



Full wwPDB EM Validation Report ⓘ

Nov 17, 2022 – 12:42 AM EST

PDB ID : 6WJJ
EMDB ID : EMD-21694
Title : Anthrax octamer prechannel bound to full-length lethal factor
Authors : Zhou, K.; Hardenbrook, N.J.; Liu, S.; Cui, Y.X.; Krantz, B.A.; Zhou, Z.H.
Deposited on : 2020-04-13
Resolution : 3.80 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

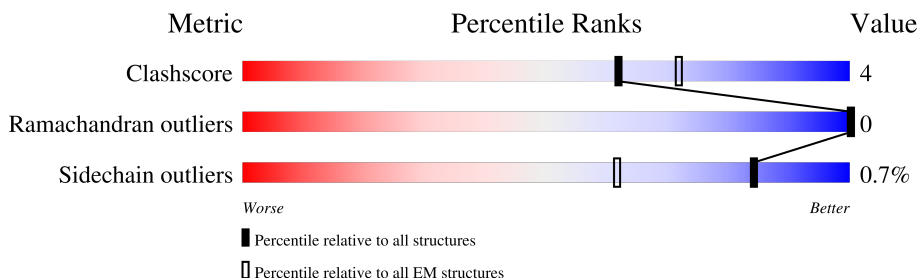
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	
1	C	735	
1	D	735	
1	E	735	
2	B	735	
2	F	735	
2	G	735	
2	H	735	

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Mol	Chain	Length	Quality of chain
3	I	776	<div><div>32%</div><div><div></div><div>80%</div><div>13%</div><div>7%</div></div></div>
3	J	776	<div><div>32%</div><div><div></div><div>80%</div><div>13%</div><div>7%</div></div></div>
3	K	776	<div><div>32%</div><div><div></div><div>79%</div><div>14%</div><div>7%</div></div></div>
3	L	776	<div><div>32%</div><div><div></div><div>80%</div><div>13%</div><div>7%</div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 56908 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	523	Total	C	N	O	S	0	0
			4144	2596	711	831	6		
1	C	523	Total	C	N	O	S	0	0
			4144	2596	711	831	6		
1	D	523	Total	C	N	O	S	0	0
			4144	2596	711	831	6		
1	E	523	Total	C	N	O	S	0	0
			4144	2596	711	831	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
D	121	ASP	ASN	conflict	UNP P13423
D	161	LEU	ARG	conflict	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
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	245	GLY	LYS	engineered mutation	UNP P13423
D	252	ASN	ARG	engineered mutation	UNP P13423
E	121	ASP	ASN	conflict	UNP P13423
E	161	LEU	ARG	conflict	UNP P13423
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

- Molecule 2 is a protein called Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	523	Total	C	N	O	S	0	0
			4150	2602	715	827	6		
2	F	523	Total	C	N	O	S	0	0
			4150	2602	715	827	6		
2	G	523	Total	C	N	O	S	0	0
			4150	2602	715	827	6		
2	H	523	Total	C	N	O	S	0	0
			4150	2602	715	827	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
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
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	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 Lethal factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	723	Total	C	N	O	S	0	0
			5923	3772	998	1146	7		
3	I	723	Total	C	N	O	S	0	0
			5923	3772	998	1146	7		
3	J	723	Total	C	N	O	S	0	0
			5923	3772	998	1146	7		
3	K	723	Total	C	N	O	S	0	0
			5923	3772	998	1146	7		

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

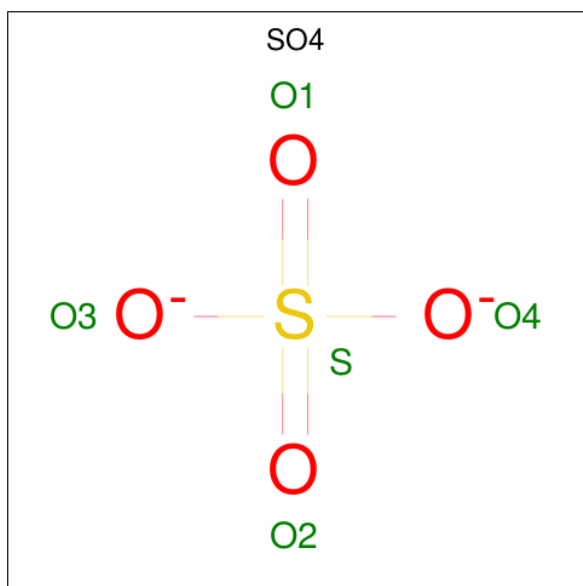
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	

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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	F	2	Total 2	Ca 2	0
4	D	2	Total 2	Ca 2	0
4	G	2	Total 2	Ca 2	0
4	E	2	Total 2	Ca 2	0
4	H	2	Total 2	Ca 2	0

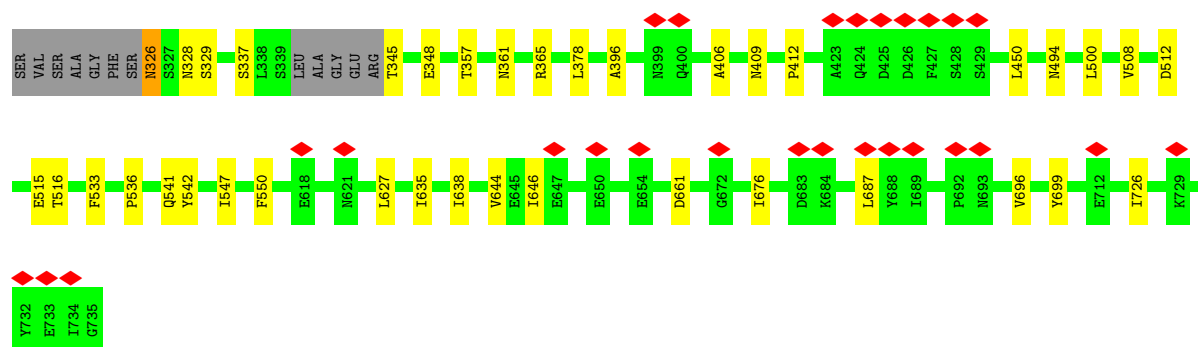
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



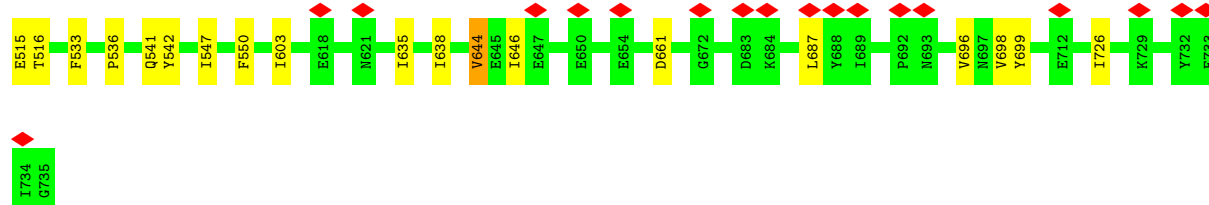
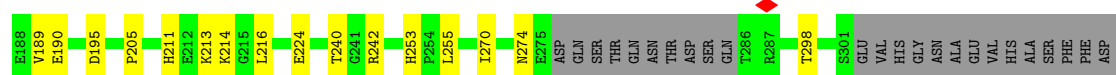
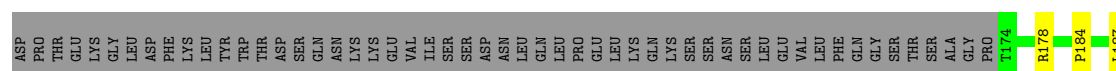
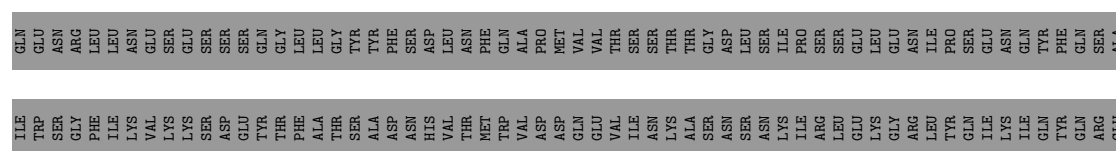
Mol	Chain	Residues	Atoms			AltConf
5	L	1	Total 5	O 4	S 1	0
5	I	1	Total 5	O 4	S 1	0
5	J	1	Total 5	O 4	S 1	0
5	K	1	Total 5	O 4	S 1	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

