



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:30 AM EST

PDB ID : 6VRA
EMDB ID : EMD-21365
Title : Anthrax octamer prechannel bound to full-length edema factor
Authors : Zhou, K.; Hardenbrook, N.J.; Liu, S.; Cui, Y.X.; Krantz, B.A.; Zhou, Z.H.
Deposited on : 2020-02-07
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

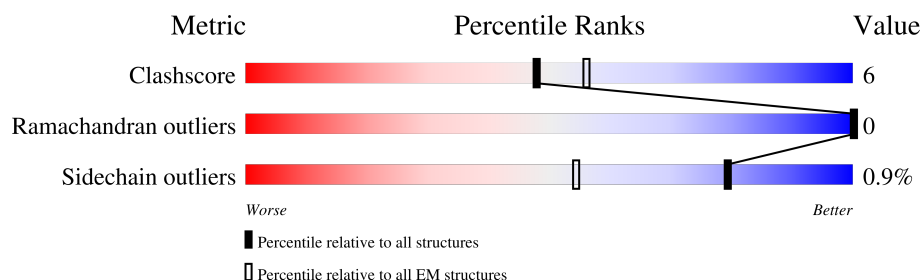
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	735	61% 12% 26%
1	C	735	61% 12% 26%
1	E	735	61% 12% 26%
1	G	735	61% 12% 26%
2	B	735	63% 10% 26%
2	D	735	63% 10% 26%
2	F	735	63% 11% 26%
2	H	735	62% 11% 26%

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Mol	Chain	Length	Quality of chain
3	I	767	<div><div>36%</div><div><div></div><div></div><div></div><div></div></div><div>75%</div><div>18%</div><div>6%</div></div>
3	J	767	<div><div>36%</div><div><div></div><div></div><div></div><div></div></div><div>76%</div><div>18%</div><div>6%</div></div>
3	K	767	<div><div>36%</div><div><div></div><div></div><div></div><div></div></div><div>76%</div><div>17%</div><div>6%</div></div>
3	L	767	<div><div>36%</div><div><div></div><div></div><div></div><div></div></div><div>77%</div><div>17%</div><div>6%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57744 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 Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	541	Total	C	N	O	S	0	0
			4274	2672	736	860	6		
1	C	541	Total	C	N	O	S	0	0
			4274	2672	736	860	6		
1	E	541	Total	C	N	O	S	0	0
			4274	2672	736	860	6		
1	G	541	Total	C	N	O	S	0	0
			4274	2672	736	860	6		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	ASP	ASN	conflict	UNP P13423
A	161	LEU	ARG	conflict	UNP P13423
A	162	GLU	LYS	conflict	UNP P13423
A	163	VAL	-	insertion	UNP P13423
A	164	LEU	-	insertion	UNP P13423
A	165	PHE	-	insertion	UNP P13423
A	166	GLN	LYS	conflict	UNP P13423
A	167	GLY	ARG	conflict	UNP P13423
A	245	GLY	LYS	engineered mutation	UNP P13423
A	252	ASN	ARG	engineered mutation	UNP P13423
C	121	ASP	ASN	conflict	UNP P13423
C	161	LEU	ARG	conflict	UNP P13423
C	162	GLU	LYS	conflict	UNP P13423
C	163	VAL	-	insertion	UNP P13423
C	164	LEU	-	insertion	UNP P13423
C	165	PHE	-	insertion	UNP P13423
C	166	GLN	LYS	conflict	UNP P13423
C	167	GLY	ARG	conflict	UNP P13423
C	245	GLY	LYS	engineered mutation	UNP P13423
C	252	ASN	ARG	engineered mutation	UNP P13423
E	121	ASP	ASN	conflict	UNP P13423
E	161	LEU	ARG	conflict	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
E	162	GLU	LYS	conflict	UNP P13423
E	163	VAL	-	insertion	UNP P13423
E	164	LEU	-	insertion	UNP P13423
E	165	PHE	-	insertion	UNP P13423
E	166	GLN	LYS	conflict	UNP P13423
E	167	GLY	ARG	conflict	UNP P13423
E	245	GLY	LYS	engineered mutation	UNP P13423
E	252	ASN	ARG	engineered mutation	UNP P13423
G	121	ASP	ASN	conflict	UNP P13423
G	161	LEU	ARG	conflict	UNP P13423
G	162	GLU	LYS	conflict	UNP P13423
G	163	VAL	-	insertion	UNP P13423
G	164	LEU	-	insertion	UNP P13423
G	165	PHE	-	insertion	UNP P13423
G	166	GLN	LYS	conflict	UNP P13423
G	167	GLY	ARG	conflict	UNP P13423
G	245	GLY	LYS	engineered mutation	UNP P13423
G	252	ASN	ARG	engineered mutation	UNP P13423

- Molecule 2 is a protein called Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	541	Total	C	N	O	S	0	0
			4283	2680	740	857	6		
2	D	541	Total	C	N	O	S	0	0
			4283	2680	740	857	6		
2	F	541	Total	C	N	O	S	0	0
			4283	2680	740	857	6		
2	H	541	Total	C	N	O	S	0	0
			4283	2680	740	857	6		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	161	LEU	ARG	conflict	UNP P13423
B	162	GLU	LYS	conflict	UNP P13423
B	163	VAL	-	insertion	UNP P13423
B	164	LEU	-	insertion	UNP P13423
B	165	PHE	-	insertion	UNP P13423
B	166	GLN	LYS	conflict	UNP P13423
B	167	GLY	ARG	conflict	UNP P13423
B	512	LYS	ASP	engineered mutation	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
D	161	LEU	ARG	conflict	UNP P13423
D	162	GLU	LYS	conflict	UNP P13423
D	163	VAL	-	insertion	UNP P13423
D	164	LEU	-	insertion	UNP P13423
D	165	PHE	-	insertion	UNP P13423
D	166	GLN	LYS	conflict	UNP P13423
D	167	GLY	ARG	conflict	UNP P13423
D	512	LYS	ASP	engineered mutation	UNP P13423
F	161	LEU	ARG	conflict	UNP P13423
F	162	GLU	LYS	conflict	UNP P13423
F	163	VAL	-	insertion	UNP P13423
F	164	LEU	-	insertion	UNP P13423
F	165	PHE	-	insertion	UNP P13423
F	166	GLN	LYS	conflict	UNP P13423
F	167	GLY	ARG	conflict	UNP P13423
F	512	LYS	ASP	engineered mutation	UNP P13423
H	161	LEU	ARG	conflict	UNP P13423
H	162	GLU	LYS	conflict	UNP P13423
H	163	VAL	-	insertion	UNP P13423
H	164	LEU	-	insertion	UNP P13423
H	165	PHE	-	insertion	UNP P13423
H	166	GLN	LYS	conflict	UNP P13423
H	167	GLY	ARG	conflict	UNP P13423
H	512	LYS	ASP	engineered mutation	UNP P13423

- Molecule 3 is a protein called Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	720	Total	C	N	O	S	0	0
			5875	3752	976	1141	6		
3	J	720	Total	C	N	O	S	0	0
			5875	3752	976	1141	6		
3	K	720	Total	C	N	O	S	0	0
			5875	3752	976	1141	6		
3	L	720	Total	C	N	O	S	0	0
			5875	3752	976	1141	6		

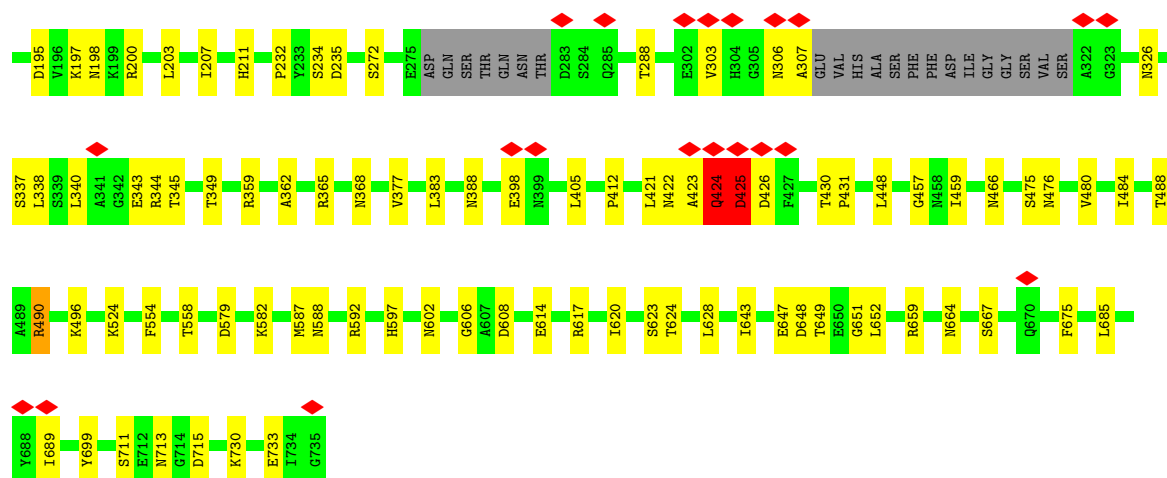
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	

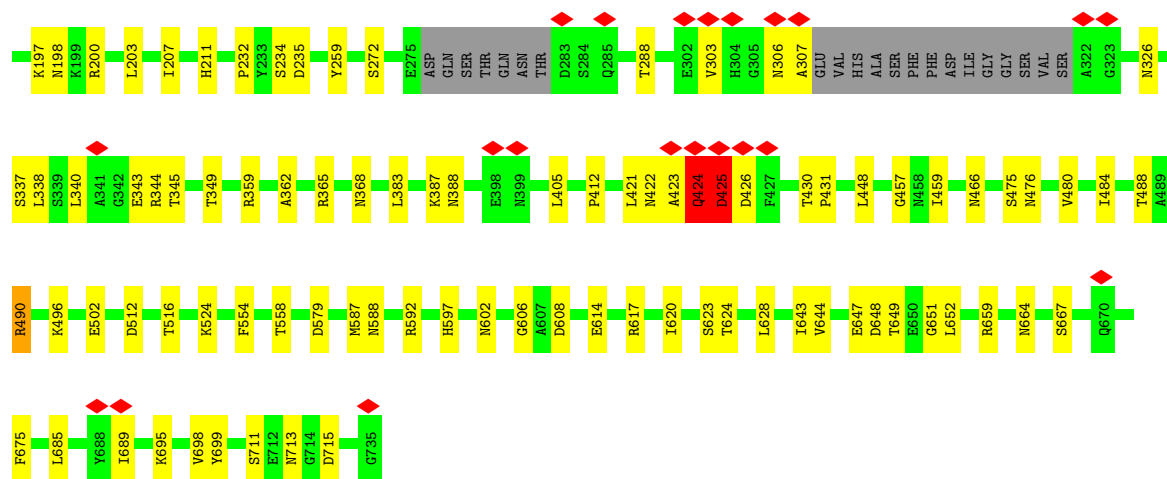
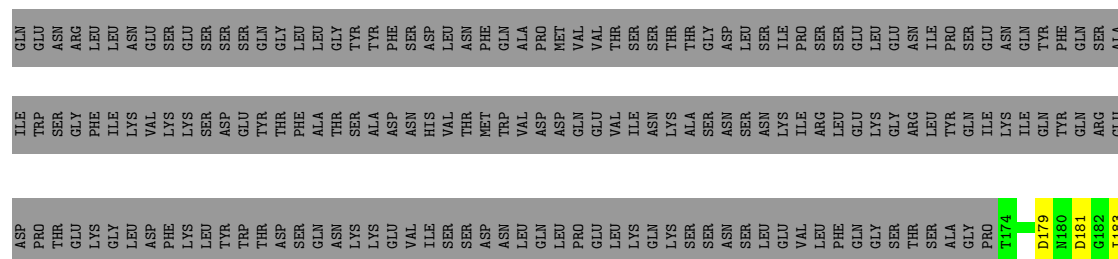
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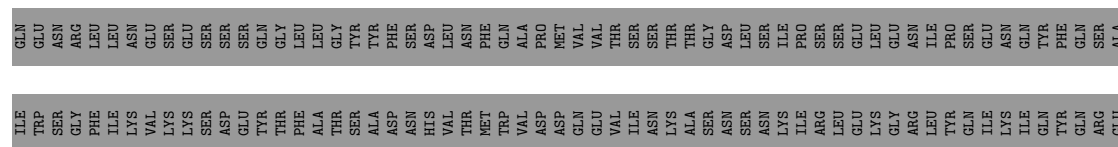
Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total 2	Ca 2	0
4	C	2	Total 2	Ca 2	0
4	D	2	Total 2	Ca 2	0
4	E	2	Total 2	Ca 2	0
4	F	2	Total 2	Ca 2	0
4	G	2	Total 2	Ca 2	0
4	H	2	Total 2	Ca 2	0

