



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:42 am BST

PDB ID : 1ZS3
Title : The crystal structure of the Lactococcus lactis MG1363 DpsB protein
Authors : Stillman, T.J.; Upadhyay, M.; Norte, V.A.; Sedelnikova, S.E.; Carradus, M.;
Tzokov, S.; Bullough, P.A.; Shearman, C.A.; Gasson, M.J.; Williams, C.H.;
Artymiuk, P.J.; Green, J.
Deposited on : 2005-05-23
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

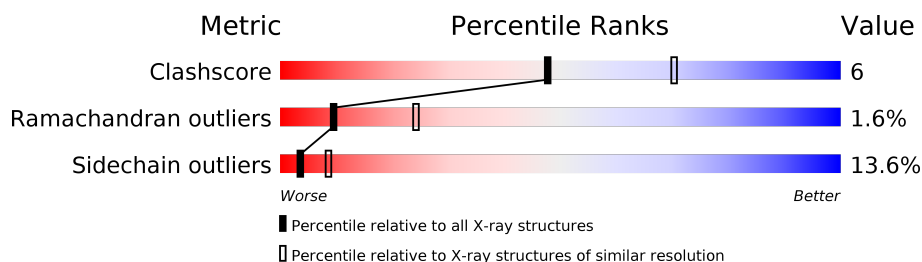
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	71% 21% 6%
1	B	182	71% 19% 6%
1	C	182	66% 20% 6%
1	D	182	70% 21% 6%
1	E	182	74% 16% 6%
1	F	182	67% 23% 6%
1	G	182	70% 19% 6%
1	H	182	71% 18% 6%

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Mol	Chain	Length	Quality of chain
1	I	182	<div><div></div><div>70%18%••6%</div></div>
1	J	182	<div><div></div><div>62%29%•6%</div></div>
1	K	182	<div><div></div><div>68%21%••6%</div></div>
1	L	182	<div><div></div><div>71%19%••6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16775 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 Lactococcus lactis MG1363 DpsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	B	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	C	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	D	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	E	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	F	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	G	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	H	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	I	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	J	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	K	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			
1	L	171	Total	C	N	O	S	0	0	0
			1387	897	223	263	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	13	Total	O	0	0
			13	13		

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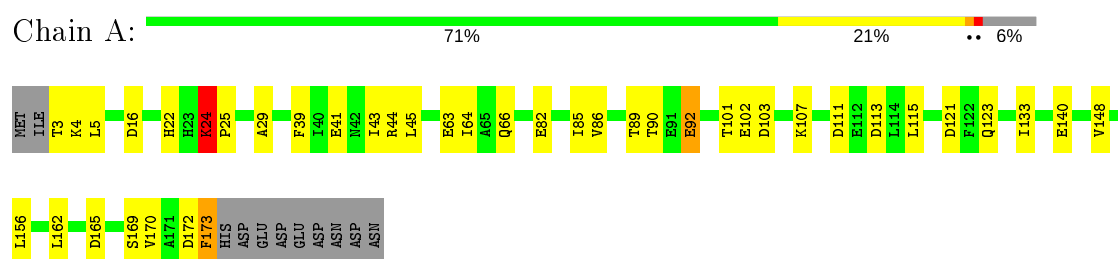
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	9	Total 9	O 9	0	0
2	D	13	Total 13	O 13	0	0
2	E	13	Total 13	O 13	0	0
2	F	10	Total 10	O 10	0	0
2	G	15	Total 15	O 15	0	0
2	H	8	Total 8	O 8	0	0
2	I	13	Total 13	O 13	0	0
2	J	6	Total 6	O 6	0	0
2	K	12	Total 12	O 12	0	0
2	L	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

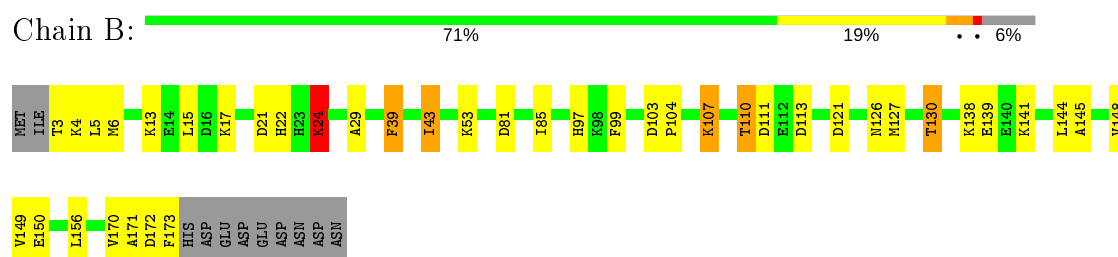
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

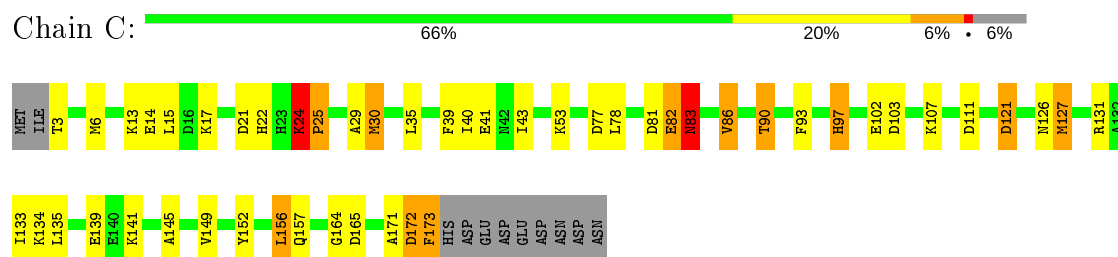
• Molecule 1: Lactococcus lactis MG1363 DpsA