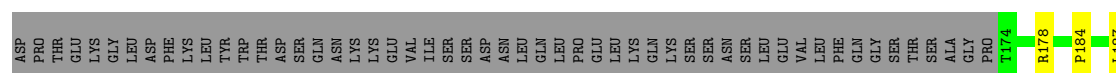
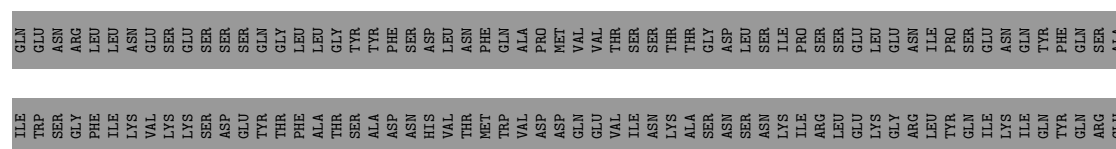
Mol	Chain	Residues	Atoms		AltConf
6	L	1	Total 1	Zn 1	0
6	I	1	Total 1	Zn 1	0
6	J	1	Total 1	Zn 1	0
6	K	1	Total 1	Zn 1	0

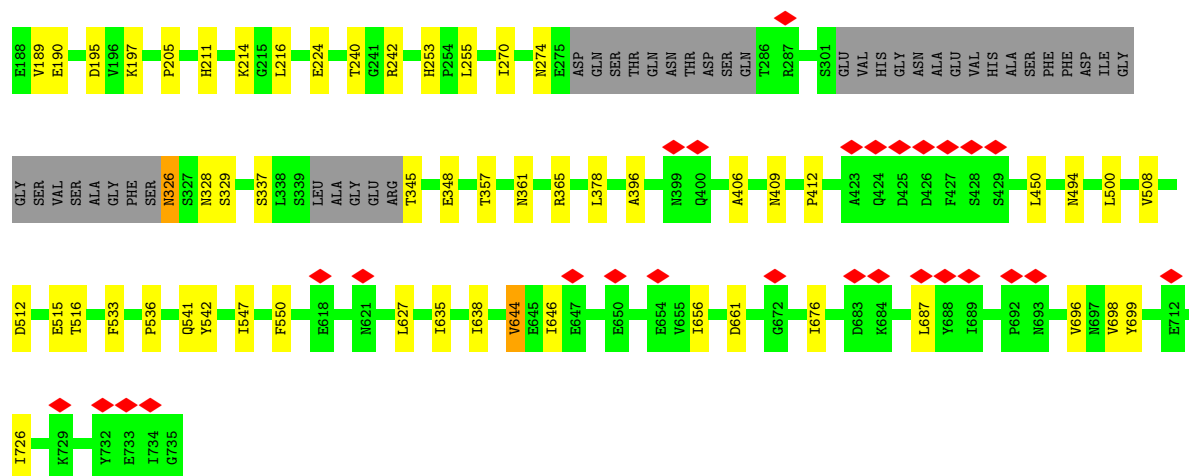


- Molecule 1: Protective antigen

