wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:58 PM BST

PDB ID	:	3IZM
EMDB ID:	:	EMD-5249
Title	:	Mm-cpn wildtype with ATP
Authors	:	Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.; Chiu, W.; Frydman, J.
Deposited on	:	2010-10-30
Resolution	:	7.20 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

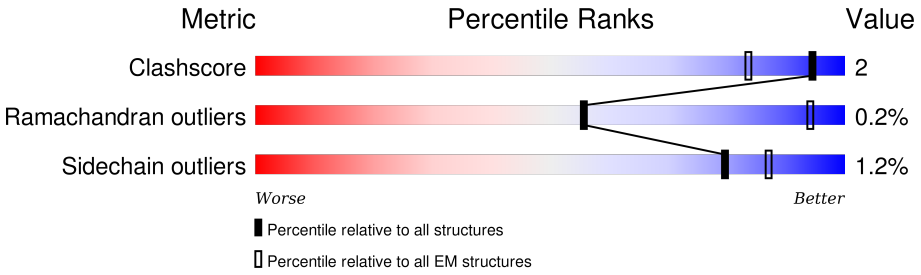
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 7.20 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 >=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	513	95%
1	B	513	95%
1	C	513	95%
1	D	513	96%
1	E	513	95%
1	F	513	96%
1	G	513	95%
1	H	513	95%
1	I	513	95%

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Mol	Chain	Length	Quality of chain
1	J	513	95%
1	K	513	95%
1	L	513	95%
1	M	513	95%
1	N	513	96%
1	O	513	95%
1	P	513	96%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 61632 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.

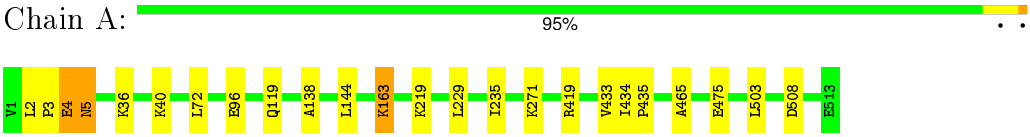
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	B	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	C	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	D	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	E	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	F	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	G	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	H	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	I	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	J	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	K	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	L	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	M	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	N	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	O	513	Total	C	N	O	S	0	0
			3852	2391	664	772	25		
1	P	513	Total	C	N	O	S	0	0
			3852	2391	664	772	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.

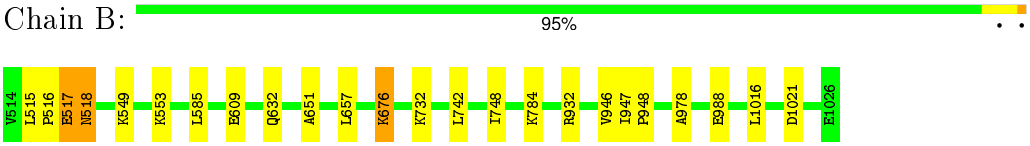
- Molecule 1: Chaperonin

Chain A:



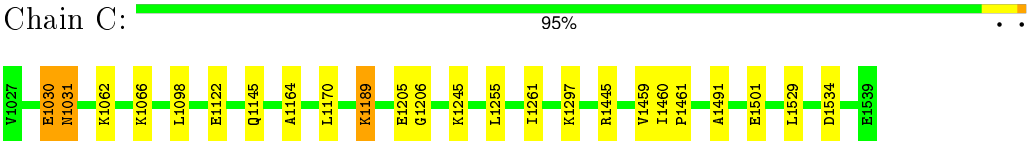
- Molecule 1: Chaperonin

Chain B:



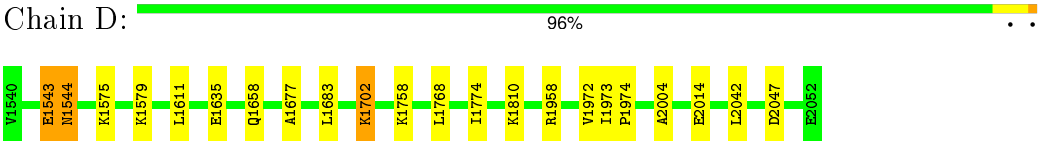
- Molecule 1: Chaperonin

Chain C:



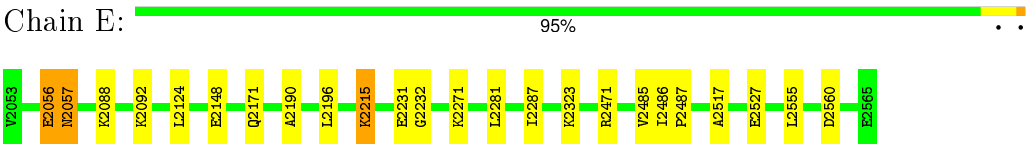
- Molecule 1: Chaperonin

Chain D:



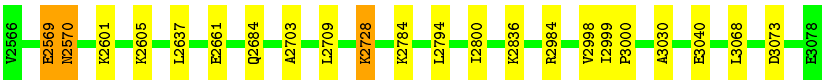
- Molecule 1: Chaperonin

Chain E:



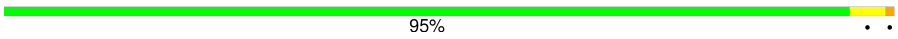
- Molecule 1: Chaperonin

Chain F:



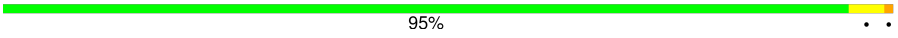
- Molecule 1: Chaperonin

Chain G:



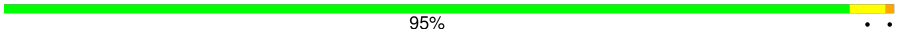
- Molecule 1: Chaperonin

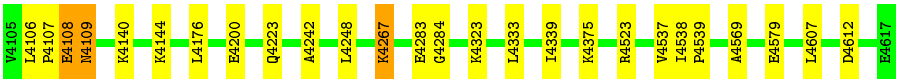
Chain H:



- Molecule 1: Chaperonin

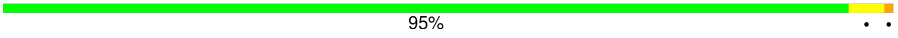
Chain I:





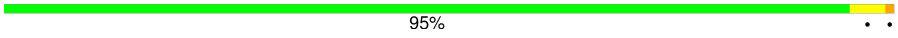
- Molecule 1: Chaperonin

Chain J:



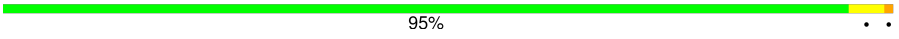
- Molecule 1: Chaperonin

Chain K:



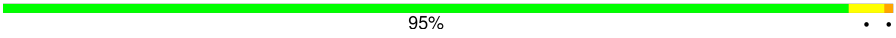
- Molecule 1: Chaperonin

Chain L:



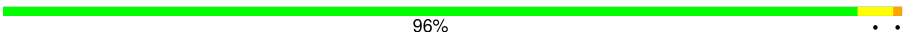
- Molecule 1: Chaperonin

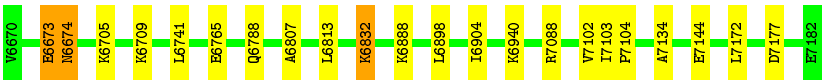
Chain M:



- Molecule 1: Chaperonin

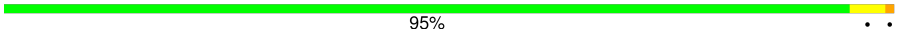
Chain N:

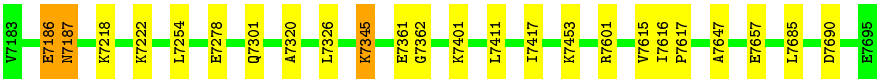




- Molecule 1: Chaperonin

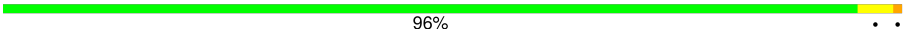
Chain O:





- Molecule 1: Chaperonin

Chain P:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 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 ($e^-/Å^2$)	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	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	B	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	C	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	D	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	E	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	F	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	G	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	H	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	I	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	J	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	K	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	L	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	M	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	N	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	O	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
1	P	0.88	2/3875 (0.1%)	0.78	2/5214 (0.0%)
All	All	0.88	32/62000 (0.1%)	0.78	32/83424 (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 (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	6160	GLU	C-O	-5.76	1.12	1.23
1	O	7186	GLU	C-O	-5.75	1.12	1.23
1	A	4	GLU	C-O	-5.72	1.12	1.23
1	C	1030	GLU	C-O	-5.72	1.12	1.23
1	E	2056	GLU	C-O	-5.72	1.12	1.23
1	G	3082	GLU	C-O	-5.72	1.12	1.23
1	K	5134	GLU	C-O	-5.72	1.12	1.23
1	B	517	GLU	C-O	-5.72	1.12	1.23
1	D	1543	GLU	C-O	-5.72	1.12	1.23
1	F	2569	GLU	C-O	-5.72	1.12	1.23
1	H	3595	GLU	C-O	-5.72	1.12	1.23
1	J	4621	GLU	C-O	-5.72	1.12	1.23
1	L	5647	GLU	C-O	-5.72	1.12	1.23
1	N	6673	GLU	C-O	-5.72	1.12	1.23
1	P	7699	GLU	C-O	-5.72	1.12	1.23
1	I	4108	GLU	C-O	-5.71	1.12	1.23
1	A	4	GLU	C-N	5.45	1.46	1.34
1	C	1030	GLU	C-N	5.45	1.46	1.34
1	E	2056	GLU	C-N	5.45	1.46	1.34
1	G	3082	GLU	C-N	5.45	1.46	1.34
1	N	6673	GLU	C-N	5.43	1.46	1.34
1	P	7699	GLU	C-N	5.43	1.46	1.34
1	B	517	GLU	C-N	5.41	1.46	1.34
1	D	1543	GLU	C-N	5.41	1.46	1.34
1	F	2569	GLU	C-N	5.41	1.46	1.34
1	H	3595	GLU	C-N	5.41	1.46	1.34
1	I	4108	GLU	C-N	5.40	1.46	1.34
1	J	4621	GLU	C-N	5.40	1.46	1.34
1	K	5134	GLU	C-N	5.40	1.46	1.34
1	L	5647	GLU	C-N	5.40	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	6160	GLU	C-N	5.40	1.46	1.34
1	O	7186	GLU	C-N	5.40	1.46	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	C	1255	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	E	2281	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	G	3307	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	I	4333	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	K	5359	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	M	6385	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	O	7411	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	B	742	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	D	1768	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	F	2794	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	H	3820	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	N	6898	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	P	7924	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	J	4846	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	L	5872	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	B	978	ALA	CB-CA-C	5.11	117.77	110.10
1	D	2004	ALA	CB-CA-C	5.11	117.77	110.10
1	F	3030	ALA	CB-CA-C	5.11	117.77	110.10
1	H	4056	ALA	CB-CA-C	5.11	117.77	110.10
1	A	465	ALA	CB-CA-C	5.11	117.76	110.10
1	C	1491	ALA	CB-CA-C	5.11	117.76	110.10
1	E	2517	ALA	CB-CA-C	5.11	117.76	110.10
1	G	3543	ALA	CB-CA-C	5.11	117.76	110.10
1	K	5595	ALA	CB-CA-C	5.11	117.76	110.10
1	M	6621	ALA	CB-CA-C	5.10	117.75	110.10
1	N	7134	ALA	CB-CA-C	5.09	117.74	110.10
1	P	8160	ALA	CB-CA-C	5.09	117.74	110.10
1	J	5082	ALA	CB-CA-C	5.08	117.73	110.10
1	L	6108	ALA	CB-CA-C	5.08	117.73	110.10
1	I	4569	ALA	CB-CA-C	5.07	117.70	110.10
1	O	7647	ALA	CB-CA-C	5.06	117.69	110.10

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	475	GLU	Mainchain
1	B	632	GLN	Mainchain
1	B	651	ALA	Mainchain
1	B	988	GLU	Mainchain
1	C	1145	GLN	Mainchain
1	C	1164	ALA	Mainchain
1	C	1501	GLU	Mainchain
1	D	1658	GLN	Mainchain
1	D	1677	ALA	Mainchain
1	D	2014	GLU	Mainchain
1	E	2171	GLN	Mainchain
1	E	2190	ALA	Mainchain
1	E	2527	GLU	Mainchain
1	F	2684	GLN	Mainchain
1	F	2703	ALA	Mainchain
1	F	3040	GLU	Mainchain
1	G	3197	GLN	Mainchain
1	G	3216	ALA	Mainchain
1	G	3553	GLU	Mainchain
1	H	3710	GLN	Mainchain
1	H	3729	ALA	Mainchain
1	H	4066	GLU	Mainchain
1	I	4223	GLN	Mainchain
1	I	4242	ALA	Mainchain
1	I	4579	GLU	Mainchain
1	J	4736	GLN	Mainchain
1	J	4755	ALA	Mainchain
1	J	5092	GLU	Mainchain
1	K	5249	GLN	Mainchain
1	K	5268	ALA	Mainchain
1	K	5605	GLU	Mainchain
1	L	5762	GLN	Mainchain
1	L	5781	ALA	Mainchain
1	L	6118	GLU	Mainchain
1	M	6275	GLN	Mainchain
1	M	6294	ALA	Mainchain
1	M	6631	GLU	Mainchain
1	N	6788	GLN	Mainchain
1	N	6807	ALA	Mainchain
1	N	7144	GLU	Mainchain
1	O	7301	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	O	7320	ALA	Mainchain
1	O	7657	GLU	Mainchain
1	P	7814	GLN	Mainchain
1	P	7833	ALA	Mainchain
1	P	8170	GLU	Mainchain