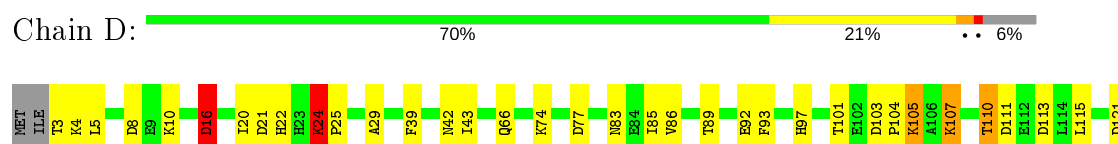
• Molecule 1: Lactococcus lactis MG1363 DpsA



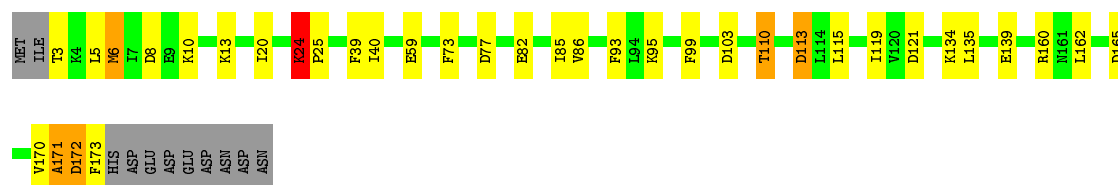
• Molecule 1: Lactococcus lactis MG1363 DpsA



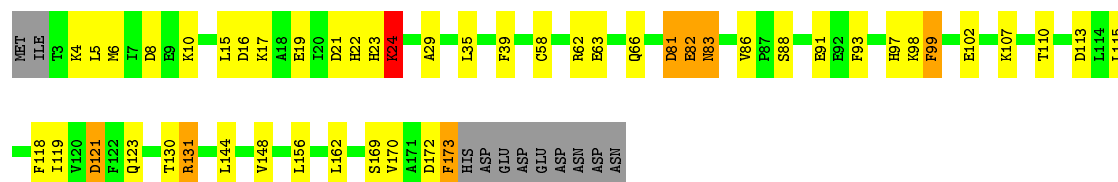
• Molecule 1: Lactococcus lactis MG1363 DpsA



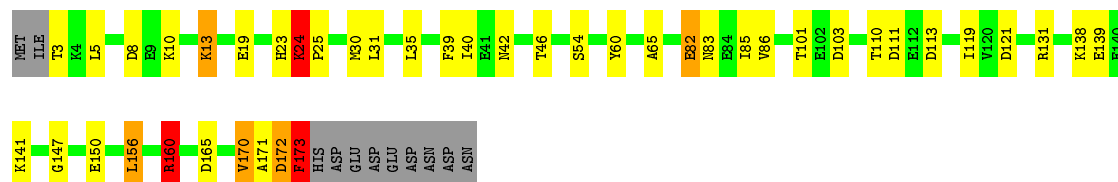
- Molecule 1: *Lactococcus lactis* MG1363 DpsA



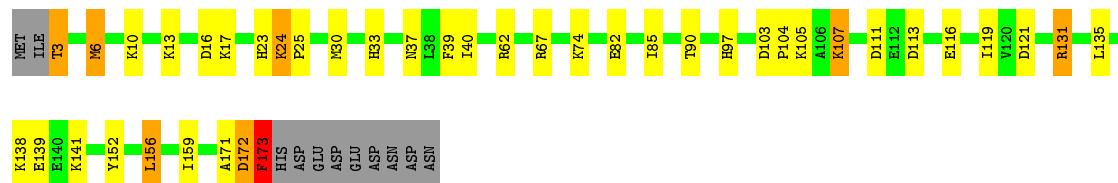
- Molecule 1: *Lactococcus lactis* MG1363 DpsA



- Molecule 1: *Lactococcus lactis* MG1363 DpsA



- Molecule 1: *Lactococcus lactis* MG1363 DpsA

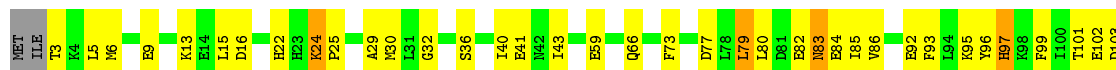


- Molecule 1: *Lactococcus lactis* MG1363 DpsA

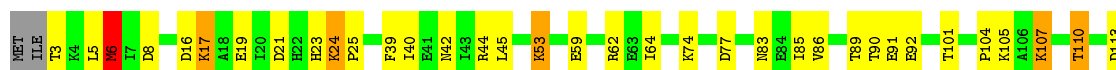




- Molecule 1: *Lactococcus lactis* MG1363 DpsA



- Molecule 1: *Lactococcus lactis* MG1363 DpsA



- Molecule 1: *Lactococcus lactis* MG1363 DpsA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.98Å 128.38Å 193.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.3 (15.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16775	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

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	0.86	0/1414	0.91	5/1907 (0.3%)
1	B	0.98	2/1414 (0.1%)	0.96	3/1907 (0.2%)
1	C	0.90	1/1414 (0.1%)	0.95	7/1907 (0.4%)
1	D	1.01	2/1414 (0.1%)	1.01	6/1907 (0.3%)
1	E	0.96	2/1414 (0.1%)	0.95	7/1907 (0.4%)
1	F	0.94	0/1414	1.00	6/1907 (0.3%)
1	G	1.00	4/1414 (0.3%)	1.03	7/1907 (0.4%)
1	H	0.95	2/1414 (0.1%)	0.98	7/1907 (0.4%)
1	I	1.72	6/1414 (0.4%)	1.04	9/1907 (0.5%)
1	J	0.91	1/1414 (0.1%)	0.96	6/1907 (0.3%)
1	K	1.04	5/1414 (0.4%)	1.13	13/1907 (0.7%)
1	L	0.87	0/1414	0.91	5/1907 (0.3%)
All	All	1.03	25/16968 (0.1%)	0.99	81/22884 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	2
1	L	0	1
All	All	0	13

