



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:48 PM UTC

PDB ID : 4D64 / pdb_00004d64
Title : Structure of porin Omp-Pst1 from *P. stuartii*; the crystallographic symmetry generates a dimer of trimers.
Authors : Nasrallah, C.; Colletier, J.P.
Deposited on : 2014-11-08
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

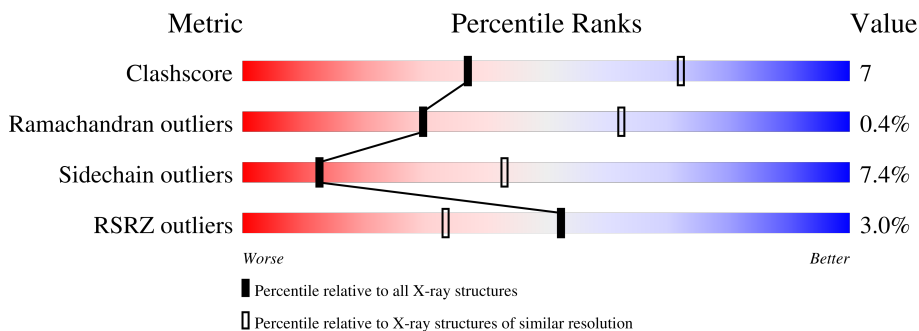
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	 3% 78% 19%
1	B	352	 4% 80% 18%
1	C	352	 3% 78% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8459 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 PORIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2775	1739	473	558	5	0	2	0
1	B	352	2757	1728	469	555	5	0	0	0
1	C	352	2766	1733	470	558	5	0	1	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	69	Total	O	0	0
			69	69		
3	C	41	Total	O	0	0
			41	41		



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.52Å 142.02Å 113.32Å 90.00° 131.00° 90.00°	Depositor
Resolution (Å)	36.25 – 3.20 36.25 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (36.25-3.20) 91.1 (36.25-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.207 , 0.261 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8459	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.41	0/2832	0.78	2/3823 (0.1%)
1	B	0.40	0/2814	0.78	2/3800 (0.1%)
1	C	0.39	0/2823	0.79	1/3812 (0.0%)
All	All	0.40	0/8469	0.78	5/11435 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	GLY	N-CA-C	-5.74	104.46	111.35
1	B	349	VAL	N-CA-C	5.45	115.71	107.75
1	A	125	PHE	CB-CA-C	-5.26	110.53	116.63
1	B	83	GLY	N-CA-C	5.10	118.92	110.55
1	C	125	PHE	CB-CA-C	-5.10	110.72	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2775	0	2610	40	0
1	B	2757	0	2591	41	0
1	C	2766	0	2596	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	50	0	0	2	0
3	B	69	0	0	3	0
3	C	41	0	0	1	0
All	All	8459	0	7797	114	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 7.

