



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:07 AM UTC

PDB ID : 4NJ6 / pdb_00004nj6
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 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
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

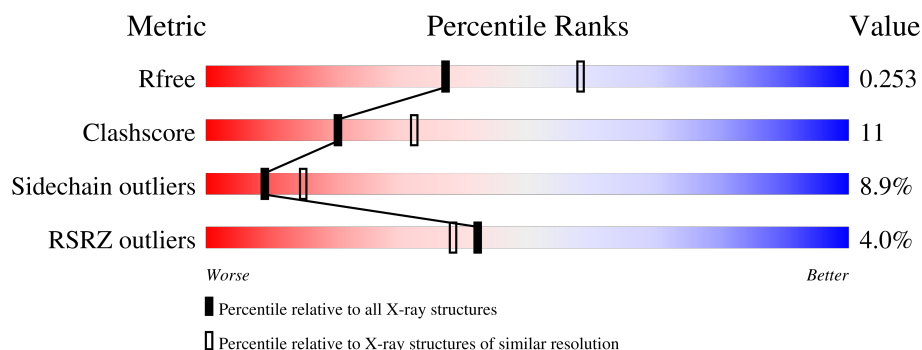
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



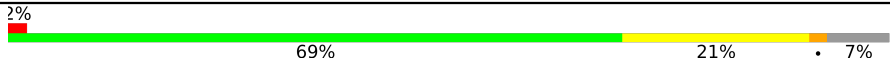
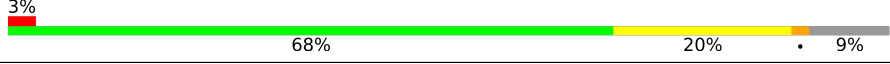
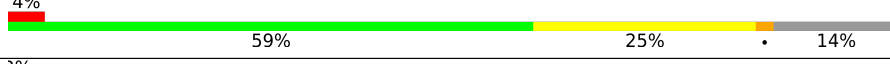
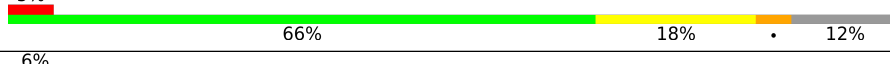
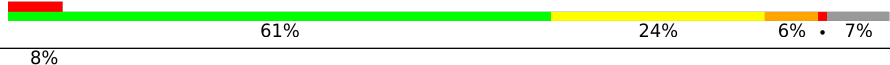
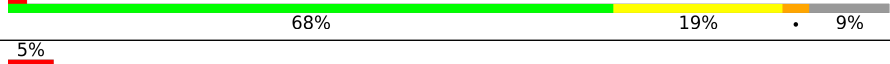
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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	4% 71% 20% • 7%
1	B	95	3% 68% 20% 5% 6%
1	C	95	2% 66% 23% • 6%
1	D	95	% 73% 18% • 7%
1	E	95	3% 75% 15% 11%
1	F	95	2% 72% 19% • 6%

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Mol	Chain	Length	Quality of chain
1	G	95	
1	H	95	
1	I	95	
1	J	95	
1	K	95	
1	L	95	
1	M	95	
1	N	95	
1	O	95	
1	P	95	

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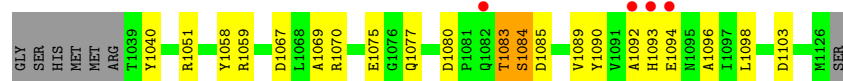
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	24	Total 24	O 24	0	0
2	G	38	Total 38	O 38	0	0
2	H	24	Total 24	O 24	0	0
2	I	27	Total 27	O 27	0	0
2	J	24	Total 24	O 24	0	0
2	K	43	Total 43	O 43	0	0
2	L	31	Total 31	O 31	0	0
2	M	17	Total 17	O 17	0	0
2	N	16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

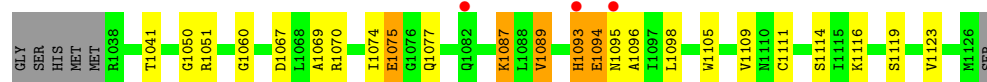
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

