



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 04:01 AM EDT

PDB ID : 6VJ2
Title : 3.10 Angstrom Resolution Crystal Structure of Foldase Protein (PrsA) from *Lactococcus lactis*
Authors : Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Endres, M.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2020-01-14
Resolution : 3.10 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

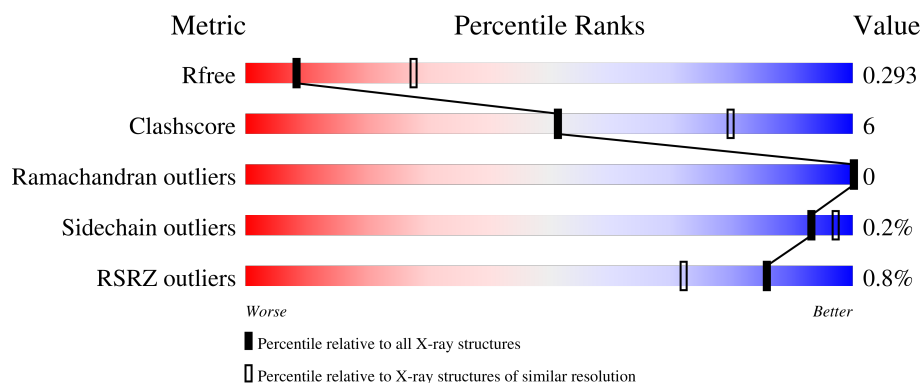
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	284	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 85%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 10% 5% </div> </div>
1	B	284	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 85%, yellow 10%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 10% 5% </div> </div>
1	C	284	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 83%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 83% 11% 5% </div> </div>
1	D	284	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 84%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 11% • 5% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8570 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 Foldase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	Se	0	1	0
			2128	1335	345	443	5			
1	B	270	Total	C	N	O	Se	0	1	0
			2122	1332	343	442	5			
1	C	269	Total	C	N	O	Se	0	1	0
			2117	1329	342	441	5			
1	D	270	Total	C	N	O	Se	0	0	0
			2115	1328	342	440	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	-	expression tag	UNP Q9CEV9
A	26	ASN	-	expression tag	UNP Q9CEV9
A	27	ALA	-	expression tag	UNP Q9CEV9
B	25	SER	-	expression tag	UNP Q9CEV9
B	26	ASN	-	expression tag	UNP Q9CEV9
B	27	ALA	-	expression tag	UNP Q9CEV9
C	25	SER	-	expression tag	UNP Q9CEV9
C	26	ASN	-	expression tag	UNP Q9CEV9
C	27	ALA	-	expression tag	UNP Q9CEV9
D	25	SER	-	expression tag	UNP Q9CEV9
D	26	ASN	-	expression tag	UNP Q9CEV9
D	27	ALA	-	expression tag	UNP Q9CEV9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	22	Total	O	0	0
			22	22		

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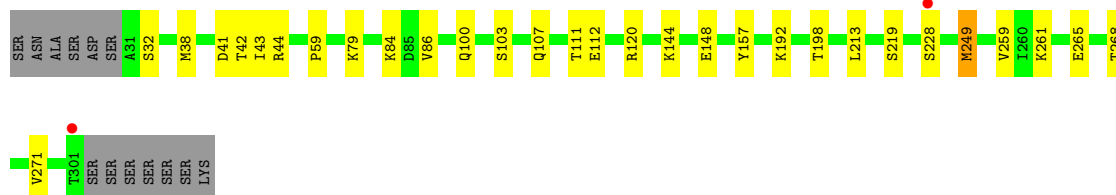
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	32	Total 32	O 32	0	0
2	D	11	Total 11	O 11	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

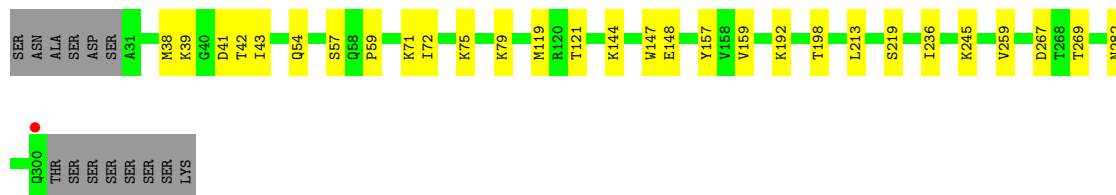
- Molecule 1: Foldase

Chain A: 




