



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2022 – 12:11 PM JST

PDB ID : 7WAP
Title : Mevo lectin mutant D134A
Authors : Sivaji, N.; Vijayan, M.
Deposited on : 2021-12-14
Resolution : 3.10 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

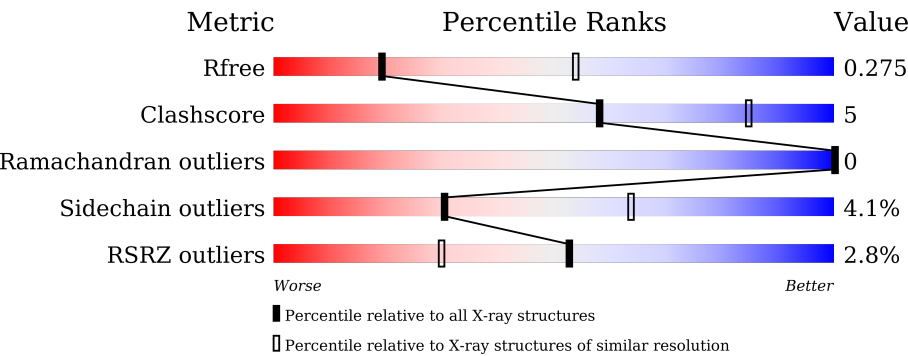
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	145	<div><div></div><div>89%7% ..</div></div>
1	B	145	<div><div>6%</div><div>83%12% ..</div></div>
1	C	145	<div><div>%</div><div>87%8% ..</div></div>
1	D	145	<div><div>3%</div><div>87%10% .</div></div>
1	E	145	<div><div>12%</div><div>86%10% ..</div></div>
1	F	145	<div><div></div><div>86%9% ..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	145	<div><div>%</div><div><div></div><div>84%</div><div>8%</div><div>7%</div></div></div>
1	H	145	<div><div>3%</div><div><div></div><div>81%</div><div>14%</div><div></div></div></div>
1	I	145	<div><div></div><div><div></div><div>84%</div><div>8%</div><div>7%</div></div></div>
1	J	145	<div><div>3%</div><div><div></div><div>86%</div><div>10%</div><div></div></div></div>
1	K	145	<div><div>2%</div><div><div></div><div>79%</div><div>16%</div><div></div></div></div>
1	L	145	<div><div>4%</div><div><div></div><div>83%</div><div>12%</div><div></div></div></div>
1	M	145	<div><div>3%</div><div><div></div><div>88%</div><div>8%</div><div></div></div></div>
1	N	145	<div><div></div><div><div></div><div>71%</div><div>22%</div><div></div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14478 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 Mevo lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	140	Total	C	N	O	S	0	0	0
			1054	672	172	207	3			
1	G	135	Total	C	N	O	S	0	0	0
			974	624	158	190	2			
1	A	140	Total	C	N	O	S	0	0	0
			1029	658	171	198	2			
1	D	140	Total	C	N	O	S	0	0	0
			1048	670	171	204	3			
1	E	140	Total	C	N	O	S	0	0	0
			1043	664	169	207	3			
1	F	140	Total	C	N	O	S	0	0	0
			1046	671	171	201	3			
1	C	140	Total	C	N	O	S	0	0	0
			1043	665	170	205	3			
1	H	140	Total	C	N	O	S	0	0	0
			1058	675	173	207	3			
1	I	135	Total	C	N	O	S	0	0	0
			978	627	159	190	2			
1	J	140	Total	C	N	O	S	0	0	0
			1025	655	170	198	2			
1	K	140	Total	C	N	O	S	0	0	0
			1040	664	169	204	3			
1	L	140	Total	C	N	O	S	0	0	0
			1051	670	171	207	3			
1	M	140	Total	C	N	O	S	0	0	0
			1042	668	170	201	3			
1	N	140	Total	C	N	O	S	0	0	0
			1047	668	171	205	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	134	ALA	ASP	engineered mutation	UNP D7DTD6

