



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:18 PM GMT

PDB ID : 1A0T  
Title : SUCROSE-SPECIFIC PORIN, WITH BOUND SUCROSE MOLECULES  
Authors : Diederichs, K.; Welte, W.  
Deposited on : 1997-12-08  
Resolution : 2.40 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 (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

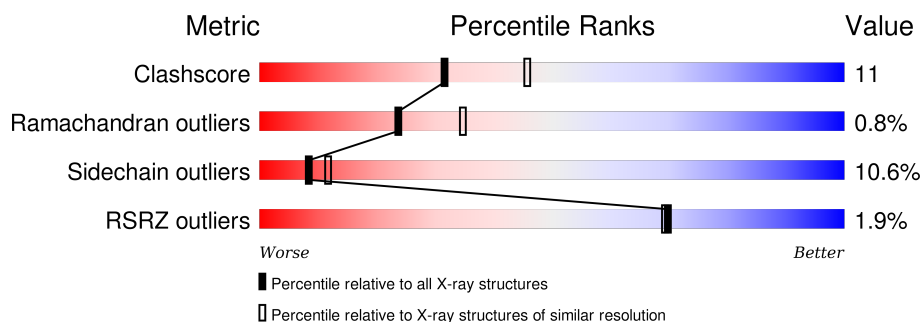
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	P	413	
1	Q	413	
1	R	413	

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	SUC	P	1	-	-	-	X
2	SUC	P	2	-	-	-	X
2	SUC	Q	1	-	-	-	X
2	SUC	Q	2	-	-	-	X
2	SUC	R	1	-	-	-	X
2	SUC	R	2	-	-	-	X

## 2 Entry composition [i](#)

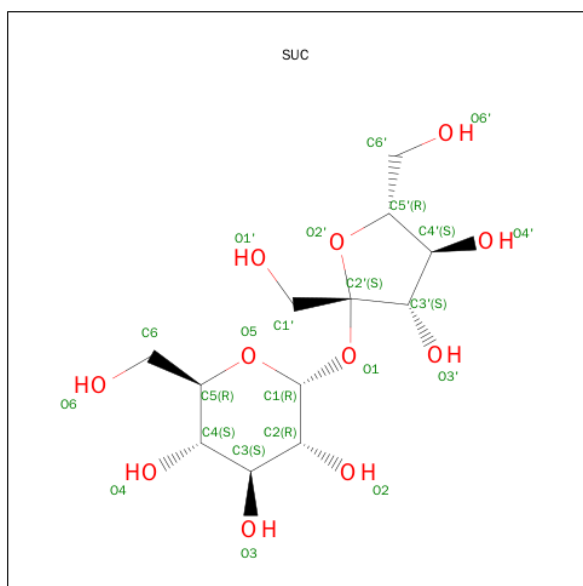
There are 4 unique types of molecules in this entry. The entry contains 10077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUCROSE-SPECIFIC PORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	413	Total	C	N	O	S	0	0	0
			3202	2011	553	628	10			
1	Q	413	Total	C	N	O	S	0	0	0
			3202	2011	553	628	10			
1	R	413	Total	C	N	O	S	0	0	0
			3202	2011	553	628	10			

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	C	O	0	0
			23	12	11		
2	P	1	Total	C	O	0	0
			23	12	11		
2	Q	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	C	O	0	0
			23	12	11		
2	R	1	Total	C	O	0	0
			23	12	11		
2	R	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Ca	0	0
			1	1		
3	R	1	Total	Ca	0	0
			1	1		
3	Q	1	Total	Ca	0	0
			1	1		

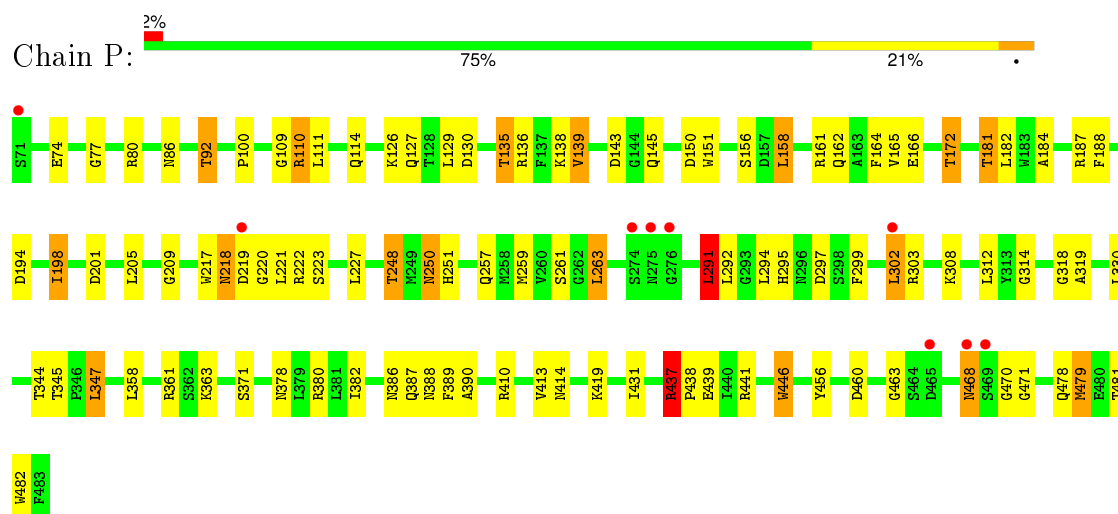
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	109	Total	O	0	0
			109	109		
4	Q	111	Total	O	0	0
			111	111		
4	R	110	Total	O	0	0
			110	110		

