wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:52 PM BST

PDB ID	:	3IZI
EMDB ID:	:	EMD-5245
Title	:	Mm-cpn rls with ATP
Authors	:	Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.; Chiu, W.; Frydman, J.
Deposited on	:	2010-10-29
Resolution	:	6.70 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

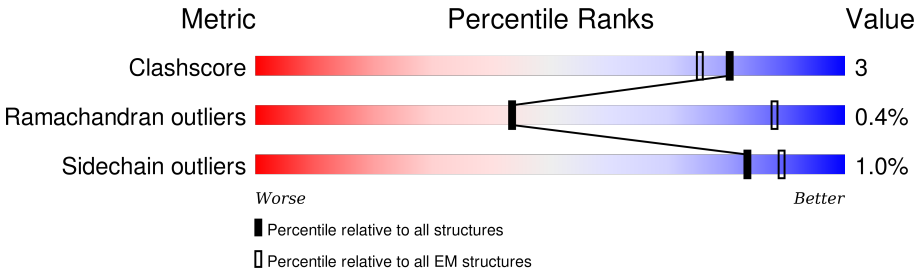
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 6.70 Å.

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



Metric	Whole archive (#Entries)	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	90% 9% •
1	B	513	91% 9% •
1	C	513	91% 9% •
1	D	513	90% 9% •
1	E	513	90% 9% •
1	F	513	89% 10% •
1	G	513	89% 10% •
1	H	513	90% 9% •
1	I	513	90% 9% •

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Mol	Chain	Length	Quality of chain
1	J	513	91% 9%
1	K	513	91% 9%
1	L	513	91% 9%
1	M	513	90% 9%
1	N	513	90% 9%
1	O	513	89% 10%
1	P	513	90% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 61440 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
			3840	2385	662	768	25		
1	B	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	C	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	D	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	E	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	F	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	G	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	H	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	I	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	J	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	K	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	L	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	M	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	N	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	O	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	P	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
A	322	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
A	324	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
A	325	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
B	834	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
B	835	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
B	837	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
B	838	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
C	1347	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
C	1348	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
C	1350	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
C	1351	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
D	1860	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
D	1861	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
D	1863	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
D	1864	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
E	2373	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
E	2374	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
E	2376	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
E	2377	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
F	2886	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
F	2887	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
F	2889	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
F	2890	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
G	3399	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
G	3400	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
G	3402	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
G	3403	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
H	3912	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
H	3913	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
H	3915	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
H	3916	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
I	4425	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
I	4426	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
I	4428	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
I	4429	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
J	4938	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
J	4939	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
J	4941	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
J	4942	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
K	5451	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
K	5452	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
K	5454	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8

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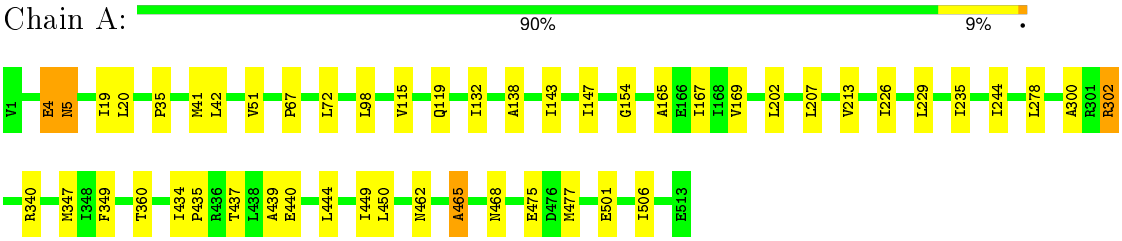
Chain	Residue	Modelled	Actual	Comment	Reference
K	5455	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
L	5964	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
L	5965	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
L	5967	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
L	5968	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
M	6477	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
M	6478	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
M	6480	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
M	6481	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
N	6990	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
N	6991	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
N	6993	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
N	6994	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
O	7503	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
O	7504	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
O	7506	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
O	7507	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
P	8016	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
P	8017	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
P	8019	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
P	8020	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

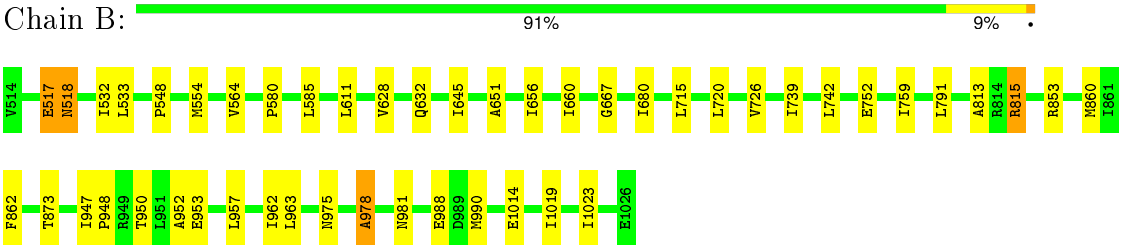
- Molecule 1: Chaperonin

Chain A:



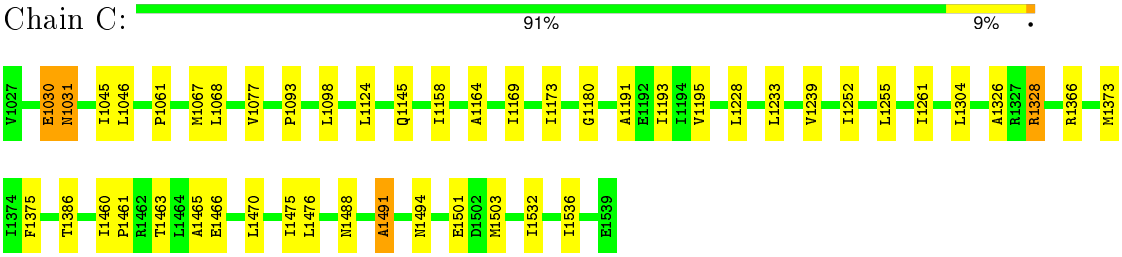
- Molecule 1: Chaperonin

Chain B:



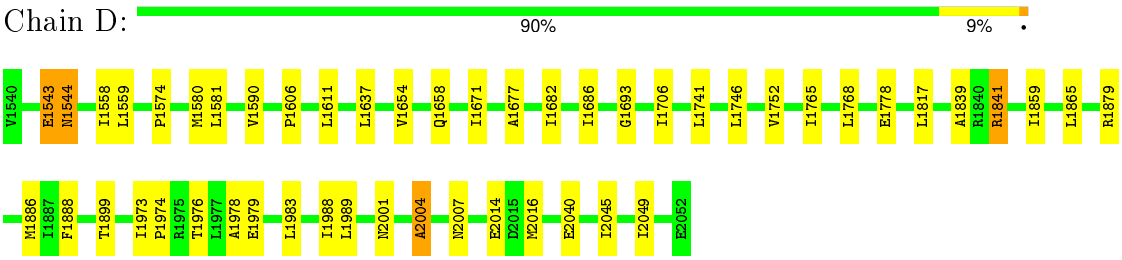
- Molecule 1: Chaperonin

Chain C:



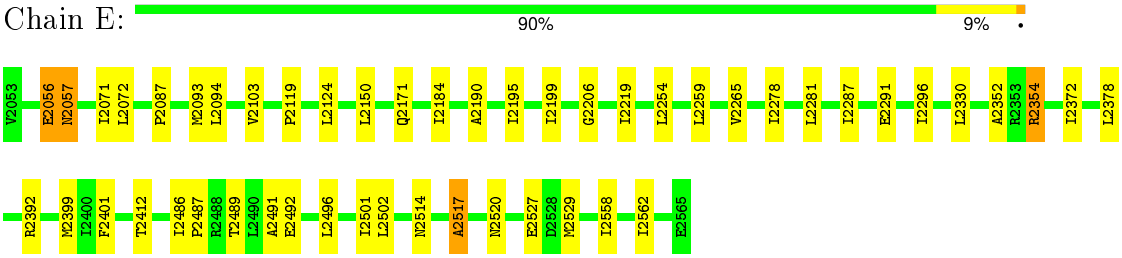
- Molecule 1: Chaperonin

Chain D:



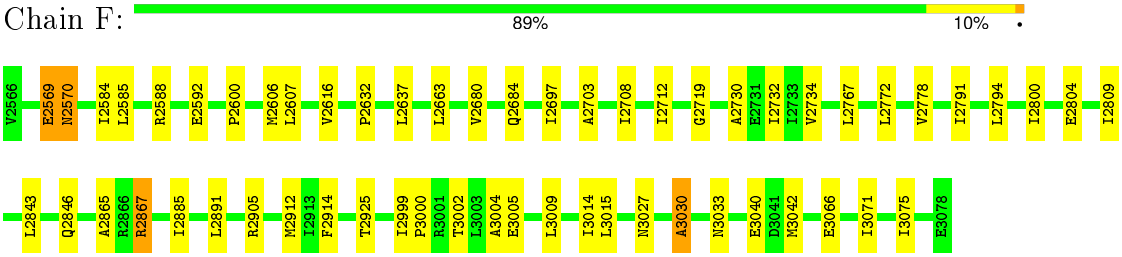
• Molecule 1: Chaperonin

Chain E:



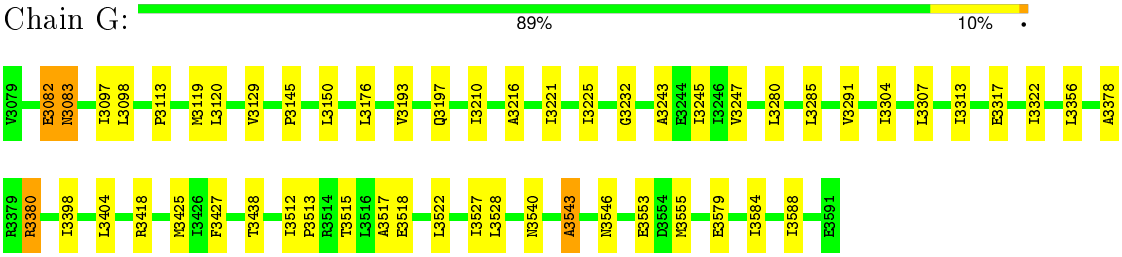
• Molecule 1: Chaperonin

Chain F:



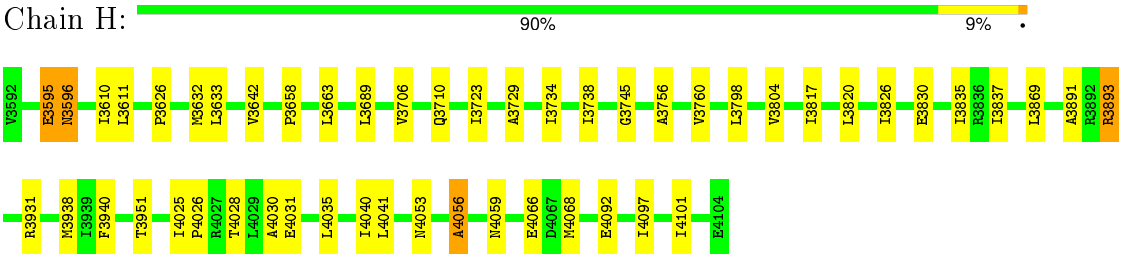
• Molecule 1: Chaperonin

Chain G:



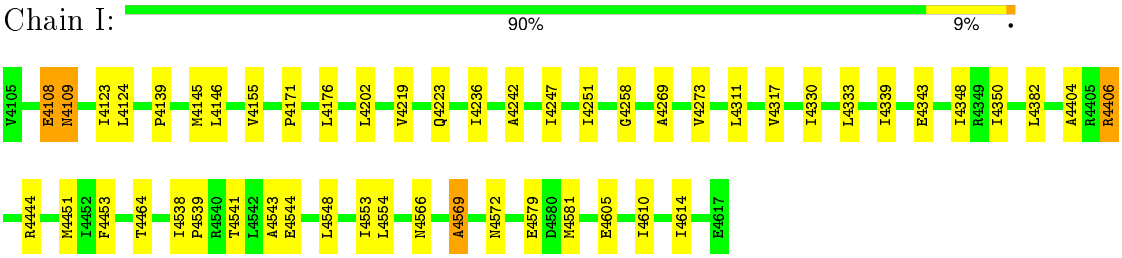
• Molecule 1: Chaperonin

Chain H:



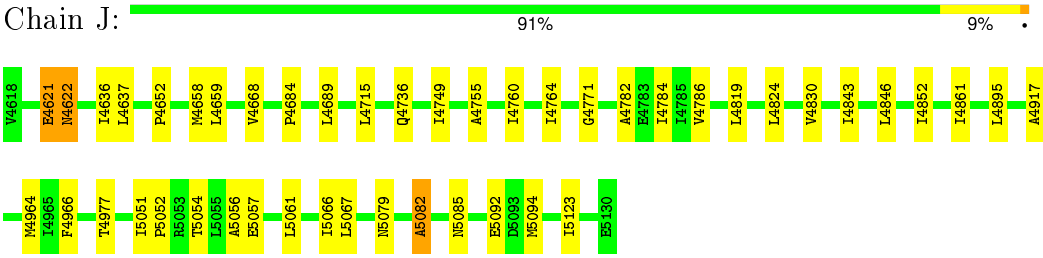
• Molecule 1: Chaperonin

Chain I:



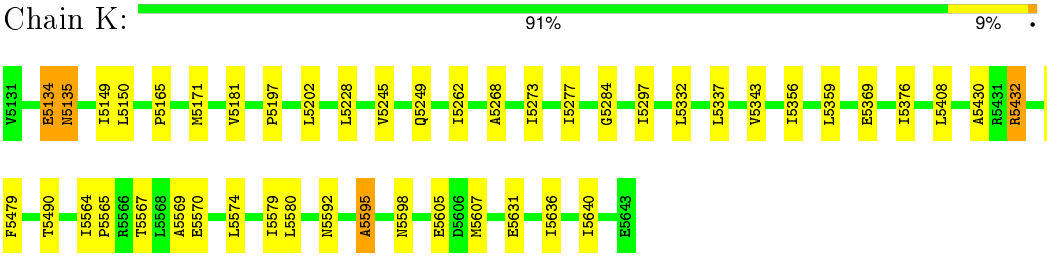
- Molecule 1: Chaperonin

Chain J:



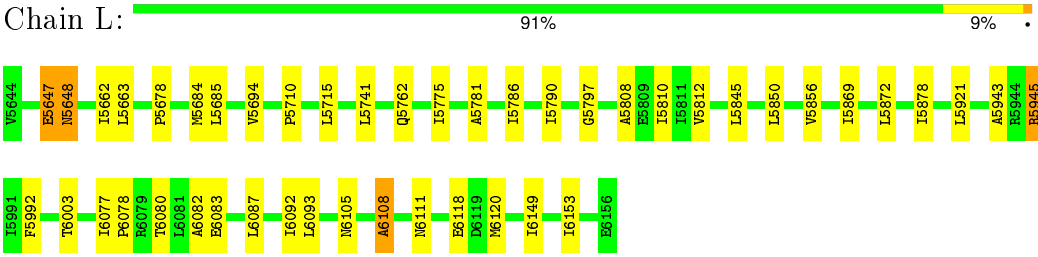
- Molecule 1: Chaperonin

Chain K:



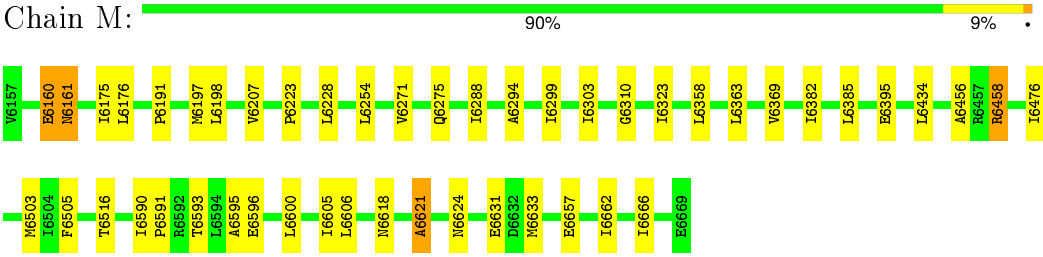
- Molecule 1: Chaperonin

Chain L:



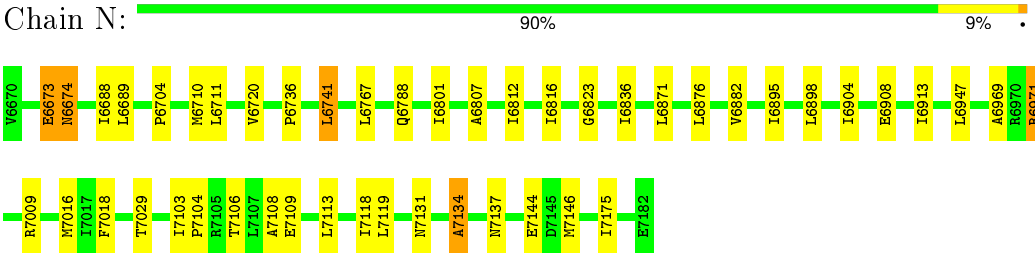
- Molecule 1: Chaperonin

Chain M:



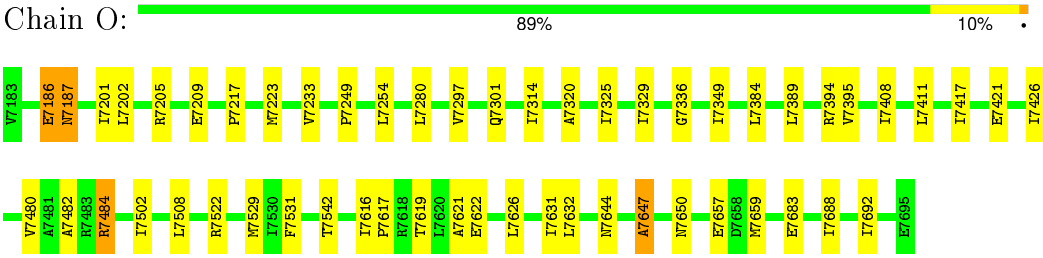
- Molecule 1: Chaperonin

Chain N:



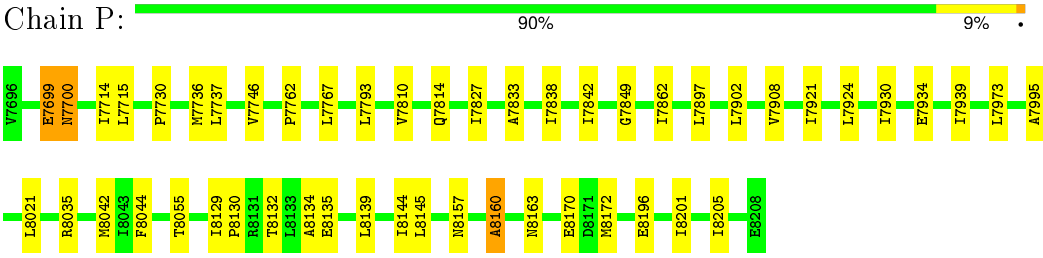
- Molecule 1: Chaperonin

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)	Not provided	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	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	B	0.88	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	C	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	D	0.88	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	E	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	F	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	G	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	H	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	I	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	J	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	K	0.88	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	L	0.88	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	M	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	N	0.88	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	O	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	P	0.87	2/3863 (0.1%)	0.78	2/5199 (0.0%)
All	All	0.87	32/61808 (0.1%)	0.78	32/83184 (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	E	2056	GLU	C-O	-6.03	1.11	1.23
1	D	1543	GLU	C-O	-5.98	1.11	1.23
1	P	7699	GLU	C-O	-5.97	1.12	1.23
1	J	4621	GLU	C-O	-5.97	1.12	1.23
1	O	7186	GLU	C-O	-5.96	1.12	1.23
1	C	1030	GLU	C-O	-5.96	1.12	1.23
1	B	517	GLU	C-O	-5.96	1.12	1.23
1	K	5134	GLU	C-O	-5.96	1.12	1.23
1	A	4	GLU	C-O	-5.94	1.12	1.23
1	G	3082	GLU	C-O	-5.94	1.12	1.23
1	L	5647	GLU	C-O	-5.94	1.12	1.23
1	N	6673	GLU	C-O	-5.94	1.12	1.23
1	M	6160	GLU	C-O	-5.92	1.12	1.23
1	F	2569	GLU	C-O	-5.91	1.12	1.23
1	H	3595	GLU	C-O	-5.91	1.12	1.23
1	I	4108	GLU	C-O	-5.91	1.12	1.23
1	E	2056	GLU	C-N	5.70	1.47	1.34
1	J	4621	GLU	C-N	5.70	1.47	1.34
1	B	517	GLU	C-N	5.70	1.47	1.34
1	D	1543	GLU	C-N	5.69	1.47	1.34
1	C	1030	GLU	C-N	5.68	1.47	1.34
1	L	5647	GLU	C-N	5.68	1.47	1.34
1	P	7699	GLU	C-N	5.68	1.47	1.34
1	F	2569	GLU	C-N	5.67	1.47	1.34
1	H	3595	GLU	C-N	5.67	1.47	1.34
1	I	4108	GLU	C-N	5.67	1.47	1.34
1	K	5134	GLU	C-N	5.67	1.47	1.34
1	M	6160	GLU	C-N	5.67	1.47	1.34
1	O	7186	GLU	C-N	5.67	1.47	1.34
1	A	4	GLU	C-N	5.64	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	3082	GLU	C-N	5.64	1.47	1.34
1	N	6673	GLU	C-N	5.64	1.47	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	5872	LEU	CB-CG-CD2	-5.29	102.02	111.00
1	O	7411	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	A	229	LEU	CB-CG-CD2	-5.27	102.03	111.00
1	F	2794	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	H	3820	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	K	5359	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	M	6385	LEU	CB-CG-CD2	-5.27	102.05	111.00
1	C	1255	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	G	3307	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	P	7924	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	742	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	D	1768	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	I	4333	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	J	4846	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	E	2281	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	N	6898	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	J	5082	ALA	CB-CA-C	5.06	117.69	110.10
1	L	6108	ALA	CB-CA-C	5.05	117.68	110.10
1	P	8160	ALA	CB-CA-C	5.05	117.68	110.10
1	B	978	ALA	CB-CA-C	5.04	117.66	110.10
1	E	2517	ALA	CB-CA-C	5.04	117.66	110.10
1	G	3543	ALA	CB-CA-C	5.04	117.66	110.10
1	A	465	ALA	CB-CA-C	5.04	117.66	110.10
1	F	3030	ALA	CB-CA-C	5.03	117.65	110.10
1	H	4056	ALA	CB-CA-C	5.03	117.65	110.10
1	I	4569	ALA	CB-CA-C	5.03	117.65	110.10
1	M	6621	ALA	CB-CA-C	5.03	117.65	110.10
1	O	7647	ALA	CB-CA-C	5.03	117.65	110.10
1	N	7134	ALA	CB-CA-C	5.03	117.64	110.10
1	C	1491	ALA	CB-CA-C	5.02	117.64	110.10
1	D	2004	ALA	CB-CA-C	5.00	117.61	110.10
1	K	5595	ALA	CB-CA-C	5.00	117.61	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	3840	0	3986	30	0
1	B	3840	0	3983	28	0
1	C	3840	0	3983	28	0
1	D	3840	0	3983	30	0
1	E	3840	0	3983	31	0
1	F	3840	0	3983	33	0
1	G	3840	0	3983	32	0
1	H	3840	0	3983	31	0
1	I	3840	0	3983	31	0
1	J	3840	0	3983	29	0
1	K	3840	0	3983	28	0
1	L	3840	0	3983	28	0
1	M	3840	0	3983	29	0
1	N	3840	0	3983	31	0
1	O	3840	0	3983	32	0
1	P	3840	0	3983	31	0
All	All	61440	0	63731	407	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 3.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3380:ARG:HE	1:G:3380:ARG:HA	1.60	0.67
1:A:302:ARG:HA	1:A:302:ARG:HE	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7997:ARG:HA	1:P:7997:ARG:HE	1.60	0.67
1:J:4919:ARG:HA	1:J:4919:ARG:HE	1.60	0.67
1:H:3893:ARG:HA	1:H:3893:ARG:HE	1.60	0.66
1:I:4406:ARG:HE	1:I:4406:ARG:HA	1.60	0.66
1:B:815:ARG:HE	1:B:815:ARG:HA	1.60	0.66
1:K:5432:ARG:HE	1:K:5432:ARG:HA	1.60	0.66
1:C:1328:ARG:HE	1:C:1328:ARG:HA	1.60	0.66
1:L:5945:ARG:HE	1:L:5945:ARG:HA	1.60	0.66
1:F:2867:ARG:HA	1:F:2867:ARG:HE	1.60	0.65
1:M:6458:ARG:HA	1:M:6458:ARG:HE	1.60	0.65
1:O:7484:ARG:HA	1:O:7484:ARG:HE	1.60	0.65
1:D:1841:ARG:HE	1:D:1841:ARG:HA	1.60	0.65
1:E:2354:ARG:HE	1:E:2354:ARG:HA	1.60	0.65
1:N:6971:ARG:HE	1:N:6971:ARG:HA	1.60	0.65
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:I:4538:ILE:HB	1:I:4539:PRO:HD3	1.84	0.60
1:H:4025:ILE:HB	1:H:4026:PRO:HD3	1.84	0.60
1:P:8129:ILE:HB	1:P:8130:PRO:HD3	1.84	0.60
1:G:3512:ILE:HB	1:G:3513:PRO:HD3	1.84	0.60
1:N:7103:ILE:HB	1:N:7104:PRO:HD3	1.84	0.59
1:E:2486:ILE:HB	1:E:2487:PRO:HD3	1.84	0.59
1:J:5051:ILE:HB	1:J:5052:PRO:HD3	1.84	0.59
1:A:434:ILE:HB	1:A:435:PRO:HD3	1.84	0.59
1:B:947:ILE:HB	1:B:948:PRO:HD3	1.84	0.58
1:K:5564:ILE:HB	1:K:5565:PRO:HD3	1.84	0.58
1:D:1973:ILE:HB	1:D:1974:PRO:HD3	1.84	0.58
1:M:6590:ILE:HB	1:M:6591:PRO:HD3	1.84	0.58
1:C:1465:ALA:HB1	1:C:1470:LEU:HB2	1.86	0.58
1:L:6082:ALA:HB1	1:L:6087:LEU:HB2	1.86	0.58
1:F:3004:ALA:HB1	1:F:3009:LEU:HB2	1.86	0.58
1:O:7621:ALA:HB1	1:O:7626:LEU:HB2	1.86	0.58
