



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:18 AM UTC

PDB ID : 3KOP / pdb_00003kop
Title : Crystal structure of Protein with a cyclophilin-like fold (YP_831253.1) from *Arthrobacter* sp. FB24 at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-11-13
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

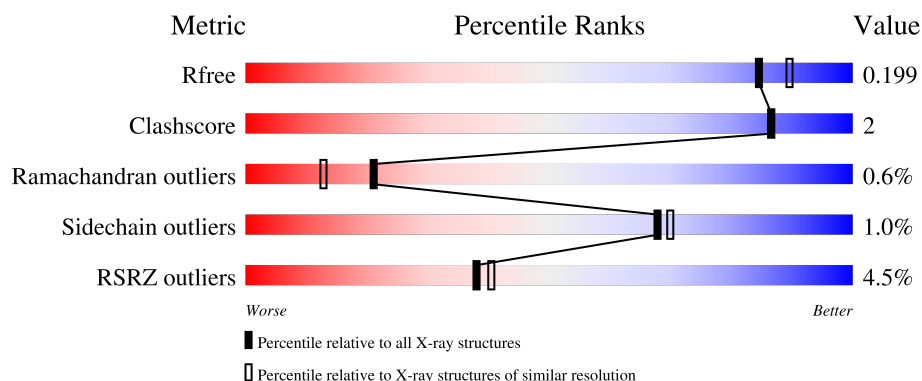
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	188	5% 79% 5% 16%
1	B	188	5% 81% • 17%
1	C	188	4% 81% 7% 12%
1	D	188	2% 78% 6% 16%
1	E	188	4% 84% • 12%

