



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:48 PM BST

PDB ID : 2YNJ
EMDB ID: : EMD-2221
Title : GroEL at sub-nanometer resolution by Constrained Single Particle Tomography
Authors : Bartesaghi, A.; Lecumberry, F.; Sapiro, G.; Subramaniam, S.
Deposited on : 2012-10-15
Resolution : 8.40 Å(reported)
Based on PDB ID : 3E76

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 : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

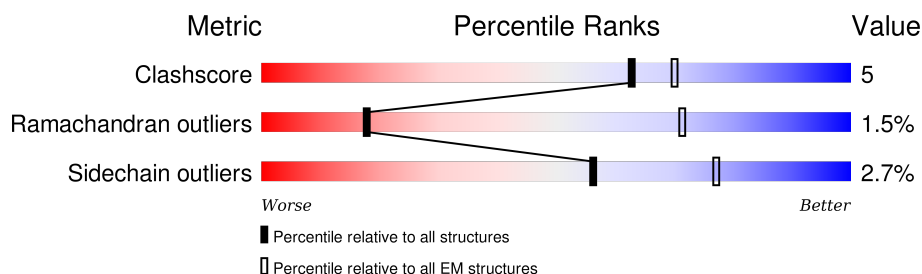
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.40 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	524	85% 14% .
1	B	524	85% 14% .
1	C	524	84% 15% .
1	D	524	85% 14% .
1	E	524	85% 14% .
1	F	524	85% 14% .
1	G	524	85% 14% .
1	H	524	85% 14% .
1	I	524	85% 14% .

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Mol	Chain	Length	Quality of chain
1	J	524	<div><div></div><div>85%</div><div>14%</div><div></div></div>
1	K	524	<div><div></div><div>84%</div><div>15%</div><div></div></div>
1	L	524	<div><div></div><div>85%</div><div>14%</div><div></div></div>
1	M	524	<div><div></div><div>85%</div><div>15%</div><div></div></div>
1	N	524	<div><div></div><div>86%</div><div>13%</div><div></div></div>

2 Entry composition [i](#)

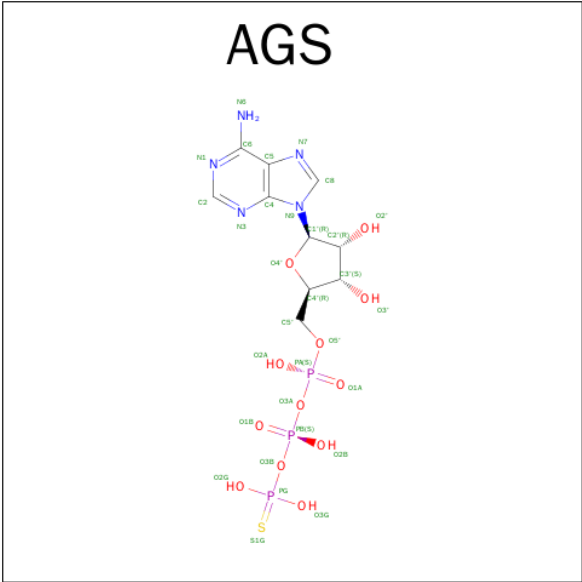
There are 4 unique types of molecules in this entry. The entry contains 54474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	B	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	C	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	D	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	E	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	F	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	G	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	H	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	I	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	J	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	K	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	L	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	M	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
1	N	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	H	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	I	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	J	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	K	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	L	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	M	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	N	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 3 is THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

Mol	Chain	Residues	Atoms		AltConf
3	G	4	Total 4	Tl 4	0
3	J	4	Total 4	Tl 4	0
3	D	4	Total 4	Tl 4	0
3	K	4	Total 4	Tl 4	0
3	E	4	Total 4	Tl 4	0
3	H	4	Total 4	Tl 4	0
3	B	4	Total 4	Tl 4	0
3	I	4	Total 4	Tl 4	0
3	C	4	Total 4	Tl 4	0
3	A	4	Total 4	Tl 4	0
3	N	4	Total 4	Tl 4	0
3	L	4	Total 4	Tl 4	0
3	F	4	Total 4	Tl 4	0
3	M	4	Total 4	Tl 4	0

- Molecule 4 is MAGNESIUM ION (three-letter code: Mg) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Mg 1	0
4	J	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	K	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0

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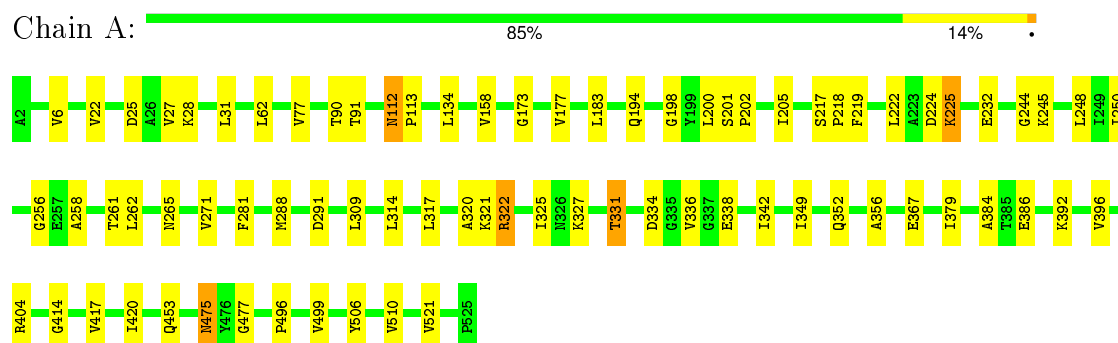
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Mol	Chain	Residues	Atoms		AltConf
4	H	1	Total 1	Mg 1	0
4	B	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	A	1	Total 1	Mg 1	0
4	N	1	Total 1	Mg 1	0
4	L	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	M	1	Total 1	Mg 1	0

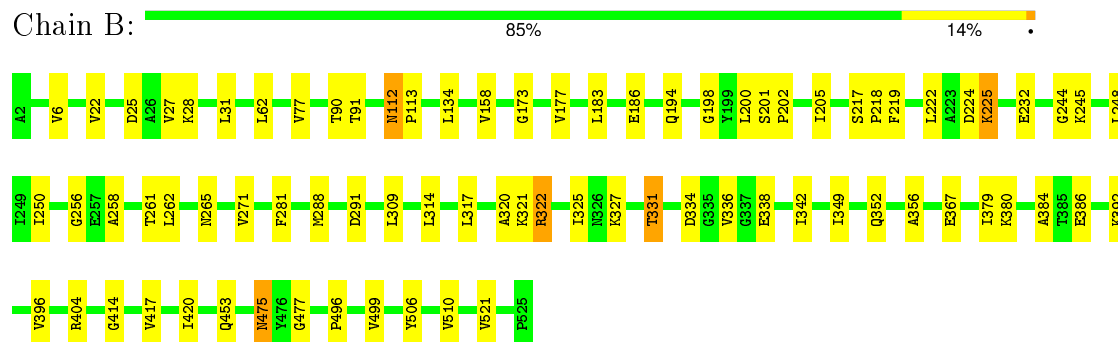
3 Residue-property plots [i](#)

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.

