



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:14 PM UTC

PDB ID : 4NJ7 / pdb_00004nj7
Title : PB1 Domain of AtARF7 - SeMet Derivative
Authors : Korasick, D.A.; Westfall, C.S.; Lee, S.G.; Nanao, M.; Jez, J.M.; Strader, L.C.
Deposited on : 2013-11-08
Resolution : 3.00 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

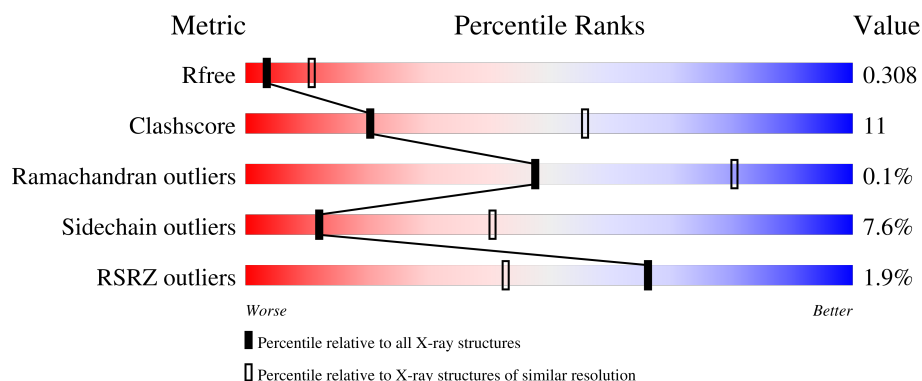
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	95	0.1% 57% 21% • 19%
1	B	95	3% 46% 28% 7% 18%
1	C	95	0.1% 66% 16% • 16%
1	D	95	0.1% 52% 19% • 26%
1	E	95	2% 61% 17% 5% 17%

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Mol	Chain	Length	Quality of chain
1	F	95	% 59% 21% 5% 15%
1	G	95	57% 23% • 18%
1	H	95	58% 17% 5% 20%
1	I	95	% 57% 22% • 17%
1	J	95	% 56% 18% • 22%
1	K	95	2% 59% 18% • 21%
1	L	95	4% 55% 19% • 25%
1	M	95	2% 58% 14% • 24%
1	N	95	2% 55% 15% • 27%
1	O	95	% 61% 20% • 16%
1	P	95	% 62% 16% • 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9822 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	77	Total	C	N	O	S	Se	0	0	0
			620	393	108	117	1	1			
1	B	78	Total	C	N	O	S	Se	0	0	0
			631	400	112	117	1	1			
1	C	80	Total	C	N	O	S	Se	0	0	0
			650	410	113	124	1	2			
1	D	70	Total	C	N	O	S	Se	0	0	0
			568	363	100	103	1	1			
1	E	79	Total	C	N	O	S	Se	0	0	0
			633	400	109	122	1	1			
1	F	81	Total	C	N	O	S	Se	0	0	0
			653	412	113	125	1	2			
1	G	78	Total	C	N	O	S	Se	0	0	0
			629	399	111	116	1	2			
1	H	76	Total	C	N	O	S	Se	0	0	0
			616	392	108	113	1	2			
1	I	79	Total	C	N	O	S	Se	0	0	0
			638	404	112	119	1	2			
1	J	74	Total	C	N	O	S	Se	0	0	0
			599	382	105	110	1	1			
1	K	75	Total	C	N	O	S	Se	0	0	0
			607	385	107	113	1	1			
1	L	71	Total	C	N	O	S	Se	0	0	0
			567	360	100	105	1	1			
1	M	72	Total	C	N	O	S	Se	0	0	0
			585	374	102	107	1	1			
1	N	69	Total	C	N	O	S	Se	0	0	0
			550	349	96	102	1	2			
1	O	80	Total	C	N	O	S	Se	0	0	0
			650	410	113	124	1	2			
1	P	77	Total	C	N	O	S	Se	0	0	0
			626	397	110	117	1	1			

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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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	MSE	-	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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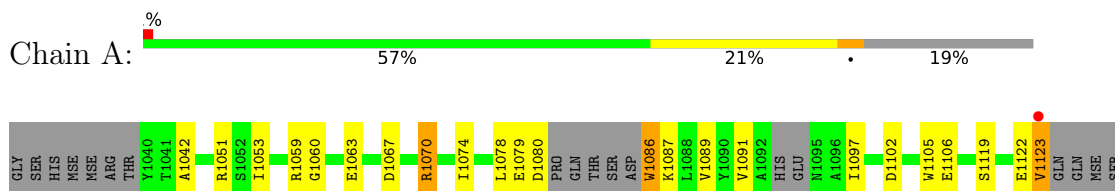
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Chain	Residue	Modelled	Actual	Comment	Reference
M	1033	GLY	-	expression tag	UNP P93022
M	1034	SER	-	expression tag	UNP P93022
M	1035	HIS	-	expression tag	UNP P93022
M	1036	MSE	-	expression tag	UNP P93022
M	1042	ALA	LYS	engineered mutation	UNP P93022
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	MSE	-	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	MSE	-	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	MSE	-	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

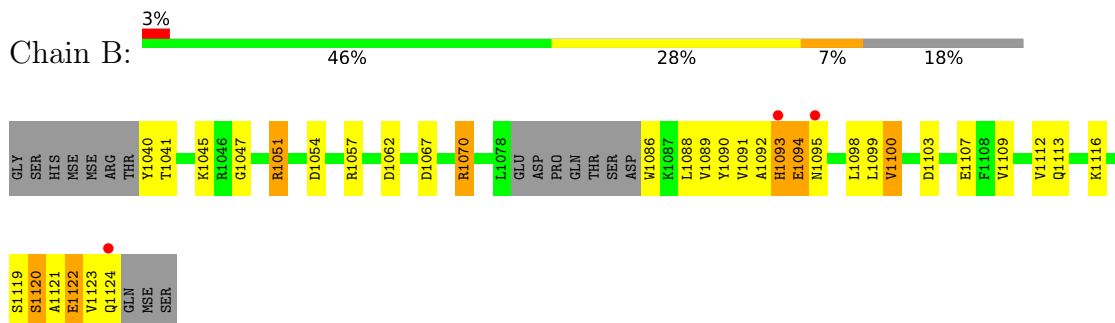
3 Residue-property plots [i](#)

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.