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Mol	Chain	Length	Quality of chain
1	F	188	4% 84% 6% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8455 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	Se	0	6	0
			1237	790	204	238	3	2			
1	B	156	Total	C	N	O	S	Se	0	4	0
			1206	769	202	230	3	2			
1	C	165	Total	C	N	O	S	Se	0	9	0
			1320	848	217	249	3	3			
1	D	158	Total	C	N	O	S	Se	0	4	0
			1228	784	203	235	3	3			
1	E	165	Total	C	N	O	S	Se	0	6	0
			1304	837	214	247	3	3			
1	F	169	Total	C	N	O	S	Se	0	6	0
			1341	855	232	248	3	3			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	expression tag	UNP A0JVT3
A	-17	GLY	-	expression tag	UNP A0JVT3
A	-16	SER	-	expression tag	UNP A0JVT3
A	-15	ASP	-	expression tag	UNP A0JVT3
A	-14	LYS	-	expression tag	UNP A0JVT3
A	-13	ILE	-	expression tag	UNP A0JVT3
A	-12	HIS	-	expression tag	UNP A0JVT3
A	-11	HIS	-	expression tag	UNP A0JVT3
A	-10	HIS	-	expression tag	UNP A0JVT3
A	-9	HIS	-	expression tag	UNP A0JVT3
A	-8	HIS	-	expression tag	UNP A0JVT3
A	-7	HIS	-	expression tag	UNP A0JVT3
A	-6	GLU	-	expression tag	UNP A0JVT3
A	-5	ASN	-	expression tag	UNP A0JVT3
A	-4	LEU	-	expression tag	UNP A0JVT3
A	-3	TYR	-	expression tag	UNP A0JVT3
A	-2	PHE	-	expression tag	UNP A0JVT3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP A0JVT3
A	0	GLY	-	expression tag	UNP A0JVT3
B	-18	MSE	-	expression tag	UNP A0JVT3
B	-17	GLY	-	expression tag	UNP A0JVT3
B	-16	SER	-	expression tag	UNP A0JVT3
B	-15	ASP	-	expression tag	UNP A0JVT3
B	-14	LYS	-	expression tag	UNP A0JVT3
B	-13	ILE	-	expression tag	UNP A0JVT3
B	-12	HIS	-	expression tag	UNP A0JVT3
B	-11	HIS	-	expression tag	UNP A0JVT3
B	-10	HIS	-	expression tag	UNP A0JVT3
B	-9	HIS	-	expression tag	UNP A0JVT3
B	-8	HIS	-	expression tag	UNP A0JVT3
B	-7	HIS	-	expression tag	UNP A0JVT3
B	-6	GLU	-	expression tag	UNP A0JVT3
B	-5	ASN	-	expression tag	UNP A0JVT3
B	-4	LEU	-	expression tag	UNP A0JVT3
B	-3	TYR	-	expression tag	UNP A0JVT3
B	-2	PHE	-	expression tag	UNP A0JVT3
B	-1	GLN	-	expression tag	UNP A0JVT3
B	0	GLY	-	expression tag	UNP A0JVT3
C	-18	MSE	-	expression tag	UNP A0JVT3
C	-17	GLY	-	expression tag	UNP A0JVT3
C	-16	SER	-	expression tag	UNP A0JVT3
C	-15	ASP	-	expression tag	UNP A0JVT3
C	-14	LYS	-	expression tag	UNP A0JVT3
C	-13	ILE	-	expression tag	UNP A0JVT3
C	-12	HIS	-	expression tag	UNP A0JVT3
C	-11	HIS	-	expression tag	UNP A0JVT3
C	-10	HIS	-	expression tag	UNP A0JVT3
C	-9	HIS	-	expression tag	UNP A0JVT3
C	-8	HIS	-	expression tag	UNP A0JVT3
C	-7	HIS	-	expression tag	UNP A0JVT3
C	-6	GLU	-	expression tag	UNP A0JVT3
C	-5	ASN	-	expression tag	UNP A0JVT3
C	-4	LEU	-	expression tag	UNP A0JVT3
C	-3	TYR	-	expression tag	UNP A0JVT3
C	-2	PHE	-	expression tag	UNP A0JVT3
C	-1	GLN	-	expression tag	UNP A0JVT3
C	0	GLY	-	expression tag	UNP A0JVT3
D	-18	MSE	-	expression tag	UNP A0JVT3
D	-17	GLY	-	expression tag	UNP A0JVT3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0JVT3
D	-15	ASP	-	expression tag	UNP A0JVT3
D	-14	LYS	-	expression tag	UNP A0JVT3
D	-13	ILE	-	expression tag	UNP A0JVT3
D	-12	HIS	-	expression tag	UNP A0JVT3
D	-11	HIS	-	expression tag	UNP A0JVT3
D	-10	HIS	-	expression tag	UNP A0JVT3
D	-9	HIS	-	expression tag	UNP A0JVT3
D	-8	HIS	-	expression tag	UNP A0JVT3
D	-7	HIS	-	expression tag	UNP A0JVT3
D	-6	GLU	-	expression tag	UNP A0JVT3
D	-5	ASN	-	expression tag	UNP A0JVT3
D	-4	LEU	-	expression tag	UNP A0JVT3
D	-3	TYR	-	expression tag	UNP A0JVT3
D	-2	PHE	-	expression tag	UNP A0JVT3
D	-1	GLN	-	expression tag	UNP A0JVT3
D	0	GLY	-	expression tag	UNP A0JVT3
E	-18	MSE	-	expression tag	UNP A0JVT3
E	-17	GLY	-	expression tag	UNP A0JVT3
E	-16	SER	-	expression tag	UNP A0JVT3
E	-15	ASP	-	expression tag	UNP A0JVT3
E	-14	LYS	-	expression tag	UNP A0JVT3
E	-13	ILE	-	expression tag	UNP A0JVT3
E	-12	HIS	-	expression tag	UNP A0JVT3
E	-11	HIS	-	expression tag	UNP A0JVT3
E	-10	HIS	-	expression tag	UNP A0JVT3
E	-9	HIS	-	expression tag	UNP A0JVT3
E	-8	HIS	-	expression tag	UNP A0JVT3
E	-7	HIS	-	expression tag	UNP A0JVT3
E	-6	GLU	-	expression tag	UNP A0JVT3
E	-5	ASN	-	expression tag	UNP A0JVT3
E	-4	LEU	-	expression tag	UNP A0JVT3
E	-3	TYR	-	expression tag	UNP A0JVT3
E	-2	PHE	-	expression tag	UNP A0JVT3
E	-1	GLN	-	expression tag	UNP A0JVT3
E	0	GLY	-	expression tag	UNP A0JVT3
F	-18	MSE	-	expression tag	UNP A0JVT3
F	-17	GLY	-	expression tag	UNP A0JVT3
F	-16	SER	-	expression tag	UNP A0JVT3
F	-15	ASP	-	expression tag	UNP A0JVT3
F	-14	LYS	-	expression tag	UNP A0JVT3
F	-13	ILE	-	expression tag	UNP A0JVT3