1:B:952:ALA:HB1	1:B:957:LEU:HB2	1.86	0.58
1:K:5569:ALA:HB1	1:K:5574:LEU:HB2	1.86	0.58
1:E:2491:ALA:HB1	1:E:2496:LEU:HB2	1.86	0.58
1:N:7108:ALA:HB1	1:N:7113:LEU:HB2	1.86	0.58
1:C:1460:ILE:HB	1:C:1461:PRO:HD3	1.84	0.57
1:L:6077:ILE:HB	1:L:6078:PRO:HD3	1.84	0.57
1:A:439:ALA:HB1	1:A:444:LEU:HB2	1.86	0.57
1:J:5056:ALA:HB1	1:J:5061:LEU:HB2	1.86	0.57
1:I:4543:ALA:HB1	1:I:4548:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3517:ALA:HB1	1:G:3522:LEU:HB2	1.86	0.57
1:H:4030:ALA:HB1	1:H:4035:LEU:HB2	1.86	0.57
1:P:8134:ALA:HB1	1:P:8139:LEU:HB2	1.86	0.56
1:D:1978:ALA:HB1	1:D:1983:LEU:HB2	1.86	0.56
1:M:6595:ALA:HB1	1:M:6600:LEU:HB2	1.86	0.56
1:D:1817:LEU:HD13	1:D:1817:LEU:C	2.32	0.50
1:M:6434:LEU:C	1:M:6434:LEU:HD13	2.32	0.50
1:L:5921:LEU:C	1:L:5921:LEU:HD13	2.32	0.50
1:C:1304:LEU:C	1:C:1304:LEU:HD13	2.32	0.50
1:E:2330:LEU:HD13	1:E:2330:LEU:C	2.32	0.50
1:K:5134:GLU:O	1:K:5135:ASN:CB	2.60	0.50
1:N:6947:LEU:HD13	1:N:6947:LEU:C	2.32	0.50
1:C:1030:GLU:O	1:C:1031:ASN:CB	2.60	0.50
1:B:517:GLU:O	1:B:518:ASN:CB	2.60	0.50
1:H:3869:LEU:HD13	1:H:3869:LEU:C	2.32	0.50
1:L:5647:GLU:O	1:L:5648:ASN:CB	2.60	0.50
1:I:4382:LEU:HD13	1:I:4382:LEU:C	2.32	0.50
1:B:791:LEU:C	1:B:791:LEU:HD13	2.32	0.50
1:P:7973:LEU:HD13	1:P:7973:LEU:C	2.32	0.50
1:M:6160:GLU:O	1:M:6161:ASN:CB	2.60	0.50
1:K:5408:LEU:HD13	1:K:5408:LEU:C	2.32	0.50
1:A:4:GLU:O	1:A:5:ASN:CB	2.60	0.50
1:D:1543:GLU:O	1:D:1544:ASN:CB	2.60	0.50
1:G:3356:LEU:C	1:G:3356:LEU:HD13	2.32	0.50
1:J:4621:GLU:O	1:J:4622:ASN:CB	2.60	0.49
1:F:2843:LEU:HD13	1:F:2843:LEU:C	2.32	0.49
1:N:6673:GLU:O	1:N:6674:ASN:CB	2.60	0.49
1:O:7460:LEU:HD13	1:O:7460:LEU:C	2.32	0.49
1:E:2056:GLU:O	1:E:2057:ASN:CB	2.60	0.49
1:I:4108:GLU:O	1:I:4109:ASN:CB	2.60	0.49
1:H:3595:GLU:O	1:H:3596:ASN:CB	2.60	0.49
1:G:3082:GLU:O	1:G:3083:ASN:CB	2.60	0.49
1:N:6736:PRO:HB2	1:O:7223:MET:SD	2.53	0.49
1:F:2569:GLU:O	1:F:2570:ASN:CB	2.60	0.49
1:C:1093:PRO:HB2	1:D:1580:MET:SD	2.53	0.49
1:J:4895:LEU:C	1:J:4895:LEU:HD13	2.32	0.49
1:L:5710:PRO:HB2	1:M:6197:MET:SD	2.53	0.49
1:E:2119:PRO:HB2	1:F:2606:MET:SD	2.53	0.49
1:P:7699:GLU:O	1:P:7700:ASN:CB	2.60	0.49
1:A:278:LEU:C	1:A:278:LEU:HD13	2.32	0.49
1:O:7186:GLU:O	1:O:7187:ASN:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6223:PRO:HB2	1:N:6710:MET:SD	2.53	0.49
1:D:1606:PRO:HB2	1:E:2093:MET:SD	2.53	0.49
1:B:580:PRO:HB2	1:C:1067:MET:SD	2.53	0.48
1:K:5197:PRO:HB2	1:L:5684:MET:SD	2.53	0.48
1:A:67:PRO:HB2	1:B:554:MET:SD	2.53	0.48
1:G:3145:PRO:HB2	1:H:3632:MET:SD	2.53	0.48
1:J:4684:PRO:HB2	1:K:5171:MET:SD	2.53	0.48
1:A:41:MET:SD	1:H:3658:PRO:HB2	2.53	0.48
1:I:4145:MET:SD	1:P:7762:PRO:HB2	2.53	0.48
1:F:2632:PRO:HB2	1:G:3119:MET:SD	2.53	0.48
1:I:4171:PRO:HB2	1:J:4658:MET:SD	2.53	0.48
1:O:7249:PRO:HB2	1:P:7736:MET:SD	2.53	0.48
1:J:4636:ILE:HG12	1:J:4715:LEU:HB3	1.99	0.45
1:A:19:ILE:HG12	1:A:98:LEU:HB3	1.99	0.45
1:G:3097:ILE:HG12	1:G:3176:LEU:HB3	1.99	0.45
1:B:532:ILE:HG12	1:B:611:LEU:HB3	1.99	0.45
1:K:5149:ILE:HG12	1:K:5228:LEU:HB3	1.99	0.45
1:H:3610:ILE:HG12	1:H:3689:LEU:HB3	1.99	0.45
1:J:4824:LEU:HB3	1:J:4977:THR:HG21	1.98	0.45
1:O:7389:LEU:HB3	1:O:7542:THR:HG21	1.98	0.45
1:O:7201:ILE:HG12	1:O:7280:LEU:HB3	1.99	0.45
1:I:4123:ILE:HG12	1:I:4202:LEU:HB3	1.99	0.45
1:L:5869:ILE:N	1:L:5869:ILE:HD12	2.32	0.45
1:P:7714:ILE:HG12	1:P:7793:LEU:HB3	1.99	0.45
1:F:2584:ILE:HG12	1:F:2663:LEU:HB3	1.99	0.45
1:F:2772:LEU:HB3	1:F:2925:THR:HG21	1.98	0.45
1:A:207:LEU:HB3	1:A:360:THR:HG21	1.98	0.45
1:I:4311:LEU:HB3	1:I:4464:THR:HG21	1.98	0.45
1:G:3285:LEU:HB3	1:G:3438:THR:HG21	1.98	0.45
1:C:1252:ILE:HD12	1:C:1252:ILE:N	2.32	0.45
1:N:6688:ILE:HG12	1:N:6767:LEU:HB3	1.99	0.45
1:P:7902:LEU:HB3	1:P:8055:THR:HG21	1.98	0.45
1:K:5337:LEU:HB3	1:K:5490:THR:HG21	1.98	0.45
1:D:1765:ILE:N	1:D:1765:ILE:HD12	2.32	0.45
1:C:1045:ILE:HG12	1:C:1124:LEU:HB3	1.99	0.45
1:L:5662:ILE:HG12	1:L:5741:LEU:HB3	1.99	0.45
1:E:2071:ILE:HG12	1:E:2150:LEU:HB3	1.99	0.45
1:H:3798:LEU:HB3	1:H:3951:THR:HG21	1.98	0.45
1:M:6382:ILE:N	1:M:6382:ILE:HD12	2.32	0.45
1:N:6876:LEU:HB3	1:N:7029:THR:HG21	1.98	0.45
1:D:1746:LEU:HB3	1:D:1899:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5850:LEU:HB3	1:L:6003:THR:HG21	1.98	0.45
1:C:1233:LEU:HB3	1:C:1386:THR:HG21	1.98	0.45
1:B:720:LEU:HB3	1:B:873:THR:HG21	1.98	0.45
1:I:4610:ILE:N	1:I:4610:ILE:HD12	2.33	0.44
1:M:6662:ILE:N	1:M:6662:ILE:HD12	2.33	0.44
1:J:5123:ILE:N	1:J:5123:ILE:HD12	2.33	0.44
1:D:2007:ASN:HB2	1:D:2016:MET:HE3	1.98	0.44
1:E:2259:LEU:HB3	1:E:2412:THR:HG21	1.98	0.44
1:D:1558:ILE:HG12	1:D:1637:LEU:HB3	1.99	0.44
1:M:6363:LEU:HB3	1:M:6516:THR:HG21	1.98	0.44
1:D:2045:ILE:HD12	1:D:2045:ILE:N	2.33	0.44
1:K:5636:ILE:HD12	1:K:5636:ILE:N	2.33	0.44
1:A:506:ILE:N	1:A:506:ILE:HD12	2.33	0.44
1:H:4097:ILE:N	1:H:4097:ILE:HD12	2.33	0.44
1:M:6175:ILE:HG12	1:M:6254:LEU:HB3	1.99	0.44
1:I:4553:ILE:HG13	1:I:4554:LEU:N	2.33	0.44
1:K:5356:ILE:N	1:K:5356:ILE:HD12	2.32	0.44
1:B:1019:ILE:N	1:B:1019:ILE:HD12	2.33	0.44
1:H:4040:ILE:HG13	1:H:4041:LEU:N	2.33	0.44
1:B:739:ILE:HD12	1:B:739:ILE:N	2.32	0.44
1:G:3584:ILE:HD12	1:G:3584:ILE:N	2.33	0.44
1:P:8201:ILE:HD12	1:P:8201:ILE:N	2.33	0.44
1:E:2489:THR:HA	1:E:2492:GLU:HB3	2.00	0.44
1:O:7688:ILE:N	1:O:7688:ILE:HD12	2.33	0.44
1:J:5066:ILE:HG13	1:J:5067:LEU:N	2.33	0.44
1:L:6149:ILE:N	1:L:6149:ILE:HD12	2.33	0.44
1:A:449:ILE:HG13	1:A:450:LEU:N	2.33	0.44
1:E:2278:ILE:N	1:E:2278:ILE:HD12	2.32	0.44
1:N:7106:THR:HA	1:N:7109:GLU:HB3	2.00	0.44
1:F:3071:ILE:N	1:F:3071:ILE:HD12	2.33	0.44
1:M:6605:ILE:HG13	1:M:6606:LEU:N	2.33	0.44
1:A:226:ILE:N	1:A:226:ILE:HD12	2.32	0.44
1:J:4843:ILE:N	1:J:4843:ILE:HD12	2.32	0.44
1:P:8144:ILE:HG13	1:P:8145:LEU:N	2.33	0.44
1:G:3527:ILE:HG13	1:G:3528:LEU:N	2.33	0.44
1:D:1988:ILE:HG13	1:D:1989:LEU:N	2.33	0.44
1:N:6895:ILE:N	1:N:6895:ILE:HD12	2.32	0.44
1:N:7118:ILE:HG13	1:N:7119:LEU:N	2.33	0.44
1:C:1532:ILE:N	1:C:1532:ILE:HD12	2.33	0.44
1:E:2558:ILE:HD12	1:E:2558:ILE:N	2.33	0.44
1:G:3515:THR:HA	1:G:3518:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4330:ILE:N	1:I:4330:ILE:HD12	2.32	0.44