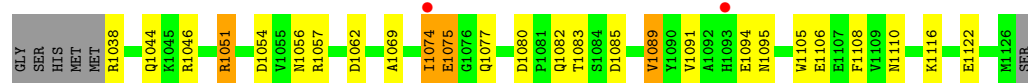
- Molecule 1: Auxin response factor 7



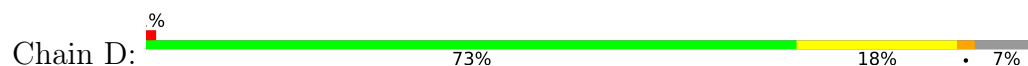
- Molecule 1: Auxin response factor 7



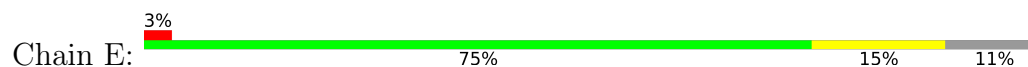
- Molecule 1: Auxin response factor 7



- Molecule 1: Auxin response factor 7



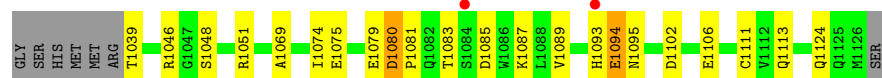
- Molecule 1: Auxin response factor 7



● Molecule 1: Auxin response factor 7



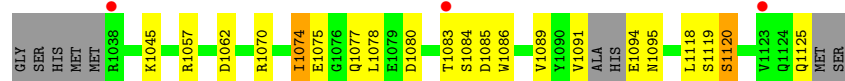
● Molecule 1: Auxin response factor 7



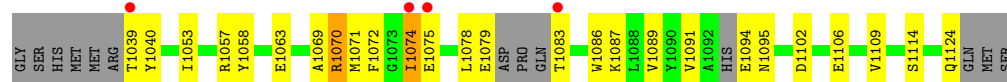
● Molecule 1: Auxin response factor 7



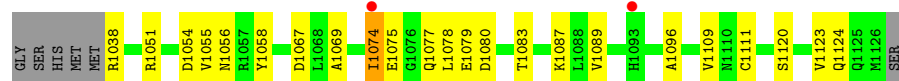
● Molecule 1: Auxin response factor 7



● Molecule 1: Auxin response factor 7

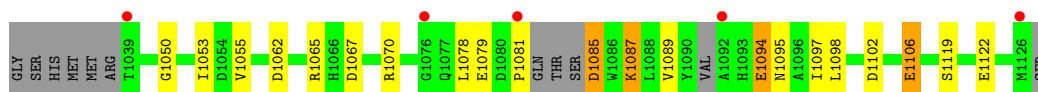


● Molecule 1: Auxin response factor 7

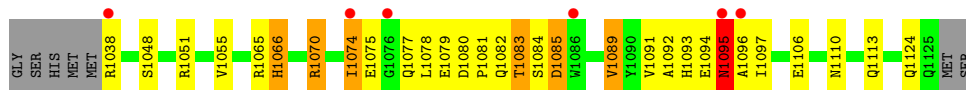


● Molecule 1: Auxin response factor 7

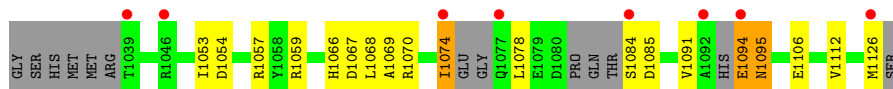




- Molecule 1: Auxin response factor 7



- 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 33.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.65-2.40) 94.2 (33.65-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.209 , 0.271 (Not available) , 0.253	Depositor DCC
R_{free} test set	1949 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for $-2/3^*h-1/3^*k+2/3^*l, -1/3^*h-2/3^*k-2/3^*l, 2/3^*h-2/3^*k+1/3^*l$ 0.016 for $-h, 1/3^*h-1/3^*k+2/3^*l, 2/3^*h+4/3^*k+1/3^*l$ 0.018 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 4.14% 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	0.65	0/722	0.96	3/977 (0.3%)
1	B	0.60	0/733	0.95	2/991 (0.2%)
1	C	0.55	0/733	0.92	2/991 (0.2%)
1	D	0.57	0/722	0.87	0/977
1	E	0.57	0/695	0.88	0/939
1	F	0.50	0/728	0.87	0/985
1	G	0.55	0/722	0.99	3/977 (0.3%)
1	H	0.50	0/710	0.92	0/959
1	I	0.57	0/708	0.84	0/956
1	J	0.47	0/667	0.87	0/899
1	K	0.54	0/733	0.89	0/991
1	L	0.52	0/691	0.86	0/931
1	M	0.58	0/725	0.91	2/981 (0.2%)
1	N	0.45	0/671	0.83	1/902 (0.1%)
1	O	0.57	0/703	0.85	0/949
1	P	0.52	0/710	0.88	0/959
All	All	0.55	0/11373	0.89	13/15364 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1094	GLU	N-CA-C	-7.08	103.74	112.38
1	G	1080	ASP	CA-C-N	6.70	128.22	119.84
1	G	1080	ASP	C-N-CA	6.70	128.22	119.84
1	A	1103	ASP	CA-C-N	-6.68	113.42	120.03
1	A	1103	ASP	C-N-CA	-6.68	113.42	120.03
1	C	1080	ASP	CA-C-N	6.00	126.43	119.47
1	C	1080	ASP	C-N-CA	6.00	126.43	119.47
1	A	1090	TYR	N-CA-C	5.87	118.10	109.24
1	M	1095	ASN	CB-CA-C	-5.73	109.99	116.63
1	B	1119	SER	N-CA-C	-5.61	103.12	110.53
1	N	1112	VAL	N-CA-C	5.60	116.49	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1055	VAL	N-CA-C	5.40	116.78	110.62
1	G	1085	ASP	N-CA-C	-5.33	106.55	113.16