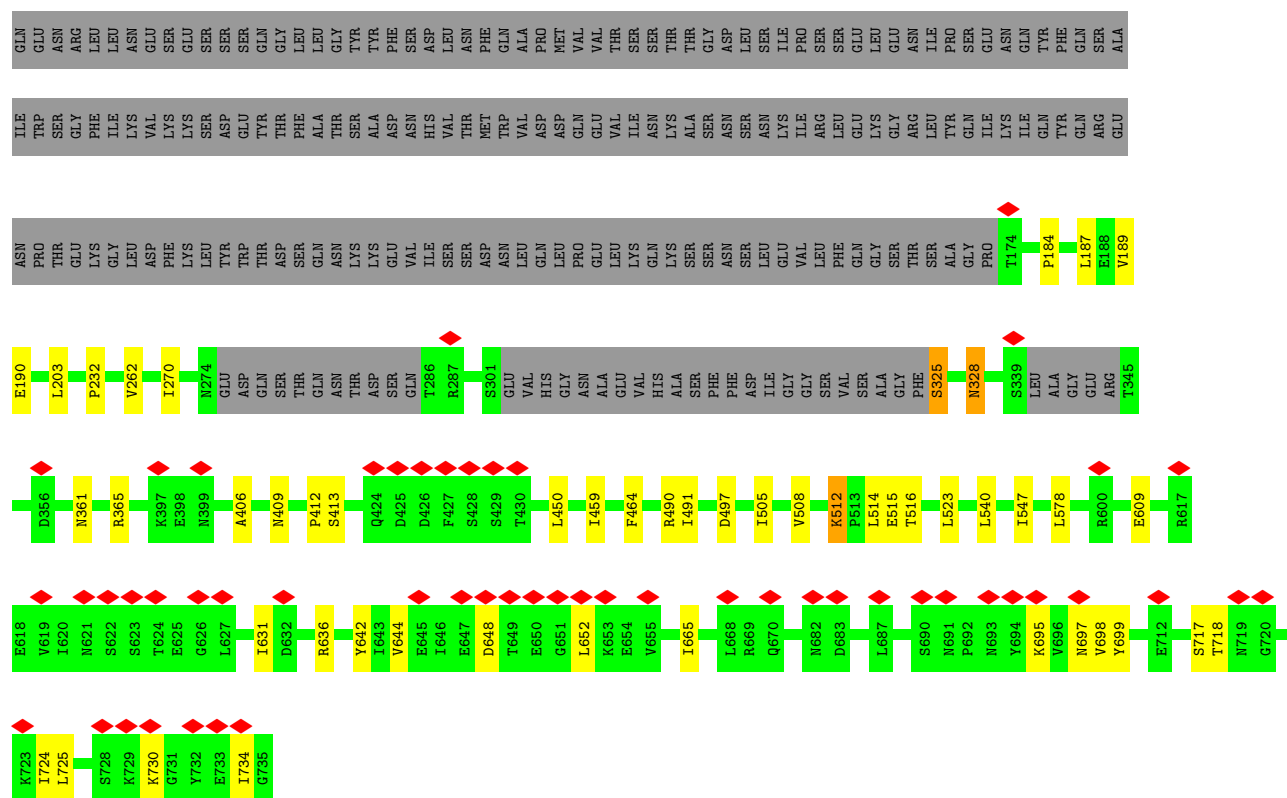


- Molecule 1: Protective antigen

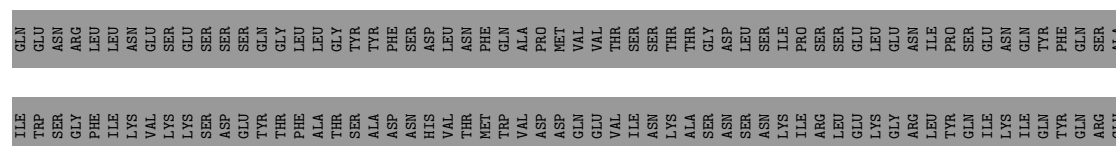


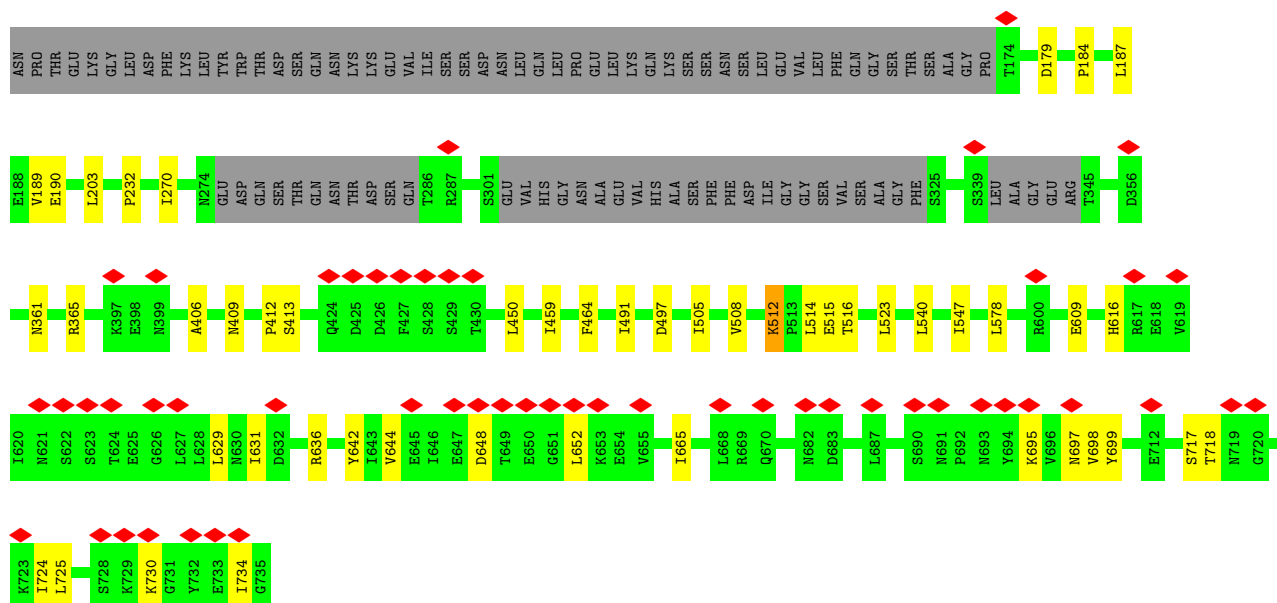


• Molecule 2: Protective antigen

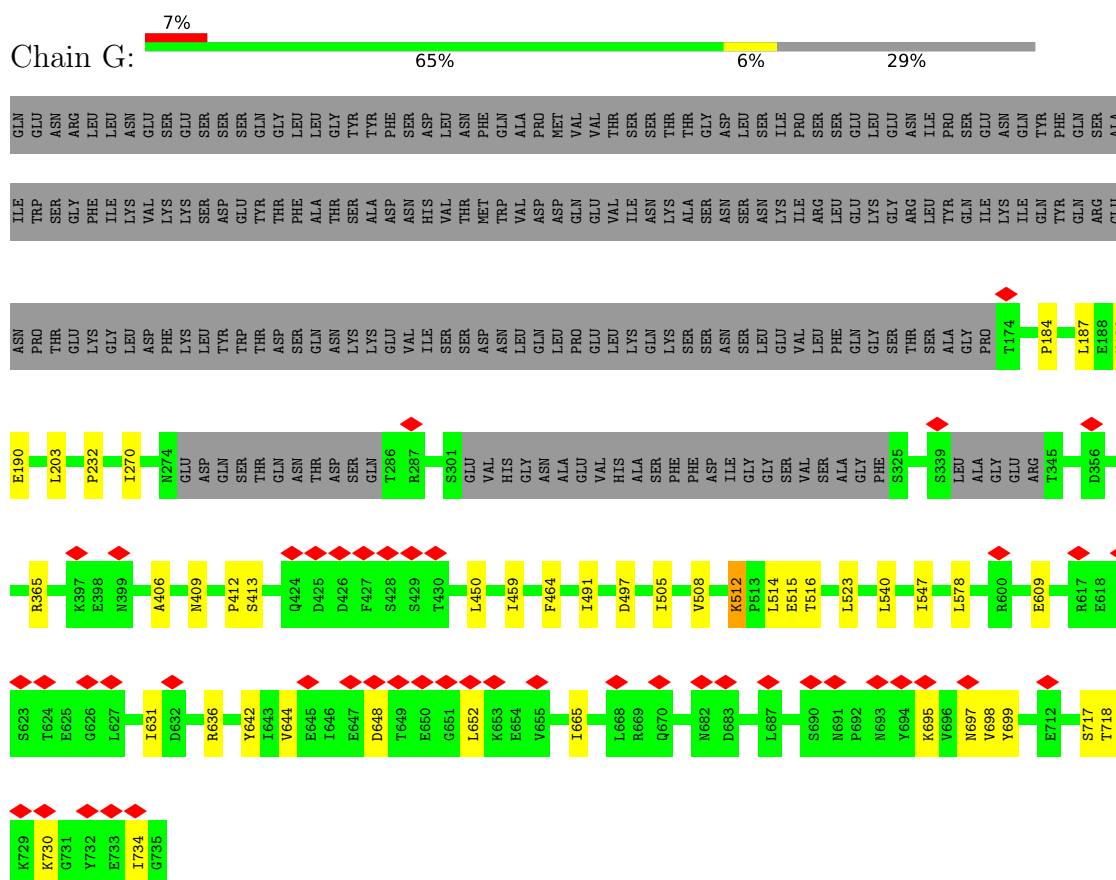