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	3852	0	3996	13	0
1	B	3852	0	3993	13	0
1	C	3852	0	3993	13	0
1	D	3852	0	3993	12	0
1	E	3852	0	3993	13	0
1	F	3852	0	3993	12	0
1	G	3852	0	3993	13	0
1	H	3852	0	3993	13	0
1	I	3852	0	3993	14	0
1	J	3852	0	3993	13	0
1	K	3852	0	3993	13	0
1	L	3852	0	3993	13	0
1	M	3852	0	3993	13	0
1	N	3852	0	3993	12	0
1	O	3852	0	3993	13	0
1	P	3852	0	3993	12	0
All	All	61632	0	63891	189	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 (189) 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:4:GLU:O	1:A:5:ASN:HB2	1.96	0.65
1:B:517:GLU:O	1:B:518:ASN:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5134:GLU:O	1:K:5135:ASN:HB2	1.96	0.65
1:L:5647:GLU:O	1:L:5648:ASN:HB2	1.96	0.65
1:C:1030:GLU:O	1:C:1031:ASN:HB2	1.96	0.65
1:H:3595:GLU:O	1:H:3596:ASN:HB2	1.96	0.65
1:J:4621:GLU:O	1:J:4622:ASN:HB2	1.96	0.65
1:M:6160:GLU:O	1:M:6161:ASN:HB2	1.96	0.64
1:D:1543:GLU:O	1:D:1544:ASN:HB2	1.96	0.64
1:N:6673:GLU:O	1:N:6674:ASN:HB2	1.96	0.64
1:I:4108:GLU:O	1:I:4109:ASN:HB2	1.96	0.64
1:G:3082:GLU:O	1:G:3083:ASN:HB2	1.96	0.64
1:P:7699:GLU:O	1:P:7700:ASN:HB2	1.96	0.64
1:F:2569:GLU:O	1:F:2570:ASN:HB2	1.96	0.64
1:O:7186:GLU:O	1:O:7187:ASN:HB2	1.96	0.64
1:E:2056:GLU:O	1:E:2057:ASN:HB2	1.96	0.64
1:E:2287:ILE:HD12	1:E:2287:ILE:H	1.65	0.62
1:O:7417:ILE:H	1:O:7417:ILE:HD12	1.65	0.62
1:C:1261:ILE:HD12	1:C:1261:ILE:H	1.65	0.61
1:M:6391:ILE:H	1:M:6391:ILE:HD12	1.65	0.61
1:G:3313:ILE:H	1:G:3313:ILE:HD12	1.65	0.61
1:I:4339:ILE:H	1:I:4339:ILE:HD12	1.65	0.61
1:N:6904:ILE:H	1:N:6904:ILE:HD12	1.65	0.60
1:K:5564:ILE:HB	1:K:5565:PRO:HD3	1.84	0.60
1:J:5051:ILE:HB	1:J:5052:PRO:HD3	1.83	0.60
1:H:4025:ILE:HB	1:H:4026:PRO:HD3	1.84	0.60
1:A:434:ILE:HB	1:A:435:PRO:HD3	1.84	0.60
1:D:1774:ILE:HD12	1:D:1774:ILE:H	1.65	0.60
1:L:6077:ILE:HB	1:L:6078:PRO:HD3	1.83	0.60
1:B:947:ILE:HB	1:B:948:PRO:HD3	1.84	0.60
1:M:6590:ILE:HB	1:M:6591:PRO:HD3	1.84	0.60
1:E:2486:ILE:HB	1:E:2487:PRO:HD3	1.84	0.60
1:D:1973:ILE:HB	1:D:1974:PRO:HD3	1.84	0.60
1:O:7616:ILE:HB	1:O:7617:PRO:HD3	1.84	0.60
1:F:2999:ILE:HB	1:F:3000:PRO:HD3	1.84	0.60
1:F:2800:ILE:HD12	1:F:2800:ILE:H	1.65	0.60
1:C:1460:ILE:HB	1:C:1461:PRO:HD3	1.84	0.60
1:J:4852:ILE:HD12	1:J:4852:ILE:H	1.65	0.60
1:N:7103:ILE:HB	1:N:7104:PRO:HD3	1.84	0.60
1:P:8129:ILE:HB	1:P:8130:PRO:HD3	1.84	0.60
1:A:235:ILE:H	1:A:235:ILE:HD12	1.65	0.60
1:P:7930:ILE:H	1:P:7930:ILE:HD12	1.65	0.60
1:G:3512:ILE:HB	1:G:3513:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5365:ILE:H	1:K:5365:ILE:HD12	1.65	0.60
