



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3IZL  
EMDB ID: : EMD-5248  
Title : Mm-cpn rls deltalid with ATP and AlFx  
Authors : Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.;  
Chiu, W.; Frydman, J.  
Deposited on : 2010-10-29  
Resolution : 6.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241



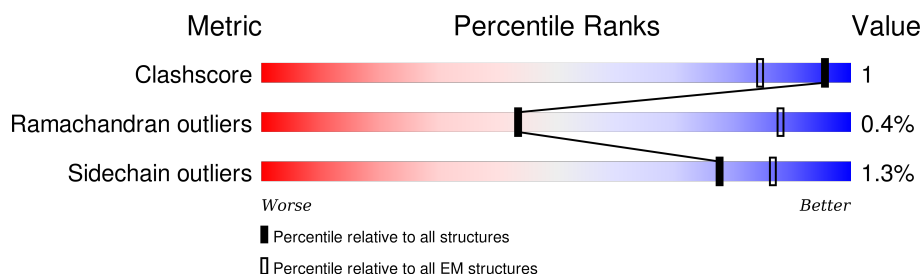
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.20 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	491	95% 5%
1	B	491	96% ..
1	C	491	96% .
1	D	491	96% .
1	E	491	96% .
1	F	491	96% .
1	G	491	96% .
1	H	491	96% ..
1	I	491	96% ..

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Mol	Chain	Length	Quality of chain
1	J	491	<div><div></div><div>95%</div><div>5%</div></div>
1	K	491	<div><div></div><div>96%</div><div></div></div>
1	L	491	<div><div></div><div>96%</div><div></div></div>
1	M	491	<div><div></div><div>96%</div><div></div></div>
1	N	491	<div><div></div><div>96%</div><div></div></div>
1	O	491	<div><div></div><div>96%</div><div></div></div>
1	P	491	<div><div></div><div>96%</div><div></div></div>



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 58448 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Mm-cpn rls deltalid.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	B	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	C	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	D	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	E	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	F	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	G	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	H	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	I	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	J	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	K	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	L	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	M	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	N	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	O	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		
1	P	491	Total	C	N	O	S	0	0
			3653	2266	633	730	24		