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	9	GLU	CD-OE1	41.07	1.70	1.25
1	I	9	GLU	CD-OE2	29.05	1.57	1.25
1	K	173	PHE	N-CA	14.25	1.74	1.46
1	I	91	GLU	CD-OE2	10.75	1.37	1.25
1	I	6	MET	SD-CE	9.91	2.33	1.77
1	I	91	GLU	CD-OE1	9.16	1.35	1.25
1	G	13	LYS	CE-NZ	8.41	1.70	1.49
1	D	173	PHE	C-O	-8.10	1.07	1.23
1	G	173	PHE	N-CA	6.82	1.59	1.46
1	I	172	ASP	CB-CG	6.78	1.66	1.51
1	K	62	ARG	NE-CZ	-6.66	1.24	1.33
1	K	172	ASP	C-N	5.96	1.47	1.34
1	E	173	PHE	N-CA	5.77	1.57	1.46
1	J	9	GLU	CD-OE2	5.70	1.31	1.25
1	E	173	PHE	C-O	5.60	1.33	1.23
1	H	173	PHE	N-CA	5.58	1.57	1.46
1	B	13	LYS	CD-CE	5.47	1.65	1.51
1	H	173	PHE	CG-CD1	5.45	1.47	1.38
1	D	173	PHE	CB-CG	5.43	1.60	1.51
1	B	150	GLU	CD-OE1	5.31	1.31	1.25
1	G	60	TYR	CD2-CE2	5.29	1.47	1.39
1	G	173	PHE	CB-CG	5.25	1.60	1.51
1	K	173	PHE	CE2-CZ	5.18	1.47	1.37
1	C	127	MET	SD-CE	5.04	2.06	1.77
1	K	6	MET	SD-CE	5.01	2.05	1.77

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	62	ARG	NE-CZ-NH2	16.21	128.41	120.30
1	K	172	ASP	CB-CG-OD2	11.62	128.76	118.30
1	I	9	GLU	OE1-CD-OE2	10.75	136.20	123.30
1	G	172	ASP	CB-CG-OD2	10.58	127.83	118.30
1	F	172	ASP	CB-CG-OD2	10.37	127.64	118.30
1	G	8	ASP	CB-CG-OD2	9.87	127.19	118.30
1	C	172	ASP	CB-CG-OD2	8.83	126.25	118.30
1	D	121	ASP	CB-CG-OD2	8.73	126.15	118.30
1	K	77	ASP	CB-CG-OD2	8.51	125.96	118.30
1	H	172	ASP	CB-CG-OD2	8.40	125.86	118.30
1	F	16	ASP	CB-CG-OD2	8.37	125.83	118.30
1	B	103	ASP	CB-CG-OD2	8.20	125.68	118.30
1	J	121	ASP	CB-CG-OD2	8.08	125.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	173	PHE	N-CA-C	7.78	132.01	111.00
1	I	165	ASP	CB-CG-OD2	7.70	125.23	118.30
1	I	121	ASP	CB-CG-OD2	7.67	125.20	118.30
1	B	121	ASP	CB-CG-OD2	7.67	125.20	118.30
1	J	165	ASP	CB-CG-OD2	7.62	125.16	118.30
1	J	77	ASP	CB-CG-OD2	7.43	124.99	118.30
1	E	8	ASP	CB-CG-OD2	7.24	124.82	118.30
1	E	165	ASP	CB-CG-OD2	7.09	124.68	118.30
1	D	111	ASP	CB-CG-OD2	7.04	124.64	118.30
1	E	103	ASP	CB-CG-OD2	7.04	124.63	118.30
1	C	121	ASP	CB-CG-OD2	6.99	124.59	118.30
1	D	21	ASP	CB-CG-OD1	6.98	124.58	118.30
1	J	103	ASP	CB-CG-OD2	6.90	124.51	118.30
1	G	111	ASP	CB-CG-OD2	6.88	124.49	118.30
1	K	44	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	K	172	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	K	16	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	77	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	113	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	103	ASP	CB-CG-OD2	6.58	124.22	118.30
1	D	16	ASP	CB-CG-OD2	6.54	124.19	118.30
1	K	8	ASP	CB-CG-OD2	6.53	124.17	118.30
1	K	160	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	K	62	ARG	CD-NE-CZ	6.49	132.69	123.60
1	L	16	ASP	CB-CG-OD2	6.38	124.05	118.30
1	E	121	ASP	CB-CG-OD2	6.17	123.86	118.30
1	F	121	ASP	CB-CG-OD2	6.16	123.84	118.30
1	I	81	ASP	CB-CG-OD2	6.12	123.80	118.30
1	E	77	ASP	CB-CG-OD2	6.05	123.75	118.30
1	L	8	ASP	CB-CG-OD2	6.04	123.74	118.30
1	K	62	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	I	44	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	F	81	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	165	ASP	CB-CG-OD2	5.97	123.68	118.30
1	G	121	ASP	CB-CG-OD2	5.95	123.65	118.30
1	G	160	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	103	ASP	CB-CG-OD2	5.87	123.58	118.30
1	K	121	ASP	CB-CG-OD2	5.85	123.56	118.30
1	L	173	PHE	CB-CG-CD1	5.84	124.89	120.80
1	C	165	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	44	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	111	ASP	CB-CG-OD2	5.80	123.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	131	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	I	103	ASP	CB-CG-OD2	5.67	123.40	118.30
1	J	111	ASP	CB-CG-OD2	5.67	123.40	118.30
1	H	103	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	111	ASP	CB-CG-OD2	5.64	123.38	118.30
1	G	103	ASP	CB-CG-OD2	5.62	123.36	118.30
1	I	172	ASP	CB-CG-OD1	5.59	123.33	118.30
1	H	16	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	21	ASP	CB-CG-OD2	5.58	123.32	118.30
1	I	6	MET	CG-SD-CE	-5.58	91.28	100.20
1	H	131	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	D	77	ASP	CB-CG-OD2	5.55	123.29	118.30
1	H	113	ASP	CB-CG-OD2	5.47	123.23	118.30
1	H	111	ASP	CB-CG-OD2	5.46	123.22	118.30
1	K	172	ASP	C-N-CA	-5.41	108.19	121.70
1	F	21	ASP	CB-CG-OD2	5.37	123.14	118.30
1	I	111	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	165	ASP	CB-CG-OD2	5.32	123.09	118.30
1	J	173	PHE	CB-CG-CD1	5.29	124.50	120.80
1	L	77	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	172	ASP	CB-CG-OD2	5.17	122.96	118.30
1	G	165	ASP	CB-CG-OD2	5.06	122.86	118.30
1	L	121	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	111	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	113	ASP	CB-CG-OD1	5.02	122.82	118.30
1	H	121	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	LYS	Peptide
1	B	24	LYS	Peptide
1	C	24	LYS	Peptide
1	D	24	LYS	Peptide
1	E	24	LYS	Peptide
1	F	24	LYS	Peptide
1	G	24	LYS	Peptide
1	H	24	LYS	Peptide
1	I	24	LYS	Peptide
1	J	24	LYS	Peptide
1	K	172	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	K	24	LYS	Peptide
1	L	24	LYS	Peptide

