wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:31 PM BST

PDB ID	:	3JC1
EMDB ID:	:	EMD-6461
Title	:	Electron cryo-microscopy of the IST1-CHMP1B ESCRT-III copolymer
Authors	:	McCullough, J.; Clippinger, A.K.; Talledge, N.; Skowyra, M.L.; Saunders, M.G.; Naismith, T.V.; Colf, L.A.; Afonine, P.; Arthur, C.; Sundquist, W.I.; Hanson, P.I.; Frost, A.
Deposited on	:	2015-11-09
Resolution	:	4.00 Å(reported)
Based on PDB ID	:	3FRR

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

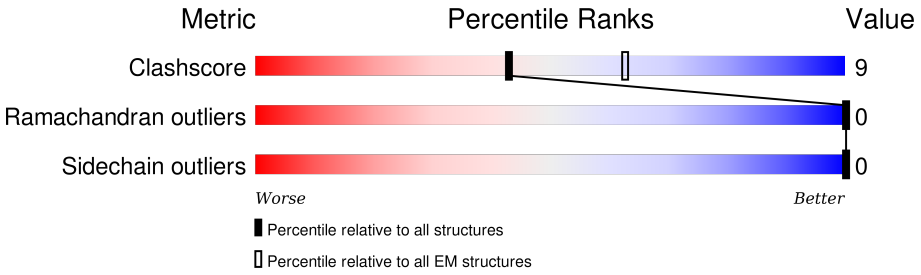
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	Aa	182	100%
1	Ac	182	100%
1	Ae	182	100%
1	Ag	182	100%
1	Ai	182	100%
1	Ak	182	100%
1	Am	182	100%
1	Ao	182	100%
1	Aq	182	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	As	182	100%
1	Au	182	100%
1	Aw	182	100%
1	Ay	182	100%
1	Ba	182	100%
1	Bc	182	100%
1	Be	182	100%
1	Bg	182	100%
1	Bi	182	100%
1	Bk	182	100%
1	Bm	182	100%
1	Bo	182	100%
1	Bq	182	100%
1	Bs	182	100%
1	Bu	182	100%
1	Bw	182	100%
1	By	182	100%
1	Ca	182	100%
1	Cc	182	100%
1	Ce	182	100%
1	Cg	182	100%
1	Ci	182	100%
1	Ck	182	100%
1	Cm	182	100%
1	Co	182	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Ab	160	100%
2	Ad	160	100%
2	Af	160	100%
2	Ah	160	100%
2	Aj	160	100%
2	Al	160	100%
2	An	160	100%
2	Ap	160	100%
2	Ar	160	100%
2	At	160	100%
2	Av	160	100%
2	Ax	160	100%
2	Az	160	100%
2	Bb	160	100%
2	Bd	160	100%
2	Bf	160	100%
2	Bh	160	100%
2	Bj	160	100%
2	Bl	160	100%
2	Bn	160	100%
2	Bp	160	100%
2	Br	160	100%
2	Bt	160	100%
2	Bv	160	100%
2	Bx	160	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Bz	160	100%
2	Cb	160	100%
2	Cd	160	100%
2	Cf	160	100%
2	Ch	160	100%
2	Cj	160	100%
2	Cl	160	100%
2	Cn	160	100%
2	Cp	160	100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 92106 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 Increased Sodium Tolerance 1 (IST1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ac	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ae	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ag	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ai	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ak	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Am	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ao	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Aq	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	As	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Au	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Aw	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ay	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ba	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bc	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Be	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bg	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bk	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bm	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bo	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bq	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bs	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bu	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bw	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	By	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ca	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Cc	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ce	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Cg	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ci	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ck	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Cm	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Co	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		

- Molecule 2 is a protein called Charged multivesicular body protein 1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ad	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Af	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ah	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Aj	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Al	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	An	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ap	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ar	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	At	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Av	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ax	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Az	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bb	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bd	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bf	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bh	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bj	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bl	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bn	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bp	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Br	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bt	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bv	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bx	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bz	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cb	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cd	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cf	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ch	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cj	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cl	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cn	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cp	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Ad	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Af	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Ah	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Aj	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Al	34	GLU	LYS	CONFLICT	UNP Q7LBR1
An	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Ap	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Ar	34	GLU	LYS	CONFLICT	UNP Q7LBR1
At	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Av	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Ax	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Az	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bb	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bd	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bf	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bh	34	GLU	LYS	CONFLICT	UNP Q7LBR1

Continued on next page...