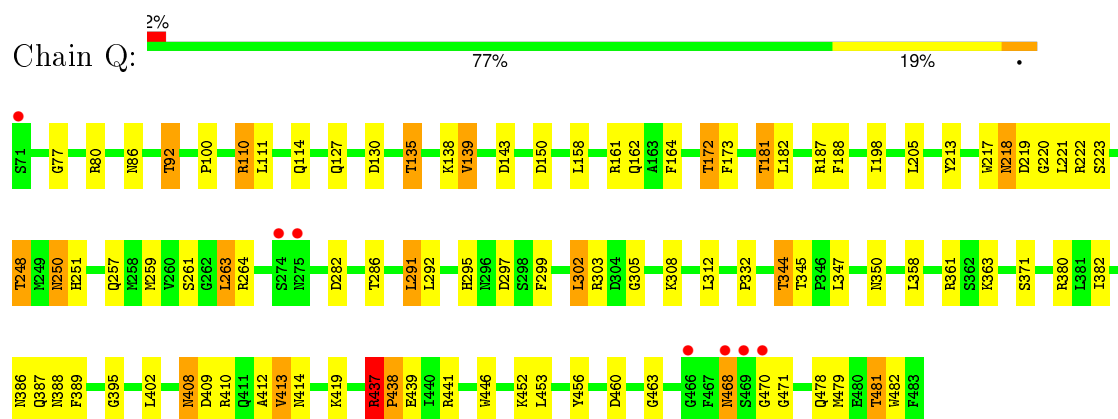
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

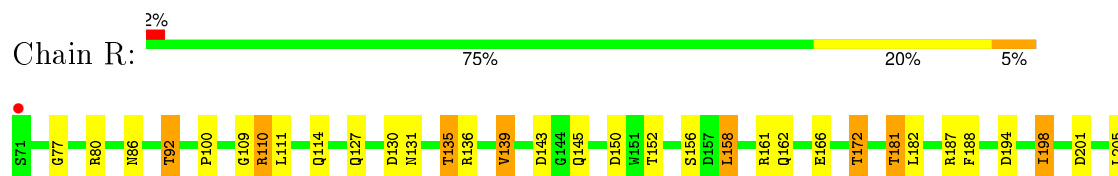
#### • Molecule 1: SUCROSE-SPECIFIC PORIN

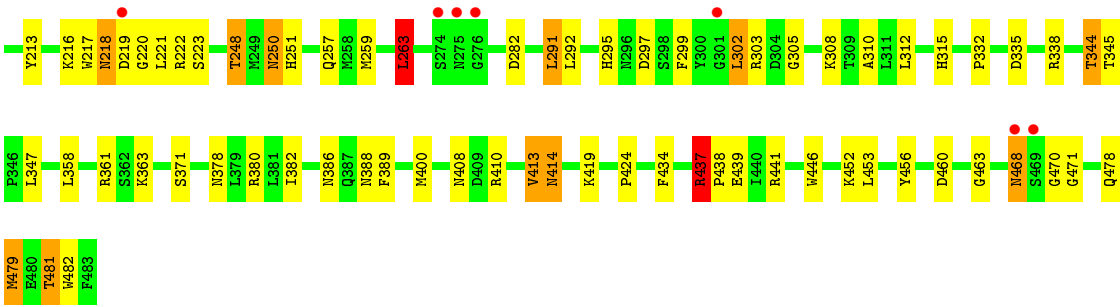


#### • Molecule 1: SUCROSE-SPECIFIC PORIN



#### • Molecule 1: SUCROSE-SPECIFIC PORIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.80Å 111.80Å 147.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.40 15.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	67.4 (100.00-2.40) 66.9 (15.76-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.19 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.207 , 0.246 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.050 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 72892 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 56.29 % 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 2.7954e-05. 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, 0.375 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: CA, SUC