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	709	0	684	13	0
1	B	720	0	697	15	0
1	C	720	0	697	17	0
1	D	709	0	684	17	0
1	E	684	0	660	11	0
1	F	715	0	689	12	0
1	G	709	0	684	14	0
1	H	699	0	676	18	0
1	I	697	0	675	21	0
1	J	658	0	639	20	0
1	K	720	0	697	23	0
1	L	680	0	653	11	0
1	M	712	0	688	33	0
1	N	663	0	643	9	0
1	O	692	0	669	9	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	247	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 (247) 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:HG13	1:J:1074:ILE:O	1.41	1.17
1:K:1074:ILE:HG12	1:K:1074:ILE:O	1.41	1.14
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
1:D:1093:HIS:C	1:D:1094:GLU:HG2	1.96	0.90
1:B:1094:GLU:O	1:B:1095:ASN:HB2	1.72	0.88
1:G:1111:CYS:HB3	2:G:1234:HOH:O	1.74	0.87
1:K:1074:ILE:HD11	1:K:1077:GLN:HB2	1.57	0.87
1:K:1074:ILE:CD1	1:K:1077:GLN:HB2	2.06	0.86
1:I:1070:ARG:HG2	1:I:1075:GLU:CD	2.00	0.85
1:H:1066:HIS:HB3	2:H:1218:HOH:O	1.76	0.85
1:M:1077:GLN:O	1:M:1084:SER:HB2	1.79	0.82
1:G:1093:HIS:CE1	1:G:1113:GLN:CD	2.60	0.79
1:P:1080:ASP:O	1:P:1083:THR:CG2	2.30	0.79
1:P:1080:ASP:O	1:P:1083:THR:HG23	1.83	0.78
1:K:1074:ILE:HG12	1:K:1077:GLN:HB2	1.66	0.78
1:L:1094:GLU:O	1:L:1095:ASN:HB2	1.83	0.78
1:J:1074:ILE:O	1:J:1074:ILE:CG1	2.30	0.76
1:D:1083:THR:HG22	1:D:1085:ASP:H	1.51	0.75
1:M:1094:GLU:C	1:M:1095:ASN:OD1	2.31	0.74
1:B:1087:LYS:HD2	1:B:1123:VAL:HG21	1.68	0.74
1:J:1074:ILE:HD11	1:J:1078:LEU:HD21	1.68	0.74
1:B:1093:HIS:CD2	1:B:1093:HIS:H	2.07	0.73
1:C:1074:ILE:HG23	1:C:1077:GLN:HB2	1.71	0.72
1:D:1093:HIS:O	1:D:1094:GLU:CG	2.36	0.72
1:C:1074:ILE:HG23	1:C:1074:ILE:O	1.87	0.72
1:J:1074:ILE:HD11	1:J:1078:LEU:CD2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1054:ASP:HB3	1:P:1057:ARG:HD2	1.73	0.70
1:F:1093:HIS:ND1	1:F:1113:GLN:OE1	2.25	0.70
1:K:1038:ARG:NH1	2:K:1220:HOH:O	2.23	0.69
1:G:1069:ALA:HB1	1:G:1075:GLU:HA	1.75	0.69
1:H:1106:GLU:CD	1:H:1106:GLU:H	2.01	0.68
1:B:1067:ASP:OD1	1:B:1070:ARG:NH1	2.27	0.68
1:G:1039:THR:N	2:G:1222:HOH:O	2.27	0.67
1:N:1106:GLU:N	1:N:1106:GLU:OE1	2.24	0.67
1:D:1092:ALA:O	1:D:1093:HIS:CB	2.43	0.67
1:O:1070:ARG:HA	1:O:1075:GLU:HG2	1.76	0.67
1:L:1085:ASP:OD1	1:L:1085:ASP:N	2.26	0.66
1:J:1040:TYR:OH	1:J:1057:ARG:NH2	2.29	0.65
1:D:1093:HIS:O	1:D:1094:GLU:HG2	1.95	0.65
1:M:1093:HIS:HB2	1:M:1094:GLU:OE2	1.96	0.65
1:A:1077:GLN:O	1:A:1084:SER:CB	2.40	0.64
1:M:1095:ASN:OD1	1:M:1095:ASN:N	2.30	0.64
1:I:1094:GLU:OE2	1:I:1094:GLU:N	2.30	0.64
1:E:1070:ARG:HG3	2:E:1207:HOH:O	1.97	0.63
1:K:1074:ILE:O	1:K:1074:ILE:CG1	2.30	0.63
1:M:1094:GLU:OE2	1:M:1094:GLU:N	2.30	0.63
1:A:1067:ASP:OD1	1:A:1070:ARG:NH1	2.32	0.63
1:I:1083:THR:CG2	1:I:1083:THR:O	2.46	0.63
1:N:1054:ASP:HB3	1:N:1057:ARG:HD2	1.78	0.63
1:J:1069:ALA:O	1:J:1074:ILE:HG23	1.98	0.62
1:L:1079:GLU:N	1:L:1079:GLU:OE1	2.32	0.62
1:O:1067:ASP:OD1	1:O:1070:ARG:NH1	2.33	0.62
1:N:1069:ALA:HA	1:N:1074:ILE:HG22	1.81	0.62
1:I:1077:GLN:O	1:I:1084:SER:HB2	1.99	0.62
1:M:1093:HIS:H	1:M:1113:GLN:HG3	1.65	0.61
1:D:1067:ASP:OD1	1:D:1070:ARG:NH1	2.33	0.61
1:I:1057:ARG:NH1	2:I:1212:HOH:O	2.21	0.61