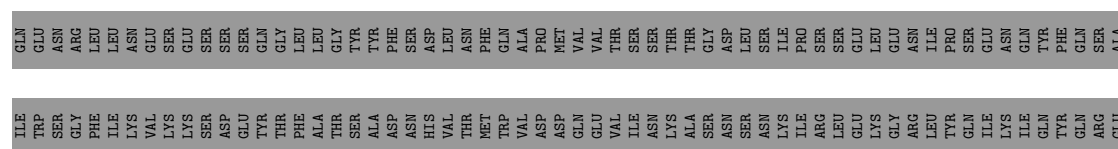


- Molecule 1: Protective antigen

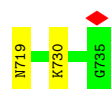


- Molecule 1: Protective antigen

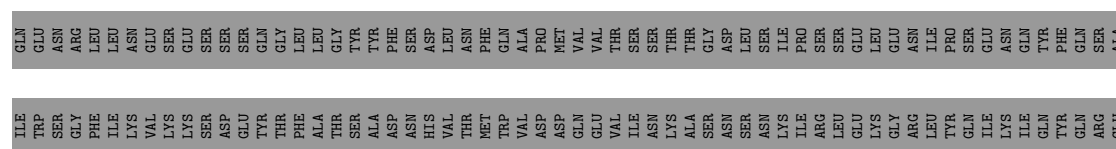


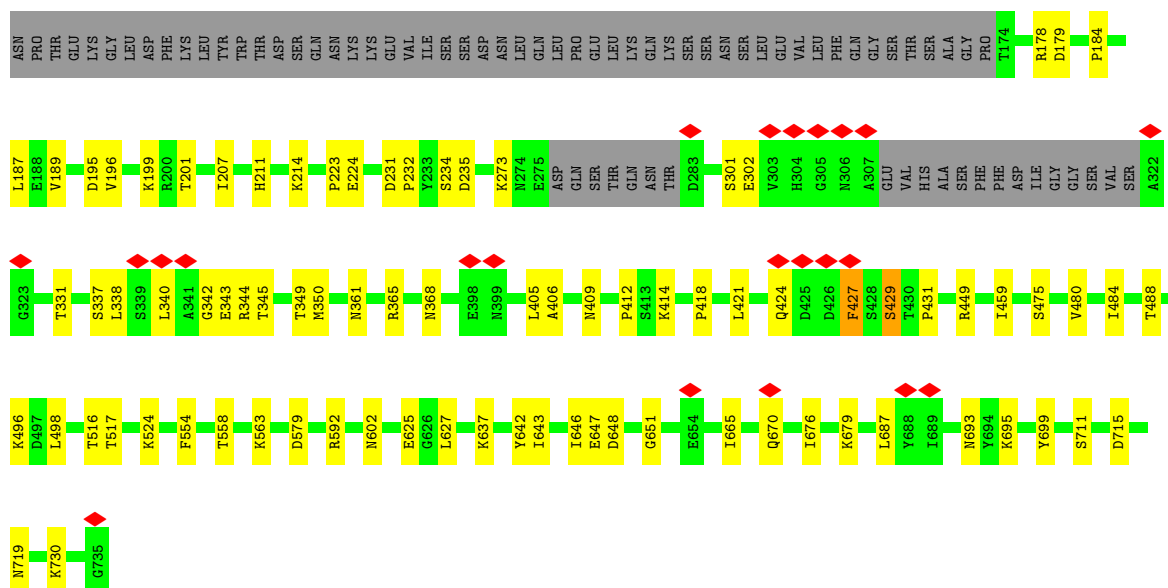


- Molecule 2: Protective antigen

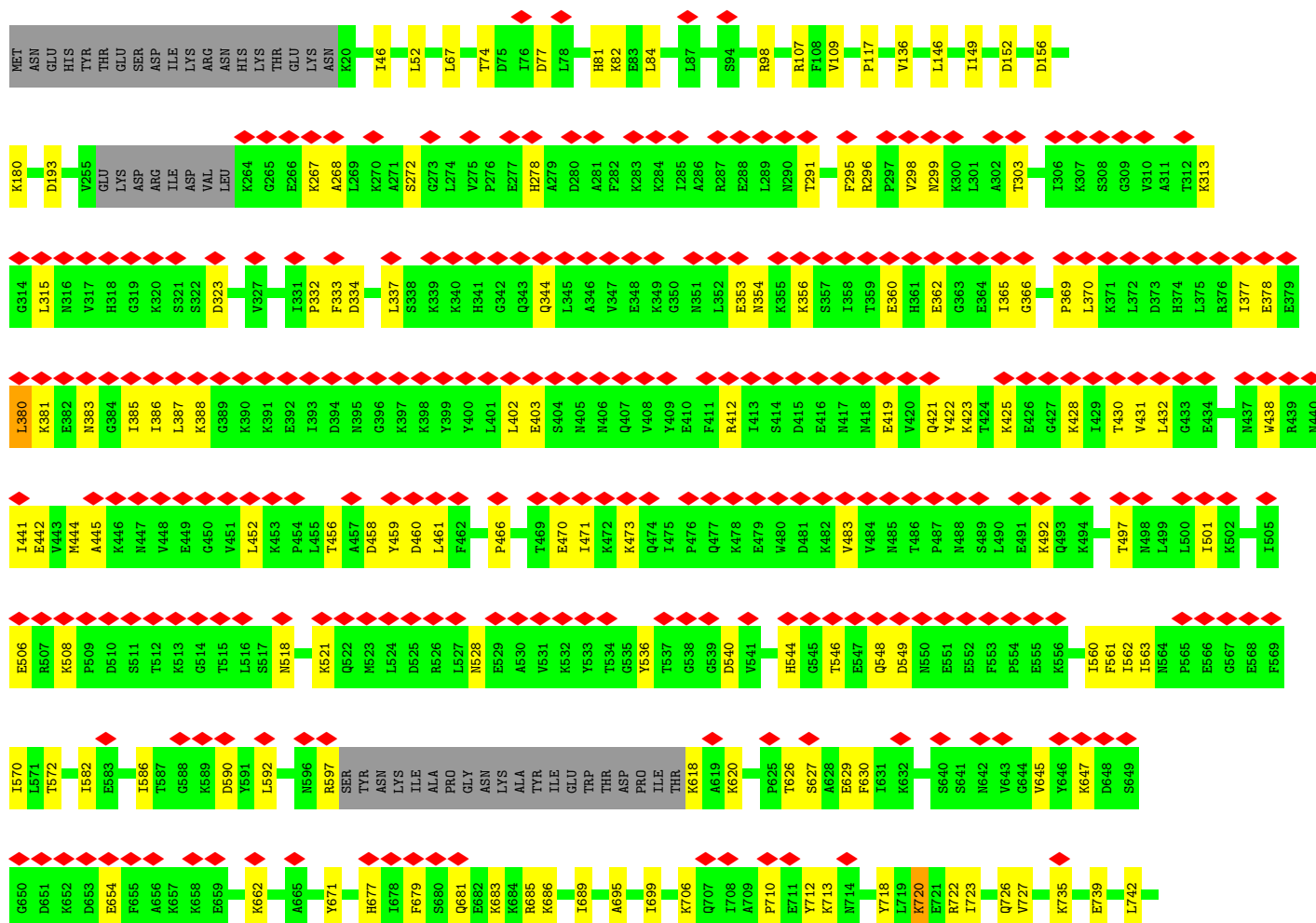
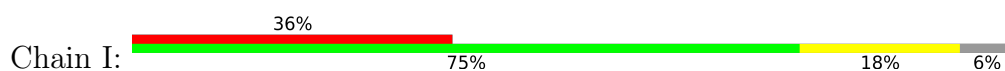


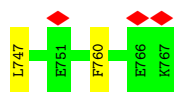
- Molecule 2: Protective antigen





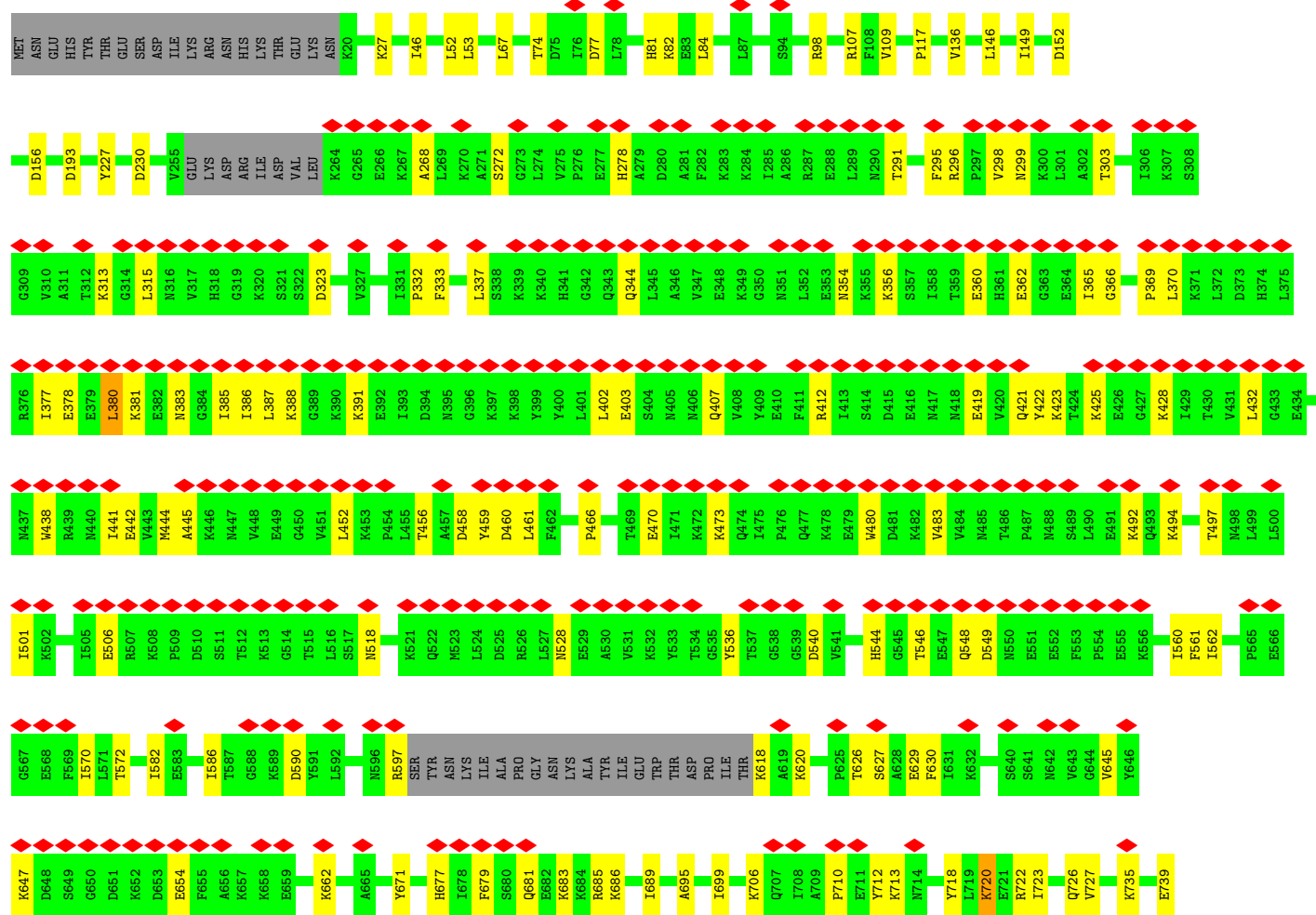
• Molecule 3: Calmodulin-sensitive adenylate cyclase





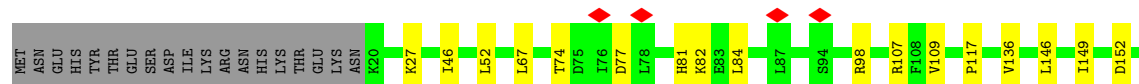
• Molecule 3: Calmodulin-sensitive adenylate cyclase

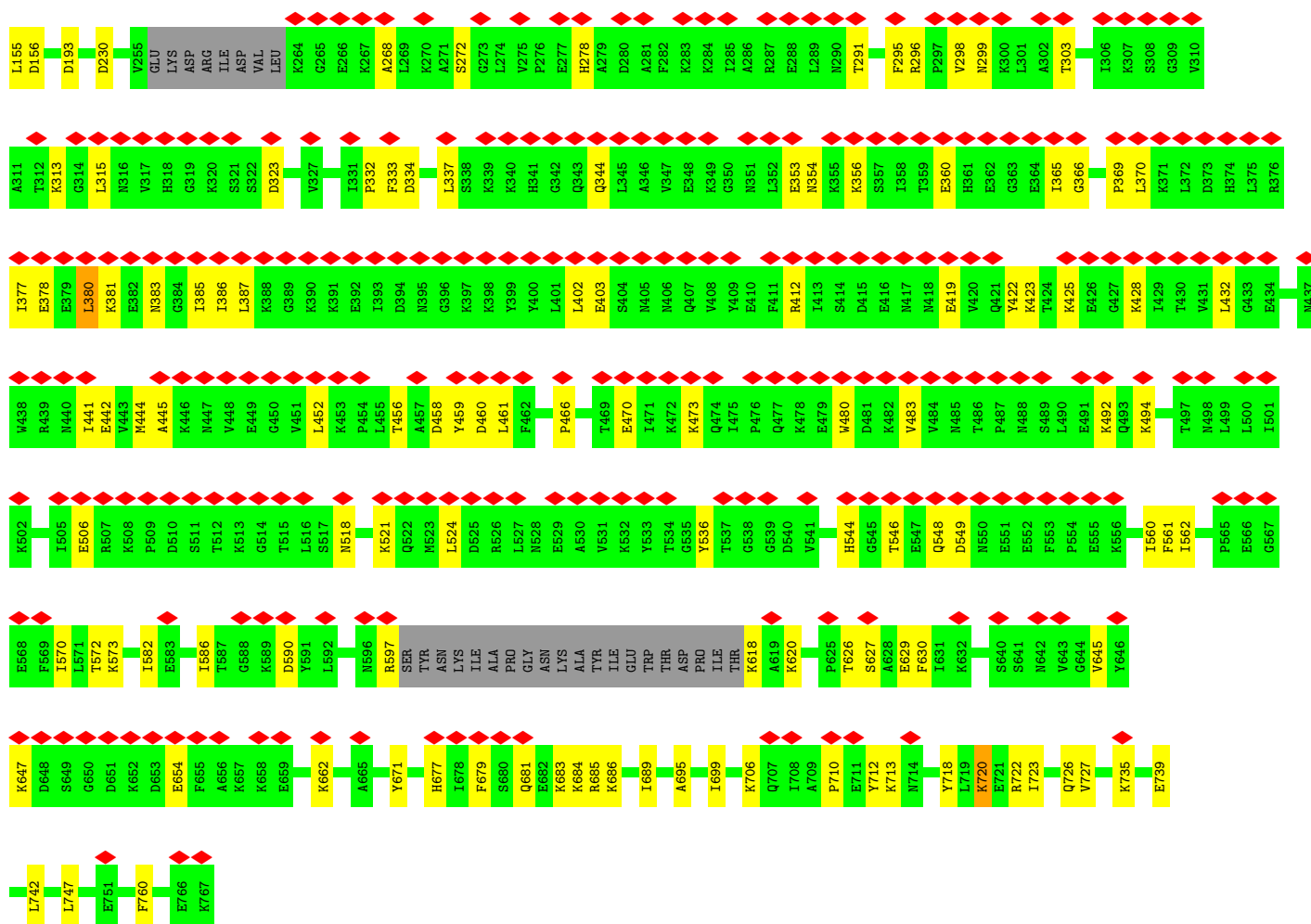
Chain J: 36% 76% 18% 6%



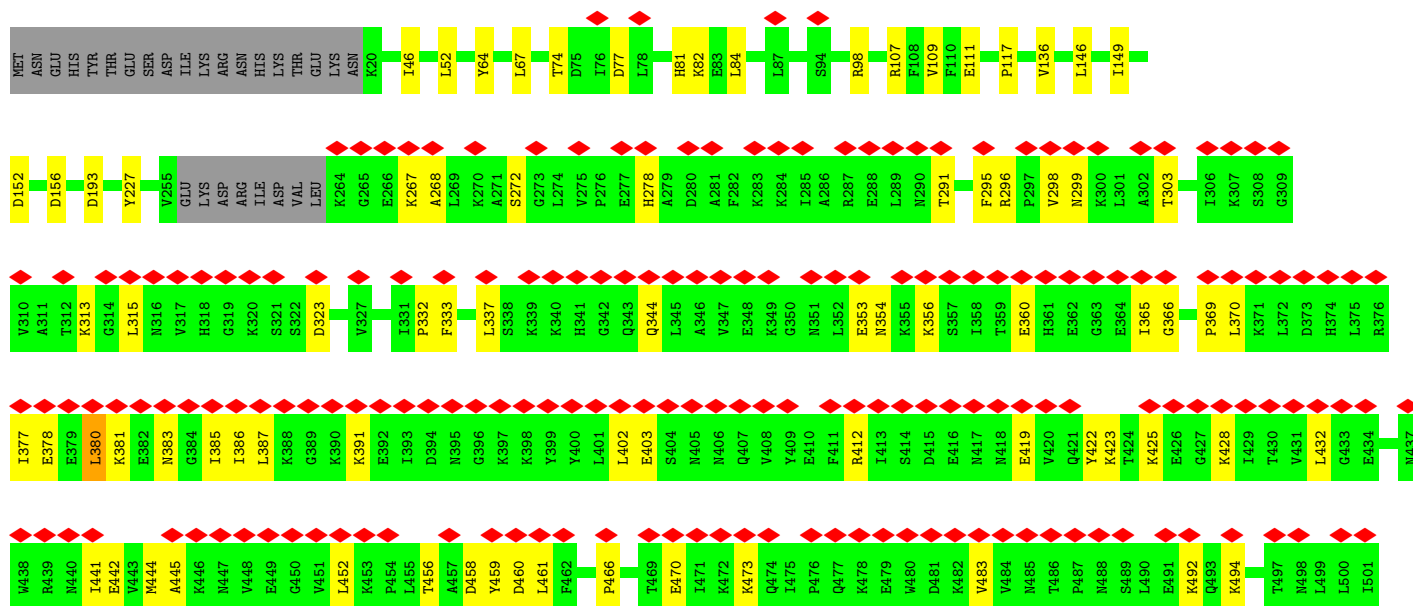
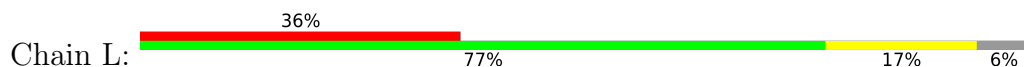
• Molecule 3: Calmodulin-sensitive adenylate cyclase

