



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2018 – 05:47 AM EDT

PDB ID : 1A0S  
Title : SUCROSE-SPECIFIC PORIN  
Authors : Diederichs, K.; Welte, W.  
Deposited on : 1997-12-07  
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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : rb-20031021  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031021

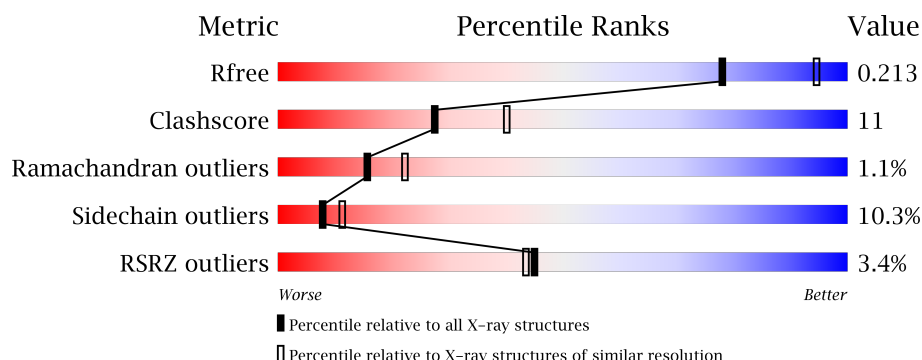
# 1 Overall quality at a glance

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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (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	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>•</div> </div> </div>
1	Q	413	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>•</div> </div> </div>
1	R	413	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9939 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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

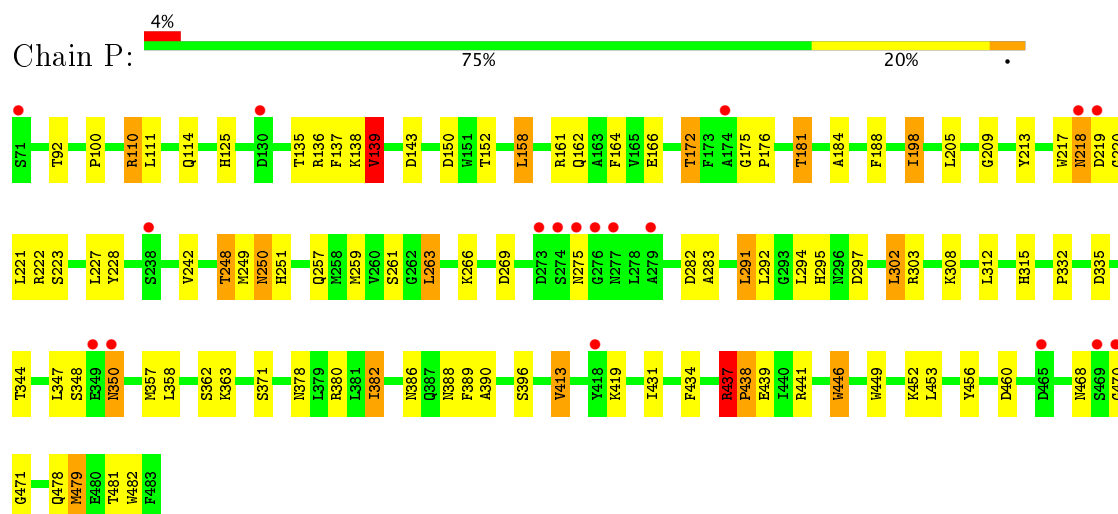
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	108	Total	O	0	0
			108	108		
3	Q	112	Total	O	0	0
			112	112		
3	R	110	Total	O	0	0
			110	110		