There are 144 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	LINKER	UNP Q877G8
A	236	THR	-	LINKER	UNP Q877G8
A	237	ALA	-	LINKER	UNP Q877G8
A	238	SER	-	LINKER	UNP Q877G8
A	239	GLU	-	LINKER	UNP Q877G8
A	299	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
A	300	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
A	302	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
A	303	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
B	726	GLU	-	LINKER	UNP Q877G8
B	727	THR	-	LINKER	UNP Q877G8
B	728	ALA	-	LINKER	UNP Q877G8
B	729	SER	-	LINKER	UNP Q877G8
B	730	GLU	-	LINKER	UNP Q877G8
B	790	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
B	791	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
B	793	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
B	794	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
C	1217	GLU	-	LINKER	UNP Q877G8
C	1218	THR	-	LINKER	UNP Q877G8
C	1219	ALA	-	LINKER	UNP Q877G8
C	1220	SER	-	LINKER	UNP Q877G8
C	1221	GLU	-	LINKER	UNP Q877G8
C	1281	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
C	1282	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
C	1284	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
C	1285	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
D	1708	GLU	-	LINKER	UNP Q877G8
D	1709	THR	-	LINKER	UNP Q877G8
D	1710	ALA	-	LINKER	UNP Q877G8
D	1711	SER	-	LINKER	UNP Q877G8
D	1712	GLU	-	LINKER	UNP Q877G8
D	1772	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
D	1773	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
D	1775	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
D	1776	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
E	2199	GLU	-	LINKER	UNP Q877G8
E	2200	THR	-	LINKER	UNP Q877G8
E	2201	ALA	-	LINKER	UNP Q877G8
E	2202	SER	-	LINKER	UNP Q877G8
E	2203	GLU	-	LINKER	UNP Q877G8
E	2263	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
E	2264	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2266	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
E	2267	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
F	2690	GLU	-	LINKER	UNP Q877G8
F	2691	THR	-	LINKER	UNP Q877G8
F	2692	ALA	-	LINKER	UNP Q877G8
F	2693	SER	-	LINKER	UNP Q877G8
F	2694	GLU	-	LINKER	UNP Q877G8
F	2754	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
F	2755	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
F	2757	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
F	2758	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
G	3181	GLU	-	LINKER	UNP Q877G8
G	3182	THR	-	LINKER	UNP Q877G8
G	3183	ALA	-	LINKER	UNP Q877G8
G	3184	SER	-	LINKER	UNP Q877G8
G	3185	GLU	-	LINKER	UNP Q877G8
G	3245	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
G	3246	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
G	3248	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
G	3249	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
H	3672	GLU	-	LINKER	UNP Q877G8
H	3673	THR	-	LINKER	UNP Q877G8
H	3674	ALA	-	LINKER	UNP Q877G8
H	3675	SER	-	LINKER	UNP Q877G8
H	3676	GLU	-	LINKER	UNP Q877G8
H	3736	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
H	3737	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
H	3739	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
H	3740	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
I	4163	GLU	-	LINKER	UNP Q877G8
I	4164	THR	-	LINKER	UNP Q877G8
I	4165	ALA	-	LINKER	UNP Q877G8
I	4166	SER	-	LINKER	UNP Q877G8
I	4167	GLU	-	LINKER	UNP Q877G8
I	4227	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
I	4228	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
I	4230	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
I	4231	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
J	4654	GLU	-	LINKER	UNP Q877G8
J	4655	THR	-	LINKER	UNP Q877G8
J	4656	ALA	-	LINKER	UNP Q877G8
J	4657	SER	-	LINKER	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	4658	GLU	-	LINKER	UNP Q877G8
J	4718	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
J	4719	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
J	4721	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
J	4722	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
K	5145	GLU	-	LINKER	UNP Q877G8
K	5146	THR	-	LINKER	UNP Q877G8
K	5147	ALA	-	LINKER	UNP Q877G8
K	5148	SER	-	LINKER	UNP Q877G8
K	5149	GLU	-	LINKER	UNP Q877G8
K	5209	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
K	5210	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
K	5212	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
K	5213	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
L	5636	GLU	-	LINKER	UNP Q877G8
L	5637	THR	-	LINKER	UNP Q877G8
L	5638	ALA	-	LINKER	UNP Q877G8
L	5639	SER	-	LINKER	UNP Q877G8
L	5640	GLU	-	LINKER	UNP Q877G8
L	5700	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
L	5701	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
L	5703	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
L	5704	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
M	6127	GLU	-	LINKER	UNP Q877G8
M	6128	THR	-	LINKER	UNP Q877G8
M	6129	ALA	-	LINKER	UNP Q877G8
M	6130	SER	-	LINKER	UNP Q877G8
M	6131	GLU	-	LINKER	UNP Q877G8
M	6191	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
M	6192	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
M	6194	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
M	6195	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
N	6618	GLU	-	LINKER	UNP Q877G8
N	6619	THR	-	LINKER	UNP Q877G8
N	6620	ALA	-	LINKER	UNP Q877G8
N	6621	SER	-	LINKER	UNP Q877G8
N	6622	GLU	-	LINKER	UNP Q877G8
N	6682	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
N	6683	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
N	6685	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
N	6686	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
O	7109	GLU	-	LINKER	UNP Q877G8

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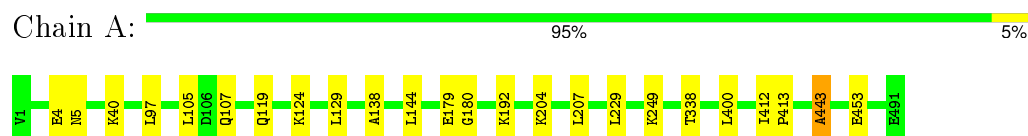
Chain	Residue	Modelled	Actual	Comment	Reference
O	7110	THR	-	LINKER	UNP Q877G8
O	7111	ALA	-	LINKER	UNP Q877G8
O	7112	SER	-	LINKER	UNP Q877G8
O	7113	GLU	-	LINKER	UNP Q877G8
O	7173	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
O	7174	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
O	7176	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
O	7177	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
P	7600	GLU	-	LINKER	UNP Q877G8
P	7601	THR	-	LINKER	UNP Q877G8
P	7602	ALA	-	LINKER	UNP Q877G8
P	7603	SER	-	LINKER	UNP Q877G8
P	7604	GLU	-	LINKER	UNP Q877G8
P	7664	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
P	7665	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
P	7667	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
P	7668	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8



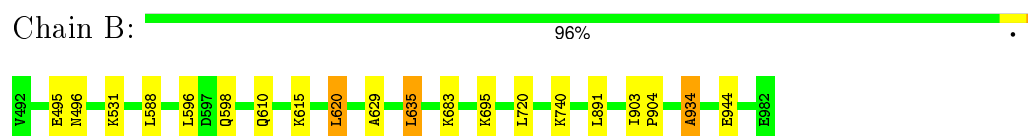
### 3 Residue-property plots [i](#)