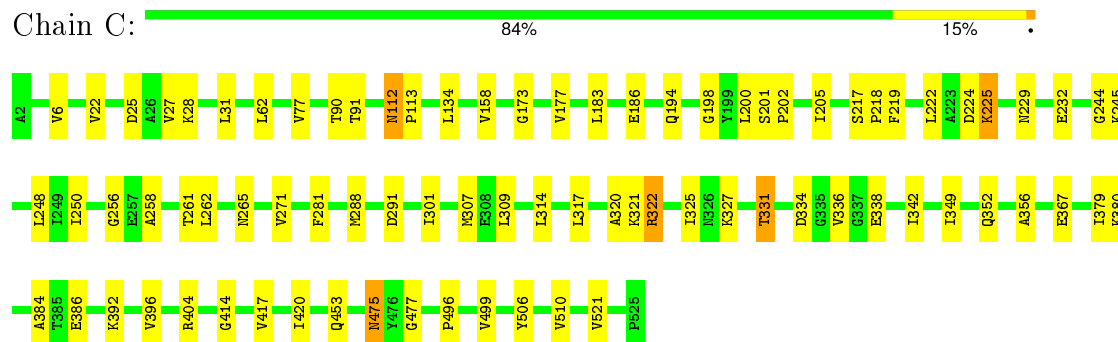
- Molecule 1: 60 KDA CHAPERONIN



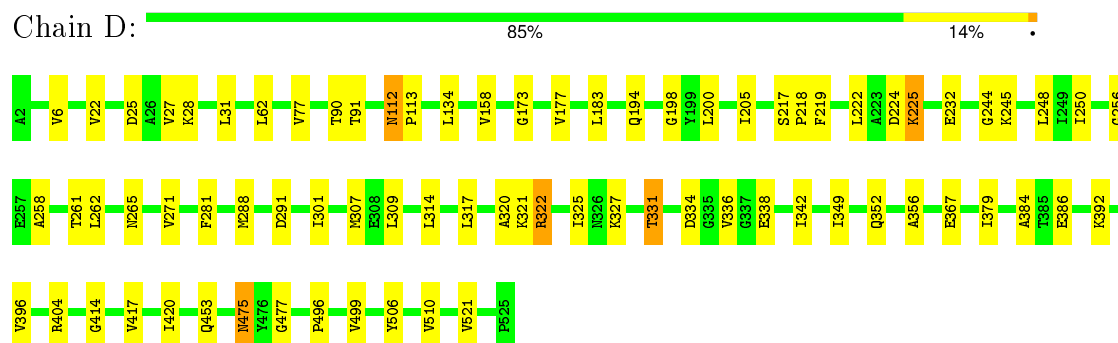
- Molecule 1: 60 KDA CHAPERONIN



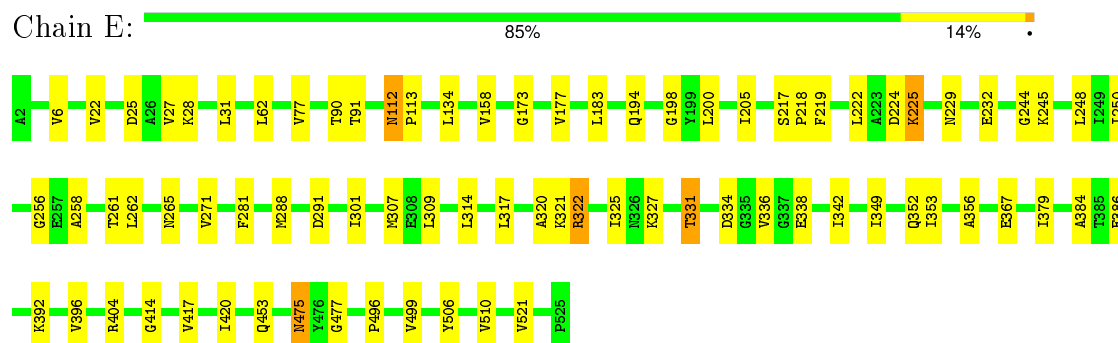
- Molecule 1: 60 KDA CHAPERONIN



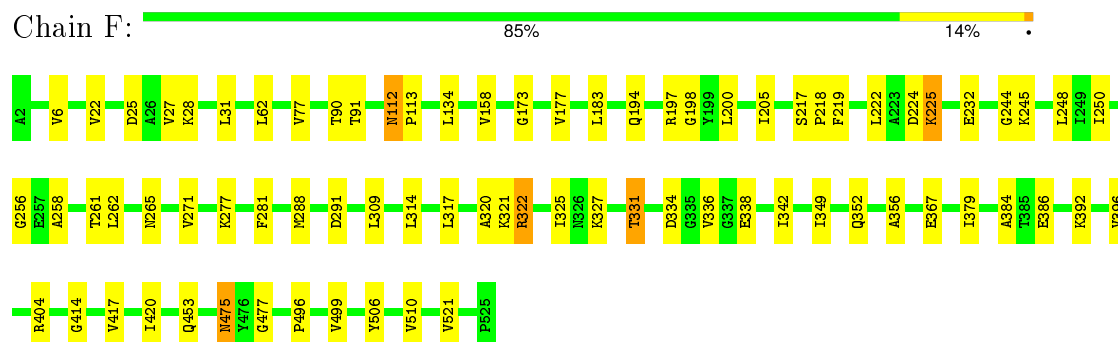
- Molecule 1: 60 KDA CHAPERONIN



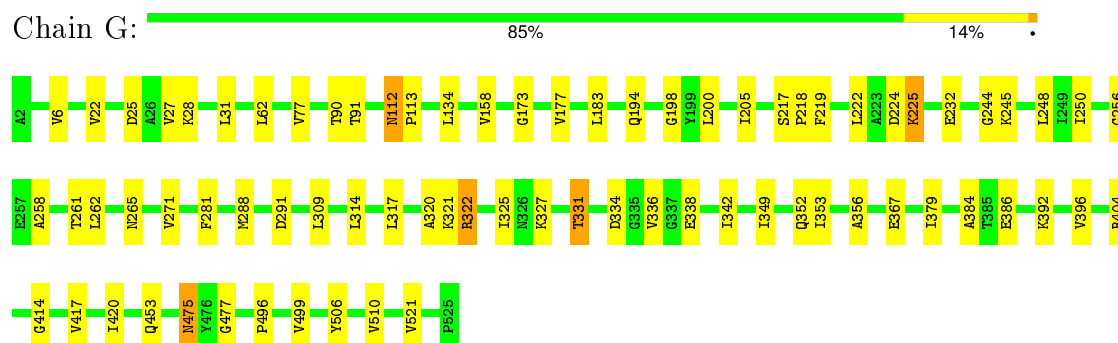
- Molecule 1: 60 KDA CHAPERONIN



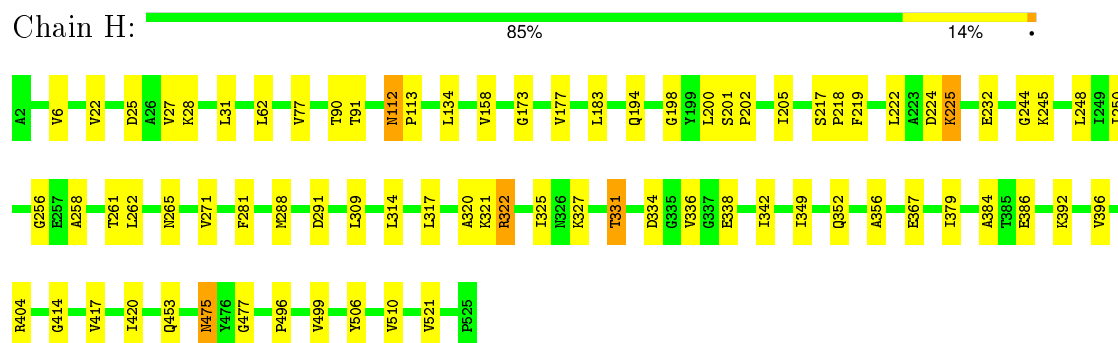
- Molecule 1: 60 KDA CHAPERONIN



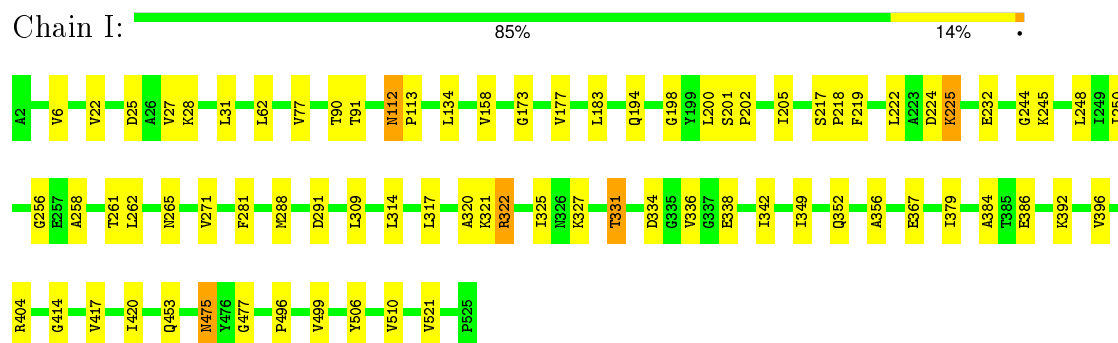
- Molecule 1: 60 KDA CHAPERONIN



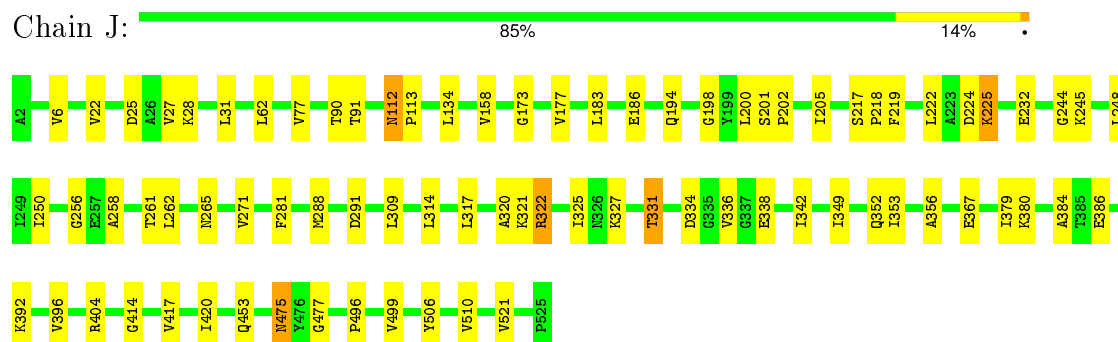
- Molecule 1: 60 KDA CHAPERONIN



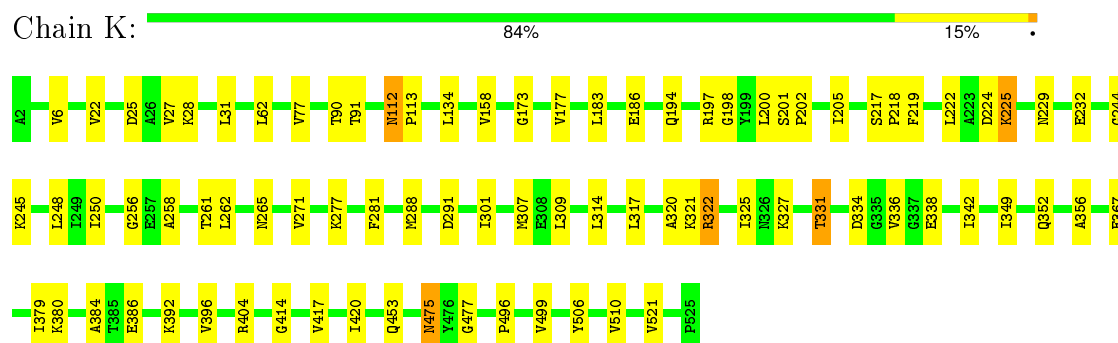
- Molecule 1: 60 KDA CHAPERONIN



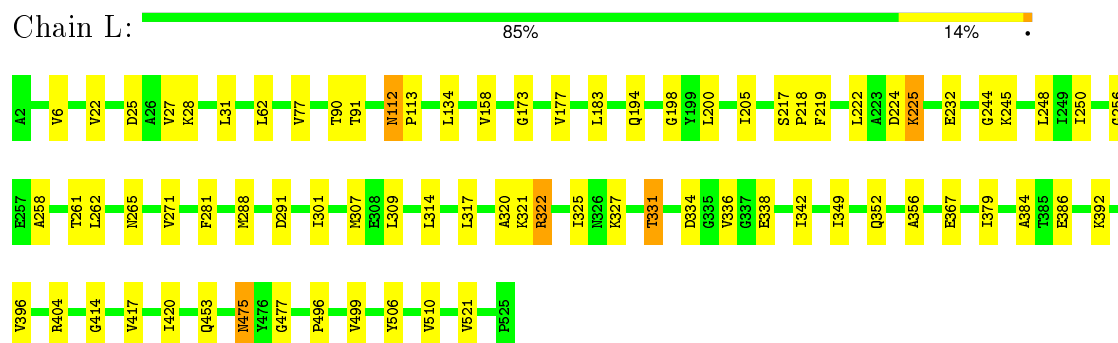
- Molecule 1: 60 KDA CHAPERONIN



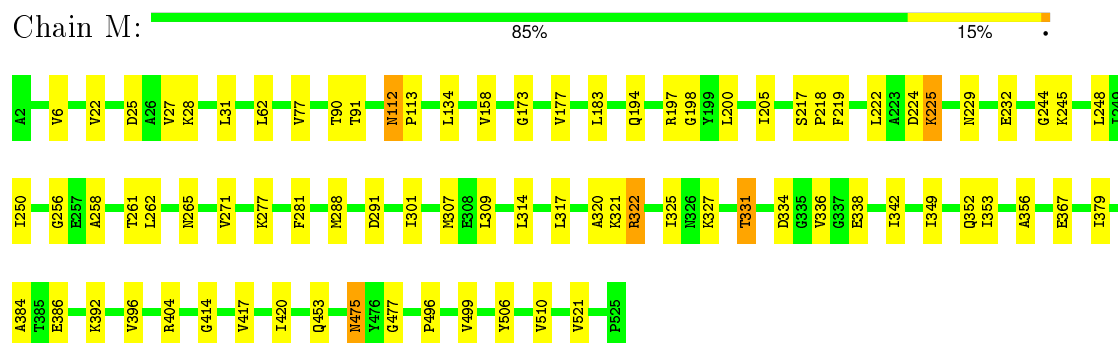
- Molecule 1: 60 KDA CHAPERONIN



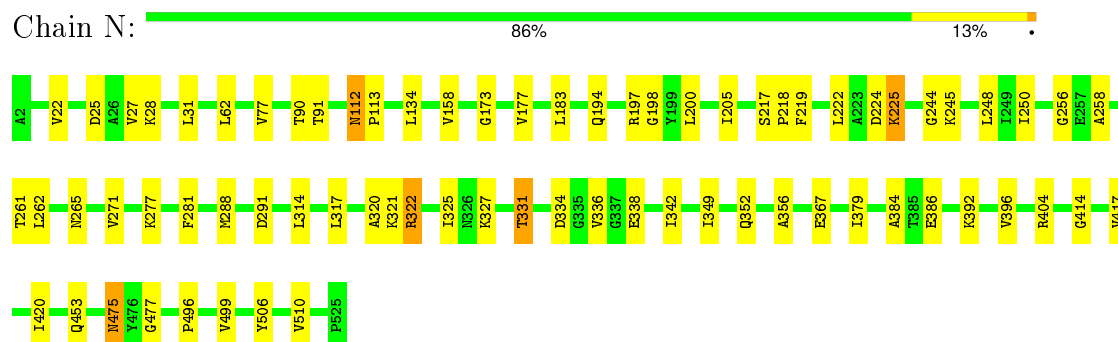
- Molecule 1: 60 KDA CHAPERONIN



- Molecule 1: 60 KDA CHAPERONIN



- Molecule 1: 60 KDA CHAPERONIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS VALUES WERE ASSIGNED TO EACH PARTICLE PROJECTION BASED ON THE DEFOCUS AT THE UNTILTED PLANE OF EACH TILT- SERIES AND A CORRECTION ACCORDING TO THE RELATIVE HEIGHT OF EACH PARTICLE. TO THIS PLANE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	80	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47000	Depositor
Image detector	CCD	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, TL