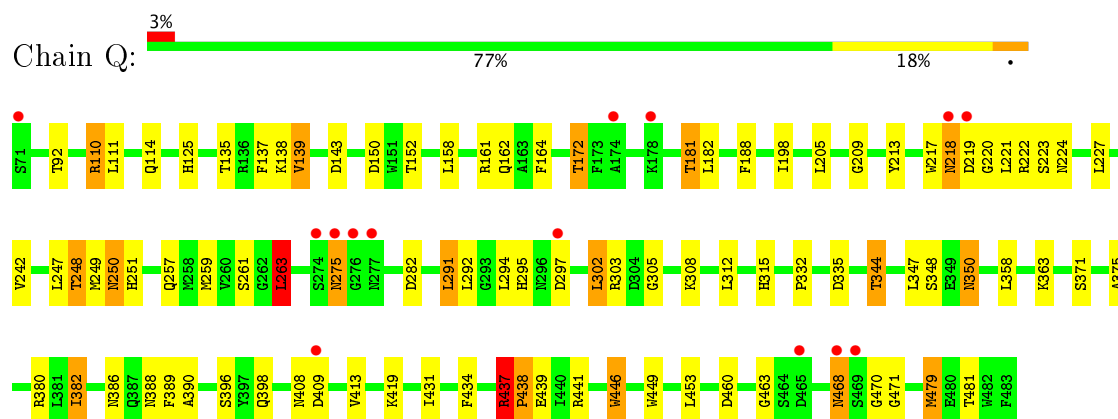
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

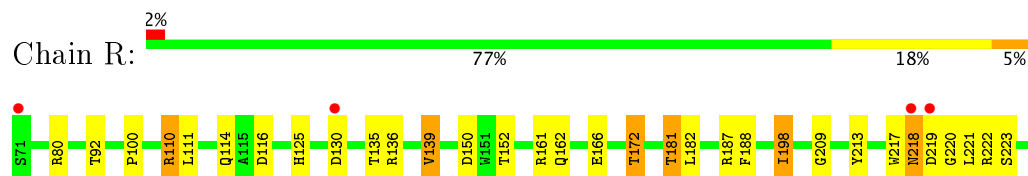
#### • Molecule 1: SUCROSE-SPECIFIC PORIN

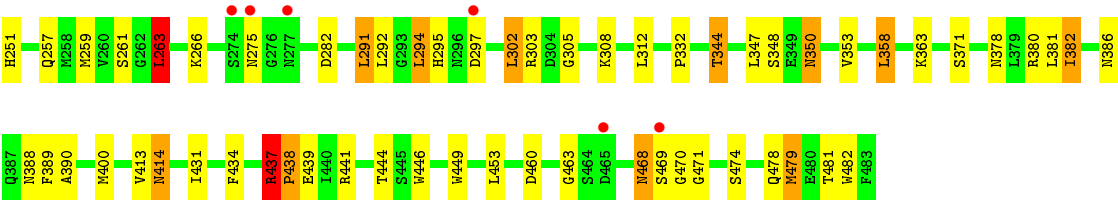


#### • Molecule 1: SUCROSE-SPECIFIC PORIN



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.10Å 112.10Å 147.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.40 9.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	78.3 (100.00-2.40) 82.6 (9.99-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.214 , 0.228 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	795 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 66.9	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.040 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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 56.53 % 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 2.6999e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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	0.55	0/3283	0.80	3/4443 (0.1%)
1	Q	0.52	0/3283	0.80	4/4443 (0.1%)
1	R	0.54	0/3283	0.80	4/4443 (0.1%)
All	All	0.54	0/9849	0.80	11/13329 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	437	ARG	N-CA-C	7.30	130.70	111.00
1	R	437	ARG	N-CA-C	6.96	129.78	111.00
1	Q	139	VAL	CB-CA-C	-6.87	98.35	111.40
1	Q	437	ARG	N-CA-C	6.86	129.51	111.00
1	R	139	VAL	CB-CA-C	-6.41	99.22	111.40
1	P	291	LEU	CA-CB-CG	6.19	129.53	115.30
1	P	139	VAL	CB-CA-C	-6.17	99.67	111.40
1	R	263	LEU	CA-CB-CG	5.69	128.38	115.30
1	R	291	LEU	CA-CB-CG	5.58	128.14	115.30
1	Q	291	LEU	CA-CB-CG	5.52	127.99	115.30
1	Q	263	LEU	CA-CB-CG	5.37	127.65	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	228	TYR	Sidechain