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	P	0.56	0/3283	0.81	4/4443 (0.1%)
1	Q	0.55	0/3283	0.82	4/4443 (0.1%)
1	R	0.56	0/3283	0.82	4/4443 (0.1%)
All	All	0.56	0/9849	0.82	12/13329 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	437	ARG	N-CA-C	8.26	133.31	111.00
1	Q	437	ARG	N-CA-C	8.26	133.29	111.00
1	P	437	ARG	N-CA-C	8.23	133.22	111.00
1	P	263	LEU	CA-CB-CG	6.31	129.82	115.30
1	P	291	LEU	CA-CB-CG	6.02	129.15	115.30
1	P	139	VAL	CB-CA-C	-5.97	100.05	111.40
1	R	291	LEU	CA-CB-CG	5.78	128.60	115.30
1	Q	263	LEU	CA-CB-CG	5.74	128.49	115.30
1	Q	139	VAL	CB-CA-C	-5.64	100.69	111.40
1	Q	291	LEU	CA-CB-CG	5.57	128.10	115.30
1	R	263	LEU	CA-CB-CG	5.36	127.62	115.30
1	R	139	VAL	CB-CA-C	-5.17	101.57	111.40

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	P	3202	0	2985	69	0
1	Q	3202	0	2985	66	0
1	R	3202	0	2985	75	0
2	P	46	0	44	3	0
2	Q	46	0	44	5	0
2	R	46	0	44	3	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	P	109	0	0	3	0
4	Q	111	0	0	4	0
4	R	110	0	0	5	0
All	All	10077	0	9087	201	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 11.

