wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:59 PM BST

PDB ID	:	3J3X
EMDB ID:	:	EMD-5645
Title	:	Independent reconstruction of Mm-cpn cryo-EM density map from half dataset in the closed state (training map)
Authors	:	DiMaio, F.; Zhang, J.; Chiu, W.; Baker, D.
Deposited on	:	2013-05-02
Resolution	:	4.30 Å(reported)
Based on PDB ID	:	1Q3Q

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

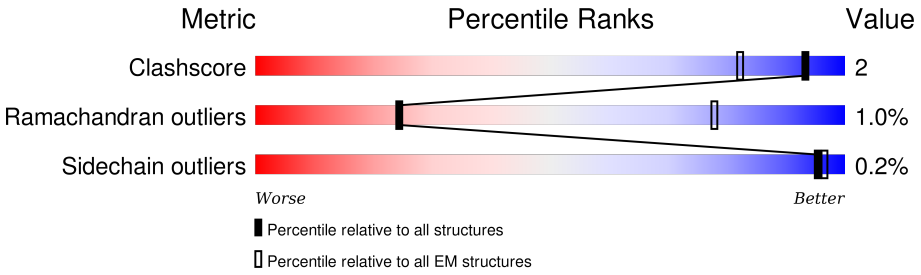
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 4.30 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	A	532	91%
1	B	532	91%
1	C	532	92%
1	D	532	91%
1	E	532	91%
1	F	532	91%
1	G	532	91%
1	H	532	91%
1	I	532	91%

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Mol	Chain	Length	Quality of chain
1	J	532	91%
1	K	532	91%
1	L	532	91%
1	M	532	92%
1	N	532	91%
1	O	532	91%
1	P	532	91%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 61264 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 Chaperonin.

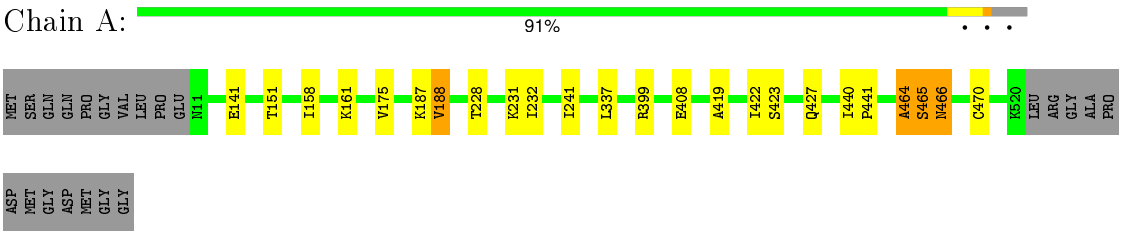
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	B	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	C	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	D	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	E	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	F	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	G	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	H	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	I	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	J	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	K	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	L	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	M	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	N	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	O	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		
1	P	510	Total	C	N	O	S	0	0
			3829	2376	662	766	25		

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.

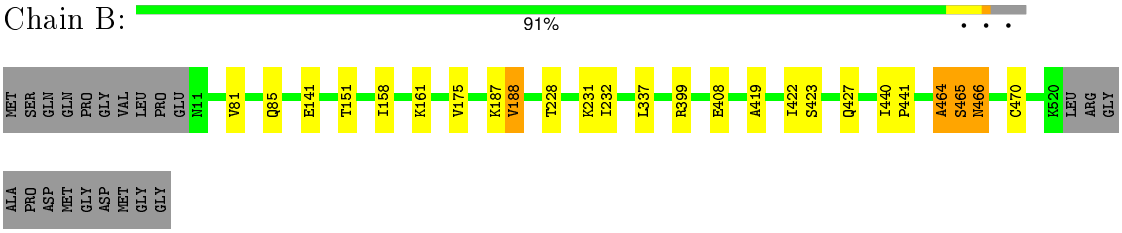
- Molecule 1: Chaperonin

Chain A:



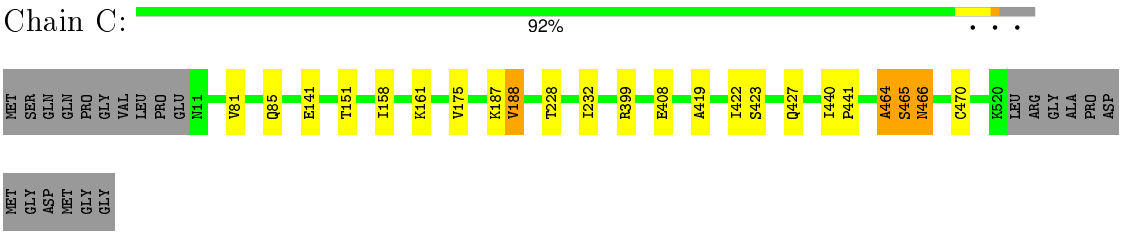
- Molecule 1: Chaperonin

Chain B:



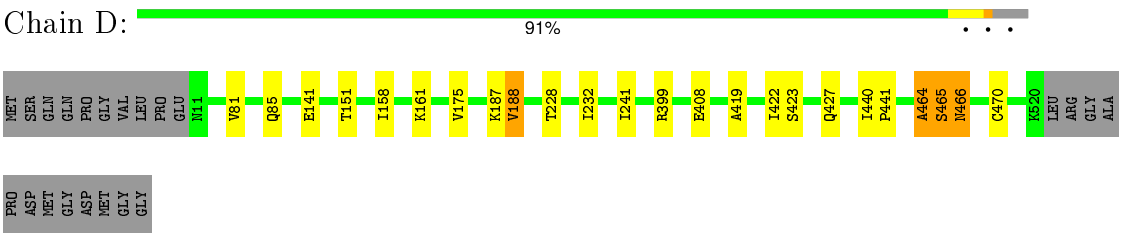
- Molecule 1: Chaperonin

Chain C:



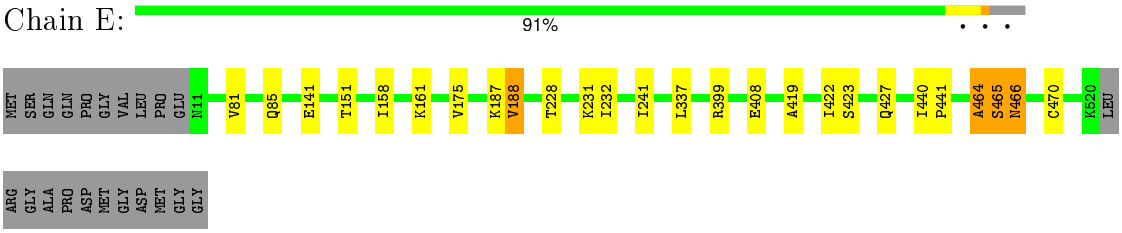
- Molecule 1: Chaperonin

Chain D:



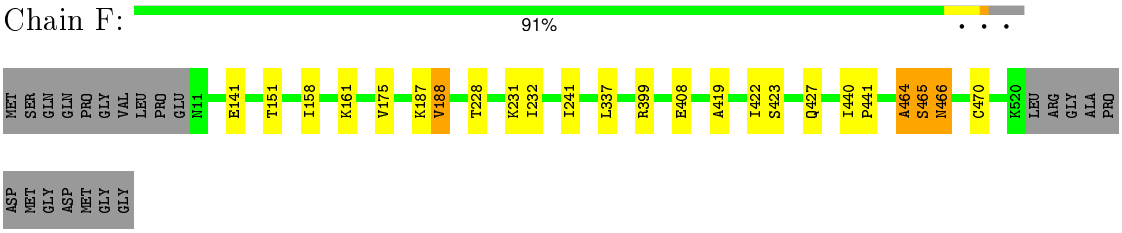
- Molecule 1: Chaperonin

Chain E:



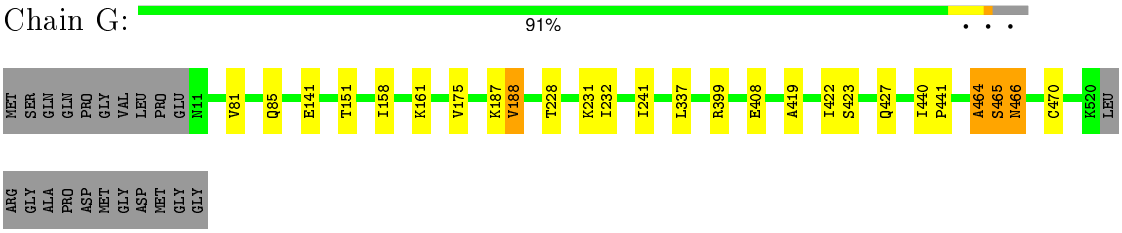
• Molecule 1: Chaperonin

Chain F:



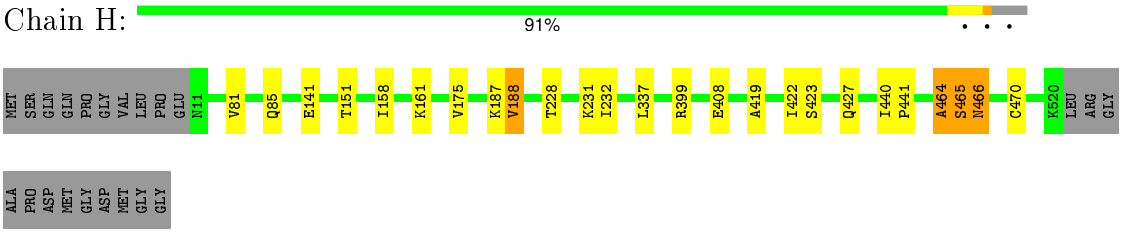
• Molecule 1: Chaperonin

Chain G:



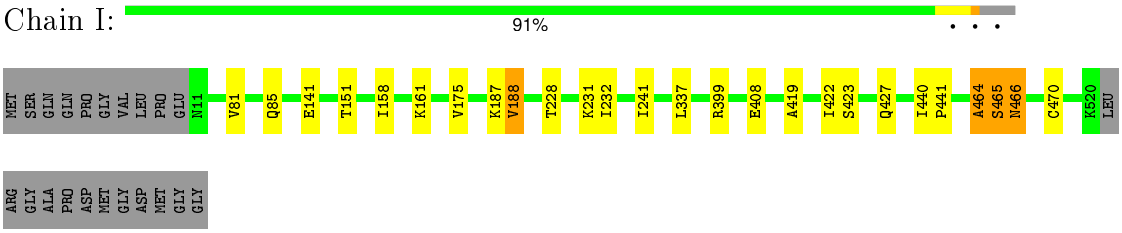
• Molecule 1: Chaperonin

Chain H:



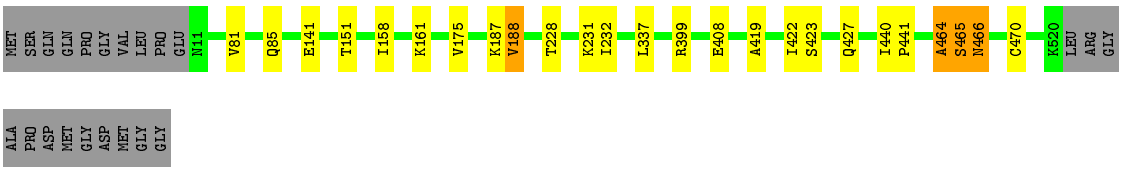
• Molecule 1: Chaperonin

Chain I:



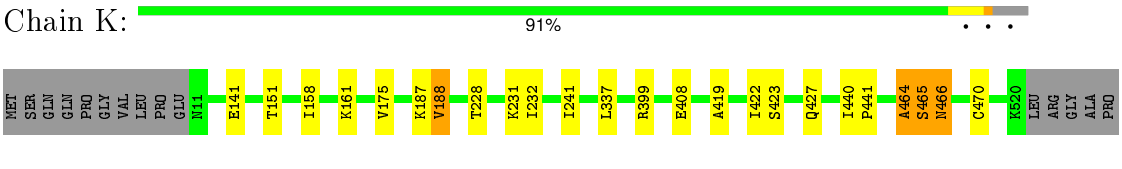
• Molecule 1: Chaperonin

Chain J:



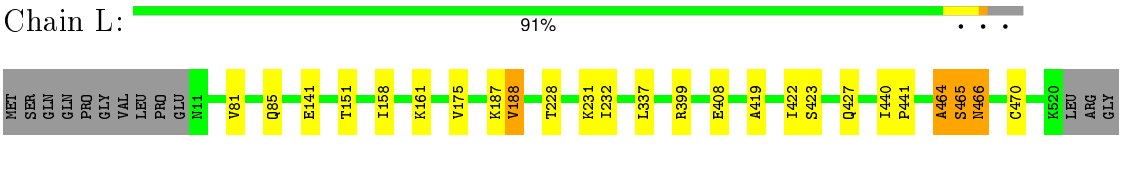
• Molecule 1: Chaperonin

Chain K:



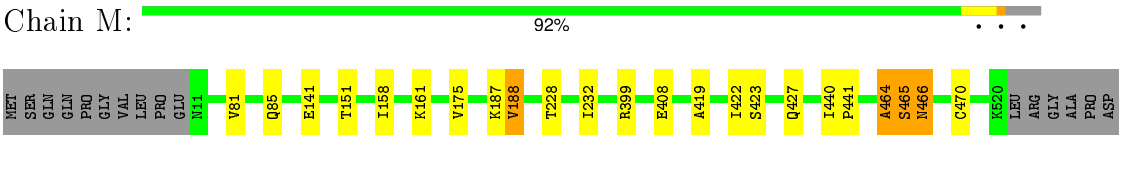
• Molecule 1: Chaperonin

Chain L:



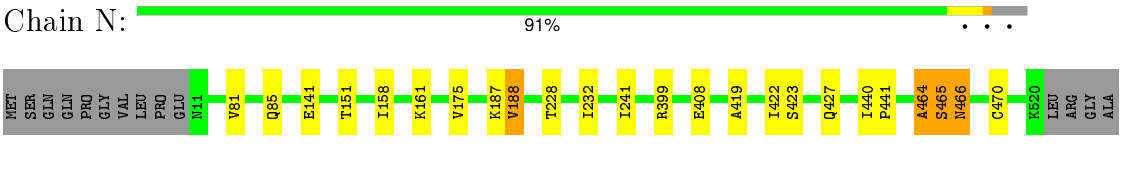
• Molecule 1: Chaperonin

Chain M:



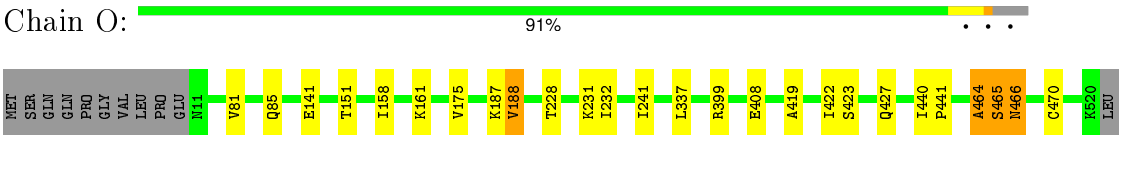
• Molecule 1: Chaperonin

Chain N:



• Molecule 1: Chaperonin

Chain O:



- Molecule 1: Chaperonin

Chain P:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	22571	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	80000	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	0.78	0/3851	0.66	1/5180 (0.0%)
1	B	0.78	0/3851	0.66	1/5180 (0.0%)
1	C	0.78	0/3851	0.66	1/5180 (0.0%)
1	D	0.78	0/3851	0.66	1/5180 (0.0%)
1	E	0.78	0/3851	0.66	1/5180 (0.0%)
1	F	0.78	0/3851	0.66	1/5180 (0.0%)
1	G	0.78	0/3851	0.66	1/5180 (0.0%)
1	H	0.78	0/3851	0.66	1/5180 (0.0%)
1	I	0.78	0/3851	0.66	1/5180 (0.0%)
1	J	0.78	0/3851	0.66	1/5180 (0.0%)
1	K	0.78	0/3851	0.66	1/5180 (0.0%)
1	L	0.78	0/3851	0.66	1/5180 (0.0%)
1	M	0.78	0/3851	0.66	1/5180 (0.0%)
1	N	0.78	0/3851	0.66	1/5180 (0.0%)
1	O	0.78	0/3851	0.66	1/5180 (0.0%)
1	P	0.78	0/3851	0.66	1/5180 (0.0%)
All	All	0.78	0/61616	0.66	16/82880 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	470	CYS	N-CA-CB	-5.52	100.66	110.60
1	B	470	CYS	N-CA-CB	-5.51	100.69	110.60
1	M	470	CYS	N-CA-CB	-5.51	100.69	110.60
1	E	470	CYS	N-CA-CB	-5.50	100.70	110.60
1	J	470	CYS	N-CA-CB	-5.50	100.70	110.60
1	I	470	CYS	N-CA-CB	-5.50	100.71	110.60
1	H	470	CYS	N-CA-CB	-5.49	100.71	110.60
1	O	470	CYS	N-CA-CB	-5.49	100.71	110.60
1	F	470	CYS	N-CA-CB	-5.49	100.72	110.60
1	D	470	CYS	N-CA-CB	-5.48	100.73	110.60
1	P	470	CYS	N-CA-CB	-5.48	100.73	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	CYS	N-CA-CB	-5.48	100.74	110.60
1	G	470	CYS	N-CA-CB	-5.48	100.74	110.60
1	N	470	CYS	N-CA-CB	-5.48	100.74	110.60
1	C	470	CYS	N-CA-CB	-5.47	100.75	110.60
1	K	470	CYS	N-CA-CB	-5.46	100.78	110.60

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	A	3829	0	3973	13	0
1	B	3829	0	3973	13	0
1	C	3829	0	3973	12	0
1	D	3829	0	3973	13	0
1	E	3829	0	3973	14	0
1	F	3829	0	3973	13	0
1	G	3829	0	3973	14	0
1	H	3829	0	3973	13	0
1	I	3829	0	3973	14	0
1	J	3829	0	3973	13	0
1	K	3829	0	3973	13	0
1	L	3829	0	3973	13	0
1	M	3829	0	3973	12	0
1	N	3829	0	3973	13	0
1	O	3829	0	3973	14	0
1	P	3829	0	3973	13	0
All	All	61264	0	63568	210	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 2.