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

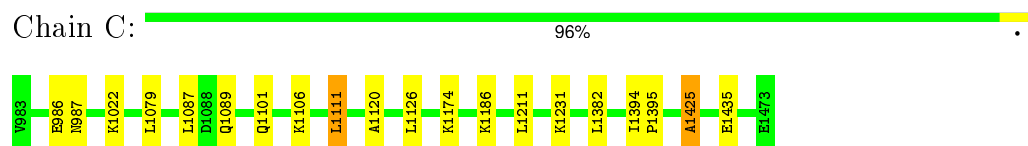
- Molecule 1: Mm-cpn rls deltalid



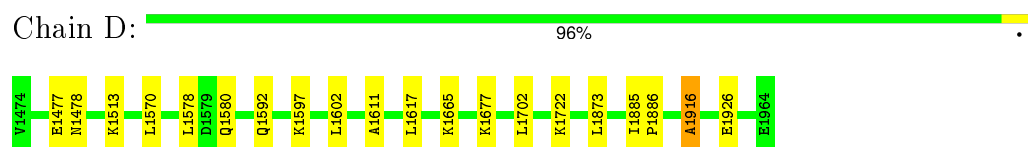
- Molecule 1: Mm-cpn rls deltalid



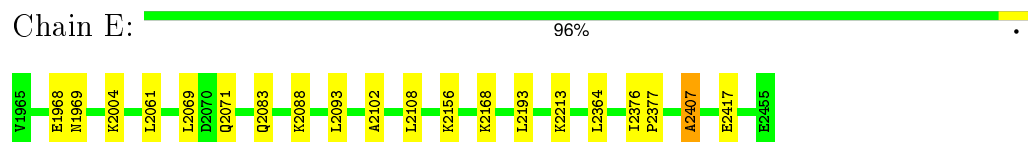
- Molecule 1: Mm-cpn rls deltalid



- Molecule 1: Mm-cpn rls deltalid



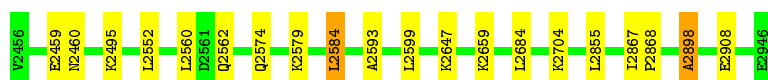
- Molecule 1: Mm-cpn rls deltalid



- Molecule 1: Mm-cpn rls deltalid







- Molecule 1: Mm-cpn rls deltalid

Chain G: 96% .



- Molecule 1: Mm-cpn rls deltalid

Chain H: 96% ..



- Molecule 1: Mm-cpn rls deltalid

Chain I: 96% ..



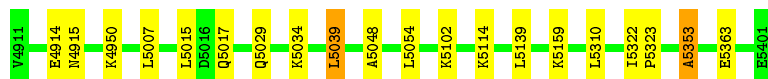
- Molecule 1: Mm-cpn rls deltalid

Chain J: 95% 5%



- Molecule 1: Mm-cpn rls deltalid

Chain K: 96% .



- Molecule 1: Mm-cpn rls deltalid

Chain L: 96% ..



- Molecule 1: Mm-cpn rls deltalid

Chain M: 96% .





- Molecule 1: Mm-cpn rls deltalid

Chain N: 96%



- Molecule 1: Mm-cpn rls deltalid

Chain O: 96%



- Molecule 1: Mm-cpn rls deltalid

Chain P: 96%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEM3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Gatan 4Kx4K CCD camera	Depositor



## 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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	B	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	C	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	D	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	E	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	F	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	G	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	H	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	I	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	J	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	K	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	L	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	M	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	N	0.87	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	O	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
1	P	0.88	1/3674 (0.0%)	0.76	2/4946 (0.0%)
All	All	0.88	16/58784 (0.0%)	0.76	32/79136 (0.0%)