## 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	76	0
1	Q	3202	0	2985	67	0
1	R	3202	0	2985	68	1
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
3	P	108	0	0	5	0
3	Q	112	0	0	6	0
3	R	110	0	0	6	1
All	All	9939	0	8955	201	1

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:250:ASN:HD21	1:P:257:GLN:HE21	1.10	0.99
1:R:110:ARG:HH11	1:R:114:GLN:HE22	1.15	0.94
1:Q:250:ASN:HD21	1:Q:257:GLN:HE21	1.07	0.91
1:Q:110:ARG:HH11	1:Q:114:GLN:HE22	1.17	0.91
1:P:110:ARG:HH11	1:P:114:GLN:HE22	1.19	0.87
1:R:250:ASN:HD21	1:R:257:GLN:HE21	1.23	0.85
1:R:386:ASN:HB2	1:R:389:PHE:H	1.42	0.83
1:P:302:LEU:HD13	3:P:498:HOH:O	1.86	0.76
1:P:172:THR:HB	1:R:388:ASN:OD1	1.84	0.76
1:P:438:PRO:HA	1:P:481:THR:HG22	1.66	0.75
1:Q:438:PRO:HA	1:Q:481:THR:HG22	1.69	0.74
1:P:161:ARG:HD2	1:R:150:ASP:O	1.86	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:386:ASN:HB2	1:P:389:PHE:H	1.51	0.74
1:R:162:GLN:NE2	1:R:188:PHE:H	1.86	0.74
1:Q:181:THR:HG22	3:Q:527:HOH:O	1.88	0.73
1:Q:386:ASN:HB2	1:Q:389:PHE:H	1.52	0.72
1:P:150:ASP:O	1:Q:161:ARG:HD2	1.90	0.72
1:Q:388:ASN:OD1	1:R:172:THR:HB	1.90	0.72
1:R:438:PRO:HA	1:R:481:THR:HG22	1.72	0.71
1:R:181:THR:HG22	3:R:529:HOH:O	1.90	0.70
1:Q:302:LEU:HD13	3:Q:502:HOH:O	1.92	0.69
1:R:302:LEU:HD13	3:R:504:HOH:O	1.91	0.69
1:P:181:THR:HG22	3:P:522:HOH:O	1.92	0.68
1:P:295:HIS:HD2	1:P:308:LYS:NZ	1.92	0.67
1:P:437:ARG:HE	1:P:437:ARG:HA	1.61	0.66
1:R:437:ARG:HA	1:R:437:ARG:HE	1.62	0.64
1:Q:295:HIS:HD2	1:Q:308:LYS:NZ	1.96	0.64
1:R:217:TRP:HD1	1:R:221:LEU:HD12	1.63	0.63
1:P:388:ASN:OD1	1:Q:172:THR:HB	1.97	0.63
3:Q:594:HOH:O	1:R:125:HIS:HD2	1.80	0.63
1:Q:217:TRP:HD1	1:Q:221:LEU:HD12	1.64	0.62
1:Q:437:ARG:HE	1:Q:437:ARG:HA	1.65	0.62
1:R:295:HIS:HD2	1:R:308:LYS:NZ	1.98	0.61
1:R:449:TRP:HB2	1:R:453:LEU:HD12	1.81	0.61
1:Q:437:ARG:HD3	1:Q:437:ARG:O	2.00	0.61
1:R:110:ARG:HH11	1:R:114:GLN:NE2	1.94	0.61
1:Q:110:ARG:NH1	1:Q:114:GLN:HE22	1.96	0.60
1:R:217:TRP:O	1:R:219:ASP:N	2.35	0.60
1:P:125:HIS:HD2	3:R:485:HOH:O	1.84	0.60
1:Q:223:SER:OG	1:Q:251:HIS:HD2	1.84	0.60
1:Q:259:MET:HB3	1:Q:291:LEU:HB3	1.83	0.60
1:R:437:ARG:O	1:R:439:GLU:N	2.35	0.59
1:Q:437:ARG:O	1:Q:439:GLU:N	2.37	0.57
1:P:438:PRO:HA	1:P:481:THR:CG2	2.35	0.57
1:Q:438:PRO:HA	1:Q:481:THR:CG2	2.33	0.57