1:N:7175:ILE:N	1:N:7175:ILE:HD12	2.33	0.43
1:P:8132:THR:HA	1:P:8135:GLU:HB3	2.00	0.43
1:E:2501:ILE:HG13	1:E:2502:LEU:N	2.33	0.43
1:H:3817:ILE:N	1:H:3817:ILE:HD12	2.32	0.43
1:C:1463:THR:HA	1:C:1466:GLU:HB3	2.00	0.43
1:O:7619:THR:HA	1:O:7622:GLU:HB3	2.00	0.43
1:E:2520:ASN:HB2	1:E:2529:MET:HE3	1.99	0.43
1:L:6080:THR:HA	1:L:6083:GLU:HB3	2.00	0.43
1:F:3014:ILE:HG13	1:F:3015:LEU:N	2.33	0.43
1:O:7631:ILE:HG13	1:O:7632:LEU:N	2.33	0.43
1:N:7137:ASN:HB2	1:N:7146:MET:HE3	1.99	0.43
1:L:6092:ILE:HG13	1:L:6093:LEU:N	2.33	0.43
1:F:2791:ILE:N	1:F:2791:ILE:HD12	2.32	0.43
1:B:962:ILE:HG13	1:B:963:LEU:N	2.33	0.43
1:N:6704:PRO:O	1:N:6823:GLY:HA2	2.19	0.43
1:A:35:PRO:O	1:A:154:GLY:HA2	2.19	0.43
1:J:4652:PRO:O	1:J:4771:GLY:HA2	2.19	0.43
1:K:5579:ILE:HG13	1:K:5580:LEU:N	2.33	0.43
1:G:3304:ILE:N	1:G:3304:ILE:HD12	2.32	0.43
1:O:7408:ILE:N	1:O:7408:ILE:HD12	2.32	0.43
1:F:3002:THR:HA	1:F:3005:GLU:HB3	2.00	0.43
1:P:7921:ILE:HD12	1:P:7921:ILE:N	2.32	0.43
1:C:1475:ILE:HG13	1:C:1476:LEU:N	2.33	0.43
1:B:548:PRO:O	1:B:667:GLY:HA2	2.19	0.43
1:E:2087:PRO:O	1:E:2206:GLY:HA2	2.19	0.43
1:H:3626:PRO:O	1:H:3745:GLY:HA2	2.19	0.43
1:I:4139:PRO:O	1:I:4258:GLY:HA2	2.19	0.43
1:M:6191:PRO:O	1:M:6310:GLY:HA2	2.19	0.43
1:K:5165:PRO:O	1:K:5284:GLY:HA2	2.19	0.43
1:D:1574:PRO:O	1:D:1693:GLY:HA2	2.19	0.43
1:L:5678:PRO:O	1:L:5797:GLY:HA2	2.19	0.43
1:C:1061:PRO:O	1:C:1180:GLY:HA2	2.19	0.43
1:A:132:ILE:HD11	1:A:462:ASN:HB3	2.01	0.43
1:O:7217:PRO:O	1:O:7336:GLY:HA2	2.19	0.43
1:A:437:THR:HA	1:A:440:GLU:HB3	2.00	0.43
1:P:7730:PRO:O	1:P:7849:GLY:HA2	2.19	0.42
1:J:4749:ILE:HD11	1:J:5079:ASN:HB3	2.01	0.42
1:J:5054:THR:HA	1:J:5057:GLU:HB3	2.00	0.42
1:M:6593:THR:HA	1:M:6596:GLU:HB3	2.00	0.42
1:F:2600:PRO:O	1:F:2719:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3113:PRO:O	1:G:3232:GLY:HA2	2.19	0.42
1:D:1976:THR:HA	1:D:1979:GLU:HB3	2.00	0.42
1:H:4028:THR:HA	1:H:4031:GLU:HB3	2.00	0.42
1:A:51:VAL:HG11	1:H:4097:ILE:HD11	2.01	0.42
1:I:4541:THR:HA	1:I:4544:GLU:HB3	2.00	0.42
1:A:340:ARG:HD2	1:A:349:PHE:CD1	2.55	0.42
1:E:2392:ARG:HD2	1:E:2401:PHE:CD1	2.55	0.42
1:J:4957:ARG:HD2	1:J:4966:PHE:CD1	2.55	0.42
1:N:7009:ARG:HD2	1:N:7018:PHE:CD1	2.55	0.42
1:I:4610:ILE:HD11	1:J:4668:VAL:HG11	2.02	0.42
1:H:3931:ARG:HD2	1:H:3940:PHE:CD1	2.55	0.42
1:I:4236:ILE:HD11	1:I:4566:ASN:HB3	2.01	0.42
1:C:1366:ARG:HD2	1:C:1375:PHE:CD1	2.55	0.42
1:B:1019:ILE:HD11	1:C:1077:VAL:HG11	2.02	0.42
1:N:6801:ILE:HD11	1:N:7131:ASN:HB3	2.01	0.42
1:B:853:ARG:HD2	1:B:862:PHE:CD1	2.55	0.42
1:I:4444:ARG:HD2	1:I:4453:PHE:CD1	2.55	0.42
1:K:5470:ARG:HD2	1:K:5479:PHE:CD1	2.55	0.42
1:M:6299:ILE:O	1:M:6303:ILE:HG12	2.20	0.42
1:K:5636:ILE:HD11	1:L:5694:VAL:HG11	2.02	0.42
1:D:1682:ILE:O	1:D:1686:ILE:HG12	2.20	0.42
1:G:3418:ARG:HD2	1:G:3427:PHE:CD1	2.55	0.42
1:P:7827:ILE:HD11	1:P:8157:ASN:HB3	2.01	0.42
1:B:726:VAL:HG13	1:B:813:ALA:HA	2.02	0.42
1:K:5343:VAL:HG13	1:K:5430:ALA:HA	2.02	0.42
1:L:5983:ARG:HD2	1:L:5992:PHE:CD1	2.55	0.42
1:H:3723:ILE:HD11	1:H:4053:ASN:HB3	2.01	0.42
1:B:656:ILE:O	1:B:660:ILE:HG12	2.20	0.42
1:G:3210:ILE:HD11	1:G:3540:ASN:HB3	2.01	0.42
1:D:1671:ILE:HD11	1:D:2001:ASN:HB3	2.01	0.42
1:E:2184:ILE:HD11	1:E:2514:ASN:HB3	2.01	0.42
1:M:6288:ILE:HD11	1:M:6618:ASN:HB3	2.01	0.42
1:P:8035:ARG:HD2	1:P:8044:PHE:CD1	2.55	0.42
1:C:1158:ILE:HD11	1:C:1488:ASN:HB3	2.01	0.42
1:A:143:ILE:O	1:A:147:ILE:HG12	2.20	0.42
1:K:5567:THR:HA	1:K:5570:GLU:HB3	2.00	0.42
1:J:4760:ILE:O	1:J:4764:ILE:HG12	2.20	0.42
1:D:1879:ARG:HD2	1:D:1888:PHE:CD1	2.55	0.42
1:M:6496:ARG:HD2	1:M:6505:PHE:CD1	2.55	0.42
1:K:5273:ILE:O	1:K:5277:ILE:HG12	2.20	0.42
1:L:5775:ILE:HD11	1:L:6105:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:THR:HA	1:B:953:GLU:HB3	2.00	0.42
1:G:3584:ILE:HD11	1:H:3642:VAL:HG11	2.02	0.41
1:C:1169:ILE:O	1:C:1173:ILE:HG12	2.20	0.41
1:K:5262:ILE:HD11	1:K:5592:ASN:HB3	2.01	0.41
1:L:6149:ILE:HG12	1:M:6197:MET:HB2	2.02	0.41
1:B:1019:ILE:HG12	1:C:1067:MET:HB2	2.02	0.41
1:K:5636:ILE:HG12	1:L:5684:MET:HB2	2.02	0.41
1:J:5123:ILE:HD11	1:K:5181:VAL:HG11	2.01	0.41
1:I:4155:VAL:HG11	1:P:8201:ILE:HD11	2.02	0.41
1:B:645:ILE:HD11	1:B:975:ASN:HB3	2.01	0.41
1:B:981:ASN:HB2	1:B:990:MET:CE	2.51	0.41
1:K:5598:ASN:HB2	1:K:5607:MET:CE	2.51	0.41
1:L:5786:ILE:O	1:L:5790:ILE:HG12	2.20	0.41
1:H:3734:ILE:O	1:H:3738:ILE:HG12	2.20	0.41
1:C:1532:ILE:HG12	1:D:1580:MET:HB2	2.03	0.41
1:D:2007:ASN:HB2	1:D:2016:MET:CE	2.51	0.41
1:E:2520:ASN:HB2	1:E:2529:MET:CE	2.51	0.41
1:N:7137:ASN:HB2	1:N:7146:MET:CE	2.50	0.41
1:M:6395:GLU:HB2	1:N:6904:ILE:HB	2.03	0.41
1:E:2219:ILE:HG23	1:E:2254:LEU:HB2	2.03	0.41
1:H:4059:ASN:HB2	1:H:4068:MET:CE	2.50	0.41
1:F:2804:GLU:HB2	1:G:3313:ILE:HB	2.03	0.41
1:D:1778:GLU:HB2	1:E:2287:ILE:HB	2.03	0.41
1:O:7522:ARG:HD2	1:O:7531:PHE:CD1	2.55	0.41
1:F:2708:ILE:O	1:F:2712:ILE:HG12	2.20	0.41
1:M:6624:ASN:HB2	1:M:6633:MET:CE	2.51	0.41
1:J:4830:VAL:HG13	1:J:4917:ALA:HA	2.02	0.41
1:I:4572:ASN:HB2	1:I:4581:MET:CE	2.50	0.41
1:N:6836:ILE:HG23	1:N:6871:LEU:HB2	2.03	0.41
1:C:1193:ILE:HG23	1:C:1228:LEU:HB2	2.03	0.41
1:A:213:VAL:HG13	1:A:300:ALA:HA	2.02	0.41
1:G:3221:ILE:O	1:G:3225:ILE:HG12	2.20	0.41
1:O:7314:ILE:HD11	1:O:7644:ASN:HB3	2.01	0.41
1:F:2697:ILE:HD11	1:F:3027:ASN:HB3	2.01	0.41
1:O:7325:ILE:O	1:O:7329:ILE:HG12	2.20	0.41
1:I:4247:ILE:O	1:I:4251:ILE:HG12	2.20	0.41
1:F:2905:ARG:HD2	1:F:2914:PHE:CD1	2.55	0.41
1:D:2045:ILE:HG12	1:E:2093:MET:HB2	2.02	0.41
1:O:7688:ILE:HD11	1:P:7746:VAL:HG11	2.01	0.41
1:D:1752:VAL:HG13	1:D:1839:ALA:HA	2.02	0.41
1:I:4317:VAL:HG13	1:I:4404:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2778:VAL:HG13	1:F:2865:ALA:HA	2.02	0.41
1:M:6369:VAL:HG13	1:M:6456:ALA:HA	2.02	0.41
1:M:6662:ILE:HG12	1:N:6710:MET:HB2	2.02	0.41
1:O:7395:VAL:HG13	1:O:7482:ALA:HA	2.02	0.41
1:P:7838:ILE:O	1:P:7842:ILE:HG12	2.20	0.41
1:P:7862:ILE:HG23	1:P:7897:LEU:HB2	2.03	0.41
1:P:8163:ASN:HB2	1:P:8172:MET:CE	2.50	0.41
1:E:2195:ILE:O	1:E:2199:ILE:HG12	2.20	0.41
1:L:5810:ILE:HG23	1:L:5845:LEU:HB2	2.03	0.41