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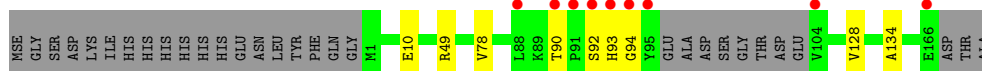
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	HIS	-	expression tag	UNP A0JVT3
F	-11	HIS	-	expression tag	UNP A0JVT3
F	-10	HIS	-	expression tag	UNP A0JVT3
F	-9	HIS	-	expression tag	UNP A0JVT3
F	-8	HIS	-	expression tag	UNP A0JVT3
F	-7	HIS	-	expression tag	UNP A0JVT3
F	-6	GLU	-	expression tag	UNP A0JVT3
F	-5	ASN	-	expression tag	UNP A0JVT3
F	-4	LEU	-	expression tag	UNP A0JVT3
F	-3	TYR	-	expression tag	UNP A0JVT3
F	-2	PHE	-	expression tag	UNP A0JVT3
F	-1	GLN	-	expression tag	UNP A0JVT3
F	0	GLY	-	expression tag	UNP A0JVT3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	132	Total O 133 133	0	1
2	B	143	Total O 144 144	0	1
2	C	153	Total O 154 154	0	1
2	D	93	Total O 93 93	0	0
2	E	144	Total O 145 145	0	1
2	F	149	Total O 150 150	0	1

- Molecule 1: Uncharacterized protein



MSE	GLY	SER	ASP	LVS	ILE	HIS	HIS	HIS	HIS	HIS	GLU	ASN	THR	THR	GLY	GLY	M1	R49	S85	N86	D87	L88	K89	T90	P91	S92	H93	GLY	THR	GLU	ALA	ASP	SER	THR	THR	ASP	GLU	V104	Q148	E166	ASP	THR	ALA
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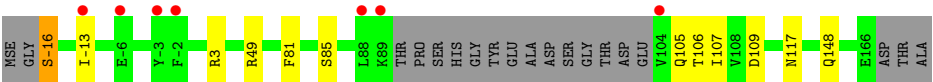
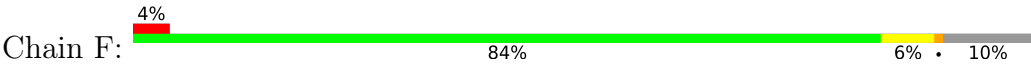
MSE	GLY	SER	ASP	LYS	ILE	HIS	HIS	HIS	HIS	HIS	HIS	E-6	E-6	N-5	N-5	L-4	L-4	Y-3	Y-3	M1	M1	K30	K30	R49	R49	T72	T72	V78	V78	F81	F81	S85	S85	F88	F88	K89	K89	S92	S92	H93	H93	G94	G94	Y95	Y95	E96	E96	ALA	ALA	ASP	ASP	SER	SER	GLY	GLY	THR	THR	ASP	ASP	GLU	GLU	VAL	VAL	Q105	Q105	D109	D109	A134	A134	Q148	Q148	E166	E166	ASP	ASP	THR	THR
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MSE	GLY	SER	ASP	LVS	ILE	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	PHE	GLN	G0	R49	L88	P91	G94	Y95	E96	ALA	ASP	SER	GLY	THR	ASP	GLU	VAL	T105	T106	I107	L121	G126	V137	E138	A165	GLU	ASP	THR	ALA
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MSE	GLY	SER	ASP	LVS	ILE	HIS	HIS	HIS	HIS	GLU	ILE-6	L-4	Y-3	R49	V78	P91	S92	H93	G94	Y95	E96	ALA	ASP	GLY	THR	ASP	GLU	V104	L121	G126	A134	Q148	E166	ASP	THR	ALA
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WORLD WIDE
PDB
PROTEIN DATA BANK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.29Å 98.10Å 84.50Å 90.00° 93.19° 90.00°	Depositor
Resolution (Å)	29.91 – 1.90 29.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.91-1.90) 92.0 (29.91-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0053, PHENIX	Depositor
R, R_{free}	0.160 , 0.196 0.167 , 0.199	Depositor DCC
R_{free} test set	4416 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8455	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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](#)