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	0.43	2/3883 (0.1%)	0.50	0/5243
1	B	0.43	2/3883 (0.1%)	0.50	0/5243
1	C	0.43	2/3883 (0.1%)	0.50	0/5243
1	D	0.43	2/3883 (0.1%)	0.50	0/5243
1	E	0.43	2/3883 (0.1%)	0.50	0/5243
1	F	0.43	2/3883 (0.1%)	0.50	0/5243
1	G	0.43	2/3883 (0.1%)	0.50	0/5243
1	H	0.43	2/3883 (0.1%)	0.50	0/5243
1	I	0.43	2/3883 (0.1%)	0.50	0/5243
1	J	0.43	2/3883 (0.1%)	0.50	0/5243
1	K	0.43	2/3883 (0.1%)	0.50	0/5243
1	L	0.43	2/3883 (0.1%)	0.50	0/5243
1	M	0.43	2/3883 (0.1%)	0.50	0/5243
1	N	0.43	2/3883 (0.1%)	0.50	0/5243
All	All	0.43	28/54362 (0.1%)	0.50	0/73402

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	GLU	CD-OE2	10.29	1.36	1.25
1	E	367	GLU	CD-OE2	10.27	1.36	1.25
1	J	367	GLU	CD-OE2	10.26	1.36	1.25
1	M	367	GLU	CD-OE2	10.26	1.36	1.25
1	F	367	GLU	CD-OE2	10.24	1.36	1.25
1	K	367	GLU	CD-OE2	10.24	1.36	1.25
1	N	367	GLU	CD-OE2	10.23	1.36	1.25
1	A	367	GLU	CD-OE2	10.20	1.36	1.25
1	D	367	GLU	CD-OE2	10.19	1.36	1.25
1	I	367	GLU	CD-OE2	10.17	1.36	1.25
1	C	367	GLU	CD-OE2	10.17	1.36	1.25
1	G	367	GLU	CD-OE2	10.17	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	367	GLU	CD-OE2	10.16	1.36	1.25
1	L	367	GLU	CD-OE2	10.12	1.36	1.25
1	C	367	GLU	CD-OE1	9.49	1.36	1.25
1	F	367	GLU	CD-OE1	9.49	1.36	1.25
1	H	367	GLU	CD-OE1	9.49	1.36	1.25
1	I	367	GLU	CD-OE1	9.49	1.36	1.25
1	L	367	GLU	CD-OE1	9.47	1.36	1.25
1	E	367	GLU	CD-OE1	9.47	1.36	1.25
1	J	367	GLU	CD-OE1	9.46	1.36	1.25
1	A	367	GLU	CD-OE1	9.46	1.36	1.25
1	N	367	GLU	CD-OE1	9.45	1.36	1.25
1	B	367	GLU	CD-OE1	9.44	1.36	1.25
1	G	367	GLU	CD-OE1	9.42	1.36	1.25
1	K	367	GLU	CD-OE1	9.42	1.36	1.25
1	M	367	GLU	CD-OE1	9.39	1.35	1.25
1	D	367	GLU	CD-OE1	9.35	1.35	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	46	0
1	B	3855	0	3976	47	0
1	C	3855	0	3976	49	0
1	D	3855	0	3976	46	0
1	E	3855	0	3976	48	0
1	F	3855	0	3976	46	0
1	G	3855	0	3976	46	0
1	H	3855	0	3976	46	0
1	I	3855	0	3976	46	0
1	J	3855	0	3976	47	0
1	K	3855	0	3976	49	0
1	L	3855	0	3976	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3855	0	3976	49	0
1	N	3855	0	3976	44	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
2	I	31	0	12	0	0
2	J	31	0	12	0	0
2	K	31	0	12	0	0
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
3	M	4	0	0	0	0
3	N	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1	0	0	0	0
4	N	1	0	0	0	0
All	All	54474	0	55832	600	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 5.