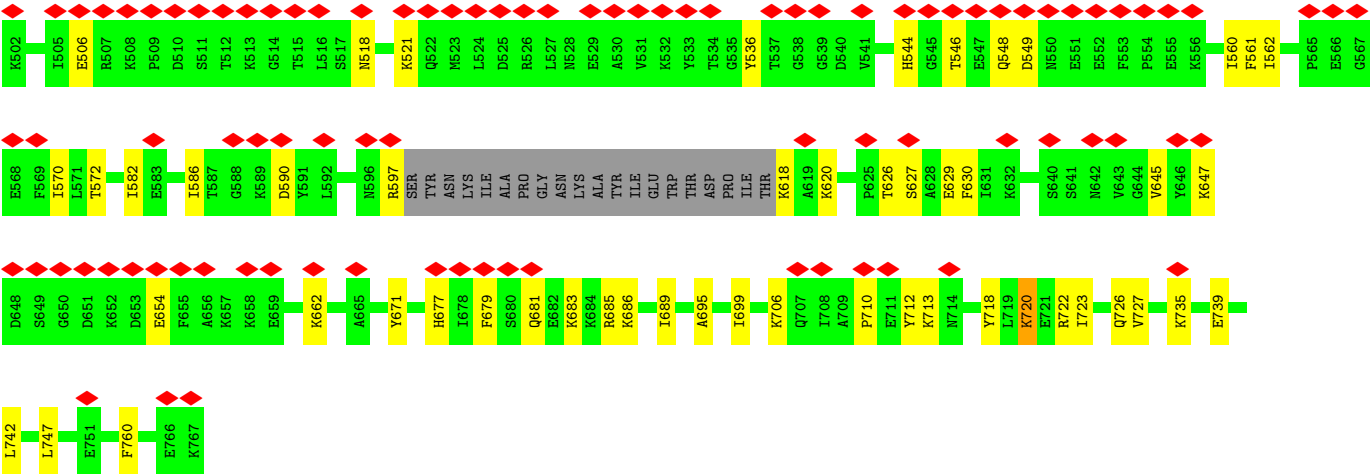
Chain K: 36% 76% 17% 6%





• Molecule 3: Calmodulin-sensitive adenylylate cyclase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	78465	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size (\AA)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/4346	0.60	4/5894 (0.1%)
1	C	0.45	0/4346	0.60	4/5894 (0.1%)
1	E	0.45	0/4346	0.60	4/5894 (0.1%)
1	G	0.45	0/4346	0.60	4/5894 (0.1%)
2	B	0.46	0/4355	0.55	0/5903
2	D	0.46	0/4355	0.55	0/5903
2	F	0.46	0/4355	0.55	0/5903
2	H	0.46	0/4355	0.55	0/5903
3	I	0.33	0/5980	0.56	2/8028 (0.0%)
3	J	0.33	0/5980	0.56	2/8028 (0.0%)
3	K	0.33	0/5980	0.56	2/8028 (0.0%)
3	L	0.33	0/5980	0.56	2/8028 (0.0%)
All	All	0.41	0/58724	0.57	24/79300 (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	1
1	C	0	1
1	E	0	1
1	G	0	1
3	I	0	2
3	J	0	2
3	K	0	2
3	L	0	2
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	GLN	O-C-N	-7.02	111.47	122.70
1	C	424	GLN	O-C-N	-7.02	111.47	122.70
1	E	424	GLN	O-C-N	-7.02	111.47	122.70
1	G	424	GLN	O-C-N	-7.02	111.47	122.70
3	I	380	LEU	CA-CB-CG	6.99	131.38	115.30
3	J	380	LEU	CA-CB-CG	6.99	131.38	115.30
3	K	380	LEU	CA-CB-CG	6.99	131.38	115.30
3	L	380	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	425	ASP	CB-CA-C	5.75	121.89	110.40
1	C	425	ASP	CB-CA-C	5.75	121.89	110.40
1	E	425	ASP	CB-CA-C	5.75	121.89	110.40
1	G	425	ASP	CB-CA-C	5.75	121.89	110.40
3	I	337	LEU	CA-CB-CG	5.61	128.21	115.30
3	J	337	LEU	CA-CB-CG	5.61	128.21	115.30
3	K	337	LEU	CA-CB-CG	5.61	128.21	115.30
3	L	337	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	424	GLN	CA-C-N	5.25	128.76	117.20
1	C	424	GLN	CA-C-N	5.25	128.76	117.20
1	E	424	GLN	CA-C-N	5.25	128.76	117.20
1	G	424	GLN	CA-C-N	5.25	128.76	117.20
1	A	685	LEU	CA-CB-CG	5.21	127.27	115.30
1	C	685	LEU	CA-CB-CG	5.21	127.27	115.30
1	E	685	LEU	CA-CB-CG	5.21	127.27	115.30
1	G	685	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ASN	Peptide
1	C	198	ASN	Peptide
1	E	198	ASN	Peptide
1	G	198	ASN	Peptide
3	I	156	ASP	Peptide
3	I	735	LYS	Peptide
3	J	156	ASP	Peptide
3	J	735	LYS	Peptide
3	K	156	ASP	Peptide
3	K	735	LYS	Peptide
3	L	156	ASP	Peptide
3	L	735	LYS	Peptide

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	4274	0	4224	58	0
1	C	4274	0	4224	57	0
1	E	4274	0	4224	59	0
1	G	4274	0	4224	56	0
2	B	4283	0	4250	46	0
2	D	4283	0	4250	43	0
2	F	4283	0	4250	49	0
2	H	4283	0	4250	51	0
3	I	5875	0	5901	82	0
3	J	5875	0	5901	83	0
3	K	5875	0	5901	81	0
3	L	5875	0	5901	76	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
All	All	57744	0	57500	727	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 6.