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	0.85	0/1281	0.81	0/1748
1	B	0.86	0/1243	0.84	0/1697
1	C	0.86	0/1374	0.81	0/1867
1	D	0.79	0/1265	0.81	0/1724
1	E	0.85	0/1349	0.82	0/1836
1	F	0.84	0/1389	0.80	0/1890
All	All	0.84	0/7901	0.81	0/10762

There are no bond length outliers.

There are no bond angle outliers.

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	1237	0	1205	6	0
1	B	1206	0	1177	2	0
1	C	1320	0	1313	11	0
1	D	1228	0	1201	7	0
1	E	1304	0	1285	6	0
1	F	1341	0	1299	8	0
2	A	133	0	0	3	0
2	B	144	0	0	0	0
2	C	154	0	0	3	0
2	D	93	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	145	0	0	0	0
2	F	150	0	0	0	0
All	All	8455	0	7480	31	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 2.

All (31) 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:A:90:THR:HG22	2:A:696:HOH:O	1.96	0.66
1:C:94:GLY:HA3	1:E:148[A]:GLN:HE22	1.64	0.62
1:C:148[A]:GLN:NE2	1:E:94:GLY:HA3	2.14	0.62
2:A:258:HOH:O	1:B:92:SER:HA	2.00	0.61
1:A:92:SER:HA	2:A:192:HOH:O	2.02	0.59
1:C:94:GLY:HA3	1:E:148[A]:GLN:NE2	2.17	0.59
1:A:94:GLY:HA3	1:B:148:GLN:NE2	2.21	0.55
1:C:148[A]:GLN:HE22	1:E:94:GLY:HA3	1.73	0.52
1:F:-16:SER:O	1:F:-13[B]:ILE:HG22	2.11	0.51
1:C:78:VAL:HB	1:C:134:ALA:HB3	1.92	0.50
1:C:1:MSE:HG3	2:C:813[B]:HOH:O	2.12	0.50
1:F:106:THR:O	1:F:107:ILE:HD13	2.13	0.48
1:F:106:THR:C	1:F:107:ILE:HD13	2.38	0.48
1:D:94:GLY:HA3	1:F:148[A]:GLN:NE2	2.29	0.47
1:C:30[A]:LYS:CE	2:C:368:HOH:O	2.63	0.47
1:D:96:GLU:HG2	1:F:148[B]:GLN:CD	2.39	0.46
1:C:30[A]:LYS:HE3	2:C:368:HOH:O	2.15	0.46
1:C:85[A]:SER:HG	1:C:105:GLN:N	2.13	0.46
1:A:10[A]:GLU:HA	1:A:10[A]:GLU:OE1	2.16	0.46
1:D:137:VAL:HG23	1:D:138:GLU:HG3	1.98	0.45
1:E:121:LEU:HD12	1:E:126:GLY:C	2.42	0.45
1:D:94:GLY:HA3	1:F:148[A]:GLN:HE22	1.83	0.44
1:D:106:THR:O	1:D:107[A]:ILE:HD13	2.17	0.44
1:F:81:PHE:HB2	1:F:109:ASP:HB3	2.00	0.43
1:C:81:PHE:HB2	1:C:109:ASP:HB3	2.00	0.43
1:C:72:THR:OG1	1:F:117:ASN:HA	2.19	0.43
1:D:88:LEU:HD12	1:D:107[B]:ILE:HD12	2.00	0.42
1:A:78:VAL:HB	1:A:134:ALA:HB3	2.02	0.41
1:E:78:VAL:HB	1:E:134:ALA:HB3	2.03	0.41
1:D:121:LEU:HD12	1:D:126:GLY:C	2.46	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	160/188 (85%)	158 (99%)	1 (1%)	1 (1%)	21	13
1	B	156/188 (83%)	153 (98%)	2 (1%)	1 (1%)	21	13
1	C	170/188 (90%)	166 (98%)	3 (2%)	1 (1%)	21	13
1	D	158/188 (84%)	155 (98%)	2 (1%)	1 (1%)	21	13
1	E	167/188 (89%)	164 (98%)	2 (1%)	1 (1%)	21	13
1	F	171/188 (91%)	170 (99%)	0	1 (1%)	21	13
All	All	982/1128 (87%)	966 (98%)	10 (1%)	6 (1%)	21	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	ARG
1	A	49	ARG
1	B	49	ARG
1	D	49	ARG
1	E	49	ARG
1	F	49	ARG