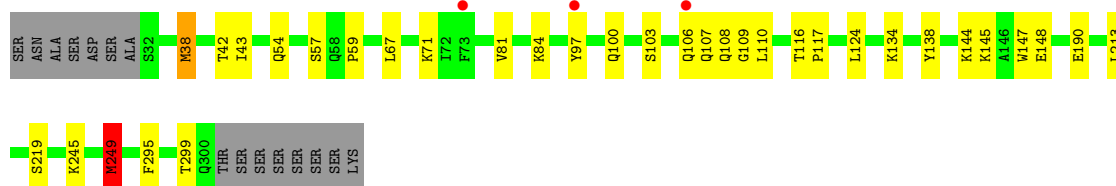
- Molecule 1: Foldase

Chain B: 




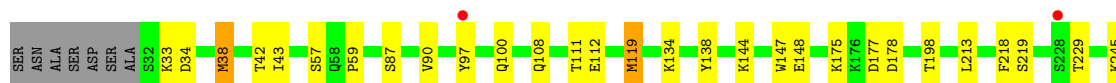
- Molecule 1: Foldase

Chain C: 



- Molecule 1: Foldase

Chain D: 



V259	V256	A292	T301	SER	SER	SER	SER	SER	SER	SER	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.51Å 117.61Å 149.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 3.10 29.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.40-3.10) 99.9 (29.39-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.290 0.236 , 0.293	Depositor DCC
R_{free} test set	1307 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 17.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8570	wwPDB-VP
Average B, all atoms (Å ²)	78.0	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 45.91 % 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 1.2351e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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	0.67	0/2155	0.75	1/2895 (0.0%)
1	B	0.67	0/2149	0.71	0/2886
1	C	0.67	0/2144	0.75	2/2879 (0.1%)
1	D	0.67	0/2142	0.74	2/2877 (0.1%)
All	All	0.67	0/8590	0.74	5/11537 (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	C	249	MSE	CG-SE-CE	7.53	115.45	98.90
1	C	38	MSE	CG-SE-CE	6.75	113.74	98.90
1	D	38	MSE	CG-SE-CE	5.69	111.41	98.90
1	D	119	MSE	CG-SE-CE	5.17	110.27	98.90
1	A	249	MSE	CG-SE-CE	5.03	109.96	98.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2128	0	2111	22	0
1	B	2122	0	2104	26	0
1	C	2117	0	2099	33	0
1	D	2115	0	2101	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	0	0	0	0
2	B	22	0	0	2	0
2	C	32	0	0	1	0
2	D	11	0	0	0	0
All	All	8570	0	8415	95	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 6.