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	1387	0	1386	14	0
1	B	1387	0	1386	19	0
1	C	1387	0	1386	22	0
1	D	1387	0	1386	13	0
1	E	1387	0	1386	18	0
1	F	1387	0	1386	24	0
1	G	1387	0	1386	17	0
1	H	1387	0	1386	15	0
1	I	1387	0	1386	21	0
1	J	1387	0	1386	23	0
1	K	1387	0	1386	20	0
1	L	1387	0	1386	15	0
2	A	12	0	0	0	0
2	B	13	0	0	1	0
2	C	9	0	0	0	0
2	D	13	0	0	0	0
2	E	13	0	0	3	0
2	F	10	0	0	3	0
2	G	15	0	0	4	0
2	H	8	0	0	4	0
2	I	13	0	0	1	0
2	J	6	0	0	5	0
2	K	12	0	0	4	0
2	L	7	0	0	1	0
All	All	16775	0	16632	202	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 6.

All (202) 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:G:13:LYS:CE	1:G:13:LYS:NZ	1.70	1.52
1:K:173:PHE:CA	1:K:173:PHE:N	1.74	1.47
1:E:6:MET:CE	1:E:6:MET:SD	2.03	1.46
1:B:127:MET:SD	1:B:127:MET:CE	2.05	1.44
1:K:6:MET:CE	1:K:6:MET:SD	2.05	1.43
1:C:127:MET:CE	1:C:127:MET:SD	2.06	1.43
1:I:9:GLU:OE1	1:I:9:GLU:CD	1.70	1.29
1:G:119:ILE:HG21	2:G:183:HOH:O	1.33	1.23
1:J:173:PHE:CD1	2:J:183:HOH:O	1.92	1.23
1:G:173:PHE:CG	2:G:183:HOH:O	1.88	1.23
1:I:6:MET:CE	1:I:6:MET:SD	2.33	1.17
1:H:119:ILE:HG21	2:H:183:HOH:O	1.51	1.10
1:H:173:PHE:CG	2:H:183:HOH:O	2.08	1.06
1:I:82:GLU:HG2	1:I:141:LYS:HD2	1.50	0.94
1:B:139:GLU:OE2	1:B:141:LYS:HE3	1.69	0.93
1:D:110:THR:HG22	1:D:113:ASP:H	1.39	0.87
1:G:173:PHE:CD2	2:G:183:HOH:O	2.14	0.86
1:I:82:GLU:HG2	1:I:141:LYS:CD	2.07	0.85
1:B:173:PHE:HB3	2:B:186:HOH:O	1.78	0.83
1:K:173:PHE:HB3	2:K:183:HOH:O	1.78	0.83
1:K:173:PHE:HD2	2:K:183:HOH:O	1.67	0.77
1:F:173:PHE:CD1	2:F:192:HOH:O	2.36	0.77
1:E:119:ILE:HG21	2:E:188:HOH:O	1.83	0.77
1:K:173:PHE:CD2	2:K:183:HOH:O	2.38	0.77
1:L:173:PHE:CD1	2:L:183:HOH:O	2.38	0.76
1:B:104:PRO:O	1:B:107:LYS:HE2	1.86	0.75
1:I:171:ALA:O	1:I:172:ASP:C	2.29	0.71
1:J:173:PHE:CG	2:J:183:HOH:O	2.29	0.71
1:I:173:PHE:O	2:I:185:HOH:O	2.08	0.70
1:F:24:LYS:O	1:F:24:LYS:HG2	1.90	0.70
1:F:119:ILE:O	1:F:123:GLN:HG3	1.91	0.69
1:K:172:ASP:C	1:K:173:PHE:CA	2.61	0.69
1:F:22:HIS:ND1	1:F:29:ALA:HB1	2.08	0.69
1:J:119:ILE:HG21	2:J:183:HOH:O	1.92	0.69
1:F:24:LYS:O	1:F:24:LYS:CG	2.41	0.69
1:K:89:THR:OG1	1:K:92:GLU:HG3	1.93	0.68
1:C:82:GLU:OE2	1:C:141:LYS:HB3	1.95	0.67
1:F:110:THR:HG23	1:F:113:ASP:H	1.60	0.66
1:H:173:PHE:CD1	2:H:183:HOH:O	2.42	0.66
1:J:171:ALA:O	1:J:172:ASP:C	2.35	0.65
1:D:104:PRO:O	1:D:107:LYS:HE2	1.96	0.65
1:C:152:TYR:OH	1:J:82:GLU:OE1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ASP:OD2	1:D:105:LYS:HD3	1.99	0.63
1:H:104:PRO:O	1:H:107:LYS:HE2	1.99	0.62
1:K:173:PHE:N	1:K:173:PHE:CB	2.60	0.62
1:F:102:GLU:OE2	1:H:90:THR:OG1	2.12	0.61
1:J:22:HIS:ND1	1:J:29:ALA:HB1	2.14	0.61
1:E:110:THR:HG22	1:E:113:ASP:H	1.64	0.61
1:F:83:ASN:C	1:F:83:ASN:HD22	2.04	0.61
1:D:16:ASP:O	1:D:20:ILE:HD12	2.00	0.61
1:E:119:ILE:HD13	2:E:188:HOH:O	2.02	0.60
1:J:173:PHE:C	2:J:188:HOH:O	2.40	0.60
1:K:110:THR:HG22	1:K:113:ASP:H	1.65	0.60
1:C:78:LEU:O	1:C:81:ASP:HB2	2.02	0.60
1:C:134:LYS:HE2	1:J:140:GLU:OE2	2.00	0.60
1:K:173:PHE:N	1:K:173:PHE:CG	2.70	0.60
1:E:119:ILE:CG2	2:E:188:HOH:O	2.43	0.59
1:F:173:PHE:CD1	1:F:173:PHE:N	2.70	0.59
1:H:152:TYR:CZ	1:H:156:LEU:HD11	2.37	0.59
1:C:135:LEU:O	1:C:139:GLU:HG3	2.04	0.58
1:G:139:GLU:OE2	1:G:141:LYS:NZ	2.37	0.57
1:I:24:LYS:CG	1:I:24:LYS:O	2.52	0.57
1:D:110:THR:HG22	1:D:113:ASP:N	2.17	0.56