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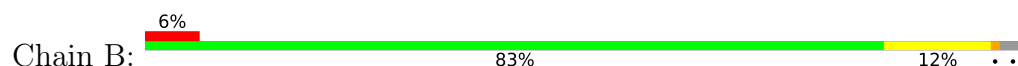
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Chain	Residue	Modelled	Actual	Comment	Reference
G	134	ALA	ASP	engineered mutation	UNP D7DTD6
A	134	ALA	ASP	engineered mutation	UNP D7DTD6
D	134	ALA	ASP	engineered mutation	UNP D7DTD6
E	134	ALA	ASP	engineered mutation	UNP D7DTD6
F	134	ALA	ASP	engineered mutation	UNP D7DTD6
C	134	ALA	ASP	engineered mutation	UNP D7DTD6
H	134	ALA	ASP	engineered mutation	UNP D7DTD6
I	134	ALA	ASP	engineered mutation	UNP D7DTD6
J	134	ALA	ASP	engineered mutation	UNP D7DTD6
K	134	ALA	ASP	engineered mutation	UNP D7DTD6
L	134	ALA	ASP	engineered mutation	UNP D7DTD6
M	134	ALA	ASP	engineered mutation	UNP D7DTD6
N	134	ALA	ASP	engineered mutation	UNP D7DTD6

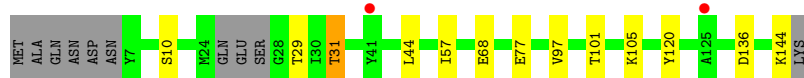
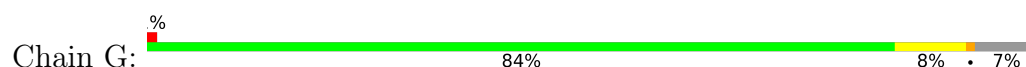
3 Residue-property plots [i](#)

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.

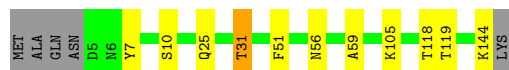
- Molecule 1: Mevo lectin



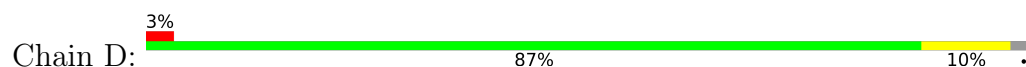
- Molecule 1: Mevo lectin



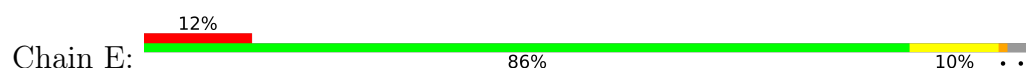
- Molecule 1: Mevo lectin




- Molecule 1: Mevo lectin



- Molecule 1: Mevo lectin




- Molecule 1: Mevo lectin

Chain F:  86% 9% ..




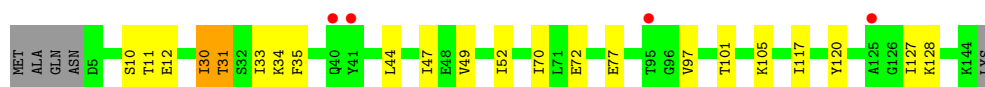
• Molecule 1: Mevo lectin

Chain C:  87% 8% ..




• Molecule 1: Mevo lectin

Chain H:  81% 14% ..




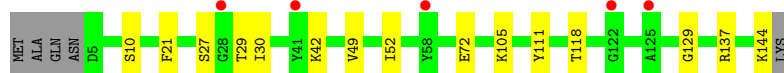
• Molecule 1: Mevo lectin

Chain I:  84% 8% 7%




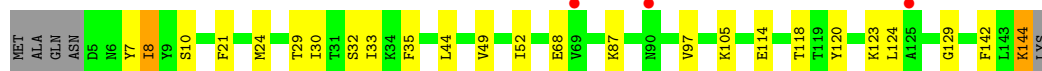
• Molecule 1: Mevo lectin

Chain J:  86% 10% .