All (114) 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:C:101:VAL:HG22	1:C:127:THR:HA	1.63	0.81
1:C:131:ARG:NH2	1:C:170:LYS:O	2.15	0.78
1:A:169:ALA:HB1	1:A:251:ARG:HD3	1.67	0.77
1:C:160:ASP:OD1	1:C:161:ASN:N	2.21	0.74
1:A:213:ASP:N	1:A:213:ASP:OD1	2.21	0.74
1:C:169:ALA:HB1	1:C:251:ARG:HD3	1.70	0.74
1:B:117:ASP:OD2	1:B:303:TYR:OH	2.07	0.73
1:B:169:ALA:HB1	1:B:251:ARG:HD3	1.71	0.73
1:B:196:SER:OG	1:B:222:ARG:NH1	2.23	0.71
1:A:37:ASP:O	1:A:39:ARG:NH1	2.26	0.69
1:B:14:TYR:OH	1:B:59:ARG:NH1	2.28	0.67
1:A:6:LYS:NZ	1:A:7:ASP:OD2	2.24	0.66
1:B:118:THR:HB	1:B:264:ASN:HB3	1.76	0.66
1:A:169:ALA:O	1:A:251:ARG:NH1	2.28	0.65
1:B:238:TYR:HB3	1:B:270:GLN:HG3	1.79	0.63
1:B:88:ASP:OD1	1:B:140:ASN:ND2	2.31	0.63
1:C:287:LYS:HB3	1:C:289:LYS:HZ3	1.63	0.63
1:A:238:TYR:HB3	1:A:270:GLN:HG3	1.80	0.63
1:A:4:TYR:HB3	1:A:11:LEU:HG	1.82	0.61
1:C:238:TYR:HB3	1:C:270:GLN:HG3	1.83	0.61
1:A:163:LYS:NZ	1:C:33:GLU:OE1	2.31	0.60
1:A:34:ASP:OD1	1:A:35:GLY:N	2.35	0.60
1:B:27:ASP:HB2	1:B:30:LYS:HD2	1.84	0.59
1:A:139:ASN:HA	1:A:149:SER:HB3	1.83	0.59
1:B:216:TYR:H	1:B:293:ASN:HD21	1.51	0.57
1:A:285:GLN:NE2	1:A:287:LYS:HE2	2.20	0.57
1:C:221:LYS:H	1:C:221:LYS:HZ1	1.51	0.57
1:C:139:ASN:HA	1:C:149:SER:HB3	1.87	0.57
1:A:56:GLY:HA3	1:C:316:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:HD3	1:B:223:ALA:HB2	1.88	0.56
1:C:199:ARG:HD3	1:C:223:ALA:HB2	1.88	0.55
1:C:281:ILE:HD12	1:C:305:SER:O	2.07	0.54
1:A:199:ARG:HD3	1:A:223:ALA:HB2	1.88	0.54
1:C:221:LYS:H	1:C:221:LYS:NZ	2.06	0.54
1:B:285:GLN:NE2	1:B:287:LYS:HE2	2.24	0.53
1:A:140:ASN:N	1:A:140:ASN:OD1	2.41	0.53
1:C:125:PHE:O	1:C:130:ASN:ND2	2.23	0.53
1:C:162:ASN:OD1	1:C:165:SER:OG	2.27	0.53
1:B:194:TYR:HD1	1:B:226:TRP:HB3	1.74	0.52
1:A:33:GLU:OE1	1:B:163:LYS:NZ	2.31	0.52
1:A:159:GLY:HA2	1:A:171:ASP:OD2	2.10	0.52
1:C:133:LEU:HG	1:C:153:GLN:NE2	2.26	0.51
1:A:45[B]:LYS:NZ	1:A:57:PHE:HB2	2.25	0.51
1:B:37:ASP:O	1:B:39:ARG:NH1	2.44	0.51
1:A:194:TYR:HD1	1:A:226:TRP:HB3	1.76	0.51
1:C:218:ALA:HA	1:C:260:ASN:ND2	2.26	0.51
1:B:327:LEU:HB3	1:B:340:THR:HG22	1.92	0.50
1:A:32:SER:HB3	1:B:162:ASN:HA	1.94	0.50
1:A:117:ASP:OD2	1:A:303:TYR:OH	2.24	0.49
1:C:178:PHE:CE1	1:C:194:TYR:HB3	2.49	0.48
1:C:146:ASP:OD1	1:C:146:ASP:N	2.38	0.48
1:C:325:ASN:ND2	1:C:339:ASN:O	2.45	0.48
1:B:2:GLU:HA	1:B:12:ASP:HA	1.96	0.48
1:A:27:ASP:HB2	1:A:30:LYS:HD3	1.95	0.48
1:C:316:MET:HE1	1:C:350:TYR:HB2	1.95	0.48
1:A:50:ILE:HD13	1:C:312:PHE:HB3	1.95	0.47
1:C:194:TYR:HD1	1:C:226:TRP:HB3	1.79	0.47