All (600) 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:F:281:PHE:CZ	1:H:384:ALA:O	2.26	0.89
1:G:384:ALA:O	1:N:281:PHE:CZ	2.26	0.89
1:A:384:ALA:O	1:H:281:PHE:CZ	2.26	0.89
1:G:281:PHE:CZ	1:I:384:ALA:O	2.26	0.89
1:M:281:PHE:CZ	1:N:384:ALA:O	2.26	0.88
1:E:281:PHE:CZ	1:F:384:ALA:O	2.26	0.88
1:A:281:PHE:CZ	1:B:384:ALA:O	2.26	0.88
1:I:281:PHE:CZ	1:J:384:ALA:O	2.26	0.88
1:B:281:PHE:CZ	1:C:384:ALA:O	2.26	0.88
1:J:281:PHE:CZ	1:K:384:ALA:O	2.26	0.87
1:D:281:PHE:CZ	1:E:384:ALA:O	2.26	0.87
1:L:281:PHE:CZ	1:M:384:ALA:O	2.26	0.87
1:C:281:PHE:CZ	1:D:384:ALA:O	2.26	0.87
1:K:281:PHE:CZ	1:L:384:ALA:O	2.26	0.87
1:N:349:ILE:HA	1:N:352:GLN:HG2	1.68	0.76
1:F:349:ILE:HA	1:F:352:GLN:HG2	1.68	0.76
1:K:349:ILE:HA	1:K:352:GLN:HG2	1.68	0.76
1:E:349:ILE:HA	1:E:352:GLN:HG2	1.68	0.76
1:J:349:ILE:HA	1:J:352:GLN:HG2	1.68	0.76
1:A:384:ALA:O	1:H:281:PHE:CE1	2.39	0.76
1:M:349:ILE:HA	1:M:352:GLN:HG2	1.68	0.76
1:C:349:ILE:HA	1:C:352:GLN:HG2	1.68	0.76
1:L:349:ILE:HA	1:L:352:GLN:HG2	1.68	0.76
1:G:384:ALA:O	1:N:281:PHE:CE1	2.39	0.76
1:G:281:PHE:CE1	1:I:384:ALA:O	2.39	0.76
1:A:349:ILE:HA	1:A:352:GLN:HG2	1.68	0.76
1:H:349:ILE:HA	1:H:352:GLN:HG2	1.68	0.76
1:B:349:ILE:HA	1:B:352:GLN:HG2	1.68	0.76
1:D:349:ILE:HA	1:D:352:GLN:HG2	1.68	0.76
1:F:281:PHE:CE1	1:H:384:ALA:O	2.39	0.76
1:G:349:ILE:HA	1:G:352:GLN:HG2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:ILE:HA	1:I:352:GLN:HG2	1.68	0.75
1:L:281:PHE:CE1	1:M:384:ALA:O	2.39	0.75
1:M:281:PHE:CE1	1:N:384:ALA:O	2.39	0.75
1:E:281:PHE:CE1	1:F:384:ALA:O	2.39	0.75
1:D:281:PHE:CE1	1:E:384:ALA:O	2.39	0.75
1:C:281:PHE:CE1	1:D:384:ALA:O	2.39	0.74
1:J:281:PHE:CE1	1:K:384:ALA:O	2.39	0.74
1:B:281:PHE:CE1	1:C:384:ALA:O	2.39	0.74
1:K:281:PHE:CE1	1:L:384:ALA:O	2.39	0.74
1:A:281:PHE:CE1	1:B:384:ALA:O	2.39	0.74
1:I:281:PHE:CE1	1:J:384:ALA:O	2.39	0.73
1:I:219:PHE:HE2	1:I:245:LYS:HB2	1.56	0.71
1:G:219:PHE:HE2	1:G:245:LYS:HB2	1.56	0.71
1:A:219:PHE:HE2	1:A:245:LYS:HB2	1.56	0.71
1:H:219:PHE:HE2	1:H:245:LYS:HB2	1.56	0.71
1:M:219:PHE:HE2	1:M:245:LYS:HB2	1.56	0.71
1:H:321:LYS:O	1:H:322:ARG:HB2	1.90	0.71
1:B:219:PHE:HE2	1:B:245:LYS:HB2	1.56	0.71
1:J:219:PHE:HE2	1:J:245:LYS:HB2	1.56	0.71
1:C:321:LYS:O	1:C:322:ARG:HB2	1.90	0.71
1:E:219:PHE:HE2	1:E:245:LYS:HB2	1.56	0.71
1:L:219:PHE:HE2	1:L:245:LYS:HB2	1.56	0.71
1:G:321:LYS:O	1:G:322:ARG:HB2	1.90	0.71
1:D:219:PHE:HE2	1:D:245:LYS:HB2	1.56	0.70
1:K:321:LYS:O	1:K:322:ARG:HB2	1.90	0.70
1:B:321:LYS:O	1:B:322:ARG:HB2	1.90	0.70
1:J:321:LYS:O	1:J:322:ARG:HB2	1.90	0.70
1:E:321:LYS:O	1:E:322:ARG:HB2	1.90	0.70
1:D:321:LYS:O	1:D:322:ARG:HB2	1.90	0.70
1:M:321:LYS:O	1:M:322:ARG:HB2	1.90	0.70
1:A:321:LYS:O	1:A:322:ARG:HB2	1.90	0.70
1:C:219:PHE:HE2	1:C:245:LYS:HB2	1.56	0.70
1:N:219:PHE:HE2	1:N:245:LYS:HB2	1.56	0.69
1:I:321:LYS:O	1:I:322:ARG:HB2	1.90	0.69
1:L:321:LYS:O	1:L:322:ARG:HB2	1.90	0.69
1:I:219:PHE:CE2	1:I:245:LYS:HB2	2.27	0.69
1:K:219:PHE:HE2	1:K:245:LYS:HB2	1.56	0.69
1:H:219:PHE:CE2	1:H:245:LYS:HB2	2.27	0.69
1:M:219:PHE:CE2	1:M:245:LYS:HB2	2.27	0.69
1:G:219:PHE:CE2	1:G:245:LYS:HB2	2.27	0.69
1:L:219:PHE:CE2	1:L:245:LYS:HB2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:CE2	1:C:245:LYS:HB2	2.27	0.69
1:K:219:PHE:CE2	1:K:245:LYS:HB2	2.27	0.69
1:N:321:LYS:O	1:N:322:ARG:HB2	1.90	0.69
1:F:219:PHE:HE2	1:F:245:LYS:HB2	1.56	0.69
1:A:219:PHE:CE2	1:A:245:LYS:HB2	2.27	0.69
1:D:219:PHE:CE2	1:D:245:LYS:HB2	2.27	0.69
1:N:219:PHE:CE2	1:N:245:LYS:HB2	2.27	0.69
1:E:219:PHE:CE2	1:E:245:LYS:HB2	2.27	0.69
1:F:219:PHE:CE2	1:F:245:LYS:HB2	2.27	0.69
1:F:321:LYS:O	1:F:322:ARG:HB2	1.90	0.69
1:B:219:PHE:CE2	1:B:245:LYS:HB2	2.27	0.69
1:J:219:PHE:CE2	1:J:245:LYS:HB2	2.27	0.69
1:B:281:PHE:HZ	1:C:384:ALA:O	1.76	0.69
1:J:281:PHE:HZ	1:K:384:ALA:O	1.76	0.68
1:C:281:PHE:HZ	1:D:384:ALA:O	1.76	0.68
1:A:281:PHE:HZ	1:B:384:ALA:O	1.76	0.67
1:I:281:PHE:HZ	1:J:384:ALA:O	1.76	0.67
1:A:384:ALA:O	1:H:281:PHE:HZ	1.75	0.67
1:G:281:PHE:HZ	1:I:384:ALA:O	1.75	0.67
1:M:288:MET:HA	1:M:291:ASP:HB2	1.77	0.67
1:D:288:MET:HA	1:D:291:ASP:HB2	1.77	0.67
1:E:288:MET:HA	1:E:291:ASP:HB2	1.77	0.67
1:N:288:MET:HA	1:N:291:ASP:HB2	1.77	0.67
1:L:288:MET:HA	1:L:291:ASP:HB2	1.77	0.67
1:C:288:MET:HA	1:C:291:ASP:HB2	1.77	0.67
1:M:281:PHE:HZ	1:N:384:ALA:O	1.75	0.66
1:K:288:MET:HA	1:K:291:ASP:HB2	1.77	0.66
1:F:288:MET:HA	1:F:291:ASP:HB2	1.77	0.66
1:B:288:MET:HA	1:B:291:ASP:HB2	1.77	0.66
1:J:288:MET:HA	1:J:291:ASP:HB2	1.77	0.66
1:G:384:ALA:O	1:N:281:PHE:HZ	1.76	0.66
1:E:281:PHE:HZ	1:F:384:ALA:O	1.76	0.66
1:G:288:MET:HA	1:G:291:ASP:HB2	1.77	0.66
1:F:281:PHE:HZ	1:H:384:ALA:O	1.75	0.66
1:A:288:MET:HA	1:A:291:ASP:HB2	1.77	0.66
1:L:281:PHE:HZ	1:M:384:ALA:O	1.76	0.66
1:I:288:MET:HA	1:I:291:ASP:HB2	1.77	0.66
1:H:288:MET:HA	1:H:291:ASP:HB2	1.77	0.66
1:D:281:PHE:HZ	1:E:384:ALA:O	1.76	0.66
1:N:349:ILE:HA	1:N:352:GLN:CG	2.27	0.65
1:E:349:ILE:HA	1:E:352:GLN:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ILE:HA	1:F:352:GLN:CG	2.27	0.65
1:M:349:ILE:HA	1:M:352:GLN:CG	2.27	0.65
1:D:349:ILE:HA	1:D:352:GLN:CG	2.27	0.65
1:L:349:ILE:HA	1:L:352:GLN:CG	2.27	0.65
1:C:349:ILE:HA	1:C:352:GLN:CG	2.27	0.65
1:K:349:ILE:HA	1:K:352:GLN:CG	2.27	0.65
1:H:349:ILE:HA	1:H:352:GLN:CG	2.26	0.65
1:G:349:ILE:HA	1:G:352:GLN:CG	2.27	0.65
1:K:281:PHE:HZ	1:L:384:ALA:O	1.76	0.65
1:B:349:ILE:HA	1:B:352:GLN:CG	2.27	0.64
1:J:349:ILE:HA	1:J:352:GLN:CG	2.27	0.64
1:I:349:ILE:HA	1:I:352:GLN:CG	2.26	0.64
1:A:349:ILE:HA	1:A:352:GLN:CG	2.26	0.64
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.81	0.63
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.81	0.63
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.81	0.63
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.81	0.63
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.80	0.63
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.81	0.63
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.81	0.63
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.81	0.63
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.81	0.63
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.81	0.63
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.80	0.62
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.81	0.62
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.81	0.62
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.81	0.62
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.82	0.62
1:N:417:VAL:HA	1:N:420:ILE:HG22	1.82	0.62
1:F:417:VAL:HA	1:F:420:ILE:HG22	1.82	0.62
1:H:417:VAL:HA	1:H:420:ILE:HG22	1.82	0.62
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.82	0.62
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.82	0.62
1:I:417:VAL:HA	1:I:420:ILE:HG22	1.82	0.62
1:J:417:VAL:HA	1:J:420:ILE:HG22	1.82	0.62
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.82	0.62
1:K:417:VAL:HA	1:K:420:ILE:HG22	1.82	0.61
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.82	0.61
1:E:417:VAL:HA	1:E:420:ILE:HG22	1.82	0.61
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.82	0.60
1:D:417:VAL:HA	1:D:420:ILE:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:VAL:HG21	1:D:510:VAL:HG11	1.83	0.60
1:L:77:VAL:HG21	1:L:510:VAL:HG11	1.83	0.60
1:C:77:VAL:HG21	1:C:510:VAL:HG11	1.83	0.60
1:K:77:VAL:HG21	1:K:510:VAL:HG11	1.83	0.60
1:I:77:VAL:HG21	1:I:510:VAL:HG11	1.83	0.60
1:A:77:VAL:HG21	1:A:510:VAL:HG11	1.83	0.60
1:B:77:VAL:HG21	1:B:510:VAL:HG11	1.83	0.60
1:J:77:VAL:HG21	1:J:510:VAL:HG11	1.83	0.59
1:E:77:VAL:HG21	1:E:510:VAL:HG11	1.83	0.59
1:H:77:VAL:HG21	1:H:510:VAL:HG11	1.83	0.59
1:M:77:VAL:HG21	1:M:510:VAL:HG11	1.83	0.59
1:G:77:VAL:HG21	1:G:510:VAL:HG11	1.83	0.59
1:N:77:VAL:HG21	1:N:510:VAL:HG11	1.83	0.59
1:F:77:VAL:HG21	1:F:510:VAL:HG11	1.83	0.59
1:E:173:GLY:O	1:E:404:ARG:NH2	2.37	0.58
1:M:173:GLY:O	1:M:404:ARG:NH2	2.37	0.58
1:D:173:GLY:O	1:D:404:ARG:NH2	2.37	0.57
1:H:173:GLY:O	1:H:404:ARG:NH2	2.37	0.57
1:L:173:GLY:O	1:L:404:ARG:NH2	2.37	0.57
1:G:173:GLY:O	1:G:404:ARG:NH2	2.37	0.57
1:A:173:GLY:O	1:A:404:ARG:NH2	2.37	0.57
1:I:173:GLY:O	1:I:404:ARG:NH2	2.37	0.57
1:K:173:GLY:O	1:K:404:ARG:NH2	2.37	0.57
1:J:173:GLY:O	1:J:404:ARG:NH2	2.37	0.57
1:C:173:GLY:O	1:C:404:ARG:NH2	2.37	0.57
1:B:173:GLY:O	1:B:404:ARG:NH2	2.37	0.57
1:N:173:GLY:O	1:N:404:ARG:NH2	2.37	0.56
1:F:173:GLY:O	1:F:404:ARG:NH2	2.37	0.56
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.89	0.55
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.89	0.55
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.89	0.55
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.89	0.55
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.89	0.55
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.89	0.55
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.89	0.55
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.89	0.54
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.89	0.54
1:I:22:VAL:HG11	1:I:62:LEU:HD21	1.89	0.54
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.89	0.53
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.89	0.53
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.89	0.53
1:F:77:VAL:HG12	1:F:506:TYR:HB3	1.92	0.52
1:N:77:VAL:HG12	1:N:506:TYR:HB3	1.92	0.52
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.92	0.52
1:M:77:VAL:HG12	1:M:506:TYR:HB3	1.92	0.52
1:E:496:PRO:O	1:E:499:VAL:HG12	2.10	0.52
1:F:496:PRO:O	1:F:499:VAL:HG12	2.10	0.52
1:L:77:VAL:HG12	1:L:506:TYR:HB3	1.92	0.52
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.92	0.52
1:M:496:PRO:O	1:M:499:VAL:HG12	2.10	0.52
1:N:496:PRO:O	1:N:499:VAL:HG12	2.10	0.52
1:H:496:PRO:O	1:H:499:VAL:HG12	2.10	0.52
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.92	0.52
1:H:77:VAL:HG12	1:H:506:TYR:HB3	1.92	0.52
1:G:496:PRO:O	1:G:499:VAL:HG12	2.10	0.52
1:A:496:PRO:O	1:A:499:VAL:HG12	2.10	0.51
1:L:496:PRO:O	1:L:499:VAL:HG12	2.10	0.51
1:D:496:PRO:O	1:D:499:VAL:HG12	2.10	0.51
1:I:496:PRO:O	1:I:499:VAL:HG12	2.10	0.51
1:C:496:PRO:O	1:C:499:VAL:HG12	2.10	0.51
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.92	0.51
1:K:77:VAL:HG12	1:K:506:TYR:HB3	1.92	0.51
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.92	0.51
1:K:496:PRO:O	1:K:499:VAL:HG12	2.10	0.51
1:B:496:PRO:O	1:B:499:VAL:HG12	2.10	0.51
1:J:496:PRO:O	1:J:499:VAL:HG12	2.10	0.51
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.92	0.51
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.92	0.51
1:J:77:VAL:HG12	1:J:506:TYR:HB3	1.92	0.50
1:H:194:GLN:HG3	1:H:331:THR:HB	1.95	0.49
1:G:194:GLN:HG3	1:G:331:THR:HB	1.95	0.49
1:J:194:GLN:HG3	1:J:331:THR:HB	1.95	0.49
1:E:392:LYS:O	1:E:396:VAL:HG23	2.13	0.49
1:C:194:GLN:HG3	1:C:331:THR:HB	1.95	0.49
1:F:392:LYS:O	1:F:396:VAL:HG23	2.13	0.49
1:M:392:LYS:O	1:M:396:VAL:HG23	2.13	0.49
1:F:194:GLN:HG3	1:F:331:THR:HB	1.95	0.49
1:N:392:LYS:O	1:N:396:VAL:HG23	2.13	0.49
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.94	0.49
1:I:194:GLN:HG3	1:I:331:THR:HB	1.95	0.49
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLN:HG3	1:B:331:THR:HB	1.95	0.49
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.94	0.49
1:D:194:GLN:HG3	1:D:331:THR:HB	1.95	0.49
1:N:194:GLN:HG3	1:N:331:THR:HB	1.95	0.49
1:K:194:GLN:HG3	1:K:331:THR:HB	1.95	0.49
1:L:194:GLN:HG3	1:L:331:THR:HB	1.95	0.49
1:H:392:LYS:O	1:H:396:VAL:HG23	2.13	0.49
1:G:158:VAL:HG13	1:G:396:VAL:HG22	1.94	0.49
1:G:392:LYS:O	1:G:396:VAL:HG23	2.13	0.49
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.94	0.49
1:A:194:GLN:HG3	1:A:331:THR:HB	1.95	0.49
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.94	0.49
1:D:392:LYS:O	1:D:396:VAL:HG23	2.13	0.49
1:B:158:VAL:HG13	1:B:396:VAL:HG22	1.94	0.49
1:H:198:GLY:HA3	1:H:327:LYS:O	2.13	0.49
1:G:198:GLY:HA3	1:G:327:LYS:O	2.13	0.49
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.94	0.48
1:M:194:GLN:HG3	1:M:331:THR:HB	1.95	0.48
1:F:31:LEU:HD23	1:F:453:GLN:HB3	1.96	0.48
1:L:392:LYS:O	1:L:396:VAL:HG23	2.13	0.48
1:A:158:VAL:HG13	1:A:396:VAL:HG22	1.94	0.48
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.94	0.48
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.96	0.48
1:N:31:LEU:HD23	1:N:453:GLN:HB3	1.96	0.48
1:E:194:GLN:HG3	1:E:331:THR:HB	1.95	0.48
1:E:31:LEU:HD23	1:E:453:GLN:HB3	1.95	0.48
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.94	0.48
1:D:198:GLY:HA3	1:D:327:LYS:O	2.13	0.48
1:A:198:GLY:HA3	1:A:327:LYS:O	2.13	0.48
1:I:158:VAL:HG13	1:I:396:VAL:HG22	1.94	0.48
1:L:198:GLY:HA3	1:L:327:LYS:O	2.13	0.48
1:I:198:GLY:HA3	1:I:327:LYS:O	2.13	0.48
1:M:31:LEU:HD23	1:M:453:GLN:HB3	1.96	0.48
1:I:31:LEU:HD23	1:I:453:GLN:HB3	1.96	0.48
1:C:392:LYS:O	1:C:396:VAL:HG23	2.13	0.48
1:E:198:GLY:HA3	1:E:327:LYS:O	2.14	0.48
1:F:158:VAL:HG13	1:F:396:VAL:HG22	1.94	0.48
1:M:198:GLY:HA3	1:M:327:LYS:O	2.14	0.48
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.94	0.48
1:K:392:LYS:O	1:K:396:VAL:HG23	2.13	0.48
1:N:198:GLY:HA3	1:N:327:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:414:GLY:O	1:K:417:VAL:HG22	2.14	0.48
1:B:31:LEU:HD23	1:B:453:GLN:HB3	1.96	0.48
1:G:414:GLY:O	1:G:417:VAL:HG22	2.14	0.47
1:H:414:GLY:O	1:H:417:VAL:HG22	2.14	0.47
1:C:414:GLY:O	1:C:417:VAL:HG22	2.14	0.47
1:M:414:GLY:O	1:M:417:VAL:HG22	2.14	0.47
1:I:392:LYS:O	1:I:396:VAL:HG23	2.13	0.47
1:K:198:GLY:HA3	1:K:327:LYS:O	2.13	0.47
1:L:31:LEU:HD23	1:L:453:GLN:HB3	1.96	0.47
1:F:198:GLY:HA3	1:F:327:LYS:O	2.13	0.47
1:C:198:GLY:HA3	1:C:327:LYS:O	2.13	0.47
1:J:31:LEU:HD23	1:J:453:GLN:HB3	1.96	0.47
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.96	0.47
1:B:392:LYS:O	1:B:396:VAL:HG23	2.13	0.47
1:A:392:LYS:O	1:A:396:VAL:HG23	2.13	0.47
1:B:198:GLY:HA3	1:B:327:LYS:O	2.13	0.47
1:K:183:LEU:HG	1:K:183:LEU:O	2.15	0.47
1:E:414:GLY:O	1:E:417:VAL:HG22	2.14	0.47
1:J:198:GLY:HA3	1:J:327:LYS:O	2.13	0.47
1:F:414:GLY:O	1:F:417:VAL:HG22	2.14	0.47
1:J:392:LYS:O	1:J:396:VAL:HG23	2.13	0.47
1:D:183:LEU:O	1:D:183:LEU:HG	2.15	0.47