• Molecule 1: Mevo lectin

Chain K:  79% 16% ..

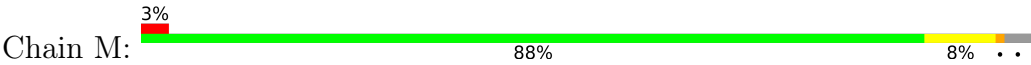


• Molecule 1: Mevo lectin

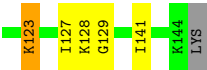
Chain L:  83% 12% ..



• Molecule 1: Mevo lectin



● Molecule 1: Mevo lectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.81Å 169.26Å 160.94Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	84.62 – 3.10 84.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (84.62-3.10) 91.5 (84.63-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.275 0.232 , 0.275	Depositor DCC
R_{free} test set	2114 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	1.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14478	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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	0.88	0/1048	1.15	2/1418 (0.1%)
1	B	0.79	0/1073	1.03	0/1449
1	C	0.86	0/1062	1.06	0/1437
1	D	0.87	0/1067	1.08	1/1441 (0.1%)
1	E	0.84	0/1062	1.03	1/1438 (0.1%)
1	F	0.88	0/1065	1.11	2/1437 (0.1%)
1	G	0.90	0/990	1.08	2/1340 (0.1%)
1	H	0.80	0/1077	1.05	0/1453
1	I	0.92	0/994	1.07	0/1344
1	J	0.81	0/1044	1.08	2/1414 (0.1%)
1	K	0.82	0/1059	1.06	1/1433 (0.1%)
1	L	0.83	0/1070	1.06	0/1446
1	M	0.85	0/1061	1.05	2/1433 (0.1%)
1	N	0.93	2/1066 (0.2%)	1.09	1/1441 (0.1%)
All	All	0.86	2/14738 (0.0%)	1.07	14/19924 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	48	GLU	CD-OE1	-5.16	1.20	1.25
1	N	77	GLU	CD-OE2	-5.13	1.20	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	THR	CB-CA-C	-6.38	94.37	111.60
1	M	144	LYS	CA-C-O	5.97	132.65	120.10
1	G	144	LYS	CA-C-O	5.86	132.41	120.10
1	A	144	LYS	CA-C-O	5.73	132.13	120.10
1	F	144	LYS	CA-C-O	5.55	131.76	120.10
1	J	144	LYS	CA-C-O	5.50	131.65	120.10
1	K	144	LYS	CA-C-O	5.45	131.54	120.10
1	N	69	VAL	CA-CB-CG1	5.38	118.98	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	137	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	144	LYS	CA-C-O	5.10	130.81	120.10
1	M	136	ASP	CB-CA-C	5.04	120.49	110.40
1	G	136	ASP	CB-CA-C	5.04	120.47	110.40
1	F	137	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	E	120	TYR	CB-CA-C	-5.00	100.39	110.40

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	1029	0	994	14	0
1	B	1054	0	1030	12	0
1	C	1043	0	1006	10	0
1	D	1048	0	1024	7	0
1	E	1043	0	999	9	0
1	F	1046	0	1029	11	0
1	G	974	0	933	7	0
1	H	1058	0	1041	15	0
1	I	978	0	944	9	0
1	J	1025	0	983	11	0
1	K	1040	0	1002	19	0
1	L	1051	0	1021	15	0
1	M	1042	0	1018	8	0
1	N	1047	0	1017	27	0
All	All	14478	0	14041	137	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 5.

