



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:03 AM GMT

PDB ID : 3KOP
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

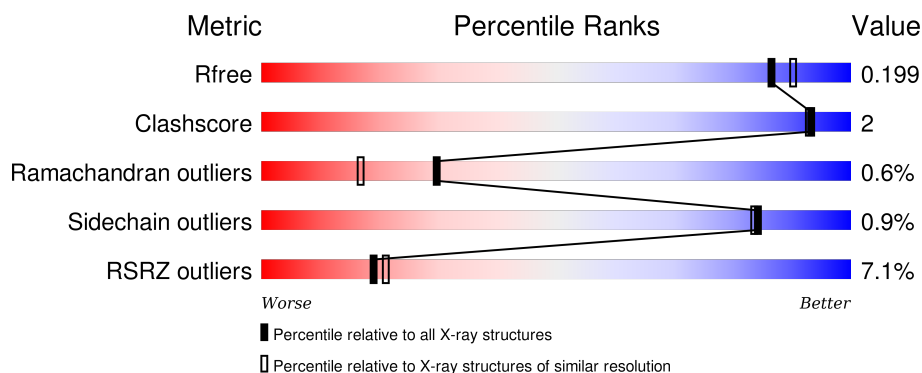
1 Overall quality at a glance

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	A	188	<div> <div>7%</div> <div>79% 5% 16%</div> </div>
1	B	188	<div> <div>6%</div> <div>81% • 17%</div> </div>
1	C	188	<div> <div>3%</div> <div>81% 7% 12%</div> </div>
1	D	188	<div> <div>5%</div> <div>79% 5% 16%</div> </div>
1	E	188	<div> <div>5%</div> <div>85% • 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	188	<div> <div>10%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>

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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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

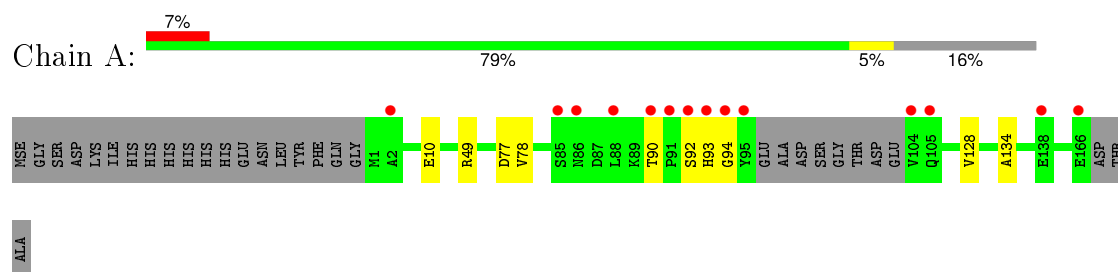
- Molecule 2 is water.

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

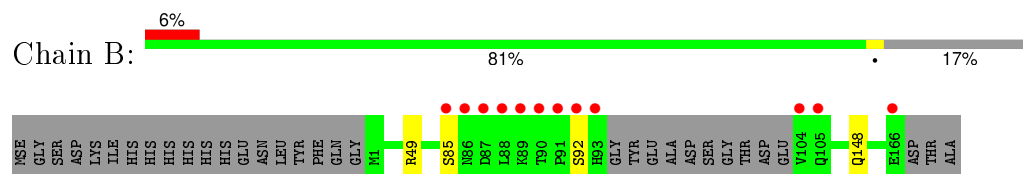
3 Residue-property plots [i](#)

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.