1:L:183:LEU:O	1:L:183:LEU:HG	2.15	0.47
1:C:183:LEU:O	1:C:183:LEU:HG	2.15	0.47
1:K:31:LEU:HD23	1:K:453:GLN:HB3	1.96	0.47
1:L:321:LYS:O	1:L:322:ARG:CB	2.62	0.47
1:I:414:GLY:O	1:I:417:VAL:HG22	2.14	0.47
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.96	0.47
1:D:321:LYS:O	1:D:322:ARG:CB	2.62	0.47
1:L:414:GLY:O	1:L:417:VAL:HG22	2.14	0.47
1:D:414:GLY:O	1:D:417:VAL:HG22	2.14	0.47
1:C:218:PRO:HD2	1:C:320:ALA:O	2.15	0.47
1:K:321:LYS:O	1:K:322:ARG:CB	2.62	0.47
1:N:414:GLY:O	1:N:417:VAL:HG22	2.14	0.47
1:A:414:GLY:O	1:A:417:VAL:HG22	2.14	0.47
1:C:77:VAL:CG1	1:C:506:TYR:HB3	2.45	0.47
1:K:77:VAL:CG1	1:K:506:TYR:HB3	2.45	0.47
1:J:77:VAL:CG1	1:J:506:TYR:HB3	2.45	0.47
1:H:338:GLU:O	1:H:342:ILE:HG13	2.15	0.47
1:I:218:PRO:HD2	1:I:320:ALA:O	2.15	0.47
1:K:218:PRO:HD2	1:K:320:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:LEU:HG	1:F:183:LEU:O	2.15	0.47
1:A:218:PRO:HD2	1:A:320:ALA:O	2.15	0.47
1:C:321:LYS:O	1:C:322:ARG:CB	2.62	0.47
1:B:77:VAL:CG1	1:B:506:TYR:HB3	2.45	0.47
1:E:218:PRO:HD2	1:E:320:ALA:O	2.15	0.47
1:D:338:GLU:O	1:D:342:ILE:HG13	2.15	0.47
1:E:183:LEU:O	1:E:183:LEU:HG	2.14	0.47
1:N:183:LEU:O	1:N:183:LEU:HG	2.15	0.47
1:M:218:PRO:HD2	1:M:320:ALA:O	2.15	0.47
1:K:338:GLU:O	1:K:342:ILE:HG13	2.15	0.47
1:C:338:GLU:O	1:C:342:ILE:HG13	2.15	0.47
1:G:183:LEU:HG	1:G:183:LEU:O	2.15	0.47
1:G:338:GLU:O	1:G:342:ILE:HG13	2.15	0.47
1:G:31:LEU:HD23	1:G:453:GLN:HB3	1.96	0.47
1:H:31:LEU:HD23	1:H:453:GLN:HB3	1.96	0.47
1:L:338:GLU:O	1:L:342:ILE:HG13	2.15	0.47
1:M:183:LEU:O	1:M:183:LEU:HG	2.15	0.46
1:H:183:LEU:HG	1:H:183:LEU:O	2.15	0.46
1:B:414:GLY:O	1:B:417:VAL:HG22	2.14	0.46
1:N:218:PRO:HD2	1:N:320:ALA:O	2.15	0.46
1:F:218:PRO:HD2	1:F:320:ALA:O	2.15	0.46
1:F:222:LEU:HD23	1:F:250:ILE:HB	1.97	0.46
1:N:222:LEU:HD23	1:N:250:ILE:HB	1.97	0.46
1:J:414:GLY:O	1:J:417:VAL:HG22	2.14	0.46
1:J:183:LEU:HG	1:J:183:LEU:O	2.14	0.46
1:B:183:LEU:HG	1:B:183:LEU:O	2.15	0.46
1:G:77:VAL:CG1	1:G:506:TYR:HB3	2.45	0.46
1:B:112:ASN:HD22	1:B:113:PRO:HD2	1.81	0.46
1:G:218:PRO:HD2	1:G:320:ALA:O	2.15	0.46
1:J:338:GLU:O	1:J:342:ILE:HG13	2.15	0.46
1:A:183:LEU:HG	1:A:183:LEU:O	2.15	0.46
1:I:183:LEU:O	1:I:183:LEU:HG	2.14	0.46
1:H:77:VAL:CG1	1:H:506:TYR:HB3	2.45	0.46
1:M:77:VAL:CG1	1:M:506:TYR:HB3	2.45	0.46
1:M:338:GLU:O	1:M:342:ILE:HG13	2.15	0.46
1:J:112:ASN:HD22	1:J:113:PRO:HD2	1.81	0.46
1:B:338:GLU:O	1:B:342:ILE:HG13	2.15	0.46
1:D:218:PRO:HD2	1:D:320:ALA:O	2.15	0.46
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.97	0.46
1:E:338:GLU:O	1:E:342:ILE:HG13	2.15	0.46
1:E:77:VAL:CG1	1:E:506:TYR:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:CG1	1:F:506:TYR:HB3	2.45	0.46
1:C:112:ASN:HD22	1:C:113:PRO:HD2	1.81	0.46
1:C:222:LEU:HD23	1:C:250:ILE:HB	1.97	0.46
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.97	0.46
1:K:112:ASN:HD22	1:K:113:PRO:HD2	1.81	0.46
1:G:222:LEU:HD23	1:G:250:ILE:HB	1.97	0.46
1:I:77:VAL:CG1	1:I:506:TYR:HB3	2.45	0.46
1:A:77:VAL:CG1	1:A:506:TYR:HB3	2.45	0.46
1:N:77:VAL:CG1	1:N:506:TYR:HB3	2.45	0.46
1:H:218:PRO:HD2	1:H:320:ALA:O	2.15	0.46
1:J:218:PRO:HD2	1:J:320:ALA:O	2.15	0.46
1:A:112:ASN:HD22	1:A:113:PRO:HD2	1.81	0.46
1:L:218:PRO:HD2	1:L:320:ALA:O	2.15	0.46
1:I:112:ASN:HD22	1:I:113:PRO:HD2	1.81	0.46
1:M:222:LEU:HD23	1:M:250:ILE:HB	1.97	0.46
1:E:222:LEU:HD23	1:E:250:ILE:HB	1.97	0.46
1:L:77:VAL:CG1	1:L:506:TYR:HB3	2.45	0.45
1:B:218:PRO:HD2	1:B:320:ALA:O	2.15	0.45
1:N:338:GLU:O	1:N:342:ILE:HG13	2.15	0.45
1:J:222:LEU:HD23	1:J:250:ILE:HB	1.97	0.45
1:B:321:LYS:O	1:B:322:ARG:CB	2.62	0.45
1:D:77:VAL:CG1	1:D:506:TYR:HB3	2.45	0.45
1:I:338:GLU:O	1:I:342:ILE:HG13	2.15	0.45
1:F:338:GLU:O	1:F:342:ILE:HG13	2.15	0.45
1:B:222:LEU:HD23	1:B:250:ILE:HB	1.97	0.45
1:A:338:GLU:O	1:A:342:ILE:HG13	2.15	0.45
1:D:222:LEU:HD23	1:D:250:ILE:HB	1.97	0.45
1:J:25:ASP:HA	1:J:28:LYS:HG2	1.98	0.45
1:H:321:LYS:O	1:H:322:ARG:CB	2.62	0.45
1:I:25:ASP:HA	1:I:28:LYS:HG2	1.98	0.45
1:L:222:LEU:HD23	1:L:250:ILE:HB	1.97	0.45
1:K:25:ASP:HA	1:K:28:LYS:HG2	1.98	0.45
1:G:321:LYS:O	1:G:322:ARG:CB	2.62	0.45
1:A:321:LYS:O	1:A:322:ARG:CB	2.62	0.45
1:I:321:LYS:O	1:I:322:ARG:CB	2.62	0.45
1:B:25:ASP:HA	1:B:28:LYS:HG2	1.98	0.45
1:A:25:ASP:HA	1:A:28:LYS:HG2	1.98	0.45
1:L:112:ASN:HD22	1:L:113:PRO:HD2	1.81	0.45
1:L:25:ASP:HA	1:L:28:LYS:HG2	1.98	0.45
1:I:222:LEU:HD23	1:I:250:ILE:HB	1.97	0.45
1:A:222:LEU:HD23	1:A:250:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASN:HD22	1:D:113:PRO:HD2	1.81	0.45
1:C:25:ASP:HA	1:C:28:LYS:HG2	1.98	0.45
1:D:25:ASP:HA	1:D:28:LYS:HG2	1.98	0.44
1:G:25:ASP:HA	1:G:28:LYS:HG2	1.98	0.44
1:M:25:ASP:HA	1:M:28:LYS:HG2	1.98	0.44
1:E:25:ASP:HA	1:E:28:LYS:HG2	1.98	0.44
1:H:25:ASP:HA	1:H:28:LYS:HG2	1.98	0.44
1:H:112:ASN:HD22	1:H:113:PRO:HD2	1.81	0.44
1:G:112:ASN:HD22	1:G:113:PRO:HD2	1.81	0.44
1:M:112:ASN:HD22	1:M:113:PRO:HD2	1.81	0.44
1:N:417:VAL:HG11	1:N:477:GLY:HA3	2.00	0.44
1:E:112:ASN:HD22	1:E:113:PRO:HD2	1.81	0.44
1:N:25:ASP:HA	1:N:28:LYS:HG2	1.98	0.44
1:N:112:ASN:HD22	1:N:113:PRO:HD2	1.81	0.44
1:F:112:ASN:HD22	1:F:113:PRO:HD2	1.81	0.44
1:F:417:VAL:HG11	1:F:477:GLY:HA3	2.00	0.44
1:N:321:LYS:O	1:N:322:ARG:CB	2.62	0.44
1:G:417:VAL:HG11	1:G:477:GLY:HA3	2.00	0.44
1:F:25:ASP:HA	1:F:28:LYS:HG2	1.98	0.44
1:B:258:ALA:O	1:B:262:LEU:HG	2.18	0.44
1:E:248:LEU:HD13	1:E:325:ILE:HD11	2.00	0.44
1:M:248:LEU:HD13	1:M:325:ILE:HD11	2.00	0.44
1:F:321:LYS:O	1:F:322:ARG:CB	2.62	0.44
1:H:417:VAL:HG11	1:H:477:GLY:HA3	2.00	0.44
1:I:417:VAL:HG11	1:I:477:GLY:HA3	2.00	0.44
1:F:248:LEU:HD13	1:F:325:ILE:HD11	2.00	0.44
1:B:248:LEU:HD13	1:B:325:ILE:HD11	2.00	0.44
1:J:258:ALA:O	1:J:262:LEU:HG	2.18	0.44
1:F:258:ALA:O	1:F:262:LEU:HG	2.18	0.44
1:A:417:VAL:HG11	1:A:477:GLY:HA3	2.00	0.43
1:J:417:VAL:HG11	1:J:477:GLY:HA3	2.00	0.43
1:N:248:LEU:HD13	1:N:325:ILE:HD11	2.00	0.43
1:G:261:THR:O	1:G:265:ASN:HB2	2.18	0.43
1:N:258:ALA:O	1:N:262:LEU:HG	2.18	0.43
1:J:224:ASP:O	1:J:225:LYS:HB3	2.19	0.43
1:H:261:THR:O	1:H:265:ASN:HB2	2.18	0.43
1:J:248:LEU:HD13	1:J:325:ILE:HD11	2.00	0.43
1:H:258:ALA:O	1:H:262:LEU:HG	2.18	0.43
1:C:248:LEU:HD13	1:C:325:ILE:HD11	2.00	0.43
1:M:417:VAL:HG11	1:M:477:GLY:HA3	2.00	0.43
1:E:417:VAL:HG11	1:E:477:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASP:O	1:B:225:LYS:HB3	2.19	0.43
1:G:258:ALA:O	1:G:262:LEU:HG	2.18	0.43
1:A:258:ALA:O	1:A:262:LEU:HG	2.18	0.43
1:I:224:ASP:O	1:I:225:LYS:HB3	2.18	0.43
1:I:258:ALA:O	1:I:262:LEU:HG	2.18	0.43
1:E:258:ALA:O	1:E:262:LEU:HG	2.18	0.43
1:K:248:LEU:HD13	1:K:325:ILE:HD11	2.00	0.43
1:B:417:VAL:HG11	1:B:477:GLY:HA3	2.00	0.43
1:L:261:THR:O	1:L:265:ASN:HB2	2.18	0.43
1:M:258:ALA:O	1:M:262:LEU:HG	2.18	0.43
1:N:261:THR:O	1:N:265:ASN:HB2	2.18	0.43
1:A:224:ASP:O	1:A:225:LYS:HB3	2.19	0.43
1:F:261:THR:O	1:F:265:ASN:HB2	2.18	0.43
1:C:258:ALA:O	1:C:262:LEU:HG	2.18	0.43
1:C:261:THR:O	1:C:265:ASN:HB2	2.18	0.43
1:D:261:THR:O	1:D:265:ASN:HB2	2.18	0.43
1:K:261:THR:O	1:K:265:ASN:HB2	2.18	0.43
1:K:417:VAL:HG11	1:K:477:GLY:HA3	2.00	0.43
1:A:261:THR:O	1:A:265:ASN:HB2	2.18	0.43
1:K:224:ASP:O	1:K:225:LYS:HB3	2.19	0.43
1:I:261:THR:O	1:I:265:ASN:HB2	2.18	0.43
1:K:258:ALA:O	1:K:262:LEU:HG	2.19	0.43
1:L:417:VAL:HG11	1:L:477:GLY:HA3	2.00	0.43
1:H:248:LEU:HD13	1:H:325:ILE:HD11	2.00	0.43
1:I:248:LEU:HD13	1:I:325:ILE:HD11	2.00	0.43
1:C:417:VAL:HG11	1:C:477:GLY:HA3	2.00	0.43
1:G:248:LEU:HD13	1:G:325:ILE:HD11	2.00	0.43
1:D:258:ALA:O	1:D:262:LEU:HG	2.18	0.43
1:J:321:LYS:O	1:J:322:ARG:CB	2.62	0.43
1:D:417:VAL:HG11	1:D:477:GLY:HA3	2.00	0.43
1:A:248:LEU:HD13	1:A:325:ILE:HD11	2.00	0.43
1:C:224:ASP:O	1:C:225:LYS:HB3	2.19	0.43
1:M:229:ASN:HA	1:M:229:ASN:HD22	1.75	0.43
1:B:112:ASN:HD22	1:B:113:PRO:CD	2.32	0.42
1:L:258:ALA:O	1:L:262:LEU:HG	2.19	0.42
1:M:261:THR:O	1:M:265:ASN:HB2	2.18	0.42
1:G:224:ASP:O	1:G:225:LYS:HB3	2.19	0.42
1:J:112:ASN:HD22	1:J:113:PRO:CD	2.32	0.42
1:H:224:ASP:O	1:H:225:LYS:HB3	2.19	0.42
1:L:224:ASP:O	1:L:225:LYS:HB3	2.19	0.42
1:E:261:THR:O	1:E:265:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:O	1:B:265:ASN:HB2	2.18	0.42
1:M:224:ASP:O	1:M:225:LYS:HB3	2.18	0.42
1:E:229:ASN:HD22	1:E:229:ASN:HA	1.75	0.42
1:L:112:ASN:HD22	1:L:113:PRO:CD	2.32	0.42
1:F:177:VAL:HG22	1:F:379:ILE:HB	2.01	0.42
1:D:224:ASP:O	1:D:225:LYS:HB3	2.19	0.42
1:C:112:ASN:HD22	1:C:113:PRO:CD	2.32	0.42
1:I:112:ASN:HD22	1:I:113:PRO:CD	2.33	0.42
1:D:112:ASN:HD22	1:D:113:PRO:CD	2.32	0.42
1:H:177:VAL:HG22	1:H:379:ILE:HB	2.01	0.42
1:D:248:LEU:HD13	1:D:325:ILE:HD11	2.00	0.42
1:N:177:VAL:HG22	1:N:379:ILE:HB	2.01	0.42
1:F:224:ASP:O	1:F:225:LYS:HB3	2.19	0.42
1:J:261:THR:O	1:J:265:ASN:HB2	2.18	0.42
1:L:281:PHE:HZ	1:M:384:ALA:C	2.23	0.42
1:C:281:PHE:HZ	1:D:384:ALA:C	2.23	0.42
1:K:112:ASN:HD22	1:K:113:PRO:CD	2.32	0.42
1:A:112:ASN:HD22	1:A:113:PRO:CD	2.32	0.42
1:N:112:ASN:HD22	1:N:113:PRO:CD	2.32	0.42
1:L:248:LEU:HD13	1:L:325:ILE:HD11	2.00	0.42
1:E:224:ASP:O	1:E:225:LYS:HB3	2.19	0.42
1:C:475:ASN:N	1:C:475:ASN:HD22	2.18	0.42
1:K:475:ASN:N	1:K:475:ASN:HD22	2.18	0.42
1:N:224:ASP:O	1:N:225:LYS:HB3	2.19	0.42
1:D:281:PHE:HZ	1:E:384:ALA:C	2.23	0.42
1:E:112:ASN:HD22	1:E:113:PRO:CD	2.32	0.42
1:G:177:VAL:HG22	1:G:379:ILE:HB	2.01	0.42
1:E:475:ASN:N	1:E:475:ASN:HD22	2.18	0.42
1:A:281:PHE:HZ	1:B:384:ALA:C	2.23	0.42
1:I:281:PHE:HZ	1:J:384:ALA:C	2.23	0.42
1:K:281:PHE:HZ	1:L:384:ALA:C	2.23	0.42
1:H:112:ASN:HD22	1:H:113:PRO:CD	2.32	0.42
1:M:112:ASN:HD22	1:M:113:PRO:CD	2.33	0.42
1:F:112:ASN:HD22	1:F:113:PRO:CD	2.33	0.42
1:M:475:ASN:HD22	1:M:475:ASN:N	2.18	0.42
1:H:475:ASN:N	1:H:475:ASN:HD22	2.18	0.42
1:K:177:VAL:HG22	1:K:379:ILE:HB	2.01	0.42
1:G:112:ASN:HD22	1:G:113:PRO:CD	2.32	0.42
1:E:177:VAL:HG22	1:E:379:ILE:HB	2.01	0.42
1:A:177:VAL:HG22	1:A:379:ILE:HB	2.01	0.42
1:M:177:VAL:HG22	1:M:379:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:475:ASN:HD22	1:L:475:ASN:N	2.18	0.42
1:F:475:ASN:N	1:F:475:ASN:HD22	2.18	0.42
1:G:475:ASN:HD22	1:G:475:ASN:N	2.18	0.42
1:N:475:ASN:N	1:N:475:ASN:HD22	2.18	0.42
1:K:6:VAL:HG22	1:K:521:VAL:HG22	2.02	0.41
1:C:177:VAL:HG22	1:C:379:ILE:HB	2.01	0.41
1:K:229:ASN:HA	1:K:229:ASN:HD22	1.74	0.41
1:B:475:ASN:N	1:B:475:ASN:HD22	2.18	0.41
1:I:177:VAL:HG22	1:I:379:ILE:HB	2.01	0.41
1:F:281:PHE:HZ	1:H:384:ALA:C	2.23	0.41
1:B:6:VAL:HG22	1:B:521:VAL:HG22	2.03	0.41
1:B:177:VAL:HG22	1:B:379:ILE:HB	2.01	0.41
1:J:6:VAL:HG22	1:J:521:VAL:HG22	2.03	0.41
1:J:475:ASN:N	1:J:475:ASN:HD22	2.18	0.41
1:D:475:ASN:N	1:D:475:ASN:HD22	2.18	0.41
1:J:177:VAL:HG22	1:J:379:ILE:HB	2.01	0.41
1:G:384:ALA:C	1:N:281:PHE:HZ	2.23	0.41
1:A:384:ALA:C	1:H:281:PHE:HZ	2.23	0.41
1:G:281:PHE:HZ	1:I:384:ALA:C	2.23	0.41
1:C:6:VAL:HG22	1:C:521:VAL:HG22	2.03	0.41
1:C:229:ASN:HA	1:C:229:ASN:HD22	1.74	0.41
1:D:232:GLU:HB3	1:D:309:LEU:HB2	2.03	0.41
1:L:6:VAL:HG22	1:L:521:VAL:HG22	2.02	0.41
1:D:177:VAL:HG22	1:D:379:ILE:HB	2.01	0.41
1:A:6:VAL:HG22	1:A:521:VAL:HG22	2.03	0.41
1:L:177:VAL:HG22	1:L:379:ILE:HB	2.01	0.41
1:C:232:GLU:HB3	1:C:309:LEU:HB2	2.03	0.41
1:I:6:VAL:HG22	1:I:521:VAL:HG22	2.03	0.41
1:L:232:GLU:HB3	1:L:309:LEU:HB2	2.03	0.41
1:M:353:ILE:H	1:M:353:ILE:HG13	1.66	0.41
1:D:6:VAL:HG22	1:D:521:VAL:HG22	2.03	0.41
1:B:232:GLU:HB3	1:B:309:LEU:HB2	2.03	0.41
1:M:321:LYS:O	1:M:322:ARG:CB	2.62	0.41
1:K:232:GLU:HB3	1:K:309:LEU:HB2	2.03	0.41
1:M:281:PHE:HZ	1:N:384:ALA:C	2.23	0.41
1:E:281:PHE:HZ	1:F:384:ALA:C	2.23	0.41
1:E:321:LYS:O	1:E:322:ARG:CB	2.62	0.41
1:H:6:VAL:HG22	1:H:521:VAL:HG22	2.02	0.41
1:E:301:ILE:HG23	1:E:307:MET:HB3	2.03	0.41
1:J:232:GLU:HB3	1:J:309:LEU:HB2	2.03	0.41
1:E:232:GLU:HB3	1:E:309:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:475:ASN:N	1:I:475:ASN:HD22	2.18	0.41
1:A:232:GLU:HB3	1:A:309:LEU:HB2	2.03	0.41
1:E:353:ILE:HG13	1:E:353:ILE:H	1.66	0.41
1:A:475:ASN:HD22	1:A:475:ASN:N	2.18	0.41
1:M:232:GLU:HB3	1:M:309:LEU:HB2	2.03	0.41
1:M:301:ILE:HG23	1:M:307:MET:HB3	2.03	0.41
1:D:301:ILE:HG23	1:D:307:MET:HB3	2.03	0.41
1:N:197:ARG:HD2	1:N:277:LYS:HB2	2.03	0.41
1:L:301:ILE:HG23	1:L:307:MET:HB3	2.03	0.41
1:C:301:ILE:HG23	1:C:307:MET:HB3	2.03	0.40
1:F:197:ARG:HD2	1:F:277:LYS:HB2	2.03	0.40
1:I:232:GLU:HB3	1:I:309:LEU:HB2	2.03	0.40
1:E:6:VAL:HG22	1:E:521:VAL:HG22	2.03	0.40
1:G:6:VAL:HG22	1:G:521:VAL:HG22	2.03	0.40
1:C:201:SER:HA	1:C:202:PRO:HD3	1.94	0.40
1:K:186:GLU:HB2	1:K:380:LYS:HB2	2.04	0.40
1:K:301:ILE:HG23	1:K:307:MET:HB3	2.03	0.40
1:M:6:VAL:HG22	1:M:521:VAL:HG22	2.03	0.40
1:J:186:GLU:HB2	1:J:380:LYS:HB2	2.03	0.40
1:F:232:GLU:HB3	1:F:309:LEU:HB2	2.03	0.40
1:J:353:ILE:H	1:J:353:ILE:HG13	1.66	0.40
1:B:281:PHE:HZ	1:C:384:ALA:C	2.23	0.40
1:K:197:ARG:HD2	1:K:277:LYS:HB2	2.03	0.40
1:J:201:SER:HA	1:J:202:PRO:HD3	1.94	0.40
1:K:201:SER:HA	1:K:202:PRO:HD3	1.93	0.40
1:F:6:VAL:HG22	1:F:521:VAL:HG22	2.03	0.40
1:A:201:SER:HA	1:A:202:PRO:HD3	1.93	0.40
1:G:353:ILE:HG13	1:G:353:ILE:H	1.66	0.40
1:C:186:GLU:HB2	1:C:380:LYS:HB2	2.04	0.40
1:H:232:GLU:HB3	1:H:309:LEU:HB2	2.03	0.40
1:M:197:ARG:HD2	1:M:277:LYS:HB2	2.03	0.40
1:B:186:GLU:HB2	1:B:380:LYS:HB2	2.04	0.40
1:H:201:SER:HA	1:H:202:PRO:HD3	1.93	0.40
1:B:201:SER:HA	1:B:202:PRO:HD3	1.94	0.40
1:G:232:GLU:HB3	1:G:309:LEU:HB2	2.03	0.40
1:I:201:SER:HA	1:I:202:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	B	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	C	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	D	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	E	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	F	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	G	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	H	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	I	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	J	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	K	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	L	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	M	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
1	N	522/524 (100%)	496 (95%)	18 (3%)	8 (2%)	13	57
All	All	7308/7336 (100%)	6944 (95%)	252 (3%)	112 (2%)	18	57