1:C:35:LEU:CD1	1:C:86:VAL:HG22	2.36	0.56
1:D:171:ALA:O	1:D:172:ASP:C	2.45	0.55
1:H:171:ALA:O	1:H:172:ASP:C	2.44	0.55
1:J:73:PHE:CZ	1:L:46:THR:HG23	2.41	0.55
1:J:173:PHE:CE1	2:J:183:HOH:O	2.39	0.54
1:B:81:ASP:HB3	1:G:156:LEU:HB3	1.89	0.54
1:E:135:LEU:O	1:E:139:GLU:HG3	2.06	0.54
1:C:22:HIS:ND1	1:C:29:ALA:HB1	2.23	0.54
1:H:173:PHE:CD2	2:H:183:HOH:O	2.47	0.54
1:I:93:PHE:O	1:I:97:HIS:HB3	2.07	0.54
1:H:23:HIS:O	1:H:25:PRO:HD3	2.09	0.53
1:J:144:LEU:O	1:J:148:VAL:HG23	2.09	0.53
1:L:171:ALA:O	1:L:172:ASP:C	2.46	0.53
1:B:24:LYS:O	1:B:24:LYS:CG	2.56	0.53
1:K:17:LYS:HE3	1:K:21:ASP:OD2	2.09	0.53
1:A:90:THR:OG1	1:C:102:GLU:OE2	2.23	0.53
1:C:173:PHE:CD1	1:C:173:PHE:N	2.77	0.53
1:G:110:THR:HG23	1:G:113:ASP:H	1.74	0.53
1:L:110:THR:HG22	1:L:113:ASP:CG	2.29	0.52
1:J:41:GLU:OE2	1:J:125:GLN:NE2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:O	1:F:83:ASN:ND2	2.44	0.51
1:C:41:GLU:OE2	1:C:121:ASP:HB3	2.11	0.51
1:E:115:LEU:HG	1:E:162:LEU:HD22	1.93	0.51
1:I:110:THR:CG2	1:I:113:ASP:H	2.23	0.51
1:C:93:PHE:O	1:C:97:HIS:HB3	2.11	0.51
1:D:22:HIS:ND1	1:D:29:ALA:HB1	2.25	0.51
1:J:116:GLU:HA	1:J:119:ILE:HD12	1.92	0.51
1:J:93:PHE:O	1:J:97:HIS:HB3	2.11	0.51
1:K:173:PHE:CB	2:K:183:HOH:O	2.48	0.51
1:K:45:LEU:HD13	1:K:64:ILE:HG22	1.93	0.50
1:A:133:ILE:CG1	1:A:148:VAL:HG12	2.41	0.50
1:E:110:THR:CG2	1:E:113:ASP:H	2.24	0.50
1:G:82:GLU:HG2	1:G:141:LYS:CE	2.41	0.50
1:A:45:LEU:HD13	1:A:64:ILE:HG22	1.93	0.49
1:B:110:THR:HG22	1:B:113:ASP:OD2	2.12	0.49
1:E:110:THR:HG22	1:E:113:ASP:CB	2.42	0.49
1:H:119:ILE:HG23	1:H:159:ILE:HG23	1.94	0.49
1:A:102:GLU:OE2	1:C:90:THR:OG1	2.25	0.49
1:I:99:PHE:HE1	1:I:128:PHE:CE1	2.31	0.49
1:D:89:THR:OG1	1:D:92:GLU:HG3	2.12	0.48
1:G:42:ASN:HD22	1:G:65:ALA:HB1	1.79	0.48
1:B:145:ALA:O	1:B:149:VAL:HG23	2.13	0.48
1:F:115:LEU:HG	1:F:162:LEU:HD22	1.95	0.48
1:A:133:ILE:HG13	1:A:148:VAL:HG12	1.94	0.48
1:I:82:GLU:HG2	1:I:141:LYS:HD3	1.92	0.48
1:F:93:PHE:O	1:F:97:HIS:HB3	2.14	0.48
1:I:110:THR:HG22	1:I:113:ASP:CG	2.34	0.48
1:C:171:ALA:O	1:C:172:ASP:C	2.52	0.48
1:G:171:ALA:O	1:G:172:ASP:C	2.53	0.47
1:K:39:PHE:O	1:K:42:ASN:HB3	2.14	0.47
1:E:110:THR:HG22	1:E:113:ASP:CG	2.34	0.47
1:H:3:THR:HA	1:H:6:MET:HG2	1.95	0.47
1:I:110:THR:HG22	1:I:113:ASP:H	1.79	0.47
1:D:93:PHE:O	1:D:97:HIS:HB3	2.13	0.47
1:B:139:GLU:OE2	1:B:141:LYS:CE	2.53	0.47
1:C:83:ASN:C	1:C:83:ASN:HD22	2.18	0.47
1:L:126:ASN:HD21	1:L:156:LEU:HD13	1.79	0.47
1:G:173:PHE:CD1	2:G:183:HOH:O	2.41	0.47
1:H:33:HIS:O	1:H:37:ASN:ND2	2.48	0.47
1:L:51:TYR:CG	1:L:107:LYS:HB2	2.50	0.47
1:L:106:ALA:HA	1:L:109:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HB3	1:L:81:ASP:HB3	1.97	0.46
1:A:3:THR:O	1:A:5:LEU:N	2.48	0.46
1:F:58:CYS:O	1:F:62:ARG:HG3	2.15	0.46
1:J:168:LYS:HG2	1:J:172:ASP:OD2	2.14	0.46
1:G:147:GLY:O	1:G:150:GLU:HB2	2.16	0.46
1:F:82:GLU:OE1	1:K:152:TYR:OH	2.26	0.46
1:K:171:ALA:O	1:K:172:ASP:C	2.54	0.46
1:F:81:ASP:HB3	1:K:156:LEU:HB3	1.98	0.46
1:G:82:GLU:HG2	1:G:141:LYS:CD	2.46	0.46
1:K:53:LYS:HD3	1:K:53:LYS:N	2.31	0.46
1:L:173:PHE:CD1	1:L:173:PHE:N	2.83	0.46
1:A:115:LEU:HG	1:A:162:LEU:HD22	1.97	0.45
1:B:22:HIS:ND1	1:B:29:ALA:HB1	2.32	0.45
1:J:95:LYS:HD3	1:J:96:TYR:CE2	2.51	0.45
1:I:41:GLU:OE2	1:I:121:ASP:HB3	2.16	0.45
1:E:110:THR:HG22	1:E:113:ASP:N	2.32	0.45