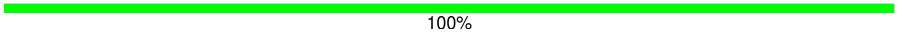
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bj	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bl	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bn	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bp	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Br	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bt	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bv	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bx	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Bz	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cb	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cd	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cf	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Ch	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cj	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cl	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cn	34	GLU	LYS	CONFLICT	UNP Q7LBR1
Cp	34	GLU	LYS	CONFLICT	UNP Q7LBR1

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: Increased Sodium Tolerance 1 (IST1)

Chain Aa: 

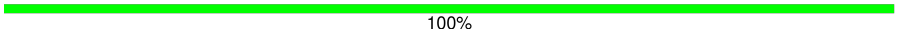
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ac: 

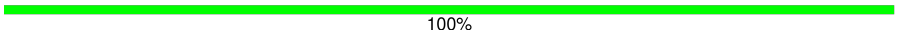
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ae: 

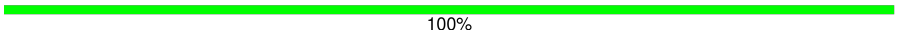
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ag: 

There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ai: 

There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ak: 

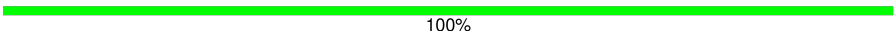
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Am: 

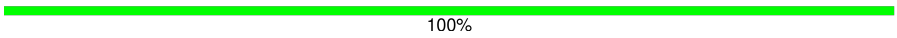
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ao: 

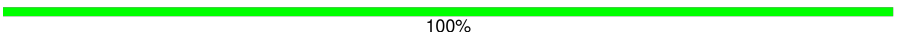
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Aq: 

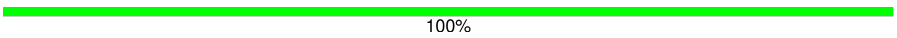
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain As: 

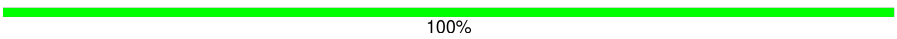
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Au: 

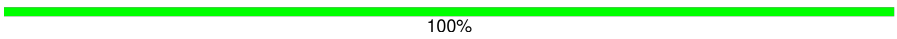
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Aw: 

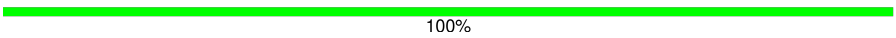
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ay: 

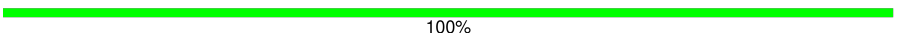
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ba: 

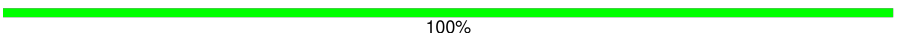
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bc: 

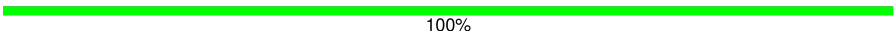
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Be: 

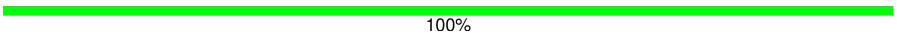
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bg: 

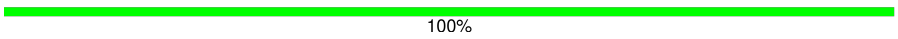
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bi: 

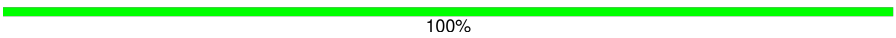
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bk: 

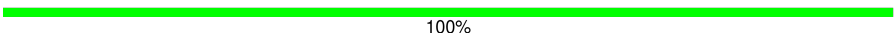
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bm: 

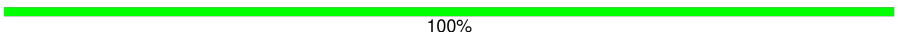
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bo: 

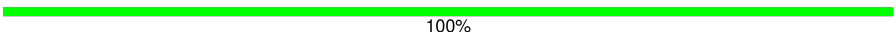
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bq: 

