



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:08 AM 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 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/ValidationPDFNotes.html>

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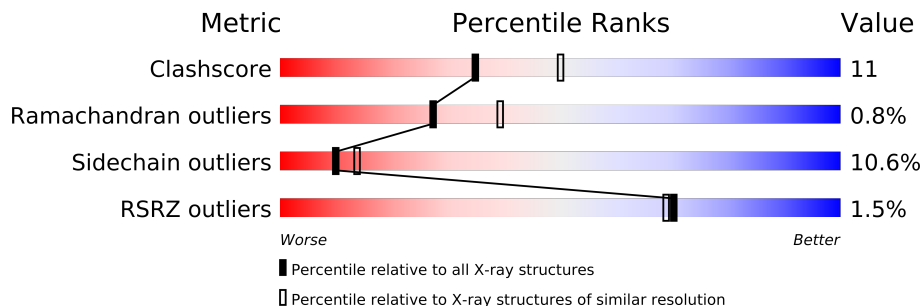
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	P	413	
1	Q	413	
1	R	413	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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

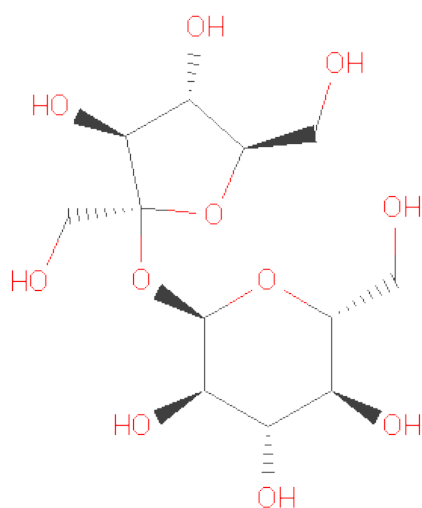
There are 4 unique types of molecules in this entry. The entry contains 10077 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ( $RSRZ > 2$ ). 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.

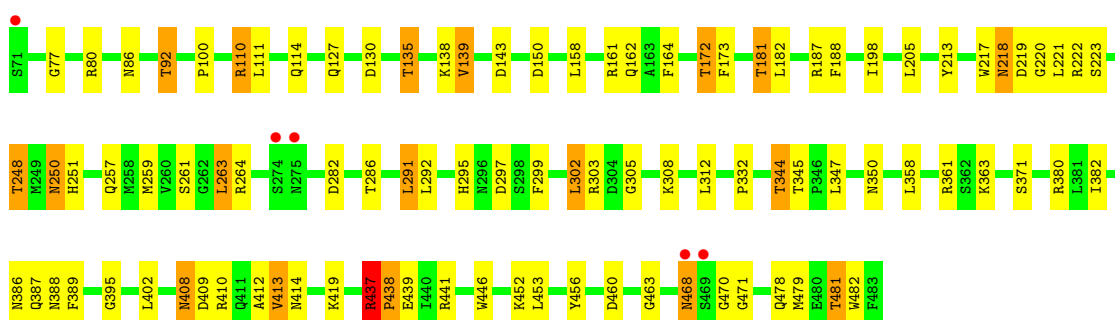
#### • Molecule 1: SUCROSE-SPECIFIC PORIN

Chain P: 



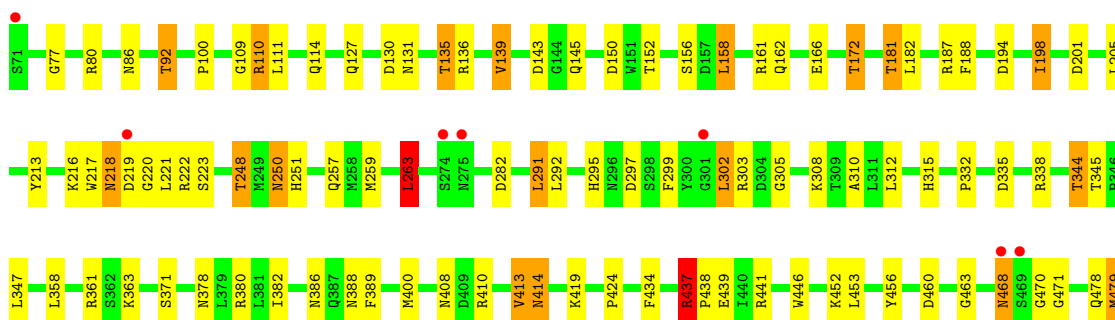
#### • Molecule 1: SUCROSE-SPECIFIC PORIN