1:J:1069:ALA:HB1	1:J:1075:GLU:HA	1.82	0.61
1:I:1084:SER:OG	1:I:1086:TRP:O	2.20	0.60
1:I:1084:SER:O	1:I:1085:ASP:HB2	2.01	0.60
1:I:1070:ARG:HG2	1:I:1075:GLU:CG	2.32	0.60
1:K:1051:ARG:NH2	2:K:1222:HOH:O	2.35	0.60
1:B:1075:GLU:CD	1:B:1075:GLU:H	2.09	0.59
1:K:1074:ILE:HG13	1:K:1077:GLN:CD	2.26	0.59
1:M:1092:ALA:O	1:M:1094:GLU:N	2.36	0.59
1:K:1069:ALA:HB1	1:K:1075:GLU:HA	1.85	0.58
1:D:1106:GLU:CD	1:D:1106:GLU:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1083:THR:O	1:I:1083:THR:HG22	2.02	0.58
1:P:1077:GLN:O	1:P:1084:SER:HB2	2.03	0.58
1:A:1070:ARG:HD3	1:C:1094:GLU:HG2	1.84	0.58
1:N:1084:SER:OG	1:N:1085:ASP:N	2.35	0.58
1:I:1080:ASP:O	1:I:1084:SER:HB3	2.05	0.57
1:C:1106:GLU:CD	1:C:1106:GLU:H	2.13	0.56
1:I:1091:VAL:HG13	1:I:1095:ASN:HA	1.88	0.56
1:P:1069:ALA:HA	1:P:1074:ILE:HG22	1.86	0.56
1:N:1067:ASP:HA	1:N:1070:ARG:HH11	1.70	0.56
1:J:1072:PHE:HB2	1:J:1074:ILE:CG2	2.34	0.56
1:J:1074:ILE:CD1	1:J:1078:LEU:HD21	2.35	0.56
1:C:1074:ILE:O	1:C:1074:ILE:CG2	2.54	0.56
1:F:1058:TYR:OH	1:F:1067:ASP:OD2	2.23	0.56
1:M:1082:GLN:H	1:M:1082:GLN:CD	2.13	0.56
1:H:1094:GLU:OE2	1:H:1094:GLU:N	2.38	0.56
1:D:1090:TYR:CE1	1:D:1092:ALA:HB2	2.41	0.56
1:P:1080:ASP:O	1:P:1083:THR:HG22	2.07	0.55
1:K:1074:ILE:HD11	1:K:1077:GLN:CB	2.33	0.55
1:L:1106:GLU:H	1:L:1106:GLU:CD	2.13	0.55
1:M:1077:GLN:O	1:M:1084:SER:CB	2.53	0.54
1:F:1057:ARG:NH1	2:F:1211:HOH:O	2.40	0.54
1:M:1081:PRO:HA	1:M:1084:SER:OG	2.07	0.54
1:F:1055:VAL:HG12	1:F:1109:VAL:HG22	1.89	0.54
1:B:1060:GLY:HA2	1:B:1105:TRP:CD2	2.43	0.53
1:B:1089:VAL:HG12	1:B:1116:LYS:HB2	1.90	0.53
1:I:1045:LYS:HE3	1:I:1074:ILE:HD13	1.90	0.53
1:A:1093:HIS:O	1:A:1094:GLU:HB2	2.08	0.53
1:F:1067:ASP:OD1	1:F:1070:ARG:NH1	2.34	0.53
1:D:1093:HIS:O	1:D:1094:GLU:CB	2.56	0.53
1:E:1089:VAL:HG11	1:E:1097:ILE:HG23	1.90	0.53
1:D:1092:ALA:O	1:D:1093:HIS:HB2	2.08	0.53
1:K:1074:ILE:CG1	1:K:1077:GLN:CB	2.81	0.53
1:H:1077:GLN:HG2	1:H:1086:TRP:HE1	1.73	0.52
1:H:1062:ASP:O	1:H:1066:HIS:ND1	2.42	0.52
1:I:1084:SER:O	1:I:1085:ASP:CB	2.55	0.52
1:J:1072:PHE:CB	1:J:1074:ILE:HG22	2.40	0.52
1:K:1058:TYR:OH	1:K:1067:ASP:OD2	2.22	0.52
1:B:1098:LEU:HD23	1:O:1050:GLY:C	2.35	0.52
1:A:1059:ARG:HE	1:D:1059:ARG:HH21	1.57	0.52
1:D:1069:ALA:HB1	1:D:1075:GLU:HA	1.91	0.51
1:E:1057:ARG:NH2	1:H:1083:THR:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1106:GLU:OE1	1:G:1106:GLU:N	2.32	0.51
1:B:1093:HIS:C	1:B:1095:ASN:N	2.67	0.51
1:I:1086:TRP:CZ3	1:I:1119:SER:HB3	2.46	0.51
1:M:1066:HIS:CE1	1:M:1079:GLU:HG2	2.45	0.51
1:C:1044:GLN:OE1	1:C:1116:LYS:NZ	2.37	0.51
1:M:1096:ALA:O	1:M:1097:ILE:C	2.53	0.51
1:M:1093:HIS:H	1:M:1113:GLN:CG	2.25	0.50
1:P:1040:TYR:CZ	1:P:1054:ASP:HB2	2.46	0.50
1:A:1059:ARG:HH21	1:D:1059:ARG:HH22	1.59	0.50
1:C:1051:ARG:NH1	1:G:1102:ASP:OD1	2.45	0.50
1:E:1057:ARG:HH21	1:H:1083:THR:HG23	1.75	0.50
1:L:1065:ARG:HD3	1:L:1078:LEU:O	2.11	0.49
1:O:1122:GLU:O	1:O:1126:MET:HG2	2.11	0.49
1:F:1091:VAL:O	1:F:1113:GLN:HG2	2.13	0.49
1:E:1089:VAL:CG1	1:E:1097:ILE:HG23	2.43	0.49
1:A:1080:ASP:HB3	1:A:1083:THR:HB	1.95	0.49
1:K:1079:GLU:OE1	1:K:1079:GLU:N	2.36	0.49