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
All	All	0	48

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	6826	ALA	C-O	5.13	1.33	1.23
1	B	934	ALA	C-O	5.10	1.33	1.23
1	I	4371	ALA	C-O	5.09	1.33	1.23
1	A	443	ALA	C-O	5.09	1.33	1.23
1	C	1425	ALA	C-O	5.09	1.33	1.23
1	P	7808	ALA	C-O	5.09	1.33	1.23
1	J	4862	ALA	C-O	5.08	1.33	1.23
1	O	7317	ALA	C-O	5.08	1.32	1.23
1	F	2898	ALA	C-O	5.08	1.32	1.23
1	K	5353	ALA	C-O	5.08	1.32	1.23
1	E	2407	ALA	C-O	5.05	1.32	1.23
1	L	5844	ALA	C-O	5.05	1.32	1.23
1	D	1916	ALA	C-O	5.05	1.32	1.23
1	G	3389	ALA	C-O	5.05	1.32	1.23
1	H	3880	ALA	C-O	5.05	1.32	1.23
1	M	6335	ALA	C-O	5.05	1.32	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	GLU	CA-C-O	-6.67	106.10	120.10
1	F	2459	GLU	CA-C-O	-6.66	106.12	120.10
1	K	4914	GLU	CA-C-O	-6.66	106.12	120.10
1	C	986	GLU	CA-C-O	-6.65	106.13	120.10
1	E	1968	GLU	CA-C-O	-6.65	106.13	120.10
1	G	2950	GLU	CA-C-O	-6.65	106.13	120.10
1	D	1477	GLU	CA-C-O	-6.65	106.14	120.10
1	H	3441	GLU	CA-C-O	-6.65	106.14	120.10
1	I	3932	GLU	CA-C-O	-6.65	106.14	120.10
1	J	4423	GLU	CA-C-O	-6.65	106.14	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	5405	GLU	CA-C-O	-6.64	106.15	120.10
1	O	6878	GLU	CA-C-O	-6.63	106.17	120.10
1	P	7369	GLU	CA-C-O	-6.63	106.19	120.10
1	B	495	GLU	CA-C-O	-6.62	106.19	120.10
1	N	6387	GLU	CA-C-O	-6.62	106.21	120.10
1	M	5896	GLU	CA-C-O	-6.61	106.21	120.10
1	I	4157	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	J	4648	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	H	3666	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	N	6612	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	K	5139	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	C	1211	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	720	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	M	6121	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	O	7103	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	229	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	E	2193	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	G	3175	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	L	5630	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	F	2684	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	P	7594	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	D	1702	LEU	CB-CG-CD2	-5.07	102.38	111.00

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLN	Mainchain
1	A	138	ALA	Mainchain
1	A	453	GLU	Mainchain
1	B	610	GLN	Mainchain
1	B	629	ALA	Mainchain
1	B	944	GLU	Mainchain
1	C	1101	GLN	Mainchain
1	C	1120	ALA	Mainchain
1	C	1435	GLU	Mainchain
1	D	1592	GLN	Mainchain
1	D	1611	ALA	Mainchain
1	D	1926	GLU	Mainchain
1	E	2083	GLN	Mainchain
1	E	2102	ALA	Mainchain
1	E	2417	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	F	2574	GLN	Mainchain
1	F	2593	ALA	Mainchain
1	F	2908	GLU	Mainchain
1	G	3065	GLN	Mainchain
1	G	3084	ALA	Mainchain
1	G	3399	GLU	Mainchain
1	H	3556	GLN	Mainchain
1	H	3575	ALA	Mainchain
1	H	3890	GLU	Mainchain
1	I	4047	GLN	Mainchain
1	I	4066	ALA	Mainchain
1	I	4381	GLU	Mainchain
1	J	4538	GLN	Mainchain
1	J	4557	ALA	Mainchain
1	J	4872	GLU	Mainchain
1	K	5029	GLN	Mainchain
1	K	5048	ALA	Mainchain
1	K	5363	GLU	Mainchain
1	L	5520	GLN	Mainchain
1	L	5539	ALA	Mainchain
1	L	5854	GLU	Mainchain
1	M	6011	GLN	Mainchain
1	M	6030	ALA	Mainchain
1	M	6345	GLU	Mainchain
1	N	6502	GLN	Mainchain
1	N	6521	ALA	Mainchain
1	N	6836	GLU	Mainchain
1	O	6993	GLN	Mainchain
1	O	7012	ALA	Mainchain
1	O	7327	GLU	Mainchain
1	P	7484	GLN	Mainchain
1	P	7503	ALA	Mainchain
1	P	7818	GLU	Mainchain