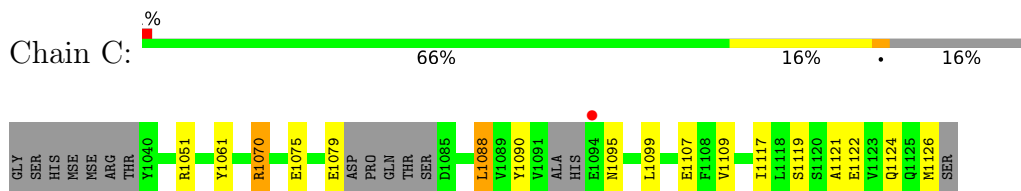
- Molecule 1: Auxin response factor 7



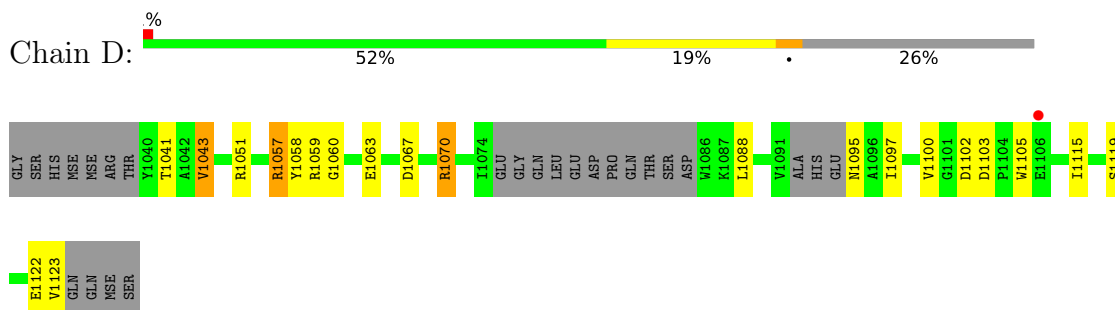
- Molecule 1: Auxin response factor 7



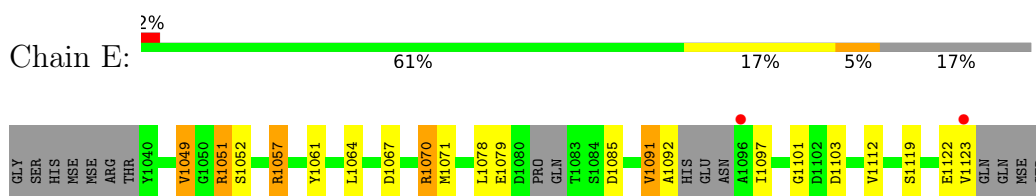
- Molecule 1: Auxin response factor 7



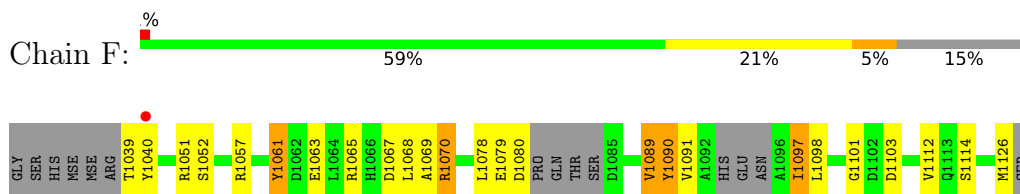
- Molecule 1: Auxin response factor 7



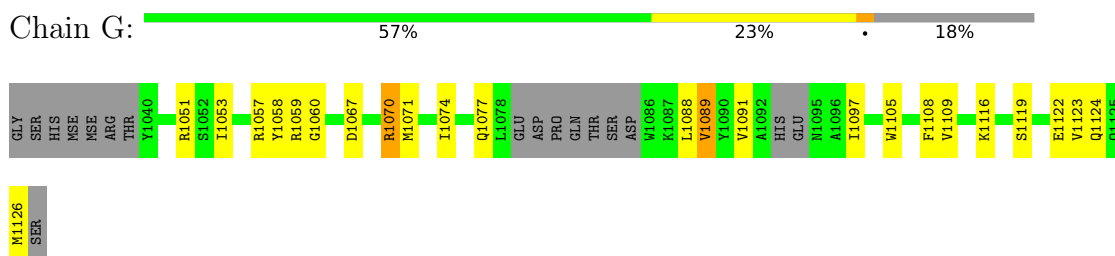
- Molecule 1: Auxin response factor 7



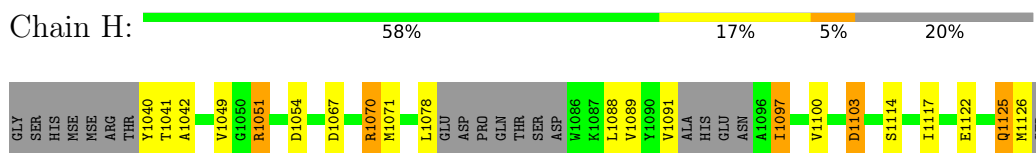
- Molecule 1: Auxin response factor 7



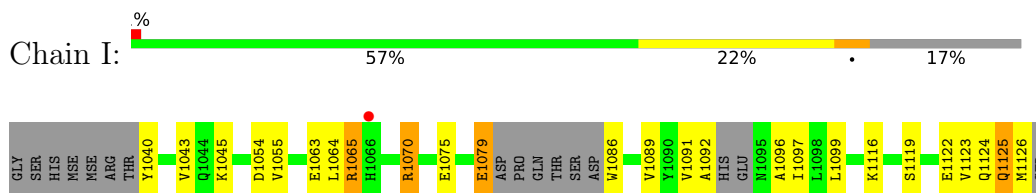
- Molecule 1: Auxin response factor 7



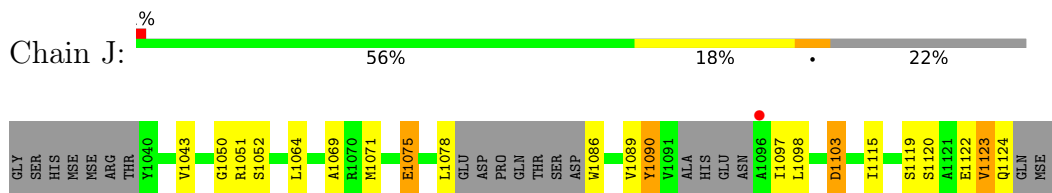
- Molecule 1: Auxin response factor 7



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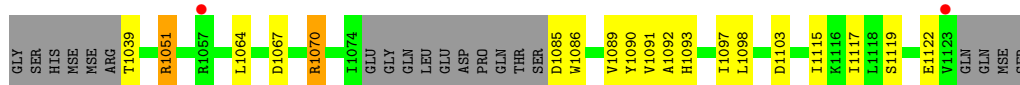


