



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:38 PM GMT

PDB ID : 4YEE  
Title : beta2 carbohydrate binding module (CBM) of AMP-activated protein kinase (AMPK) in complex with glucosyl-beta-cyclodextrin  
Authors : Mobbs, J.; Gorman, M.A.; Parker, M.W.; Gooley, P.R.; Griffin, M.  
Deposited on : 2015-02-24  
Resolution : 2.00 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

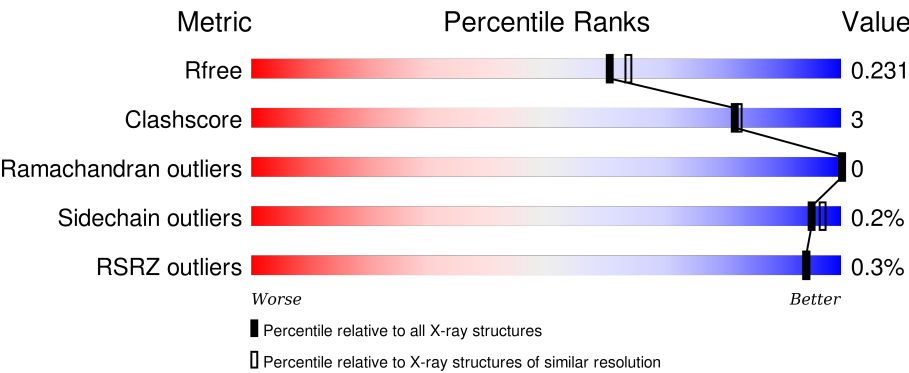
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.













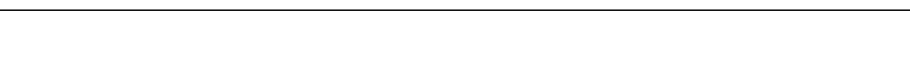
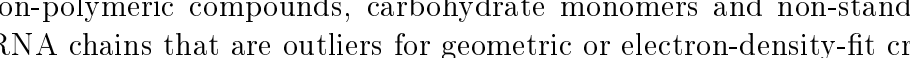

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 >=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 <=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	90	<div><div></div><div>79%12%9%</div></div>
1	B	90	<div><div>%</div><div>81%11%8%</div></div>
1	C	90	<div><div></div><div>84%8%8%</div></div>
1	D	90	<div><div></div><div>84%.12%</div></div>
1	E	90	<div><div></div><div>86%9%6%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	90	
1	G	90	
1	H	90	
1	I	90	
1	J	90	
1	K	90	
1	L	90	
1	M	90	
1	N	90	
1	O	90	
1	P	90	
1	Q	90	
1	R	90	