1:A:130:ASN:ND2	1:A:155:GLN:HE22	2.12	0.47
1:B:131:ARG:NH2	1:B:164:SER:O	2.48	0.47
1:B:266:GLU:O	1:B:267:LEU:HD23	2.15	0.47
1:A:118:THR:HB	1:A:264:ASN:HB3	1.97	0.47
1:B:88:ASP:HA	1:B:140:ASN:HD21	1.79	0.47
1:A:160:ASP:OD1	1:A:200:THR:HB	2.15	0.46
1:C:111:PHE:HE1	1:C:268:VAL:HB	1.80	0.46
1:C:101:VAL:HG13	1:C:126:MET:O	2.16	0.46
1:B:169:ALA:O	1:B:251:ARG:NH1	2.49	0.46
1:B:30:LYS:HD3	3:B:2013:HOH:O	2.15	0.45
1:C:27:ASP:OD1	1:C:30:LYS:HE2	2.17	0.45
1:A:45[B]:LYS:HE2	3:A:2013:HOH:O	2.17	0.45
1:B:199:ARG:O	1:B:204:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ASN:ND2	1:C:155:GLN:HE22	2.15	0.45
1:A:175:GLY:HA3	1:A:197:SER:OG	2.17	0.44
1:C:288:GLY:C	1:C:289:LYS:HD2	2.42	0.44
1:A:210:SER:O	1:A:212:GLY:N	2.45	0.44
1:A:45[B]:LYS:HZ1	1:A:57:PHE:HB2	1.83	0.44
1:B:315:ASN:OD1	1:C:9:ASN:ND2	2.51	0.44
1:B:281:ILE:O	1:B:281:ILE:HG13	2.18	0.44
1:C:88:ASP:C	1:C:89:PHE:HD1	2.26	0.44
1:C:111:PHE:CE1	1:C:268:VAL:HB	2.53	0.43
1:A:94:TYR:HA	1:A:133:LEU:O	2.18	0.43
1:A:138:ASN:HB3	1:A:150:PHE:CE1	2.53	0.43
1:B:70:GLU:HG2	1:C:76:LYS:HB3	2.01	0.43
1:A:310:TYR:N	1:A:318:ALA:O	2.49	0.43
1:B:159:GLY:HA3	1:B:200:THR:HG21	2.00	0.43
1:B:10:LYS:HB2	1:B:47:ASP:HB2	2.01	0.43
1:C:267:LEU:HB2	1:C:283:TYR:HB3	2.01	0.43
1:A:351[B]:GLN:NE2	1:A:352:PHE:O	2.52	0.43
1:B:6:LYS:HB2	1:B:7:ASP:H	1.62	0.43
1:A:4:TYR:O	1:A:10:LYS:HA	2.19	0.42
1:A:201:PRO:HG2	1:C:28:LYS:HD3	2.01	0.42
1:B:232:PHE:CZ	1:B:234:ALA:HB3	2.55	0.42
1:C:85:LYS:HG3	1:C:91:SER:HB3	2.02	0.42
1:A:53:GLN:HG3	1:A:87:ALA:HB3	2.02	0.42
1:A:1:ALA:O	1:A:3:VAL:HG13	2.20	0.42
1:C:10:LYS:HE2	1:C:10:LYS:HB3	1.80	0.42
1:A:157:LYS:O	1:A:162:ASN:ND2	2.44	0.42
1:C:135:THR:HG23	1:C:153:GLN:HB2	2.02	0.41
1:B:175:GLY:HA3	1:B:197:SER:OG	2.20	0.41
1:B:216:TYR:O	1:B:257:LEU:HD22	2.20	0.41
1:B:45:LYS:HG3	1:B:59:ARG:HD3	2.03	0.41
1:C:118:THR:HB	1:C:264:ASN:CB	2.49	0.41
1:B:70:GLU:CD	1:C:129:ARG:HH21	2.28	0.41
1:B:327:LEU:HD12	1:B:327:LEU:HA	1.85	0.41
1:A:122:THR:HG21	3:A:2039:HOH:O	2.19	0.41
1:B:285:GLN:HE22	1:B:287:LYS:HE2	1.85	0.41
1:C:118:THR:HB	1:C:264:ASN:HB3	2.03	0.41
1:C:14:TYR:HE2	1:C:45:LYS:HG3	1.86	0.41
1:C:139:ASN:OD1	1:C:140:ASN:ND2	2.54	0.41
1:B:4:TYR:O	1:B:10:LYS:HA	2.21	0.41
1:B:211:GLU:HB3	3:B:2045:HOH:O	2.21	0.41
1:C:45:LYS:NZ	3:C:2008:HOH:O	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:NH1	3:B:2044:HOH:O	2.52	0.40
1:A:69:ALA:HB2	1:B:166:ALA:HB1	2.03	0.40
1:B:330:ASN:O	1:B:334:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