- Molecule 1: Auxin response factor 7

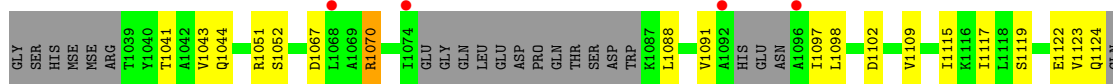


- Molecule 1: Auxin response factor 7

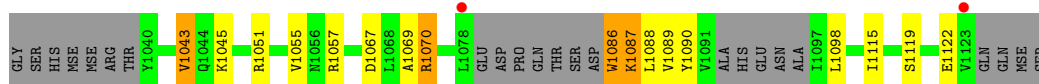




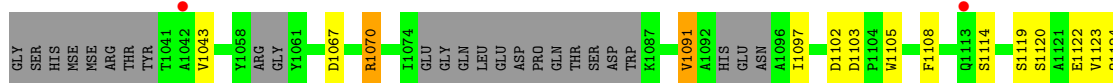
- Molecule 1: Auxin response factor 7



- 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	150.94Å 150.94Å 184.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.60 – 3.00 47.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.60-3.00) 98.5 (47.60-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.257 , 0.304 0.258 , 0.308	Depositor DCC
R_{free} test set	2029 reflections (6.47%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 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 0.028 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.035 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.028 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.028 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.038 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 0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 ⓘ

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	1.41	3/628 (0.5%)	1.46	4/844 (0.5%)
1	B	1.40	2/641 (0.3%)	1.36	3/863 (0.3%)
1	C	1.51	4/657 (0.6%)	1.38	2/880 (0.2%)
1	D	1.35	2/576 (0.3%)	1.31	2/774 (0.3%)
1	E	1.52	3/641 (0.5%)	1.47	7/862 (0.8%)
1	F	1.31	3/660 (0.5%)	1.37	3/885 (0.3%)
1	G	1.37	2/636 (0.3%)	1.40	6/852 (0.7%)
1	H	1.40	4/623 (0.6%)	1.29	3/834 (0.4%)
1	I	1.32	2/645 (0.3%)	1.34	3/864 (0.3%)
1	J	1.31	2/607 (0.3%)	1.32	6/815 (0.7%)
1	K	1.39	4/617 (0.6%)	1.28	0/832
1	L	1.35	4/573 (0.7%)	1.29	2/769 (0.3%)
1	M	1.30	3/593 (0.5%)	1.32	4/796 (0.5%)
1	N	1.29	2/553 (0.4%)	1.30	1/738 (0.1%)
1	O	1.44	3/657 (0.5%)	1.42	6/880 (0.7%)
1	P	1.35	2/637 (0.3%)	1.35	1/859 (0.1%)
All	All	1.38	45/9944 (0.5%)	1.36	53/13347 (0.4%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1091	VAL	CA-CB	8.92	1.66	1.54
1	C	1117	ILE	CA-CB	-8.72	1.43	1.53
1	A	1042	ALA	CA-CB	-7.75	1.40	1.53
1	C	1088	LEU	C-O	7.11	1.32	1.24
1	B	1100	VAL	CA-CB	7.04	1.62	1.53
1	O	1079	GLU	CA-C	6.90	1.62	1.52
1	E	1049	VAL	CA-CB	-6.89	1.45	1.54
1	H	1117	ILE	CA-CB	-6.83	1.45	1.53
1	L	1097	ILE	N-CA	6.83	1.53	1.46
1	B	1116	LYS	C-O	6.76	1.32	1.23
1	F	1112	VAL	CA-CB	6.75	1.62	1.54
1	K	1115	ILE	CA-CB	-6.67	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1064	LEU	CG-CD1	6.48	1.74	1.52
1	K	1117	ILE	CA-CB	-6.36	1.46	1.53
1	M	1043	VAL	CA-CB	-6.34	1.46	1.54
1	N	1097	ILE	CA-CB	6.26	1.61	1.54
1	D	1041	THR	CA-CB	6.26	1.63	1.53
1	P	1080	ASP	CA-C	6.07	1.60	1.52
1	F	1089	VAL	CA-C	6.05	1.59	1.53
1	K	1115	ILE	CA-C	6.01	1.59	1.52
1	H	1125	GLN	CA-C	5.95	1.60	1.52
1	C	1095	ASN	CA-C	5.76	1.60	1.52
1	P	1043	VAL	CA-CB	-5.63	1.47	1.54
1	A	1074	ILE	CA-C	5.61	1.59	1.52
1	L	1044	GLN	CA-C	-5.61	1.45	1.52
1	I	1043	VAL	CA-CB	-5.60	1.47	1.54
1	L	1088	LEU	N-CA	5.60	1.53	1.46
1	O	1086	TRP	N-CA	5.54	1.56	1.46
1	H	1042	ALA	CA-CB	-5.49	1.44	1.53
1	H	1126	MSE	CG-SE	5.44	2.11	1.95
1	L	1098	LEU	C-O	5.44	1.30	1.23
1	F	1090	TYR	CA-CB	-5.35	1.44	1.53
1	M	1069	ALA	CA-CB	-5.22	1.45	1.53
1	N	1043	VAL	CA-CB	-5.20	1.48	1.54
1	G	1088	LEU	CA-C	5.15	1.59	1.52
1	O	1078	LEU	CA-C	-5.15	1.45	1.52
1	J	1052	SER	CA-C	-5.14	1.46	1.52
1	K	1051	ARG	N-CA	5.14	1.52	1.45
1	C	1099	LEU	C-O	-5.14	1.17	1.24
1	J	1097	ILE	CA-CB	5.11	1.60	1.54
1	I	1116	LYS	CA-C	-5.10	1.46	1.52
1	D	1043	VAL	CA-C	-5.08	1.46	1.52
1	M	1088	LEU	N-CA	5.07	1.52	1.46
1	E	1051	ARG	CG-CD	-5.06	1.37	1.52
1	A	1053	ILE	CA-CB	-5.03	1.47	1.55