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
2	GOL	A	202	-	-	-	X
2	GOL	B	201	-	-	-	X
2	GOL	C	201	-	-	-	X
2	GOL	H	201	-	-	-	X
2	GOL	H	202	-	-	-	X
2	GOL	I	202	-	-	-	X
2	GOL	K	201	-	-	-	X
2	GOL	L	201	-	-	-	X
2	GOL	M	201	-	-	-	X
2	GOL	N	202	-	-	-	X
2	GOL	P	201	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15355 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-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	0	0	0
			652	421	110	121			
1	B	83	Total	C	N	O	0	0	0
			667	429	114	124			
1	C	83	Total	C	N	O	0	1	0
			662	428	111	123			
1	D	79	Total	C	N	O	0	0	0
			630	408	104	118			
1	E	85	Total	C	N	O	0	1	0
			685	440	118	127			
1	F	85	Total	C	N	O	0	0	0
			682	438	117	127			
1	G	83	Total	C	N	O	0	1	0
			666	429	113	124			
1	H	85	Total	C	N	O	0	0	0
			675	434	114	127			
1	I	85	Total	C	N	O	0	0	0
			666	429	113	124			
1	J	85	Total	C	N	O	0	0	0
			671	431	114	126			
1	K	82	Total	C	N	O	0	0	0
			639	414	103	122			
1	L	82	Total	C	N	O	0	0	0
			654	422	111	121			
1	M	85	Total	C	N	O	0	0	0
			679	437	116	126			
1	N	84	Total	C	N	O	0	0	0
			672	432	115	125			
1	O	84	Total	C	N	O	0	0	0
			675	433	116	126			
1	P	85	Total	C	N	O	0	0	0
			678	435	116	127			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	84	Total	C	N	O	0	0	0
			665	427	113	125			
1	R	84	Total	C	N	O	0	0	0
			662	425	111	126			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	GLY	-	expression tag	UNP Q9QZH4
A	68	PRO	-	expression tag	UNP Q9QZH4
A	69	LEU	-	expression tag	UNP Q9QZH4
A	70	GLY	-	expression tag	UNP Q9QZH4
A	71	SER	-	expression tag	UNP Q9QZH4
A	72	PRO	-	expression tag	UNP Q9QZH4
A	73	ASN	-	expression tag	UNP Q9QZH4
A	74	SER	-	expression tag	UNP Q9QZH4
B	67	GLY	-	expression tag	UNP Q9QZH4
B	68	PRO	-	expression tag	UNP Q9QZH4
B	69	LEU	-	expression tag	UNP Q9QZH4
B	70	GLY	-	expression tag	UNP Q9QZH4
B	71	SER	-	expression tag	UNP Q9QZH4
B	72	PRO	-	expression tag	UNP Q9QZH4
B	73	ASN	-	expression tag	UNP Q9QZH4
B	74	SER	-	expression tag	UNP Q9QZH4
C	67	GLY	-	expression tag	UNP Q9QZH4
C	68	PRO	-	expression tag	UNP Q9QZH4
C	69	LEU	-	expression tag	UNP Q9QZH4
C	70	GLY	-	expression tag	UNP Q9QZH4
C	71	SER	-	expression tag	UNP Q9QZH4
C	72	PRO	-	expression tag	UNP Q9QZH4
C	73	ASN	-	expression tag	UNP Q9QZH4
C	74	SER	-	expression tag	UNP Q9QZH4
D	67	GLY	-	expression tag	UNP Q9QZH4
D	68	PRO	-	expression tag	UNP Q9QZH4
D	69	LEU	-	expression tag	UNP Q9QZH4
D	70	GLY	-	expression tag	UNP Q9QZH4
D	71	SER	-	expression tag	UNP Q9QZH4
D	72	PRO	-	expression tag	UNP Q9QZH4
D	73	ASN	-	expression tag	UNP Q9QZH4
D	74	SER	-	expression tag	UNP Q9QZH4
E	67	GLY	-	expression tag	UNP Q9QZH4
E	68	PRO	-	expression tag	UNP Q9QZH4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	69	LEU	-	expression tag	UNP Q9QZH4
E	70	GLY	-	expression tag	UNP Q9QZH4
E	71	SER	-	expression tag	UNP Q9QZH4
E	72	PRO	-	expression tag	UNP Q9QZH4
E	73	ASN	-	expression tag	UNP Q9QZH4
E	74	SER	-	expression tag	UNP Q9QZH4
F	67	GLY	-	expression tag	UNP Q9QZH4
F	68	PRO	-	expression tag	UNP Q9QZH4
F	69	LEU	-	expression tag	UNP Q9QZH4
F	70	GLY	-	expression tag	UNP Q9QZH4
F	71	SER	-	expression tag	UNP Q9QZH4
F	72	PRO	-	expression tag	UNP Q9QZH4
F	73	ASN	-	expression tag	UNP Q9QZH4
F	74	SER	-	expression tag	UNP Q9QZH4
G	67	GLY	-	expression tag	UNP Q9QZH4
G	68	PRO	-	expression tag	UNP Q9QZH4
G	69	LEU	-	expression tag	UNP Q9QZH4
G	70	GLY	-	expression tag	UNP Q9QZH4
G	71	SER	-	expression tag	UNP Q9QZH4
G	72	PRO	-	expression tag	UNP Q9QZH4
G	73	ASN	-	expression tag	UNP Q9QZH4
G	74	SER	-	expression tag	UNP Q9QZH4
H	67	GLY	-	expression tag	UNP Q9QZH4
H	68	PRO	-	expression tag	UNP Q9QZH4
H	69	LEU	-	expression tag	UNP Q9QZH4
H	70	GLY	-	expression tag	UNP Q9QZH4
H	71	SER	-	expression tag	UNP Q9QZH4
H	72	PRO	-	expression tag	UNP Q9QZH4
H	73	ASN	-	expression tag	UNP Q9QZH4
H	74	SER	-	expression tag	UNP Q9QZH4
I	67	GLY	-	expression tag	UNP Q9QZH4
I	68	PRO	-	expression tag	UNP Q9QZH4
I	69	LEU	-	expression tag	UNP Q9QZH4
I	70	GLY	-	expression tag	UNP Q9QZH4
I	71	SER	-	expression tag	UNP Q9QZH4
I	72	PRO	-	expression tag	UNP Q9QZH4
I	73	ASN	-	expression tag	UNP Q9QZH4
I	74	SER	-	expression tag	UNP Q9QZH4
J	67	GLY	-	expression tag	UNP Q9QZH4
J	68	PRO	-	expression tag	UNP Q9QZH4
J	69	LEU	-	expression tag	UNP Q9QZH4
J	70	GLY	-	expression tag	UNP Q9QZH4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	71	SER	-	expression tag	UNP Q9QZH4
J	72	PRO	-	expression tag	UNP Q9QZH4
J	73	ASN	-	expression tag	UNP Q9QZH4
J	74	SER	-	expression tag	UNP Q9QZH4
K	67	GLY	-	expression tag	UNP Q9QZH4
K	68	PRO	-	expression tag	UNP Q9QZH4
K	69	LEU	-	expression tag	UNP Q9QZH4
K	70	GLY	-	expression tag	UNP Q9QZH4
K	71	SER	-	expression tag	UNP Q9QZH4
K	72	PRO	-	expression tag	UNP Q9QZH4
K	73	ASN	-	expression tag	UNP Q9QZH4
K	74	SER	-	expression tag	UNP Q9QZH4
L	67	GLY	-	expression tag	UNP Q9QZH4
L	68	PRO	-	expression tag	UNP Q9QZH4
L	69	LEU	-	expression tag	UNP Q9QZH4
L	70	GLY	-	expression tag	UNP Q9QZH4
L	71	SER	-	expression tag	UNP Q9QZH4
L	72	PRO	-	expression tag	UNP Q9QZH4
L	73	ASN	-	expression tag	UNP Q9QZH4
L	74	SER	-	expression tag	UNP Q9QZH4
M	67	GLY	-	expression tag	UNP Q9QZH4
M	68	PRO	-	expression tag	UNP Q9QZH4
M	69	LEU	-	expression tag	UNP Q9QZH4
M	70	GLY	-	expression tag	UNP Q9QZH4
M	71	SER	-	expression tag	UNP Q9QZH4
M	72	PRO	-	expression tag	UNP Q9QZH4
M	73	ASN	-	expression tag	UNP Q9QZH4
M	74	SER	-	expression tag	UNP Q9QZH4
N	67	GLY	-	expression tag	UNP Q9QZH4
N	68	PRO	-	expression tag	UNP Q9QZH4
N	69	LEU	-	expression tag	UNP Q9QZH4
N	70	GLY	-	expression tag	UNP Q9QZH4
N	71	SER	-	expression tag	UNP Q9QZH4
N	72	PRO	-	expression tag	UNP Q9QZH4
N	73	ASN	-	expression tag	UNP Q9QZH4
N	74	SER	-	expression tag	UNP Q9QZH4
O	67	GLY	-	expression tag	UNP Q9QZH4
O	68	PRO	-	expression tag	UNP Q9QZH4
O	69	LEU	-	expression tag	UNP Q9QZH4
O	70	GLY	-	expression tag	UNP Q9QZH4
O	71	SER	-	expression tag	UNP Q9QZH4
O	72	PRO	-	expression tag	UNP Q9QZH4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
O	73	ASN	-	expression tag	UNP Q9QZH4
O	74	SER	-	expression tag	UNP Q9QZH4
P	67	GLY	-	expression tag	UNP Q9QZH4
P	68	PRO	-	expression tag	UNP Q9QZH4
P	69	LEU	-	expression tag	UNP Q9QZH4
P	70	GLY	-	expression tag	UNP Q9QZH4
P	71	SER	-	expression tag	UNP Q9QZH4
P	72	PRO	-	expression tag	UNP Q9QZH4
P	73	ASN	-	expression tag	UNP Q9QZH4
P	74	SER	-	expression tag	UNP Q9QZH4
Q	67	GLY	-	expression tag	UNP Q9QZH4
Q	68	PRO	-	expression tag	UNP Q9QZH4
Q	69	LEU	-	expression tag	UNP Q9QZH4
Q	70	GLY	-	expression tag	UNP Q9QZH4
Q	71	SER	-	expression tag	UNP Q9QZH4
Q	72	PRO	-	expression tag	UNP Q9QZH4
Q	73	ASN	-	expression tag	UNP Q9QZH4
Q	74	SER	-	expression tag	UNP Q9QZH4
R	67	GLY	-	expression tag	UNP Q9QZH4
R	68	PRO	-	expression tag	UNP Q9QZH4
R	69	LEU	-	expression tag	UNP Q9QZH4
R	70	GLY	-	expression tag	UNP Q9QZH4
R	71	SER	-	expression tag	UNP Q9QZH4
R	72	PRO	-	expression tag	UNP Q9QZH4
R	73	ASN	-	expression tag	UNP Q9QZH4
R	74	SER	-	expression tag	UNP Q9QZH4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