1:Q:449:TRP:HB2	1:Q:453:LEU:HD12	1.87	0.57
1:R:110:ARG:HD2	3:R:576:HOH:O	2.03	0.57
1:Q:150:ASP:O	1:R:161:ARG:HD2	2.05	0.57
1:P:217:TRP:HD1	1:P:221:LEU:HD12	1.70	0.56
1:R:438:PRO:HA	1:R:481:THR:CG2	2.35	0.56
1:P:217:TRP:O	1:P:219:ASP:N	2.38	0.56
1:P:437:ARG:O	1:P:439:GLU:N	2.39	0.56
1:R:181:THR:HG23	1:R:213:TYR:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:437:ARG:O	1:R:437:ARG:HD3	2.05	0.56
1:R:446:TRP:CZ3	1:R:471:GLY:HA3	2.39	0.56
1:P:449:TRP:HB2	1:P:453:LEU:HD12	1.88	0.56
1:Q:217:TRP:O	1:Q:219:ASP:N	2.38	0.56
1:R:217:TRP:CD1	1:R:221:LEU:HD12	2.40	0.56
1:P:291:LEU:HD23	1:P:312:LEU:HG	1.87	0.56
1:Q:249:MET:SD	1:Q:251:HIS:HE1	2.29	0.56
1:R:110:ARG:NH1	1:R:114:GLN:HE22	1.94	0.56
1:Q:162:GLN:NE2	1:Q:188:PHE:H	2.03	0.55
1:Q:248:THR:HB	1:Q:261:SER:OG	2.06	0.55
1:P:438:PRO:CA	1:P:481:THR:HG22	2.36	0.55
1:P:282:ASP:O	1:P:332:PRO:HD3	2.06	0.55
1:R:223:SER:OG	1:R:251:HIS:HD2	1.89	0.55
1:Q:282:ASP:O	1:Q:332:PRO:HD3	2.07	0.55
1:P:386:ASN:HD22	1:Q:172:THR:HG21	1.72	0.55
1:P:437:ARG:HD3	1:P:437:ARG:O	2.06	0.55
1:P:110:ARG:HD2	3:P:569:HOH:O	2.07	0.54
1:Q:110:ARG:HH11	1:Q:114:GLN:NE2	1.95	0.54
1:Q:217:TRP:CD1	1:Q:221:LEU:HD12	2.41	0.54
1:Q:446:TRP:CZ3	1:Q:471:GLY:HA3	2.42	0.54
1:R:479:MET:SD	1:R:479:MET:C	2.87	0.53
1:Q:438:PRO:CA	1:Q:481:THR:HG22	2.37	0.53
1:Q:350:ASN:N	1:Q:350:ASN:HD22	2.07	0.53
1:P:217:TRP:CD1	1:P:221:LEU:HD12	2.44	0.53
1:Q:181:THR:HG23	1:Q:213:TYR:HB2	1.90	0.53
1:R:162:GLN:HE21	1:R:187:ARG:HA	1.73	0.53
1:P:110:ARG:HH11	1:P:114:GLN:NE2	1.99	0.53
1:P:248:THR:HB	1:P:261:SER:OG	2.09	0.53
1:P:110:ARG:NH1	1:P:114:GLN:HE22	1.98	0.52
1:Q:152:THR:HG23	3:Q:521:HOH:O	2.09	0.52
1:Q:295:HIS:HD2	1:Q:308:LYS:HZ3	1.58	0.52
1:Q:382:ILE:HD11	1:Q:434:PHE:CE1	2.45	0.52
1:R:282:ASP:O	1:R:332:PRO:HD3	2.09	0.52
1:P:382:ILE:HD11	1:P:434:PHE:CE1	2.44	0.52
1:R:303:ARG:HB2	1:R:303:ARG:HH11	1.74	0.52
1:P:143:ASP:HB2	1:P:158:LEU:HD13	1.90	0.52
1:P:263:LEU:N	1:P:263:LEU:HD23	2.24	0.52
1:Q:303:ARG:HH11	1:Q:303:ARG:HB2	1.74	0.51
1:P:143:ASP:HB2	1:P:158:LEU:CD1	2.40	0.51
1:R:438:PRO:CA	1:R:481:THR:HG22	2.39	0.51
1:Q:437:ARG:O	1:Q:438:PRO:C	2.49	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:80:ARG:HD2	1:R:116:ASP:OD1	2.10	0.51
1:P:110:ARG:HD3	1:P:114:GLN:NE2	2.25	0.51
1:Q:390:ALA:HB2	1:Q:431:ILE:HD13	1.91	0.51