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ARG
1	A	336	VAL
1	B	322	ARG
1	B	336	VAL
1	C	322	ARG
1	C	336	VAL
1	D	322	ARG
1	D	336	VAL
1	E	322	ARG

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Mol	Chain	Res	Type
1	E	336	VAL
1	F	322	ARG
1	F	336	VAL
1	G	322	ARG
1	G	336	VAL
1	H	322	ARG
1	H	336	VAL
1	I	322	ARG
1	I	336	VAL
1	J	322	ARG
1	J	336	VAL
1	K	322	ARG
1	K	336	VAL
1	L	322	ARG
1	L	336	VAL
1	M	322	ARG
1	M	336	VAL
1	N	322	ARG
1	N	336	VAL
1	A	271	VAL
1	A	334	ASP
1	B	271	VAL
1	B	334	ASP
1	C	271	VAL
1	C	334	ASP
1	D	271	VAL
1	D	334	ASP
1	E	271	VAL
1	E	334	ASP
1	F	271	VAL
1	F	334	ASP
1	G	271	VAL
1	G	334	ASP
1	H	271	VAL
1	H	334	ASP
1	I	271	VAL
1	I	334	ASP
1	J	271	VAL
1	J	334	ASP
1	K	271	VAL
1	K	334	ASP
1	L	271	VAL