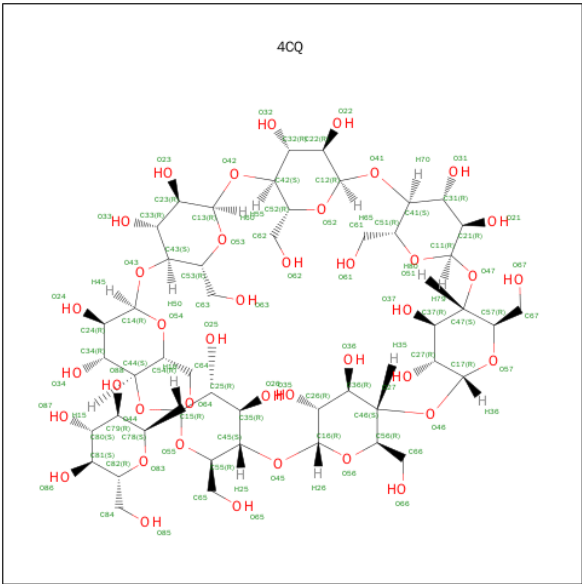
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			88	48	40		
3	B	1	Total	C	O	0	0
			88	48	40		
3	C	1	Total	C	O	0	0
			88	48	40		
3	D	1	Total	C	O	0	0
			88	48	40		
3	E	1	Total	C	O	0	0
			88	48	40		
3	F	1	Total	C	O	0	0
			88	48	40		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 88 48 40	0	0
3	H	1	Total C O 88 48 40	0	0
3	I	1	Total C O 88 48 40	0	0
3	J	1	Total C O 88 48 40	0	0
3	K	1	Total C O 88 48 40	0	0
3	L	1	Total C O 88 48 40	0	0
3	M	1	Total C O 88 48 40	0	0
3	N	1	Total C O 88 48 40	0	0
3	O	1	Total C O 88 48 40	0	0
3	P	1	Total C O 88 48 40	0	0
3	Q	1	Total C O 88 48 40	0	0
3	R	1	Total C O 88 48 40	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	126	Total O 126 126	0	0
4	B	110	Total O 110 110	0	0
4	C	112	Total O 112 112	0	0
4	D	107	Total O 107 107	0	0
4	E	120	Total O 120 120	0	0
4	F	101	Total O 101 101	0	0
4	G	97	Total O 97 97	0	0

*Continued on next page...*


*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	86	Total 86	O 86	0	0
4	I	87	Total 87	O 87	0	0
4	J	84	Total 84	O 84	0	0
4	K	70	Total 70	O 70	0	0
4	L	79	Total 79	O 79	0	0
4	M	112	Total 112	O 112	0	0
4	N	75	Total 75	O 75	0	0
4	O	94	Total 94	O 94	0	0
4	P	80	Total 80	O 80	0	0
4	Q	76	Total 76	O 76	0	0
4	R	61	Total 61	O 61	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-2

Chain A: 




- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain B: 




- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain C: 




- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain D: 



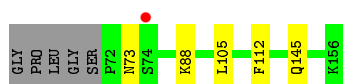
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain E: 



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain F: 



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain G: 89% 8%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain H: 86% 8% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain I: 92% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain J: 89% 6% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain K: 82% 9% 9%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain L: 83% 8% 9%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain M: 87% 8% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain N: 87% 7% 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain O: 88% 6% 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain P: 88% 7% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain Q: 89% • 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain R: 89% • 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.54 Å   96.43 Å   118.72 Å 90.00°   125.46°   90.00°	Depositor
Resolution (Å)	43.38 – 2.00 48.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.38-2.00) 99.9 (48.38-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.169 , 0.225 0.177 , 0.231	Depositor DCC
$R_{free}$ test set	6370 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.5	EDS
Estimated twinning fraction	0.027 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 127114 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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, 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	0.69	0/672	0.79	2/916 (0.2%)
1	B	0.72	0/687	0.77	0/934
1	C	0.76	1/685 (0.1%)	0.73	0/934
1	D	0.71	0/650	0.71	0/886
1	E	0.64	0/710	0.74	0/967
1	F	0.61	0/703	0.71	0/956
1	G	0.60	0/689	0.69	0/938
1	H	0.59	0/695	0.70	1/946 (0.1%)
1	I	0.60	0/687	0.71	0/938
1	J	0.60	0/692	0.68	0/944
1	K	0.59	0/658	0.70	0/899
1	L	0.66	0/674	0.77	1/918 (0.1%)
1	M	0.63	0/700	0.72	0/952
1	N	0.65	0/692	0.74	1/941 (0.1%)
1	O	0.63	0/695	0.69	0/945
1	P	0.60	0/699	0.73	0/952
1	Q	0.57	0/685	0.70	0/934
1	R	0.48	0/682	0.64	0/931
All	All	0.63	1/12355 (0.0%)	0.72	5/16831 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	SER	CB-OG	5.32	1.49	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	N	111	ASP	CB-CG-OD1	5.70	123.43	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	136	ASP	CB-CG-OD1	5.67	123.41	118.30
1	L	111	ASP	CB-CG-OD1	5.45	123.21	118.30
1	H	146	LEU	CA-CB-CG	5.10	127.03	115.30

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	652	0	618	7	0
1	B	667	0	645	9	0
1	C	662	0	632	6	0
1	D	630	0	597	2	0
1	E	685	0	655	6	0
1	F	682	0	659	4	0
1	G	666	0	638	2	0
1	H	675	0	647	8	0
1	I	666	0	624	1	0
1	J	671	0	633	3	0
1	K	639	0	597	4	1
1	L	654	0	625	4	0
1	M	679	0	655	6	0
1	N	672	0	647	4	0
1	O	675	0	651	3	0
1	P	678	0	648	5	0
1	Q	665	0	627	2	0
1	R	662	0	620	2	0
2	A	12	0	16	1	0
2	B	12	0	16	2	0
2	C	12	0	16	2	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	H	12	0	16	2	0
2	I	12	0	16	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	6	0	8	1	0
2	L	6	0	8	0	0
2	M	6	0	8	0	0
2	N	12	0	16	0	0
2	P	6	0	8	2	0
3	A	88	0	80	0	0
3	B	88	0	80	0	0
3	C	88	0	80	0	0
3	D	88	0	80	1	0
3	E	88	0	80	0	0
3	F	88	0	80	0	0
3	G	88	0	80	0	0
3	H	88	0	80	3	0
3	I	88	0	80	1	0
3	J	88	0	80	0	0
3	K	88	0	80	0	0
3	L	88	0	80	1	0
3	M	88	0	80	1	0
3	N	88	0	80	3	0
3	O	88	0	80	2	0
3	P	88	0	80	0	0
3	Q	88	0	80	1	0
3	R	88	0	80	0	0
4	A	126	0	0	1	0
4	B	110	0	0	1	0
4	C	112	0	0	0	0
4	D	107	0	0	1	0
4	E	120	0	0	0	0
4	F	101	0	0	3	0
4	G	97	0	0	1	0
4	H	86	0	0	2	0
4	I	87	0	0	0	0
4	J	84	0	0	1	0
4	K	70	0	0	1	0
4	L	79	0	0	1	1
4	M	112	0	0	3	0
4	N	75	0	0	2	0
4	O	94	0	0	0	1
4	P	80	0	0	0	1
4	Q	76	0	0	1	0
4	R	61	0	0	0	0
All	All	15355	0	13010	86	3

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 3.