• Molecule 2: Protective antigen



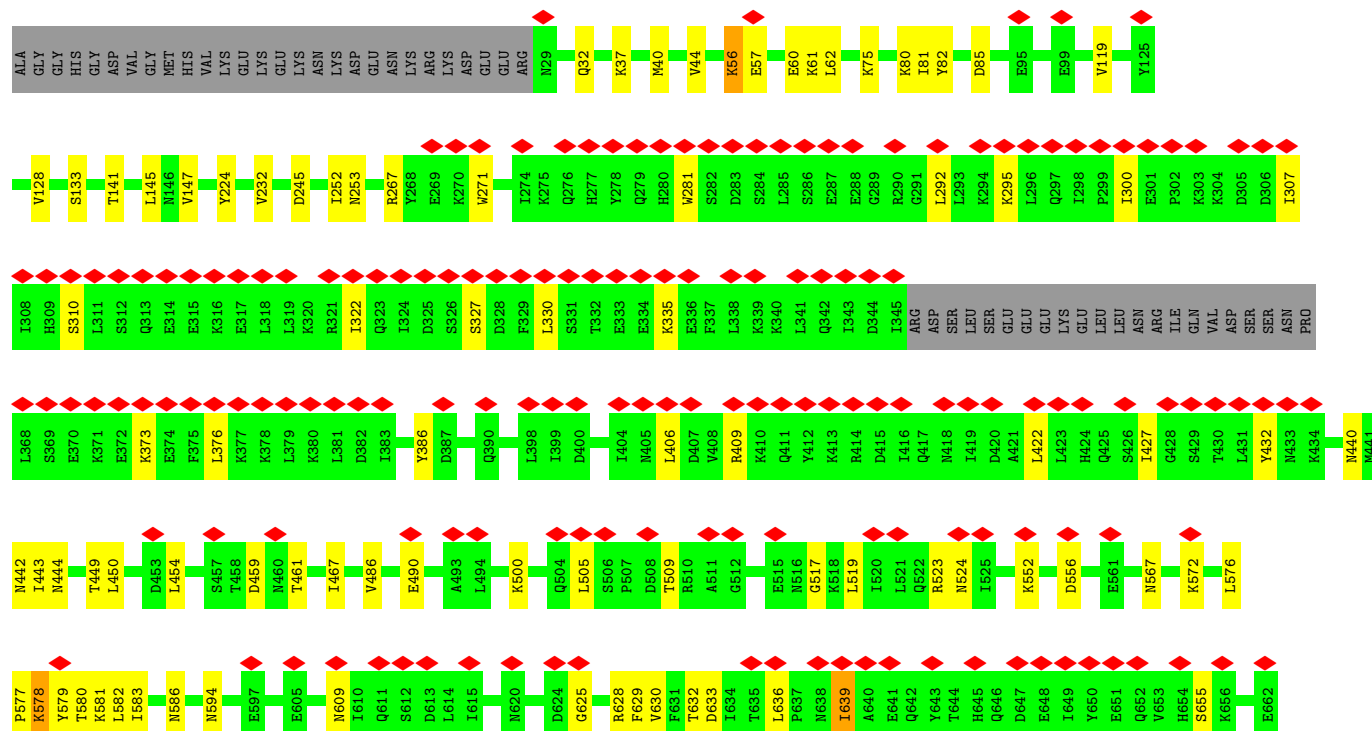


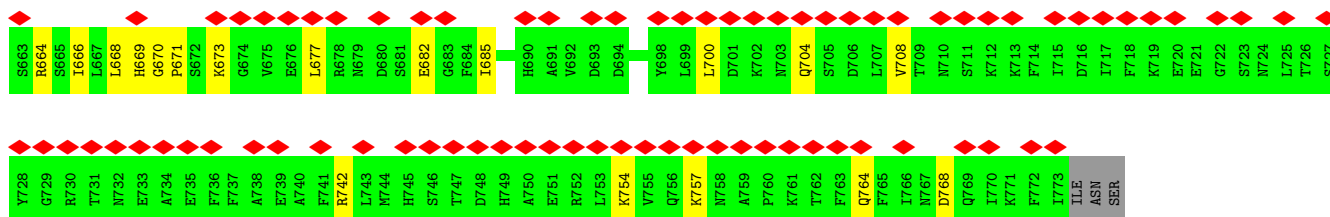
• Molecule 2: Protective antigen



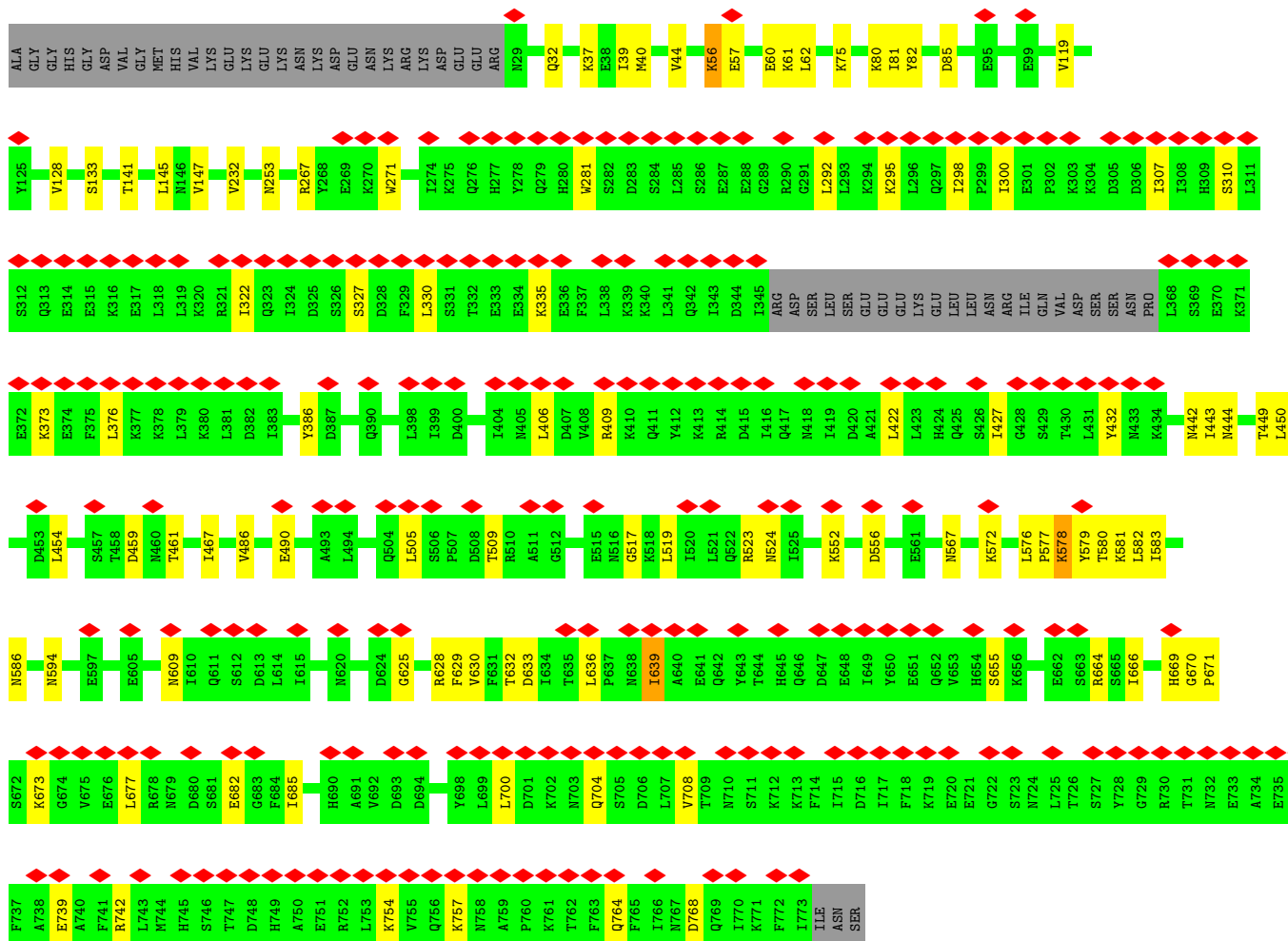
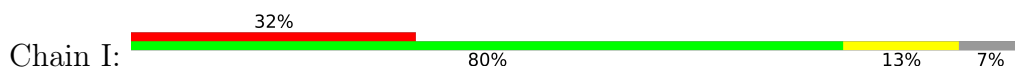
• Molecule 2: Protective antigen