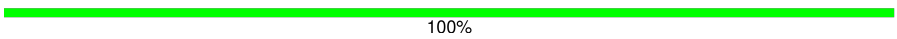
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bs: 

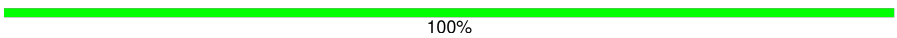
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bu: 

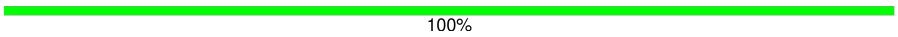
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Bw: 

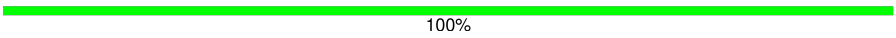
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain By: 

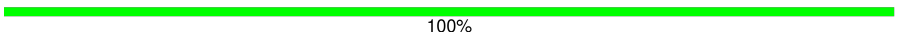
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ca: 

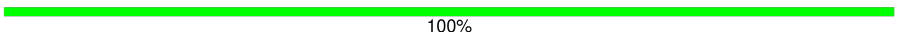
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Cc: 

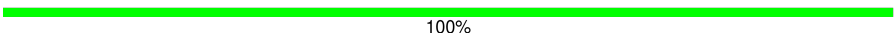
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ce: 

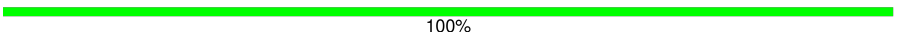
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Cg: 

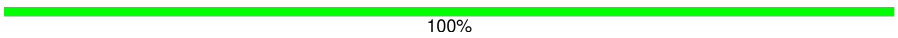
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ci: 

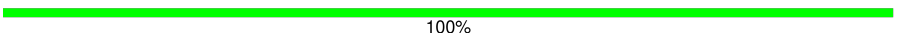
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Ck: 

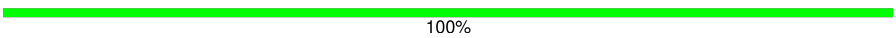
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Cm: 

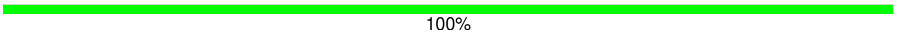
There are no outlier residues recorded for this chain.

- Molecule 1: Increased Sodium Tolerance 1 (IST1)

Chain Co: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Ab: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Ad: 

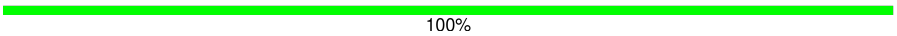
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Af: 

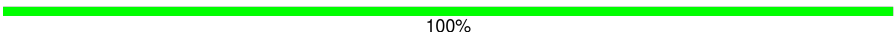
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Ah: 

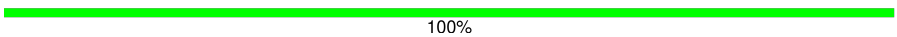
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Aj: 

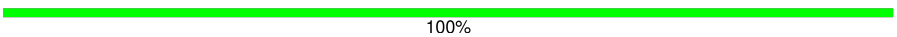
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Al: 

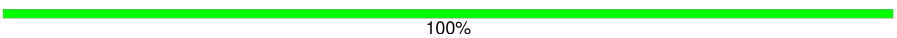
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain An: 

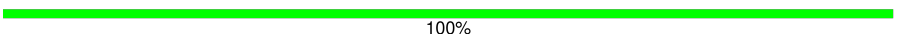
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Ap: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Ar: 

There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain At: 

There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Av: 

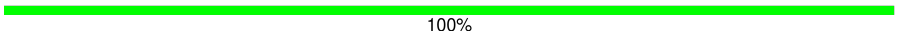
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Ax: 

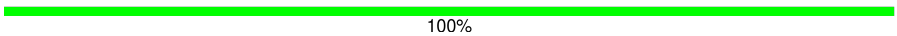
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Az: 

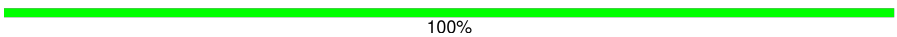
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Bb: 

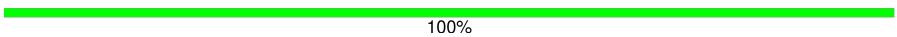
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Bd: 

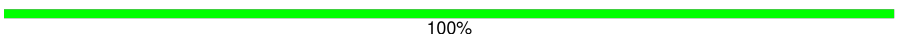
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Bf: 

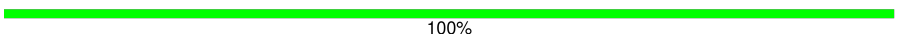
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Bh: 

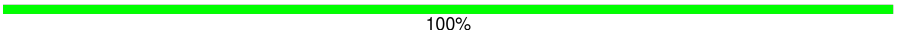
There are no outlier residues recorded for this chain.