All (727) 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:C:424:GLN:HE21	1:C:424:GLN:HA	1.36	0.91
1:A:424:GLN:HE21	1:A:424:GLN:HA	1.36	0.91
1:G:424:GLN:HE21	1:G:424:GLN:HA	1.36	0.91
1:E:424:GLN:HA	1:E:424:GLN:HE21	1.36	0.91
3:K:618:LYS:N	3:K:718:TYR:HH	1.77	0.83
1:E:424:GLN:HA	1:E:424:GLN:NE2	1.95	0.82
1:G:424:GLN:HA	1:G:424:GLN:NE2	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:618:LYS:N	3:L:718:TYR:HH	1.79	0.81
1:A:424:GLN:HA	1:A:424:GLN:NE2	1.95	0.80
1:C:424:GLN:HA	1:C:424:GLN:NE2	1.95	0.80
3:J:618:LYS:N	3:J:718:TYR:HH	1.82	0.76
3:I:618:LYS:N	3:I:718:TYR:HH	1.87	0.71
3:I:689:ILE:HD12	3:I:727:VAL:HG23	1.76	0.67
3:J:689:ILE:HD12	3:J:727:VAL:HG23	1.76	0.67
3:K:689:ILE:HD12	3:K:727:VAL:HG23	1.76	0.67
3:I:296:ARG:HB3	3:I:460:ASP:HB3	1.75	0.67
3:L:689:ILE:HD12	3:L:727:VAL:HG23	1.76	0.67
3:J:296:ARG:HB3	3:J:460:ASP:HB3	1.75	0.67
3:L:296:ARG:HB3	3:L:460:ASP:HB3	1.75	0.67
2:H:648:ASP:HB3	2:H:651:GLY:H	1.61	0.66
3:K:296:ARG:HB3	3:K:460:ASP:HB3	1.75	0.66
2:F:648:ASP:HB3	2:F:651:GLY:H	1.61	0.65
2:D:648:ASP:HB3	2:D:651:GLY:H	1.61	0.65
2:B:648:ASP:HB3	2:B:651:GLY:H	1.61	0.65
2:B:643:ILE:HB	2:B:699:TYR:HB2	1.81	0.63
2:D:643:ILE:HB	2:D:699:TYR:HB2	1.81	0.63
2:F:646:ILE:HD11	2:F:687:LEU:HD11	1.79	0.63
2:H:646:ILE:HD11	2:H:687:LEU:HD11	1.79	0.63
2:B:646:ILE:HD11	2:B:687:LEU:HD11	1.79	0.63
2:D:340:LEU:HD23	2:D:342:GLY:H	1.64	0.62
2:B:340:LEU:HD23	2:B:342:GLY:H	1.64	0.62
3:J:645:VAL:H	3:J:712:TYR:HD2	1.47	0.62
2:F:643:ILE:HB	2:F:699:TYR:HB2	1.81	0.62
2:H:643:ILE:HB	2:H:699:TYR:HB2	1.81	0.62
3:K:645:VAL:H	3:K:712:TYR:HD2	1.47	0.62
2:D:646:ILE:HD11	2:D:687:LEU:HD11	1.79	0.62
1:A:232:PRO:HD3	1:A:480:VAL:HG11	1.82	0.62
1:C:232:PRO:HD3	1:C:480:VAL:HG11	1.82	0.62
1:C:365:ARG:HG2	1:C:412:PRO:HD2	1.82	0.62
2:H:340:LEU:HD23	2:H:342:GLY:H	1.64	0.62
3:L:645:VAL:H	3:L:712:TYR:HD2	1.47	0.61
1:G:232:PRO:HD3	1:G:480:VAL:HG11	1.82	0.61
2:H:406:ALA:HB3	2:H:409:ASN:HD22	1.66	0.61
2:D:406:ALA:HB3	2:D:409:ASN:HD22	1.66	0.61
1:A:365:ARG:HG2	1:A:412:PRO:HD2	1.82	0.61
1:E:179:ASP:N	1:E:179:ASP:OD1	2.33	0.61
2:B:406:ALA:HB3	2:B:409:ASN:HD22	1.66	0.61
1:E:232:PRO:HD3	1:E:480:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:406:ALA:HB3	2:F:409:ASN:HD22	1.66	0.61
1:C:179:ASP:OD1	1:C:179:ASP:N	2.33	0.61
1:E:365:ARG:HG2	1:E:412:PRO:HD2	1.82	0.61
2:F:331:THR:HG22	2:F:449:ARG:HG3	1.83	0.61
2:B:331:THR:HG22	2:B:449:ARG:HG3	1.83	0.60
2:F:340:LEU:HD23	2:F:342:GLY:H	1.64	0.60
1:G:365:ARG:HG2	1:G:412:PRO:HD2	1.82	0.60
2:H:331:THR:HG22	2:H:449:ARG:HG3	1.83	0.60
3:I:645:VAL:H	3:I:712:TYR:HD2	1.47	0.60
3:J:67:LEU:HD22	3:J:117:PRO:HG3	1.84	0.60
2:D:331:THR:HG22	2:D:449:ARG:HG3	1.83	0.60
1:E:307:ALA:H	2:F:670:GLN:HB2	1.67	0.60
3:I:82:LYS:NZ	3:I:739:GLU:OE2	2.34	0.60
3:L:67:LEU:HD22	3:L:117:PRO:HG3	1.84	0.60
1:G:307:ALA:H	2:H:670:GLN:HB2	1.67	0.59
3:I:67:LEU:HD22	3:I:117:PRO:HG3	1.84	0.59
3:J:332:PRO:O	3:J:354:ASN:ND2	2.35	0.59
3:L:332:PRO:O	3:L:354:ASN:ND2	2.35	0.59
3:I:344:GLN:HB3	3:I:432:LEU:HD13	1.84	0.59
3:K:332:PRO:O	3:K:354:ASN:ND2	2.35	0.59
3:K:67:LEU:HD22	3:K:117:PRO:HG3	1.84	0.59
3:K:344:GLN:HB3	3:K:432:LEU:HD13	1.84	0.59
1:A:272:SER:HB3	1:A:288:THR:HG22	1.84	0.59
2:B:524:LYS:HD2	2:B:579:ASP:HB3	1.85	0.59
2:D:207:ILE:H	2:D:211:HIS:HD2	1.50	0.59
3:I:332:PRO:O	3:I:354:ASN:ND2	2.35	0.59
1:A:179:ASP:OD1	1:A:179:ASP:N	2.33	0.59
1:E:272:SER:HB3	1:E:288:THR:HG22	1.84	0.59
3:J:679:PHE:HB3	3:J:683:LYS:HG3	1.84	0.59
3:K:82:LYS:NZ	3:K:739:GLU:OE2	2.34	0.59
3:L:546:THR:H	3:L:549:ASP:HB2	1.68	0.59
2:F:207:ILE:H	2:F:211:HIS:HD2	1.50	0.59
2:D:232:PRO:HD3	2:D:480:VAL:HG11	1.85	0.59
2:D:524:LYS:HD2	2:D:579:ASP:HB3	1.85	0.59
1:E:423:ALA:O	1:E:425:ASP:OD2	2.21	0.59
3:I:546:THR:H	3:I:549:ASP:HB2	1.68	0.59
3:K:546:THR:H	3:K:549:ASP:HB2	1.68	0.59
1:C:459:ILE:HD12	1:C:475:SER:HB3	1.85	0.58
2:F:232:PRO:HD3	2:F:480:VAL:HG11	1.85	0.58
2:H:232:PRO:HD3	2:H:480:VAL:HG11	1.85	0.58
1:C:307:ALA:H	2:D:670:GLN:HB2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ALA:H	2:B:670:GLN:HB2	1.67	0.58
1:C:423:ALA:O	1:C:425:ASP:OD2	2.21	0.58
2:H:524:LYS:HD2	2:H:579:ASP:HB3	1.85	0.58
3:J:82:LYS:NZ	3:J:739:GLU:OE2	2.34	0.58
3:J:344:GLN:HB3	3:J:432:LEU:HD13	1.84	0.58
3:I:679:PHE:HB3	3:I:683:LYS:HG3	1.84	0.58
3:L:82:LYS:NZ	3:L:739:GLU:OE2	2.34	0.58
1:G:423:ALA:O	1:G:425:ASP:OD2	2.21	0.58
2:D:365:ARG:HH21	2:D:418:PRO:HG3	1.69	0.58
2:B:232:PRO:HD3	2:B:480:VAL:HG11	1.85	0.58
1:A:459:ILE:HD12	1:A:475:SER:HB3	1.85	0.58
1:E:459:ILE:HD12	1:E:475:SER:HB3	1.85	0.58
3:L:679:PHE:HB3	3:L:683:LYS:HG3	1.84	0.58
1:A:423:ALA:O	1:A:425:ASP:OD2	2.21	0.58
1:C:272:SER:HB3	1:C:288:THR:HG22	1.84	0.58
2:F:365:ARG:HH21	2:F:418:PRO:HG3	1.69	0.58
3:K:620:LYS:HG3	3:K:722:ARG:HH11	1.69	0.58
3:L:620:LYS:HG3	3:L:722:ARG:HH11	1.69	0.57
2:F:524:LYS:HD2	2:F:579:ASP:HB3	1.85	0.57
1:G:272:SER:HB3	1:G:288:THR:HG22	1.84	0.57
3:K:679:PHE:HB3	3:K:683:LYS:HG3	1.84	0.57
1:A:592:ARG:NH1	1:A:602:ASN:OD1	2.37	0.57
1:E:592:ARG:NH1	1:E:602:ASN:OD1	2.37	0.57
1:G:592:ARG:NH1	1:G:602:ASN:OD1	2.37	0.57
2:H:207:ILE:H	2:H:211:HIS:HD2	1.50	0.57
2:B:207:ILE:H	2:B:211:HIS:HD2	1.50	0.57
3:I:620:LYS:HG3	3:I:722:ARG:HH11	1.69	0.57
3:J:620:LYS:HG3	3:J:722:ARG:HH11	1.69	0.57
3:L:344:GLN:HB3	3:L:432:LEU:HD13	1.84	0.57
1:C:303:VAL:O	2:D:670:GLN:NE2	2.37	0.57
1:C:592:ARG:NH1	1:C:602:ASN:OD1	2.37	0.57
3:J:546:THR:H	3:J:549:ASP:HB2	1.68	0.57
1:G:303:VAL:O	2:H:670:GLN:NE2	2.37	0.57
1:G:179:ASP:N	1:G:179:ASP:OD1	2.33	0.56
1:G:459:ILE:HD12	1:G:475:SER:HB3	1.85	0.56
2:H:344:ARG:O	2:H:349:THR:OG1	2.23	0.56
2:B:365:ARG:HH21	2:B:418:PRO:HG3	1.69	0.56
2:H:365:ARG:HH21	2:H:418:PRO:HG3	1.69	0.56
2:B:234:SER:OG	2:B:235:ASP:N	2.39	0.56
2:F:234:SER:OG	2:F:235:ASP:N	2.39	0.56
2:D:344:ARG:O	2:D:349:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:ARG:O	2:F:349:THR:OG1	2.23	0.56
1:G:234:SER:OG	1:G:235:ASP:N	2.40	0.56
2:D:234:SER:OG	2:D:235:ASP:N	2.39	0.55
2:H:234:SER:OG	2:H:235:ASP:N	2.39	0.55
3:J:483:VAL:HA	3:J:492:LYS:HZ1	1.72	0.55
2:B:344:ARG:O	2:B:349:THR:OG1	2.23	0.55
1:E:234:SER:OG	1:E:235:ASP:N	2.40	0.55
1:C:234:SER:OG	1:C:235:ASP:N	2.40	0.54
2:H:693:ASN:O	2:H:695:LYS:NZ	2.40	0.54
3:K:483:VAL:HA	3:K:492:LYS:HZ1	1.72	0.54
3:L:46:ILE:HD11	3:L:742:LEU:HD12	1.89	0.54
1:A:344:ARG:HB3	1:A:345:THR:HG23	1.90	0.54
2:F:693:ASN:O	2:F:695:LYS:NZ	2.40	0.54
1:G:620:ILE:HB	1:G:628:LEU:HB3	1.89	0.54
1:A:303:VAL:O	2:B:670:GLN:NE2	2.37	0.54
1:C:344:ARG:O	1:C:349:THR:OG1	2.26	0.54
1:G:344:ARG:HB3	1:G:345:THR:HG23	1.90	0.54
2:B:693:ASN:O	2:B:695:LYS:NZ	2.40	0.54
1:C:620:ILE:HB	1:C:628:LEU:HB3	1.89	0.54
2:D:693:ASN:O	2:D:695:LYS:NZ	2.40	0.54
1:E:303:VAL:O	2:F:670:GLN:NE2	2.37	0.54
2:F:337:SER:OG	2:F:338:LEU:N	2.41	0.54
3:I:385:ILE:HG23	3:I:386:ILE:HG12	1.90	0.54
1:A:620:ILE:HB	1:A:628:LEU:HB3	1.89	0.54
1:E:344:ARG:O	1:E:349:THR:OG1	2.26	0.54
3:L:298:VAL:HG21	3:L:459:TYR:HA	1.90	0.54
2:D:337:SER:OG	2:D:338:LEU:N	2.41	0.53
3:I:46:ILE:HD11	3:I:742:LEU:HD12	1.89	0.53
3:J:387:LEU:HD22	3:J:403:GLU:HB2	1.90	0.53
3:K:299:ASN:ND2	3:K:323:ASP:OD1	2.42	0.53
3:K:506:GLU:OE2	3:K:518:ASN:ND2	2.42	0.53
2:B:337:SER:OG	2:B:338:LEU:N	2.41	0.53
1:C:344:ARG:HB3	1:C:345:THR:HG23	1.90	0.53
3:J:299:ASN:ND2	3:J:323:ASP:OD1	2.42	0.53
1:A:554:PHE:HB3	1:A:558:THR:HB	1.90	0.53
1:E:620:ILE:HB	1:E:628:LEU:HB3	1.89	0.53
1:G:554:PHE:HB3	1:G:558:THR:HB	1.90	0.53
3:L:483:VAL:HA	3:L:492:LYS:HZ1	1.72	0.53
3:I:298:VAL:HG21	3:I:459:TYR:HA	1.90	0.53
1:A:344:ARG:O	1:A:349:THR:OG1	2.26	0.53
3:J:46:ILE:HD11	3:J:742:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:337:SER:OG	2:H:338:LEU:N	2.41	0.53
3:I:483:VAL:HA	3:I:492:LYS:HZ1	1.72	0.53
3:I:506:GLU:OE2	3:I:518:ASN:ND2	2.42	0.53
3:J:506:GLU:OE2	3:J:518:ASN:ND2	2.42	0.53
3:K:46:ILE:HD11	3:K:742:LEU:HD12	1.89	0.53
3:L:295:PHE:HA	3:L:461:LEU:HA	1.91	0.53
3:K:295:PHE:HA	3:K:461:LEU:HA	1.91	0.53
3:J:295:PHE:HA	3:J:461:LEU:HA	1.91	0.53
3:L:299:ASN:ND2	3:L:323:ASP:OD1	2.42	0.53
1:E:554:PHE:HB3	1:E:558:THR:HB	1.90	0.53
3:I:387:LEU:HD22	3:I:403:GLU:HB2	1.90	0.53
3:K:385:ILE:HG23	3:K:386:ILE:HG12	1.90	0.53
3:L:387:LEU:HD22	3:L:403:GLU:HB2	1.90	0.53
1:A:234:SER:OG	1:A:235:ASP:N	2.40	0.52
3:L:506:GLU:OE2	3:L:518:ASN:ND2	2.42	0.52
1:E:344:ARG:HB3	1:E:345:THR:HG23	1.90	0.52
3:I:299:ASN:ND2	3:I:323:ASP:OD1	2.42	0.52
1:E:368:ASN:HB2	1:E:405:LEU:HG	1.92	0.52
3:J:298:VAL:HG21	3:J:459:TYR:HA	1.90	0.52
3:L:385:ILE:HG23	3:L:386:ILE:HG12	1.90	0.52
3:I:295:PHE:HA	3:I:461:LEU:HA	1.91	0.52
3:L:385:ILE:HD11	3:L:402:LEU:HD13	1.92	0.52
1:A:368:ASN:HB2	1:A:405:LEU:HG	1.92	0.52
1:C:368:ASN:HB2	1:C:405:LEU:HG	1.92	0.52
1:G:344:ARG:O	1:G:349:THR:OG1	2.26	0.52
3:K:387:LEU:HD22	3:K:403:GLU:HB2	1.90	0.52
1:E:608:ASP:OD1	1:E:608:ASP:N	2.41	0.52
3:J:385:ILE:HG23	3:J:386:ILE:HG12	1.90	0.52
3:K:298:VAL:HG21	3:K:459:TYR:HA	1.90	0.52
1:G:368:ASN:HB2	1:G:405:LEU:HG	1.92	0.52
3:I:385:ILE:HD11	3:I:402:LEU:HD13	1.92	0.52
3:K:385:ILE:HD11	3:K:402:LEU:HD13	1.92	0.52
2:D:695:LYS:HE3	2:D:730:LYS:HD3	1.92	0.52
2:F:695:LYS:HE3	2:F:730:LYS:HD3	1.92	0.52
2:H:592:ARG:NH1	2:H:602:ASN:OD1	2.43	0.52
3:J:385:ILE:HD11	3:J:402:LEU:HD13	1.92	0.52
3:K:107:ARG:NH2	3:K:109:VAL:O	2.43	0.52
1:C:554:PHE:HB3	1:C:558:THR:HB	1.90	0.51
2:F:592:ARG:NH1	2:F:602:ASN:OD1	2.43	0.51
2:H:695:LYS:HE3	2:H:730:LYS:HD3	1.92	0.51
3:J:77:ASP:HB2	3:J:81:HIS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:683:LYS:HD3	3:L:686:LYS:HD3	1.93	0.51
3:I:77:ASP:HB2	3:I:81:HIS:HB2	1.92	0.51
3:J:626:THR:OG1	3:J:627:SER:N	2.44	0.51
2:D:189:VAL:HG21	1:E:200:ARG:HH11	1.76	0.51
1:G:181:ASP:OD1	1:G:181:ASP:N	2.41	0.51
3:K:412:ARG:HB2	3:K:422:TYR:HA	1.93	0.51
2:B:695:LYS:HE3	2:B:730:LYS:HD3	1.92	0.51
3:I:107:ARG:NH2	3:I:109:VAL:O	2.43	0.51
3:J:193:ASP:OD1	3:J:193:ASP:N	2.44	0.51
3:K:626:THR:OG1	3:K:627:SER:N	2.44	0.51
3:L:77:ASP:HB2	3:L:81:HIS:HB2	1.92	0.51
3:K:193:ASP:OD1	3:K:193:ASP:N	2.44	0.50
2:D:196:VAL:HG22	2:D:201:THR:HG22	1.94	0.50
3:I:683:LYS:HD3	3:I:686:LYS:HD3	1.93	0.50
3:J:291:THR:HG23	3:J:466:PRO:HB3	1.93	0.50
1:A:623:SER:OG	1:A:624:THR:N	2.45	0.50
2:B:592:ARG:NH1	2:B:602:ASN:OD1	2.43	0.50
3:K:291:THR:HG23	3:K:466:PRO:HB3	1.93	0.50
3:L:313:LYS:HG2	3:L:458:ASP:HB2	1.94	0.50
1:A:326:ASN:OD1	1:A:490:ARG:NH2	2.44	0.50
1:A:337:SER:OG	1:A:338:LEU:N	2.45	0.50
1:C:608:ASP:OD1	1:C:608:ASP:N	2.41	0.50
2:D:592:ARG:NH1	2:D:602:ASN:OD1	2.43	0.50
3:I:291:THR:HG23	3:I:466:PRO:HB3	1.93	0.50
3:J:377:ILE:HD11	3:J:385:ILE:HG12	1.94	0.50
1:A:200:ARG:HH11	2:H:189:VAL:HG21	1.76	0.50
1:C:623:SER:OG	1:C:624:THR:N	2.45	0.50
3:I:313:LYS:HG2	3:I:458:ASP:HB2	1.94	0.50
3:I:548:GLN:NE2	3:I:629:GLU:OE2	2.45	0.50
3:K:313:LYS:HG2	3:K:458:ASP:HB2	1.94	0.50
3:L:291:THR:HG23	3:L:466:PRO:HB3	1.93	0.50
1:C:337:SER:OG	1:C:338:LEU:N	2.45	0.50
3:J:107:ARG:NH2	3:J:109:VAL:O	2.43	0.50
3:J:313:LYS:HG2	3:J:458:ASP:HB2	1.94	0.50
3:K:377:ILE:HD11	3:K:385:ILE:HG12	1.94	0.50
3:K:683:LYS:HD3	3:K:686:LYS:HD3	1.93	0.50
3:K:747:LEU:HD11	3:K:760:PHE:HD1	1.77	0.50
2:B:196:VAL:HG22	2:B:201:THR:HG22	1.94	0.50
1:C:326:ASN:OD1	1:C:490:ARG:NH2	2.44	0.50
2:D:195:ASP:OD2	2:D:214:LYS:NZ	2.45	0.50
1:E:326:ASN:OD1	1:E:490:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:747:LEU:HD11	3:L:760:PHE:HD1	1.77	0.50
2:B:189:VAL:HG21	1:C:200:ARG:HH11	1.76	0.50
2:D:498:LEU:HB2	2:D:637:LYS:HD3	1.94	0.50
1:E:337:SER:OG	1:E:338:LEU:N	2.45	0.50
2:F:196:VAL:HG22	2:F:201:THR:HG22	1.94	0.50
1:G:623:SER:OG	1:G:624:THR:N	2.45	0.50
3:I:377:ILE:HD11	3:I:385:ILE:HG12	1.94	0.50
3:L:412:ARG:HB2	3:L:422:TYR:HA	1.93	0.50
3:L:548:GLN:NE2	3:L:629:GLU:OE2	2.45	0.50
3:L:626:THR:OG1	3:L:627:SER:N	2.44	0.50
3:J:412:ARG:HB2	3:J:422:TYR:HA	1.93	0.50
3:J:548:GLN:NE2	3:J:629:GLU:OE2	2.45	0.50
3:K:77:ASP:HB2	3:K:81:HIS:HB2	1.92	0.50
3:K:548:GLN:NE2	3:K:629:GLU:OE2	2.45	0.50
1:E:623:SER:OG	1:E:624:THR:N	2.45	0.49
2:H:498:LEU:HB2	2:H:637:LYS:HD3	1.94	0.49
3:I:152:ASP:OD1	3:I:152:ASP:N	2.43	0.49
3:J:671:TYR:OH	3:J:726:GLN:NE2	2.45	0.49
2:B:195:ASP:OD2	2:B:214:LYS:NZ	2.45	0.49
2:B:498:LEU:HB2	2:B:637:LYS:HD3	1.94	0.49
2:F:498:LEU:HB2	2:F:637:LYS:HD3	1.94	0.49
2:F:195:ASP:OD2	2:F:214:LYS:NZ	2.45	0.49
3:I:295:PHE:HB2	3:I:561:PHE:HB3	1.95	0.49
3:J:683:LYS:HD3	3:J:686:LYS:HD3	1.93	0.49
3:K:268:ALA:O	3:K:272:SER:HB3	2.13	0.49
2:F:189:VAL:HG21	1:G:200:ARG:HH11	1.76	0.49
3:I:268:ALA:O	3:I:272:SER:HB3	2.13	0.49
3:I:671:TYR:OH	3:I:726:GLN:NE2	2.45	0.49
3:J:230:ASP:OD1	3:J:230:ASP:N	2.44	0.49
3:K:412:ARG:HH21	3:K:423:LYS:HB3	1.78	0.49
3:L:412:ARG:HH21	3:L:423:LYS:HB3	1.78	0.49
3:I:412:ARG:HB2	3:I:422:TYR:HA	1.93	0.49
3:L:377:ILE:HD11	3:L:385:ILE:HG12	1.94	0.49
3:L:107:ARG:NH2	3:L:109:VAL:O	2.43	0.49
3:L:295:PHE:HB2	3:L:561:PHE:HB3	1.95	0.49
2:H:196:VAL:HG22	2:H:201:THR:HG22	1.94	0.49
3:J:597:ARG:HB2	3:J:626:THR:HG21	1.95	0.49
3:K:671:TYR:OH	3:K:726:GLN:NE2	2.45	0.49
2:H:195:ASP:OD2	2:H:214:LYS:NZ	2.45	0.49
3:I:193:ASP:OD1	3:I:193:ASP:N	2.44	0.49
3:I:747:LEU:HD11	3:I:760:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:671:TYR:OH	3:L:726:GLN:NE2	2.45	0.49
3:I:626:THR:OG1	3:I:627:SER:N	2.44	0.49
3:J:295:PHE:HB2	3:J:561:PHE:HB3	1.95	0.49
3:L:268:ALA:O	3:L:272:SER:HB3	2.13	0.49
3:J:268:ALA:O	3:J:272:SER:HB3	2.13	0.49
3:K:597:ARG:HB2	3:K:626:THR:HG21	1.95	0.49
1:A:422:ASN:ND2	1:A:430:THR:O	2.39	0.48
1:C:424:GLN:NE2	1:C:424:GLN:CA	2.73	0.48
2:F:661:ASP:OD1	2:F:661:ASP:N	2.45	0.48
3:I:597:ARG:HB2	3:I:626:THR:HG21	1.95	0.48
3:J:747:LEU:HD11	3:J:760:PHE:HD1	1.77	0.48
3:K:562:ILE:HB	3:K:570:ILE:HB	1.95	0.48
3:J:412:ARG:HH21	3:J:423:LYS:HB3	1.78	0.48
3:K:295:PHE:HB2	3:K:561:PHE:HB3	1.95	0.48
3:I:412:ARG:HH21	3:I:423:LYS:HB3	1.78	0.48
3:L:152:ASP:OD1	3:L:152:ASP:N	2.43	0.48
1:C:614:GLU:HG2	1:C:617:ARG:HH22	1.78	0.48
1:E:614:GLU:HG2	1:E:617:ARG:HH22	1.78	0.48
1:G:614:GLU:HG2	1:G:617:ARG:HH22	1.78	0.48
1:A:207:ILE:H	1:A:211:HIS:HD2	1.62	0.48
1:C:207:ILE:H	1:C:211:HIS:HD2	1.62	0.48
1:E:524:LYS:HD2	1:E:579:ASP:HB3	1.95	0.48
1:E:197:LYS:HD2	1:E:197:LYS:HA	1.76	0.48
1:G:337:SER:OG	1:G:338:LEU:N	2.45	0.48
3:L:562:ILE:HB	3:L:570:ILE:HB	1.95	0.48
2:B:178:ARG:NH1	2:B:224:GLU:OE2	2.47	0.48
2:D:429:SER:O	2:D:431:PRO:HD3	2.14	0.48
1:G:422:ASN:ND2	1:G:430:THR:O	2.39	0.48
3:J:562:ILE:HB	3:J:570:ILE:HB	1.95	0.48
3:L:597:ARG:HB2	3:L:626:THR:HG21	1.95	0.48
1:A:183:ILE:HG23	1:A:203:LEU:HD21	1.95	0.48
3:I:52:LEU:HD21	3:I:136:VAL:HG11	1.96	0.48
3:L:193:ASP:OD1	3:L:193:ASP:N	2.44	0.48
2:D:484:ILE:O	2:D:488:THR:OG1	2.28	0.47
1:G:524:LYS:HD2	1:G:579:ASP:HB3	1.95	0.47
2:D:178:ARG:NH1	2:D:224:GLU:OE2	2.47	0.47
2:D:179:ASP:OD1	2:D:179:ASP:N	2.37	0.47
3:K:560:ILE:H	3:K:572:THR:HG22	1.79	0.47
1:C:524:LYS:HD2	1:C:579:ASP:HB3	1.95	0.47
1:E:422:ASN:ND2	1:E:430:THR:O	2.39	0.47
3:L:52:LEU:HD21	3:L:136:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:ILE:H	1:G:211:HIS:HD2	1.62	0.47
1:A:614:GLU:HG2	1:A:617:ARG:HH22	1.78	0.47
1:E:207:ILE:H	1:E:211:HIS:HD2	1.62	0.47
2:F:429:SER:O	2:F:431:PRO:HD3	2.14	0.47
2:H:711:SER:HB2	2:H:715:ASP:HB2	1.97	0.47
3:I:365:ILE:HD11	3:I:444:MET:HG3	1.97	0.47
3:J:52:LEU:HD21	3:J:136:VAL:HG11	1.96	0.47
3:K:52:LEU:HD21	3:K:136:VAL:HG11	1.96	0.47
3:K:366:GLY:H	3:K:445:ALA:HB3	1.79	0.47
1:A:524:LYS:HD2	1:A:579:ASP:HB3	1.95	0.47
2:H:178:ARG:NH1	2:H:224:GLU:OE2	2.47	0.47
3:I:562:ILE:HB	3:I:570:ILE:HB	1.95	0.47
3:J:365:ILE:HD11	3:J:444:MET:HG3	1.97	0.47
3:K:365:ILE:HD11	3:K:444:MET:HG3	1.97	0.47
2:B:429:SER:O	2:B:431:PRO:HD3	2.14	0.47
2:B:711:SER:HB2	2:B:715:ASP:HB2	1.97	0.47
1:C:183:ILE:HG23	1:C:203:LEU:HD21	1.95	0.47
2:F:178:ARG:NH1	2:F:224:GLU:OE2	2.47	0.47
2:H:554:PHE:HB3	2:H:558:THR:HB	1.97	0.47
3:K:152:ASP:OD1	3:K:152:ASP:N	2.43	0.47
3:L:365:ILE:HD11	3:L:444:MET:HG3	1.97	0.47
1:G:344:ARG:HD3	1:G:659:ARG:HH12	1.80	0.47
1:G:608:ASP:OD1	1:G:608:ASP:N	2.41	0.47
3:L:560:ILE:H	3:L:572:THR:HG22	1.79	0.47
1:E:183:ILE:HG23	1:E:203:LEU:HD21	1.95	0.47
1:E:484:ILE:O	1:E:488:THR:OG1	2.30	0.47
2:B:361:ASN:ND2	2:B:421:LEU:O	2.48	0.47
2:B:554:PHE:HB3	2:B:558:THR:HB	1.97	0.47
1:C:647:GLU:HG2	1:C:651:GLY:HA2	1.97	0.47
1:G:183:ILE:HG23	1:G:203:LEU:HD21	1.95	0.47
3:J:560:ILE:H	3:J:572:THR:HG22	1.79	0.47
1:C:484:ILE:O	1:C:488:THR:OG1	2.30	0.46
2:F:711:SER:HB2	2:F:715:ASP:HB2	1.97	0.46
2:H:429:SER:O	2:H:431:PRO:HD3	2.14	0.46
2:B:365:ARG:HH12	2:B:414:LYS:HA	1.81	0.46
1:E:713:ASN:OD1	1:E:713:ASN:N	2.49	0.46
3:L:366:GLY:H	3:L:445:ALA:HB3	1.79	0.46
2:B:484:ILE:O	2:B:488:THR:OG1	2.28	0.46
2:D:554:PHE:HB3	2:D:558:THR:HB	1.97	0.46
1:E:344:ARG:HD3	1:E:659:ARG:HH12	1.80	0.46
1:G:326:ASN:OD1	1:G:490:ARG:NH2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:366:GLY:H	3:J:445:ALA:HB3	1.79	0.46