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1090	TYR	N-CA-C	9.28	120.50	108.34
1	M	1087	LYS	CA-C-N	-8.62	111.31	122.77
1	M	1087	LYS	C-N-CA	-8.62	111.31	122.77
1	F	1097	ILE	N-CA-C	7.97	120.43	108.23
1	H	1097	ILE	N-CA-C	7.28	119.31	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1059	ARG	N-CA-C	-7.05	104.49	113.23
1	B	1091	VAL	CB-CA-C	-6.68	101.95	111.31
1	B	1062	ASP	N-CA-C	6.65	118.18	111.07
1	O	1078	LEU	N-CA-C	-6.39	106.06	114.31
1	J	1097	ILE	N-CA-C	6.35	117.94	108.54
1	A	1097	ILE	N-CA-C	6.32	117.90	108.23
1	D	1057	ARG	N-CA-C	-6.31	104.40	111.28
1	G	1059	ARG	N-CA-C	-6.29	104.66	112.90
1	I	1089	VAL	N-CA-C	6.20	118.09	109.29
1	C	1061	TYR	N-CA-C	6.12	118.74	111.33
1	E	1097	ILE	N-CA-C	6.09	117.34	108.58
1	I	1096	ALA	N-CA-C	-6.06	99.47	108.99
1	D	1097	ILE	N-CA-C	6.01	116.78	108.84
1	J	1090	TYR	N-CA-C	5.92	118.87	109.81
1	E	1057	ARG	N-CA-C	-5.90	104.92	111.71
1	J	1071	MSE	N-CA-C	5.87	118.43	111.33
1	O	1086	TRP	CB-CA-C	-5.81	99.07	110.10
1	I	1097	ILE	N-CA-C	5.81	116.47	107.99
1	M	1089	VAL	N-CA-C	5.69	115.77	108.82
1	E	1103	ASP	CA-C-N	5.66	125.67	119.90
1	E	1103	ASP	C-N-CA	5.66	125.67	119.90
1	E	1112	VAL	N-CA-C	5.57	116.24	108.89
1	E	1078	LEU	N-CA-C	-5.50	107.58	114.56
1	G	1108	PHE	N-CA-C	5.47	117.67	111.11
1	G	1071	MSE	N-CA-C	5.46	118.73	111.75
1	O	1079	GLU	CB-CA-C	5.39	120.61	110.63
1	O	1065	ARG	N-CA-C	5.38	116.83	111.07
1	L	1117	ILE	N-CA-C	5.37	115.05	106.88
1	O	1041	THR	N-CA-C	5.31	117.05	108.34
1	N	1097	ILE	N-CA-C	5.30	116.34	108.23
1	E	1071	MSE	N-CA-C	5.29	118.52	111.75
1	L	1109	VAL	N-CA-C	5.27	118.44	111.17
1	H	1071	MSE	N-CA-C	5.26	118.48	111.75
1	A	1087	LYS	CA-C-N	-5.25	115.55	122.85
1	A	1087	LYS	C-N-CA	-5.25	115.55	122.85
1	F	1061	TYR	N-CA-C	5.22	116.97	111.28
1	G	1089	VAL	CB-CA-C	-5.19	103.77	111.19
1	J	1103	ASP	CA-C-N	5.18	125.17	119.89
1	J	1103	ASP	C-N-CA	5.18	125.17	119.89
1	B	1112	VAL	N-CA-C	5.16	115.69	108.89
1	A	1089	VAL	O-C-N	-5.12	117.92	122.69
1	F	1068	LEU	N-CA-C	5.10	117.23	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1049	VAL	N-CA-C	-5.08	103.03	109.58
1	J	1086	TRP	CB-CA-C	-5.05	100.51	110.10
1	M	1086	TRP	CB-CA-C	-5.04	100.52	110.10
1	O	1095	ASN	N-CA-C	5.03	118.89	112.26
1	G	1053	ILE	CA-C-N	-5.02	115.75	122.42
1	G	1053	ILE	C-N-CA	-5.02	115.75	122.42

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	620	0	606	37	0
1	B	631	0	618	55	0
1	C	650	0	632	8	0
1	D	568	0	563	10	0
1	E	633	0	616	8	0
1	F	653	0	636	16	0
1	G	629	0	621	13	0
1	H	616	0	610	11	0
1	I	638	0	627	25	0
1	J	599	0	593	11	0
1	K	607	0	593	14	0
1	L	567	0	567	5	0
1	M	585	0	580	7	0
1	N	550	0	551	15	0
1	O	650	0	632	13	0
1	P	626	0	609	8	0
All	All	9822	0	9654	219	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.