All (137) 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:N:42:LYS:NZ	1:N:113:GLU:OE2	1.89	1.04
1:D:12:GLU:OE1	1:D:128:LYS:HE3	1.54	1.04
1:L:30:ILE:HD13	1:L:49:VAL:HG13	1.34	1.04
1:K:29:THR:HG21	1:K:123:LYS:HE2	1.42	1.01
1:N:25:GLN:HE22	1:N:54:ASN:HD22	1.04	0.96
1:L:30:ILE:HD13	1:L:49:VAL:CG1	2.04	0.87
1:B:105:LYS:HD2	1:E:118:THR:HG22	1.58	0.86
1:N:25:GLN:NE2	1:N:54:ASN:HD22	1.79	0.81
1:J:42:LYS:CB	1:J:111:TYR:HD2	1.98	0.77
1:K:8:ILE:HD11	1:K:144:LYS:HG2	1.69	0.74
1:L:101:THR:OG1	1:L:105:LYS:HB2	1.88	0.73
1:C:33:ILE:HG13	1:C:49:VAL:HG22	1.69	0.73
1:E:34:LYS:HG3	1:E:70:ILE:HG12	1.69	0.72
1:K:29:THR:HG21	1:K:123:LYS:CE	2.19	0.72
1:N:42:LYS:NZ	1:N:113:GLU:CD	2.44	0.71
1:F:31:THR:HG23	1:C:120:TYR:OH	1.92	0.69
1:H:77:GLU:OE2	1:H:105:LYS:HD3	1.93	0.69
1:I:117:ILE:HD11	1:N:72:GLU:OE2	1.92	0.69
1:A:31:THR:HG22	1:F:120:TYR:OH	1.93	0.69
1:B:71:LEU:HB2	1:B:107:ILE:HG21	1.76	0.68
1:K:120:TYR:CD2	1:L:72:GLU:OE2	2.47	0.67
1:J:30:ILE:HG12	1:J:49:VAL:HG13	1.76	0.67
1:J:42:LYS:CB	1:J:111:TYR:CD2	2.78	0.66
1:A:105:LYS:HG2	1:F:118:THR:CG2	2.27	0.65
1:J:29:THR:O	1:J:52:ILE:HG23	1.97	0.64
1:N:128:LYS:HG2	1:N:141:ILE:HD11	1.78	0.64
1:C:30:ILE:HD13	1:C:49:VAL:HG13	1.79	0.63
1:B:37:TRP:CE3	1:B:109:ALA:HB1	2.33	0.62
1:H:31:THR:HG23	1:L:120:TYR:OH	1.98	0.62
1:H:120:TYR:OH	1:I:31:THR:HG23	1.99	0.62
1:E:30:ILE:HD13	1:E:49:VAL:HG13	1.80	0.61
1:G:31:THR:HG23	1:G:31:THR:O	2.02	0.59
1:A:7:TYR:OH	1:A:25:GLN:O	2.21	0.59
1:J:105:LYS:HG2	1:M:118:THR:CG2	2.31	0.59
1:I:33:ILE:HG12	1:I:35:PHE:CE1	2.37	0.59
1:N:74:ASP:OD2	1:N:103:LYS:HE3	2.02	0.59
1:E:34:LYS:HG3	1:E:70:ILE:CG1	2.34	0.58
1:B:30:ILE:HD13	1:B:49:VAL:HG13	1.87	0.57
1:N:12:GLU:OE1	1:N:128:LYS:HD3	2.04	0.57
1:N:36:ASN:HB2	1:N:46:HIS:HB3	1.86	0.56
1:B:37:TRP:CZ3	1:B:109:ALA:HB1	2.41	0.56
1:I:30:ILE:HD13	1:I:49:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ILE:HG12	1:H:35:PHE:CE1	2.41	0.56
1:B:96:GLY:HA2	1:B:110:GLY:HA3	1.88	0.56
1:K:7:TYR:CE2	1:K:24:MET:CE	2.90	0.55
1:G:120:TYR:CE1	1:C:72:GLU:HB3	2.42	0.55
1:A:59:ALA:HB3	1:N:56:ASN:HD21	1.72	0.55
1:A:105:LYS:HG2	1:F:118:THR:HG21	1.89	0.54
1:F:30:ILE:HD12	1:F:124:LEU:HG	1.90	0.54
1:B:101:THR:OG1	1:B:105:LYS:HB2	2.08	0.53
1:H:30:ILE:HD13	1:H:49:VAL:HG13	1.89	0.53
1:B:107:ILE:HG13	1:B:107:ILE:O	2.09	0.53
1:M:31:THR:O	1:M:31:THR:HG23	2.09	0.53
1:A:59:ALA:CB	1:N:56:ASN:HD21	2.22	0.53
1:N:39:ASP:OD1	1:N:111:TYR:OH	2.25	0.52
1:A:31:THR:CG2	1:F:120:TYR:OH	2.58	0.52