All (210) 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:H:464:ALA:O	1:H:465:SER:C	2.34	0.66
1:J:464:ALA:O	1:J:465:SER:C	2.34	0.66
1:A:464:ALA:O	1:A:465:SER:C	2.34	0.66
1:N:464:ALA:O	1:N:465:SER:C	2.34	0.65
1:O:464:ALA:O	1:O:465:SER:C	2.34	0.65
1:D:464:ALA:O	1:D:465:SER:C	2.34	0.65
1:K:464:ALA:O	1:K:465:SER:C	2.34	0.65
1:E:464:ALA:O	1:E:465:SER:C	2.34	0.65
1:I:464:ALA:O	1:I:465:SER:C	2.34	0.64
1:F:464:ALA:O	1:F:465:SER:C	2.34	0.64
1:P:464:ALA:O	1:P:465:SER:C	2.34	0.64
1:M:464:ALA:O	1:M:465:SER:C	2.34	0.64
1:B:464:ALA:O	1:B:465:SER:C	2.34	0.64
1:C:464:ALA:O	1:C:465:SER:C	2.34	0.64
1:L:464:ALA:O	1:L:465:SER:C	2.34	0.64
1:G:464:ALA:O	1:G:465:SER:C	2.34	0.64
1:M:465:SER:O	1:M:466:ASN:C	2.37	0.63
1:C:465:SER:O	1:C:466:ASN:C	2.37	0.63
1:N:465:SER:O	1:N:466:ASN:C	2.37	0.63
1:D:465:SER:O	1:D:466:ASN:C	2.37	0.63
1:H:465:SER:O	1:H:466:ASN:C	2.37	0.63
1:J:465:SER:O	1:J:466:ASN:C	2.37	0.63
1:B:465:SER:O	1:B:466:ASN:C	2.37	0.63
1:I:465:SER:O	1:I:466:ASN:C	2.37	0.63
1:L:465:SER:O	1:L:466:ASN:C	2.37	0.63
1:G:465:SER:O	1:G:466:ASN:C	2.37	0.63
1:O:465:SER:O	1:O:466:ASN:C	2.37	0.62
1:E:465:SER:O	1:E:466:ASN:C	2.37	0.62
1:P:465:SER:O	1:P:466:ASN:C	2.37	0.62
1:F:465:SER:O	1:F:466:ASN:C	2.37	0.62
1:A:465:SER:O	1:A:466:ASN:C	2.37	0.62
1:K:465:SER:O	1:K:466:ASN:C	2.37	0.62
1:K:187:LYS:O	1:K:188:VAL:C	2.44	0.56
1:P:187:LYS:O	1:P:188:VAL:C	2.44	0.56
1:F:187:LYS:O	1:F:188:VAL:C	2.44	0.56
1:A:187:LYS:O	1:A:188:VAL:C	2.44	0.56
1:D:187:LYS:O	1:D:188:VAL:C	2.44	0.56
1:G:187:LYS:O	1:G:188:VAL:C	2.44	0.56
1:N:187:LYS:O	1:N:188:VAL:C	2.44	0.56
1:I:187:LYS:O	1:I:188:VAL:C	2.44	0.56
1:O:187:LYS:O	1:O:188:VAL:C	2.44	0.56
1:M:187:LYS:O	1:M:188:VAL:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LYS:O	1:E:188:VAL:C	2.44	0.55
1:C:187:LYS:O	1:C:188:VAL:C	2.44	0.55
1:J:187:LYS:O	1:J:188:VAL:C	2.44	0.55
1:H:187:LYS:O	1:H:188:VAL:C	2.44	0.55
1:L:187:LYS:O	1:L:188:VAL:C	2.44	0.54
1:B:187:LYS:O	1:B:188:VAL:C	2.44	0.54
1:G:408:GLU:N	1:G:408:GLU:OE1	2.42	0.51
1:I:408:GLU:OE1	1:I:408:GLU:N	2.42	0.51
1:I:141:GLU:HA	1:I:399:ARG:HG2	1.93	0.50
1:H:141:GLU:HA	1:H:399:ARG:HG2	1.93	0.50
1:J:141:GLU:HA	1:J:399:ARG:HG2	1.93	0.50
1:C:408:GLU:OE1	1:C:408:GLU:N	2.42	0.50
1:M:141:GLU:HA	1:M:399:ARG:HG2	1.93	0.50
1:M:408:GLU:N	1:M:408:GLU:OE1	2.42	0.50
1:G:141:GLU:HA	1:G:399:ARG:HG2	1.93	0.50
1:P:141:GLU:HA	1:P:399:ARG:HG2	1.93	0.50
1:C:141:GLU:HA	1:C:399:ARG:HG2	1.93	0.50
1:F:141:GLU:HA	1:F:399:ARG:HG2	1.93	0.50
1:K:141:GLU:HA	1:K:399:ARG:HG2	1.93	0.50
1:A:141:GLU:HA	1:A:399:ARG:HG2	1.93	0.50
1:O:141:GLU:HA	1:O:399:ARG:HG2	1.93	0.49
1:A:408:GLU:OE1	1:A:408:GLU:N	2.42	0.49
1:E:141:GLU:HA	1:E:399:ARG:HG2	1.93	0.49
1:D:408:GLU:OE1	1:D:408:GLU:N	2.42	0.49
1:K:408:GLU:N	1:K:408:GLU:OE1	2.42	0.49
1:N:141:GLU:HA	1:N:399:ARG:HG2	1.93	0.49
1:B:141:GLU:HA	1:B:399:ARG:HG2	1.93	0.49
1:N:408:GLU:OE1	1:N:408:GLU:N	2.42	0.49
1:D:141:GLU:HA	1:D:399:ARG:HG2	1.93	0.49
1:L:141:GLU:HA	1:L:399:ARG:HG2	1.93	0.49