## 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	3653	0	3794	11	0
1	B	3653	0	3791	11	0
1	C	3653	0	3791	10	0
1	D	3653	0	3791	9	0
1	E	3653	0	3791	9	0
1	F	3653	0	3791	9	0
1	G	3653	0	3791	9	0
1	H	3653	0	3791	10	0
1	I	3653	0	3791	10	0
1	J	3653	0	3791	11	0
1	K	3653	0	3791	10	0
1	L	3653	0	3791	11	0
1	M	3653	0	3791	9	0
1	N	3653	0	3791	9	0
1	O	3653	0	3791	9	0
1	P	3653	0	3791	9	0
All	All	58448	0	60659	156	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 1.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:HA	1:A:124:LYS:HE2	1.76	0.68
1:J:4543:LYS:HA	1:J:4543:LYS:HE2	1.76	0.68
1:L:5525:LYS:HE2	1:L:5525:LYS:HA	1.76	0.67
1:C:1106:LYS:HE2	1:C:1106:LYS:HA	1.76	0.67
1:G:3070:LYS:HE2	1:G:3070:LYS:HA	1.76	0.67
1:P:7489:LYS:HE2	1:P:7489:LYS:HA	1.76	0.67
1:E:2088:LYS:HE2	1:E:2088:LYS:HA	1.76	0.66
1:B:615:LYS:HA	1:B:615:LYS:HE2	1.76	0.66
1:I:4052:LYS:HA	1:I:4052:LYS:HE2	1.76	0.66
1:N:6507:LYS:HE2	1:N:6507:LYS:HA	1.76	0.66
1:H:3561:LYS:HA	1:H:3561:LYS:HE2	1.76	0.66
1:K:5034:LYS:HA	1:K:5034:LYS:HE2	1.76	0.65
1:F:2579:LYS:HA	1:F:2579:LYS:HE2	1.76	0.65
1:D:1677:LYS:O	1:D:1677:LYS:HG3	1.97	0.65
1:M:6096:LYS:O	1:M:6096:LYS:HG3	1.97	0.65
1:O:6998:LYS:HA	1:O:6998:LYS:HE2	1.76	0.65
1:L:5605:LYS:O	1:L:5605:LYS:HG3	1.97	0.65
1:D:1597:LYS:HA	1:D:1597:LYS:HE2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1186:LYS:HG3	1:C:1186:LYS:O	1.97	0.65
1:N:6587:LYS:O	1:N:6587:LYS:HG3	1.97	0.65
1:E:2168:LYS:HG3	1:E:2168:LYS:O	1.97	0.64
1:M:6016:LYS:HA	1:M:6016:LYS:HE2	1.76	0.64
1:J:4623:LYS:HG3	1:J:4623:LYS:O	1.97	0.64
1:A:204:LYS:HG3	1:A:204:LYS:O	1.97	0.64
1:K:5114:LYS:HG3	1:K:5114:LYS:O	1.97	0.64
1:B:695:LYS:O	1:B:695:LYS:HG3	1.97	0.63
1:H:3641:LYS:O	1:H:3641:LYS:HG3	1.97	0.63
1:I:4132:LYS:HG3	1:I:4132:LYS:O	1.97	0.63
1:G:3150:LYS:O	1:G:3150:LYS:HG3	1.97	0.63
1:O:7078:LYS:O	1:O:7078:LYS:HG3	1.97	0.63
1:P:7569:LYS:O	1:P:7569:LYS:HG3	1.97	0.63
1:F:2659:LYS:O	1:F:2659:LYS:HG3	1.97	0.62
1:D:1722:LYS:HD3	1:D:1722:LYS:O	2.03	0.59
1:N:6632:LYS:O	1:N:6632:LYS:HD3	2.03	0.59
1:M:6141:LYS:O	1:M:6141:LYS:HD3	2.03	0.59
1:G:3195:LYS:HD3	1:G:3195:LYS:O	2.03	0.59
1:L:5650:LYS:HD3	1:L:5650:LYS:O	2.03	0.59
1:P:7614:LYS:O	1:P:7614:LYS:HD3	2.03	0.59
1:E:2213:LYS:O	1:E:2213:LYS:HD3	2.03	0.59
1:C:1231:LYS:HD3	1:C:1231:LYS:O	2.03	0.58
1:F:2704:LYS:O	1:F:2704:LYS:HD3	2.03	0.58
1:O:7123:LYS:HD3	1:O:7123:LYS:O	2.03	0.58
1:H:3686:LYS:HD3	1:H:3686:LYS:O	2.03	0.58
1:I:4177:LYS:HD3	1:I:4177:LYS:O	2.03	0.58
1:K:5159:LYS:HD3	1:K:5159:LYS:O	2.03	0.58