2:D:361:ASN:ND2	2:D:421:LEU:O	2.48	0.46
1:G:195:ASP:OD2	3:L:227:TYR:OH	2.30	0.46
2:H:361:ASN:ND2	2:H:421:LEU:O	2.48	0.46
1:C:383:LEU:HD21	1:C:448:LEU:HD13	1.98	0.46
1:E:490:ARG:HG2	1:E:588:ASN:HD22	1.80	0.46
3:I:366:GLY:H	3:I:445:ALA:HB3	1.79	0.46
3:L:64:TYR:OH	3:L:111:GLU:OE2	2.29	0.46
3:L:582:ILE:HG23	3:L:586:ILE:HD12	1.98	0.46
1:C:197:LYS:HD2	1:C:197:LYS:HA	1.76	0.46
2:F:361:ASN:ND2	2:F:421:LEU:O	2.48	0.46
1:A:647:GLU:HG2	1:A:651:GLY:HA2	1.97	0.46
1:E:383:LEU:HD21	1:E:448:LEU:HD13	1.98	0.46
1:E:647:GLU:HG2	1:E:651:GLY:HA2	1.97	0.46
1:E:648:ASP:HB3	1:E:651:GLY:H	1.81	0.46
2:F:554:PHE:HB3	2:F:558:THR:HB	1.97	0.46
1:G:490:ARG:HG2	1:G:588:ASN:HD22	1.80	0.46
3:I:582:ILE:HG23	3:I:586:ILE:HD12	1.98	0.46
1:A:344:ARG:HD3	1:A:659:ARG:HH12	1.80	0.46
1:A:457:GLY:O	1:A:476:ASN:ND2	2.49	0.46
1:C:344:ARG:HD3	1:C:659:ARG:HH12	1.80	0.46
2:D:711:SER:HB2	2:D:715:ASP:HB2	1.97	0.46
3:J:470:GLU:HA	3:J:473:LYS:HG2	1.98	0.46
3:K:380:LEU:O	3:K:383:ASN:ND2	2.49	0.46
1:A:648:ASP:HB3	1:A:651:GLY:H	1.81	0.46
2:B:301:SER:OG	2:B:302:GLU:N	2.49	0.46
2:F:459:ILE:HD12	2:F:475:SER:HB3	1.98	0.46
2:H:301:SER:OG	2:H:302:GLU:N	2.49	0.46
1:C:195:ASP:OD2	3:J:227:TYR:OH	2.30	0.45
3:I:560:ILE:H	3:I:572:THR:HG22	1.79	0.45
3:J:378:GLU:HA	3:J:381:LYS:HG2	1.98	0.45
3:K:230:ASP:OD1	3:K:230:ASP:N	2.44	0.45
3:L:299:ASN:O	3:L:303:THR:OG1	2.34	0.45
2:H:365:ARG:HH12	2:H:414:LYS:HA	1.81	0.45
2:H:459:ILE:HD12	2:H:475:SER:HB3	1.98	0.45
3:I:356:LYS:O	3:I:360:GLU:HB2	2.16	0.45
3:J:356:LYS:O	3:J:360:GLU:HB2	2.16	0.45
3:J:369:PRO:HG3	3:J:419:GLU:HG3	1.98	0.45
3:J:582:ILE:HG23	3:J:586:ILE:HD12	1.98	0.45
3:K:470:GLU:HA	3:K:473:LYS:HG2	1.98	0.45
3:L:470:GLU:HA	3:L:473:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ASP:OD1	1:A:608:ASP:N	2.41	0.45
1:E:457:GLY:O	1:E:476:ASN:ND2	2.49	0.45
2:F:484:ILE:O	2:F:488:THR:OG1	2.28	0.45
1:G:383:LEU:HD21	1:G:448:LEU:HD13	1.98	0.45
3:J:380:LEU:O	3:J:383:ASN:ND2	2.49	0.45
3:K:378:GLU:HA	3:K:381:LYS:HG2	1.98	0.45
1:C:422:ASN:ND2	1:C:430:THR:O	2.39	0.45
2:H:179:ASP:OD1	2:H:179:ASP:N	2.37	0.45
1:G:647:GLU:HG2	1:G:651:GLY:HA2	1.97	0.45
2:H:484:ILE:O	2:H:488:THR:OG1	2.28	0.45
3:L:356:LYS:O	3:L:360:GLU:HB2	2.16	0.45
3:L:380:LEU:O	3:L:383:ASN:ND2	2.49	0.45
1:A:424:GLN:NE2	1:A:424:GLN:CA	2.73	0.45
2:D:365:ARG:HH12	2:D:414:LYS:HA	1.81	0.45
2:F:365:ARG:HH12	2:F:414:LYS:HA	1.81	0.45
1:G:648:ASP:HB3	1:G:651:GLY:H	1.81	0.45
3:I:470:GLU:HA	3:I:473:LYS:HG2	1.98	0.45
3:J:152:ASP:OD1	3:J:152:ASP:N	2.43	0.45
1:C:490:ARG:HG2	1:C:588:ASN:HD22	1.80	0.45
1:C:713:ASN:OD1	1:C:713:ASN:N	2.49	0.45
2:D:459:ILE:HD12	2:D:475:SER:HB3	1.98	0.45
1:A:383:LEU:HD21	1:A:448:LEU:HD13	1.98	0.45
2:D:301:SER:OG	2:D:302:GLU:N	2.49	0.45
1:E:587:MET:O	1:E:588:ASN:ND2	2.50	0.45
3:I:380:LEU:O	3:I:383:ASN:ND2	2.49	0.45
3:K:356:LYS:O	3:K:360:GLU:HB2	2.16	0.45
3:K:369:PRO:HG3	3:K:419:GLU:HG3	1.98	0.45
1:C:362:ALA:HB3	1:C:421:LEU:HD12	1.99	0.45
1:E:362:ALA:HB3	1:E:421:LEU:HD12	1.99	0.45
2:F:344:ARG:HB3	2:F:345:THR:HG23	1.99	0.45
2:H:365:ARG:HB2	2:H:412:PRO:HD2	1.99	0.45
3:I:299:ASN:O	3:I:303:THR:OG1	2.34	0.45
1:C:648:ASP:HB3	1:C:651:GLY:H	1.81	0.44
2:D:344:ARG:HB3	2:D:345:THR:HG23	1.99	0.44
3:K:582:ILE:HG23	3:K:586:ILE:HD12	1.98	0.44
2:B:459:ILE:HD12	2:B:475:SER:HB3	1.98	0.44
3:I:378:GLU:HA	3:I:381:LYS:HG2	1.98	0.44
3:L:378:GLU:HA	3:L:381:LYS:HG2	1.98	0.44
1:G:587:MET:O	1:G:588:ASN:ND2	2.50	0.44
3:J:590:ASP:OD1	3:J:677:HIS:ND1	2.51	0.44
1:A:484:ILE:O	1:A:488:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ARG:HG2	1:A:588:ASN:HD22	1.80	0.44
2:B:365:ARG:HB2	2:B:412:PRO:HD2	1.99	0.44
1:C:457:GLY:O	1:C:476:ASN:ND2	2.49	0.44
3:I:425:LYS:HD2	3:I:428:LYS:HD3	2.00	0.44
3:L:369:PRO:HG3	3:L:419:GLU:HG3	1.98	0.44
3:L:391:LYS:HA	3:L:391:LYS:HD2	1.79	0.44
1:G:362:ALA:HB3	1:G:421:LEU:HD12	1.99	0.44
1:A:362:ALA:HB3	1:A:421:LEU:HD12	1.99	0.44
1:A:587:MET:O	1:A:588:ASN:ND2	2.50	0.44
1:A:667:SER:O	1:A:675:PHE:N	2.51	0.44
1:C:587:MET:O	1:C:588:ASN:ND2	2.50	0.44
1:E:424:GLN:NE2	1:E:424:GLN:CA	2.73	0.44
2:F:365:ARG:HB2	2:F:412:PRO:HD2	1.99	0.44
1:G:457:GLY:O	1:G:476:ASN:ND2	2.49	0.44
1:A:648:ASP:OD1	1:A:649:THR:N	2.51	0.44
1:C:597:HIS:N	1:C:606:GLY:O	2.49	0.44
1:E:597:HIS:N	1:E:606:GLY:O	2.49	0.44
3:K:425:LYS:HD2	3:K:428:LYS:HD3	2.00	0.44
2:D:365:ARG:HB2	2:D:412:PRO:HD2	1.99	0.44
3:I:369:PRO:HG3	3:I:419:GLU:HG3	1.98	0.44
3:K:155:LEU:HD23	3:K:155:LEU:HA	1.82	0.44
1:E:340:LEU:HD12	1:E:343:GLU:HB3	2.00	0.44
1:G:340:LEU:HD12	1:G:343:GLU:HB3	2.00	0.44
3:J:681:GLN:OE1	3:J:685:ARG:NH1	2.51	0.44
3:K:82:LYS:HE3	3:K:84:LEU:HB3	2.00	0.44
3:L:590:ASP:OD1	3:L:677:HIS:ND1	2.51	0.44
1:A:197:LYS:HA	1:A:197:LYS:HD2	1.76	0.43
1:C:340:LEU:HD12	1:C:343:GLU:HB3	2.00	0.43
1:E:667:SER:O	1:E:675:PHE:N	2.51	0.43
3:I:313:LYS:HE2	3:I:458:ASP:H	1.84	0.43
3:I:590:ASP:OD1	3:I:677:HIS:ND1	2.51	0.43
3:I:681:GLN:OE1	3:I:685:ARG:NH1	2.51	0.43
3:J:82:LYS:HE3	3:J:84:LEU:HB3	2.00	0.43
1:A:340:LEU:HD12	1:A:343:GLU:HB3	2.00	0.43
1:A:259:TYR:OH	1:A:502:GLU:OE2	2.35	0.43
2:B:223:PRO:HD2	2:B:517:THR:HG22	2.01	0.43
1:G:484:ILE:O	1:G:488:THR:OG1	2.30	0.43
2:H:642:TYR:HB2	2:H:665:ILE:HD11	2.01	0.43
3:I:146:LEU:HA	3:I:149:ILE:HG22	2.00	0.43
2:B:344:ARG:HB3	2:B:345:THR:HG23	1.99	0.43
2:F:179:ASP:N	2:F:179:ASP:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:301:SER:OG	2:F:302:GLU:N	2.49	0.43
2:H:223:PRO:HD2	2:H:517:THR:HG22	2.01	0.43
2:H:344:ARG:HB3	2:H:345:THR:HG23	1.99	0.43
3:K:590:ASP:OD1	3:K:677:HIS:ND1	2.51	0.43
1:C:466:ASN:OD1	1:C:466:ASN:N	2.52	0.43
3:I:647:LYS:N	3:I:654:GLU:OE1	2.51	0.43
3:J:425:LYS:HD2	3:J:428:LYS:HD3	2.00	0.43
3:K:299:ASN:O	3:K:303:THR:OG1	2.34	0.43
3:K:334:ASP:OD1	3:K:334:ASP:N	2.52	0.43
2:D:642:TYR:HB2	2:D:665:ILE:HD11	2.01	0.43
3:J:74:THR:HA	3:J:739:GLU:HG3	2.01	0.43
3:J:146:LEU:HA	3:J:149:ILE:HG22	2.00	0.43
3:J:313:LYS:HE2	3:J:458:ASP:H	1.84	0.43
1:A:689:ILE:HD12	1:A:689:ILE:HA	1.97	0.43
1:C:648:ASP:OD1	1:C:649:THR:N	2.51	0.43
2:F:719:ASN:OD1	2:F:719:ASN:N	2.51	0.43
3:L:313:LYS:HE2	3:L:458:ASP:H	1.84	0.43
1:E:466:ASN:OD1	1:E:466:ASN:N	2.52	0.43
1:G:648:ASP:OD1	1:G:649:THR:N	2.51	0.43
3:J:299:ASN:O	3:J:303:THR:OG1	2.34	0.43
3:L:425:LYS:HD2	3:L:428:LYS:HD3	2.00	0.43
3:L:647:LYS:N	3:L:654:GLU:OE1	2.51	0.43
2:B:719:ASN:OD1	2:B:719:ASN:N	2.51	0.43
1:E:648:ASP:OD1	1:E:649:THR:N	2.51	0.43
1:C:181:ASP:OD1	1:C:181:ASP:N	2.41	0.43
2:D:223:PRO:HD2	2:D:517:THR:HG22	2.01	0.43
2:F:223:PRO:HD2	2:F:517:THR:HG22	2.01	0.43
2:H:273:LYS:NZ	2:H:350:MET:O	2.45	0.43
3:L:82:LYS:HE3	3:L:84:LEU:HB3	2.00	0.43
2:D:625:GLU:HG2	2:D:679:LYS:HD3	2.01	0.42
3:K:74:THR:HA	3:K:739:GLU:HG3	2.01	0.42
3:L:710:PRO:HA	3:L:713:LYS:HB3	2.01	0.42
2:B:424:GLN:N	2:B:424:GLN:CD	2.73	0.42
2:B:427:PHE:CD2	2:B:427:PHE:N	2.86	0.42
2:F:199:LYS:HD3	2:F:199:LYS:HA	1.81	0.42
2:B:184:PRO:HG2	2:B:187:LEU:HG	2.01	0.42
2:B:627:LEU:HD12	2:B:676:ILE:HD12	2.01	0.42
2:F:184:PRO:HG2	2:F:187:LEU:HG	2.01	0.42
2:H:184:PRO:HG2	2:H:187:LEU:HG	2.01	0.42
3:I:388:LYS:HD2	3:I:388:LYS:HA	1.80	0.42
3:I:618:LYS:HD3	3:I:718:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:315:LEU:HD12	3:L:544:HIS:HB2	2.01	0.42
1:A:359:ARG:HH21	1:A:431:PRO:HB3	1.85	0.42
1:C:359:ARG:HH21	1:C:431:PRO:HB3	1.85	0.42
1:C:689:ILE:HD12	1:C:689:ILE:HA	1.97	0.42
1:C:711:SER:HB2	1:C:715:ASP:HB2	2.01	0.42
1:E:359:ARG:HH21	1:E:431:PRO:HB3	1.85	0.42
2:H:427:PHE:CD2	2:H:427:PHE:N	2.86	0.42
2:H:719:ASN:OD1	2:H:719:ASN:N	2.51	0.42
3:J:445:ALA:HB1	3:J:452:LEU:HD22	2.02	0.42
2:B:642:TYR:HB2	2:B:665:ILE:HD11	2.01	0.42
2:D:424:GLN:CD	2:D:424:GLN:N	2.73	0.42
2:D:627:LEU:HD12	2:D:676:ILE:HD12	2.01	0.42
1:E:711:SER:HB2	1:E:715:ASP:HB2	2.01	0.42
2:F:627:LEU:HD12	2:F:676:ILE:HD12	2.01	0.42
3:I:82:LYS:HE3	3:I:84:LEU:HB3	2.00	0.42
3:K:710:PRO:HA	3:K:713:LYS:HB3	2.01	0.42
3:L:618:LYS:HD3	3:L:718:TYR:HE1	1.84	0.42
2:F:427:PHE:CD2	2:F:427:PHE:N	2.86	0.42
3:I:74:THR:HA	3:I:739:GLU:HG3	2.01	0.42
3:I:370:LEU:HD23	3:I:441:ILE:HG21	2.02	0.42
3:K:313:LYS:HE2	3:K:458:ASP:H	1.84	0.42
3:K:445:ALA:HB1	3:K:452:LEU:HD22	2.02	0.42
3:K:684:LYS:HE3	3:K:684:LYS:HB2	1.89	0.42
3:L:494:LYS:HA	3:L:494:LYS:HD3	1.84	0.42
2:D:184:PRO:HG2	2:D:187:LEU:HG	2.01	0.42
2:F:625:GLU:HG2	2:F:679:LYS:HD3	2.01	0.42
2:F:642:TYR:HB2	2:F:665:ILE:HD11	2.01	0.42
1:G:667:SER:O	1:G:675:PHE:N	2.51	0.42
2:H:424:GLN:N	2:H:424:GLN:CD	2.73	0.42
3:I:521:LYS:HD2	3:I:521:LYS:HA	1.88	0.42
3:J:377:ILE:HD12	3:J:377:ILE:HA	1.90	0.42
3:K:27:LYS:HA	3:K:27:LYS:HD3	1.85	0.42
3:L:146:LEU:HA	3:L:149:ILE:HG22	2.00	0.42
2:H:579:ASP:OD1	2:H:579:ASP:N	2.44	0.42
2:H:625:GLU:HG2	2:H:679:LYS:HD3	2.01	0.42
3:J:494:LYS:HA	3:J:494:LYS:HD3	1.84	0.42
3:K:315:LEU:HD12	3:K:544:HIS:HB2	2.01	0.42
3:L:720:LYS:HA	3:L:723:ILE:HG22	2.02	0.42
1:G:711:SER:HB2	1:G:715:ASP:HB2	2.01	0.42
3:I:315:LEU:HD12	3:I:544:HIS:HB2	2.01	0.42
3:J:647:LYS:N	3:J:654:GLU:OE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:681:GLN:OE1	3:K:685:ARG:NH1	2.51	0.42
3:K:720:LYS:HA	3:K:723:ILE:HG22	2.02	0.42
3:L:77:ASP:OD1	3:L:77:ASP:N	2.53	0.42
1:A:664:ASN:OD1	1:A:664:ASN:N	2.53	0.42
1:C:664:ASN:OD1	1:C:664:ASN:N	2.53	0.42
2:F:424:GLN:CD	2:F:424:GLN:N	2.73	0.42
3:I:710:PRO:HA	3:I:713:LYS:HB3	2.01	0.42
3:I:720:LYS:HA	3:I:723:ILE:HG22	2.02	0.42
3:J:27:LYS:HD3	3:J:27:LYS:HA	1.85	0.42
3:K:77:ASP:OD1	3:K:77:ASP:N	2.53	0.42
3:L:267:LYS:HE3	3:L:267:LYS:HB3	1.88	0.42
3:J:278:HIS:CE1	3:J:536:TYR:HB2	2.55	0.41
3:J:720:LYS:HA	3:J:723:ILE:HG22	2.02	0.41
3:K:494:LYS:HA	3:K:494:LYS:HD3	1.84	0.41
3:L:74:THR:HA	3:L:739:GLU:HG3	2.01	0.41
3:L:278:HIS:CE1	3:L:536:TYR:HB2	2.55	0.41
1:A:639:LEU:HD13	1:A:639:LEU:HA	1.96	0.41
1:A:653:LYS:HA	1:A:653:LYS:HD3	1.88	0.41
1:A:730:LYS:HB2	1:A:733:GLU:HG3	2.02	0.41
2:B:231:ASP:N	2:B:231:ASP:OD1	2.49	0.41
1:E:259:TYR:OH	1:E:502:GLU:OE2	2.35	0.41
1:E:689:ILE:HD12	1:E:689:ILE:HA	1.97	0.41
1:G:723:LYS:HE2	1:G:723:LYS:HB2	1.89	0.41
3:I:278:HIS:CE1	3:I:536:TYR:HB2	2.55	0.41
3:K:146:LEU:HA	3:K:149:ILE:HG22	2.00	0.41
1:A:711:SER:HB2	1:A:715:ASP:HB2	2.01	0.41
2:B:214:LYS:HB3	2:B:214:LYS:HE2	1.89	0.41
1:C:643:ILE:HB	1:C:699:TYR:HB2	2.02	0.41
1:C:648:ASP:HB2	1:C:652:LEU:HB2	2.03	0.41
1:E:648:ASP:HB2	1:E:652:LEU:HB2	2.03	0.41
2:H:199:LYS:HA	2:H:199:LYS:HD3	1.81	0.41
3:J:370:LEU:HD23	3:J:441:ILE:HG21	2.02	0.41
3:L:445:ALA:HB1	3:L:452:LEU:HD22	2.02	0.41
3:L:681:GLN:OE1	3:L:685:ARG:NH1	2.51	0.41
1:E:643:ILE:HB	1:E:699:TYR:HB2	2.02	0.41
2:F:368:ASN:HB2	2:F:405:LEU:HG	2.03	0.41
3:K:278:HIS:CE1	3:K:536:TYR:HB2	2.55	0.41
1:A:647:GLU:HB3	1:A:695:LYS:HB2	2.02	0.41
1:A:648:ASP:HB2	1:A:652:LEU:HB2	2.03	0.41
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.92	0.41
1:A:719:ASN:OD1	1:A:719:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:ASP:OD1	1:E:181:ASP:N	2.41	0.41
1:G:306:ASN:OD1	1:G:306:ASN:N	2.54	0.41
3:K:521:LYS:HA	3:K:521:LYS:HD2	1.88	0.41
3:K:573:LYS:HE2	3:K:573:LYS:HB2	1.89	0.41
3:L:370:LEU:HD23	3:L:441:ILE:HG21	2.02	0.41
1:A:644:VAL:HG23	1:A:698:VAL:HG22	2.02	0.41
2:B:340:LEU:HB3	2:B:343:GLU:HB3	2.03	0.41
1:C:667:SER:O	1:C:675:PHE:N	2.51	0.41
1:C:730:LYS:HB2	1:C:733:GLU:HG3	2.02	0.41
1:E:387:LYS:HE2	1:E:387:LYS:HB3	1.96	0.41
1:G:648:ASP:HB2	1:G:652:LEU:HB2	2.03	0.41
2:H:273:LYS:H	2:H:273:LYS:HG2	1.75	0.41
2:H:627:LEU:HD12	2:H:676:ILE:HD12	2.01	0.41
3:I:445:ALA:HB1	3:I:452:LEU:HD22	2.02	0.41
3:J:407:GLN:O	3:J:428:LYS:NZ	2.43	0.41
3:K:377:ILE:HD12	3:K:377:ILE:HA	1.90	0.41
1:E:388:ASN:OD1	1:E:388:ASN:N	2.54	0.41
1:E:647:GLU:HB3	1:E:695:LYS:HB2	2.02	0.41
1:G:359:ARG:HH21	1:G:431:PRO:HB3	1.85	0.41
1:G:719:ASN:OD1	1:G:719:ASN:N	2.54	0.41
3:I:333:PHE:HB2	3:I:442:GLU:HB2	2.02	0.41
3:K:370:LEU:HD23	3:K:441:ILE:HG21	2.02	0.41
3:L:353:GLU:HA	3:L:356:LYS:HE3	2.03	0.41
3:L:521:LYS:HA	3:L:521:LYS:HD2	1.88	0.41
1:A:643:ILE:HB	1:A:699:TYR:HB2	2.02	0.41
2:B:625:GLU:HG2	2:B:679:LYS:HD3	2.01	0.41
2:D:647:GLU:HB3	2:D:695:LYS:HB2	2.03	0.41
1:E:306:ASN:OD1	1:E:306:ASN:N	2.54	0.41
2:F:647:GLU:HB3	2:F:695:LYS:HB2	2.03	0.41
1:G:388:ASN:OD1	1:G:388:ASN:N	2.54	0.41
2:H:231:ASP:N	2:H:231:ASP:OD1	2.49	0.41
2:H:368:ASN:HB2	2:H:405:LEU:HG	2.03	0.41
3:I:77:ASP:N	3:I:77:ASP:OD1	2.53	0.41
3:I:334:ASP:OD1	3:I:334:ASP:N	2.52	0.41
3:J:710:PRO:HA	3:J:713:LYS:HB3	2.01	0.41
3:K:353:GLU:HA	3:K:356:LYS:HE3	2.03	0.41
3:L:627:SER:HA	3:L:630:PHE:HB3	2.03	0.41
1:A:259:TYR:HA	1:A:260:PRO:HD3	1.91	0.41
2:B:647:GLU:HB3	2:B:695:LYS:HB2	2.03	0.41
2:D:368:ASN:HB2	2:D:405:LEU:HG	2.03	0.41
1:E:512:ASP:O	1:E:516:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:664:ASN:OD1	1:E:664:ASN:N	2.53	0.41
2:F:414:LYS:HA	2:F:414:LYS:HD3	1.90	0.41
1:G:466:ASN:OD1	1:G:466:ASN:N	2.52	0.41
1:G:647:GLU:HB3	1:G:695:LYS:HB2	2.02	0.41
1:G:664:ASN:OD1	1:G:664:ASN:N	2.53	0.41
2:H:340:LEU:HB3	2:H:343:GLU:HB3	2.03	0.41
2:H:563:LYS:HE3	2:H:563:LYS:HB2	1.90	0.41
2:H:647:GLU:HB3	2:H:695:LYS:HB2	2.03	0.41
3:I:353:GLU:HA	3:I:356:LYS:HE3	2.03	0.41
3:I:528:ASN:ND2	3:I:540:ASP:OD1	2.54	0.41
3:I:627:SER:HA	3:I:630:PHE:HB3	2.03	0.41
3:J:77:ASP:OD1	3:J:77:ASP:N	2.53	0.41
3:J:315:LEU:HD12	3:J:544:HIS:HB2	2.01	0.41
3:J:333:PHE:HB2	3:J:442:GLU:HB2	2.02	0.41
3:K:627:SER:HA	3:K:630:PHE:HB3	2.03	0.41
3:K:695:ALA:O	3:K:699:ILE:HG12	2.21	0.41
3:L:695:ALA:O	3:L:699:ILE:HG12	2.21	0.41
1:A:306:ASN:OD1	1:A:306:ASN:N	2.54	0.41
1:A:582:LYS:HA	1:A:582:LYS:HD3	1.92	0.41
1:G:377:VAL:HG13	1:G:398:GLU:HG3	2.03	0.41
3:I:180:LYS:HE3	3:I:180:LYS:HB3	1.96	0.41
3:I:267:LYS:HE3	3:I:267:LYS:HB3	1.88	0.41
3:J:618:LYS:HD3	3:J:718:TYR:HE1	1.84	0.40
3:K:618:LYS:HD3	3:K:718:TYR:HE1	1.84	0.40
2:B:273:LYS:H	2:B:273:LYS:HG2	1.75	0.40
2:D:645:GLU:OE2	2:D:699:TYR:OH	2.36	0.40
1:E:644:VAL:HG23	1:E:698:VAL:HG22	2.02	0.40
3:I:362:GLU:HA	3:I:365:ILE:HG22	2.04	0.40
3:I:421:GLN:HG2	3:I:438:TRP:HB2	2.03	0.40
3:I:497:THR:O	3:I:501:ILE:HG12	2.21	0.40
3:I:563:ILE:HD13	3:I:563:ILE:HA	1.93	0.40
3:I:695:ALA:O	3:I:699:ILE:HG12	2.21	0.40
3:J:391:LYS:HA	3:J:391:LYS:HD2	1.79	0.40
3:J:480:TRP:HA	3:J:483:VAL:HG23	2.03	0.40
3:K:461:LEU:HD21	3:K:524:LEU:HD11	2.04	0.40
3:K:647:LYS:N	3:K:654:GLU:OE1	2.51	0.40
3:L:333:PHE:HB2	3:L:442:GLU:HB2	2.02	0.40
3:L:383:ASN:HD21	3:L:385:ILE:HB	1.86	0.40
1:E:652:LEU:HD23	1:E:652:LEU:HA	1.92	0.40
1:G:334:ILE:H	1:G:334:ILE:HG13	1.74	0.40
3:I:471:ILE:HD13	3:I:592:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:383:ASN:HD21	3:J:385:ILE:HB	1.86	0.40
3:J:528:ASN:ND2	3:J:540:ASP:OD1	2.54	0.40
3:J:627:SER:HA	3:J:630:PHE:HB3	2.03	0.40
3:J:695:ALA:O	3:J:699:ILE:HG12	2.21	0.40
1:C:306:ASN:OD1	1:C:306:ASN:N	2.54	0.40
1:C:377:VAL:HG13	1:C:398:GLU:HG3	2.03	0.40
2:F:537:ASN:OD1	2:F:537:ASN:N	2.55	0.40
1:G:730:LYS:HB2	1:G:733:GLU:HG3	2.02	0.40
3:I:508:LYS:HB2	3:I:508:LYS:HE2	1.93	0.40
3:J:497:THR:O	3:J:501:ILE:HG12	2.21	0.40
3:K:333:PHE:HB2	3:K:442:GLU:HB2	2.02	0.40
3:K:480:TRP:HA	3:K:483:VAL:HG23	2.03	0.40
1:C:388:ASN:OD1	1:C:388:ASN:N	2.54	0.40
1:C:582:LYS:HA	1:C:582:LYS:HD3	1.92	0.40
2:F:563:LYS:HE3	2:F:563:LYS:HB2	1.90	0.40
1:G:643:ILE:HB	1:G:699:TYR:HB2	2.02	0.40
1:G:644:VAL:HG23	1:G:698:VAL:HG22	2.02	0.40
3:I:430:THR:OG1	3:I:431:VAL:N	2.55	0.40
3:J:53:LEU:HD23	3:J:53:LEU:HA	1.86	0.40
3:J:362:GLU:HA	3:J:365:ILE:HG22	2.04	0.40
3:J:388:LYS:HD2	3:J:388:LYS:HA	1.80	0.40
3:J:421:GLN:HG2	3:J:438:TRP:HB2	2.03	0.40
3:K:383:ASN:HD21	3:K:385:ILE:HB	1.86	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	535/735 (73%)	499 (93%)	36 (7%)	0	100	100
1	C	535/735 (73%)	499 (93%)	36 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	535/735 (73%)	499 (93%)	36 (7%)	0	100	100
1	G	535/735 (73%)	499 (93%)	36 (7%)	0	100	100
2	B	535/735 (73%)	493 (92%)	42 (8%)	0	100	100
2	D	535/735 (73%)	493 (92%)	42 (8%)	0	100	100
2	F	535/735 (73%)	493 (92%)	42 (8%)	0	100	100
2	H	535/735 (73%)	493 (92%)	42 (8%)	0	100	100
3	I	714/767 (93%)	640 (90%)	74 (10%)	0	100	100
3	J	714/767 (93%)	640 (90%)	74 (10%)	0	100	100
3	K	714/767 (93%)	640 (90%)	74 (10%)	0	100	100
3	L	714/767 (93%)	640 (90%)	74 (10%)	0	100	100
All	All	7136/8948 (80%)	6528 (92%)	608 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	482/659 (73%)	477 (99%)	5 (1%)	76	86
1	C	482/659 (73%)	477 (99%)	5 (1%)	76	86
1	E	482/659 (73%)	477 (99%)	5 (1%)	76	86
1	G	482/659 (73%)	477 (99%)	5 (1%)	76	86
2	B	483/660 (73%)	479 (99%)	4 (1%)	81	89
2	D	483/660 (73%)	479 (99%)	4 (1%)	81	89
2	F	483/660 (73%)	479 (99%)	4 (1%)	81	89
2	H	483/660 (73%)	479 (99%)	4 (1%)	81	89
3	I	652/698 (93%)	647 (99%)	5 (1%)	81	89
3	J	652/698 (93%)	647 (99%)	5 (1%)	81	89
3	K	652/698 (93%)	647 (99%)	5 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	652/698 (93%)	647 (99%)	5 (1%)	81	89
All	All	6468/8068 (80%)	6412 (99%)	56 (1%)	79	87