All (86) 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:J:139:GLU:OE1	4:J:370:HOH:O	1.95	0.82
3:H:203:4CQ:H76	3:H:203:4CQ:H67	0.80	0.78
1:B:142:VAL:HG11	1:B:152:LEU:HD22	1.71	0.71
1:H:148:THR:HG21	3:H:203:4CQ:H58	1.75	0.69
1:B:89:GLU:OE2	2:B:201:GOL:O2	2.14	0.66
1:F:145:GLN:NE2	4:F:301:HOH:O	2.28	0.65
1:I:122:GLU:OE2	1:I:154:HIS:NE2	2.32	0.61
3:H:203:4CQ:O31	3:H:203:4CQ:O22	2.02	0.61
1:C:107:LYS:HE2	1:C:109:HIS:O	2.02	0.59
3:N:203:4CQ:O25	4:N:330:HOH:O	2.17	0.59
1:E:122:GLU:CG	1:E:152:LEU:HD11	2.33	0.58
1:C:107:LYS:HD3	1:C:112:PHE:CZ	2.39	0.57
1:P:122:GLU:HG3	1:P:152:LEU:HD11	1.87	0.57
1:E:122:GLU:HG3	1:E:152:LEU:HD11	1.87	0.56
2:K:201:GOL:O1	4:K:343:HOH:O	2.18	0.56
1:P:122:GLU:CG	1:P:152:LEU:HD11	2.35	0.55
1:A:117:ASP:OD2	4:A:386:HOH:O	2.18	0.54
1:H:139:GLU:HG3	2:H:201:GOL:H12	1.89	0.53
1:M:120:GLU:HG2	4:M:366:HOH:O	2.09	0.52
1:E:97:ASN:ND2	1:E:101:THR:HG22	2.26	0.51
1:F:88:LYS:NZ	4:F:384:HOH:O	2.25	0.51
1:A:89:GLU:HG2	2:A:202:GOL:H11	1.91	0.51
3:I:203:4CQ:O21	3:I:203:4CQ:O37	2.22	0.51
1:H:122:GLU:HG2	1:H:154:HIS:CD2	2.47	0.50
1:M:148:THR:HG21	3:M:202:4CQ:H58	1.94	0.49
1:B:105:LEU:HG	1:B:114:ALA:HB2	1.94	0.49
1:R:126:LYS:HE2	1:R:133:TRP:HB3	1.95	0.49
1:B:89:GLU:HB2	2:B:201:GOL:H12	1.93	0.49
1:H:139:GLU:HG3	2:H:201:GOL:C1	2.43	0.48
3:N:203:4CQ:O67	3:N:203:4CQ:O51	2.31	0.48
1:C:105:LEU:HB3	1:C:112:PHE:HB3	1.94	0.48
1:N:154:HIS:HB2	4:N:364:HOH:O	2.14	0.48
1:F:73:ASN:HB3	4:F:304:HOH:O	2.13	0.48
1:P:106:ILE:HD11	2:P:201:GOL:H12	1.94	0.48
1:R:105:LEU:HG	1:R:114:ALA:HB2	1.95	0.48
3:O:201:4CQ:C11	3:O:201:4CQ:H44	2.27	0.47
1:L:83:TRP:CZ2	1:L:85:GLU:HB2	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:106:ILE:HD11	2:P:201:GOL:C1	2.45	0.47
1:G:78:PRO:HD2	4:G:339:HOH:O	2.15	0.47
3:Q:201:4CQ:C17	3:Q:201:4CQ:H34	2.27	0.47
1:O:122:GLU:HG2	1:O:154:HIS:CD2	2.50	0.47
1:O:148:THR:HG21	3:O:201:4CQ:H58	1.98	0.46
3:N:203:4CQ:C11	3:N:203:4CQ:H44	2.29	0.46
1:F:105:LEU:HB3	1:F:112:PHE:HB3	1.97	0.46
1:B:141:VAL:HG23	1:N:141:VAL:HG23	1.97	0.46
1:K:83:TRP:CZ2	1:K:85:GLU:HB2	2.51	0.46
1:H:134:VAL:CG2	4:H:308:HOH:O	2.63	0.46
1:E:107:LYS:HD3	1:E:112:PHE:CZ	2.50	0.46
1:J:105:LEU:HB3	1:J:112:PHE:HB3	1.97	0.45
1:D:105:LEU:HG	1:D:114:ALA:HB2	1.97	0.45
1:B:83:TRP:CZ2	1:B:85:GLU:HB2	2.52	0.45
1:H:146:LEU:HD13	1:H:148:THR:HG23	1.97	0.45
1:J:122:GLU:HG3	1:J:152:LEU:HD11	1.99	0.45
1:G:83:TRP:CZ2	1:G:85:GLU:HB2	2.52	0.45
1:C:114:ALA:HB1	2:C:202:GOL:H12	1.97	0.45
1:D:148:THR:HG21	3:D:202:4CQ:H58	1.99	0.45
1:M:120:GLU:CG	4:M:366:HOH:O	2.65	0.44
1:B:105:LEU:HB3	1:B:112:PHE:HB3	1.99	0.44
1:L:105:LEU:HG	1:L:114:ALA:HB2	1.99	0.44
1:M:105:LEU:HB3	1:M:112:PHE:HB3	2.00	0.44
1:E:81:ILE:HG21	1:E:92:ILE:HD12	1.97	0.44
1:L:134:VAL:HG22	4:L:379:HOH:O	2.17	0.44
1:A:107:LYS:HD2	1:A:109:HIS:O	2.17	0.44
3:L:202:4CQ:O67	3:L:202:4CQ:O51	2.35	0.44
1:E:107:LYS:CD	1:E:112:PHE:CZ	3.01	0.43
1:H:83:TRP:CZ2	1:H:85:GLU:HB2	2.53	0.43
1:A:115:ILE:HD12	2:C:202:GOL:O2	2.18	0.43
1:A:83:TRP:CZ2	1:A:85:GLU:HB2	2.53	0.43
1:H:154:HIS:CD2	4:H:307:HOH:O	2.72	0.43
1:M:154:HIS:HB3	4:M:381:HOH:O	2.18	0.43
1:B:142:VAL:CG1	1:B:152:LEU:HD22	2.44	0.42
1:O:105:LEU:HB3	1:O:112:PHE:HB3	2.02	0.42
1:Q:105:LEU:HB3	1:Q:112:PHE:HB3	2.02	0.42
1:M:122:GLU:CG	1:M:152:LEU:HD11	2.49	0.42
1:Q:120:GLU:OE1	4:Q:301:HOH:O	2.22	0.42
1:K:94:GLY:HA2	1:K:99:TRP:CH2	2.55	0.42
1:L:105:LEU:HB3	1:L:112:PHE:HB3	2.01	0.42
1:B:138:SER:OG	4:B:375:HOH:O	2.22	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:HG	1:C:114:ALA:HB2	2.03	0.41
1:A:113:VAL:HG23	1:C:115:ILE:HD11	2.02	0.41
1:P:128:PHE:CZ	1:P:131:GLY:HA2	2.56	0.41
1:N:105:LEU:HB3	1:N:112:PHE:HB3	2.01	0.41
1:K:105:LEU:HB3	1:K:112:PHE:HB3	2.03	0.41
4:D:396:HOH:O	1:N:88:LYS:HE3	2.21	0.41
1:A:105:LEU:HB3	1:A:112:PHE:HB3	2.03	0.41
1:K:105:LEU:HG	1:K:114:ALA:HB2	2.02	0.40