1:H:105:LYS:HE3	1:L:118:THR:HG22	1.90	0.52
1:N:39:ASP:OD2	1:N:67:HIS:NE2	2.40	0.52
1:K:21:PHE:CE1	1:K:129:GLY:C	2.83	0.52
1:N:21:PHE:CE1	1:N:129:GLY:C	2.83	0.51
1:N:77:GLU:HG3	1:N:103:LYS:HG3	1.92	0.51
1:D:30:ILE:HG12	1:D:49:VAL:HG13	1.92	0.51
1:C:30:ILE:CD1	1:C:49:VAL:HG13	2.41	0.51
1:I:117:ILE:HG13	1:N:70:ILE:HB	1.93	0.51
1:J:21:PHE:CE1	1:J:129:GLY:C	2.84	0.51
1:N:31:THR:O	1:N:31:THR:HG23	2.11	0.51
1:H:72:GLU:OE1	1:L:120:TYR:CD2	2.64	0.51
1:A:105:LYS:HG2	1:F:118:THR:HG22	1.93	0.50
1:H:117:ILE:HD11	1:I:72:GLU:OE2	2.11	0.50
1:M:31:THR:HG23	1:N:120:TYR:OH	2.12	0.49
1:D:128:LYS:HG2	1:D:141:ILE:HD11	1.94	0.49
1:H:101:THR:OG1	1:H:105:LYS:HB2	2.11	0.49
1:J:105:LYS:HG2	1:M:118:THR:HG22	1.94	0.49
1:E:76:ASP:OD1	1:E:103:LYS:NZ	2.45	0.49
1:N:34:LYS:HB3	1:N:48:GLU:HB2	1.95	0.49
1:G:120:TYR:CD1	1:C:72:GLU:HB3	2.48	0.49
1:B:118:THR:CG2	1:G:105:LYS:HG2	2.43	0.48
1:A:118:THR:CG2	1:D:105:LYS:HG2	2.43	0.48
1:J:30:ILE:HG12	1:J:49:VAL:CG1	2.43	0.48
1:F:8:ILE:HD11	1:F:144:LYS:HE3	1.95	0.48
1:J:118:THR:HG22	1:K:105:LYS:HE3	1.96	0.48
1:N:47:ILE:HG21	1:N:127:ILE:CD1	2.44	0.48
1:L:101:THR:HG1	1:L:105:LYS:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:LYS:HE3	1:E:48:GLU:CD	2.34	0.47
1:N:36:ASN:CB	1:N:46:HIS:HB3	2.45	0.47
1:A:119:THR:HA	1:D:72:GLU:OE1	2.14	0.47
1:A:31:THR:HG22	1:A:31:THR:O	2.13	0.47
1:L:30:ILE:CD1	1:L:49:VAL:CG1	2.86	0.47
1:M:33:ILE:HG13	1:M:49:VAL:HG22	1.96	0.47
1:K:29:THR:HG22	1:K:124:LEU:O	2.16	0.46
1:H:31:THR:CG2	1:L:120:TYR:OH	2.64	0.46
1:K:29:THR:HG21	1:K:123:LYS:HG3	1.97	0.45
1:K:30:ILE:HG12	1:K:49:VAL:HG13	1.97	0.45
1:N:25:GLN:HG3	1:N:51:PHE:CD2	2.51	0.45
1:F:105:LYS:HG2	1:C:118:THR:CG2	2.47	0.45
1:C:31:THR:O	1:C:31:THR:HG23	2.16	0.45
1:K:118:THR:CG2	1:L:105:LYS:HG2	2.46	0.45
1:M:72:GLU:OE1	1:N:119:THR:HA	2.17	0.45
1:J:105:LYS:HG2	1:M:118:THR:HG21	1.98	0.45
1:A:31:THR:OG1	1:A:51:PHE:C	2.55	0.44
1:I:30:ILE:CD1	1:I:49:VAL:HG13	2.47	0.44
1:K:33:ILE:HG12	1:K:35:PHE:CE1	2.52	0.44
1:K:7:TYR:CD2	1:K:24:MET:CE	3.01	0.44
1:G:77:GLU:OE1	1:G:105:LYS:HD3	2.18	0.43
1:B:88:LYS:HD3	1:G:68:GLU:HG2	2.01	0.43
1:A:56:ASN:HD21	1:N:59:ALA:CB	2.31	0.43
1:L:82:SER:HB3	1:L:119:THR:OG1	2.19	0.43
1:A:56:ASN:ND2	1:N:46:HIS:HE1	2.17	0.43
1:K:7:TYR:HA	1:K:142:PHE:O	2.18	0.42
1:B:68:GLU:HG2	1:E:88:LYS:HD3	2.01	0.42
1:H:44:LEU:HD11	1:H:97:VAL:HG23	2.01	0.42
1:G:44:LEU:HD11	1:G:97:VAL:HG23	2.02	0.42
1:E:33:ILE:HG13	1:E:49:VAL:HG22	2.00	0.42
1:N:33:ILE:O	1:N:33:ILE:HG23	2.19	0.42