All (219) 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:1059:ARG:HG3	1:B:1095:ASN:CB	1.35	1.51
1:A:1059:ARG:CG	1:B:1095:ASN:HB3	1.57	1.31
1:A:1059:ARG:HG3	1:B:1095:ASN:CG	1.63	1.20
1:A:1105:TRP:CB	1:B:1094:GLU:HG2	1.73	1.19
1:B:1120:SER:O	1:B:1123:VAL:HG22	1.46	1.16
1:A:1105:TRP:HB2	1:B:1094:GLU:HG2	1.27	1.11
1:A:1059:ARG:HB2	1:B:1095:ASN:ND2	1.76	1.01
1:B:1119:SER:OG	1:B:1122:GLU:HG3	1.60	1.00
1:A:1059:ARG:CB	1:B:1095:ASN:ND2	2.25	0.99
1:A:1059:ARG:CA	1:B:1095:ASN:HD22	1.75	0.98
1:A:1059:ARG:CG	1:B:1095:ASN:CB	2.27	0.97
1:N:1123:VAL:O	1:N:1126:MSE:HG3	1.64	0.96
1:A:1059:ARG:HA	1:B:1095:ASN:HD22	1.27	0.96
1:I:1065:ARG:HG3	1:I:1065:ARG:HH11	1.29	0.95
1:A:1059:ARG:CG	1:B:1095:ASN:CG	2.40	0.94
1:I:1124:GLN:C	1:I:1125:GLN:HG3	1.97	0.89
1:B:1090:TYR:CE1	1:B:1098:LEU:HB2	2.08	0.88
1:A:1105:TRP:HB3	1:B:1094:GLU:HG2	1.54	0.85
1:A:1059:ARG:HG3	1:B:1095:ASN:HB3	0.87	0.85
1:G:1124:GLN:OE1	1:G:1124:GLN:N	2.11	0.83
1:B:1120:SER:O	1:B:1123:VAL:CG2	2.27	0.82
1:I:1079:GLU:N	1:I:1079:GLU:OE1	2.14	0.80
1:I:1124:GLN:OE1	1:I:1125:GLN:CG	2.30	0.79
1:B:1123:VAL:O	1:B:1124:GLN:CG	2.30	0.79
1:J:1075:GLU:CD	1:J:1075:GLU:H	1.92	0.78
1:A:1059:ARG:CB	1:B:1095:ASN:HD22	1.91	0.78
1:A:1059:ARG:HG2	1:B:1095:ASN:HB3	1.66	0.75
1:I:1065:ARG:HG3	1:I:1065:ARG:NH1	1.99	0.74
1:I:1124:GLN:O	1:I:1125:GLN:CD	2.30	0.74
1:B:1123:VAL:O	1:B:1124:GLN:CD	2.30	0.74
1:N:1120:SER:O	1:N:1124:GLN:HG2	1.87	0.73
1:M:1067:ASP:OD1	1:M:1070:ARG:NH2	2.22	0.73
1:E:1079:GLU:OE1	1:E:1079:GLU:N	2.22	0.73
1:B:1121:ALA:C	1:B:1123:VAL:H	1.97	0.72
1:A:1067:ASP:OD1	1:A:1070:ARG:NH2	2.22	0.72
1:O:1067:ASP:OD1	1:O:1070:ARG:NH2	2.22	0.72
1:D:1088:LEU:HD23	1:D:1100:VAL:HB	1.71	0.72
1:A:1106:GLU:HG3	1:B:1113:GLN:HE22	1.55	0.71
1:C:1070:ARG:HA	1:C:1075:GLU:HG3	1.72	0.71
1:E:1091:VAL:HG12	1:E:1092:ALA:H	1.56	0.70
1:N:1067:ASP:OD1	1:N:1070:ARG:NH2	2.24	0.69
1:A:1106:GLU:CG	1:B:1113:GLN:HE22	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1067:ASP:OD1	1:L:1070:ARG:NH2	2.27	0.68
1:I:1124:GLN:C	1:I:1125:GLN:CG	2.67	0.68
1:B:1121:ALA:O	1:B:1123:VAL:N	2.27	0.68
1:F:1067:ASP:OD1	1:F:1070:ARG:NH2	2.27	0.67
1:K:1089:VAL:HB	1:K:1097:ILE:CG2	2.25	0.66
1:B:1123:VAL:O	1:B:1124:GLN:CB	2.42	0.66
1:H:1103:ASP:OD1	1:H:1103:ASP:N	2.30	0.65
1:F:1079:GLU:O	1:F:1080:ASP:OD1	2.15	0.65
1:A:1078:LEU:C	1:A:1079:GLU:OE2	2.41	0.64
1:F:1079:GLU:N	1:F:1079:GLU:OE1	2.30	0.64
1:I:1124:GLN:OE1	1:I:1125:GLN:HG3	1.98	0.64
1:J:1075:GLU:OE1	1:J:1075:GLU:N	2.30	0.64
1:P:1079:GLU:N	1:P:1079:GLU:OE1	2.30	0.64
1:I:1124:GLN:OE1	1:I:1125:GLN:NE2	2.30	0.64
1:A:1059:ARG:N	1:A:1063:GLU:OE1	2.28	0.63
1:B:1095:ASN:OD1	1:B:1095:ASN:O	2.15	0.63
1:K:1119:SER:OG	1:K:1122:GLU:HG3	1.98	0.63
1:I:1070:ARG:HA	1:I:1075:GLU:HG3	1.81	0.63
1:I:1124:GLN:O	1:I:1125:GLN:CG	2.48	0.62
1:P:1067:ASP:OD1	1:P:1070:ARG:NH2	2.34	0.61
1:A:1106:GLU:CD	1:B:1113:GLN:HE22	2.09	0.61
1:F:1065:ARG:HG3	1:F:1065:ARG:HH11	1.66	0.61
1:N:1124:GLN:C	1:N:1125:GLN:HG2	2.24	0.61
1:A:1059:ARG:HA	1:B:1095:ASN:ND2	2.08	0.60
1:A:1086:TRP:CE3	1:A:1086:TRP:HA	2.37	0.60
1:A:1059:ARG:CG	1:B:1095:ASN:ND2	2.62	0.60
1:G:1067:ASP:OD1	1:G:1070:ARG:NH2	2.33	0.60
1:F:1069:ALA:HB2	1:F:1078:LEU:HB2	1.83	0.60
1:A:1106:GLU:OE2	1:B:1113:GLN:NE2	2.34	0.59
1:N:1124:GLN:OE1	1:N:1124:GLN:HA	2.01	0.59
1:D:1102:ASP:OD2	1:E:1052:SER:N	2.31	0.59
1:C:1107:GLU:OE2	1:P:1039:THR:HG22	2.03	0.59
1:H:1122:GLU:HA	1:H:1125:GLN:HG2	1.84	0.59
1:F:1065:ARG:HG3	1:F:1065:ARG:NH1	2.18	0.58
1:N:1123:VAL:C	1:N:1126:MSE:HG3	2.27	0.58
1:N:1123:VAL:HA	1:N:1126:MSE:CG	2.32	0.58
1:A:1105:TRP:CB	1:B:1094:GLU:CG	2.66	0.58
1:J:1090:TYR:CE1	1:J:1098:LEU:HB2	2.38	0.58
1:K:1085:ASP:N	1:K:1085:ASP:OD1	2.36	0.58
1:F:1065:ARG:HD3	1:F:1078:LEU:O	2.03	0.58
1:M:1090:TYR:CE1	1:M:1098:LEU:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:TYR:CE2	1:B:1092:ALA:HB2	2.39	0.58
1:P:1060:GLY:HA2	1:P:1105:TRP:CD2	2.39	0.58
1:B:1090:TYR:CE1	1:B:1098:LEU:CB	2.87	0.57
1:O:1090:TYR:CE1	1:O:1098:LEU:HB2	2.40	0.57
1:I:1123:VAL:O	1:I:1126:MSE:HG2	2.05	0.56
1:A:1105:TRP:HB3	1:B:1094:GLU:CG	2.31	0.56
1:J:1120:SER:O	1:J:1123:VAL:HG23	2.05	0.56
1:P:1045:LYS:HE2	1:P:1086:TRP:CH2	2.40	0.56
1:M:1057:ARG:NH1	1:O:1080:ASP:OD1	2.39	0.55
1:H:1040:TYR:CE1	1:H:1054:ASP:HB2	2.42	0.55
1:G:1074:ILE:O	1:G:1074:ILE:HG13	2.07	0.55
1:H:1067:ASP:OD1	1:H:1070:ARG:NH2	2.40	0.54
1:F:1090:TYR:CE1	1:F:1098:LEU:HB2	2.42	0.54
1:G:1123:VAL:HG12	1:G:1126:MSE:SE	2.57	0.54
1:B:1090:TYR:HB3	1:B:1100:VAL:HG22	1.89	0.54
1:F:1040:TYR:HB3	1:F:1052:SER:HB3	1.89	0.53
1:A:1086:TRP:HA	1:A:1086:TRP:HE3	1.73	0.53
1:H:1051:ARG:NH1	1:L:1102:ASP:OD1	2.42	0.53
1:G:1119:SER:OG	1:G:1122:GLU:HG3	2.08	0.53
1:N:1119:SER:OG	1:N:1122:GLU:HG3	2.09	0.53
1:K:1089:VAL:HB	1:K:1097:ILE:HG21	1.90	0.53
1:E:1091:VAL:HG12	1:E:1092:ALA:N	2.24	0.53
1:A:1078:LEU:C	1:A:1079:GLU:CD	2.77	0.52
1:O:1119:SER:OG	1:O:1122:GLU:HG3	2.10	0.52
1:I:1065:ARG:NH1	1:I:1065:ARG:CG	2.70	0.52
1:G:1058:TYR:OH	1:G:1067:ASP:OD2	2.24	0.52
1:G:1074:ILE:C	1:G:1077:GLN:HG3	2.35	0.52
1:I:1124:GLN:OE1	1:I:1125:GLN:HG2	2.10	0.51
1:K:1067:ASP:OD1	1:K:1070:ARG:NH2	2.43	0.51
1:B:1107:GLU:OE2	1:K:1039:THR:HG22	2.11	0.51
1:B:1067:ASP:OD1	1:B:1070:ARG:NH2	2.43	0.51
1:B:1090:TYR:OH	1:B:1098:LEU:HD12	2.11	0.51
1:F:1089:VAL:HB	1:F:1097:ILE:HG23	1.93	0.51
1:I:1091:VAL:O	1:I:1092:ALA:C	2.53	0.51
1:A:1078:LEU:O	1:A:1079:GLU:CD	2.54	0.51
1:G:1074:ILE:HB	1:G:1077:GLN:HG3	1.92	0.50