1:K:1074:ILE:O	1:K:1077:GLN:HG3	2.13	0.48
1:M:1085:ASP:O	1:M:1085:ASP:OD2	2.30	0.48
1:I:1070:ARG:HG2	1:I:1075:GLU:HG2	1.94	0.48
1:P:1094:GLU:OE2	1:P:1094:GLU:N	2.46	0.48
1:M:1066:HIS:ND1	1:M:1079:GLU:HG2	2.28	0.48
1:J:1069:ALA:HA	1:J:1074:ILE:HG23	1.94	0.48
1:I:1125:GLN:HG2	1:P:1085:ASP:HB3	1.96	0.48
1:K:1080:ASP:HB3	1:K:1083:THR:HG23	1.94	0.48
1:E:1040:TYR:N	2:E:1222:HOH:O	2.46	0.48
1:H:1070:ARG:NH2	2:H:1218:HOH:O	2.21	0.48
1:J:1069:ALA:HB2	1:J:1078:LEU:HD12	1.96	0.48
1:C:1082:GLN:N	1:C:1082:GLN:OE1	2.47	0.47
1:G:1051:ARG:HD2	1:J:1102:ASP:OD2	2.15	0.47
1:J:1070:ARG:HG2	1:J:1071:MET:N	2.30	0.47
1:J:1094:GLU:N	1:J:1094:GLU:OE2	2.46	0.47
1:K:1055:VAL:HG12	1:K:1109:VAL:HG22	1.96	0.47
1:M:1084:SER:O	1:M:1085:ASP:HB3	2.15	0.47
1:P:1062:ASP:HA	2:P:1216:HOH:O	2.14	0.47
1:A:1069:ALA:HB1	1:A:1075:GLU:HA	1.97	0.47
1:O:1080:ASP:O	1:O:1083:THR:HG22	2.15	0.47
1:A:1040:TYR:HB2	2:P:1211:HOH:O	2.14	0.47
1:C:1074:ILE:HG13	1:C:1077:GLN:CD	2.39	0.47
1:O:1089:VAL:HG21	1:O:1097:ILE:HG23	1.96	0.47
1:N:1091:VAL:HG13	1:N:1095:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1120:SER:O	1:H:1124:GLN:HG3	2.15	0.46
1:M:1089:VAL:HG13	1:M:1097:ILE:HG23	1.97	0.46
1:O:1091:VAL:HG13	1:O:1095:ASN:HA	1.98	0.46
1:H:1039:THR:HA	2:H:1223:HOH:O	2.15	0.46
1:K:1120:SER:O	1:K:1124:GLN:HG3	2.16	0.46
1:B:1050:GLY:HA3	1:L:1098:LEU:HD23	1.97	0.46
1:B:1094:GLU:HG2	1:B:1096:ALA:H	1.80	0.46
1:F:1069:ALA:HB1	1:F:1075:GLU:HA	1.98	0.46
1:E:1045:LYS:HE2	2:E:1217:HOH:O	2.16	0.46
1:G:1087:LYS:HD3	1:G:1087:LYS:HA	1.74	0.46
1:K:1111:CYS:SG	1:M:1038:ARG:HD3	2.56	0.46
1:P:1079:GLU:N	1:P:1079:GLU:OE1	2.49	0.46
1:F:1074:ILE:HG13	1:F:1077:GLN:CD	2.41	0.45
1:H:1053:ILE:HG21	1:H:1071:MET:HE1	1.97	0.45
1:L:1067:ASP:HA	1:L:1070:ARG:NH1	2.32	0.45
1:C:1106:GLU:O	1:C:1110:ASN:ND2	2.49	0.45
1:H:1091:VAL:HG13	1:H:1095:ASN:HA	1.99	0.45
1:C:1038:ARG:NH2	1:G:1094:GLU:OE1	2.40	0.45
1:H:1087:LYS:HA	1:H:1087:LYS:HD3	1.65	0.45
1:M:1065:ARG:HD3	1:M:1078:LEU:O	2.17	0.45
1:M:1070:ARG:HA	1:M:1075:GLU:HG2	1.98	0.45
1:M:1106:GLU:O	1:M:1110:ASN:ND2	2.50	0.45
1:N:1094:GLU:OE2	1:N:1094:GLU:N	2.50	0.44
1:P:1089:VAL:HG13	1:P:1097:ILE:HG23	1.99	0.44
1:E:1094:GLU:N	1:E:1094:GLU:OE2	2.50	0.44
1:G:1093:HIS:CE1	1:G:1113:GLN:OE1	2.69	0.44
1:H:1079:GLU:OE1	1:H:1079:GLU:N	2.45	0.44
1:J:1072:PHE:HB2	1:J:1074:ILE:HG22	1.98	0.44
1:M:1083:THR:HA	2:M:1214:HOH:O	2.17	0.44
1:P:1069:ALA:HB1	1:P:1075:GLU:HA	1.99	0.44
1:I:1125:GLN:N	1:I:1125:GLN:OE1	2.50	0.44
1:P:1091:VAL:HG13	1:P:1095:ASN:HA	1.98	0.44
1:D:1087:LYS:HD3	1:D:1087:LYS:HA	1.74	0.44
1:H:1077:GLN:HB3	1:H:1086:TRP:CD1	2.53	0.44
1:K:1096:ALA:HB3	2:K:1239:HOH:O	2.16	0.44
1:A:1098:LEU:HD23	1:L:1050:GLY:HA3	2.00	0.44
1:P:1060:GLY:HA2	1:P:1105:TRP:CD2	2.53	0.44
1:I:1086:TRP:HE3	1:I:1118:LEU:O	2.01	0.44
1:J:1091:VAL:HG13	1:J:1095:ASN:HA	1.99	0.44
1:B:1041:THR:HG23	1:B:1114:SER:HA	1.99	0.44
1:M:1092:ALA:HA	1:M:1113:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1097:ILE:H	1:M:1097:ILE:HD12	1.83	0.43
1:L:1081:PRO:HB3	1:L:1087:LYS:NZ	2.33	0.43
1:O:1065:ARG:HD3	1:O:1078:LEU:O	2.17	0.43