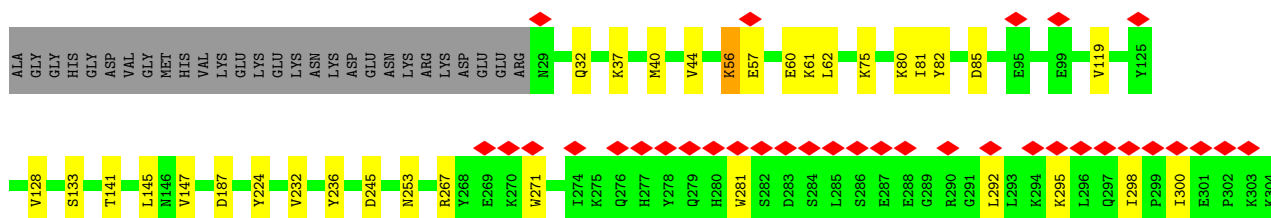
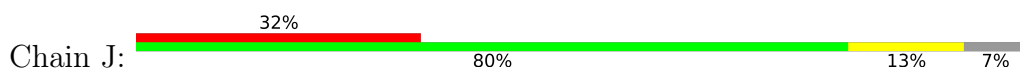


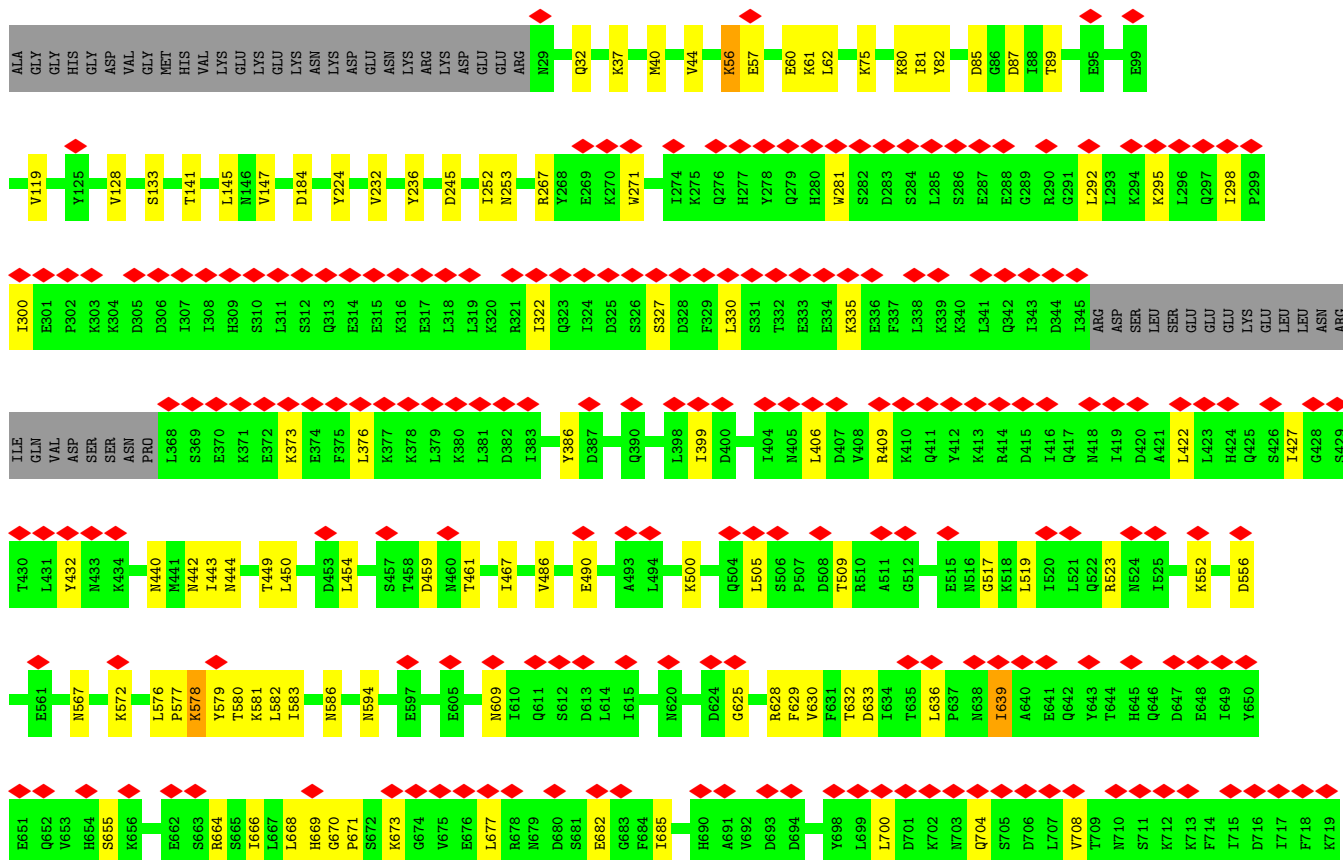


• Molecule 3: Lethal factor



• Molecule 3: Lethal factor





E720	E721	G722	S723	N724	L725	T726	S727	Y728	G729	R730	T731	N732	E733	A734	E735	F736	F737	A738	E739	A740	F741	R742	L743	M744	H745	S746	T747	D748	H749	A750	E751	R752	L753	K754	V755	Q756	K757	N758	A759	P760	K761	T762	F763	Q764	F765	I766	N767	D768	Q769	I770	K771	F772	I773	I774	ASU	SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	23839	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	0.154	Depositor
Minimum map value	-0.081	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	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, ZN, SO4

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	0.44	0/4213	0.59	0/5715
1	C	0.44	0/4213	0.59	0/5715
1	D	0.44	0/4213	0.59	0/5715
1	E	0.44	0/4213	0.59	0/5715
2	B	0.43	0/4219	0.60	1/5720 (0.0%)
2	F	0.43	0/4219	0.60	1/5720 (0.0%)
2	G	0.43	0/4219	0.60	1/5720 (0.0%)
2	H	0.43	0/4219	0.60	1/5720 (0.0%)
3	I	0.34	0/6029	0.55	1/8122 (0.0%)
3	J	0.34	0/6029	0.55	1/8122 (0.0%)
3	K	0.34	0/6029	0.55	1/8122 (0.0%)
3	L	0.34	0/6029	0.55	1/8122 (0.0%)
All	All	0.40	0/57844	0.58	8/78228 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	LEU	CA-CB-CG	5.69	128.39	115.30
2	F	450	LEU	CA-CB-CG	5.69	128.39	115.30
2	G	450	LEU	CA-CB-CG	5.69	128.39	115.30
2	H	450	LEU	CA-CB-CG	5.69	128.39	115.30
3	L	639	ILE	CG1-CB-CG2	-5.07	100.24	111.40
3	I	639	ILE	CG1-CB-CG2	-5.07	100.24	111.40
3	J	639	ILE	CG1-CB-CG2	-5.07	100.24	111.40
3	K	639	ILE	CG1-CB-CG2	-5.07	100.24	111.40

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	4144	0	4110	28	0
1	C	4144	0	4110	30	0
1	D	4144	0	4110	31	0
1	E	4144	0	4110	33	0
2	B	4150	0	4135	27	0
2	F	4150	0	4135	27	0
2	G	4150	0	4135	25	0
2	H	4150	0	4135	27	0
3	I	5923	0	5915	80	0
3	J	5923	0	5915	83	0
3	K	5923	0	5915	85	0
3	L	5923	0	5915	80	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
5	I	5	0	0	0	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
All	All	56908	0	56640	506	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 4.