1:H:408:GLU:N	1:H:408:GLU:OE1	2.42	0.48
1:J:408:GLU:N	1:J:408:GLU:OE1	2.42	0.48
1:B:408:GLU:N	1:B:408:GLU:OE1	2.42	0.48
1:M:232:ILE:N	1:M:232:ILE:HD12	2.30	0.47
1:C:232:ILE:HD12	1:C:232:ILE:N	2.30	0.47
1:L:408:GLU:N	1:L:408:GLU:OE1	2.42	0.47
1:N:232:ILE:HD12	1:N:232:ILE:N	2.30	0.47
1:D:232:ILE:HD12	1:D:232:ILE:N	2.30	0.47
1:E:408:GLU:OE1	1:E:408:GLU:N	2.42	0.47
1:A:232:ILE:N	1:A:232:ILE:HD12	2.30	0.47
1:L:232:ILE:N	1:L:232:ILE:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:408:GLU:N	1:O:408:GLU:OE1	2.42	0.47
1:K:232:ILE:N	1:K:232:ILE:HD12	2.30	0.47
1:B:232:ILE:HD12	1:B:232:ILE:N	2.30	0.47
1:O:232:ILE:N	1:O:232:ILE:HD12	2.30	0.46
1:H:232:ILE:HD12	1:H:232:ILE:N	2.30	0.46
1:J:232:ILE:N	1:J:232:ILE:HD12	2.30	0.46
1:E:232:ILE:HD12	1:E:232:ILE:N	2.30	0.46
1:F:232:ILE:HD12	1:F:232:ILE:N	2.30	0.46
1:P:232:ILE:N	1:P:232:ILE:HD12	2.30	0.46
1:G:232:ILE:N	1:G:232:ILE:HD12	2.30	0.45
1:I:232:ILE:N	1:I:232:ILE:HD12	2.30	0.45
1:L:151:THR:HA	1:L:175:VAL:HG21	1.99	0.45
1:K:151:THR:HA	1:K:175:VAL:HG21	1.99	0.45
1:A:151:THR:HA	1:A:175:VAL:HG21	1.99	0.45
1:B:151:THR:HA	1:B:175:VAL:HG21	1.99	0.45
1:O:151:THR:HA	1:O:175:VAL:HG21	1.99	0.45
1:E:151:THR:HA	1:E:175:VAL:HG21	1.99	0.45
1:F:408:GLU:OE1	1:F:408:GLU:N	2.42	0.45
1:D:151:THR:HA	1:D:175:VAL:HG21	1.99	0.44
1:P:408:GLU:OE1	1:P:408:GLU:N	2.42	0.44
1:E:440:ILE:HB	1:E:441:PRO:CD	2.48	0.44
1:L:440:ILE:HB	1:L:441:PRO:CD	2.48	0.44
1:N:151:THR:HA	1:N:175:VAL:HG21	1.99	0.44
1:O:440:ILE:HB	1:O:441:PRO:CD	2.48	0.44
1:J:151:THR:HA	1:J:175:VAL:HG21	1.99	0.44
1:H:151:THR:HA	1:H:175:VAL:HG21	1.99	0.44
1:A:440:ILE:HB	1:A:441:PRO:CD	2.48	0.44
1:N:440:ILE:HB	1:N:441:PRO:CD	2.48	0.44
1:B:440:ILE:HB	1:B:441:PRO:CD	2.48	0.44
1:D:440:ILE:HB	1:D:441:PRO:CD	2.48	0.44
1:K:440:ILE:HB	1:K:441:PRO:CD	2.48	0.44
1:C:440:ILE:HB	1:C:441:PRO:CD	2.48	0.44
1:M:440:ILE:HB	1:M:441:PRO:CD	2.48	0.44
1:J:440:ILE:HB	1:J:441:PRO:CD	2.48	0.44
1:H:440:ILE:HB	1:H:441:PRO:CD	2.48	0.44
1:P:151:THR:HA	1:P:175:VAL:HG21	1.99	0.44
1:F:151:THR:HA	1:F:175:VAL:HG21	1.99	0.44
1:G:151:THR:HA	1:G:175:VAL:HG21	1.99	0.44
1:G:440:ILE:HB	1:G:441:PRO:CD	2.47	0.44
1:I:151:THR:HA	1:I:175:VAL:HG21	1.99	0.44
1:P:440:ILE:HB	1:P:441:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:ILE:O	1:E:423:SER:HB3	2.18	0.43
1:M:151:THR:HA	1:M:175:VAL:HG21	1.99	0.43
1:O:422:ILE:O	1:O:423:SER:HB3	2.18	0.43
1:I:440:ILE:HB	1:I:441:PRO:CD	2.48	0.43
1:C:151:THR:HA	1:C:175:VAL:HG21	1.99	0.43
1:F:440:ILE:HB	1:F:441:PRO:CD	2.48	0.43
1:N:422:ILE:O	1:N:423:SER:HB3	2.18	0.43
1:D:422:ILE:O	1:D:423:SER:HB3	2.18	0.43
1:I:422:ILE:O	1:I:423:SER:HB3	2.18	0.43
1:G:422:ILE:O	1:G:423:SER:HB3	2.19	0.43
1:C:422:ILE:O	1:C:423:SER:HB3	2.18	0.42
1:F:422:ILE:O	1:F:423:SER:HB3	2.18	0.42
1:A:158:ILE:HG22	1:A:158:ILE:O	2.20	0.42
1:K:158:ILE:O	1:K:158:ILE:HG22	2.20	0.42
1:M:422:ILE:O	1:M:423:SER:HB3	2.18	0.42
1:J:422:ILE:O	1:J:423:SER:HB3	2.18	0.42
1:G:158:ILE:HG22	1:G:158:ILE:O	2.20	0.42
