



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:54 am GMT

PDB ID : 4NJ6
Title : PB1 Domain of AtARF7
Authors : Korasick, D.A.; Westfall, C.S.; Lee, S.G.; Nanao, M.; Jez, J.M.; Strader, L.C.
Deposited on : 2013-11-08
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

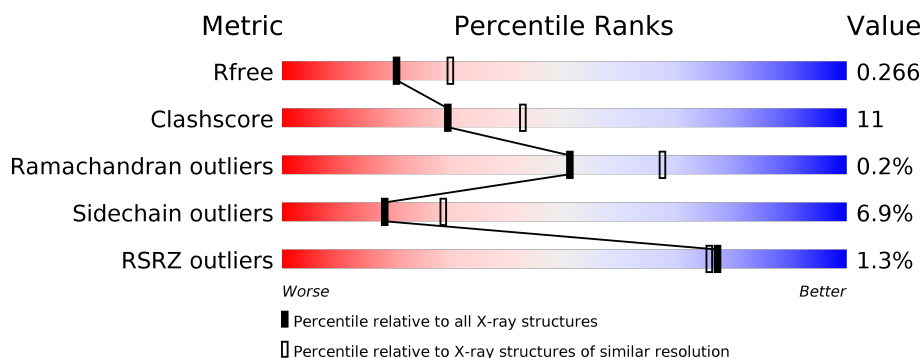
1 Overall quality at a glance

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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 ≥ 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	95	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	95	<div> <div></div> <div>72%</div> <div>19%</div> <div>• 6%</div> </div>
1	C	95	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	D	95	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	E	95	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>11%</div> </div> </div>
1	F	95	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	95	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>72%</div><div>19%</div><div>• 7%</div></div></div>
1	H	95	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>68%</div><div>21%</div><div>• 8%</div></div></div>
1	I	95	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>21%</div><div>• 9%</div></div></div>
1	J	95	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>61%</div><div>23%</div><div>• 14%</div></div></div>
1	K	95	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>72%</div><div>21%</div><div>• 6%</div></div></div>
1	L	95	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>16%</div><div>• 12%</div></div></div>
1	M	95	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>24%</div><div>5% 7%</div></div></div>
1	N	95	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>67%</div><div>19%</div><div>14%</div></div></div>
1	O	95	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>69%</div><div>19%</div><div>• 9%</div></div></div>
1	P	95	<div><div><div></div><div></div><div></div></div><div><div></div><div>66%</div><div>23%</div><div>• 8%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11676 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 Auxin response factor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			709	444	124	138	3			
1	B	89	Total	C	N	O	S	0	0	0
			720	450	128	139	3			
1	C	89	Total	C	N	O	S	0	0	0
			720	450	128	139	3			
1	D	88	Total	C	N	O	S	0	0	0
			709	444	124	138	3			
1	E	85	Total	C	N	O	S	0	0	0
			684	429	119	134	2			
1	F	89	Total	C	N	O	S	0	0	0
			715	447	125	140	3			
1	G	88	Total	C	N	O	S	0	0	0
			709	444	124	138	3			
1	H	87	Total	C	N	O	S	0	0	0
			699	438	121	137	3			
1	I	86	Total	C	N	O	S	0	0	0
			697	436	123	136	2			
1	J	82	Total	C	N	O	S	0	0	0
			658	414	114	128	2			
1	K	89	Total	C	N	O	S	0	0	0
			720	450	128	139	3			
1	L	84	Total	C	N	O	S	0	0	0
			680	427	119	131	3			
1	M	88	Total	C	N	O	S	0	0	0
			712	445	127	138	2			
1	N	82	Total	C	N	O	S	0	0	0
			663	417	115	128	3			
1	O	86	Total	C	N	O	S	0	0	0
			692	434	120	135	3			
1	P	87	Total	C	N	O	S	0	0	0
			699	438	121	137	3			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	GLY	-	EXPRESSION TAG	UNP P93022
A	1034	SER	-	EXPRESSION TAG	UNP P93022
A	1035	HIS	-	EXPRESSION TAG	UNP P93022
A	1036	MET	-	EXPRESSION TAG	UNP P93022
A	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
A	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
A	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
B	1033	GLY	-	EXPRESSION TAG	UNP P93022
B	1034	SER	-	EXPRESSION TAG	UNP P93022
B	1035	HIS	-	EXPRESSION TAG	UNP P93022
B	1036	MET	-	EXPRESSION TAG	UNP P93022
B	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
B	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
B	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
C	1033	GLY	-	EXPRESSION TAG	UNP P93022
C	1034	SER	-	EXPRESSION TAG	UNP P93022
C	1035	HIS	-	EXPRESSION TAG	UNP P93022
C	1036	MET	-	EXPRESSION TAG	UNP P93022
C	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
C	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
C	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
D	1033	GLY	-	EXPRESSION TAG	UNP P93022
D	1034	SER	-	EXPRESSION TAG	UNP P93022
D	1035	HIS	-	EXPRESSION TAG	UNP P93022