• Molecule 2: Charged multivesicular body protein 1b

Chain Bj: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bl: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bn: 

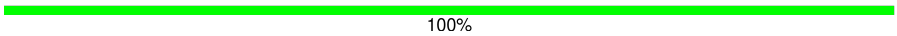
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bp: 

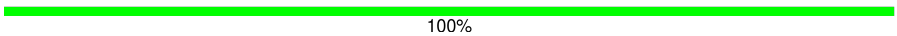
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Br: 

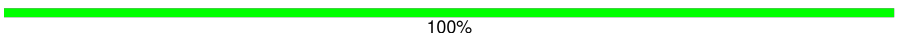
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bt: 

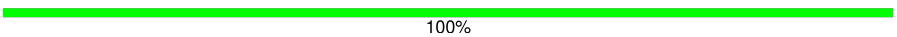
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bv: 

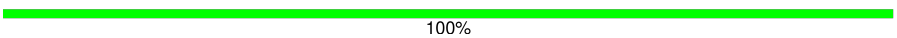
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bx: 

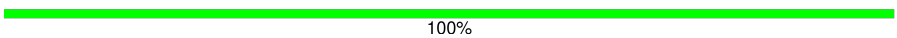
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Bz: 

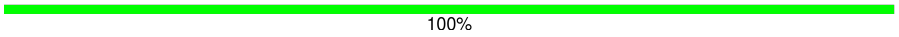
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cb: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cd: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cf: 

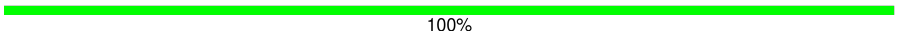
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Ch: 

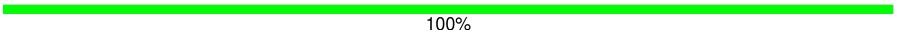
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cj: 

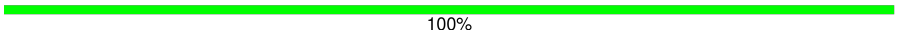
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cl: 

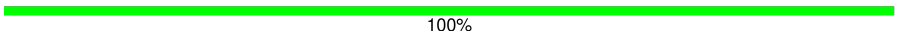
There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cn: 

There are no outlier residues recorded for this chain.

- Molecule 2: Charged multivesicular body protein 1b

Chain Cp: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	188713	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS, FEI TECNAI F20, JEOL 3200FSC	Depositor
Voltage (kV)	300, 200, 300	Depositor
Electron dose ($e^-/Å^2$)	15, 10, 20	Depositor
Minimum defocus (nm)	600, 600, 600	Depositor
Maximum defocus (nm)	3000, 3000, 3000	Depositor
Magnification	59000, 50000, 59000	Depositor
Image detector	FEI Falcon I (4k x 4k), KODAK SO-163 film, DIRECT ELECTRON DE-12 (4k x 3k)	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	Aa	0.38	0/1484	0.52	0/1997
1	Ac	0.38	0/1484	0.52	0/1997
1	Ae	0.38	0/1484	0.52	0/1997
1	Ag	0.38	0/1484	0.52	0/1997
1	Ai	0.38	0/1484	0.52	0/1997
1	Ak	0.38	0/1484	0.52	0/1997
1	Am	0.38	0/1484	0.52	0/1997
1	Ao	0.38	0/1484	0.52	0/1997
1	Aq	0.38	0/1484	0.52	0/1997
1	As	0.38	0/1484	0.52	0/1997
1	Au	0.38	0/1484	0.52	0/1997
1	Aw	0.38	0/1484	0.52	0/1997
1	Ay	0.38	0/1484	0.52	0/1997
1	Ba	0.38	0/1484	0.52	0/1997
1	Bc	0.38	0/1484	0.52	0/1997
1	Be	0.38	0/1484	0.52	0/1997
1	Bg	0.38	0/1484	0.52	0/1997
1	Bi	0.38	0/1484	0.52	0/1997
1	Bk	0.38	0/1484	0.52	0/1997
1	Bm	0.38	0/1484	0.52	0/1997
1	Bo	0.38	0/1484	0.52	0/1997
1	Bq	0.38	0/1484	0.52	0/1997
1	Bs	0.38	0/1484	0.52	0/1997
1	Bu	0.38	0/1484	0.52	0/1997
1	Bw	0.38	0/1484	0.52	0/1997
1	By	0.38	0/1484	0.52	0/1997
1	Ca	0.38	0/1484	0.52	0/1997
1	Cc	0.38	0/1484	0.52	0/1997
1	Ce	0.38	0/1484	0.52	0/1997
1	Cg	0.38	0/1484	0.52	0/1997
1	Ci	0.38	0/1484	0.52	0/1997
1	Ck	0.38	0/1484	0.52	0/1997
1	Cm	0.38	0/1484	0.52	0/1997
1	Co	0.38	0/1484	0.52	0/1997