All (201) 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:P:110:ARG:HH11	1:P:114:GLN:HE22	1.15	0.93
1:Q:250:ASN:HD21	1:Q:257:GLN:HE21	1.21	0.88
1:R:110:ARG:HH11	1:R:114:GLN:HE22	1.21	0.88
1:P:150:ASP:O	1:Q:161:ARG:HD2	1.76	0.86
1:Q:110:ARG:HH11	1:Q:114:GLN:HE22	1.24	0.85
1:P:188:PHE:HE2	2:P:1:SUC:H6'1	1.45	0.80
1:P:161:ARG:HD2	1:R:150:ASP:O	1.83	0.79
1:P:188:PHE:CE2	2:P:1:SUC:H6'1	2.19	0.77
1:P:143:ASP:HB2	1:P:158:LEU:HD13	1.67	0.77
1:P:217:TRP:HD1	1:P:221:LEU:HD12	1.50	0.75
1:P:250:ASN:HD21	1:P:257:GLN:HE21	1.33	0.73
1:P:181:THR:HG22	4:P:521:HOH:O	1.86	0.73
1:R:143:ASP:HB2	1:R:158:LEU:HD13	1.70	0.73
1:R:303:ARG:HB2	1:R:303:ARG:HH11	1.55	0.71
1:R:217:TRP:HD1	1:R:221:LEU:HD12	1.54	0.71
1:P:217:TRP:CD1	1:P:221:LEU:HD12	2.26	0.71
1:P:86:ASN:HB3	1:P:92:THR:HG23	1.73	0.70
1:Q:150:ASP:O	1:R:161:ARG:HD2	1.92	0.70
1:R:295:HIS:HD2	1:R:308:LYS:NZ	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:143:ASP:HB2	1:Q:158:LEU:HD13	1.74	0.69
1:R:437:ARG:HG3	1:R:482:TRP:CE3	2.28	0.68
1:R:217:TRP:CD1	1:R:221:LEU:HD12	2.28	0.68
1:Q:181:THR:HG22	4:Q:528:HOH:O	1.93	0.68
1:P:303:ARG:HB2	1:P:303:ARG:NH1	2.09	0.68
1:R:162:GLN:NE2	1:R:188:PHE:H	1.93	0.67
1:Q:303:ARG:HB2	1:Q:303:ARG:NH1	2.10	0.67
1:R:250:ASN:HD21	1:R:257:GLN:HE21	1.41	0.66
1:Q:259:MET:HB3	1:Q:291:LEU:HB3	1.78	0.66
1:P:437:ARG:HG3	1:P:482:TRP:CE3	2.30	0.66
1:Q:437:ARG:HG3	1:Q:482:TRP:CE3	2.31	0.66
1:Q:223:SER:OG	1:Q:251:HIS:HD2	1.80	0.65
1:Q:86:ASN:HB3	1:Q:92:THR:HG23	1.78	0.65
1:Q:388:ASN:OD1	1:R:172:THR:HB	1.97	0.65
1:R:181:THR:HG22	4:R:524:HOH:O	1.97	0.65
1:R:223:SER:OG	1:R:251:HIS:HD2	1.79	0.65
1:Q:217:TRP:CD1	1:Q:221:LEU:HD12	2.32	0.64
1:P:223:SER:OG	1:P:251:HIS:HD2	1.81	0.64
1:P:172:THR:HB	1:R:388:ASN:OD1	1.96	0.64
1:Q:217:TRP:HD1	1:Q:221:LEU:HD12	1.63	0.64
1:Q:438:PRO:HA	1:Q:481:THR:CG2	2.29	0.63
1:P:110:ARG:HH11	1:P:114:GLN:NE2	1.93	0.63
1:R:303:ARG:HB2	1:R:303:ARG:NH1	2.13	0.62
1:P:259:MET:HB3	1:P:291:LEU:HB3	1.81	0.62
1:P:110:ARG:HD3	1:P:114:GLN:NE2	2.14	0.62
1:R:295:HIS:HD2	1:R:308:LYS:HZ2	1.47	0.62
1:R:437:ARG:O	1:R:437:ARG:HD3	2.00	0.62
1:Q:303:ARG:HB2	1:Q:303:ARG:HH11	1.65	0.62
1:Q:217:TRP:O	1:Q:219:ASP:N	2.34	0.61
1:Q:302:LEU:HB2	4:Q:504:HOH:O	2.00	0.61
1:P:86:ASN:HB3	1:P:92:THR:CG2	2.31	0.61
1:R:86:ASN:HB3	1:R:92:THR:HG23	1.83	0.60
1:Q:188:PHE:CE2	2:R:1:SUC:H6'1	2.36	0.60
2:Q:1:SUC:H6'1	1:R:188:PHE:HE2	1.67	0.60
1:R:259:MET:HB3	1:R:291:LEU:HB3	1.82	0.60
1:P:295:HIS:HD2	1:P:308:LYS:NZ	2.00	0.60
1:Q:100:PRO:HA	4:Q:562:HOH:O	2.02	0.59
1:P:303:ARG:HB2	1:P:303:ARG:HH11	1.66	0.59
1:R:217:TRP:O	1:R:219:ASP:N	2.35	0.59
1:R:302:LEU:HB2	4:R:500:HOH:O	2.02	0.59
1:P:438:PRO:HA	1:P:481:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:217:TRP:O	1:P:219:ASP:N	2.36	0.58
1:P:162:GLN:NE2	1:P:188:PHE:H	2.02	0.57
1:P:437:ARG:HG3	1:P:482:TRP:CD2	2.39	0.57
1:Q:438:PRO:HA	1:Q:481:THR:HG23	1.86	0.57
1:P:100:PRO:HA	4:P:555:HOH:O	2.04	0.57
1:Q:386:ASN:HB2	1:Q:389:PHE:H	1.69	0.56