1:L:5878:ILE:HD12	1:L:5878:ILE:H	1.65	0.59
1:I:4538:ILE:HB	1:I:4539:PRO:HD3	1.84	0.59
1:H:3826:ILE:HD12	1:H:3826:ILE:H	1.65	0.59
1:B:748:ILE:H	1:B:748:ILE:HD12	1.65	0.59
1:A:163:LYS:HE3	1:A:163:LYS:HA	1.90	0.54
1:K:5293:LYS:HA	1:K:5293:LYS:HE3	1.90	0.54
1:I:4267:LYS:HE3	1:I:4267:LYS:HA	1.90	0.54
1:G:3241:LYS:HE3	1:G:3241:LYS:HA	1.90	0.54
1:F:2728:LYS:HA	1:F:2728:LYS:HE3	1.90	0.54
1:C:1189:LYS:HE3	1:C:1189:LYS:HA	1.90	0.54
1:M:6319:LYS:HE3	1:M:6319:LYS:HA	1.90	0.53
1:P:7858:LYS:HA	1:P:7858:LYS:HE3	1.90	0.53
1:H:3754:LYS:HA	1:H:3754:LYS:HE3	1.90	0.53
1:J:4780:LYS:HA	1:J:4780:LYS:HE3	1.90	0.53
1:L:5806:LYS:HA	1:L:5806:LYS:HE3	1.90	0.53
1:E:2215:LYS:HE3	1:E:2215:LYS:HA	1.90	0.53
1:O:7345:LYS:HA	1:O:7345:LYS:HE3	1.90	0.53
1:B:676:LYS:HA	1:B:676:LYS:HE3	1.90	0.53
1:O:7685:LEU:C	1:O:7685:LEU:HD23	2.30	0.53
1:E:2555:LEU:C	1:E:2555:LEU:HD23	2.30	0.53
1:M:6659:LEU:C	1:M:6659:LEU:HD23	2.30	0.52
1:D:2042:LEU:HD23	1:D:2042:LEU:C	2.29	0.52
1:C:1529:LEU:HD23	1:C:1529:LEU:C	2.30	0.52
1:N:7172:LEU:HD23	1:N:7172:LEU:C	2.29	0.52
1:L:6146:LEU:HD23	1:L:6146:LEU:C	2.29	0.52
1:G:3581:LEU:HD23	1:G:3581:LEU:C	2.30	0.52
1:I:4607:LEU:C	1:I:4607:LEU:HD23	2.30	0.52
1:B:1016:LEU:C	1:B:1016:LEU:HD23	2.29	0.52
1:F:3068:LEU:C	1:F:3068:LEU:HD23	2.29	0.52
1:D:1702:LYS:HE3	1:D:1702:LYS:HA	1.90	0.52
1:P:8198:LEU:HD23	1:P:8198:LEU:C	2.29	0.52
1:N:6832:LYS:HE3	1:N:6832:LYS:HA	1.90	0.52
1:J:5120:LEU:HD23	1:J:5120:LEU:C	2.29	0.51
1:H:4094:LEU:C	1:H:4094:LEU:HD23	2.29	0.51
1:K:5633:LEU:C	1:K:5633:LEU:HD23	2.30	0.51
1:A:503:LEU:HD23	1:A:503:LEU:C	2.30	0.51
1:I:4108:GLU:O	1:I:4109:ASN:CB	2.60	0.50
1:G:3082:GLU:O	1:G:3083:ASN:CB	2.60	0.50
1:F:2569:GLU:O	1:F:2570:ASN:CB	2.60	0.49
1:J:4852:ILE:HD12	1:J:4852:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3826:ILE:HD12	1:H:3826:ILE:N	2.27	0.49
1:J:4621:GLU:O	1:J:4622:ASN:CB	2.60	0.49
1:P:7699:GLU:O	1:P:7700:ASN:CB	2.60	0.49
1:H:3595:GLU:O	1:H:3596:ASN:CB	2.60	0.49
1:C:1030:GLU:O	1:C:1031:ASN:CB	2.60	0.49
1:M:6160:GLU:O	1:M:6161:ASN:CB	2.60	0.49
1:B:517:GLU:O	1:B:518:ASN:CB	2.60	0.49
1:L:5878:ILE:N	1:L:5878:ILE:HD12	2.27	0.49
1:B:748:ILE:HD12	1:B:748:ILE:N	2.27	0.49
1:L:5647:GLU:O	1:L:5648:ASN:CB	2.60	0.49
1:N:6673:GLU:O	1:N:6674:ASN:CB	2.60	0.49
1:D:1543:GLU:O	1:D:1544:ASN:CB	2.60	0.49
1:E:2056:GLU:O	1:E:2057:ASN:CB	2.60	0.49
1:I:4339:ILE:N	1:I:4339:ILE:HD12	2.27	0.49
1:K:5134:GLU:O	1:K:5135:ASN:CB	2.60	0.49
1:G:3313:ILE:HD12	1:G:3313:ILE:N	2.27	0.49