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
2	Ab	0.43	0/1251	0.59	0/1671
2	Ad	0.43	0/1251	0.59	0/1671
2	Af	0.43	0/1251	0.59	0/1671
2	Ah	0.43	0/1251	0.59	0/1671
2	Aj	0.43	0/1251	0.58	0/1671
2	Al	0.43	0/1251	0.59	0/1671
2	An	0.43	0/1251	0.58	0/1671
2	Ap	0.43	0/1251	0.59	0/1671
2	Ar	0.43	0/1251	0.59	0/1671
2	At	0.43	0/1251	0.59	0/1671
2	Av	0.43	0/1251	0.59	0/1671
2	Ax	0.43	0/1251	0.59	0/1671
2	Az	0.43	0/1251	0.59	0/1671
2	Bb	0.43	0/1251	0.59	0/1671
2	Bd	0.43	0/1251	0.59	0/1671
2	Bf	0.43	0/1251	0.59	0/1671
2	Bh	0.44	0/1251	0.59	0/1671
2	Bj	0.43	0/1251	0.58	0/1671
2	Bl	0.43	0/1251	0.59	0/1671
2	Bn	0.43	0/1251	0.59	0/1671
2	Bp	0.43	0/1251	0.59	0/1671
2	Br	0.43	0/1251	0.59	0/1671
2	Bt	0.43	0/1251	0.59	0/1671
2	Bv	0.43	0/1251	0.59	0/1671
2	Bx	0.43	0/1251	0.59	0/1671
2	Bz	0.43	0/1251	0.59	0/1671
2	Cb	0.43	0/1251	0.59	0/1671
2	Cd	0.43	0/1251	0.59	0/1671
2	Cf	0.43	0/1251	0.59	0/1671
2	Ch	0.43	0/1251	0.59	0/1671
2	Cj	0.43	0/1251	0.58	0/1671
2	Cl	0.43	0/1251	0.58	0/1671
2	Cn	0.43	0/1251	0.59	0/1671
2	Cp	0.43	0/1251	0.59	0/1671
All	All	0.41	0/92990	0.55	0/124712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	Aa	1466	0	1541	0	0
1	Ac	1466	0	1541	0	0
1	Ae	1466	0	1541	0	0
1	Ag	1466	0	1541	0	0
1	Ai	1466	0	1541	0	0
1	Ak	1466	0	1541	0	0
1	Am	1466	0	1541	0	0
1	Ao	1466	0	1541	0	0
1	Aq	1466	0	1541	0	0
1	As	1466	0	1541	0	0
1	Au	1466	0	1541	0	0
1	Aw	1466	0	1541	0	0
1	Ay	1466	0	1541	0	0
1	Ba	1466	0	1541	0	0
1	Bc	1466	0	1541	0	0
1	Be	1466	0	1541	0	0
1	Bg	1466	0	1541	0	0
1	Bi	1466	0	1541	0	0
1	Bk	1466	0	1541	0	0
1	Bm	1466	0	1541	0	0
1	Bo	1466	0	1541	0	0
1	Bq	1466	0	1541	0	0
1	Bs	1466	0	1541	0	0
1	Bu	1466	0	1541	0	0
1	Bw	1466	0	1541	0	0
1	By	1466	0	1541	0	0
1	Ca	1466	0	1541	0	0
1	Cc	1466	0	1541	0	0
1	Ce	1466	0	1541	0	0
1	Cg	1466	0	1541	0	0
1	Ci	1466	0	1541	0	0
1	Ck	1466	0	1541	0	0
1	Cm	1466	0	1541	0	0
1	Co	1466	0	1541	0	0
2	Ab	1243	0	1279	0	0
2	Ad	1243	0	1279	0	0
2	Af	1243	0	1279	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ah	1243	0	1279	0	0
2	Aj	1243	0	1279	0	0
2	Al	1243	0	1279	0	0
2	An	1243	0	1279	0	0
2	Ap	1243	0	1279	0	0
2	Ar	1243	0	1279	0	0
2	At	1243	0	1279	0	0
2	Av	1243	0	1279	0	0
2	Ax	1243	0	1279	0	0
2	Az	1243	0	1279	0	0
2	Bb	1243	0	1279	0	0
2	Bd	1243	0	1279	0	0
2	Bf	1243	0	1279	0	0
2	Bh	1243	0	1279	0	0
2	Bj	1243	0	1279	0	0
2	Bl	1243	0	1279	0	0
2	Bn	1243	0	1279	0	0
2	Bp	1243	0	1279	0	0
2	Br	1243	0	1279	0	0
2	Bt	1243	0	1279	0	0
2	Bv	1243	0	1279	0	0
2	Bx	1243	0	1279	0	0
2	Bz	1243	0	1279	0	0
2	Cb	1243	0	1279	0	0
2	Cd	1243	0	1279	0	0
2	Cf	1243	0	1279	0	0
2	Ch	1243	0	1279	0	0
2	Cj	1243	0	1279	0	0
2	Cl	1243	0	1279	0	0
2	Cn	1243	0	1279	0	0
2	Cp	1243	0	1279	0	0
All	All	92106	0	95880	0	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 9.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	Aa	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ac	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ae	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ag	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ai	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ak	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Am	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ao	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Aq	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	