1:P:1059:ARG:N	1:P:1063:GLU:OE1	2.32	0.50
1:G:1074:ILE:O	1:G:1077:GLN:HG3	2.11	0.50
1:O:1060:GLY:HA2	1:O:1105:TRP:CD2	2.46	0.50
1:A:1078:LEU:O	1:A:1079:GLU:OE2	2.30	0.49
1:N:1091:VAL:CG2	1:N:1114:SER:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1058:TYR:OH	1:D:1067:ASP:OD2	2.24	0.49
1:I:1124:GLN:O	1:I:1125:GLN:HG3	2.12	0.49
1:L:1119:SER:OG	1:L:1122:GLU:HG3	2.13	0.49
1:I:1124:GLN:O	1:I:1125:GLN:OE1	2.30	0.49
1:J:1120:SER:O	1:J:1123:VAL:CG2	2.60	0.49
1:I:1040:TYR:CE1	1:I:1054:ASP:HB2	2.47	0.48
1:A:1060:GLY:HA2	1:A:1105:TRP:CD2	2.47	0.48
1:B:1123:VAL:O	1:B:1124:GLN:OE1	2.30	0.48
1:A:1123:VAL:HG11	1:O:1049:VAL:HG23	1.95	0.48
1:O:1090:TYR:HD1	1:O:1090:TYR:H	1.60	0.48
1:A:1119:SER:OG	1:A:1122:GLU:HG3	2.13	0.48
1:I:1119:SER:OG	1:I:1122:GLU:HG3	2.14	0.48
1:A:1123:VAL:HG11	1:O:1049:VAL:CG2	2.44	0.48
1:G:1060:GLY:HA2	1:G:1105:TRP:CD2	2.49	0.48
1:F:1091:VAL:HB	1:F:1114:SER:HB3	1.96	0.47
1:E:1119:SER:OG	1:E:1122:GLU:HG3	2.14	0.47
1:J:1050:GLY:HA3	1:O:1098:LEU:HD23	1.96	0.47
1:C:1121:ALA:HA	1:C:1124:GLN:HB2	1.96	0.47
1:H:1091:VAL:CG2	1:H:1114:SER:HB3	2.44	0.47
1:K:1090:TYR:CE1	1:K:1098:LEU:HB2	2.50	0.47
1:C:1075:GLU:OE1	1:C:1075:GLU:N	2.30	0.47
1:I:1123:VAL:HA	1:I:1126:MSE:SE	2.65	0.47
1:G:1123:VAL:HA	1:G:1126:MSE:CG	2.45	0.47
1:B:1093:HIS:HA	1:B:1094:GLU:HA	1.49	0.46
1:N:1124:GLN:C	1:N:1125:GLN:CG	2.88	0.46
1:B:1090:TYR:CZ	1:B:1098:LEU:HD12	2.51	0.46
1:B:1123:VAL:O	1:B:1124:GLN:HB2	2.15	0.46
1:K:1097:ILE:CG2	1:K:1098:LEU:N	2.78	0.46
1:O:1091:VAL:HA	1:O:1096:ALA:O	2.15	0.46
1:P:1039:THR:HG23	1:P:1040:TYR:HD1	1.81	0.46
1:B:1121:ALA:C	1:B:1123:VAL:N	2.64	0.46
1:G:1089:VAL:HG23	1:G:1116:LYS:HB2	1.98	0.46
1:H:1088:LEU:HG	1:H:1100:VAL:HG21	1.98	0.46
1:J:1119:SER:OG	1:J:1122:GLU:HG3	2.16	0.45
1:A:1106:GLU:HG3	1:B:1113:GLN:NE2	2.28	0.45
1:B:1045:LYS:HE2	1:B:1086:TRP:CH2	2.52	0.45
1:F:1079:GLU:O	1:F:1080:ASP:CG	2.60	0.45
1:A:1102:ASP:HB3	1:O:1052:SER:HB2	1.99	0.45
1:J:1069:ALA:HB1	1:J:1075:GLU:HA	1.98	0.45
1:O:1090:TYR:CD1	1:O:1090:TYR:N	2.85	0.45
1:B:1107:GLU:OE2	1:K:1039:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1095:ASN:O	1:D:1095:ASN:CG	2.61	0.44
1:K:1097:ILE:O	1:K:1098:LEU:HD23	2.17	0.44
1:C:1119:SER:OG	1:C:1122:GLU:HG3	2.17	0.44
1:B:1040:TYR:CE1	1:B:1054:ASP:HB2	2.52	0.44
1:D:1119:SER:OG	1:D:1122:GLU:HG3	2.17	0.44
1:B:1088:LEU:O	1:B:1099:LEU:HD12	2.18	0.44
1:H:1040:TYR:HB3	1:H:1041:THR:H	1.67	0.44
1:K:1091:VAL:CG1	1:K:1092:ALA:O	2.66	0.44
1:M:1045:LYS:HE2	1:M:1086:TRP:CH2	2.52	0.44
1:B:1123:VAL:O	1:B:1124:GLN:HG3	2.14	0.44
1:F:1061:TYR:CZ	1:F:1101:GLY:HA2	2.52	0.44
1:M:1119:SER:OG	1:M:1122:GLU:HG3	2.17	0.44
1:B:1093:HIS:O	1:B:1093:HIS:ND1	2.51	0.44
1:I:1064:LEU:HD12	1:I:1064:LEU:HA	1.78	0.43
1:B:1090:TYR:HE2	1:B:1092:ALA:HB2	1.83	0.43
1:D:1067:ASP:OD1	1:D:1070:ARG:NH2	2.51	0.43
1:I:1065:ARG:HH11	1:I:1065:ARG:CG	2.10	0.43
1:E:1067:ASP:OD1	1:E:1070:ARG:NH2	2.51	0.43
1:D:1060:GLY:HA2	1:D:1105:TRP:CD2	2.53	0.43
1:F:1065:ARG:HH11	1:F:1065:ARG:CG	2.32	0.43
1:C:1079:GLU:OE1	1:C:1079:GLU:N	2.52	0.43
1:D:1043:VAL:HA	1:D:1115:ILE:O	2.18	0.43
1:K:1064:LEU:HA	1:K:1064:LEU:HD12	1.61	0.43
1:N:1091:VAL:HG23	1:N:1114:SER:HB3	2.01	0.43
1:H:1089:VAL:HB	1:H:1097:ILE:HG23	2.00	0.43
1:H:1091:VAL:HG23	1:H:1114:SER:HB3	2.01	0.43
1:J:1043:VAL:HG22	1:J:1115:ILE:HB	2.01	0.42
1:J:1064:LEU:HD12	1:J:1064:LEU:HA	1.68	0.42
1:B:1040:TYR:HB3	1:B:1041:THR:H	1.77	0.42
1:F:1065:ARG:CD	1:F:1078:LEU:O	2.67	0.42
1:B:1047:GLY:HA2	1:N:1126:MSE:HB2	2.02	0.42
1:B:1051:ARG:NH1	1:N:1102:ASP:OD1	2.53	0.42
1:D:1123:VAL:HG11	1:E:1049:VAL:HG23	2.01	0.42
1:J:1078:LEU:HD23	1:J:1078:LEU:HA	1.81	0.42
1:N:1123:VAL:HA	1:N:1126:MSE:HG2	2.00	0.42
1:D:1059:ARG:N	1:D:1063:GLU:OE1	2.38	0.42
1:C:1088:LEU:HD12	1:C:1088:LEU:HA	1.38	0.42
1:F:1097:ILE:HD12	1:F:1126:MSE:HE3	2.00	0.41
1:M:1087:LYS:HA	1:M:1087:LYS:HD3	1.90	0.41
1:L:1041:THR:O	1:L:1052:SER:HA	2.19	0.41
1:L:1043:VAL:HG22	1:L:1115:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1105:TRP:O	1:P:1108:PHE:HB3	2.21	0.41
1:H:1078:LEU:HD23	1:H:1078:LEU:HA	1.82	0.41
1:I:1124:GLN:OE1	1:I:1125:GLN:CD	2.64	0.41
1:O:1078:LEU:HD23	1:O:1078:LEU:HA	1.79	0.41
1:C:1122:GLU:O	1:C:1126:MSE:HG3	2.21	0.41
1:I:1045:LYS:HE2	1:I:1086:TRP:CH2	2.56	0.41
1:I:1099:LEU:HD12	1:I:1099:LEU:HA	1.91	0.41
1:M:1043:VAL:HA	1:M:1115:ILE:O	2.21	0.41
1:N:1105:TRP:O	1:N:1108:PHE:HB3	2.21	0.40
1:G:1089:VAL:HB	1:G:1097:ILE:HG23	2.03	0.40
1:E:1061:TYR:CZ	1:E:1101:GLY:HA2	2.56	0.40
1:K:1097:ILE:HG22	1:K:1098:LEU:N	2.36	0.40
1:K:1086:TRP:CZ3	1:K:1119:SER:HB3	2.56	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	71/95 (75%)	69 (97%)	2 (3%)	0	100	100
1	B	74/95 (78%)	71 (96%)	2 (3%)	1 (1%)	9	36
1	C	74/95 (78%)	73 (99%)	1 (1%)	0	100	100
1	D	64/95 (67%)	64 (100%)	0	0	100	100
1	E	73/95 (77%)	72 (99%)	1 (1%)	0	100	100
1	F	75/95 (79%)	74 (99%)	1 (1%)	0	100	100
1	G	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
1	H	70/95 (74%)	68 (97%)	2 (3%)	0	100	100
1	I	73/95 (77%)	69 (94%)	4 (6%)	0	100	100
1	J	68/95 (72%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	71/95 (75%)	71 (100%)	0	0	100	100
1	L	65/95 (68%)	64 (98%)	1 (2%)	0	100	100
1	M	66/95 (70%)	65 (98%)	1 (2%)	0	100	100
1	N	61/95 (64%)	60 (98%)	1 (2%)	0	100	100
1	O	74/95 (78%)	72 (97%)	2 (3%)	0	100	100
1	P	73/95 (77%)	72 (99%)	1 (1%)	0	100	100
All	All	1124/1520 (74%)	1101 (98%)	22 (2%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1122	GLU