1:R:259:MET:HB3	1:R:291:LEU:HB3	1.93	0.51
1:P:295:HIS:HD2	1:P:308:LYS:HZ2	1.56	0.50
1:P:446:TRP:CZ3	1:P:471:GLY:HA3	2.46	0.50
1:R:263:LEU:HD23	1:R:263:LEU:N	2.27	0.50
1:P:184:ALA:HB3	1:R:479:MET:HB3	1.93	0.50
1:P:181:THR:HG23	1:P:213:TYR:HB2	1.94	0.50
3:P:588:HOH:O	1:Q:125:HIS:HD2	1.95	0.50
1:R:152:THR:HG23	3:R:523:HOH:O	2.12	0.50
1:P:479:MET:SD	1:P:479:MET:C	2.90	0.49
1:P:350:ASN:N	1:P:350:ASN:HD22	2.11	0.49
1:R:295:HIS:HD2	1:R:308:LYS:HZ2	1.60	0.49
1:R:437:ARG:HA	1:R:437:ARG:NE	2.27	0.49
1:P:250:ASN:ND2	1:P:257:GLN:HE21	1.94	0.49
1:Q:382:ILE:HD11	1:Q:434:PHE:CD1	2.48	0.49
1:Q:110:ARG:HD2	3:Q:575:HOH:O	2.10	0.49
1:P:396:SER:HB2	1:P:419:LYS:HB3	1.95	0.49
1:P:437:ARG:HG2	1:P:482:TRP:CE2	2.47	0.49
1:R:291:LEU:HD23	1:R:312:LEU:HG	1.94	0.49
1:R:350:ASN:HD22	1:R:350:ASN:N	2.11	0.49
1:P:205:LEU:HD21	1:P:248:THR:HG21	1.95	0.48
1:Q:137:PHE:CZ	1:Q:139:VAL:HG22	2.48	0.48
1:P:223:SER:OG	1:P:251:HIS:HD2	1.97	0.48
1:P:259:MET:HB3	1:P:291:LEU:HB3	1.95	0.48
1:Q:396:SER:HB2	1:Q:419:LYS:HB3	1.94	0.48
1:Q:263:LEU:N	1:Q:263:LEU:HD23	2.28	0.48
1:R:437:ARG:O	1:R:438:PRO:C	2.50	0.48
1:Q:291:LEU:HD23	1:Q:312:LEU:HG	1.95	0.48
1:P:382:ILE:HD11	1:P:434:PHE:CD1	2.49	0.48
1:P:162:GLN:NE2	1:P:188:PHE:H	2.12	0.47
1:P:249:MET:SD	1:P:251:HIS:HE1	2.37	0.47
1:Q:408:ASN:O	1:Q:409:ASP:HB2	2.14	0.47
1:P:315:HIS:HD2	1:P:335:ASP:OD1	1.97	0.47
1:P:209:GLY:HA3	1:P:227:LEU:O	2.14	0.47
1:P:437:ARG:HA	1:P:437:ARG:NE	2.29	0.46
1:R:446:TRP:CH2	1:R:471:GLY:HA3	2.50	0.46
1:Q:350:ASN:N	1:Q:350:ASN:ND2	2.63	0.46
1:R:209:GLY:HA3	1:R:227:LEU:O	2.15	0.45
1:R:266:LYS:HD3	3:R:554:HOH:O	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:315:HIS:HD2	1:Q:335:ASP:OD1	2.00	0.45
1:Q:143:ASP:HB2	1:Q:158:LEU:HD13	1.99	0.45
1:R:363:LYS:HD3	1:R:371:SER:HB2	1.98	0.45
1:R:390:ALA:HB2	1:R:431:ILE:HD13	1.97	0.45
1:R:382:ILE:HD11	1:R:434:PHE:CE1	2.51	0.45
1:P:150:ASP:O	1:Q:161:ARG:CD	2.63	0.45
1:P:295:HIS:HD2	1:P:308:LYS:HZ3	1.61	0.45
1:P:350:ASN:N	1:P:350:ASN:ND2	2.65	0.45
1:P:390:ALA:HB2	1:P:431:ILE:HD13	1.97	0.45
1:Q:446:TRP:CH2	1:Q:471:GLY:HA3	2.52	0.45
1:R:249:MET:SD	1:R:251:HIS:HE1	2.39	0.45
1:P:172:THR:HG21	1:R:386:ASN:HD22	1.82	0.44
1:Q:223:SER:OG	1:Q:251:HIS:CD2	2.69	0.44
1:P:434:PHE:O	1:P:437:ARG:NH2	2.50	0.44