1:A:4:GLU:O	1:A:5:ASN:CB	2.60	0.48
1:O:7186:GLU:O	1:O:7187:ASN:CB	2.60	0.48
1:C:1261:ILE:HD12	1:C:1261:ILE:N	2.27	0.48
1:A:235:ILE:N	1:A:235:ILE:HD12	2.27	0.48
1:M:6391:ILE:HD12	1:M:6391:ILE:N	2.27	0.48
1:K:5365:ILE:N	1:K:5365:ILE:HD12	2.27	0.48
1:N:6904:ILE:N	1:N:6904:ILE:HD12	2.27	0.48
1:E:2287:ILE:N	1:E:2287:ILE:HD12	2.27	0.48
1:O:7417:ILE:N	1:O:7417:ILE:HD12	2.27	0.48
1:D:1774:ILE:HD12	1:D:1774:ILE:N	2.27	0.48
1:F:2800:ILE:HD12	1:F:2800:ILE:N	2.27	0.48
1:P:7930:ILE:N	1:P:7930:ILE:HD12	2.27	0.47
1:O:7690:ASP:HB3	1:P:7735:LYS:HD2	1.98	0.45
1:D:2047:ASP:HB3	1:E:2092:LYS:HD2	1.98	0.45
1:M:6664:ASP:HB3	1:N:6709:LYS:HD2	1.98	0.45
1:E:2560:ASP:HB3	1:F:2605:LYS:HD2	1.98	0.45
1:C:1534:ASP:HB3	1:D:1579:LYS:HD2	1.98	0.45
1:N:7177:ASP:HB3	1:O:7222:LYS:HD2	1.99	0.45
1:F:3073:ASP:HB3	1:G:3118:LYS:HD2	1.98	0.45
1:B:1021:ASP:HB3	1:C:1066:LYS:HD2	1.98	0.45
1:I:4612:ASP:HB3	1:J:4657:LYS:HD2	1.98	0.44
1:I:4144:LYS:HD2	1:P:8203:ASP:HB3	1.99	0.44
1:L:6151:ASP:HB3	1:M:6196:LYS:HD2	1.99	0.44
1:G:3586:ASP:HB3	1:H:3631:LYS:HD2	1.98	0.44
1:K:5638:ASP:HB3	1:L:5683:LYS:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HD2	1:H:4099:ASP:HB3	1.98	0.44
1:A:508:ASP:HB3	1:B:553:LYS:HD2	1.98	0.43
1:M:6335:GLU:HA	1:M:6336:GLY:HA3	1.81	0.43
1:J:5125:ASP:HB3	1:K:5170:LYS:HD2	1.99	0.43
1:F:2836:LYS:O	1:F:2836:LYS:HD3	2.19	0.43
1:P:7966:LYS:O	1:P:7966:LYS:HD3	2.19	0.43
1:C:1205:GLU:HA	1:C:1206:GLY:HA3	1.81	0.43
1:E:2323:LYS:O	1:E:2323:LYS:HD3	2.19	0.43
1:N:6940:LYS:HD3	1:N:6940:LYS:O	2.19	0.43
1:P:7791:GLU:HG2	1:P:8128:VAL:HB	2.01	0.43
1:B:609:GLU:HG2	1:B:946:VAL:HB	2.01	0.43
1:F:2661:GLU:HG2	1:F:2998:VAL:HB	2.01	0.43
1:O:7453:LYS:O	1:O:7453:LYS:HD3	2.19	0.43
1:N:6765:GLU:HG2	1:N:7102:VAL:HB	2.01	0.43
1:L:5739:GLU:HG2	1:L:6076:VAL:HB	2.01	0.43
1:D:1635:GLU:HG2	1:D:1972:VAL:HB	2.01	0.43
1:D:1810:LYS:HD3	1:D:1810:LYS:O	2.19	0.43
1:G:3349:LYS:O	1:G:3349:LYS:HD3	2.19	0.42
1:L:5862:LYS:HE2	1:L:5862:LYS:HA	2.02	0.42
1:J:4619:LEU:HA	1:J:4620:PRO:HD3	1.91	0.42
1:I:4375:LYS:HD3	1:I:4375:LYS:O	2.19	0.42
1:H:3862:LYS:O	1:H:3862:LYS:HD3	2.19	0.42
1:K:5349:LYS:HA	1:K:5349:LYS:HE2	2.02	0.42
1:J:4713:GLU:HG2	1:J:5050:VAL:HB	2.01	0.42
1:H:3687:GLU:HG2	1:H:4024:VAL:HB	2.01	0.42
1:H:3593:LEU:HA	1:H:3594:PRO:HD3	1.91	0.42
1:A:219:LYS:HE2	1:A:219:LYS:HA	2.02	0.42
1:K:5401:LYS:HD3	1:K:5401:LYS:O	2.19	0.42
1:A:271:LYS:HD3	1:A:271:LYS:O	2.19	0.42
1:M:6427:LYS:HD3	1:M:6427:LYS:O	2.19	0.42
1:J:4888:LYS:O	1:J:4888:LYS:HD3	2.19	0.42