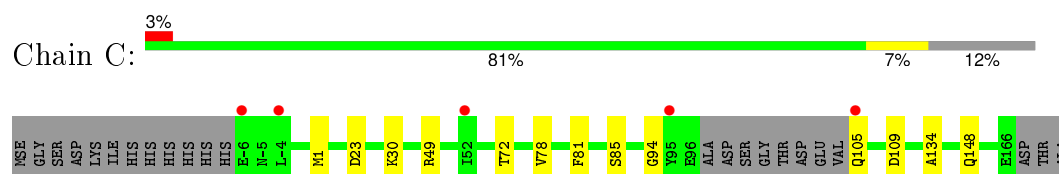
- Molecule 1: Uncharacterized protein



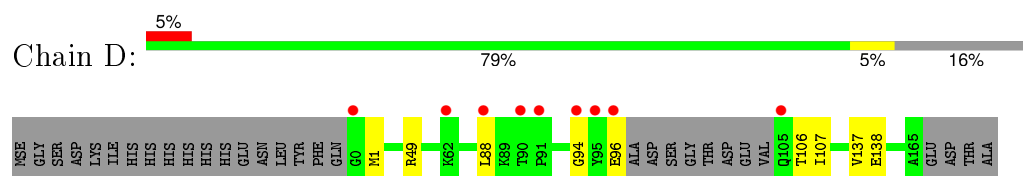
- Molecule 1: Uncharacterized protein



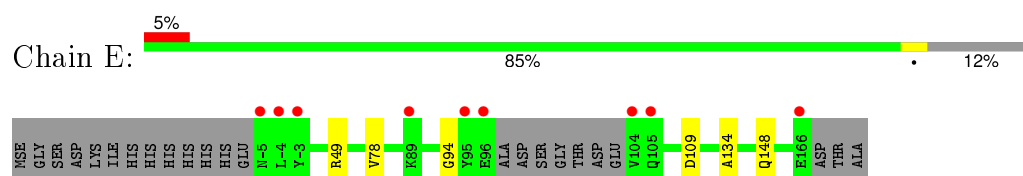
- Molecule 1: Uncharacterized protein



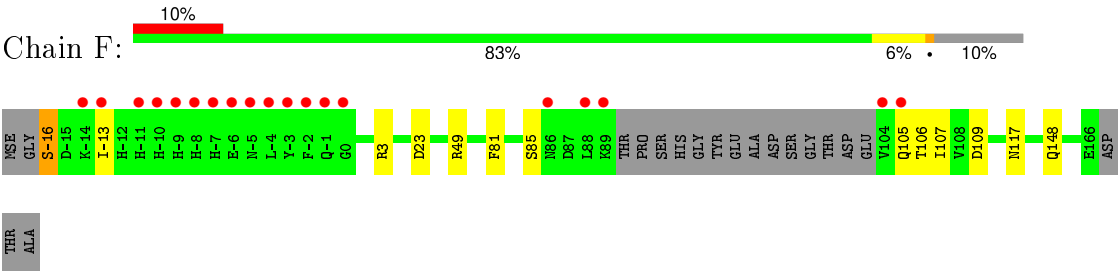
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



● Molecule 1: Uncharacterized protein



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) 99.3 (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	Depositor
R, R_{free}	0.160 , 0.196 0.167 , 0.199	Depositor DCC
R_{free} test set	4416 reflections (5.27%)	DCC
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 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 88235 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.73	0/1281	0.73	1/1748 (0.1%)
1	B	0.73	0/1243	0.73	0/1697
1	C	0.72	0/1374	0.69	1/1867 (0.1%)
1	D	0.65	0/1265	0.69	0/1724
1	E	0.73	0/1349	0.74	2/1836 (0.1%)
1	F	0.72	0/1389	0.71	1/1890 (0.1%)
All	All	0.71	0/7901	0.71	5/10762 (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	E	109	ASP	CB-CG-OD1	6.14	123.82	118.30
1	E	109	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	F	23	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	23	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	77	ASP	CB-CG-OD1	5.16	122.94	118.30

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1320	0	1313	11	0
1	D	1228	0	1201	6	0
1	E	1304	0	1285	5	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
2	E	145	0	0	0	0
2	F	150	0	0	0	0
All	All	8455	0	7480	29	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 (29) 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:85[A]:SER:HG	1:C:105:GLN:N	2.09	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: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:C:30[A]:LYS:HE3	2:C:368:HOH:O	2.15	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: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:F:106:THR:C	1:F:107:ILE:HD13	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:96:GLU:HG2	1:F:148[B]:GLN:CD	2.39	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