All (95) 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:108:GLN:HE21	1:D:108:GLN:HE21	1.17	0.91
1:B:121:THR:HG22	2:B:418:HOH:O	1.87	0.74
1:D:175:LYS:HE2	1:D:218:PHE:HB2	1.70	0.74
1:A:32:SER:HB2	1:A:44:ARG:NH2	2.06	0.71
1:C:67:LEU:O	1:C:71:LYS:HG3	1.91	0.70
1:B:71:LYS:O	1:B:75:LYS:CG	2.41	0.69
1:C:109:GLY:C	1:C:110:LEU:HD12	2.15	0.67
1:D:38:MSE:HE1	1:D:43:ILE:HG13	1.77	0.66
1:A:84:LYS:HA	1:A:84:LYS:HE2	1.79	0.65
1:D:175:LYS:CE	1:D:218:PHE:HB2	2.29	0.62
1:B:71:LYS:O	1:B:75:LYS:HG2	2.00	0.61
1:D:100:GLN:N	1:D:100:GLN:OE1	2.34	0.61
1:B:38:MSE:HE1	1:B:43:ILE:HG13	1.82	0.60
1:C:81:VAL:HG23	1:C:81:VAL:O	2.01	0.60
1:A:38:MSE:HE1	1:A:43:ILE:HG13	1.84	0.60
1:D:87:SER:HA	1:D:90:VAL:HG22	1.83	0.60
1:C:38:MSE:HE1	1:C:43:ILE:HG13	1.82	0.60
1:A:79:LYS:HA	1:A:79:LYS:HE2	1.84	0.59
1:C:116:THR:OG1	1:C:117:PRO:CD	2.52	0.58
1:B:71:LYS:O	1:B:75:LYS:HG3	2.02	0.58
1:D:33:LYS:CD	1:D:34:ASP:H	2.17	0.57
1:C:299:THR:HG23	1:C:299:THR:O	2.04	0.57
1:C:116:THR:OG1	1:C:117:PRO:HD3	2.05	0.57
1:C:81:VAL:CG2	1:C:124:LEU:CD2	2.87	0.53
1:C:54:GLN:OE1	1:D:229:THR:HG22	2.09	0.52
1:A:268:THR:HA	1:A:271:VAL:HG22	1.91	0.52
1:B:79:LYS:HG2	2:B:410:HOH:O	2.08	0.52
1:B:59:PRO:HA	1:D:59:PRO:HA	1.92	0.52
1:C:38:MSE:HE3	1:C:42:THR:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:TYR:HE2	1:D:97:TYR:CE2	2.29	0.51
1:A:86:VAL:HG21	1:A:120:ARG:HG3	1.94	0.50
1:B:57:SER:O	1:D:59:PRO:HB3	2.12	0.49
1:C:100:GLN:NE2	1:D:119:MSE:HE3	2.28	0.49
1:C:190[B]:GLU:HG3	1:C:190[B]:GLU:O	2.13	0.49
1:C:145:LYS:O	1:C:148:GLU:HG2	2.13	0.49
1:D:87:SER:HA	1:D:90:VAL:CG2	2.43	0.48
1:C:81:VAL:CG2	1:C:124:LEU:HD23	2.44	0.48
1:A:32:SER:CB	1:A:44:ARG:NH2	2.74	0.48
1:C:84:LYS:N	2:C:403:HOH:O	2.47	0.47
1:B:159:VAL:CG2	1:B:236:ILE:HB	2.44	0.47
1:C:97:TYR:CE2	1:D:97:TYR:HE2	2.31	0.47
1:C:103:SER:HA	1:C:106:GLN:HG2	1.96	0.47
1:C:97:TYR:HE2	1:D:97:TYR:HE2	1.62	0.46
1:C:144:LYS:HG2	1:C:249:MSE:HE1	1.96	0.46
1:C:213:LEU:HD11	1:C:219:SER:HB3	1.98	0.46
1:B:41:ASP:O	1:B:42:THR:CG2	2.64	0.46
1:B:144:LYS:O	1:B:148:GLU:HG2	2.16	0.46
1:B:72:ILE:HA	1:B:75:LYS:HD2	1.98	0.45
1:A:144:LYS:O	1:A:148:GLU:HG2	2.16	0.45
1:C:295:PHE:O	1:C:299:THR:HG22	2.16	0.45
1:D:134:LYS:HA	1:D:138:TYR:CE2	2.51	0.45
1:A:59:PRO:HA	1:C:59:PRO:HA	1.98	0.45
1:D:144:LYS:O	1:D:148:GLU:HG3	2.17	0.45
1:B:39:LYS:HD3	1:B:282:ASN:HA	1.98	0.45
1:B:213:LEU:HD11	1:B:219:SER:HB3	1.98	0.45
1:A:100:GLN:HE22	1:B:119:MSE:CE	2.30	0.45
1:A:103:SER:O	1:A:107:GLN:HG2	2.17	0.45
1:D:33:LYS:HD3	1:D:34:ASP:H	1.81	0.45
1:C:134:LYS:HA	1:C:138:TYR:CE2	2.52	0.44
1:A:261:LYS:HE2	1:A:265:GLU:OE2	2.17	0.44
1:A:32:SER:HB2	1:A:44:ARG:CZ	2.47	0.44
1:D:87:SER:CA	1:D:90:VAL:HG22	2.48	0.44
1:D:33:LYS:HD2	1:D:34:ASP:H	1.83	0.44
1:A:157:TYR:CE1	1:A:192:LYS:HB2	2.53	0.43