D	1036	MET	-	EXPRESSION TAG	UNP P93022
D	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
D	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
D	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
E	1033	GLY	-	EXPRESSION TAG	UNP P93022
E	1034	SER	-	EXPRESSION TAG	UNP P93022
E	1035	HIS	-	EXPRESSION TAG	UNP P93022
E	1036	MET	-	EXPRESSION TAG	UNP P93022
E	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
E	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
E	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
F	1033	GLY	-	EXPRESSION TAG	UNP P93022
F	1034	SER	-	EXPRESSION TAG	UNP P93022
F	1035	HIS	-	EXPRESSION TAG	UNP P93022
F	1036	MET	-	EXPRESSION TAG	UNP P93022
F	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
F	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
F	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1033	GLY	-	EXPRESSION TAG	UNP P93022
G	1034	SER	-	EXPRESSION TAG	UNP P93022
G	1035	HIS	-	EXPRESSION TAG	UNP P93022
G	1036	MET	-	EXPRESSION TAG	UNP P93022
G	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
G	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
G	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
H	1033	GLY	-	EXPRESSION TAG	UNP P93022
H	1034	SER	-	EXPRESSION TAG	UNP P93022
H	1035	HIS	-	EXPRESSION TAG	UNP P93022
H	1036	MET	-	EXPRESSION TAG	UNP P93022
H	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
H	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
H	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
I	1033	GLY	-	EXPRESSION TAG	UNP P93022
I	1034	SER	-	EXPRESSION TAG	UNP P93022
I	1035	HIS	-	EXPRESSION TAG	UNP P93022
I	1036	MET	-	EXPRESSION TAG	UNP P93022
I	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
I	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
I	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
J	1033	GLY	-	EXPRESSION TAG	UNP P93022
J	1034	SER	-	EXPRESSION TAG	UNP P93022
J	1035	HIS	-	EXPRESSION TAG	UNP P93022
J	1036	MET	-	EXPRESSION TAG	UNP P93022
J	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
J	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
J	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
K	1033	GLY	-	EXPRESSION TAG	UNP P93022
K	1034	SER	-	EXPRESSION TAG	UNP P93022
K	1035	HIS	-	EXPRESSION TAG	UNP P93022
K	1036	MET	-	EXPRESSION TAG	UNP P93022
K	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
K	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
K	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
L	1033	GLY	-	EXPRESSION TAG	UNP P93022
L	1034	SER	-	EXPRESSION TAG	UNP P93022
L	1035	HIS	-	EXPRESSION TAG	UNP P93022
L	1036	MET	-	EXPRESSION TAG	UNP P93022
L	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
L	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
L	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1033	GLY	-	EXPRESSION TAG	UNP P93022
M	1034	SER	-	EXPRESSION TAG	UNP P93022
M	1035	HIS	-	EXPRESSION TAG	UNP P93022
M	1036	MET	-	EXPRESSION TAG	UNP P93022
M	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
M	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
M	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
N	1033	GLY	-	EXPRESSION TAG	UNP P93022
N	1034	SER	-	EXPRESSION TAG	UNP P93022
N	1035	HIS	-	EXPRESSION TAG	UNP P93022
N	1036	MET	-	EXPRESSION TAG	UNP P93022
N	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
N	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
N	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
O	1033	GLY	-	EXPRESSION TAG	UNP P93022
O	1034	SER	-	EXPRESSION TAG	UNP P93022
O	1035	HIS	-	EXPRESSION TAG	UNP P93022
O	1036	MET	-	EXPRESSION TAG	UNP P93022
O	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
O	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
O	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022
P	1033	GLY	-	EXPRESSION TAG	UNP P93022
P	1034	SER	-	EXPRESSION TAG	UNP P93022
P	1035	HIS	-	EXPRESSION TAG	UNP P93022
P	1036	MET	-	EXPRESSION TAG	UNP P93022
P	1042	ALA	LYS	ENGINEERED MUTATION	UNP P93022
P	1092	ALA	ASP	ENGINEERED MUTATION	UNP P93022
P	1096	ALA	ASP	ENGINEERED MUTATION	UNP P93022