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%)	30	17
1	B	156/188 (83%)	153 (98%)	2 (1%)	1 (1%)	30	17
1	C	170/188 (90%)	166 (98%)	3 (2%)	1 (1%)	30	17
1	D	158/188 (84%)	155 (98%)	2 (1%)	1 (1%)	30	17
1	E	167/188 (89%)	164 (98%)	2 (1%)	1 (1%)	30	17
1	F	171/188 (91%)	170 (99%)	0	1 (1%)	30	17
All	All	982/1128 (87%)	966 (98%)	10 (1%)	6 (1%)	30	17

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 ⓘ

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%)	86	86
1	B	128/151 (85%)	127 (99%)	1 (1%)	86	86
1	C	143/151 (95%)	143 (100%)	0	100	100
1	D	131/151 (87%)	130 (99%)	1 (1%)	86	86
1	E	140/151 (93%)	140 (100%)	0	100	100
1	F	142/151 (94%)	138 (97%)	4 (3%)	51	41
All	All	816/906 (90%)	809 (99%)	7 (1%)	84	83

All (7) residues with a non-rotameric sidechain are listed below:

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no carbohydrates 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 ⓘ

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%)	0.10	14 (9%) 12 13	10, 16, 44, 58	0
1	B	153/188 (81%)	0.07	12 (7%) 16 17	10, 16, 37, 50	0
1	C	162/188 (86%)	-0.00	5 (3%) 52 56	10, 16, 34, 45	0
1	D	155/188 (82%)	0.05	9 (5%) 26 29	10, 16, 37, 46	0
1	E	162/188 (86%)	0.08	9 (5%) 28 31	10, 16, 36, 45	0
1	F	166/188 (88%)	0.26	19 (11%) 7 7	10, 16, 39, 45	0
All	All	953/1128 (84%)	0.10	68 (7%) 19 21	10, 16, 39, 58	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	VAL	7.3
1	A	94	GLY	6.9
1	A	95	TYR	6.8
1	F	88	LEU	6.6
1	A	104	VAL	6.2
1	B	90	THR	6.2
1	B	91	PRO	6.2
1	F	104	VAL	6.0
1	F	-3	TYR	5.7
1	E	104	VAL	5.6
1	B	88	LEU	5.4
1	F	-4	LEU	5.3
1	F	-13[A]	ILE	5.1
1	B	92	SER	4.9
1	F	-2	PHE	4.5
1	C	-6	GLU	4.4
1	A	90	THR	4.3
1	F	-10	HIS	4.2
1	B	93	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	94	GLY	4.0
1	F	-5[A]	ASN	4.0
1	F	89	LYS	3.9
1	E	-4[A]	LEU	3.9
1	F	-6	GLU	3.9
1	A	93	HIS	3.8
1	E	105	GLN	3.8
1	D	105	GLN	3.8
1	A	105	GLN	3.7
1	E	-5	ASN	3.7
1	F	-9	HIS	3.5
1	F	-7	HIS	3.5
1	A	88	LEU	3.5
1	B	87	ASP	3.4
1	B	86	ASN	3.4
1	D	95	TYR	3.4
1	B	166	GLU	3.4
1	B	89	LYS	3.2
1	F	86	ASN	3.2
1	F	105	GLN	3.2
1	D	91	PRO	3.1
1	E	166	GLU	3.1
1	C	-4	LEU	3.1
1	A	166	GLU	3.1
1	A	86	ASN	3.1
1	E	96	GLU	3.0
1	D	0	GLY	3.0
1	D	96	GLU	3.0
1	A	92	SER	3.0
1	F	-11	HIS	3.0
1	F	-1	GLN	2.9
1	D	90	THR	2.8
1	F	-8	HIS	2.7
1	B	105	GLN	2.6
1	C	105	GLN	2.6
1	A	91	PRO	2.6
1	C	52	ILE	2.4
1	C	95	TYR	2.3
1	A	2	ALA	2.3
1	A	85	SER	2.2
1	D	88	LEU	2.2
1	A	138[A]	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	-3	TYR	2.1
1	E	95	TYR	2.1
1	F	0	GLY	2.1
1	B	85	SER	2.1
1	F	-14	LYS	2.1
1	D	62	LYS	2.1
1	E	89	LYS	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 carbohydrates 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.