As	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Au	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Aw	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ay	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ba	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bc	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Be	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bg	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bi	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bk	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bm	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bo	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bq	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bs	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bu	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bw	180/182 (99%)	173 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	By	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ca	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Cc	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ce	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Cg	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ci	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ck	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Cm	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Co	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
2	Ab	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ad	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Af	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ah	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Aj	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Al	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	An	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ap	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ar	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	At	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Av	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ax	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Az	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bb	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bd	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bf	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bh	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bj	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bl	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bn	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bp	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Br	158/160 (99%)	152 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bt	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bv	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bx	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bz	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cb	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cd	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cf	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ch	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cj	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cl	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cn	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cp	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
All	All	11492/11628 (99%)	11050 (96%)	442 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 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	Aa	158/158 (100%)	158 (100%)	0	100	100
1	Ac	158/158 (100%)	158 (100%)	0	100	100
1	Ae	158/158 (100%)	158 (100%)	0	100	100
1	Ag	158/158 (100%)	158 (100%)	0	100	100
1	Ai	158/158 (100%)	158 (100%)	0	100	100
1	Ak	158/158 (100%)	158 (100%)	0	100	100
1	Am	158/158 (100%)	158 (100%)	0	100	100
1	Ao	158/158 (100%)	158 (100%)	0	100	100
1	Aq	158/158 (100%)	158 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	As	158/158 (100%)	158 (100%)	0	100	100
1	Au	158/158 (100%)	158 (100%)	0	100	100
1	Aw	158/158 (100%)	158 (100%)	0	100	100
1	Ay	158/158 (100%)	158 (100%)	0	100	100
1	Ba	158/158 (100%)	158 (100%)	0	100	100
1	Bc	158/158 (100%)	158 (100%)	0	100	100
1	Be	158/158 (100%)	158 (100%)	0	100	100
1	Bg	158/158 (100%)	158 (100%)	0	100	100
1	Bi	158/158 (100%)	158 (100%)	0	100	100
1	Bk	158/158 (100%)	158 (100%)	0	100	100
1	Bm	158/158 (100%)	158 (100%)	0	100	100
1	Bo	158/158 (100%)	158 (100%)	0	100	100
1	Bq	158/158 (100%)	158 (100%)	0	100	100
1	Bs	158/158 (100%)	158 (100%)	0	100	100
1	Bu	158/158 (100%)	158 (100%)	0	100	100
1	Bw	158/158 (100%)	158 (100%)	0	100	100
1	By	158/158 (100%)	158 (100%)	0	100	100
1	Ca	158/158 (100%)	158 (100%)	0	100	100
1	Cc	158/158 (100%)	158 (100%)	0	100	100
1	Ce	158/158 (100%)	158 (100%)	0	100	100
1	Cg	158/158 (100%)	158 (100%)	0	100	100
1	Ci	158/158 (100%)	158 (100%)	0	100	100
1	Ck	158/158 (100%)	158 (100%)	0	100	100
1	Cm	158/158 (100%)	158 (100%)	0	100	100
1	Co	158/158 (100%)	158 (100%)	0	100	100
2	Ab	136/136 (100%)	136 (100%)	0	100	100
2	Ad	136/136 (100%)	136 (100%)	0	100	100
2	Af	136/136 (100%)	136 (100%)	0	100	100
2	Ah	136/136 (100%)	136 (100%)	0	100	100
2	Aj	136/136 (100%)	136 (100%)	0	100	100
2	Al	136/136 (100%)	136 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	An	136/136 (100%)	136 (100%)	0	100	100
2	Ap	136/136 (100%)	136 (100%)	0	100	100
2	Ar	136/136 (100%)	136 (100%)	0	100	100
2	At	136/136 (100%)	136 (100%)	0	100	100
2	Av	136/136 (100%)	136 (100%)	0	100	100
2	Ax	136/136 (100%)	136 (100%)	0	100	100
2	Az	136/136 (100%)	136 (100%)	0	100	100
2	Bb	136/136 (100%)	136 (100%)	0	100	100
2	Bd	136/136 (100%)	136 (100%)	0	100	100
2	Bf	136/136 (100%)	136 (100%)	0	100	100
2	Bh	136/136 (100%)	136 (100%)	0	100	100
2	Bj	136/136 (100%)	136 (100%)	0	100	100
2	Bl	136/136 (100%)	136 (100%)	0	100	100
2	Bn	136/136 (100%)	136 (100%)	0	100	100
2	Bp	136/136 (100%)	136 (100%)	0	100	100
2	Br	136/136 (100%)	136 (100%)	0	100	100
2	Bt	136/136 (100%)	136 (100%)	0	100	100
2	Bv	136/136 (100%)	136 (100%)	0	100	100
2	Bx	136/136 (100%)	136 (100%)	0	100	100
2	Bz	136/136 (100%)	136 (100%)	0	100	100
2	Cb	136/136 (100%)	136 (100%)	0	100	100
2	Cd	136/136 (100%)	136 (100%)	0	100	100
2	Cf	136/136 (100%)	136 (100%)	0	100	100
2	Ch	136/136 (100%)	136 (100%)	0	100	100
2	Cj	136/136 (100%)	136 (100%)	0	100	100
2	Cl	136/136 (100%)	136 (100%)	0	100	100
2	Cn	136/136 (100%)	136 (100%)	0	100	100
2	Cp	136/136 (100%)	136 (100%)	0	100	100
All	All	9996/9996 (100%)	9996 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such

sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	123	GLN
2	Ab	4	HIS
2	Ab	48	HIS
2	Ab	58	GLN
2	Ab	118	GLN
1	Ac	123	GLN
2	Ad	4	HIS
2	Ad	48	HIS
2	Ad	58	GLN
2	Ad	118	GLN
1	Ae	20	ASN
1	Ae	123	GLN
2	Af	4	HIS
2	Af	48	HIS
2	Af	57	ASN
2	Af	58	GLN
2	Af	118	GLN
1	Ag	123	GLN
2	Ah	4	HIS
2	Ah	48	HIS
2	Ah	57	ASN
2	Ah	58	GLN
2	Ah	118	GLN
1	Ai	123	GLN
2	Aj	4	HIS
2	Aj	48	HIS
2	Aj	58	GLN
2	Aj	118	GLN
1	Ak	123	GLN
2	Al	4	HIS
2	Al	48	HIS
2	Al	58	GLN
2	Al	118	GLN
1	Am	123	GLN
2	An	4	HIS
2	An	48	HIS
2	An	58	GLN
2	An	118	GLN
1	Ao	123	GLN
2	Ap	4	HIS
2	Ap	48	HIS
2	Ap	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ap	118	GLN
1	Aq	123	GLN
2	Ar	4	HIS
2	Ar	48	HIS
2	Ar	57	ASN
2	Ar	58	GLN
2	Ar	118	GLN
1	As	123	GLN
2	At	4	HIS
2	At	48	HIS
2	At	57	ASN
2	At	58	GLN
2	At	118	GLN
1	Au	123	GLN
2	Av	4	HIS
2	Av	48	HIS
2	Av	58	GLN
2	Av	118	GLN
1	Aw	123	GLN
2	Ax	4	HIS
2	Ax	48	HIS
2	Ax	58	GLN
2	Ax	118	GLN
1	Ay	123	GLN
2	Az	4	HIS
2	Az	48	HIS
2	Az	58	GLN
2	Az	118	GLN
1	Ba	123	GLN
2	Bb	4	HIS
2	Bb	48	HIS
2	Bb	58	GLN
2	Bb	118	GLN
1	Bc	123	GLN
2	Bd	4	HIS
2	Bd	48	HIS
2	Bd	58	GLN
2	Bd	118	GLN
1	Be	123	GLN
2	Bf	48	HIS
2	Bf	57	ASN
2	Bf	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Bf	118	GLN
1	Bg	123	GLN
2	Bh	4	HIS
2	Bh	48	HIS
2	Bh	58	GLN
2	Bh	118	GLN
1	Bi	123	GLN
2	Bj	4	HIS
2	Bj	48	HIS
2	Bj	57	ASN
2	Bj	58	GLN
2	Bj	118	GLN
1	Bk	20	ASN
1	Bk	123	GLN
2	Bl	4	HIS
2	Bl	48	HIS
2	Bl	58	GLN
2	Bl	118	GLN
1	Bm	123	GLN
2	Bn	4	HIS
2	Bn	48	HIS
2	Bn	58	GLN
2	Bn	118	GLN
1	Bo	123	GLN
2	Bp	4	HIS
2	Bp	48	HIS
2	Bp	58	GLN
2	Bp	118	GLN
1	Bq	123	GLN
2	Br	4	HIS
2	Br	48	HIS
2	Br	58	GLN
2	Br	118	GLN
1	Bs	123	GLN
2	Bt	4	HIS
2	Bt	48	HIS
2	Bt	58	GLN
2	Bt	118	GLN
1	Bu	20	ASN
1	Bu	123	GLN
2	Bv	4	HIS
2	Bv	48	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Bv	58	GLN
2	Bv	118	GLN
1	Bw	123	GLN
2	Bx	4	HIS
2	Bx	48	HIS
2	Bx	58	GLN
2	Bx	118	GLN
1	By	123	GLN
2	Bz	4	HIS
2	Bz	48	HIS
2	Bz	58	GLN
2	Bz	118	GLN
1	Ca	123	GLN
2	Cb	4	HIS
2	Cb	48	HIS
2	Cb	58	GLN
2	Cb	118	GLN
1	Cc	20	ASN
1	Cc	123	GLN
2	Cd	4	HIS
2	Cd	48	HIS
2	Cd	58	GLN
2	Cd	118	GLN
1	Ce	123	GLN
2	Cf	4	HIS
2	Cf	48	HIS
2	Cf	58	GLN
2	Cf	118	GLN
1	Cg	123	GLN
2	Ch	4	HIS
2	Ch	48	HIS
2	Ch	57	ASN
2	Ch	58	GLN
2	Ch	118	GLN
1	Ci	123	GLN
2	Cj	4	HIS
2	Cj	48	HIS
2	Cj	58	GLN
2	Cj	118	GLN
1	Ck	123	GLN
2	Cl	4	HIS
2	Cl	48	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Cl	57	ASN
2	Cl	58	GLN
2	Cl	118	GLN
1	Cm	123	GLN
2	Cn	4	HIS
2	Cn	48	HIS
2	Cn	57	ASN
2	Cn	58	GLN
2	Cn	118	GLN
1	Co	123	GLN
2	Cp	4	HIS
2	Cp	48	HIS
2	Cp	57	ASN
2	Cp	58	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no 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.