1:R:479:MET:SD	1:R:479:MET:C	2.84	0.56
1:Q:437:ARG:HG3	1:Q:482:TRP:CD2	2.40	0.56
1:R:437:ARG:HG3	1:R:482:TRP:CD2	2.40	0.56
1:R:386:ASN:HB2	1:R:389:PHE:H	1.70	0.56
1:P:205:LEU:HD21	1:P:248:THR:HG21	1.89	0.56
1:Q:437:ARG:O	1:Q:438:PRO:C	2.44	0.55
1:Q:188:PHE:HE2	2:R:1:SUC:H6'1	1.71	0.55
1:R:438:PRO:HA	1:R:481:THR:CG2	2.35	0.55
1:Q:299:PHE:O	1:Q:302:LEU:HD12	2.06	0.55
1:Q:295:HIS:HD2	1:Q:308:LYS:NZ	2.03	0.55
2:Q:1:SUC:H6'1	1:R:188:PHE:CE2	2.41	0.55
1:P:302:LEU:HB2	4:P:498:HOH:O	2.06	0.55
1:R:446:TRP:CZ3	1:R:471:GLY:HA3	2.42	0.55
1:Q:205:LEU:HD21	1:Q:248:THR:HG21	1.89	0.55
1:R:299:PHE:O	1:R:302:LEU:HD12	2.06	0.54
1:P:77:GLY:O	1:P:482:TRP:HA	2.07	0.54
1:P:248:THR:HB	1:P:261:SER:OG	2.07	0.54
1:R:77:GLY:O	1:R:482:TRP:HA	2.08	0.54
1:R:162:GLN:HE21	1:R:187:ARG:HA	1.72	0.54
1:Q:162:GLN:HE21	1:Q:187:ARG:HA	1.74	0.53
1:P:437:ARG:HD3	1:P:437:ARG:O	2.08	0.53
1:Q:162:GLN:NE2	1:Q:188:PHE:H	2.05	0.53
1:P:184:ALA:HB3	1:R:479:MET:HB3	1.89	0.53
1:P:143:ASP:HB2	1:P:158:LEU:CD1	2.38	0.53
1:Q:446:TRP:CZ3	1:Q:471:GLY:HA3	2.44	0.53
1:P:363:LYS:HD3	1:P:371:SER:HB2	1.91	0.53
1:P:386:ASN:HB2	1:P:389:PHE:H	1.72	0.53
1:R:438:PRO:HA	1:R:481:THR:HG23	1.91	0.52
1:P:388:ASN:OD1	1:Q:172:THR:HB	2.10	0.52
1:Q:361:ARG:HG2	1:Q:361:ARG:HH11	1.73	0.52
1:R:100:PRO:HA	4:R:558:HOH:O	2.08	0.52
1:R:110:ARG:HD3	1:R:114:GLN:NE2	2.25	0.51
1:R:181:THR:HG23	1:R:213:TYR:HB2	1.91	0.51
1:R:303:ARG:HG2	1:R:345:THR:OG1	2.11	0.51
1:P:291:LEU:HD23	1:P:312:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:437:ARG:O	1:R:439:GLU:N	2.44	0.51
1:R:205:LEU:HD21	1:R:248:THR:HG21	1.91	0.51
1:Q:264:ARG:HG3	1:Q:286:THR:HG22	1.93	0.51
1:P:299:PHE:O	1:P:302:LEU:HD12	2.11	0.50
1:P:303:ARG:HG2	1:P:345:THR:OG1	2.11	0.50
1:P:437:ARG:O	1:P:438:PRO:C	2.48	0.50
1:Q:110:ARG:HD3	1:Q:114:GLN:NE2	2.25	0.50
1:P:314:GLY:HA3	1:P:318:GLY:O	2.11	0.50
1:R:217:TRP:HD1	1:R:221:LEU:CD1	2.22	0.49
1:R:437:ARG:O	1:R:438:PRO:C	2.47	0.49
1:P:162:GLN:HE21	1:P:187:ARG:HA	1.77	0.49
1:Q:181:THR:HG23	1:Q:213:TYR:HB2	1.94	0.49
1:R:136:ARG:HD3	1:R:166:GLU:OE1	2.12	0.49
1:R:86:ASN:HB3	1:R:92:THR:CG2	2.43	0.49
1:P:446:TRP:CZ3	1:P:471:GLY:HA3	2.47	0.49
1:P:198:ILE:HD11	1:P:378:ASN:HB2	1.95	0.49
1:R:110:ARG:NH1	1:R:114:GLN:HE22	2.02	0.48
1:Q:282:ASP:O	1:Q:332:PRO:HD3	2.13	0.48
1:P:80:ARG:NH2	2:P:1:SUC:O3	2.44	0.48
1:Q:437:ARG:HD3	1:Q:437:ARG:O	2.13	0.48
1:Q:248:THR:HB	1:Q:261:SER:OG	2.13	0.48
1:Q:291:LEU:HD23	1:Q:312:LEU:HG	1.95	0.48
1:Q:77:GLY:O	1:Q:482:TRP:HA	2.13	0.48
1:Q:86:ASN:HB3	1:Q:92:THR:CG2	2.42	0.48
1:P:437:ARG:O	1:P:439:GLU:N	2.47	0.48
1:P:145:GLN:NE2	1:P:156:SER:HA	2.29	0.48
1:Q:408:ASN:O	1:Q:409:ASP:HB2	2.14	0.47
1:P:151:TRP:CE3	1:Q:161:ARG:HD3	2.49	0.47
1:Q:217:TRP:HD1	1:Q:221:LEU:CD1	2.26	0.47
1:Q:437:ARG:O	1:Q:439:GLU:N	2.47	0.47
1:P:295:HIS:HD2	1:P:308:LYS:HZ2	1.62	0.47
1:Q:295:HIS:HD2	1:Q:308:LYS:HZ2	1.63	0.47
1:P:438:PRO:HA	1:P:481:THR:HG23	1.96	0.47