1:F:3071:ILE:HD11	1:G:3129:VAL:HG11	2.02	0.41
1:I:4339:ILE:HB	1:P:7934:GLU:HB2	2.02	0.41
1:O:7692:ILE:O	1:P:7737:LEU:HA	2.21	0.41
1:G:3245:ILE:HG23	1:G:3280:LEU:HB2	2.03	0.41
1:O:7421:GLU:HB2	1:P:7930:ILE:HB	2.03	0.41
1:H:3804:VAL:HG13	1:H:3891:ALA:HA	2.02	0.41
1:G:3546:ASN:HB2	1:G:3555:MET:CE	2.51	0.41
1:N:6812:ILE:O	1:N:6816:ILE:HG12	2.20	0.41
1:E:2558:ILE:HD11	1:F:2616:VAL:HG11	2.01	0.41
1:M:6662:ILE:HD11	1:N:6720:VAL:HG11	2.02	0.41
1:D:2045:ILE:HD11	1:E:2103:VAL:HG11	2.02	0.41
1:C:1536:ILE:O	1:D:1581:LEU:HA	2.21	0.41
1:F:3075:ILE:O	1:G:3120:LEU:HA	2.21	0.41
1:K:5245:VAL:HB	1:K:5631:GLU:HG3	2.03	0.41
1:H:3835:ILE:N	1:H:3835:ILE:HD12	2.36	0.41
1:I:4348:ILE:N	1:I:4348:ILE:HD12	2.36	0.41
1:L:6153:ILE:O	1:M:6198:LEU:HA	2.21	0.41
1:C:1532:ILE:HD11	1:D:1590:VAL:HG11	2.01	0.41
1:A:506:ILE:HD11	1:B:564:VAL:HG11	2.02	0.41
1:A:506:ILE:HG12	1:B:554:MET:HB2	2.02	0.41
1:J:5123:ILE:HG12	1:K:5171:MET:HB2	2.03	0.41
1:I:4219:VAL:HB	1:I:4605:GLU:HG3	2.03	0.41
1:C:1239:VAL:HG13	1:C:1326:ALA:HA	2.02	0.41
1:B:628:VAL:HB	1:B:1014:GLU:HG3	2.03	0.41
1:P:7939:ILE:N	1:P:7939:ILE:HD12	2.36	0.41
1:A:167:ILE:HG23	1:A:202:LEU:HB2	2.03	0.41
1:D:2049:ILE:O	1:E:2094:LEU:HA	2.21	0.41
1:M:6666:ILE:O	1:N:6711:LEU:HA	2.21	0.41
1:J:4784:ILE:HG23	1:J:4819:LEU:HB2	2.03	0.41
1:G:3291:VAL:HG13	1:G:3378:ALA:HA	2.02	0.41
1:G:3317:GLU:HB2	1:H:3826:ILE:HB	2.02	0.41
1:P:7908:VAL:HG13	1:P:7995:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1191:ALA:O	1:C:1195:VAL:HG23	2.21	0.41
1:L:5856:VAL:HG13	1:L:5943:ALA:HA	2.02	0.41
1:G:3322:ILE:HD12	1:G:3322:ILE:N	2.36	0.41
1:A:468:ASN:HB2	1:A:477:MET:HE3	2.02	0.41
1:N:6882:VAL:HG13	1:N:6969:ALA:HA	2.02	0.41
1:H:3706:VAL:HB	1:H:4092:GLU:HG3	2.03	0.41
1:E:2296:ILE:N	1:E:2296:ILE:HD12	2.36	0.41
1:N:6913:ILE:N	1:N:6913:ILE:HD12	2.36	0.41
1:N:6908:GLU:HB2	1:O:7417:ILE:HB	2.02	0.41
1:G:3588:ILE:O	1:H:3633:LEU:HA	2.21	0.41
1:I:4343:GLU:HB2	1:J:4852:ILE:HB	2.03	0.41
1:K:5297:ILE:HG23	1:K:5332:LEU:HB2	2.03	0.41
1:E:2265:VAL:HG13	1:E:2352:ALA:HA	2.02	0.41
1:F:2809:ILE:HD12	1:F:2809:ILE:N	2.36	0.41
1:O:7650:ASN:HB2	1:O:7659:MET:CE	2.50	0.41
1:L:6149:ILE:HD11	1:M:6207:VAL:HG11	2.01	0.40
1:I:4350:ILE:HB	1:P:7939:ILE:HG13	2.04	0.40
1:I:4146:LEU:HA	1:P:8205:ILE:O	2.21	0.40
1:F:2732:ILE:HG23	1:F:2767:LEU:HB2	2.03	0.40
1:H:3756:ALA:O	1:H:3760:VAL:HG23	2.22	0.40
1:J:5085:ASN:HB2	1:J:5094:MET:CE	2.51	0.40
1:O:7349:ILE:HG23	1:O:7384:LEU:HB2	2.03	0.40
1:L:5808:ALA:O	1:L:5812:VAL:HG23	2.22	0.40
1:B:680:ILE:HG23	1:B:715:LEU:HB2	2.03	0.40
1:A:235:ILE:HB	1:H:3830:GLU:HB2	2.03	0.40
1:N:7175:ILE:HD11	1:O:7233:VAL:HG11	2.02	0.40
1:A:41:MET:HB2	1:H:4097:ILE:HG12	2.03	0.40
1:I:4145:MET:HB2	1:P:8201:ILE:HG12	2.02	0.40
1:I:4610:ILE:HG12	1:J:4658:MET:HB2	2.03	0.40
1:A:468:ASN:HB2	1:A:477:MET:CE	2.50	0.40
1:J:5085:ASN:HB2	1:J:5094:MET:HE3	2.02	0.40
1:F:2588:ARG:O	1:F:2592:GLU:N	2.49	0.40
1:B:1023:ILE:O	1:C:1068:LEU:HA	2.21	0.40
1:M:6323:ILE:HG23	1:M:6358:LEU:HB2	2.03	0.40
1:I:4269:ALA:O	1:I:4273:VAL:HG23	2.22	0.40
1:O:7426:ILE:N	1:O:7426:ILE:HD12	2.36	0.40
1:F:3033:ASN:HB2	1:F:3042:MET:CE	2.50	0.40
1:N:7175:ILE:HG12	1:O:7223:MET:HB2	2.02	0.40
1:E:2558:ILE:HG12	1:F:2606:MET:HB2	2.02	0.40
1:G:3584:ILE:HG12	1:H:3632:MET:HB2	2.02	0.40
1:A:244:ILE:HG13	1:B:759:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6476:ILE:HG13	1:M:6482:LEU:HD23	2.04	0.40
1:K:5369:GLU:HB2	1:L:5878:ILE:HB	2.03	0.40
1:A:42:LEU:HA	1:H:4101:ILE:O	2.21	0.40
1:P:7810:VAL:HB	1:P:8196:GLU:HG3	2.03	0.40
1:A:115:VAL:HB	1:A:501:GLU:HG3	2.03	0.40
1:G:3193:VAL:HB	1:G:3579:GLU:HG3	2.03	0.40
1:O:7297:VAL:HB	1:O:7683:GLU:HG3	2.03	0.40
1:F:2846:GLN:OE1	1:F:2867:ARG:NH2	2.55	0.40
1:O:7463:GLN:OE1	1:O:7484:ARG:NH2	2.55	0.40
1:E:2291:GLU:HB2	1:F:2800:ILE:HB	2.03	0.40
1:I:4614:ILE:O	1:J:4659:LEU:HA	2.21	0.40
1:A:165:ALA:O	1:A:169:VAL:HG23	2.22	0.40
1:O:7205:ARG:O	1:O:7209:GLU:N	2.49	0.40
1:C:1494:ASN:HB2	1:C:1503:MET:CE	2.51	0.40
1:D:1859:ILE:HG13	1:D:1865:LEU:HD23	2.04	0.40
1:F:2680:VAL:HB	1:F:3066:GLU:HG3	2.03	0.40
1:K:5640:ILE:O	1:L:5685:LEU:HA	2.21	0.40
1:J:4782:ALA:O	1:J:4786:VAL:HG23	2.21	0.40
1:N:6989:ILE:HG13	1:N:6995:LEU:HD23	2.04	0.40
1:E:2562:ILE:O	1:F:2607:LEU:HA	2.21	0.40
1:B:752:GLU:HB2	1:C:1261:ILE:HB	2.03	0.40
1:J:4861:ILE:HG13	1:K:5376:ILE:HB	2.04	0.40
1:P:8015:ILE:HG13	1:P:8021:LEU:HD23	2.04	0.40
1:D:1706:ILE:HG23	1:D:1741:LEU:HB2	2.03	0.40
1:M:6271:VAL:HB	1:M:6657:GLU:HG3	2.03	0.40
1:L:6111:ASN:HB2	1:L:6120:MET:CE	2.51	0.40
1:D:1654:VAL:HB	1:D:2040:GLU:HG3	2.03	0.40
1:G:3398:ILE:HG13	1:G:3404:LEU:HD23	2.04	0.40
1:G:3322:ILE:HG13	1:H:3837:ILE:HB	2.04	0.40
1:O:7394:ARG:HD2	1:O:7480:VAL:HB	2.04	0.40
1:E:2372:ILE:HG13	1:E:2378:LEU:HD23	2.04	0.40
1:G:3243:ALA:O	1:G:3247:VAL:HG23	2.21	0.40
1:O:7502:ILE:HG13	1:O:7508:LEU:HD23	2.04	0.40
1:F:2885:ILE:HG13	1:F:2891:LEU:HD23	2.04	0.40
1:N:6741:LEU:HD23	1:N:6741:LEU:O	2.22	0.40
1:F:2730:ALA:O	1:F:2734:VAL:HG23	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	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	B	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	C	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	D	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	E	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	F	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	G	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	H	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	I	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	J	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	K	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	L	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	M	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	N	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	O	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	P	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
All	All	8176/8208 (100%)	7888 (96%)	256 (3%)	32 (0%)	43	80