1:L:422:ILE:O	1:L:423:SER:HB3	2.18	0.42
1:I:158:ILE:O	1:I:158:ILE:HG22	2.20	0.42
1:P:422:ILE:O	1:P:423:SER:HB3	2.18	0.42
1:B:422:ILE:O	1:B:423:SER:HB3	2.19	0.42
1:M:158:ILE:O	1:M:158:ILE:HG22	2.20	0.42
1:C:158:ILE:O	1:C:158:ILE:HG22	2.19	0.42
1:H:422:ILE:O	1:H:423:SER:HB3	2.18	0.42
1:B:158:ILE:HG22	1:B:158:ILE:O	2.20	0.42
1:N:158:ILE:HG22	1:N:158:ILE:O	2.19	0.42
1:D:158:ILE:HG22	1:D:158:ILE:O	2.20	0.42
1:A:422:ILE:O	1:A:423:SER:HB3	2.18	0.42
1:K:422:ILE:O	1:K:423:SER:HB3	2.18	0.42
1:L:158:ILE:HG22	1:L:158:ILE:O	2.20	0.42
1:H:158:ILE:HG22	1:H:158:ILE:O	2.20	0.41
1:J:158:ILE:O	1:J:158:ILE:HG22	2.20	0.41
1:A:419:ALA:HB1	1:A:427:GLN:HG3	2.03	0.41
1:K:419:ALA:HB1	1:K:427:GLN:HG3	2.03	0.41
1:D:81:VAL:O	1:D:85:GLN:HG2	2.21	0.41
1:L:419:ALA:HB1	1:L:427:GLN:HG3	2.03	0.41
1:P:231:LYS:HB3	1:P:337:LEU:HD13	2.03	0.41
1:F:419:ALA:HB1	1:F:427:GLN:HG3	2.03	0.41
1:M:419:ALA:HB1	1:M:427:GLN:HG3	2.03	0.41
1:B:419:ALA:HB1	1:B:427:GLN:HG3	2.03	0.41
1:O:231:LYS:HB3	1:O:337:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:419:ALA:HB1	1:P:427:GLN:HG3	2.03	0.41
1:F:231:LYS:HB3	1:F:337:LEU:HD13	2.02	0.41
1:P:158:ILE:HG22	1:P:158:ILE:O	2.20	0.41
1:N:81:VAL:O	1:N:85:GLN:HG2	2.21	0.41
1:C:419:ALA:HB1	1:C:427:GLN:HG3	2.03	0.41
1:E:231:LYS:HB3	1:E:337:LEU:HD13	2.02	0.41
1:F:158:ILE:HG22	1:F:158:ILE:O	2.20	0.41
1:A:231:LYS:HB3	1:A:337:LEU:HD13	2.02	0.41
1:L:81:VAL:O	1:L:85:GLN:HG2	2.21	0.41
1:K:231:LYS:HB3	1:K:337:LEU:HD13	2.02	0.41
1:B:81:VAL:O	1:B:85:GLN:HG2	2.21	0.41
1:J:419:ALA:HB1	1:J:427:GLN:HG3	2.03	0.41
1:E:419:ALA:HB1	1:E:427:GLN:HG3	2.03	0.41
1:O:81:VAL:O	1:O:85:GLN:HG2	2.21	0.41
1:I:81:VAL:O	1:I:85:GLN:HG2	2.21	0.41
1:H:419:ALA:HB1	1:H:427:GLN:HG3	2.03	0.41
1:G:81:VAL:O	1:G:85:GLN:HG2	2.21	0.41
1:G:241:ILE:N	1:G:241:ILE:HD12	2.37	0.40
1:H:81:VAL:O	1:H:85:GLN:HG2	2.21	0.40
1:N:419:ALA:HB1	1:N:427:GLN:HG3	2.03	0.40
1:E:81:VAL:O	1:E:85:GLN:HG2	2.21	0.40
1:E:158:ILE:O	1:E:158:ILE:HG22	2.20	0.40
1:I:241:ILE:HD12	1:I:241:ILE:N	2.37	0.40
1:G:419:ALA:HB1	1:G:427:GLN:HG3	2.03	0.40
1:H:231:LYS:HB3	1:H:337:LEU:HD13	2.02	0.40
1:J:81:VAL:O	1:J:85:GLN:HG2	2.21	0.40
1:O:419:ALA:HB1	1:O:427:GLN:HG3	2.03	0.40
1:I:419:ALA:HB1	1:I:427:GLN:HG3	2.03	0.40
1:I:231:LYS:HB3	1:I:337:LEU:HD13	2.03	0.40
1:D:419:ALA:HB1	1:D:427:GLN:HG3	2.03	0.40
1:O:158:ILE:HG22	1:O:158:ILE:O	2.20	0.40
1:E:241:ILE:N	1:E:241:ILE:HD12	2.36	0.40
1:G:231:LYS:HB3	1:G:337:LEU:HD13	2.03	0.40
1:L:231:LYS:HB3	1:L:337:LEU:HD13	2.02	0.40
1:A:241:ILE:N	1:A:241:ILE:HD12	2.37	0.40
1:N:241:ILE:N	1:N:241:ILE:HD12	2.37	0.40
1:B:231:LYS:HB3	1:B:337:LEU:HD13	2.02	0.40
1:J:231:LYS:HB3	1:J:337:LEU:HD13	2.02	0.40
1:F:241:ILE:HD12	1:F:241:ILE:N	2.37	0.40
1:O:241:ILE:HD12	1:O:241:ILE:N	2.37	0.40
1:P:241:ILE:HD12	1:P:241:ILE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:HD12	1:D:241:ILE:N	2.37	0.40
1:K:241:ILE:HD12	1:K:241:ILE:N	2.37	0.40
1:M:81:VAL:O	1:M:85:GLN:HG2	2.21	0.40
1:C:81:VAL:O	1:C:85:GLN:HG2	2.21	0.40