1:C:100:GLN:HE22	1:D:119:MSE:SE	2.51	0.43
1:D:213:LEU:HD11	1:D:219:SER:HB3	2.00	0.43
1:B:198:THR:HG21	1:B:259:VAL:HG22	1.99	0.43
1:C:106:GLN:HG3	1:C:107:GLN:N	2.33	0.43
1:A:213:LEU:HD11	1:A:219:SER:HB3	2.00	0.43
1:A:198:THR:HG21	1:A:259:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:SER:O	1:C:106:GLN:HG2	2.19	0.43
1:C:100:GLN:NE2	1:D:119:MSE:CE	2.81	0.42
1:A:32:SER:CB	1:A:44:ARG:HH22	2.33	0.42
1:D:198:THR:HG21	1:D:259:VAL:HG22	2.01	0.42
1:A:228:SER:O	1:B:54:GLN:HG3	2.20	0.42
1:B:59:PRO:HB3	1:D:57:SER:O	2.19	0.42
1:D:286:VAL:HG21	1:D:292:ALA:HA	2.02	0.42
1:B:159:VAL:HG23	1:B:236:ILE:HB	2.01	0.41
1:B:267:ASP:OD1	1:B:269:THR:OG1	2.31	0.41
1:B:157:TYR:CZ	1:B:192:LYS:HD2	2.55	0.41
1:D:111:THR:HG22	1:D:112:GLU:N	2.35	0.41
1:B:41:ASP:C	1:B:42:THR:HG23	2.41	0.41
1:D:147:TRP:CH2	1:D:245:LYS:HB2	2.56	0.41
1:A:100:GLN:HE22	1:B:119:MSE:HE3	1.85	0.41
1:C:103:SER:O	1:C:107:GLN:HG2	2.20	0.41
1:A:59:PRO:HB3	1:C:57:SER:O	2.21	0.41
1:C:110:LEU:HD12	1:C:110:LEU:N	2.36	0.41
1:A:111:THR:HG22	1:A:112:GLU:N	2.36	0.41
1:B:147:TRP:CH2	1:B:245:LYS:HB2	2.56	0.41
1:C:147:TRP:CH2	1:C:245:LYS:HB2	2.55	0.41
1:D:177:ASP:OD1	1:D:178:ASP:N	2.53	0.41
1:A:41:ASP:OD1	1:A:42:THR:N	2.50	0.41
1:B:41:ASP:OD1	1:B:42:THR:N	2.51	0.40
1:B:41:ASP:O	1:B:42:THR:HG23	2.22	0.40
1:D:38:MSE:HE3	1:D:42:THR:HA	2.03	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	A	270/284 (95%)	262 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/284 (95%)	260 (97%)	9 (3%)	0	100	100
1	C	268/284 (94%)	260 (97%)	8 (3%)	0	100	100
1	D	268/284 (94%)	261 (97%)	7 (3%)	0	100	100
All	All	1075/1136 (95%)	1043 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/246 (98%)	239 (100%)	1 (0%)	91	96
1	B	239/246 (97%)	239 (100%)	0	100	100
1	C	239/246 (97%)	238 (100%)	1 (0%)	91	96
1	D	239/246 (97%)	239 (100%)	0	100	100
All	All	957/984 (97%)	955 (100%)	2 (0%)	93	97

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

Mol	Chain	Res	Type
1	A	249	MSE
1	C	249	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	282	ASN
1	B	108	GLN
1	B	282	ASN
1	C	282	ASN
1	D	108	GLN

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Mol	Chain	Res	Type
1	D	282	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	266/284 (93%)	-0.41	2 (0%) 86 72	51, 69, 110, 152	0
1	B	265/284 (93%)	-0.46	1 (0%) 92 84	51, 72, 99, 169	0
1	C	264/284 (92%)	-0.34	3 (1%) 80 64	50, 80, 115, 145	0
1	D	265/284 (93%)	-0.38	2 (0%) 86 72	53, 84, 119, 151	0
All	All	1060/1136 (93%)	-0.40	8 (0%) 86 72	50, 76, 113, 169	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	THR	4.3
1	C	106	GLN	3.4
1	D	97	TYR	2.6
1	C	97	TYR	2.5
1	A	228	SER	2.5
1	B	300	GLN	2.2
1	C	73	PHE	2.1
1	D	228	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.