All (32) 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

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Mol	Chain	Res	Type
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
1	A	465	ALA
1	B	978	ALA
1	C	1491	ALA
1	D	2004	ALA
1	E	2517	ALA
1	F	3030	ALA
1	G	3543	ALA
1	H	4056	ALA
1	I	4569	ALA
1	J	5082	ALA
1	K	5595	ALA
1	L	6108	ALA
1	M	6621	ALA
1	N	7134	ALA
1	O	7647	ALA
1	P	8160	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	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	B	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	C	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	D	410/410 (100%)	406 (99%)	4 (1%)	82 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	F	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	G	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	H	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	I	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	J	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	K	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	L	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	M	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	N	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	O	410/410 (100%)	406 (99%)	4 (1%)	82 92
1	P	410/410 (100%)	406 (99%)	4 (1%)	82 92
All	All	6560/6560 (100%)	6496 (99%)	64 (1%)	83 92

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	72	LEU
1	A	302	ARG
1	A	347	MET
1	B	533	LEU
1	B	585	LEU
1	B	815	ARG
1	B	860	MET
1	C	1046	LEU
1	C	1098	LEU
1	C	1328	ARG
1	C	1373	MET
1	D	1559	LEU
1	D	1611	LEU
1	D	1841	ARG
1	D	1886	MET
1	E	2072	LEU
1	E	2124	LEU
1	E	2354	ARG
1	E	2399	MET
1	F	2585	LEU

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Mol	Chain	Res	Type
1	F	2637	LEU
1	F	2867	ARG
1	F	2912	MET
1	G	3098	LEU
1	G	3150	LEU
1	G	3380	ARG
1	G	3425	MET
1	H	3611	LEU
1	H	3663	LEU
1	H	3893	ARG
1	H	3938	MET
1	I	4124	LEU
1	I	4176	LEU
1	I	4406	ARG
1	I	4451	MET
1	J	4637	LEU
1	J	4689	LEU
1	J	4919	ARG
1	J	4964	MET
1	K	5150	LEU
1	K	5202	LEU
1	K	5432	ARG
1	K	5477	MET
1	L	5663	LEU
1	L	5715	LEU
1	L	5945	ARG
1	L	5990	MET
1	M	6176	LEU
1	M	6228	LEU
1	M	6458	ARG
1	M	6503	MET
1	N	6689	LEU
1	N	6741	LEU
1	N	6971	ARG
1	N	7016	MET
1	O	7202	LEU
1	O	7254	LEU
1	O	7484	ARG
1	O	7529	MET
1	P	7715	LEU
1	P	7767	LEU
1	P	7997	ARG

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Mol	Chain	Res	Type
1	P	8042	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	468	ASN
1	B	620	GLN
1	B	981	ASN
1	C	1133	GLN
1	C	1494	ASN
1	D	1646	GLN
1	D	2007	ASN
1	E	2159	GLN
1	E	2520	ASN
1	F	2672	GLN
1	F	3033	ASN
1	G	3185	GLN
1	G	3546	ASN
1	H	3698	GLN
1	H	4059	ASN
1	I	4211	GLN
1	I	4572	ASN
1	J	4724	GLN
1	J	5085	ASN
1	K	5237	GLN
1	K	5598	ASN
1	L	5750	GLN
1	L	6111	ASN
1	M	6263	GLN
1	M	6624	ASN
1	N	6776	GLN
1	N	7137	ASN
1	O	7289	GLN
1	O	7650	ASN
1	P	7802	GLN
1	P	8163	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.