1:E:6:MET:CE	1:E:6:MET:CG	2.92	0.45
1:F:35:LEU:CD1	1:F:86:VAL:HG22	2.47	0.45
1:H:139:GLU:OE2	1:H:141:LYS:CE	2.65	0.45
1:I:24:LYS:HG3	1:I:24:LYS:O	2.16	0.45
1:L:104:PRO:O	1:L:107:LYS:HE2	2.17	0.45
1:B:110:THR:HG23	1:B:113:ASP:H	1.82	0.45
1:I:99:PHE:CE1	1:I:128:PHE:CE1	3.04	0.44
1:J:173:PHE:CD1	1:J:173:PHE:N	2.85	0.44
1:A:41:GLU:OE1	1:A:121:ASP:OD1	2.35	0.44
1:E:40:ILE:CD1	1:E:93:PHE:HB3	2.47	0.44
1:B:43:ILE:HD13	1:D:39:PHE:CE2	2.53	0.44
1:J:85:ILE:HG23	1:J:86:VAL:N	2.32	0.44
1:A:89:THR:OG1	1:A:92:GLU:HG3	2.17	0.44
1:F:118:PHE:HA	1:F:121:ASP:HB2	2.00	0.44
1:E:73:PHE:CZ	1:G:46:THR:HG23	2.53	0.44
1:J:32:GLY:O	1:J:36:SER:OG	2.28	0.44
1:C:145:ALA:O	1:C:149:VAL:HG23	2.17	0.44
1:C:24:LYS:HG3	1:C:24:LYS:O	2.17	0.44
1:E:171:ALA:O	1:E:172:ASP:C	2.56	0.44
1:L:110:THR:HG22	1:L:113:ASP:OD2	2.18	0.43
1:C:133:ILE:HD13	1:J:142:PHE:CD1	2.53	0.43
1:F:23:HIS:CD2	2:F:191:HOH:O	2.71	0.43
1:D:4:LYS:O	1:D:8:ASP:OD2	2.36	0.43
1:E:170:VAL:O	1:E:171:ALA:C	2.56	0.43
1:K:104:PRO:O	1:K:107:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ASN:HD21	1:C:156:LEU:HD13	1.84	0.43
1:I:24:LYS:O	1:I:25:PRO:C	2.57	0.43
1:D:74:LYS:NZ	1:D:150:GLU:OE2	2.52	0.43
1:J:79:LEU:O	1:J:82:GLU:N	2.51	0.43
1:I:98:LYS:O	1:I:99:PHE:HB2	2.19	0.42
1:J:102:GLU:HB3	1:L:89:THR:HG22	2.00	0.42
1:A:22:HIS:CE1	1:A:29:ALA:HB1	2.54	0.42
1:B:17:LYS:HE2	1:B:21:ASP:OD2	2.19	0.42
1:H:135:LEU:O	1:H:139:GLU:HG3	2.19	0.42
1:F:173:PHE:HD1	2:F:192:HOH:O	1.88	0.42
1:F:98:LYS:O	1:F:99:PHE:HB2	2.19	0.42
1:C:134:LYS:CE	1:J:140:GLU:OE2	2.65	0.42
1:K:173:PHE:N	1:K:173:PHE:HA	2.10	0.42
1:A:140:GLU:OE1	1:E:134:LYS:NZ	2.52	0.42
1:F:162:LEU:HD23	1:F:162:LEU:HA	1.74	0.42
1:C:30:MET:CE	1:C:131:ARG:HB3	2.50	0.42
1:F:35:LEU:HD13	1:F:86:VAL:HG22	2.02	0.42
1:B:15:LEU:HA	1:B:15:LEU:HD23	1.78	0.42
1:A:22:HIS:ND1	1:A:29:ALA:HB1	2.35	0.41
1:G:160:ARG:HA	1:G:170:VAL:HG23	2.02	0.41
1:A:140:GLU:CD	1:E:134:LYS:NZ	2.74	0.41
1:H:139:GLU:OE2	1:H:141:LYS:HE2	2.21	0.41
1:I:51:TYR:CD1	1:I:107:LYS:HB2	2.56	0.41
1:L:40:ILE:HD13	1:L:97:HIS:HB3	2.03	0.41
1:F:144:LEU:O	1:F:148:VAL:HG23	2.20	0.41
1:G:31:LEU:O	1:G:35:LEU:HG	2.21	0.41
1:B:144:LEU:O	1:B:148:VAL:HG23	2.21	0.41
1:C:164:GLY:HA3	1:L:53:LYS:O	2.21	0.41
1:B:126:ASN:O	1:B:130:THR:HB	2.21	0.40
1:B:171:ALA:O	1:B:172:ASP:C	2.59	0.40
1:B:39:PHE:CE2	1:D:43:ILE:HD13	2.57	0.40
1:F:173:PHE:HD1	1:F:173:PHE:H	1.67	0.40
1:I:104:PRO:O	1:I:107:LYS:HE2	2.21	0.40
1:G:82:GLU:HG2	1:G:141:LYS:HD3	2.03	0.40
1:I:41:GLU:OE1	1:I:121:ASP:OD1	2.40	0.40
1:A:173:PHE:N	1:A:173:PHE:CD1	2.86	0.40
1:L:71:TYR:O	1:L:75:ILE:HG12	2.22	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	169/182 (93%)	160 (95%)	5 (3%)	4 (2%)	6	15
1	B	169/182 (93%)	162 (96%)	6 (4%)	1 (1%)	25	50
1	C	169/182 (93%)	157 (93%)	9 (5%)	3 (2%)	8	21
1	D	169/182 (93%)	161 (95%)	6 (4%)	2 (1%)	13	32
1	E	169/182 (93%)	158 (94%)	7 (4%)	4 (2%)	6	15
1	F	169/182 (93%)	160 (95%)	7 (4%)	2 (1%)	13	32
1	G	169/182 (93%)	161 (95%)	6 (4%)	2 (1%)	13	32
1	H	169/182 (93%)	159 (94%)	9 (5%)	1 (1%)	25	50
1	I	169/182 (93%)	158 (94%)	7 (4%)	4 (2%)	6	15
1	J	169/182 (93%)	160 (95%)	4 (2%)	5 (3%)	4	10
1	K	169/182 (93%)	162 (96%)	5 (3%)	2 (1%)	13	32
1	L	169/182 (93%)	158 (94%)	9 (5%)	2 (1%)	13	32
All	All	2028/2184 (93%)	1916 (94%)	80 (4%)	32 (2%)	9	24