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	GLN
1	A	425	ASP
1	A	426	ASP
1	A	490	ARG
1	A	496	LYS
2	B	427	PHE
2	B	429	SER
2	B	496	LYS
2	B	516	THR
1	C	424	GLN
1	C	425	ASP
1	C	426	ASP
1	C	490	ARG
1	C	496	LYS
2	D	427	PHE
2	D	429	SER
2	D	496	LYS
2	D	516	THR
1	E	424	GLN
1	E	425	ASP
1	E	426	ASP
1	E	490	ARG
1	E	496	LYS
2	F	427	PHE
2	F	429	SER
2	F	496	LYS
2	F	516	THR
1	G	424	GLN
1	G	425	ASP
1	G	426	ASP
1	G	490	ARG
1	G	496	LYS
2	H	427	PHE
2	H	429	SER
2	H	496	LYS
2	H	516	THR

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Mol	Chain	Res	Type
3	I	98	ARG
3	I	456	THR
3	I	662	LYS
3	I	706	LYS
3	I	720	LYS
3	J	98	ARG
3	J	456	THR
3	J	662	LYS
3	J	706	LYS
3	J	720	LYS
3	K	98	ARG
3	K	456	THR
3	K	662	LYS
3	K	706	LYS
3	K	720	LYS
3	L	98	ARG
3	L	456	THR
3	L	662	LYS
3	L	706	LYS
3	L	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	GLN
1	A	458	ASN
1	A	483	GLN
1	A	537	ASN
1	A	543	GLN
1	A	584	ASN
1	A	588	ASN
2	B	211	HIS
2	B	361	ASN
2	B	376	ASN
2	B	409	ASN
2	B	458	ASN
2	B	543	GLN
2	B	573	ASN
2	B	584	ASN
2	B	588	ASN
2	B	693	ASN
1	C	424	GLN