All (3) 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)
1:K:110:ASN:OD1	1:K:110:ASN:OD1[2_656]	1.85	0.35
4:O:322:HOH:O	4:O:322:HOH:O[2_655]	2.08	0.12
4:L:302:HOH:O	4:P:311:HOH:O[2_655]	2.15	0.05

## 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	80/90 (89%)	79 (99%)	1 (1%)	0	100	100
1	B	81/90 (90%)	78 (96%)	3 (4%)	0	100	100
1	C	82/90 (91%)	80 (98%)	2 (2%)	0	100	100
1	D	77/90 (86%)	76 (99%)	1 (1%)	0	100	100
1	E	84/90 (93%)	83 (99%)	1 (1%)	0	100	100
1	F	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	G	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	H	83/90 (92%)	81 (98%)	2 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	J	83/90 (92%)	82 (99%)	1 (1%)	0	100	100
1	K	80/90 (89%)	79 (99%)	1 (1%)	0	100	100
1	L	80/90 (89%)	79 (99%)	1 (1%)	0	100	100
1	M	83/90 (92%)	82 (99%)	1 (1%)	0	100	100
1	N	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	O	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	P	83/90 (92%)	81 (98%)	2 (2%)	0	100	100
1	Q	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
1	R	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
All	All	1472/1620 (91%)	1447 (98%)	25 (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	71/80 (89%)	71 (100%)	0	100	100
1	B	75/80 (94%)	75 (100%)	0	100	100
1	C	73/80 (91%)	73 (100%)	0	100	100
1	D	70/80 (88%)	70 (100%)	0	100	100
1	E	77/80 (96%)	77 (100%)	0	100	100
1	F	77/80 (96%)	77 (100%)	0	100	100
1	G	74/80 (92%)	74 (100%)	0	100	100
1	H	75/80 (94%)	75 (100%)	0	100	100
1	I	72/80 (90%)	72 (100%)	0	100	100
1	J	74/80 (92%)	74 (100%)	0	100	100
1	K	69/80 (86%)	69 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	72/80 (90%)	72 (100%)	0	100	100
1	M	76/80 (95%)	76 (100%)	0	100	100
1	N	75/80 (94%)	75 (100%)	0	100	100
1	O	76/80 (95%)	76 (100%)	0	100	100
1	P	76/80 (95%)	75 (99%)	1 (1%)	76	79
1	Q	73/80 (91%)	72 (99%)	1 (1%)	74	77
1	R	73/80 (91%)	73 (100%)	0	100	100
All	All	1328/1440 (92%)	1326 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	89	GLU
1	Q	122	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	ASN
1	C	110	ASN
1	F	145	GLN
1	N	75	GLN
1	Q	73	ASN

### 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 carbohydrates in this entry.



## 5.6 Ligand geometry

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	$\# Z  > 2$
2	GOL	A	201	-	5,5,5	0.47	0	5,5,5	0.46	0
2	GOL	A	202	-	5,5,5	0.80	0	5,5,5	1.23	1 (20%)
3	4CQ	A	203	-	96,96,96	0.58	0	144,144,144	0.98	6 (4%)
2	GOL	B	201	-	5,5,5	0.60	0	5,5,5	0.86	0
2	GOL	B	202	-	5,5,5	0.34	0	5,5,5	0.53	0
3	4CQ	B	203	-	96,96,96	0.55	0	144,144,144	1.03	9 (6%)
2	GOL	C	201	-	5,5,5	0.32	0	5,5,5	0.16	0
2	GOL	C	202	-	5,5,5	0.36	0	5,5,5	0.57	0
3	4CQ	C	203	-	96,96,96	0.58	1 (1%)	144,144,144	1.09	9 (6%)
2	GOL	D	201	-	5,5,5	0.29	0	5,5,5	0.88	0
3	4CQ	D	202	-	96,96,96	0.56	1 (1%)	144,144,144	1.08	9 (6%)
2	GOL	E	201	-	5,5,5	0.32	0	5,5,5	0.45	0
3	4CQ	E	202	-	96,96,96	0.65	1 (1%)	144,144,144	1.02	5 (3%)
2	GOL	F	201	-	5,5,5	0.34	0	5,5,5	0.75	0
3	4CQ	F	202	-	96,96,96	0.63	1 (1%)	144,144,144	1.15	15 (10%)
3	4CQ	G	201	-	96,96,96	0.44	0	144,144,144	0.94	4 (2%)
2	GOL	H	201	-	5,5,5	0.51	0	5,5,5	1.02	0
2	GOL	H	202	-	5,5,5	0.31	0	5,5,5	0.77	0
3	4CQ	H	203	-	96,96,96	0.54	1 (1%)	144,144,144	1.09	12 (8%)
2	GOL	I	201	-	5,5,5	0.29	0	5,5,5	0.44	0
2	GOL	I	202	-	5,5,5	0.72	0	5,5,5	0.82	0
3	4CQ	I	203	-	96,96,96	0.55	0	144,144,144	1.05	9 (6%)
3	4CQ	J	201	-	96,96,96	0.57	1 (1%)	144,144,144	1.04	6 (4%)
2	GOL	K	201	-	5,5,5	0.31	0	5,5,5	0.74	0
3	4CQ	K	202	-	96,96,96	0.48	0	144,144,144	1.00	9 (6%)
2	GOL	L	201	-	5,5,5	0.28	0	5,5,5	0.52	0
3	4CQ	L	202	-	96,96,96	0.63	1 (1%)	144,144,144	1.11	11 (7%)
2	GOL	M	201	-	5,5,5	0.34	0	5,5,5	0.45	0
3	4CQ	M	202	-	96,96,96	0.48	0	144,144,144	1.06	6 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	N	201	-	5,5,5	0.53	0	5,5,5	0.88	0
2	GOL	N	202	-	5,5,5	0.34	0	5,5,5	0.80	0
3	4CQ	N	203	-	96,96,96	0.62	1 (1%)	144,144,144	1.40	23 (15%)
3	4CQ	O	201	-	96,96,96	0.52	0	144,144,144	0.99	5 (3%)
2	GOL	P	201	-	5,5,5	0.30	0	5,5,5	0.45	0
3	4CQ	P	202	-	96,96,96	0.51	1 (1%)	144,144,144	0.96	6 (4%)
3	4CQ	Q	201	-	96,96,96	0.58	1 (1%)	144,144,144	0.99	6 (4%)
3	4CQ	R	201	-	96,96,96	0.56	1 (1%)	144,144,144	1.16	12 (8%)