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	66/79 (84%)	60 (91%)	6 (9%)	9	33
1	B	67/79 (85%)	58 (87%)	9 (13%)	4	18
1	C	70/79 (89%)	67 (96%)	3 (4%)	26	60
1	D	61/79 (77%)	57 (93%)	4 (7%)	15	46
1	E	68/79 (86%)	62 (91%)	6 (9%)	9	35
1	F	70/79 (89%)	64 (91%)	6 (9%)	10	36
1	G	67/79 (85%)	63 (94%)	4 (6%)	17	50
1	H	66/79 (84%)	63 (96%)	3 (4%)	24	59
1	I	68/79 (86%)	62 (91%)	6 (9%)	9	35
1	J	64/79 (81%)	58 (91%)	6 (9%)	8	32
1	K	65/79 (82%)	61 (94%)	4 (6%)	16	49
1	L	61/79 (77%)	56 (92%)	5 (8%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	63/79 (80%)	60 (95%)	3 (5%)	23	57
1	N	60/79 (76%)	56 (93%)	4 (7%)	15	46
1	O	70/79 (89%)	65 (93%)	5 (7%)	13	43
1	P	67/79 (85%)	61 (91%)	6 (9%)	9	34
All	All	1053/1264 (83%)	973 (92%)	80 (8%)	12	41

