
2	4CQ	G	202[A]	77/88	0.89	0.16	0.40	26,36,40,41	77
4	SO4	B	202	5/5	0.98	0.10	0.23	18,21,21,26	0
2	4CQ	E	201	77/88	0.93	0.10	0.15	15,31,47,56	0
2	4CQ	B	201	77/88	0.94	0.09	-0.05	15,30,47,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	4CQ	C	201	77/88	0.93	0.10	-0.17	15,29,44,58	0
2	4CQ	A	201	77/88	0.93	0.10	-0.20	15,28,44,54	0
4	SO4	B	203	5/5	0.98	0.08	-0.24	34,35,39,42	0
4	SO4	E	203	5/5	0.98	0.08	-0.30	34,36,41,45	0
2	4CQ	D	201	77/88	0.94	0.08	-0.41	17,28,38,45	0
2	4CQ	F	201	77/88	0.94	0.08	-0.48	17,28,38,44	0
4	SO4	E	202	5/5	0.99	0.09	-0.50	19,20,22,25	0
3	GOL	C	202	6/6	0.82	0.22	-	33,35,38,46	0
3	GOL	A	202	6/6	0.90	0.19	-	35,38,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.