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	GOL	A	201	-	-	0/4/4/4	0/0/0/0
2	GOL	A	202	-	-	0/4/4/4	0/0/0/0
3	4CQ	A	203	-	-	0/47/207/207	0/1/9/9
2	GOL	B	201	-	-	0/4/4/4	0/0/0/0
2	GOL	B	202	-	-	0/4/4/4	0/0/0/0
3	4CQ	B	203	-	-	0/47/207/207	0/1/9/9
2	GOL	C	201	-	-	0/4/4/4	0/0/0/0
2	GOL	C	202	-	-	0/4/4/4	0/0/0/0
3	4CQ	C	203	-	-	0/47/207/207	0/1/9/9
2	GOL	D	201	-	-	0/4/4/4	0/0/0/0
3	4CQ	D	202	-	-	0/47/207/207	0/1/9/9
2	GOL	E	201	-	-	0/4/4/4	0/0/0/0
3	4CQ	E	202	-	-	0/47/207/207	0/1/9/9
2	GOL	F	201	-	-	0/4/4/4	0/0/0/0
3	4CQ	F	202	-	-	0/47/207/207	0/1/9/9
3	4CQ	G	201	-	-	0/47/207/207	0/1/9/9
2	GOL	H	201	-	-	0/4/4/4	0/0/0/0
2	GOL	H	202	-	-	0/4/4/4	0/0/0/0
3	4CQ	H	203	-	-	0/47/207/207	0/1/9/9
2	GOL	I	201	-	-	0/4/4/4	0/0/0/0
2	GOL	I	202	-	-	0/4/4/4	0/0/0/0
3	4CQ	I	203	-	-	0/47/207/207	0/1/9/9
3	4CQ	J	201	-	-	0/47/207/207	0/1/9/9
2	GOL	K	201	-	-	0/4/4/4	0/0/0/0
3	4CQ	K	202	-	-	0/47/207/207	0/1/9/9
2	GOL	L	201	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4CQ	L	202	-	-	0/47/207/207	0/1/9/9
2	GOL	M	201	-	-	0/4/4/4	0/0/0/0
3	4CQ	M	202	-	-	0/47/207/207	0/1/9/9
2	GOL	N	201	-	-	0/4/4/4	0/0/0/0
2	GOL	N	202	-	-	0/4/4/4	0/0/0/0
3	4CQ	N	203	-	-	0/47/207/207	0/1/9/9
3	4CQ	O	201	-	-	0/47/207/207	0/1/9/9
2	GOL	P	201	-	-	0/4/4/4	0/0/0/0
3	4CQ	P	202	-	-	0/47/207/207	0/1/9/9
3	4CQ	Q	201	-	-	0/47/207/207	0/1/9/9
3	4CQ	R	201	-	-	0/47/207/207	0/1/9/9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	203	4CQ	O64-C78	2.09	1.43	1.40
3	Q	201	4CQ	O64-C78	2.20	1.44	1.40
3	L	202	4CQ	O64-C78	2.22	1.44	1.40
3	H	203	4CQ	O64-C78	2.29	1.44	1.40
3	D	202	4CQ	O64-C78	2.31	1.44	1.40
3	E	202	4CQ	O64-C78	2.44	1.44	1.40
3	P	202	4CQ	O64-C78	2.47	1.44	1.40
3	J	201	4CQ	O64-C78	2.62	1.44	1.40
3	R	201	4CQ	O64-C78	2.62	1.44	1.40
3	C	203	4CQ	O64-C78	2.64	1.44	1.40
3	F	202	4CQ	O64-C78	2.85	1.45	1.40