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	A	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	B	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	C	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	D	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	E	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	F	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	G	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	H	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	I	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	J	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	K	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	L	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	M	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	N	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	O	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65
1	P	508/532 (96%)	496 (98%)	7 (1%)	5 (1%)	19	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8128/8512 (96%)	7936 (98%)	112 (1%)	80 (1%)	24 65

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	465	SER
1	A	466	ASN
1	B	228	THR
1	B	465	SER
1	B	466	ASN
1	C	228	THR
1	C	465	SER
1	C	466	ASN
1	D	228	THR
1	D	465	SER
1	D	466	ASN
1	E	228	THR
1	E	465	SER
1	E	466	ASN
1	F	228	THR
1	F	465	SER
1	F	466	ASN
1	G	228	THR
1	G	465	SER
1	G	466	ASN
1	H	228	THR
1	H	465	SER
1	H	466	ASN
1	I	228	THR
1	I	465	SER
1	I	466	ASN
1	J	228	THR
1	J	465	SER
1	J	466	ASN
1	K	228	THR
1	K	465	SER
1	K	466	ASN
1	L	228	THR
1	L	465	SER
1	L	466	ASN
1	M	228	THR

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Mol	Chain	Res	Type
1	M	465	SER
1	M	466	ASN
1	N	228	THR
1	N	465	SER
1	N	466	ASN
1	O	228	THR
1	O	465	SER
1	O	466	ASN
1	P	228	THR
1	P	465	SER
1	P	466	ASN
1	A	188	VAL
1	B	188	VAL
1	C	188	VAL
1	D	188	VAL
1	E	188	VAL
1	F	188	VAL
1	G	188	VAL
1	H	188	VAL
1	I	188	VAL
1	J	188	VAL
1	K	188	VAL
1	L	188	VAL
1	M	188	VAL
1	N	188	VAL
1	O	188	VAL
1	P	188	VAL
1	A	464	ALA
1	B	464	ALA
1	C	464	ALA
1	D	464	ALA
1	E	464	ALA
1	F	464	ALA
1	G	464	ALA
1	H	464	ALA
1	I	464	ALA
1	J	464	ALA
1	K	464	ALA
1	L	464	ALA
1	M	464	ALA
1	N	464	ALA
1	O	464	ALA

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Mol	Chain	Res	Type
1	P	464	ALA

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	A	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	B	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	C	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	D	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	E	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	F	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	G	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	H	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	I	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	J	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	K	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	L	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	M	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	N	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	O	411/427 (96%)	410 (100%)	1 (0%)	95	97
1	P	411/427 (96%)	410 (100%)	1 (0%)	95	97
All	All	6576/6832 (96%)	6560 (100%)	16 (0%)	95	97

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	LYS
1	B	161	LYS
1	C	161	LYS

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Mol	Chain	Res	Type
1	D	161	LYS
1	E	161	LYS
1	F	161	LYS
1	G	161	LYS
1	H	161	LYS
1	I	161	LYS
1	J	161	LYS
1	K	161	LYS
1	L	161	LYS
1	M	161	LYS
1	N	161	LYS
1	O	161	LYS
1	P	161	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	497	GLN
1	B	497	GLN
1	C	497	GLN
1	D	497	GLN
1	E	497	GLN
1	F	497	GLN
1	G	497	GLN
1	H	497	GLN
1	I	497	GLN
1	J	497	GLN
1	K	497	GLN
1	L	497	GLN
1	M	497	GLN
1	N	497	GLN
1	O	497	GLN
1	P	497	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.