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	D	24	LYS
1	G	25	PRO
1	H	24	LYS
1	J	25	PRO
1	A	25	PRO
1	E	171	ALA
1	A	172	ASP
1	C	24	LYS
1	C	25	PRO
1	C	83	ASN
1	E	25	PRO

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Mol	Chain	Res	Type
1	J	80	LEU
1	L	52	ALA
1	F	99	PHE
1	G	24	LYS
1	J	79	LEU
1	J	83	ASN
1	B	99	PHE
1	E	99	PHE
1	F	24	LYS
1	I	24	LYS
1	I	25	PRO
1	I	52	ALA
1	I	99	PHE
1	J	99	PHE
1	D	25	PRO
1	E	24	LYS
1	K	24	LYS
1	A	24	LYS
1	K	25	PRO
1	L	25	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/159 (93%)	131 (88%)	17 (12%)	5	13
1	B	148/159 (93%)	133 (90%)	15 (10%)	7	17
1	C	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	D	148/159 (93%)	130 (88%)	18 (12%)	5	11
1	E	148/159 (93%)	133 (90%)	15 (10%)	7	17
1	F	148/159 (93%)	125 (84%)	23 (16%)	2	7
1	G	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	H	148/159 (93%)	127 (86%)	21 (14%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	J	148/159 (93%)	124 (84%)	24 (16%)	2	6
1	K	148/159 (93%)	122 (82%)	26 (18%)	2	4
1	L	148/159 (93%)	128 (86%)	20 (14%)	4	9
All	All	1776/1908 (93%)	1534 (86%)	242 (14%)	3	8

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	24	LYS
1	A	39	PHE
1	A	43	ILE
1	A	63	GLU
1	A	66	GLN
1	A	82	GLU
1	A	85	ILE
1	A	86	VAL
1	A	92	GLU
1	A	101	THR
1	A	107	LYS
1	A	123	GLN
1	A	156	LEU
1	A	169	SER
1	A	170	VAL
1	A	173	PHE
1	B	3	THR
1	B	4	LYS
1	B	5	LEU
1	B	6	MET
1	B	24	LYS
1	B	39	PHE
1	B	43	ILE
1	B	53	LYS
1	B	85	ILE
1	B	97	HIS
1	B	107	LYS
1	B	110	THR
1	B	130	THR
1	B	138	LYS
1	B	170	VAL