1:B:1069:ALA:HB1	1:B:1075:GLU:HA	2.01	0.43
1:M:1078:LEU:HD23	1:M:1078:LEU:HA	1.83	0.43
1:D:1077:GLN:O	1:D:1083:THR:HG21	2.19	0.43
1:L:1119:SER:OG	1:L:1122:GLU:HG3	2.18	0.43
1:H:1074:ILE:O	1:H:1077:GLN:HB2	2.18	0.42
1:C:1056:ASN:ND2	2:C:1235:HOH:O	2.43	0.42
1:F:1113:GLN:NE2	2:F:1209:HOH:O	2.51	0.42
1:A:1092:ALA:HB3	1:A:1096:ALA:O	2.20	0.42
1:M:1084:SER:O	1:M:1085:ASP:CB	2.67	0.42
1:M:1092:ALA:O	1:M:1094:GLU:OE2	2.38	0.42
1:B:1051:ARG:HD2	1:L:1102:ASP:OD2	2.19	0.42
1:G:1080:ASP:HA	1:G:1081:PRO:HD2	1.86	0.42
1:B:1074:ILE:HG13	1:B:1077:GLN:CD	2.44	0.42
1:K:1074:ILE:HG13	1:K:1077:GLN:NE2	2.34	0.42
1:C:1054:ASP:HB3	1:C:1057:ARG:HG3	2.02	0.42
1:C:1069:ALA:HB1	1:C:1075:GLU:HA	2.02	0.42
1:I:1119:SER:O	1:I:1120:SER:C	2.62	0.42
1:J:1106:GLU:CD	1:J:1106:GLU:H	2.28	0.42
1:G:1093:HIS:CE1	1:G:1113:GLN:CG	3.03	0.42
1:N:1067:ASP:HA	1:N:1070:ARG:NH1	2.33	0.42
1:P:1045:LYS:HE2	2:P:1202:HOH:O	2.20	0.42
1:E:1055:VAL:HG12	1:E:1109:VAL:HG22	2.02	0.42
1:O:1074:ILE:HG13	1:O:1077:GLN:CD	2.45	0.42
1:D:1080:ASP:HA	1:D:1081:PRO:HD3	1.87	0.41
1:F:1094:GLU:H	1:F:1094:GLU:CD	2.26	0.41
1:G:1079:GLU:OE1	1:G:1079:GLU:N	2.43	0.41
1:H:1055:VAL:HG12	1:H:1109:VAL:HG22	2.02	0.41
1:N:1068:LEU:HD23	1:N:1068:LEU:HA	1.82	0.41
1:J:1074:ILE:HD12	1:J:1086:TRP:CD1	2.56	0.41
1:M:1091:VAL:HG13	1:M:1095:ASN:CA	2.38	0.41
1:E:1066:HIS:O	1:E:1070:ARG:HG3	2.20	0.41
1:G:1074:ILE:HD12	1:G:1074:ILE:HA	1.91	0.41
1:I:1084:SER:C	1:I:1086:TRP:H	2.27	0.41
1:M:1074:ILE:HD12	1:M:1074:ILE:HA	1.85	0.41
1:C:1089:VAL:HG12	1:C:1116:LYS:HB2	2.02	0.41
1:P:1045:LYS:CE	1:P:1086:TRP:CH2	3.03	0.41
1:C:1105:TRP:O	1:C:1108:PHE:HB3	2.20	0.41
1:D:1065:ARG:NE	2:D:1219:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1058:TYR:HD1	1:J:1063:GLU:HG2	1.86	0.41
1:E:1059:ARG:HE	1:E:1059:ARG:HB2	1.44	0.41
1:P:1074:ILE:HD12	1:P:1074:ILE:HA	1.94	0.41
1:M:1085:ASP:O	1:M:1085:ASP:CG	2.61	0.40
1:C:1046:ARG:NH2	1:C:1122:GLU:HG2	2.36	0.40
1:H:1069:ALA:HB1	1:H:1075:GLU:HA	2.04	0.40
1:F:1060:GLY:HA2	1:F:1105:TRP:CD2	2.57	0.40
1:A:1058:TYR:OH	1:A:1067:ASP:OD2	2.32	0.40
1:F:1088:LEU:HD12	1:F:1088:LEU:HA	1.89	0.40
1:I:1070:ARG:CG	1:I:1075:GLU:HG2	2.51	0.40
1:K:1087:LYS:HG3	1:K:1123:VAL:HG21	2.04	0.40
1:M:1080:ASP:O	1:M:1084:SER:N	2.52	0.40
1:K:1054:ASP:OD1	1:K:1056:ASN:HB2	2.21	0.40
1:M:1096:ALA:O	1:M:1097:ILE:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	77/83 (93%)	72 (94%)	5 (6%)	15	27
1	B	78/83 (94%)	72 (92%)	6 (8%)	12	20
1	C	78/83 (94%)	69 (88%)	9 (12%)	5	8
1	D	77/83 (93%)	73 (95%)	4 (5%)	21	36
1	E	74/83 (89%)	71 (96%)	3 (4%)	27	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	78/83 (94%)	71 (91%)	7 (9%)	9	15
1	G	77/83 (93%)	70 (91%)	7 (9%)	9	14
1	H	76/83 (92%)	71 (93%)	5 (7%)	15	26
1	I	76/83 (92%)	71 (93%)	5 (7%)	15	26
1	J	71/83 (86%)	60 (84%)	11 (16%)	2	3
1	K	78/83 (94%)	75 (96%)	3 (4%)	29	49
1	L	73/83 (88%)	64 (88%)	9 (12%)	4	6
1	M	77/83 (93%)	67 (87%)	10 (13%)	4	5
1	N	72/83 (87%)	64 (89%)	8 (11%)	6	9
1	O	75/83 (90%)	67 (89%)	8 (11%)	6	10
1	P	76/83 (92%)	68 (90%)	8 (10%)	6	10
All	All	1213/1328 (91%)	1105 (91%)	108 (9%)	9	15