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	132/151 (87%)	131 (99%)	1 (1%)	73	75
1	B	128/151 (85%)	127 (99%)	1 (1%)	73	75
1	C	143/151 (95%)	142 (99%)	1 (1%)	76	78
1	D	131/151 (87%)	130 (99%)	1 (1%)	73	75
1	E	140/151 (93%)	140 (100%)	0	100	100
1	F	142/151 (94%)	138 (97%)	4 (3%)	38	32
All	All	816/906 (90%)	808 (99%)	8 (1%)	68	70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	B	85	SER
1	C	89	LYS
1	D	1	MSE
1	F	-16	SER
1	F	3	ARG
1	F	85	SER
1	F	105	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	38	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	155/188 (82%)	-0.17	9 (5%)	29	30	8, 15, 44, 58	6 (3%)
1	B	153/188 (81%)	-0.25	9 (5%)	28	30	8, 16, 37, 50	4 (2%)
1	C	162/188 (86%)	-0.25	8 (4%)	35	37	8, 16, 34, 45	9 (5%)
1	D	155/188 (82%)	0.10	3 (1%)	66	70	8, 16, 37, 46	4 (2%)
1	E	162/188 (86%)	-0.20	7 (4%)	40	42	8, 16, 36, 45	6 (3%)
1	F	166/188 (88%)	-0.10	7 (4%)	40	43	8, 16, 39, 45	6 (3%)
All	All	953/1128 (84%)	-0.15	43 (4%)	38	40	8, 16, 38, 58	35 (3%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	GLY	8.5
1	B	91	PRO	6.1
1	B	90	THR	5.7
1	B	92	SER	5.6
1	F	88	LEU	5.3
1	A	95	TYR	4.8
1	A	92	SER	4.5
1	B	88	LEU	4.4
1	B	93	HIS	4.3
1	D	91	PRO	4.0
1	C	95	TYR	3.9
1	A	93	HIS	3.7
1	B	104	VAL	3.4
1	C	94	GLY	3.1
1	E	93	HIS	3.1
1	C	-6	GLU	3.0
1	A	90	THR	3.0
1	A	91	PRO	2.9
1	F	-6	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	0	GLY	2.7
1	A	88	LEU	2.6
1	E	95	TYR	2.6
1	C	92	SER	2.6
1	F	-13[A]	ILE	2.6
1	C	93	HIS	2.6
1	F	104	VAL	2.6
1	E	104	VAL	2.5
1	B	87	ASP	2.5
1	A	104	VAL	2.4
1	C	-4	LEU	2.4
1	F	-2	PHE	2.4
1	B	89	LYS	2.4
1	F	-3	TYR	2.4
1	E	-5	ASN	2.3
1	E	91	PRO	2.3
1	B	166	GLU	2.3
1	A	166	GLU	2.2
1	E	-3	TYR	2.1
1	E	-4[A]	LEU	2.1
1	F	89	LYS	2.1
1	C	88	LEU	2.1
1	C	-3	TYR	2.1
1	D	95	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.