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1051	ARG
1	A	1070	ARG
1	A	1080	ASP
1	A	1086	TRP
1	A	1091	VAL
1	A	1123	VAL
1	B	1051	ARG
1	B	1057	ARG
1	B	1070	ARG
1	B	1089	VAL
1	B	1093	HIS
1	B	1094	GLU
1	B	1103	ASP
1	B	1109	VAL
1	B	1120	SER
1	C	1051	ARG
1	C	1070	ARG
1	C	1109	VAL
1	D	1051	ARG
1	D	1057	ARG
1	D	1070	ARG
1	D	1103	ASP
1	E	1051	ARG
1	E	1057	ARG
1	E	1070	ARG
1	E	1085	ASP
1	E	1091	VAL
1	E	1123	VAL
1	F	1039	THR
1	F	1051	ARG
1	F	1057	ARG
1	F	1063	GLU

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Mol	Chain	Res	Type
1	F	1070	ARG
1	F	1103	ASP
1	G	1051	ARG
1	G	1057	ARG
1	G	1070	ARG
1	G	1109	VAL
1	H	1051	ARG
1	H	1070	ARG
1	H	1103	ASP
1	I	1055	VAL
1	I	1063	GLU
1	I	1065	ARG
1	I	1070	ARG
1	I	1079	GLU
1	I	1125	GLN
1	J	1051	ARG
1	J	1075	GLU
1	J	1089	VAL
1	J	1103	ASP
1	J	1123	VAL
1	J	1124	GLN
1	K	1051	ARG
1	K	1070	ARG
1	K	1093	HIS
1	K	1103	ASP
1	L	1051	ARG
1	L	1070	ARG
1	L	1091	VAL
1	L	1123	VAL
1	L	1124	GLN
1	M	1051	ARG
1	M	1055	VAL
1	M	1070	ARG
1	N	1070	ARG
1	N	1091	VAL
1	N	1103	ASP
1	N	1125	GLN
1	O	1051	ARG
1	O	1057	ARG
1	O	1070	ARG
1	O	1090	TYR
1	O	1094	GLU

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Mol	Chain	Res	Type
1	P	1051	ARG
1	P	1057	ARG
1	P	1079	GLU
1	P	1080	ASP
1	P	1089	VAL
1	P	1095	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1110	ASN
1	B	1095	ASN
1	B	1113	GLN
1	C	1124	GLN
1	D	1066	HIS
1	E	1113	GLN
1	F	1113	GLN
1	G	1056	ASN
1	G	1066	HIS
1	H	1110	ASN
1	J	1124	GLN
1	O	1066	HIS
1	O	1124	GLN
1	P	1044	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	76/95 (80%)	0.14	1 (1%) 75 53	43, 71, 121, 148	0
1	B	77/95 (81%)	0.10	3 (3%) 43 24	40, 71, 118, 125	0
1	C	78/95 (82%)	-0.06	1 (1%) 75 53	41, 69, 120, 169	0
1	D	69/95 (72%)	0.09	1 (1%) 73 51	42, 81, 123, 144	0
1	E	78/95 (82%)	0.03	2 (2%) 57 34	45, 73, 123, 134	0
1	F	79/95 (83%)	0.10	1 (1%) 75 53	46, 79, 122, 148	0
1	G	76/95 (80%)	0.00	0 100 100	46, 81, 122, 170	0
1	H	74/95 (77%)	0.09	0 100 100	50, 77, 137, 154	0
1	I	77/95 (81%)	0.10	1 (1%) 75 53	55, 81, 146, 161	0
1	J	73/95 (76%)	0.04	1 (1%) 73 51	45, 81, 128, 165	0
1	K	74/95 (77%)	0.24	2 (2%) 56 33	39, 82, 138, 143	0
1	L	70/95 (73%)	0.30	4 (5%) 29 15	52, 91, 144, 228	0
1	M	71/95 (74%)	0.14	2 (2%) 55 32	45, 91, 135, 161	0
1	N	67/95 (70%)	0.41	2 (2%) 52 30	52, 94, 173, 213	0
1	O	78/95 (82%)	-0.07	1 (1%) 75 53	49, 74, 124, 150	0
1	P	76/95 (80%)	0.06	1 (1%) 75 53	49, 79, 128, 149	0
All	All	1193/1520 (78%)	0.10	23 (1%) 66 43	39, 79, 134, 228	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1096	ALA	3.9
1	P	1119	SER	3.8
1	L	1092	ALA	3.7
1	B	1095	ASN	3.3
1	K	1057	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	1123	VAL	3.0
1	M	1078	LEU	2.8
1	D	1106	GLU	2.7
1	K	1123	VAL	2.7
1	L	1096	ALA	2.7
1	C	1094	GLU	2.6
1	B	1093	HIS	2.6
1	F	1040	TYR	2.6
1	O	1113	GLN	2.5
1	L	1074	ILE	2.5
1	N	1113	GLN	2.4
1	I	1066	HIS	2.3
1	N	1042	ALA	2.3
1	B	1124	GLN	2.3
1	A	1123	VAL	2.3
1	L	1068	LEU	2.2
1	M	1123	VAL	2.1
1	E	1096	ALA	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.