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	202	4CQ	O62-C62-C52	-3.53	99.65	111.33
3	N	203	4CQ	O63-C63-C53	-3.42	100.03	111.33
3	R	201	4CQ	O53-C13-C23	-3.32	103.46	110.28
3	N	203	4CQ	O52-C12-C22	-3.21	103.69	110.28
3	N	203	4CQ	O56-C16-C26	-3.07	103.97	110.28
3	C	203	4CQ	O41-C12-O52	-3.04	102.98	110.68
3	D	202	4CQ	O65-C65-C55	-3.02	101.34	111.33
3	N	203	4CQ	O21-C21-C11	-3.02	103.41	110.02
3	I	203	4CQ	O44-C15-O55	-2.86	103.45	110.68
3	C	203	4CQ	O65-C65-C55	-2.85	101.92	111.33
3	C	203	4CQ	O22-C22-C32	-2.82	103.98	110.34
3	B	203	4CQ	O62-C62-C52	-2.82	102.02	111.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	202	4CQ	O43-C43-C33	-2.79	99.96	107.17
3	C	203	4CQ	O25-C25-C35	-2.77	104.10	110.34
3	R	201	4CQ	O32-C32-C42	-2.77	103.33	109.87
3	D	202	4CQ	C64-O64-C78	-2.76	108.03	113.82
3	F	202	4CQ	O27-C27-C17	-2.75	103.98	110.02
3	O	201	4CQ	O26-C26-C36	-2.71	104.24	110.34
3	H	203	4CQ	C14-O43-C43	-2.65	111.08	118.01
3	G	201	4CQ	O23-C23-C13	-2.61	104.29	110.02
3	N	203	4CQ	O86-C81-C80	-2.60	104.48	110.34
3	H	203	4CQ	C13-O42-C42	-2.57	111.29	118.01
3	F	202	4CQ	C64-O64-C78	-2.56	108.45	113.82
3	Q	201	4CQ	O88-C79-C80	-2.54	104.62	110.34
3	C	203	4CQ	O42-C13-O53	-2.53	104.27	110.68
3	F	202	4CQ	O33-C33-C43	-2.52	103.91	109.87
3	B	203	4CQ	O26-C26-C36	-2.49	104.72	110.34
3	E	202	4CQ	O25-C25-C15	-2.46	104.63	110.02
3	M	202	4CQ	O65-C65-C55	-2.46	103.21	111.33
3	A	203	4CQ	O62-C62-C52	-2.45	103.23	111.33
3	L	202	4CQ	O34-C34-C44	-2.45	104.08	109.87
3	H	203	4CQ	O51-C51-C41	-2.45	104.57	109.75
3	F	202	4CQ	O65-C65-C55	-2.45	103.24	111.33
3	N	203	4CQ	O25-C25-C15	-2.45	104.66	110.02
3	H	203	4CQ	O56-C16-C26	-2.44	105.26	110.28
3	Q	201	4CQ	O27-C27-C37	-2.44	104.85	110.34
3	F	202	4CQ	O52-C52-C42	-2.39	104.69	109.75
3	I	203	4CQ	O24-C24-C14	-2.37	104.82	110.02
3	N	203	4CQ	C35-C45-C55	-2.36	105.49	110.84
3	H	203	4CQ	O87-C80-C79	-2.36	105.02	110.34
3	F	202	4CQ	O24-C24-C14	-2.35	104.86	110.02
3	O	201	4CQ	O86-C81-C80	-2.35	105.04	110.34
3	M	202	4CQ	O44-C15-O55	-2.31	104.83	110.68
3	A	203	4CQ	O26-C26-C36	-2.31	105.14	110.34
3	R	201	4CQ	O27-C27-C37	-2.31	105.15	110.34
3	B	203	4CQ	O21-C21-C31	-2.29	105.18	110.34
3	N	203	4CQ	C64-O64-C78	-2.29	109.01	113.82
3	J	201	4CQ	O27-C27-C17	-2.27	105.04	110.02
3	F	202	4CQ	O23-C23-C13	-2.26	105.07	110.02
3	D	202	4CQ	O26-C26-C36	-2.23	105.31	110.34
3	D	202	4CQ	O21-C21-C11	-2.23	105.13	110.02
3	P	202	4CQ	O63-C63-C53	-2.22	103.98	111.33
3	L	202	4CQ	O24-C24-C14	-2.18	105.23	110.02
3	P	202	4CQ	O65-C65-C55	-2.17	104.15	111.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	203	4CQ	O47-C11-O51	-2.16	105.22	110.68
3	N	203	4CQ	C67-C57-C47	-2.15	106.98	113.25
3	N	203	4CQ	O31-C31-C41	-2.15	104.79	109.87
3	K	202	4CQ	O47-C11-O51	-2.15	105.25	110.68
3	G	201	4CQ	O21-C21-C11	-2.14	105.32	110.02
3	A	203	4CQ	C36-C46-C56	-2.14	106.00	110.84
3	O	201	4CQ	O22-C22-C12	-2.14	105.33	110.02
3	L	202	4CQ	O57-C17-C27	-2.14	105.89	110.28
3	J	201	4CQ	C64-O64-C78	-2.13	109.34	113.82
3	N	203	4CQ	O44-C15-O55	-2.13	105.29	110.68
3	J	201	4CQ	O63-C63-C53	-2.11	104.35	111.33
3	H	203	4CQ	C12-O41-C41	-2.11	112.50	118.01
3	F	202	4CQ	O37-C37-C47	-2.09	104.92	109.87
3	I	203	4CQ	O63-C63-C53	-2.09	104.42	111.33
3	R	201	4CQ	O57-C17-C27	-2.09	105.99	110.28
3	I	203	4CQ	O37-C37-C47	-2.09	104.94	109.87
3	F	202	4CQ	O87-C80-C79	-2.08	105.66	110.34
3	D	202	4CQ	C12-O52-C52	-2.07	109.72	113.75
3	M	202	4CQ	O67-C67-C57	-2.07	104.49	111.33
3	K	202	4CQ	O22-C22-C32	-2.07	105.68	110.34
3	I	203	4CQ	O62-C62-C52	-2.05	104.56	111.33
3	I	203	4CQ	C14-O43-C43	-2.04	112.67	118.01
3	H	203	4CQ	C21-C31-C41	-2.03	105.14	109.60
3	L	202	4CQ	O87-C80-C79	-2.03	105.76	110.34
3	R	201	4CQ	C84-C82-C81	-2.02	108.02	113.02
3	Q	201	4CQ	O56-C16-C26	-2.01	106.15	110.28
3	K	202	4CQ	C32-C42-C52	-2.01	106.30	110.84
3	F	202	4CQ	O33-C33-C23	2.02	114.88	110.34
3	Q	201	4CQ	C63-C53-C43	2.02	119.14	113.25
3	R	201	4CQ	O54-C54-C64	2.03	110.77	106.61
3	D	202	4CQ	O56-C56-C46	2.06	114.10	109.75
3	A	203	4CQ	O53-C53-C63	2.06	111.56	106.36
3	B	203	4CQ	O41-C41-C51	2.08	114.80	109.32
3	B	203	4CQ	O24-C24-C34	2.08	115.03	110.34
3	M	202	4CQ	C11-O51-C51	2.09	117.80	113.75
3	P	202	4CQ	C33-C43-C53	2.10	115.58	110.84
3	Q	201	4CQ	O55-C55-C45	2.10	114.19	109.75
3	N	203	4CQ	O24-C24-C34	2.10	115.08	110.34
3	N	203	4CQ	O53-C53-C43	2.13	114.23	109.75
3	G	201	4CQ	O37-C37-C47	2.13	114.90	109.87
3	I	203	4CQ	C11-O51-C51	2.13	117.88	113.75
3	B	203	4CQ	O56-C56-C66	2.14	111.75	106.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	202	4CQ	O54-C54-C64	2.15	111.00	106.61
3	E	202	4CQ	C34-C44-C54	2.16	115.72	110.84
3	H	203	4CQ	C33-C43-C53	2.16	115.73	110.84
3	K	202	4CQ	O57-C57-C47	2.18	114.34	109.75
3	Q	201	4CQ	O34-C34-C24	2.21	115.31	110.34
3	D	202	4CQ	O53-C53-C43	2.21	114.42	109.75
3	P	202	4CQ	O55-C55-C45	2.22	114.43	109.75
3	R	201	4CQ	C26-C36-C46	2.24	114.52	109.60
3	N	203	4CQ	O45-C45-C35	2.24	112.95	107.17
3	H	203	4CQ	C25-C35-C45	2.26	114.56	109.60
2	A	202	GOL	O1-C1-C2	2.26	121.17	110.18
3	D	202	4CQ	O33-C33-C23	2.27	115.44	110.34
3	M	202	4CQ	O53-C53-C63	2.27	112.09	106.36
3	C	203	4CQ	O57-C57-C67	2.28	112.11	106.36
3	L	202	4CQ	C33-C43-C53	2.28	116.00	110.84
3	K	202	4CQ	O47-C11-C21	2.29	113.68	108.10
3	C	203	4CQ	O53-C53-C43	2.30	114.60	109.75
3	O	201	4CQ	C33-C43-C53	2.32	116.08	110.84
3	K	202	4CQ	C13-O53-C53	2.33	118.27	113.75
3	R	201	4CQ	C16-C26-C36	2.34	114.58	109.97
3	R	201	4CQ	O53-C53-C63	2.35	112.30	106.36
3	H	203	4CQ	O51-C51-C61	2.39	112.39	106.36