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1051	ARG
1	A	1083	THR
1	A	1084	SER
1	A	1085	ASP
1	A	1089	VAL
1	B	1075	GLU
1	B	1087	LYS
1	B	1089	VAL
1	B	1093	HIS
1	B	1109	VAL
1	B	1111	CYS
1	C	1051	ARG
1	C	1062	ASP
1	C	1074	ILE
1	C	1075	GLU
1	C	1083	THR
1	C	1085	ASP
1	C	1089	VAL
1	C	1091	VAL
1	C	1095	ASN
1	D	1055	VAL
1	D	1075	GLU

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Mol	Chain	Res	Type
1	D	1089	VAL
1	D	1094	GLU
1	E	1075	GLU
1	E	1091	VAL
1	E	1095	ASN
1	F	1059	ARG
1	F	1075	GLU
1	F	1083	THR
1	F	1089	VAL
1	F	1093	HIS
1	F	1113	GLN
1	F	1123	VAL
1	G	1046	ARG
1	G	1048	SER
1	G	1083	THR
1	G	1089	VAL
1	G	1094	GLU
1	G	1095	ASN
1	G	1124	GLN
1	H	1048	SER
1	H	1075	GLU
1	H	1077	GLN
1	H	1089	VAL
1	H	1095	ASN
1	I	1062	ASP
1	I	1074	ILE
1	I	1078	LEU
1	I	1089	VAL
1	I	1120	SER
1	J	1039	THR
1	J	1053	ILE
1	J	1070	ARG
1	J	1074	ILE
1	J	1079	GLU
1	J	1083	THR
1	J	1087	LYS
1	J	1089	VAL
1	J	1109	VAL
1	J	1114	SER
1	J	1124	GLN
1	K	1074	ILE
1	K	1078	LEU