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Mol	Chain	Res	Type
1	L	334	ASP
1	M	271	VAL
1	M	334	ASP
1	N	271	VAL
1	N	334	ASP
1	A	356	ALA
1	B	356	ALA
1	C	356	ALA
1	D	356	ALA
1	E	356	ALA
1	F	356	ALA
1	G	356	ALA
1	H	356	ALA
1	I	356	ALA
1	J	356	ALA
1	K	356	ALA
1	L	356	ALA
1	M	356	ALA
1	N	356	ALA
1	A	244	GLY
1	B	244	GLY
1	C	244	GLY
1	D	244	GLY
1	E	244	GLY
1	F	244	GLY
1	G	244	GLY
1	H	244	GLY
1	I	244	GLY
1	J	244	GLY
1	K	244	GLY
1	L	244	GLY
1	M	244	GLY
1	N	244	GLY
1	A	205	ILE
1	B	205	ILE
1	C	205	ILE
1	D	205	ILE
1	E	205	ILE
1	F	205	ILE
1	G	205	ILE
1	H	205	ILE
1	I	205	ILE

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Mol	Chain	Res	Type
1	J	205	ILE
1	K	205	ILE
1	L	205	ILE
1	M	205	ILE
1	N	205	ILE
1	A	256	GLY
1	B	256	GLY
1	D	256	GLY
1	E	256	GLY
1	F	256	GLY
1	G	256	GLY
1	H	256	GLY
1	J	256	GLY
1	K	256	GLY
1	L	256	GLY
1	M	256	GLY
1	N	256	GLY
1	C	256	GLY
1	I	256	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	B	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	C	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	D	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	E	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	F	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	G	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	H	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	I	404/404 (100%)	393 (97%)	11 (3%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	K	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	L	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	M	404/404 (100%)	393 (97%)	11 (3%)	52	79
1	N	404/404 (100%)	393 (97%)	11 (3%)	52	79
All	All	5656/5656 (100%)	5502 (97%)	154 (3%)	56	79

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	112	ASN
1	A	134	LEU
1	A	200	LEU
1	A	217	SER
1	A	225	LYS
1	A	314	LEU
1	A	317	LEU
1	A	331	THR
1	A	386	GLU
1	A	475	ASN
1	B	91	THR
1	B	112	ASN
1	B	134	LEU
1	B	200	LEU
1	B	217	SER
1	B	225	LYS
1	B	314	LEU
1	B	317	LEU
1	B	331	THR
1	B	386	GLU
1	B	475	ASN
1	C	91	THR
1	C	112	ASN
1	C	134	LEU
1	C	200	LEU
1	C	217	SER
1	C	225	LYS
1	C	314	LEU
1	C	317	LEU

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Mol	Chain	Res	Type
1	C	331	THR
1	C	386	GLU
1	C	475	ASN
1	D	91	THR
1	D	112	ASN
1	D	134	LEU
1	D	200	LEU
1	D	217	SER
1	D	225	LYS
1	D	314	LEU
1	D	317	LEU
1	D	331	THR
1	D	386	GLU
1	D	475	ASN
1	E	91	THR
1	E	112	ASN
1	E	134	LEU
1	E	200	LEU
1	E	217	SER
1	E	225	LYS
1	E	314	LEU
1	E	317	LEU
1	E	331	THR
1	E	386	GLU
1	E	475	ASN
1	F	91	THR
1	F	112	ASN
1	F	134	LEU
1	F	200	LEU
1	F	217	SER
1	F	225	LYS
1	F	314	LEU
1	F	317	LEU
1	F	331	THR
1	F	386	GLU
1	F	475	ASN
1	G	91	THR
1	G	112	ASN
1	G	134	LEU
1	G	200	LEU
1	G	217	SER
1	G	225	LYS

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Mol	Chain	Res	Type
1	G	314	LEU
1	G	317	LEU
1	G	331	THR
1	G	386	GLU
1	G	475	ASN
1	H	91	THR
1	H	112	ASN
1	H	134	LEU
1	H	200	LEU
1	H	217	SER
1	H	225	LYS
1	H	314	LEU
1	H	317	LEU
1	H	331	THR
1	H	386	GLU
1	H	475	ASN
1	I	91	THR
1	I	112	ASN
1	I	134	LEU
1	I	200	LEU
1	I	217	SER
1	I	225	LYS
1	I	314	LEU
1	I	317	LEU
1	I	331	THR
1	I	386	GLU
1	I	475	ASN
1	J	91	THR
1	J	112	ASN
1	J	134	LEU
1	J	200	LEU
1	J	217	SER
1	J	225	LYS
1	J	314	LEU
1	J	317	LEU
1	J	331	THR
1	J	386	GLU
1	J	475	ASN
1	K	91	THR
1	K	112	ASN
1	K	134	LEU
1	K	200	LEU