3	N	203	4CQ	O41-C12-C22	2.39	113.91	108.10
3	I	203	4CQ	O34-C34-C24	2.39	115.72	110.34
3	L	202	4CQ	C63-C53-C43	2.40	120.24	113.25
3	L	202	4CQ	C11-O51-C51	2.44	118.47	113.75
3	J	201	4CQ	O53-C53-C43	2.44	114.90	109.75
3	K	202	4CQ	O43-C14-C24	2.45	114.06	108.10
3	B	203	4CQ	O53-C53-C43	2.45	114.92	109.75
3	A	203	4CQ	O53-C53-C43	2.47	114.96	109.75
3	L	202	4CQ	O51-C51-C41	2.47	114.97	109.75
3	A	203	4CQ	C33-C43-C53	2.48	116.46	110.84
3	B	203	4CQ	O53-C53-C63	2.50	112.67	106.36
3	E	202	4CQ	O51-C11-C21	2.51	115.42	110.28
3	F	202	4CQ	O53-C53-C63	2.52	112.72	106.36
3	H	203	4CQ	O53-C53-C63	2.53	112.74	106.36
3	P	202	4CQ	C11-O51-C51	2.53	118.66	113.75
3	F	202	4CQ	O53-C53-C43	2.56	115.16	109.75
3	K	202	4CQ	O53-C53-C43	2.59	115.22	109.75
3	N	203	4CQ	O43-C43-C33	2.63	113.96	107.17
3	F	202	4CQ	C13-O53-C53	2.65	118.89	113.75
3	P	202	4CQ	O53-C53-C43	2.67	115.38	109.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	201	4CQ	O45-C16-C26	2.71	114.69	108.10
3	E	202	4CQ	O53-C53-C43	2.71	115.47	109.75
3	G	201	4CQ	O53-C53-C63	2.71	113.21	106.36
3	L	202	4CQ	O24-C24-C34	2.76	116.55	110.34
3	N	203	4CQ	C21-C31-C41	2.80	115.74	109.60
3	F	202	4CQ	C22-C32-C42	2.80	115.76	109.60
3	N	203	4CQ	O56-C56-C46	2.82	115.71	109.75
3	K	202	4CQ	C11-O51-C51	2.84	119.25	113.75
3	C	203	4CQ	O53-C53-C63	2.84	113.53	106.36
3	B	203	4CQ	O44-C15-C25	2.86	115.05	108.10
3	R	201	4CQ	C78-O83-C82	2.88	119.33	113.75
3	E	202	4CQ	O83-C82-C84	2.91	113.72	106.36
3	R	201	4CQ	O83-C82-C81	2.96	115.23	109.68
3	N	203	4CQ	C63-C53-C43	2.98	121.91	113.25
3	D	202	4CQ	O53-C53-C63	2.98	113.88	106.36
3	N	203	4CQ	O23-C23-C33	3.02	117.14	110.34
3	H	203	4CQ	O37-C37-C27	3.04	117.17	110.34
3	N	203	4CQ	O57-C57-C47	3.08	116.24	109.75
3	M	202	4CQ	O64-C78-C79	3.10	111.95	108.04
3	J	201	4CQ	C11-O51-C51	3.28	120.11	113.75
3	O	201	4CQ	C11-O51-C51	3.44	120.43	113.75
3	C	203	4CQ	C11-O51-C51	3.58	120.69	113.75
3	N	203	4CQ	C15-C25-C35	3.62	117.11	109.97
3	R	201	4CQ	O42-C13-C23	3.63	116.94	108.10
3	N	203	4CQ	C11-C21-C31	4.14	118.12	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	202	GOL	1	0
2	B	201	GOL	2	0
2	C	202	GOL	2	0
3	D	202	4CQ	1	0
2	H	201	GOL	2	0
3	H	203	4CQ	3	0
3	I	203	4CQ	1	0
2	K	201	GOL	1	0
3	L	202	4CQ	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	202	4CQ	1	0
3	N	203	4CQ	3	0
3	O	201	4CQ	2	0
2	P	201	GOL	2	0
3	Q	201	4CQ	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	82/90 (91%)	-0.63	0 100 100	15, 21, 39, 51	0
1	B	83/90 (92%)	-0.39	1 (1%) 81 81	15, 24, 49, 59	0
1	C	83/90 (92%)	-0.43	0 100 100	14, 20, 45, 60	0
1	D	79/90 (87%)	-0.64	0 100 100	16, 24, 40, 52	0
1	E	85/90 (94%)	-0.41	0 100 100	17, 25, 38, 57	0
1	F	85/90 (94%)	-0.39	1 (1%) 81 81	17, 29, 49, 79	0
1	G	83/90 (92%)	-0.57	0 100 100	21, 30, 48, 67	0
1	H	85/90 (94%)	-0.49	0 100 100	24, 34, 52, 61	0
1	I	85/90 (94%)	-0.46	0 100 100	23, 33, 48, 55	0
1	J	85/90 (94%)	-0.49	0 100 100	22, 31, 50, 59	0
1	K	82/90 (91%)	-0.42	0 100 100	24, 32, 52, 68	0
1	L	82/90 (91%)	-0.51	0 100 100	20, 31, 50, 70	0
1	M	85/90 (94%)	-0.53	1 (1%) 81 81	20, 26, 47, 63	0
1	N	84/90 (93%)	-0.37	0 100 100	20, 32, 52, 67	0
1	O	84/90 (93%)	-0.63	0 100 100	20, 27, 41, 48	0
1	P	85/90 (94%)	-0.49	0 100 100	24, 33, 49, 58	0
1	Q	84/90 (93%)	-0.46	0 100 100	23, 36, 60, 73	0
1	R	84/90 (93%)	-0.19	1 (1%) 81 81	38, 49, 62, 79	0
All	All	1505/1620 (92%)	-0.47	4 (0%) 94 94	14, 30, 54, 79	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	74	SER	2.4
1	R	154	HIS	2.4
1	B	77	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	72	PRO	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
2	GOL	H	202	6/6	0.90	0.36	15.73	46,48,52,54	0
2	GOL	A	202	6/6	0.94	0.15	11.99	21,31,38,39	0
2	GOL	M	201	6/6	0.89	0.13	8.71	33,37,41,41	0
2	GOL	B	201	6/6	0.90	0.17	6.27	27,30,31,40	0
2	GOL	C	201	6/6	0.89	0.20	6.07	34,53,60,66	0
2	GOL	H	201	6/6	0.86	0.22	5.67	28,41,47,47	0
2	GOL	I	202	6/6	0.88	0.18	4.94	32,40,44,44	0
2	GOL	P	201	6/6	0.94	0.18	4.62	38,48,51,55	0
2	GOL	N	202	6/6	0.89	0.12	3.84	34,44,48,48	0
2	GOL	K	201	6/6	0.89	0.21	3.00	30,45,48,58	0
2	GOL	L	201	6/6	0.97	0.11	2.19	22,26,29,31	0
2	GOL	E	201	6/6	0.91	0.14	1.98	30,34,38,45	0
2	GOL	D	201	6/6	0.97	0.12	1.86	25,28,31,31	0
3	4CQ	N	203	88/88	0.83	0.18	1.83	35,51,75,79	0
3	4CQ	I	203	88/88	0.93	0.13	1.77	26,43,57,63	0
2	GOL	F	201	6/6	0.90	0.13	1.70	41,42,47,52	0
2	GOL	B	202	6/6	0.97	0.11	1.36	20,26,27,32	0
2	GOL	I	201	6/6	0.91	0.11	0.87	40,47,47,55	0
3	4CQ	Q	201	88/88	0.93	0.11	0.77	25,43,63,65	0
2	GOL	A	201	6/6	0.95	0.13	0.66	32,34,36,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	4CQ	L	202	88/88	0.91	0.13	0.62	23,40,53,59	0
3	4CQ	H	203	88/88	0.88	0.14	0.55	38,53,68,74	0
3	4CQ	J	201	88/88	0.94	0.10	0.36	23,38,50,57	0
3	4CQ	P	202	88/88	0.93	0.11	0.32	27,44,63,70	0
3	4CQ	R	201	88/88	0.90	0.13	0.27	35,48,60,64	0
3	4CQ	O	201	88/88	0.92	0.11	0.22	27,40,53,58	0
3	4CQ	B	203	88/88	0.95	0.10	0.20	15,27,44,53	0
3	4CQ	M	202	88/88	0.94	0.09	0.15	22,36,50,54	0
3	4CQ	K	202	88/88	0.94	0.09	0.04	28,39,52,54	0
3	4CQ	G	201	88/88	0.92	0.11	-0.05	30,43,59,63	0
3	4CQ	D	202	88/88	0.95	0.09	-0.15	21,31,43,51	0
2	GOL	C	202	6/6	0.95	0.10	-0.16	28,30,31,33	0
3	4CQ	A	203	88/88	0.96	0.09	-0.36	17,25,39,49	0
3	4CQ	E	202	88/88	0.95	0.09	-0.69	20,27,37,51	0
2	GOL	N	201	6/6	0.96	0.09	-0.75	27,31,32,35	0
3	4CQ	C	203	88/88	0.96	0.09	-0.83	14,23,42,52	0
3	4CQ	F	202	88/88	0.95	0.09	-0.95	18,24,31,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.