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Mol	Chain	Res	Type
1	K	1089	VAL
1	L	1053	ILE
1	L	1055	VAL
1	L	1062	ASP
1	L	1085	ASP
1	L	1087	LYS
1	L	1089	VAL
1	L	1094	GLU
1	L	1097	ILE
1	L	1106	GLU
1	M	1048	SER
1	M	1051	ARG
1	M	1066	HIS
1	M	1070	ARG
1	M	1074	ILE
1	M	1083	THR
1	M	1085	ASP
1	M	1089	VAL
1	M	1095	ASN
1	M	1124	GLN
1	N	1053	ILE
1	N	1059	ARG
1	N	1066	HIS
1	N	1074	ILE
1	N	1078	LEU
1	N	1094	GLU
1	N	1095	ASN
1	N	1126	MET
1	O	1051	ARG
1	O	1056	ASN
1	O	1074	ILE
1	O	1082	GLN
1	O	1083	THR
1	O	1089	VAL
1	O	1094	GLU
1	O	1109	VAL
1	P	1046	ARG
1	P	1051	ARG
1	P	1066	HIS
1	P	1074	ILE
1	P	1075	GLU
1	P	1083	THR

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Mol	Chain	Res	Type
1	P	1087	LYS
1	P	1089	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1093	HIS
1	C	1110	ASN
1	C	1124	GLN
1	D	1093	HIS
1	D	1113	GLN
1	F	1056	ASN
1	G	1056	ASN
1	G	1093	HIS
1	I	1056	ASN
1	K	1082	GLN
1	K	1125	GLN
1	L	1077	GLN
1	N	1113	GLN
1	O	1077	GLN
1	O	1110	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	-0.03	4 (4%) 38 34	24, 39, 75, 88	0
1	B	89/95 (93%)	0.04	3 (3%) 48 44	28, 45, 82, 122	0
1	C	89/95 (93%)	-0.11	2 (2%) 62 58	24, 43, 83, 113	0
1	D	88/95 (92%)	-0.16	1 (1%) 78 74	28, 43, 75, 111	0
1	E	85/95 (89%)	-0.26	3 (3%) 47 43	25, 39, 64, 95	0
1	F	89/95 (93%)	-0.01	2 (2%) 62 58	29, 48, 93, 131	0
1	G	88/95 (92%)	0.02	2 (2%) 61 57	27, 46, 81, 115	0
1	H	87/95 (91%)	0.09	4 (4%) 37 33	29, 50, 85, 121	0
1	I	86/95 (90%)	0.06	3 (3%) 47 43	23, 48, 89, 106	0
1	J	82/95 (86%)	0.05	4 (4%) 35 31	27, 51, 82, 99	0
1	K	89/95 (93%)	-0.11	2 (2%) 62 58	27, 44, 72, 100	0
1	L	84/95 (88%)	0.14	5 (5%) 27 24	26, 51, 97, 126	0
1	M	88/95 (92%)	0.35	6 (6%) 23 20	32, 62, 106, 121	0
1	N	82/95 (86%)	0.46	8 (9%) 13 10	36, 67, 109, 126	0
1	O	86/95 (90%)	-0.13	2 (2%) 61 57	28, 44, 73, 103	0
1	P	87/95 (91%)	0.38	5 (5%) 29 25	32, 62, 94, 104	0
All	All	1387/1520 (91%)	0.05	56 (4%) 42 38	23, 48, 95, 131	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	1096	ALA	7.5
1	A	1092	ALA	5.4
1	O	1126	MET	5.0
1	J	1074	ILE	4.8
1	N	1092	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	1092	ALA	4.0
1	H	1094	GLU	3.4
1	L	1076	GLY	3.2
1	L	1081	PRO	3.2
1	P	1092	ALA	3.1
1	D	1092	ALA	3.0
1	B	1093	HIS	3.0
1	A	1094	GLU	3.0
1	H	1082	GLN	2.9
1	C	1093	HIS	2.8
1	J	1075	GLU	2.7
1	M	1086	TRP	2.7
1	E	1092	ALA	2.7
1	B	1082	GLN	2.7
1	K	1074	ILE	2.6
1	M	1095	ASN	2.6
1	J	1083	THR	2.6
1	M	1074	ILE	2.6
1	P	1083	THR	2.5
1	L	1092	ALA	2.5
1	N	1094	GLU	2.4
1	G	1093	HIS	2.4
1	M	1076	GLY	2.4
1	L	1039	THR	2.4
1	C	1074	ILE	2.4
1	A	1082	GLN	2.4
1	P	1082	GLN	2.4
1	H	1066	HIS	2.3
1	O	1094	GLU	2.3
1	E	1070	ARG	2.3
1	G	1084	SER	2.3
1	N	1126	MET	2.3
1	I	1038	ARG	2.3
1	I	1123	VAL	2.2
1	E	1125	GLN	2.2
1	P	1066	HIS	2.2
1	N	1039	THR	2.1
1	A	1093	HIS	2.1
1	N	1074	ILE	2.1
1	N	1077	GLN	2.1
1	M	1038	ARG	2.1
1	F	1093	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	1093	HIS	2.1
1	L	1126	MET	2.1
1	B	1095	ASN	2.1
1	I	1083	THR	2.1
1	J	1039	THR	2.1
1	F	1082	GLN	2.0
1	P	1086	TRP	2.0
1	N	1046	ARG	2.0
1	N	1084	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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.