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	35	Total O 35 35	0	0
2	B	42	Total O 42 42	0	0
2	C	37	Total O 37 37	0	0
2	D	32	Total O 32 32	0	0
2	E	36	Total O 36 36	0	0

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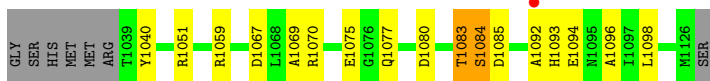
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	24	Total 24	O 24	0	0
2	G	38	Total 38	O 38	0	0
2	H	24	Total 24	O 24	0	0
2	I	27	Total 27	O 27	0	0
2	J	24	Total 24	O 24	0	0
2	K	43	Total 43	O 43	0	0
2	L	31	Total 31	O 31	0	0
2	M	17	Total 17	O 17	0	0
2	N	16	Total 16	O 16	0	0
2	O	38	Total 38	O 38	0	0
2	P	26	Total 26	O 26	0	0

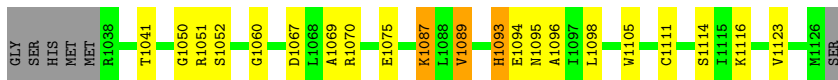
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

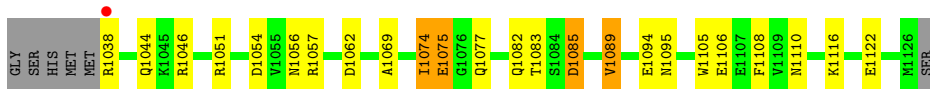
- Molecule 1: Auxin response factor 7



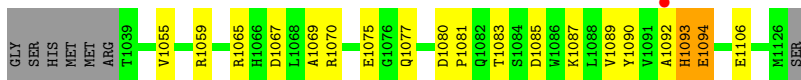
- Molecule 1: Auxin response factor 7



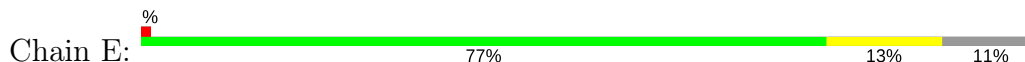
- Molecule 1: Auxin response factor 7



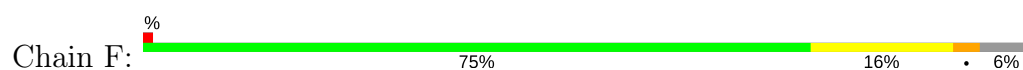
- Molecule 1: Auxin response factor 7



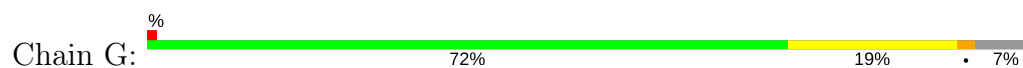
- Molecule 1: Auxin response factor 7



- Molecule 1: Auxin response factor 7



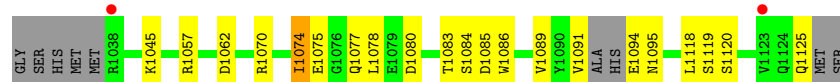
• Molecule 1: Auxin response factor 7



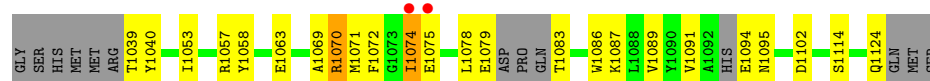
• Molecule 1: Auxin response factor 7



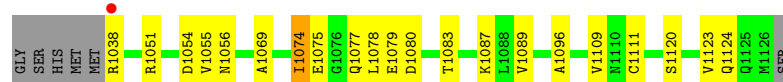
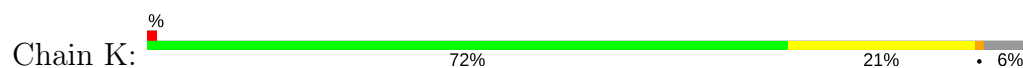
• Molecule 1: Auxin response factor 7