1:B:740:LYS:O	1:B:740:LYS:HD3	2.03	0.58
1:A:249:LYS:HD3	1:A:249:LYS:O	2.03	0.57
1:J:4668:LYS:HD3	1:J:4668:LYS:O	2.03	0.57
1:K:5159:LYS:HD3	1:K:5159:LYS:C	2.33	0.49
1:O:7123:LYS:HD3	1:O:7123:LYS:C	2.33	0.49
1:B:740:LYS:HD3	1:B:740:LYS:C	2.33	0.49
1:F:2704:LYS:C	1:F:2704:LYS:HD3	2.33	0.49
1:D:1722:LYS:HD3	1:D:1722:LYS:C	2.33	0.49
1:A:249:LYS:HD3	1:A:249:LYS:C	2.33	0.49
1:M:6141:LYS:C	1:M:6141:LYS:HD3	2.33	0.49
1:G:3195:LYS:C	1:G:3195:LYS:HD3	2.33	0.49
1:P:7614:LYS:C	1:P:7614:LYS:HD3	2.33	0.49
1:E:2213:LYS:HD3	1:E:2213:LYS:C	2.33	0.49
1:J:4668:LYS:HD3	1:J:4668:LYS:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:6632:LYS:C	1:N:6632:LYS:HD3	2.33	0.49
1:L:5650:LYS:HD3	1:L:5650:LYS:C	2.33	0.49
1:C:1231:LYS:HD3	1:C:1231:LYS:C	2.33	0.48
1:H:3686:LYS:HD3	1:H:3686:LYS:C	2.33	0.48
1:I:4177:LYS:HD3	1:I:4177:LYS:C	2.33	0.48
1:J:4623:LYS:O	1:J:4623:LYS:CG	2.66	0.43
1:A:204:LYS:CG	1:A:204:LYS:O	2.66	0.43
1:N:6587:LYS:CG	1:N:6587:LYS:O	2.66	0.43
1:E:2168:LYS:CG	1:E:2168:LYS:O	2.66	0.43
1:K:5114:LYS:CG	1:K:5114:LYS:O	2.66	0.43
1:B:695:LYS:CG	1:B:695:LYS:O	2.66	0.43
1:L:5530:LEU:HA	1:L:5530:LEU:HD12	1.83	0.43
1:O:7003:LEU:HA	1:O:7003:LEU:HD12	1.83	0.43
1:D:1677:LYS:O	1:D:1677:LYS:CG	2.66	0.43
1:M:6096:LYS:CG	1:M:6096:LYS:O	2.66	0.43
1:L:5605:LYS:O	1:L:5605:LYS:CG	2.66	0.43
1:L:5508:GLN:O	1:L:5508:GLN:HG2	2.19	0.43
1:C:1186:LYS:CG	1:C:1186:LYS:O	2.66	0.43
1:C:1089:GLN:HG2	1:C:1089:GLN:O	2.19	0.43
1:C:1111:LEU:HD12	1:C:1111:LEU:HA	1.83	0.43
1:G:3358:ILE:HB	1:G:3359:PRO:CD	2.49	0.43
1:M:5999:GLN:HG2	1:M:5999:GLN:O	2.19	0.43
1:D:1580:GLN:HG2	1:D:1580:GLN:O	2.19	0.43
1:J:4831:ILE:HB	1:J:4832:PRO:CD	2.49	0.43
1:K:5322:ILE:HB	1:K:5323:PRO:CD	2.49	0.42
1:P:7777:ILE:HB	1:P:7778:PRO:CD	2.49	0.42
1:B:903:ILE:HB	1:B:904:PRO:CD	2.49	0.42
1:B:598:GLN:HG2	1:B:598:GLN:O	2.19	0.42
1:N:6795:ILE:HB	1:N:6796:PRO:CD	2.49	0.42
1:K:5017:GLN:O	1:K:5017:GLN:HG2	2.19	0.42
1:F:2584:LEU:HD12	1:F:2584:LEU:HA	1.83	0.42
1:G:3150:LYS:O	1:G:3150:LYS:CG	2.66	0.42
1:E:2376:ILE:HB	1:E:2377:PRO:CD	2.49	0.42
1:L:5813:ILE:HB	1:L:5814:PRO:CD	2.49	0.42
1:A:412:ILE:HB	1:A:413:PRO:CD	2.49	0.42
1:P:7569:LYS:O	1:P:7569:LYS:CG	2.66	0.42
1:E:2071:GLN:O	1:E:2071:GLN:HG2	2.19	0.42
1:C:1394:ILE:HB	1:C:1395:PRO:CD	2.49	0.42
1:O:7286:ILE:HB	1:O:7287:PRO:CD	2.49	0.42
1:N:6490:GLN:HG2	1:N:6490:GLN:O	2.19	0.42
1:F:2867:ILE:HB	1:F:2868:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6304:ILE:HB	1:M:6305:PRO:CD	2.49	0.42
1:H:3849:ILE:HB	1:H:3850:PRO:CD	2.49	0.42