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Mol	Chain	Res	Type
1	C	458	ASN
1	C	483	GLN
1	C	537	ASN
1	C	543	GLN
1	C	584	ASN
1	C	588	ASN
2	D	211	HIS
2	D	361	ASN
2	D	376	ASN
2	D	409	ASN
2	D	458	ASN
2	D	543	GLN
2	D	573	ASN
2	D	584	ASN
2	D	588	ASN
2	D	693	ASN
1	E	424	GLN
1	E	458	ASN
1	E	483	GLN
1	E	537	ASN
1	E	543	GLN
1	E	584	ASN
1	E	588	ASN
1	E	601	ASN
2	F	211	HIS
2	F	285	GLN
2	F	361	ASN
2	F	376	ASN
2	F	409	ASN
2	F	458	ASN
2	F	543	GLN
2	F	573	ASN
2	F	584	ASN
2	F	588	ASN
2	F	693	ASN
1	G	424	GLN
1	G	458	ASN
1	G	483	GLN
1	G	537	ASN
1	G	543	GLN
1	G	584	ASN
1	G	588	ASN

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Mol	Chain	Res	Type
1	G	601	ASN
2	H	211	HIS
2	H	285	GLN
2	H	361	ASN
2	H	376	ASN
2	H	409	ASN
2	H	458	ASN
2	H	543	GLN
2	H	573	ASN
2	H	584	ASN
2	H	588	ASN
2	H	693	ASN
3	I	290	ASN
3	I	543	ASN
3	I	548	GLN
3	I	585	ASN
3	I	676	ASN
3	I	726	GLN
3	I	737	ASN
3	J	290	ASN
3	J	543	ASN
3	J	548	GLN
3	J	585	ASN
3	J	676	ASN
3	J	726	GLN
3	J	737	ASN
3	K	290	ASN
3	K	383	ASN
3	K	543	ASN
3	K	548	GLN
3	K	585	ASN
3	K	676	ASN
3	K	726	GLN
3	K	737	ASN
3	L	290	ASN
3	L	383	ASN
3	L	543	ASN
3	L	548	GLN
3	L	585	ASN
3	L	676	ASN
3	L	726	GLN
3	L	737	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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.

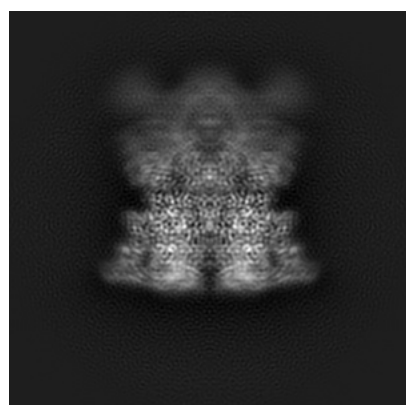
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21365. These allow visual inspection of the internal detail of the map and identification of artifacts.

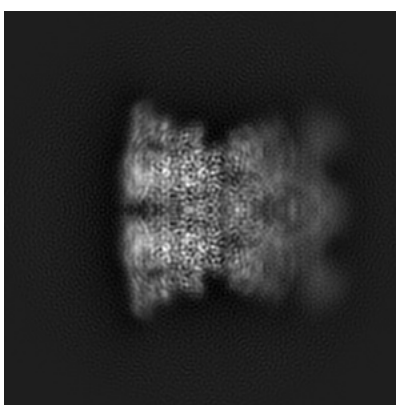
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

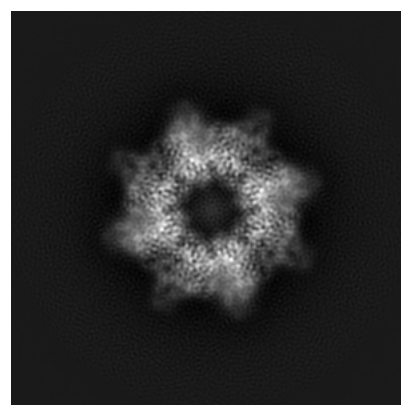
6.1.1 Primary map



X



Y

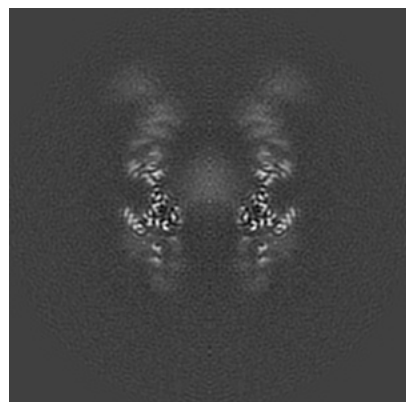


Z

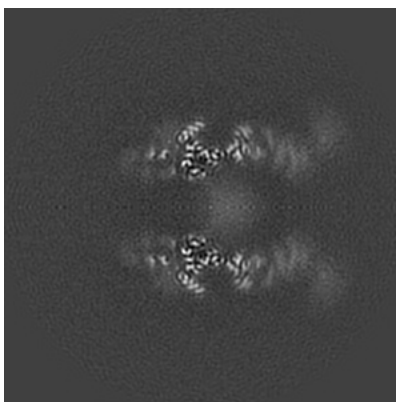
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

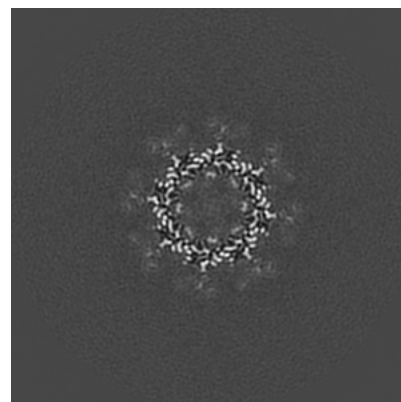
6.2.1 Primary map



X Index: 150



Y Index: 150

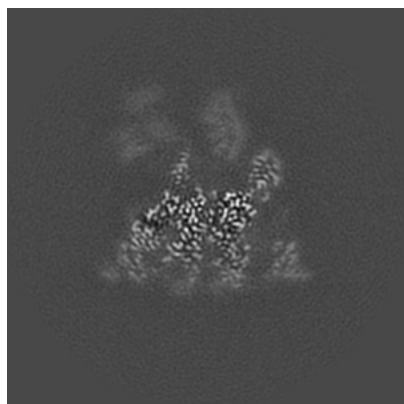


Z Index: 150

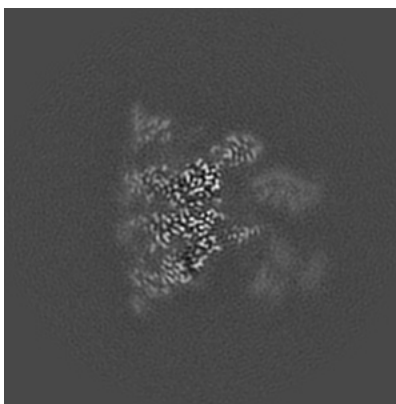
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

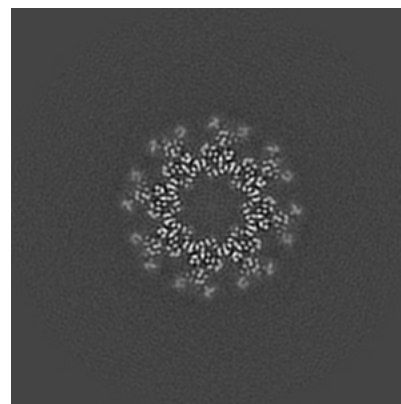
6.3.1 Primary map



X Index: 179



Y Index: 121

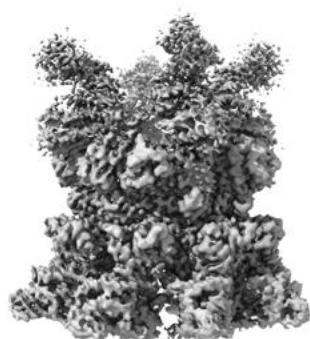


Z Index: 147

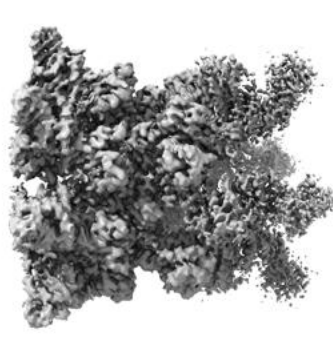
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

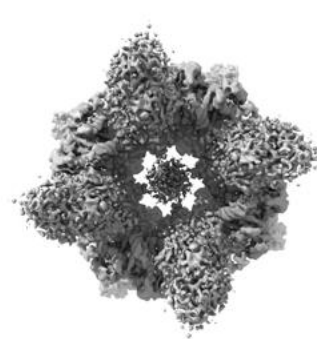
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

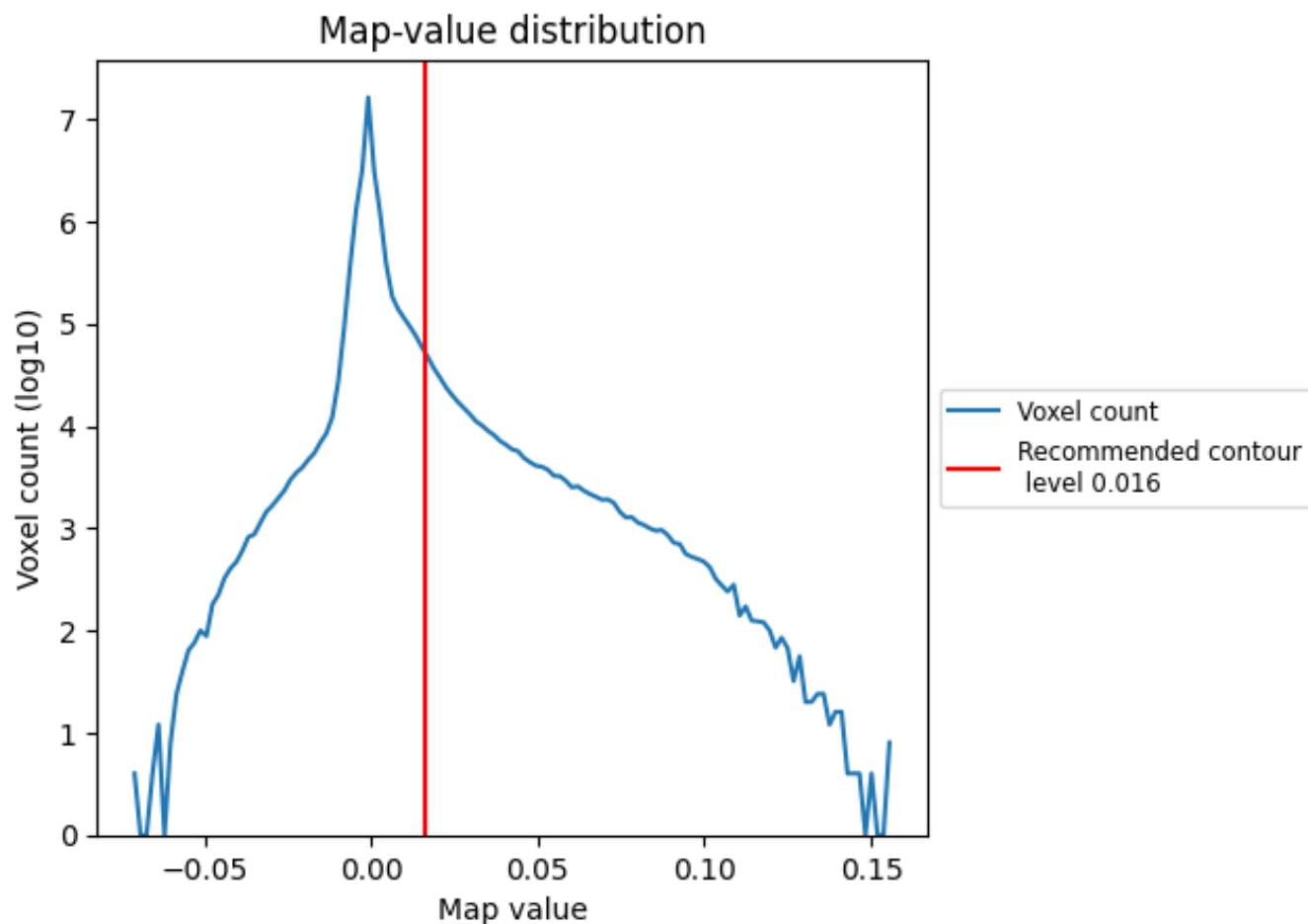
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