1:K:5132:LEU:HA	1:K:5133:PRO:HD3	1.91	0.42
1:A:2:LEU:HA	1:A:3:PRO:HD3	1.91	0.42
1:C:1297:LYS:HD3	1:C:1297:LYS:O	2.19	0.42
1:M:6252:GLU:HG2	1:M:6589:VAL:HB	2.01	0.42
1:B:732:LYS:HE2	1:B:732:LYS:HA	2.02	0.42
1:C:1122:GLU:HG2	1:C:1459:VAL:HB	2.01	0.42
1:C:1245:LYS:HA	1:C:1245:LYS:HE2	2.02	0.42
1:N:6888:LYS:HA	1:N:6888:LYS:HE2	2.02	0.42
1:O:7361:GLU:HA	1:O:7362:GLY:HA3	1.81	0.42
1:M:6375:LYS:HE2	1:M:6375:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4836:LYS:HE2	1:J:4836:LYS:HA	2.02	0.42
1:D:1758:LYS:HE2	1:D:1758:LYS:HA	2.02	0.42
1:A:96:GLU:HG2	1:A:433:VAL:HB	2.01	0.42
1:K:5226:GLU:HG2	1:K:5563:VAL:HB	2.01	0.42
1:O:7278:GLU:HG2	1:O:7615:VAL:HB	2.01	0.42
1:B:784:LYS:O	1:B:784:LYS:HD3	2.19	0.42
1:H:3810:LYS:HA	1:H:3810:LYS:HE2	2.02	0.42
1:L:5914:LYS:O	1:L:5914:LYS:HD3	2.19	0.41
1:E:2148:GLU:HG2	1:E:2485:VAL:HB	2.01	0.41
1:I:4200:GLU:HG2	1:I:4537:VAL:HB	2.01	0.41
1:O:7401:LYS:HE2	1:O:7401:LYS:HA	2.02	0.41
1:E:2271:LYS:HE2	1:E:2271:LYS:HA	2.02	0.41
1:E:2231:GLU:HA	1:E:2232:GLY:HA3	1.81	0.41
1:G:3174:GLU:HG2	1:G:3511:VAL:HB	2.01	0.41
1:I:4323:LYS:HE2	1:I:4323:LYS:HA	2.02	0.41
1:G:3297:LYS:HE2	1:G:3297:LYS:HA	2.02	0.41
1:P:7914:LYS:HE2	1:P:7914:LYS:HA	2.02	0.41
1:I:4106:LEU:HA	1:I:4107:PRO:HD3	1.91	0.41
1:G:3080:LEU:HA	1:G:3081:PRO:HD3	1.91	0.41
1:F:2784:LYS:HA	1:F:2784:LYS:HE2	2.02	0.41
1:I:4283:GLU:HA	1:I:4284:GLY:HA3	1.81	0.40
1:L:5645:LEU:HA	1:L:5646:PRO:HD3	1.91	0.40
1:B:515:LEU:HA	1:B:516:PRO:HD3	1.91	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	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52 86
1	B	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52 86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	D	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	E	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	F	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	G	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	H	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	I	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	J	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	K	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	L	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	M	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	N	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	O	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
1	P	511/513 (100%)	497 (97%)	13 (2%)	1 (0%)	52	86
All	All	8176/8208 (100%)	7952 (97%)	208 (2%)	16 (0%)	56	86