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	A	352/352 (100%)	326 (93%)	24 (7%)	2 (1%)	21	56
1	B	350/352 (99%)	324 (93%)	25 (7%)	1 (0%)	36	68
1	C	351/352 (100%)	326 (93%)	24 (7%)	1 (0%)	36	68
All	All	1053/1056 (100%)	976 (93%)	73 (7%)	4 (0%)	30	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	GLU
1	A	212	GLY
1	B	8	GLY
1	C	211	GLU

5.3.2 Protein sidechains [i](#)

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	286/284 (101%)	265 (93%)	21 (7%)	13	43
1	B	284/284 (100%)	264 (93%)	20 (7%)	14	45
1	C	285/284 (100%)	262 (92%)	23 (8%)	11	39
All	All	855/852 (100%)	791 (92%)	64 (8%)	13	42

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	39	ARG
1	A	122	THR
1	A	131	ARG
1	A	133	LEU
1	A	134	LEU
1	A	140	ASN
1	A	146	ASP
1	A	149	SER
1	A	160	ASP
1	A	165	SER
1	A	213	ASP
1	A	219	THR
1	A	221	LYS
1	A	242	MET
1	A	264	ASN
1	A	265	VAL
1	A	267	LEU
1	A	284	ASN
1	A	351[A]	GLN
1	A	351[B]	GLN
1	B	6	LYS
1	B	7	ASP
1	B	39	ARG
1	B	44	VAL
1	B	59	ARG
1	B	110	VAL
1	B	122	THR
1	B	133	LEU
1	B	134	LEU
1	B	168	MET
1	B	211	GLU
1	B	214	SER
1	B	221	LYS

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Mol	Chain	Res	Type
1	B	222	ARG
1	B	235	ASN
1	B	264	ASN
1	B	265	VAL
1	B	281	ILE
1	B	284	ASN
1	B	327	LEU
1	C	13	VAL
1	C	39	ARG
1	C	44	VAL
1	C	48	THR
1	C	101	VAL
1	C	122	THR
1	C	131	ARG
1	C	133	LEU
1	C	134	LEU
1	C	146	ASP
1	C	149	SER
1	C	152	LEU
1	C	198	SER
1	C	207	VAL
1	C	213	ASP
1	C	221	LYS
1	C	222	ARG
1	C	242	MET
1	C	264	ASN
1	C	265	VAL
1	C	281	ILE
1	C	284	ASN
1	C	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	21	HIS
1	A	49	GLN
1	A	75	ASN
1	A	139	ASN
1	A	155	GLN
1	A	260	ASN
1	A	270	GLN

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Mol	Chain	Res	Type
1	B	75	ASN
1	B	155	GLN
1	B	161	ASN
1	B	260	ASN
1	B	264	ASN
1	B	270	GLN
1	B	293	ASN
1	C	9	ASN
1	C	75	ASN
1	C	105	ASN
1	C	140	ASN
1	C	155	GLN
1	C	270	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	352/352 (100%)	0.33	10 (2%) 55 35	31, 72, 105, 140	2 (0%)
1	B	352/352 (100%)	0.31	13 (3%) 45 28	49, 73, 106, 139	0
1	C	352/352 (100%)	0.28	9 (2%) 57 37	38, 72, 105, 140	1 (0%)
All	All	1056/1056 (100%)	0.30	32 (3%) 52 33	31, 72, 105, 140	3 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.3
1	C	8	GLY	4.4
1	B	29	GLY	3.8
1	B	9	ASN	3.8
1	A	8	GLY	3.7
1	A	259	ALA	3.5
1	C	248	ASN	3.4
1	C	160	ASP	3.4
1	C	33	GLU	3.1
1	B	49	GLN	2.9
1	B	54	LEU	2.7
1	B	56	GLY	2.5
1	B	265	VAL	2.5
1	C	30	LYS	2.4
1	A	74	GLU	2.4
1	B	160	ASP	2.4
1	C	341	ASP	2.3
1	A	338	ILE	2.3
1	B	90	GLY	2.3
1	B	139	ASN	2.3
1	A	25	SER	2.2
1	C	221	LYS	2.2
1	B	299	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	340	THR	2.1
1	C	146	ASP	2.1
1	C	159	GLY	2.1
1	A	214	SER	2.1
1	A	7	ASP	2.1
1	A	205	ALA	2.1
1	B	186	TRP	2.0
1	A	26	ALA	2.0
1	B	74	GLU	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
2	CA	A	3000	1/1	0.90	0.15	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.