All (506) 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)
3:L:577:PRO:HB3	3:K:80:LYS:HG2	1.36	1.07
3:J:80:LYS:HG2	3:K:577:PRO:HB3	1.36	1.06
3:I:80:LYS:HG2	3:J:577:PRO:HB3	1.36	1.06
3:L:80:LYS:HG2	3:I:577:PRO:HB3	1.36	1.06
3:L:80:LYS:HB3	3:L:82:TYR:CE2	2.06	0.91
3:I:80:LYS:HB3	3:I:82:TYR:CE2	2.06	0.91
3:K:80:LYS:HB3	3:K:82:TYR:CE2	2.06	0.91
3:J:80:LYS:HB3	3:J:82:TYR:CE2	2.06	0.89
3:I:80:LYS:CB	3:I:82:TYR:CE2	2.69	0.76
3:L:75:LYS:HE3	3:I:579:TYR:HB2	1.67	0.76
3:J:80:LYS:CB	3:J:82:TYR:CE2	2.69	0.75
3:I:75:LYS:HE3	3:J:579:TYR:HB2	1.67	0.75
3:L:579:TYR:HB2	3:K:75:LYS:HE3	1.67	0.75
3:L:80:LYS:CB	3:L:82:TYR:CE2	2.69	0.75
3:J:75:LYS:HE3	3:K:579:TYR:HB2	1.67	0.75
3:K:80:LYS:CB	3:K:82:TYR:CE2	2.69	0.74
3:L:56:LYS:HD2	3:L:56:LYS:O	1.90	0.72
3:I:56:LYS:HD2	3:I:56:LYS:O	1.90	0.72
3:J:56:LYS:HD2	3:J:56:LYS:O	1.90	0.72
3:K:56:LYS:HD2	3:K:56:LYS:O	1.90	0.71
3:K:625:GLY:HA3	3:K:664:ARG:HD2	1.77	0.67
3:I:625:GLY:HA3	3:I:664:ARG:HD2	1.77	0.66
3:L:625:GLY:HA3	3:L:664:ARG:HD2	1.77	0.66
3:J:625:GLY:HA3	3:J:664:ARG:HD2	1.77	0.66
3:I:330:LEU:HB2	3:I:335:LYS:HE3	1.78	0.65
3:L:330:LEU:HB2	3:L:335:LYS:HE3	1.78	0.65
1:E:406:ALA:HB3	1:E:409:ASN:HD22	1.62	0.65
3:I:577:PRO:O	3:I:580:THR:HG22	1.97	0.65
1:D:326:ASN:N	1:D:326:ASN:OD1	2.30	0.65
3:K:141:THR:O	3:K:145:LEU:HB2	1.97	0.65
3:L:141:THR:O	3:L:145:LEU:HB2	1.97	0.65
3:L:62:LEU:HD21	3:L:147:VAL:HG11	1.79	0.64
3:I:62:LEU:HD21	3:I:147:VAL:HG11	1.79	0.64
3:I:141:THR:O	3:I:145:LEU:HB2	1.97	0.64
3:J:141:THR:O	3:J:145:LEU:HB2	1.97	0.64
1:A:406:ALA:HB3	1:A:409:ASN:HD22	1.62	0.64
2:B:695:LYS:HE3	2:B:697:ASN:HD21	1.63	0.64
1:C:406:ALA:HB3	1:C:409:ASN:HD22	1.62	0.64
2:F:695:LYS:HE3	2:F:697:ASN:HD21	1.63	0.64
3:J:330:LEU:HB2	3:J:335:LYS:HE3	1.78	0.64
1:D:406:ALA:HB3	1:D:409:ASN:HD22	1.62	0.64
3:J:576:LEU:HB3	3:J:577:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:62:LEU:HD21	3:K:147:VAL:HG11	1.79	0.64
3:K:577:PRO:O	3:K:580:THR:HG22	1.97	0.64
1:A:326:ASN:OD1	1:A:326:ASN:N	2.30	0.64
3:L:80:LYS:CG	3:I:577:PRO:HB3	2.23	0.64
2:G:695:LYS:HE3	2:G:697:ASN:HD21	1.63	0.64
3:K:330:LEU:HB2	3:K:335:LYS:HE3	1.78	0.64
3:K:576:LEU:HB3	3:K:577:PRO:HD2	1.80	0.64
3:L:577:PRO:O	3:L:580:THR:HG22	1.97	0.63
3:I:576:LEU:HB3	3:I:577:PRO:HD2	1.80	0.63
1:E:326:ASN:OD1	1:E:326:ASN:N	2.30	0.63
3:L:576:LEU:HB3	3:L:577:PRO:HD2	1.80	0.63
2:H:695:LYS:HE3	2:H:697:ASN:HD21	1.63	0.63
3:J:62:LEU:HD21	3:J:147:VAL:HG11	1.79	0.63
3:J:577:PRO:O	3:J:580:THR:HG22	1.97	0.63
1:C:326:ASN:OD1	1:C:326:ASN:N	2.30	0.62
2:G:184:PRO:HD2	2:G:187:LEU:HD12	1.81	0.62
2:F:184:PRO:HD2	2:F:187:LEU:HD12	1.81	0.62
3:J:80:LYS:CG	3:K:577:PRO:HB3	2.23	0.62
1:A:646:ILE:HG12	1:A:696:VAL:HG22	1.82	0.61
3:J:119:VAL:HG21	3:J:147:VAL:HG22	1.82	0.61
1:C:646:ILE:HG12	1:C:696:VAL:HG22	1.82	0.61
2:H:184:PRO:HD2	2:H:187:LEU:HD12	1.81	0.61
1:E:646:ILE:HG12	1:E:696:VAL:HG22	1.82	0.61
2:B:184:PRO:HD2	2:B:187:LEU:HD12	1.81	0.61
3:I:119:VAL:HG21	3:I:147:VAL:HG22	1.82	0.61
1:D:646:ILE:HG12	1:D:696:VAL:HG22	1.82	0.61
3:I:80:LYS:CG	3:J:577:PRO:HB3	2.23	0.60
3:L:577:PRO:HB3	3:K:80:LYS:CG	2.23	0.60
3:K:119:VAL:HG21	3:K:147:VAL:HG22	1.82	0.60
3:J:450:LEU:HD22	3:J:467:ILE:HG23	1.83	0.60
3:L:567:ASN:HD21	3:L:583:ILE:H	1.50	0.60
3:L:119:VAL:HG21	3:L:147:VAL:HG22	1.82	0.60
3:I:450:LEU:HD22	3:I:467:ILE:HG23	1.83	0.59
3:K:636:LEU:HD22	3:K:655:SER:H	1.68	0.59
3:L:450:LEU:HD22	3:L:467:ILE:HG23	1.83	0.59
3:L:636:LEU:HD22	3:L:655:SER:H	1.68	0.59
3:I:636:LEU:HD22	3:I:655:SER:H	1.68	0.59
3:J:636:LEU:HD22	3:J:655:SER:H	1.68	0.59
1:A:178:ARG:NH1	1:A:224:GLU:OE2	2.34	0.59
3:K:450:LEU:HD22	3:K:467:ILE:HG23	1.83	0.59
1:A:189:VAL:HG23	1:A:190:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:VAL:HG23	1:C:190:GLU:HG3	1.85	0.59
1:C:365:ARG:NH1	1:C:412:PRO:O	2.36	0.59