1:C:47:ILE:HG21	1:C:127:ILE:CD1	2.50	0.42
1:H:34:LYS:HE2	1:H:70:ILE:HD11	2.02	0.42
1:J:72:GLU:HB3	1:M:120:TYR:CE1	2.55	0.41
1:K:29:THR:CG2	1:K:123:LYS:HE2	2.31	0.41
1:I:47:ILE:HG21	1:I:127:ILE:CD1	2.51	0.41
1:K:44:LEU:HD11	1:K:97:VAL:HG23	2.02	0.41
1:B:30:ILE:CD1	1:B:49:VAL:HG13	2.50	0.41
1:D:44:LEU:HD11	1:D:97:VAL:HG23	2.03	0.41
1:E:77:GLU:OE2	1:E:105:LYS:HD3	2.21	0.41
1:H:47:ILE:HG21	1:H:127:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:ASN:HA	1:L:144:LYS:HE3	2.03	0.41
1:L:47:ILE:HG21	1:L:127:ILE:CD1	2.51	0.41
1:K:7:TYR:CE2	1:K:24:MET:HE1	2.56	0.40
1:D:35:PHE:O	1:D:68:GLU:HA	2.21	0.40
1:H:12:GLU:OE1	1:H:128:LYS:HE2	2.21	0.40
1:K:87:LYS:HG2	1:K:114:GLU:OE1	2.21	0.40
1:H:11:THR:HB	1:I:72:GLU:OE2	2.21	0.40
1:N:29:THR:OG1	1:N:123:LYS:HE2	2.21	0.40
1:C:77:GLU:OE2	1:C:105:LYS:HD3	2.22	0.40
1:F:45:HIS:HA	1:F:134:ALA:HA	2.04	0.40
1:F:47:ILE:HG21	1:F:127:ILE:CD1	2.51	0.40
1:K:35:PHE:O	1:K:68:GLU:HA	2.22	0.40
1:L:123:LYS:HA	1:L:123:LYS:HD2	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	138/145 (95%)	129 (94%)	9 (6%)	0	100	100
1	B	138/145 (95%)	128 (93%)	10 (7%)	0	100	100
1	C	138/145 (95%)	130 (94%)	8 (6%)	0	100	100
1	D	138/145 (95%)	129 (94%)	9 (6%)	0	100	100
1	E	138/145 (95%)	128 (93%)	10 (7%)	0	100	100
1	F	138/145 (95%)	128 (93%)	10 (7%)	0	100	100
1	G	131/145 (90%)	119 (91%)	12 (9%)	0	100	100
1	H	138/145 (95%)	129 (94%)	9 (6%)	0	100	100
1	I	131/145 (90%)	123 (94%)	8 (6%)	0	100	100
1	J	138/145 (95%)	126 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	138/145 (95%)	129 (94%)	9 (6%)	0	100	100
1	L	138/145 (95%)	130 (94%)	8 (6%)	0	100	100
1	M	138/145 (95%)	129 (94%)	9 (6%)	0	100	100
1	N	138/145 (95%)	130 (94%)	8 (6%)	0	100	100
All	All	1918/2030 (94%)	1787 (93%)	131 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	103/118 (87%)	102 (99%)	1 (1%)	76	90
1	B	110/118 (93%)	103 (94%)	7 (6%)	17	48
1	C	107/118 (91%)	102 (95%)	5 (5%)	26	59
1	D	108/118 (92%)	106 (98%)	2 (2%)	57	81
1	E	107/118 (91%)	104 (97%)	3 (3%)	43	73
1	F	107/118 (91%)	104 (97%)	3 (3%)	43	73
1	G	96/118 (81%)	91 (95%)	5 (5%)	23	55
1	H	111/118 (94%)	107 (96%)	4 (4%)	35	67
1	I	97/118 (82%)	91 (94%)	6 (6%)	18	49
1	J	102/118 (86%)	100 (98%)	2 (2%)	55	80
1	K	106/118 (90%)	102 (96%)	4 (4%)	33	66
1	L	109/118 (92%)	102 (94%)	7 (6%)	17	48
1	M	106/118 (90%)	101 (95%)	5 (5%)	26	59
1	N	108/118 (92%)	101 (94%)	7 (6%)	17	47
All	All	1477/1652 (89%)	1416 (96%)	61 (4%)	30	64