1:P:437:ARG:HG2	1:P:482:TRP:CZ2	2.52	0.44
1:Q:275:ASN:N	1:Q:275:ASN:HD22	2.16	0.44
1:Q:437:ARG:HA	1:Q:437:ARG:NE	2.30	0.44
1:P:363:LYS:HD3	1:P:371:SER:HB2	1.99	0.44
1:R:400:MET:O	1:R:414:ASN:HA	2.18	0.43
1:Q:209:GLY:HA3	1:Q:227:LEU:O	2.18	0.43
1:Q:463:GLY:HA2	1:Q:468:ASN:HB3	2.00	0.43
1:P:175:GLY:HA3	1:P:176:PRO:HD2	1.91	0.43
1:P:437:ARG:O	1:P:438:PRO:C	2.53	0.43
1:P:266:LYS:HD3	3:P:547:HOH:O	2.19	0.43
1:R:110:ARG:HD3	1:R:114:GLN:NE2	2.34	0.43
1:P:152:THR:HG23	3:Q:486:HOH:O	2.18	0.43
1:R:350:ASN:ND2	1:R:350:ASN:N	2.66	0.42
1:R:358:LEU:HD23	1:R:358:LEU:HA	1.91	0.42
1:P:413:VAL:HG22	1:P:452:LYS:HG2	2.01	0.42
1:Q:205:LEU:HD21	1:Q:248:THR:HG21	2.01	0.42
1:Q:363:LYS:HD3	1:Q:371:SER:HB2	2.02	0.42
1:R:382:ILE:HD11	1:R:434:PHE:CD1	2.55	0.42
1:R:463:GLY:HA2	1:R:468:ASN:HB3	2.01	0.42
1:P:100:PRO:HB3	1:P:456:TYR:CG	2.54	0.42
1:Q:138:LYS:HD3	1:Q:164:PHE:CE1	2.54	0.42
1:R:353:VAL:HG23	1:R:381:LEU:HD23	2.02	0.42
1:R:348:SER:OG	1:R:350:ASN:ND2	2.53	0.42
1:P:446:TRP:CH2	1:P:471:GLY:HA3	2.55	0.42
1:R:434:PHE:O	1:R:437:ARG:NH2	2.53	0.42
1:R:248:THR:HB	1:R:261:SER:OG	2.19	0.42
1:R:198:ILE:HD11	1:R:378:ASN:HB2	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:100:PRO:HB3	1:P:456:TYR:CD2	2.55	0.41
1:R:275:ASN:N	1:R:275:ASN:HD22	2.19	0.41
1:P:138:LYS:HD3	1:P:164:PHE:CE1	2.55	0.41
1:R:294:LEU:HA	1:R:294:LEU:HD23	1.83	0.41
1:P:269:ASP:HB3	1:P:283:ALA:O	2.20	0.41
1:P:275:ASN:N	1:P:275:ASN:HD22	2.18	0.41
1:Q:375:ALA:O	1:Q:398:GLN:HA	2.21	0.41
1:Q:434:PHE:O	1:Q:437:ARG:NH2	2.54	0.41
1:R:162:GLN:HE21	1:R:187:ARG:CA	2.34	0.41
1:P:378:ASN:ND2	1:P:396:SER:OG	2.53	0.41
1:Q:247:LEU:HA	1:Q:247:LEU:HD23	1.85	0.41
1:R:437:ARG:HG2	1:R:482:TRP:CE2	2.55	0.41
1:Q:305:GLY:HA3	1:Q:344:THR:O	2.21	0.41
1:Q:348:SER:OG	1:Q:350:ASN:ND2	2.54	0.41
1:R:136:ARG:HD3	1:R:166:GLU:OE1	2.20	0.41
1:Q:303:ARG:NH1	1:Q:303:ARG:HB2	2.36	0.41
1:Q:479:MET:C	1:Q:479:MET:SD	3.00	0.40
1:P:303:ARG:HB2	1:P:303:ARG:HH11	1.87	0.40
1:P:198:ILE:HD11	1:P:378:ASN:HB2	2.03	0.40
1:P:137:PHE:CE2	1:P:139:VAL:HG22	2.56	0.40
1:R:305:GLY:HA3	1:R:344:THR:O	2.22	0.40
1:R:444:THR:HA	1:R:474:SER:O	2.21	0.40
1:P:136:ARG:HD3	1:P:166:GLU:OE1	2.21	0.40
1:P:348:SER:OG	1:P:350:ASN:ND2	2.55	0.40
1:Q:224:ASN:HB2	1:Q:250:ASN:HB3	2.04	0.40