3:I:567:ASN:HD21	3:I:583:ILE:H	1.50	0.59
1:E:189:VAL:HG23	1:E:190:GLU:HG3	1.85	0.59
3:K:567:ASN:HD21	3:K:583:ILE:H	1.50	0.59
3:J:630:VAL:HG11	3:J:639:ILE:HG21	1.84	0.59
3:K:630:VAL:HG11	3:K:639:ILE:HG21	1.84	0.59
1:D:189:VAL:HG23	1:D:190:GLU:HG3	1.85	0.59
1:E:365:ARG:NH1	1:E:412:PRO:O	2.36	0.59
3:I:80:LYS:HD3	3:I:82:TYR:OH	2.03	0.58
1:E:178:ARG:NH1	1:E:224:GLU:OE2	2.34	0.58
3:K:80:LYS:HB2	3:K:82:TYR:HE2	1.68	0.58
3:K:80:LYS:HD3	3:K:82:TYR:OH	2.03	0.58
1:D:365:ARG:NH1	1:D:412:PRO:O	2.36	0.58
2:G:699:TYR:HB3	2:G:725:LEU:HD23	1.86	0.58
3:J:80:LYS:HB2	3:J:82:TYR:HE2	1.68	0.58
3:J:80:LYS:HD3	3:J:82:TYR:OH	2.03	0.58
1:A:365:ARG:NH1	1:A:412:PRO:O	2.36	0.58
2:B:699:TYR:HB3	2:B:725:LEU:HD23	1.86	0.58
3:L:630:VAL:HG11	3:L:639:ILE:HG21	1.84	0.58
3:J:567:ASN:HD21	3:J:583:ILE:H	1.50	0.58
3:I:449:THR:HG22	3:I:673:LYS:HD3	1.86	0.58
1:E:512:ASP:HB3	1:E:515:GLU:HB2	1.86	0.58
2:F:699:TYR:HB3	2:F:725:LEU:HD23	1.86	0.58
3:L:80:LYS:HD3	3:L:82:TYR:OH	2.03	0.58
3:I:630:VAL:HG11	3:I:639:ILE:HG21	1.84	0.57
3:L:449:THR:HG22	3:L:673:LYS:HD3	1.86	0.57
1:D:512:ASP:HB3	1:D:515:GLU:HB2	1.86	0.57
1:A:512:ASP:HB3	1:A:515:GLU:HB2	1.86	0.57
3:L:80:LYS:HB2	3:L:82:TYR:HE2	1.68	0.57
2:H:699:TYR:HB3	2:H:725:LEU:HD23	1.86	0.57
1:C:512:ASP:HB3	1:C:515:GLU:HB2	1.86	0.57
2:G:189:VAL:HG23	2:G:190:GLU:HG3	1.87	0.57
2:F:406:ALA:HB3	2:F:409:ASN:HD22	1.70	0.57
1:E:274:ASN:HB3	1:E:357:THR:HG23	1.86	0.57
2:B:203:LEU:HD22	3:L:44:VAL:HG23	1.87	0.57
2:B:406:ALA:HB3	2:B:409:ASN:HD22	1.70	0.57
1:D:178:ARG:NH1	1:D:224:GLU:OE2	2.34	0.57
2:H:203:LEU:HD22	3:K:44:VAL:HG23	1.87	0.57
2:F:189:VAL:HG23	2:F:190:GLU:HG3	1.87	0.57
3:I:80:LYS:HB2	3:I:82:TYR:HE2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:327:SER:O	3:J:335:LYS:NZ	2.36	0.57
2:G:203:LEU:HD22	3:J:44:VAL:HG23	1.87	0.57
2:H:406:ALA:HB3	2:H:409:ASN:HD22	1.70	0.56
2:H:609:GLU:HG2	2:H:724:ILE:HG12	1.87	0.56
2:B:609:GLU:HG2	2:B:724:ILE:HG12	1.87	0.56
3:L:673:LYS:NZ	3:L:677:LEU:O	2.39	0.56
1:C:274:ASN:HB3	1:C:357:THR:HG23	1.86	0.56
2:F:203:LEU:HD22	3:I:44:VAL:HG23	1.87	0.56
3:J:673:LYS:NZ	3:J:677:LEU:O	2.39	0.56
2:H:189:VAL:HG23	2:H:190:GLU:HG3	1.87	0.56
2:G:406:ALA:HB3	2:G:409:ASN:HD22	1.70	0.56
3:K:80:LYS:CB	3:K:82:TYR:HE2	2.18	0.56
1:A:274:ASN:HB3	1:A:357:THR:HG23	1.86	0.56
3:I:633:ASP:HA	3:I:670:GLY:H	1.71	0.56
2:B:325:SER:HA	2:B:490:ARG:HH12	1.70	0.56
3:J:292:LEU:HD23	3:J:295:LYS:HD3	1.88	0.56
3:K:292:LEU:HD23	3:K:295:LYS:HD3	1.88	0.56
3:K:449:THR:HG22	3:K:673:LYS:HD3	1.86	0.56
3:L:327:SER:O	3:L:335:LYS:NZ	2.36	0.56
1:D:274:ASN:HB3	1:D:357:THR:HG23	1.86	0.56
2:B:189:VAL:HG23	2:B:190:GLU:HG3	1.87	0.56
3:L:633:ASP:HA	3:L:670:GLY:H	1.71	0.56
3:J:633:ASP:HA	3:J:670:GLY:H	1.71	0.56
3:I:292:LEU:HD23	3:I:295:LYS:HD3	1.88	0.56
3:L:292:LEU:HD23	3:L:295:LYS:HD3	1.88	0.55
2:F:365:ARG:NH1	2:F:412:PRO:O	2.39	0.55
2:F:508:VAL:HG13	2:F:516:THR:HA	1.89	0.55
2:G:609:GLU:HG2	2:G:724:ILE:HG12	1.87	0.55
3:J:449:THR:HG22	3:J:673:LYS:HD3	1.86	0.55
3:L:764:GLN:NE2	3:L:768:ASP:OD2	2.40	0.55
1:C:337:SER:HA	1:C:661:ASP:HB2	1.89	0.55
3:I:673:LYS:NZ	3:I:677:LEU:O	2.39	0.55
2:F:609:GLU:HG2	2:F:724:ILE:HG12	1.87	0.55
3:K:673:LYS:NZ	3:K:677:LEU:O	2.39	0.55
3:I:582:LEU:HD23	3:I:583:ILE:HG13	1.89	0.55
1:E:337:SER:HA	1:E:661:ASP:HB2	1.89	0.55
2:H:365:ARG:NH1	2:H:412:PRO:O	2.39	0.55
3:I:764:GLN:NE2	3:I:768:ASP:OD2	2.40	0.55
2:G:365:ARG:NH1	2:G:412:PRO:O	2.39	0.55
2:G:508:VAL:HG13	2:G:516:THR:HA	1.89	0.55
3:J:764:GLN:NE2	3:J:768:ASP:OD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:631:ILE:HG23	2:H:636:ARG:HH11	1.72	0.55
2:B:365:ARG:NH1	2:B:412:PRO:O	2.39	0.54
3:I:427:ILE:O	3:I:432:TYR:OH	2.25	0.54
2:G:523:LEU:HD22	2:G:578:LEU:HD22	1.88	0.54
2:H:508:VAL:HG13	2:H:516:THR:HA	1.89	0.54
2:H:523:LEU:HD22	2:H:578:LEU:HD22	1.88	0.54
3:K:764:GLN:NE2	3:K:768:ASP:OD2	2.40	0.54