• Molecule 1: Auxin response factor 7



• Molecule 1: Auxin response factor 7



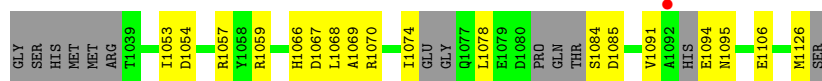
• Molecule 1: Auxin response factor 7



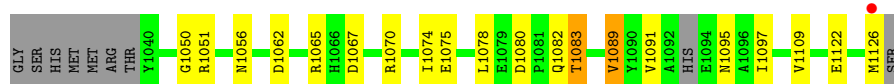
- Molecule 1: Auxin response factor 7



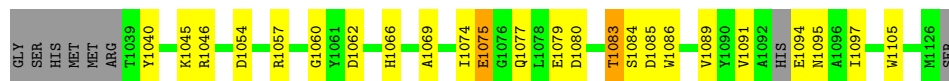
- Molecule 1: Auxin response factor 7



- Molecule 1: Auxin response factor 7



- Molecule 1: Auxin response factor 7



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	150.59Å 150.59Å 183.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.65 – 2.40 47.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.65-2.40) 94.2 (47.61-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.209 , 0.271 0.197 , 0.266	Depositor DCC
R_{free} test set	1946 reflections (3.25%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for $-2/3^*h-1/3^*k+2/3^*l, -1/3^*h-2/3^*k-2/3^*l, 2/3^*h-2/3^*k+1/3^*l$ 0.014 for $-h, 1/3^*h-1/3^*k+2/3^*l, 2/3^*h+4/3^*k+1/3^*l$ 0.016 for $-1/3^*h+1/3^*k-2/3^*l, -k, -4/3^*h-2/3^*k+1/3^*l$ 0.010 for $-h, 2/3^*h+1/3^*k-2/3^*l, -2/3^*h-4/3^*k-1/3^*l$ 0.011 for $1/3^*h+2/3^*k+2/3^*l, -k, 4/3^*h+2/3^*k-1/3^*l$ 0.016 for $-1/3^*h-2/3^*k-2/3^*l, -2/3^*h-1/3^*k+2/3^*l, -2/3^*h+2/3^*k-1/3^*l$ 0.019 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11676	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [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	0.50	0/722	0.64	0/977
1	B	0.47	0/733	0.60	0/991
1	C	0.45	0/733	0.61	0/991
1	D	0.45	0/722	0.60	0/977
1	E	0.49	0/695	0.59	0/939
1	F	0.42	0/728	0.56	0/985
1	G	0.43	0/722	0.61	0/977
1	H	0.41	0/710	0.61	0/959
1	I	0.52	0/708	0.61	0/956
1	J	0.42	0/667	0.58	0/899
1	K	0.44	0/733	0.60	0/991
1	L	0.46	0/691	0.60	0/931
1	M	0.47	0/725	0.57	0/981
1	N	0.35	0/671	0.53	0/902
1	O	0.45	0/703	0.59	0/949
1	P	0.44	0/710	0.60	0/959
All	All	0.45	0/11373	0.59	0/15364

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	709	0	684	12	0
1	B	720	0	697	14	0
1	C	720	0	697	18	0
1	D	709	0	684	17	0
1	E	684	0	660	11	0
1	F	715	0	689	10	0
1	G	709	0	684	14	0
1	H	699	0	676	17	0
1	I	697	0	675	19	0
1	J	658	0	639	19	0
1	K	720	0	697	22	0
1	L	680	0	653	11	0
1	M	712	0	688	32	0
1	N	663	0	643	9	0
1	O	692	0	669	8	0
1	P	699	0	676	18	0
2	A	35	0	0	0	0
2	B	42	0	0	0	0
2	C	37	0	0	1	0
2	D	32	0	0	1	0
2	E	36	0	0	3	0
2	F	24	0	0	2	0
2	G	38	0	0	2	0
2	H	24	0	0	3	0
2	I	27	0	0	1	0
2	J	24	0	0	0	0
2	K	43	0	0	3	0
2	L	31	0	0	0	0
2	M	17	0	0	1	0
2	N	16	0	0	0	0
2	O	38	0	0	0	0
2	P	26	0	0	3	0
All	All	11676	0	10811	237	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 11.

The worst 5 of 237 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:J:1074:ILE:O	1:J:1074:ILE:HG13	1.41	1.17
1:K:1074:ILE:O	1:K:1074:ILE:HG12	1.41	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:GLN:O	1:A:1084:SER:HB2	1.53	1.08
1:K:1074:ILE:CG1	1:K:1077:GLN:HB2	1.96	0.95
1:M:1091:VAL:HG13	1:M:1095:ASN:HA	1.52	0.90