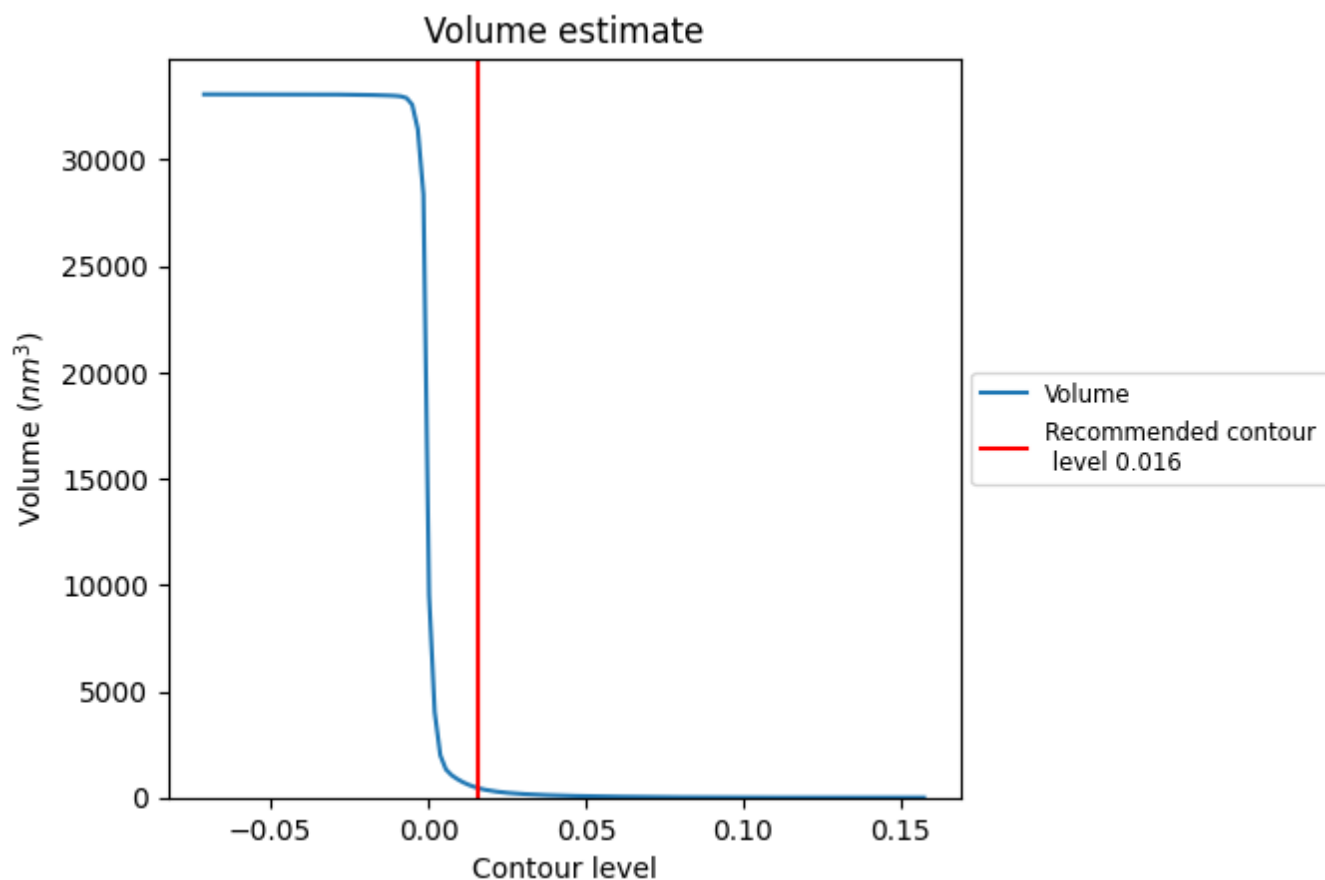
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

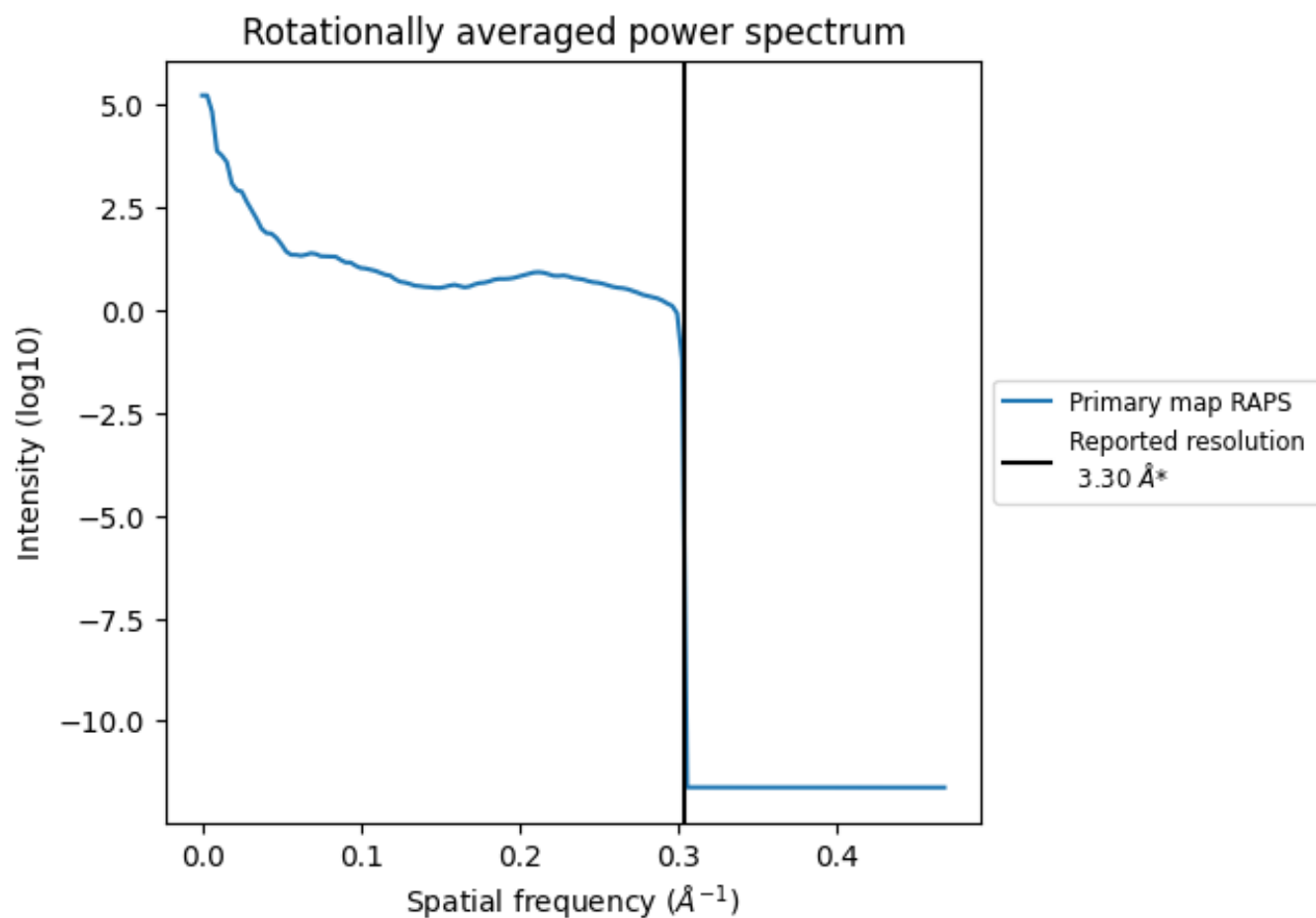
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 443 nm³; this corresponds to an approximate mass of 400 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

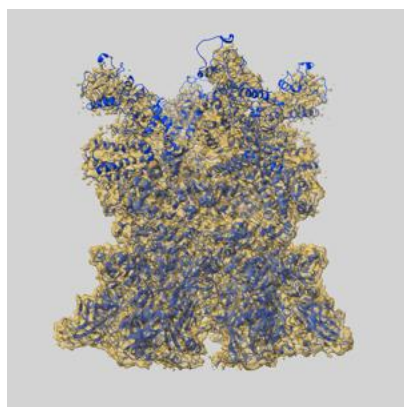
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

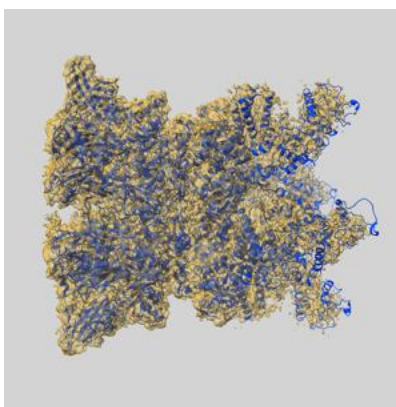
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21365 and PDB model 6VRA. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

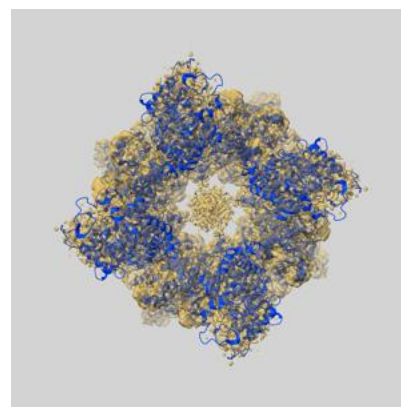
9.1 Map-model overlay [i](#)



X



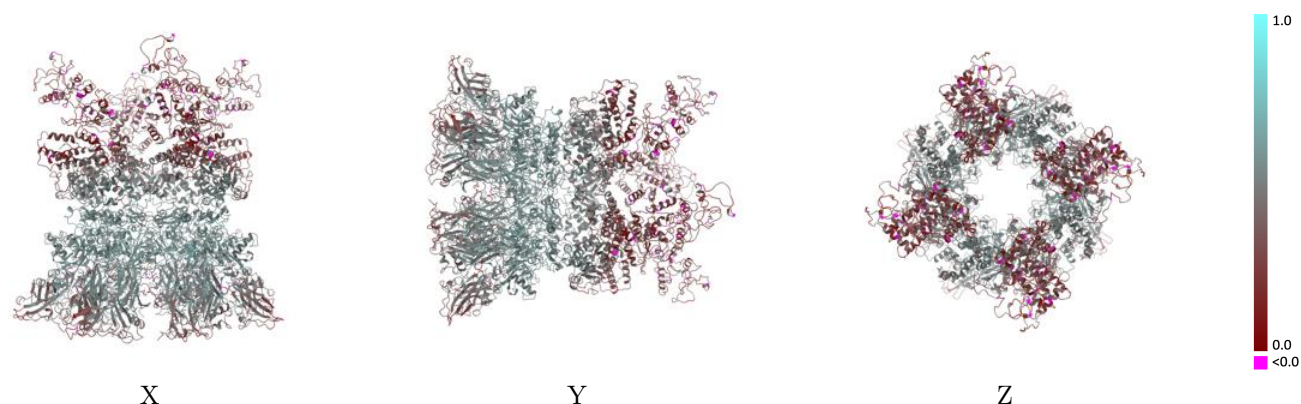
Y



Z

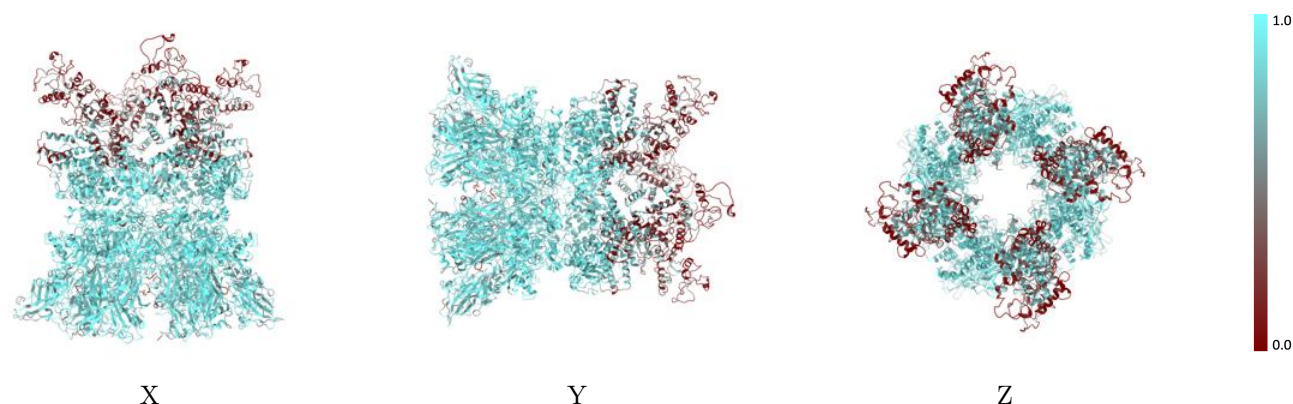
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



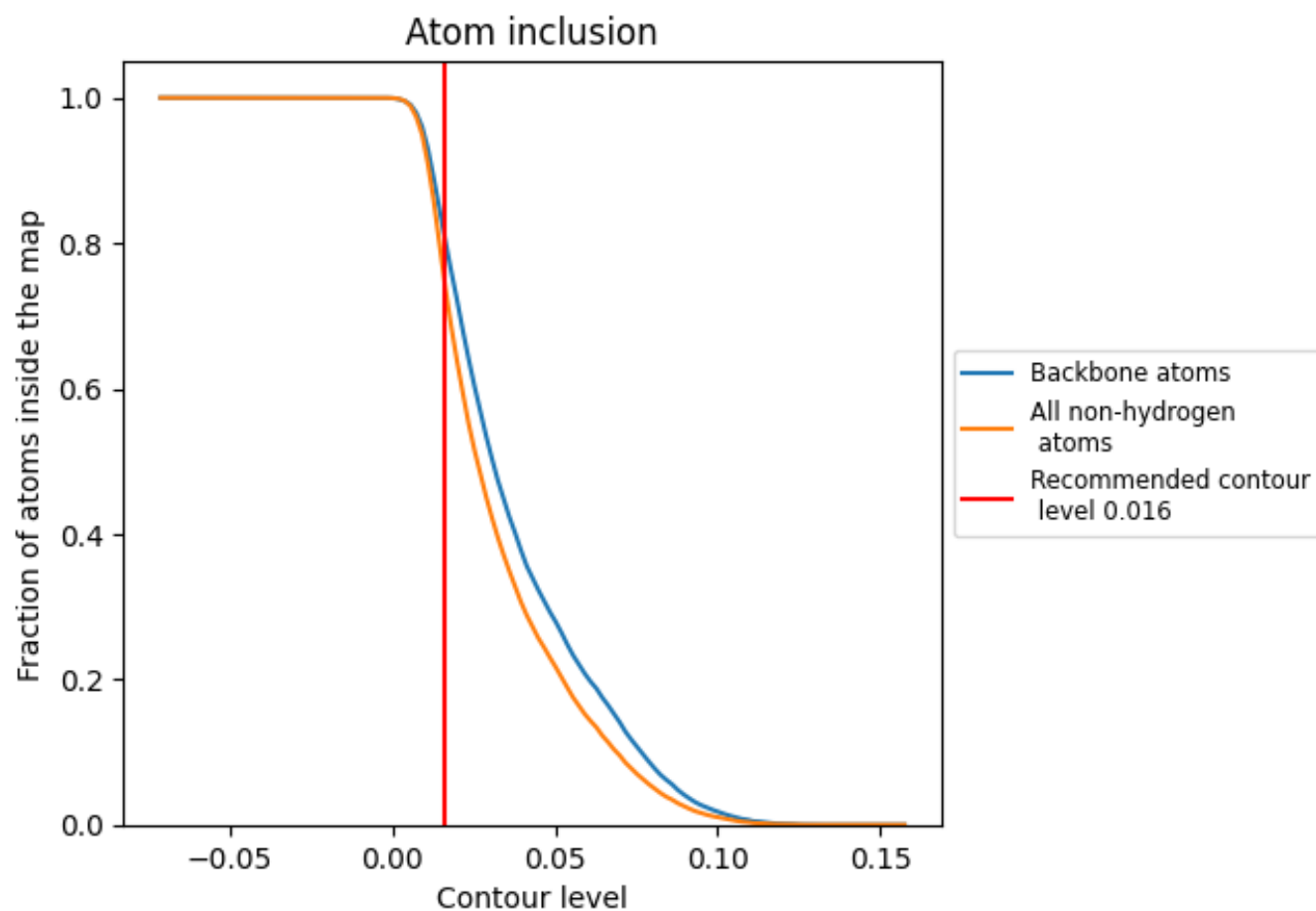
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7489	<div></div> 0.4350
A	<div></div> 0.8841	<div></div> 0.5000
B	<div></div> 0.8821	<div></div> 0.5040
C	<div></div> 0.8841	<div></div> 0.4980
D	<div></div> 0.8821	<div></div> 0.5050
E	<div></div> 0.8841	<div></div> 0.4990
F	<div></div> 0.8821	<div></div> 0.5050
G	<div></div> 0.8841	<div></div> 0.5000
H	<div></div> 0.8821	<div></div> 0.5050
I	<div></div> 0.5540	<div></div> 0.3380
J	<div></div> 0.5540	<div></div> 0.3370
K	<div></div> 0.5540	<div></div> 0.3360
L	<div></div> 0.5540	<div></div> 0.3370

1.0

0.0

<0.0