Chain Q: 



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

Chain R: 





## 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> )	0.35 , 40.8	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	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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.

## 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 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 hydrogens



added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (201) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:P:217:TRP:O	1:P:219:ASP:N	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	30	43
1	Q	411/413 (100%)	389 (95%)	18 (4%)	4 (1%)	22	32
1	R	411/413 (100%)	390 (95%)	18 (4%)	3 (1%)	30	43
All	All	1233/1239 (100%)	1166 (95%)	57 (5%)	10 (1%)	27	39

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

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Mol	Chain	Res	Type
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%)	10	13
1	Q	327/327 (100%)	293 (90%)	34 (10%)	10	14
1	R	327/327 (100%)	292 (89%)	35 (11%)	10	13
All	All	981/981 (100%)	877 (89%)	104 (11%)	10	14

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
1	P	248	THR
1	P	250	ASN
1	P	263	LEU
1	P	291	LEU
1	P	292	LEU

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Mol	Chain	Res	Type
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
1	Q	350	ASN
1	Q	358	LEU
1	Q	380	ARG
1	Q	382	ILE
1	Q	408	ASN

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Mol	Chain	Res	Type
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
1	R	437	ARG
1	R	441	ARG
1	R	460	ASP
1	R	468	ASN
1	R	478	GLN

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Mol	Chain	Res	Type
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
1	Q	468	ASN
1	Q	478	GLN
1	R	114	GLN
1	R	125	HIS
1	R	162	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	0.68	0
2	SUC	Q	2	-	24,24,24	0.39	0	36,36,36	0.67	0
2	SUC	R	1	-	24,24,24	0.70	1 (4%)	36,36,36	0.64	0
2	SUC	R	2	-	24,24,24	0.48	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	2.02	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.

## 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%)	-0.67	7 (1%) 67 65	11, 25, 52, 84	0
1	Q	413/413 (100%)	-0.65	5 (1%) 75 75	11, 24, 51, 84	0
1	R	413/413 (100%)	-0.65	7 (1%) 67 65	10, 24, 51, 83	0
All	All	1239/1239 (100%)	-0.66	19 (1%) 70 69	10, 25, 52, 84	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	71	SER	8.4
1	Q	274	SER	6.2
1	P	71	SER	5.4
1	R	274	SER	4.3
1	R	71	SER	4.3
1	Q	275	ASN	3.6
1	R	469	SER	3.5
1	Q	469	SER	3.2
1	P	274	SER	3.2
1	P	219	ASP	3.1
1	R	219	ASP	3.1
1	P	275	ASN	2.8
1	R	275	ASN	2.7
1	P	469	SER	2.2
1	P	276	GLY	2.2
1	R	301	GLY	2.1
1	P	468	ASN	2.1
1	R	468	ASN	2.1
1	Q	468	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SUC	Q	1	23/23	0.22	12.72	21,29,31,33	23
2	SUC	R	1	23/23	0.22	12.31	20,29,31,33	23
2	SUC	P	1	23/23	0.20	10.59	20,28,31,33	23
2	SUC	Q	2	23/23	0.16	7.55	29,33,35,36	23
2	SUC	P	2	23/23	0.14	4.58	29,33,35,37	23
2	SUC	R	2	23/23	0.13	4.00	29,33,35,36	23
3	CA	R	10	1/1	0.05	-2.33	27,27,27,27	0
3	CA	Q	10	1/1	0.04	-2.47	29,29,29,29	0
3	CA	P	10	1/1	0.06	-2.52	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.