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	29	THR
1	B	30	ILE
1	B	52	ILE
1	B	102	SER
1	B	108	MET
1	B	123	LYS
1	G	10	SER
1	G	29	THR
1	G	31	THR
1	G	57	ILE
1	G	101	THR
1	A	10	SER
1	D	10	SER
1	D	52	ILE
1	E	31	THR
1	E	34	LYS
1	E	57	ILE
1	F	31	THR
1	F	52	ILE
1	F	57	ILE
1	C	29	THR
1	C	30	ILE
1	C	31	THR
1	C	52	ILE
1	C	57	ILE
1	H	10	SER
1	H	30	ILE
1	H	31	THR
1	H	52	ILE
1	I	12	GLU
1	I	30	ILE
1	I	31	THR
1	I	52	ILE
1	I	57	ILE
1	I	108	MET
1	J	10	SER
1	J	27	SER
1	K	8	ILE
1	K	10	SER
1	K	32	SER
1	K	52	ILE
1	L	10	SER

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Mol	Chain	Res	Type
1	L	30	ILE
1	L	31	THR
1	L	32	SER
1	L	52	ILE
1	L	57	ILE
1	L	123	LYS
1	M	10	SER
1	M	31	THR
1	M	50	LYS
1	M	52	ILE
1	M	57	ILE
1	N	10	SER
1	N	31	THR
1	N	32	SER
1	N	52	ILE
1	N	58	TYR
1	N	103	LYS
1	N	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	D	25	GLN
1	D	40	GLN
1	D	56	ASN
1	C	25	GLN
1	C	56	ASN
1	J	25	GLN
1	J	56	ASN
1	K	56	ASN
1	M	56	ASN
1	N	25	GLN
1	N	56	ASN