1:D:1885:ILE:HB	1:D:1886:PRO:CD	2.49	0.42
1:I:4340:ILE:HB	1:I:4341:PRO:CD	2.49	0.42
1:J:4526:GLN:HG2	1:J:4526:GLN:O	2.19	0.42
1:F:2562:GLN:O	1:F:2562:GLN:HG2	2.19	0.42
1:D:1873:LEU:HD23	1:D:1873:LEU:O	2.20	0.42
1:A:107:GLN:HG2	1:A:107:GLN:O	2.19	0.41
1:L:5801:LEU:O	1:L:5801:LEU:HD23	2.20	0.41
1:C:1382:LEU:O	1:C:1382:LEU:HD23	2.20	0.41
1:O:6981:GLN:O	1:O:6981:GLN:HG2	2.19	0.41
1:M:6292:LEU:O	1:M:6292:LEU:HD23	2.20	0.41
1:O:6914:LYS:HD2	1:O:6914:LYS:N	2.35	0.41
1:F:2495:LYS:HD2	1:F:2495:LYS:N	2.35	0.41
1:P:7405:LYS:HD2	1:P:7405:LYS:N	2.35	0.41
1:N:6423:LYS:N	1:N:6423:LYS:HD2	2.35	0.41
1:G:2986:LYS:HD2	1:G:2986:LYS:N	2.35	0.41
1:H:3837:LEU:HD23	1:H:3837:LEU:O	2.20	0.41
1:P:7472:GLN:O	1:P:7472:GLN:HG2	2.19	0.41
1:G:3053:GLN:O	1:G:3053:GLN:HG2	2.19	0.41
1:E:2004:LYS:HD2	1:E:2004:LYS:N	2.35	0.41
1:H:3566:LEU:HA	1:H:3566:LEU:HD12	1.83	0.41
1:I:4328:LEU:HD23	1:I:4328:LEU:O	2.20	0.41
1:P:7765:LEU:O	1:P:7765:LEU:HD23	2.20	0.41
1:G:3346:LEU:O	1:G:3346:LEU:HD23	2.20	0.41
1:B:891:LEU:O	1:B:891:LEU:HD23	2.20	0.41
1:K:5039:LEU:HD12	1:K:5039:LEU:HA	1.83	0.41
1:K:5310:LEU:HD23	1:K:5310:LEU:O	2.20	0.41
1:D:1513:LYS:HD2	1:D:1513:LYS:N	2.35	0.41
1:F:2855:LEU:HD23	1:F:2855:LEU:O	2.20	0.41
1:M:5932:LYS:N	1:M:5932:LYS:HD2	2.35	0.41
1:N:6783:LEU:HD23	1:N:6783:LEU:O	2.20	0.41
1:E:2364:LEU:O	1:E:2364:LEU:HD23	2.20	0.41
1:O:7274:LEU:HD23	1:O:7274:LEU:O	2.20	0.41
1:H:3544:GLN:HG2	1:H:3544:GLN:O	2.19	0.41
1:I:4035:GLN:HG2	1:I:4035:GLN:O	2.19	0.41
1:B:531:LYS:N	1:B:531:LYS:HD2	2.35	0.41
1:I:4057:LEU:HA	1:I:4057:LEU:HD12	1.83	0.41
1:A:40:LYS:N	1:A:40:LYS:HD2	2.35	0.41
1:K:4950:LYS:HD2	1:K:4950:LYS:N	2.35	0.41
1:J:4598:GLU:HA	1:J:4599:GLY:HA3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4459:LYS:HD2	1:J:4459:LYS:N	2.35	0.41
1:J:4819:LEU:HD23	1:J:4819:LEU:O	2.20	0.41
1:C:1022:LYS:N	1:C:1022:LYS:HD2	2.35	0.41
1:I:3932:GLU:O	1:I:3933:ASN:HB2	2.22	0.40
1:A:400:LEU:O	1:A:400:LEU:HD23	2.20	0.40
1:H:3441:GLU:O	1:H:3442:ASN:HB2	2.22	0.40
1:H:3477:LYS:HD2	1:H:3477:LYS:N	2.35	0.40
1:B:620:LEU:HD12	1:B:620:LEU:HA	1.83	0.40
1:I:3968:LYS:HD2	1:I:3968:LYS:N	2.35	0.40
1:L:5441:LYS:N	1:L:5441:LYS:HD2	2.36	0.40
1:A:179:GLU:HA	1:A:180:GLY:HA3	1.90	0.40
1:J:4626:LEU:HB3	1:J:4757:THR:HG21	2.04	0.40
1:B:635:LEU:HD12	1:B:635:LEU:HA	1.90	0.40
1:L:5405:GLU:O	1:L:5406:ASN:HB2	2.21	0.40
1:A:207:LEU:HB3	1:A:338:THR:HG21	2.04	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 PDB entries followed by that with respect to all EM entries.