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Mol	Chain	Res	Type
1	K	217	SER
1	K	225	LYS
1	K	314	LEU
1	K	317	LEU
1	K	331	THR
1	K	386	GLU
1	K	475	ASN
1	L	91	THR
1	L	112	ASN
1	L	134	LEU
1	L	200	LEU
1	L	217	SER
1	L	225	LYS
1	L	314	LEU
1	L	317	LEU
1	L	331	THR
1	L	386	GLU
1	L	475	ASN
1	M	91	THR
1	M	112	ASN
1	M	134	LEU
1	M	200	LEU
1	M	217	SER
1	M	225	LYS
1	M	314	LEU
1	M	317	LEU
1	M	331	THR
1	M	386	GLU
1	M	475	ASN
1	N	91	THR
1	N	112	ASN
1	N	134	LEU
1	N	200	LEU
1	N	217	SER
1	N	225	LYS
1	N	314	LEU
1	N	317	LEU
1	N	331	THR
1	N	386	GLU
1	N	475	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	229	ASN
1	B	112	ASN
1	B	229	ASN
1	C	112	ASN
1	C	229	ASN
1	D	112	ASN
1	D	229	ASN
1	E	112	ASN
1	E	229	ASN
1	F	112	ASN
1	F	229	ASN
1	G	112	ASN
1	G	229	ASN
1	H	112	ASN
1	H	229	ASN
1	I	112	ASN
1	I	229	ASN
1	J	112	ASN
1	J	229	ASN
1	K	112	ASN
1	K	229	ASN
1	L	112	ASN
1	L	229	ASN
1	M	112	ASN
1	M	229	ASN
1	N	112	ASN
1	N	229	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 ⓘ

Of 84 ligands modelled in this entry, 70 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	AGS	A	549	3,4	26,33,33	1.24	3 (11%)	24,52,52	2.42	4 (16%)
2	AGS	B	549	3,4	26,33,33	1.25	3 (11%)	24,52,52	2.43	4 (16%)
2	AGS	C	549	3,4	26,33,33	1.25	3 (11%)	24,52,52	2.44	4 (16%)
2	AGS	D	549	3,4	26,33,33	1.26	3 (11%)	24,52,52	2.43	4 (16%)
2	AGS	E	549	3,4	26,33,33	1.24	3 (11%)	24,52,52	2.45	4 (16%)
2	AGS	F	549	3,4	26,33,33	1.25	3 (11%)	24,52,52	2.43	4 (16%)
2	AGS	G	549	3,4	26,33,33	1.25	3 (11%)	24,52,52	2.43	4 (16%)
2	AGS	H	549	3,4	26,33,33	1.26	3 (11%)	24,52,52	2.43	4 (16%)
2	AGS	I	549	3,4	26,33,33	1.24	3 (11%)	24,52,52	2.44	4 (16%)
2	AGS	J	549	3,4	26,33,33	1.25	3 (11%)	24,52,52	2.41	4 (16%)
2	AGS	K	549	3,4	26,33,33	1.25	3 (11%)	24,52,52	2.43	4 (16%)
2	AGS	L	549	3,4	26,33,33	1.26	3 (11%)	24,52,52	2.45	4 (16%)
2	AGS	M	549	3,4	26,33,33	1.24	3 (11%)	24,52,52	2.42	4 (16%)
2	AGS	N	549	3,4	26,33,33	1.24	3 (11%)	24,52,52	2.43	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	B	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	C	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	D	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	E	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	F	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	G	549	3,4	-	0/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	H	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	I	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	J	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	K	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	L	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	M	549	3,4	-	0/17/38/38	0/3/3/3
2	AGS	N	549	3,4	-	0/17/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	549	AGS	PG-O2G	-2.39	1.48	1.55
2	H	549	AGS	PG-O2G	-2.38	1.48	1.55
2	D	549	AGS	PG-O2G	-2.36	1.48	1.55
2	K	549	AGS	PG-O2G	-2.36	1.48	1.55
2	C	549	AGS	PG-O2G	-2.35	1.48	1.55
2	I	549	AGS	PG-O2G	-2.35	1.48	1.55
2	F	549	AGS	PG-O2G	-2.34	1.48	1.55
2	N	549	AGS	PG-O2G	-2.34	1.48	1.55
2	G	549	AGS	PG-O2G	-2.34	1.48	1.55
2	E	549	AGS	PG-O2G	-2.33	1.48	1.55
2	A	549	AGS	PG-O2G	-2.33	1.48	1.55
2	B	549	AGS	PG-O2G	-2.33	1.48	1.55
2	M	549	AGS	PG-O3G	-2.32	1.48	1.55
2	J	549	AGS	PG-O2G	-2.31	1.48	1.55
2	H	549	AGS	PG-O3G	-2.31	1.48	1.55
2	B	549	AGS	PG-O3G	-2.30	1.49	1.55
2	M	549	AGS	PG-O2G	-2.30	1.49	1.55
2	A	549	AGS	PG-O3G	-2.29	1.49	1.55
2	L	549	AGS	PG-O3G	-2.28	1.49	1.55
2	K	549	AGS	PG-O3G	-2.28	1.49	1.55
2	J	549	AGS	PG-O3G	-2.28	1.49	1.55
2	N	549	AGS	PG-O3G	-2.28	1.49	1.55
2	C	549	AGS	PG-O3G	-2.27	1.49	1.55
2	F	549	AGS	PG-O3G	-2.27	1.49	1.55
2	D	549	AGS	PG-O3G	-2.26	1.49	1.55
2	G	549	AGS	PG-O3G	-2.25	1.49	1.55
2	I	549	AGS	PG-O3G	-2.25	1.49	1.55
2	E	549	AGS	PG-O3G	-2.21	1.49	1.55
2	I	549	AGS	PG-S1G	3.52	1.96	1.90
2	A	549	AGS	PG-S1G	3.52	1.96	1.90
2	E	549	AGS	PG-S1G	3.52	1.97	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	549	AGS	PG-S1G	3.53	1.97	1.90
2	G	549	AGS	PG-S1G	3.53	1.97	1.90
2	C	549	AGS	PG-S1G	3.53	1.97	1.90
2	M	549	AGS	PG-S1G	3.53	1.97	1.90
2	B	549	AGS	PG-S1G	3.53	1.97	1.90
2	H	549	AGS	PG-S1G	3.54	1.97	1.90
2	J	549	AGS	PG-S1G	3.55	1.97	1.90
2	F	549	AGS	PG-S1G	3.56	1.97	1.90
2	N	549	AGS	PG-S1G	3.56	1.97	1.90
2	L	549	AGS	PG-S1G	3.58	1.97	1.90
2	D	549	AGS	PG-S1G	3.60	1.97	1.90

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	549	AGS	N3-C2-N1	-9.52	121.39	128.87
2	C	549	AGS	N3-C2-N1	-9.52	121.39	128.87
2	L	549	AGS	N3-C2-N1	-9.49	121.41	128.87
2	I	549	AGS	N3-C2-N1	-9.49	121.42	128.87
2	F	549	AGS	N3-C2-N1	-9.44	121.46	128.87
2	N	549	AGS	N3-C2-N1	-9.44	121.46	128.87
2	K	549	AGS	N3-C2-N1	-9.43	121.46	128.87
2	H	549	AGS	N3-C2-N1	-9.42	121.47	128.87
2	B	549	AGS	N3-C2-N1	-9.41	121.48	128.87
2	M	549	AGS	N3-C2-N1	-9.41	121.48	128.87
2	G	549	AGS	N3-C2-N1	-9.40	121.48	128.87
2	D	549	AGS	N3-C2-N1	-9.40	121.49	128.87
2	A	549	AGS	N3-C2-N1	-9.37	121.51	128.87
2	J	549	AGS	N3-C2-N1	-9.30	121.56	128.87
2	L	549	AGS	C4'-O4'-C1'	-4.92	104.43	109.64
2	D	549	AGS	C4'-O4'-C1'	-4.91	104.44	109.64
2	B	549	AGS	C4'-O4'-C1'	-4.91	104.44	109.64
2	K	549	AGS	C4'-O4'-C1'	-4.89	104.46	109.64
2	J	549	AGS	C4'-O4'-C1'	-4.89	104.46	109.64
2	I	549	AGS	C4'-O4'-C1'	-4.87	104.48	109.64
2	A	549	AGS	C4'-O4'-C1'	-4.86	104.49	109.64
2	H	549	AGS	C4'-O4'-C1'	-4.86	104.49	109.64
2	E	549	AGS	C4'-O4'-C1'	-4.86	104.49	109.64
2	F	549	AGS	C4'-O4'-C1'	-4.86	104.49	109.64
2	N	549	AGS	C4'-O4'-C1'	-4.86	104.49	109.64
2	G	549	AGS	C4'-O4'-C1'	-4.85	104.50	109.64
2	C	549	AGS	C4'-O4'-C1'	-4.83	104.53	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	549	AGS	C4'-O4'-C1'	-4.80	104.55	109.64
2	N	549	AGS	PB-O3B-PG	-2.88	122.26	132.71
2	D	549	AGS	PB-O3B-PG	-2.88	122.26	132.71
2	A	549	AGS	PB-O3B-PG	-2.87	122.31	132.71
2	F	549	AGS	PB-O3B-PG	-2.87	122.31	132.71
2	I	549	AGS	PB-O3B-PG	-2.86	122.32	132.71
2	C	549	AGS	PB-O3B-PG	-2.86	122.32	132.71
2	L	549	AGS	PB-O3B-PG	-2.86	122.33	132.71
2	E	549	AGS	PB-O3B-PG	-2.86	122.33	132.71
2	H	549	AGS	PB-O3B-PG	-2.86	122.35	132.71
2	B	549	AGS	PB-O3B-PG	-2.85	122.37	132.71
2	J	549	AGS	PB-O3B-PG	-2.85	122.38	132.71
2	K	549	AGS	PB-O3B-PG	-2.85	122.38	132.71
2	M	549	AGS	PB-O3B-PG	-2.85	122.38	132.71
2	G	549	AGS	PB-O3B-PG	-2.85	122.38	132.71
2	G	549	AGS	C5'-C4'-C3'	-2.58	105.24	115.20
2	D	549	AGS	C5'-C4'-C3'	-2.57	105.28	115.20
2	N	549	AGS	C5'-C4'-C3'	-2.56	105.28	115.20
2	E	549	AGS	C5'-C4'-C3'	-2.56	105.30	115.20
2	H	549	AGS	C5'-C4'-C3'	-2.56	105.30	115.20
2	A	549	AGS	C5'-C4'-C3'	-2.56	105.30	115.20
2	L	549	AGS	C5'-C4'-C3'	-2.56	105.31	115.20
2	I	549	AGS	C5'-C4'-C3'	-2.56	105.31	115.20
2	F	549	AGS	C5'-C4'-C3'	-2.55	105.32	115.20
2	K	549	AGS	C5'-C4'-C3'	-2.55	105.33	115.20
2	B	549	AGS	C5'-C4'-C3'	-2.55	105.34	115.20
2	C	549	AGS	C5'-C4'-C3'	-2.55	105.34	115.20
2	M	549	AGS	C5'-C4'-C3'	-2.55	105.34	115.20
2	J	549	AGS	C5'-C4'-C3'	-2.55	105.35	115.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.