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	518	ASN
1	C	1031	ASN
1	D	1544	ASN
1	E	2057	ASN
1	F	2570	ASN
1	G	3083	ASN
1	H	3596	ASN
1	I	4109	ASN
1	J	4622	ASN
1	K	5135	ASN
1	L	5648	ASN
1	M	6161	ASN
1	N	6674	ASN
1	O	7187	ASN
1	P	7700	ASN

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	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	B	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	C	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	D	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	E	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	F	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	G	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	H	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	I	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	J	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	K	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	L	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	M	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	N	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	O	414/414 (100%)	409 (99%)	5 (1%)	78	90
1	P	414/414 (100%)	409 (99%)	5 (1%)	78	90
All	All	6624/6624 (100%)	6544 (99%)	80 (1%)	79	90

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

Mol	Chain	Res	Type
1	A	36	LYS
1	A	72	LEU
1	A	144	LEU
1	A	163	LYS
1	A	419	ARG
1	B	549	LYS
1	B	585	LEU
1	B	657	LEU

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Mol	Chain	Res	Type
1	B	676	LYS
1	B	932	ARG
1	C	1062	LYS
1	C	1098	LEU
1	C	1170	LEU
1	C	1189	LYS
1	C	1445	ARG
1	D	1575	LYS
1	D	1611	LEU
1	D	1683	LEU
1	D	1702	LYS
1	D	1958	ARG
1	E	2088	LYS
1	E	2124	LEU
1	E	2196	LEU
1	E	2215	LYS
1	E	2471	ARG
1	F	2601	LYS
1	F	2637	LEU
1	F	2709	LEU
1	F	2728	LYS
1	F	2984	ARG
1	G	3114	LYS
1	G	3150	LEU
1	G	3222	LEU
1	G	3241	LYS
1	G	3497	ARG
1	H	3627	LYS
1	H	3663	LEU
1	H	3735	LEU
1	H	3754	LYS
1	H	4010	ARG
1	I	4140	LYS
1	I	4176	LEU
1	I	4248	LEU
1	I	4267	LYS
1	I	4523	ARG
1	J	4653	LYS
1	J	4689	LEU
1	J	4761	LEU
1	J	4780	LYS
1	J	5036	ARG

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Mol	Chain	Res	Type
1	K	5166	LYS
1	K	5202	LEU
1	K	5274	LEU
1	K	5293	LYS
1	K	5549	ARG
1	L	5679	LYS
1	L	5715	LEU
1	L	5787	LEU
1	L	5806	LYS
1	L	6062	ARG
1	M	6192	LYS
1	M	6228	LEU
1	M	6300	LEU
1	M	6319	LYS
1	M	6575	ARG
1	N	6705	LYS
1	N	6741	LEU
1	N	6813	LEU
1	N	6832	LYS
1	N	7088	ARG
1	O	7218	LYS
1	O	7254	LEU
1	O	7326	LEU
1	O	7345	LYS
1	O	7601	ARG
1	P	7731	LYS
1	P	7767	LEU
1	P	7839	LEU
1	P	7858	LYS
1	P	8114	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	79	GLN
1	B	531	ASN
1	B	592	GLN
1	C	1044	ASN
1	C	1105	GLN
1	D	1557	ASN
1	D	1618	GLN

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Mol	Chain	Res	Type
1	E	2070	ASN
1	E	2131	GLN
1	F	2583	ASN
1	F	2644	GLN
1	G	3096	ASN
1	G	3157	GLN
1	H	3609	ASN
1	H	3670	GLN
1	I	4122	ASN
1	I	4183	GLN
1	J	4635	ASN
1	J	4696	GLN
1	J	4907	HIS
1	K	5148	ASN
1	K	5209	GLN
1	L	5661	ASN
1	L	5722	GLN
1	M	6174	ASN
1	M	6235	GLN
1	N	6687	ASN
1	N	6748	GLN
1	O	7200	ASN
1	O	7261	GLN
1	P	7713	ASN
1	P	7774	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no 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.