1:P:361:ARG:HG2	1:P:361:ARG:HH11	1.80	0.47
1:R:361:ARG:HH11	1:R:361:ARG:HG2	1.80	0.47
1:R:152:THR:HG23	4:R:518:HOH:O	2.14	0.47
1:R:143:ASP:HB2	1:R:158:LEU:CD1	2.44	0.47
1:R:145:GLN:NE2	1:R:156:SER:HA	2.29	0.47
1:Q:80:ARG:NH2	2:R:1:SUC:O3	2.48	0.47
1:Q:302:LEU:HD13	4:Q:504:HOH:O	2.16	0.46
1:Q:410:ARG:HA	1:Q:456:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:127:GLN:OE1	1:R:135:THR:HG21	2.15	0.46
1:R:291:LEU:HD23	1:R:312:LEU:HG	1.97	0.46
1:P:74:GLU:OE2	1:P:126:LYS:HD2	2.16	0.46
1:R:363:LYS:HD3	1:R:371:SER:HB2	1.98	0.46
1:R:198:ILE:HD11	1:R:378:ASN:HB2	1.97	0.46
1:P:127:GLN:OE1	1:P:135:THR:HG21	2.16	0.45
1:R:410:ARG:HA	1:R:456:TYR:O	2.16	0.45
1:Q:127:GLN:OE1	1:Q:135:THR:HG21	2.16	0.45
1:P:319:ALA:HB3	1:P:330:LEU:HD13	1.98	0.45
1:P:136:ARG:HD3	1:P:166:GLU:OE1	2.17	0.45
1:P:463:GLY:HA2	1:P:468:ASN:HB3	1.99	0.45
1:P:151:TRP:HE3	1:Q:161:ARG:HD3	1.81	0.45
1:Q:363:LYS:HD3	1:Q:371:SER:HB2	1.97	0.45
1:Q:303:ARG:HG2	1:Q:345:THR:OG1	2.16	0.44
1:R:257:GLN:OE1	1:R:295:HIS:HE1	2.00	0.44
1:P:479:MET:SD	1:P:479:MET:C	2.95	0.44
1:R:463:GLY:HA2	1:R:468:ASN:HB3	1.99	0.44
1:R:305:GLY:HA3	1:R:344:THR:O	2.17	0.44
1:R:413:VAL:HG21	1:R:453:LEU:HA	2.00	0.44
2:Q:1:SUC:HO3	1:R:110:ARG:HH12	1.66	0.44
1:Q:387:GLN:HE22	1:R:131:ASN:ND2	2.15	0.44
1:Q:386:ASN:HB3	1:Q:387:GLN:H	1.64	0.43
1:R:109:GLY:O	1:R:419:LYS:HE2	2.17	0.43
1:R:338:ARG:NH2	4:R:544:HOH:O	2.47	0.43
1:P:194:ASP:CB	1:P:201:ASP:HA	2.48	0.43
1:R:282:ASP:O	1:R:332:PRO:HD3	2.18	0.43
1:R:216:LYS:HE2	1:R:216:LYS:HB2	1.88	0.43
1:Q:143:ASP:HB2	1:Q:158:LEU:CD1	2.45	0.43
1:P:386:ASN:HB3	1:P:387:GLN:H	1.61	0.43
1:P:410:ARG:HA	1:P:456:TYR:O	2.18	0.43
1:Q:172:THR:HG22	1:Q:173:PHE:HD1	1.84	0.43
1:P:109:GLY:O	1:P:419:LYS:HE2	2.18	0.43
2:Q:1:SUC:C2	1:R:80:ARG:NH2	2.82	0.43
2:Q:2:SUC:H1'2	2:Q:2:SUC:H1	1.83	0.42
1:Q:395:GLY:HA2	1:Q:419:LYS:O	2.19	0.42
1:Q:413:VAL:CG2	1:Q:452:LYS:HG2	2.48	0.42
1:P:390:ALA:HB2	1:P:431:ILE:HD13	2.02	0.42
1:R:194:ASP:CB	1:R:201:ASP:HA	2.49	0.42
1:R:434:PHE:O	1:R:437:ARG:NH2	2.53	0.42
1:Q:463:GLY:HA2	1:Q:468:ASN:HB3	2.01	0.42
1:R:162:GLN:HE21	1:R:187:ARG:CA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:347:LEU:HD12	1:P:347:LEU:HA	1.95	0.42
1:R:263:LEU:HD23	1:R:263:LEU:N	2.35	0.41
1:P:138:LYS:HD3	1:P:164:PHE:CE1	2.55	0.41
1:R:110:ARG:HH11	1:R:114:GLN:NE2	2.01	0.41
1:R:413:VAL:HG23	1:R:452:LYS:HG2	2.03	0.41
1:Q:413:VAL:HG21	1:Q:453:LEU:HA	2.02	0.41
1:P:209:GLY:HA3	1:P:227:LEU:O	2.21	0.41
1:Q:402:LEU:O	1:Q:412:ALA:HA	2.21	0.41
1:P:217:TRP:HD1	1:P:221:LEU:CD1	2.24	0.41
1:R:315:HIS:HD2	1:R:335:ASP:OD1	2.04	0.41
1:R:291:LEU:HD21	1:R:310:ALA:HB1	2.02	0.40
1:P:129:LEU:HD12	1:P:129:LEU:N	2.35	0.40
1:Q:305:GLY:HA3	1:Q:344:THR:O	2.22	0.40
1:R:400:MET:O	1:R:414:ASN:HA	2.21	0.40
1:P:136:ARG:O	1:P:165:VAL:HA	2.21	0.40
1:Q:162:GLN:HE21	1:Q:187:ARG:CA	2.35	0.40
1:R:361:ARG:CG	1:R:361:ARG:HH11	2.33	0.40
1:Q:138:LYS:HD3	1:Q:164:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