5.3.3 RNA ⓘ

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 monosaccharides 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	140/145 (96%)	-0.01	0 100 100	19, 36, 61, 81	0
1	B	140/145 (96%)	0.47	8 (5%) 23 11	31, 58, 90, 106	0
1	C	140/145 (96%)	0.13	1 (0%) 87 75	21, 43, 70, 110	0
1	D	140/145 (96%)	0.37	4 (2%) 51 28	25, 48, 75, 90	0
1	E	140/145 (96%)	0.83	18 (12%) 3 1	28, 61, 98, 119	0
1	F	140/145 (96%)	0.11	0 100 100	20, 42, 70, 81	0
1	G	135/145 (93%)	0.29	2 (1%) 73 54	25, 45, 70, 85	0
1	H	140/145 (96%)	0.40	4 (2%) 51 28	28, 47, 79, 109	0
1	I	135/145 (93%)	0.01	0 100 100	22, 37, 56, 72	0
1	J	140/145 (96%)	0.24	5 (3%) 42 22	24, 48, 79, 103	0
1	K	140/145 (96%)	0.25	3 (2%) 63 43	27, 45, 76, 98	0
1	L	140/145 (96%)	0.48	6 (4%) 35 17	24, 46, 73, 116	0
1	M	140/145 (96%)	0.35	4 (2%) 51 28	25, 48, 74, 92	0
1	N	140/145 (96%)	0.00	0 100 100	20, 37, 64, 76	0
All	All	1950/2030 (96%)	0.28	55 (2%) 53 30	19, 46, 77, 119	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	95	THR	4.4
1	E	26	GLU	4.3
1	E	125	ALA	4.3
1	E	135	ILE	4.1
1	E	27	SER	3.8
1	L	89	GLY	3.6
1	E	94	CYS	3.6
1	K	90	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	44	LEU	3.2
1	L	27	SER	3.0
1	E	96	GLY	3.0
1	H	95	THR	3.0
1	E	122	GLY	2.9
1	D	133	SER	2.9
1	E	127	ILE	2.9
1	E	44	LEU	2.9
1	L	28	GLY	2.8
1	J	28	GLY	2.8
1	J	122	GLY	2.8
1	B	31	THR	2.7
1	G	125	ALA	2.7
1	J	125	ALA	2.7
1	D	95	THR	2.7
1	E	118	THR	2.7
1	M	15	GLY	2.6
1	E	124	LEU	2.5
1	J	58	TYR	2.5
1	E	5	ASP	2.4
1	E	47	ILE	2.4
1	C	122	GLY	2.3
1	E	75	ASP	2.3
1	L	118	THR	2.3
1	H	41	TYR	2.3
1	M	93	ARG	2.3
1	B	35	PHE	2.3
1	E	43	LEU	2.3
1	B	123	LYS	2.3
1	G	41	TYR	2.3
1	H	40	GLN	2.3
1	B	125	ALA	2.2
1	L	109	ALA	2.2
1	L	126	GLY	2.2
1	D	94	CYS	2.2
1	B	28	GLY	2.2
1	M	94	CYS	2.2
1	K	69	VAL	2.2
1	H	125	ALA	2.2
1	B	135	ILE	2.1
1	E	86	TYR	2.1
1	K	125	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	31	THR	2.1
1	J	41	TYR	2.1
1	E	128	LYS	2.1
1	D	44	LEU	2.1
1	B	122	GLY	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 monosaccharides 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.