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Mol	Chain	Res	Type
1	C	3	THR
1	C	6	MET
1	C	13	LYS
1	C	14	GLU
1	C	15	LEU
1	C	17	LYS
1	C	25	PRO
1	C	30	MET
1	C	39	PHE
1	C	40	ILE
1	C	43	ILE
1	C	53	LYS
1	C	82	GLU
1	C	83	ASN
1	C	86	VAL
1	C	90	THR
1	C	97	HIS
1	C	107	LYS
1	C	156	LEU
1	C	157	GLN
1	C	173	PHE
1	D	3	THR
1	D	5	LEU
1	D	10	LYS
1	D	16	ASP
1	D	24	LYS
1	D	42	ASN
1	D	66	GLN
1	D	83	ASN
1	D	85	ILE
1	D	86	VAL
1	D	101	THR
1	D	105	LYS
1	D	107	LYS
1	D	110	THR
1	D	115	LEU
1	D	131	ARG
1	D	138	LYS
1	D	156	LEU
1	E	3	THR
1	E	5	LEU
1	E	6	MET

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Mol	Chain	Res	Type
1	E	10	LYS
1	E	13	LYS
1	E	20	ILE
1	E	24	LYS
1	E	39	PHE
1	E	59	GLU
1	E	82	GLU
1	E	85	ILE
1	E	86	VAL
1	E	95	LYS
1	E	110	THR
1	E	160	ARG
1	F	4	LYS
1	F	5	LEU
1	F	6	MET
1	F	8	ASP
1	F	10	LYS
1	F	15	LEU
1	F	17	LYS
1	F	19	GLU
1	F	24	LYS
1	F	39	PHE
1	F	63	GLU
1	F	66	GLN
1	F	82	GLU
1	F	83	ASN
1	F	88	SER
1	F	91	GLU
1	F	107	LYS
1	F	130	THR
1	F	131	ARG
1	F	156	LEU
1	F	169	SER
1	F	170	VAL
1	F	173	PHE
1	G	3	THR
1	G	5	LEU
1	G	10	LYS
1	G	19	GLU
1	G	23	HIS
1	G	24	LYS
1	G	30	MET

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Mol	Chain	Res	Type
1	G	39	PHE
1	G	40	ILE
1	G	54	SER
1	G	82	GLU
1	G	83	ASN
1	G	85	ILE
1	G	86	VAL
1	G	101	THR
1	G	131	ARG
1	G	138	LYS
1	G	156	LEU
1	G	160	ARG
1	G	170	VAL
1	G	173	PHE
1	H	3	THR
1	H	6	MET
1	H	10	LYS
1	H	13	LYS
1	H	17	LYS
1	H	30	MET
1	H	39	PHE
1	H	40	ILE
1	H	62	ARG
1	H	67	ARG
1	H	74	LYS
1	H	82	GLU
1	H	85	ILE
1	H	97	HIS
1	H	105	LYS
1	H	107	LYS
1	H	116	GLU
1	H	131	ARG
1	H	138	LYS
1	H	156	LEU
1	H	173	PHE
1	I	3	THR
1	I	4	LYS
1	I	6	MET
1	I	9	GLU
1	I	10	LYS
1	I	13	LYS
1	I	15	LEU

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Mol	Chain	Res	Type
1	I	17	LYS
1	I	19	GLU
1	I	39	PHE
1	I	83	ASN
1	I	85	ILE
1	I	86	VAL
1	I	91	GLU
1	I	97	HIS
1	I	105	LYS
1	I	107	LYS
1	I	138	LYS
1	I	156	LEU
1	I	170	VAL
1	I	172	ASP
1	J	3	THR
1	J	5	LEU
1	J	6	MET
1	J	13	LYS
1	J	15	LEU
1	J	16	ASP
1	J	24	LYS
1	J	30	MET
1	J	40	ILE
1	J	43	ILE
1	J	59	GLU
1	J	66	GLN
1	J	83	ASN
1	J	84	GLU
1	J	92	GLU
1	J	97	HIS
1	J	101	THR
1	J	107	LYS
1	J	127	MET
1	J	130	THR
1	J	134	LYS
1	J	138	LYS
1	J	156	LEU
1	J	169	SER
1	K	3	THR
1	K	5	LEU
1	K	6	MET
1	K	17	LYS

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Mol	Chain	Res	Type
1	K	19	GLU
1	K	23	HIS
1	K	40	ILE
1	K	53	LYS
1	K	59	GLU
1	K	74	LYS
1	K	83	ASN
1	K	85	ILE
1	K	86	VAL
1	K	90	THR
1	K	91	GLU
1	K	101	THR
1	K	105	LYS
1	K	107	LYS
1	K	110	THR
1	K	130	THR
1	K	138	LYS
1	K	157	GLN
1	K	160	ARG
1	K	165	ASP
1	K	169	SER
1	K	173	PHE
1	L	3	THR
1	L	4	LYS
1	L	6	MET
1	L	17	LYS
1	L	19	GLU
1	L	24	LYS
1	L	39	PHE
1	L	40	ILE
1	L	42	ASN
1	L	43	ILE
1	L	53	LYS
1	L	82	GLU
1	L	85	ILE
1	L	88	SER
1	L	97	HIS
1	L	101	THR
1	L	115	LEU
1	L	156	LEU
1	L	170	VAL
1	L	173	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	B	23	HIS
1	B	83	ASN
1	B	123	GLN
1	C	83	ASN
1	C	123	GLN
1	C	161	ASN
1	D	83	ASN
1	D	137	ASN
1	E	83	ASN
1	E	123	GLN
1	F	42	ASN
1	F	83	ASN
1	G	42	ASN
1	G	83	ASN
1	G	123	GLN
1	H	83	ASN
1	H	123	GLN
1	I	42	ASN
1	I	123	GLN
1	K	83	ASN
1	K	123	GLN
1	K	137	ASN
1	L	83	ASN
1	L	161	ASN

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 carbohydrates 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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.