## 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	P	411/413 (100%)	387 (94%)	21 (5%)	3 (1%)	26	38
1	Q	411/413 (100%)	389 (95%)	18 (4%)	4 (1%)	19	28
1	R	411/413 (100%)	390 (95%)	18 (4%)	3 (1%)	26	38
All	All	1233/1239 (100%)	1166 (95%)	57 (5%)	10 (1%)	24	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	218	ASN
1	Q	218	ASN
1	R	218	ASN
1	Q	220	GLY
1	R	220	GLY
1	P	220	GLY
1	P	470	GLY
1	Q	438	PRO
1	Q	470	GLY
1	R	470	GLY

### 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	P	327/327 (100%)	292 (89%)	35 (11%)	8	11
1	Q	327/327 (100%)	293 (90%)	34 (10%)	9	12
1	R	327/327 (100%)	292 (89%)	35 (11%)	8	11
All	All	981/981 (100%)	877 (89%)	104 (11%)	8	12

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	92	THR
1	P	110	ARG
1	P	111	LEU
1	P	130	ASP
1	P	135	THR
1	P	139	VAL
1	P	158	LEU
1	P	172	THR
1	P	181	THR
1	P	182	LEU
1	P	198	ILE
1	P	218	ASN
1	P	222	ARG

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Mol	Chain	Res	Type
1	P	248	THR
1	P	250	ASN
1	P	263	LEU
1	P	291	LEU
1	P	292	LEU
1	P	294	LEU
1	P	297	ASP
1	P	302	LEU
1	P	344	THR
1	P	347	LEU
1	P	358	LEU
1	P	380	ARG
1	P	382	ILE
1	P	413	VAL
1	P	414	ASN
1	P	437	ARG
1	P	441	ARG
1	P	446	TRP
1	P	460	ASP
1	P	468	ASN
1	P	478	GLN
1	P	479	MET
1	Q	92	THR
1	Q	110	ARG
1	Q	111	LEU
1	Q	130	ASP
1	Q	135	THR
1	Q	139	VAL
1	Q	172	THR
1	Q	181	THR
1	Q	182	LEU
1	Q	198	ILE
1	Q	218	ASN
1	Q	222	ARG
1	Q	248	THR
1	Q	250	ASN
1	Q	263	LEU
1	Q	292	LEU
1	Q	297	ASP
1	Q	302	LEU
1	Q	344	THR
1	Q	347	LEU

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Mol	Chain	Res	Type
1	Q	350	ASN
1	Q	358	LEU
1	Q	380	ARG
1	Q	382	ILE
1	Q	408	ASN
1	Q	413	VAL
1	Q	414	ASN
1	Q	437	ARG
1	Q	441	ARG
1	Q	460	ASP
1	Q	468	ASN
1	Q	478	GLN
1	Q	479	MET
1	Q	481	THR
1	R	92	THR
1	R	110	ARG
1	R	111	LEU
1	R	130	ASP
1	R	135	THR
1	R	139	VAL
1	R	158	LEU
1	R	172	THR
1	R	181	THR
1	R	182	LEU
1	R	198	ILE
1	R	218	ASN
1	R	222	ARG
1	R	248	THR
1	R	250	ASN
1	R	263	LEU
1	R	292	LEU
1	R	297	ASP
1	R	302	LEU
1	R	344	THR
1	R	347	LEU
1	R	358	LEU
1	R	380	ARG
1	R	382	ILE
1	R	408	ASN
1	R	413	VAL
1	R	414	ASN
1	R	424	PRO