All (1) 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:R:303:ARG:NE	3:R:552:HOH:O[3_455]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	411/413 (100%)	386 (94%)	21 (5%)	4 (1%)	17	25
1	Q	411/413 (100%)	384 (93%)	23 (6%)	4 (1%)	17	25
1	R	411/413 (100%)	388 (94%)	18 (4%)	5 (1%)	14	20
All	All	1233/1239 (100%)	1158 (94%)	62 (5%)	13 (1%)	16	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	218	ASN
1	Q	218	ASN
1	R	218	ASN
1	P	220	GLY
1	P	438	PRO
1	Q	220	GLY
1	Q	438	PRO
1	R	220	GLY
1	R	438	PRO
1	R	469	SER
1	P	470	GLY
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%)	7	10
1	Q	327/327 (100%)	295 (90%)	32 (10%)	9	13
1	R	327/327 (100%)	293 (90%)	34 (10%)	8	11
All	All	981/981 (100%)	880 (90%)	101 (10%)	8	11

All (101) 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	135	THR
1	P	139	VAL
1	P	158	LEU
1	P	172	THR
1	P	181	THR
1	P	198	ILE
1	P	218	ASN
1	P	222	ARG
1	P	242	VAL
1	P	248	THR
1	P	250	ASN
1	P	263	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	350	ASN
1	P	357	MET
1	P	358	LEU
1	P	362	SER
1	P	380	ARG
1	P	382	ILE
1	P	413	VAL
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	135	THR
1	Q	172	THR
1	Q	181	THR
1	Q	182	LEU
1	Q	198	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	218	ASN
1	Q	222	ARG
1	Q	242	VAL
1	Q	248	THR
1	Q	250	ASN
1	Q	263	LEU
1	Q	275	ASN
1	Q	292	LEU
1	Q	294	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	413	VAL
1	Q	437	ARG
1	Q	441	ARG
1	Q	446	TRP
1	Q	460	ASP
1	Q	468	ASN
1	Q	479	MET
1	R	92	THR
1	R	100	PRO
1	R	110	ARG
1	R	111	LEU
1	R	130	ASP
1	R	135	THR
1	R	139	VAL
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	294	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	R	297	ASP
1	R	302	LEU
1	R	344	THR
1	R	347	LEU
1	R	350	ASN
1	R	358	LEU
1	R	380	ARG
1	R	382	ILE
1	R	413	VAL
1	R	414	ASN
1	R	437	ARG
1	R	441	ARG
1	R	460	ASP
1	R	468	ASN
1	R	478	GLN
1	R	479	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	114	GLN
1	P	125	HIS
1	P	162	GLN
1	P	218	ASN
1	P	244	ASN
1	P	250	ASN
1	P	251	HIS
1	P	275	ASN
1	P	295	HIS
1	P	315	HIS
1	P	350	ASN
1	P	378	ASN
1	P	383	GLN
1	P	386	ASN
1	P	387	GLN
1	P	398	GLN
1	Q	114	GLN
1	Q	125	HIS
1	Q	162	GLN
1	Q	218	ASN
1	Q	244	ASN
1	Q	250	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	251	HIS
1	Q	275	ASN
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	R	114	GLN
1	R	125	HIS
1	R	162	GLN
1	R	218	ASN
1	R	244	ASN
1	R	250	ASN
1	R	251	HIS
1	R	275	ASN
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