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	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	B	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	C	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	D	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	E	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	F	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	G	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	H	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	J	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	K	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	L	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	M	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	N	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	O	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
1	P	489/491 (100%)	475 (97%)	12 (2%)	2 (0%)	39	79
All	All	7824/7856 (100%)	7600 (97%)	192 (2%)	32 (0%)	43	79

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	496	ASN
1	C	987	ASN
1	D	1478	ASN
1	E	1969	ASN
1	F	2460	ASN
1	G	2951	ASN
1	H	3442	ASN
1	I	3933	ASN
1	J	4424	ASN
1	K	4915	ASN
1	L	5406	ASN
1	M	5897	ASN
1	N	6388	ASN
1	O	6879	ASN
1	P	7370	ASN
1	A	443	ALA
1	B	934	ALA
1	C	1425	ALA
1	D	1916	ALA
1	E	2407	ALA
1	F	2898	ALA
1	G	3389	ALA
1	H	3880	ALA
1	I	4371	ALA
1	J	4862	ALA

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Mol	Chain	Res	Type
1	K	5353	ALA
1	L	5844	ALA
1	M	6335	ALA
1	N	6826	ALA
1	O	7317	ALA
1	P	7808	ALA

### 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 PDB entries followed by that with respect to all EM entries.

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	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	B	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	C	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	D	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	E	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	F	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	G	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	H	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	I	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	J	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	K	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	L	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	M	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	N	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	O	389/389 (100%)	384 (99%)	5 (1%)	76	89
1	P	389/389 (100%)	384 (99%)	5 (1%)	76	89
All	All	6224/6224 (100%)	6144 (99%)	80 (1%)	78	89

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



Mol	Chain	Res	Type
1	A	97	LEU
1	A	105	LEU
1	A	129	LEU
1	A	144	LEU
1	A	192	LYS
1	B	588	LEU
1	B	596	LEU
1	B	620	LEU
1	B	635	LEU
1	B	683	LYS
1	C	1079	LEU
1	C	1087	LEU
1	C	1111	LEU
1	C	1126	LEU
1	C	1174	LYS
1	D	1570	LEU
1	D	1578	LEU
1	D	1602	LEU
1	D	1617	LEU
1	D	1665	LYS
1	E	2061	LEU
1	E	2069	LEU
1	E	2093	LEU
1	E	2108	LEU
1	E	2156	LYS
1	F	2552	LEU
1	F	2560	LEU
1	F	2584	LEU
1	F	2599	LEU
1	F	2647	LYS
1	G	3043	LEU
1	G	3051	LEU
1	G	3075	LEU
1	G	3090	LEU
1	G	3138	LYS
1	H	3534	LEU
1	H	3542	LEU
1	H	3566	LEU
1	H	3581	LEU
1	H	3629	LYS
1	I	4025	LEU
1	I	4033	LEU
1	I	4057	LEU

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Mol	Chain	Res	Type
1	I	4072	LEU
1	I	4120	LYS
1	J	4516	LEU
1	J	4524	LEU
1	J	4548	LEU
1	J	4563	LEU
1	J	4611	LYS
1	K	5007	LEU
1	K	5015	LEU
1	K	5039	LEU
1	K	5054	LEU
1	K	5102	LYS
1	L	5498	LEU
1	L	5506	LEU
1	L	5530	LEU
1	L	5545	LEU
1	L	5593	LYS
1	M	5989	LEU
1	M	5997	LEU
1	M	6021	LEU
1	M	6036	LEU
1	M	6084	LYS
1	N	6480	LEU
1	N	6488	LEU
1	N	6512	LEU
1	N	6527	LEU
1	N	6575	LYS
1	O	6971	LEU
1	O	6979	LEU
1	O	7003	LEU
1	O	7018	LEU
1	O	7066	LYS
1	P	7462	LEU
1	P	7470	LEU
1	P	7494	LEU
1	P	7509	LEU
1	P	7557	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 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.