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	86/95 (90%)	84 (98%)	2 (2%)	0	100	100
1	B	87/95 (92%)	86 (99%)	1 (1%)	0	100	100
1	C	87/95 (92%)	86 (99%)	1 (1%)	0	100	100
1	D	86/95 (90%)	83 (96%)	2 (2%)	1 (1%)	15	21
1	E	81/95 (85%)	80 (99%)	1 (1%)	0	100	100
1	F	87/95 (92%)	85 (98%)	2 (2%)	0	100	100
1	G	86/95 (90%)	84 (98%)	1 (1%)	1 (1%)	15	21
1	H	83/95 (87%)	81 (98%)	2 (2%)	0	100	100
1	I	82/95 (86%)	79 (96%)	3 (4%)	0	100	100
1	J	76/95 (80%)	75 (99%)	1 (1%)	0	100	100
1	K	87/95 (92%)	83 (95%)	4 (5%)	0	100	100
1	L	78/95 (82%)	77 (99%)	1 (1%)	0	100	100
1	M	86/95 (90%)	83 (96%)	2 (2%)	1 (1%)	15	21
1	N	74/95 (78%)	70 (95%)	4 (5%)	0	100	100
1	O	82/95 (86%)	81 (99%)	1 (1%)	0	100	100
1	P	83/95 (87%)	80 (96%)	3 (4%)	0	100	100
All	All	1331/1520 (88%)	1297 (97%)	31 (2%)	3 (0%)	51	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	1097	ILE
1	D	1093	HIS
1	G	1081	PRO

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	77/83 (93%)	73 (95%)	4 (5%)	27	43
1	B	78/83 (94%)	73 (94%)	5 (6%)	20	32
1	C	78/83 (94%)	71 (91%)	7 (9%)	11	16
1	D	77/83 (93%)	74 (96%)	3 (4%)	37	56
1	E	74/83 (89%)	73 (99%)	1 (1%)	71	86
1	F	78/83 (94%)	72 (92%)	6 (8%)	15	23
1	G	77/83 (93%)	71 (92%)	6 (8%)	15	23
1	H	76/83 (92%)	72 (95%)	4 (5%)	26	42
1	I	76/83 (92%)	71 (93%)	5 (7%)	19	30
1	J	71/83 (86%)	61 (86%)	10 (14%)	4	4
1	K	78/83 (94%)	75 (96%)	3 (4%)	38	58
1	L	73/83 (88%)	66 (90%)	7 (10%)	10	14
1	M	77/83 (93%)	71 (92%)	6 (8%)	15	23
1	N	72/83 (87%)	67 (93%)	5 (7%)	18	28
1	O	75/83 (90%)	67 (89%)	8 (11%)	8	10
1	P	76/83 (92%)	72 (95%)	4 (5%)	26	42
All	All	1213/1328 (91%)	1129 (93%)	84 (7%)	18	28

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	1074	ILE

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Mol	Chain	Res	Type
1	J	1087	LYS
1	O	1083	THR
1	I	1089	VAL
1	J	1053	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1095	ASN
1	B	1093	HIS
1	C	1110	ASN
1	G	1093	HIS

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 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	88/95 (92%)	-0.25	1 (1%) 80 79	24, 39, 75, 88	0
1	B	89/95 (93%)	-0.32	0 100 100	28, 45, 82, 122	0
1	C	89/95 (93%)	-0.25	1 (1%) 80 79	24, 43, 83, 113	0
1	D	88/95 (92%)	-0.36	1 (1%) 80 79	28, 43, 75, 111	0
1	E	85/95 (89%)	-0.36	1 (1%) 79 77	25, 39, 64, 95	0
1	F	89/95 (93%)	-0.22	1 (1%) 80 79	29, 48, 93, 131	0
1	G	88/95 (92%)	-0.28	1 (1%) 80 79	27, 46, 81, 115	0
1	H	87/95 (91%)	-0.28	1 (1%) 80 79	29, 50, 85, 121	0
1	I	86/95 (90%)	-0.10	2 (2%) 61 58	23, 48, 89, 106	0
1	J	82/95 (86%)	-0.28	2 (2%) 59 56	27, 51, 82, 99	0
1	K	89/95 (93%)	-0.30	1 (1%) 80 79	27, 44, 72, 100	0
1	L	84/95 (88%)	-0.16	2 (2%) 59 56	26, 51, 97, 126	0
1	M	88/95 (92%)	0.01	2 (2%) 61 58	32, 62, 106, 121	0
1	N	82/95 (86%)	0.09	1 (1%) 79 77	36, 67, 109, 126	0
1	O	86/95 (90%)	-0.38	1 (1%) 79 77	28, 44, 73, 103	0
1	P	87/95 (91%)	-0.05	0 100 100	32, 62, 94, 104	0
All	All	1387/1520 (91%)	-0.22	18 (1%) 77 75	23, 48, 95, 131	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	1096	ALA	8.7
1	J	1074	ILE	4.2
1	O	1126	MET	3.7
1	A	1092	ALA	3.7
1	D	1092	ALA	3.2

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.