### 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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	P	413/413 (100%)	-0.20	18 (4%) 34 32	11, 25, 51, 84	0
1	Q	413/413 (100%)	-0.30	14 (3%) 45 43	10, 24, 50, 84	0
1	R	413/413 (100%)	-0.30	10 (2%) 59 56	10, 24, 50, 84	0
All	All	1239/1239 (100%)	-0.27	42 (3%) 45 43	10, 24, 51, 84	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	275	ASN	7.1
1	Q	71	SER	6.9
1	Q	274	SER	6.6
1	R	219	ASP	6.2
1	P	274	SER	6.1
1	Q	275	ASN	5.9
1	P	219	ASP	5.8
1	R	274	SER	5.7
1	Q	219	ASP	5.6
1	R	275	ASN	5.5
1	P	469	SER	5.3
1	Q	469	SER	4.8
1	P	71	SER	4.3
1	R	71	SER	3.8
1	P	276	GLY	3.7
1	P	218	ASN	3.7
1	R	469	SER	3.6
1	P	238	SER	3.4
1	R	297	ASP	3.1
1	P	465	ASP	3.1
1	P	349	GLU	3.1
1	P	174	ALA	3.0
1	P	350	ASN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Q	297	ASP	2.8
1	Q	276	GLY	2.8
1	Q	465	ASP	2.7
1	P	279	ALA	2.6
1	Q	468	ASN	2.6
1	P	277	ASN	2.5
1	P	273	ASP	2.5
1	Q	218	ASN	2.5
1	Q	277	ASN	2.4
1	R	465	ASP	2.4
1	R	218	ASN	2.4
1	R	130	ASP	2.3
1	P	470	GLY	2.3
1	P	130	ASP	2.3
1	Q	178	LYS	2.2
1	Q	174	ALA	2.2
1	R	277	ASN	2.1
1	P	418	TYR	2.1
1	Q	409	ASP	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	P	10	1/1	0.82	0.20	42,42,42,42	0
2	CA	Q	10	1/1	0.82	0.20	41,41,41,41	0
2	CA	R	10	1/1	0.89	0.18	45,45,45,45	0

## 6.5 Other polymers

There are no such residues in this entry.