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Mol	Chain	Res	Type
1	R	437	ARG
1	R	441	ARG
1	R	460	ASP
1	R	468	ASN
1	R	478	GLN
1	R	479	MET
1	R	481	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	114	GLN
1	P	162	GLN
1	P	196	HIS
1	P	218	ASN
1	P	244	ASN
1	P	250	ASN
1	P	251	HIS
1	P	295	HIS
1	P	315	HIS
1	P	350	ASN
1	P	378	ASN
1	P	383	GLN
1	P	387	GLN
1	P	398	GLN
1	P	468	ASN
1	P	478	GLN
1	Q	114	GLN
1	Q	162	GLN
1	Q	196	HIS
1	Q	218	ASN
1	Q	244	ASN
1	Q	250	ASN
1	Q	251	HIS
1	Q	295	HIS
1	Q	315	HIS
1	Q	350	ASN
1	Q	378	ASN
1	Q	383	GLN
1	Q	387	GLN
1	Q	398	GLN
1	Q	414	ASN

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Mol	Chain	Res	Type
1	Q	468	ASN
1	Q	478	GLN
1	R	114	GLN
1	R	125	HIS
1	R	162	GLN
1	R	196	HIS
1	R	218	ASN
1	R	244	ASN
1	R	250	ASN
1	R	251	HIS
1	R	295	HIS
1	R	315	HIS
1	R	350	ASN
1	R	378	ASN
1	R	383	GLN
1	R	387	GLN
1	R	398	GLN
1	R	468	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](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	SUC	P	1	-	24,24,24	0.67	0	36,36,36	0.61	0
2	SUC	P	2	-	24,24,24	0.47	0	36,36,36	0.58	0
2	SUC	Q	1	-	24,24,24	0.74	0	36,36,36	0.69	0
2	SUC	Q	2	-	24,24,24	0.40	0	36,36,36	0.67	0
2	SUC	R	1	-	24,24,24	0.70	1 (4%)	36,36,36	0.65	0
2	SUC	R	2	-	24,24,24	0.49	0	36,36,36	0.60	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
2	SUC	P	1	-	-	0/12/51/51	0/2/2/2
2	SUC	P	2	-	-	0/12/51/51	0/2/2/2
2	SUC	Q	1	-	-	0/12/51/51	0/2/2/2
2	SUC	Q	2	-	-	0/12/51/51	0/2/2/2
2	SUC	R	1	-	-	0/12/51/51	0/2/2/2
2	SUC	R	2	-	-	0/12/51/51	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1	SUC	O5-C1	2.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	SUC	3	0
2	Q	1	SUC	4	0
2	Q	2	SUC	1	0
2	R	1	SUC	3	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 ⓘ

### 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	P	413/413 (100%)	-0.68	9 (2%) 65 64	11, 25, 52, 84	0
1	Q	413/413 (100%)	-0.66	7 (1%) 73 72	11, 24, 51, 84	0
1	R	413/413 (100%)	-0.67	8 (1%) 70 69	10, 24, 51, 83	0
All	All	1239/1239 (100%)	-0.67	24 (1%) 70 69	10, 25, 52, 84	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	274	SER	8.5
1	Q	71	SER	8.4
1	R	274	SER	5.7
1	P	71	SER	5.1
1	Q	275	ASN	4.8
1	P	274	SER	4.5
1	R	71	SER	4.3
1	P	275	ASN	3.4
1	R	469	SER	3.4
1	Q	469	SER	3.3
1	R	275	ASN	3.2
1	P	219	ASP	3.1
1	R	219	ASP	3.1
1	R	301	GLY	2.9
1	P	276	GLY	2.7
1	Q	468	ASN	2.6
1	P	468	ASN	2.4
1	Q	466	GLY	2.4
1	R	276	GLY	2.4
1	P	469	SER	2.4
1	P	302	LEU	2.3
1	P	465	ASP	2.1
1	R	468	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	470	GLY	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	SUC	R	1	23/23	0.86	0.22	12.82	20,29,31,33	23
2	SUC	Q	1	23/23	0.83	0.23	12.06	21,29,31,33	23
2	SUC	P	1	23/23	0.87	0.20	11.21	20,28,31,33	23
2	SUC	Q	2	23/23	0.89	0.16	5.55	29,33,35,36	23
2	SUC	P	2	23/23	0.92	0.15	3.80	29,33,35,37	23
2	SUC	R	2	23/23	0.92	0.13	3.13	29,33,35,36	23
3	CA	R	10	1/1	0.99	0.06	-2.22	27,27,27,27	0
3	CA	P	10	1/1	0.97	0.07	-2.45	30,30,30,30	0
3	CA	Q	10	1/1	0.99	0.04	-2.58	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.