3:J:582:LEU:HD23	3:J:583:ILE:HG13	1.89	0.54
3:K:633:ASP:HA	3:K:670:GLY:H	1.71	0.54
3:L:582:LEU:HD23	3:L:583:ILE:HG13	1.89	0.54
3:I:80:LYS:CB	3:I:82:TYR:HE2	2.18	0.54
1:D:337:SER:HA	1:D:661:ASP:HB2	1.89	0.54
2:G:631:ILE:HG23	2:G:636:ARG:HH11	1.72	0.54
2:B:523:LEU:HD22	2:B:578:LEU:HD22	1.88	0.54
3:K:682:GLU:OE1	3:K:742:ARG:NH1	2.41	0.54
2:B:631:ILE:HG23	2:B:636:ARG:HH11	1.72	0.54
2:F:523:LEU:HD22	2:F:578:LEU:HD22	1.88	0.54
3:I:682:GLU:OE1	3:I:742:ARG:NH1	2.41	0.54
3:J:427:ILE:O	3:J:432:TYR:OH	2.25	0.54
3:L:443:ILE:HD12	3:L:454:LEU:HD22	1.90	0.54
3:J:80:LYS:CB	3:J:82:TYR:HE2	2.18	0.53
3:K:582:LEU:HD23	3:K:583:ILE:HG13	1.89	0.53
1:A:337:SER:HA	1:A:661:ASP:HB2	1.89	0.53
3:L:572:LYS:NZ	3:K:56:LYS:HB2	2.24	0.53
3:J:579:TYR:CG	3:J:579:TYR:O	2.62	0.53
3:K:443:ILE:HD12	3:K:454:LEU:HD22	1.90	0.53
1:A:211:HIS:HD2	1:A:216:LEU:HD12	1.74	0.53
2:B:508:VAL:HG13	2:B:516:THR:HA	1.89	0.53
1:C:178:ARG:NH1	1:C:224:GLU:OE2	2.34	0.53
2:F:631:ILE:HG23	2:F:636:ARG:HH11	1.72	0.53
3:I:327:SER:O	3:I:335:LYS:NZ	2.36	0.53
3:J:682:GLU:OE1	3:J:742:ARG:NH1	2.41	0.53
3:L:56:LYS:HB2	3:I:572:LYS:NZ	2.24	0.53
3:L:682:GLU:OE1	3:L:742:ARG:NH1	2.41	0.53
3:L:80:LYS:HG2	3:I:577:PRO:CB	2.26	0.53
3:L:427:ILE:O	3:L:432:TYR:OH	2.25	0.53
3:J:581:LYS:O	3:J:628:ARG:NH1	2.42	0.53
3:K:427:ILE:O	3:K:432:TYR:OH	2.25	0.53
3:K:579:TYR:CG	3:K:579:TYR:O	2.62	0.53
3:L:579:TYR:CG	3:L:579:TYR:O	2.62	0.53
3:J:56:LYS:HB2	3:K:572:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:581:LYS:O	3:K:628:ARG:NH1	2.42	0.53
3:I:56:LYS:HB2	3:J:572:LYS:NZ	2.24	0.52
1:D:211:HIS:HD2	1:D:216:LEU:HD12	1.74	0.52
1:D:508:VAL:HG13	1:D:516:THR:HA	1.91	0.52
3:J:75:LYS:CE	3:K:579:TYR:HB2	2.38	0.52
3:L:581:LYS:O	3:L:628:ARG:NH1	2.42	0.52
3:I:579:TYR:O	3:I:579:TYR:CG	2.62	0.52
1:D:205:PRO:HD2	3:J:232:VAL:HG21	1.91	0.52
3:I:75:LYS:CE	3:J:579:TYR:HB2	2.38	0.52
3:I:443:ILE:HD12	3:I:454:LEU:HD22	1.90	0.52
3:I:581:LYS:O	3:I:628:ARG:NH1	2.42	0.52
1:E:205:PRO:HD2	3:K:232:VAL:HG21	1.91	0.52
1:E:508:VAL:HG13	1:E:516:THR:HA	1.91	0.52
1:E:211:HIS:HD2	1:E:216:LEU:HD12	1.74	0.52
3:J:443:ILE:HD12	3:J:454:LEU:HD22	1.90	0.52
1:C:508:VAL:HG13	1:C:516:THR:HA	1.91	0.52
3:I:682:GLU:HB3	3:I:742:ARG:HD2	1.92	0.52
3:L:75:LYS:CE	3:I:579:TYR:HB2	2.38	0.51
1:C:211:HIS:HD2	1:C:216:LEU:HD12	1.74	0.51
1:A:205:PRO:HD2	3:L:232:VAL:HG21	1.91	0.51
2:B:648:ASP:HB2	2:B:652:LEU:H	1.76	0.51
2:F:648:ASP:HB2	2:F:652:LEU:H	1.76	0.51
3:L:682:GLU:HB3	3:L:742:ARG:HD2	1.92	0.51
1:C:205:PRO:HD2	3:I:232:VAL:HG21	1.91	0.51
3:L:579:TYR:HB2	3:K:75:LYS:CE	2.38	0.51
1:A:508:VAL:HG13	1:A:516:THR:HA	1.91	0.51
3:I:80:LYS:HG2	3:J:577:PRO:CB	2.26	0.51
2:G:514:LEU:HD13	1:E:242:ARG:HG3	1.93	0.50
2:F:514:LEU:HD13	1:D:242:ARG:HG3	1.93	0.50
2:G:642:TYR:HB2	2:G:665:ILE:HD11	1.94	0.50
3:J:682:GLU:HB3	3:J:742:ARG:HD2	1.92	0.50
2:H:642:TYR:HB2	2:H:665:ILE:HD11	1.94	0.50
3:J:80:LYS:HG2	3:K:577:PRO:CB	2.26	0.50
3:L:80:LYS:CB	3:L:82:TYR:HE2	2.18	0.50
1:A:242:ARG:HG3	2:H:514:LEU:HD13	1.93	0.50
3:K:486:VAL:N	3:K:519:LEU:O	2.45	0.50
3:K:682:GLU:HB3	3:K:742:ARG:HD2	1.92	0.50
2:F:642:TYR:HB2	2:F:665:ILE:HD11	1.94	0.50
2:H:648:ASP:HB2	2:H:652:LEU:H	1.76	0.50
3:J:486:VAL:N	3:J:519:LEU:O	2.45	0.49
2:B:642:TYR:HB2	2:B:665:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ASN:HB3	1:C:500:LEU:HD23	1.94	0.49
2:G:648:ASP:HB2	2:G:652:LEU:H	1.76	0.49
1:A:494:ASN:HB3	1:A:500:LEU:HD23	1.94	0.49
3:L:486:VAL:N	3:L:519:LEU:O	2.45	0.49
1:D:240:THR:HG21	1:D:242:ARG:HH11	1.78	0.49
3:L:57:GLU:HG2	3:L:61:LYS:HE3	1.94	0.49
2:F:365:ARG:NH1	2:F:413:SER:O	2.46	0.49
3:K:57:GLU:HG2	3:K:61:LYS:HE3	1.94	0.49
2:B:365:ARG:NH1	2:B:413:SER:O	2.46	0.49
2:B:514:LEU:HD13	1:C:242:ARG:HG3	1.93	0.49
1:A:635:ILE:HG23	1:A:638:ILE:HD11	1.95	0.49
1:C:635:ILE:HG23	1:C:638:ILE:HD11	1.95	0.49
3:J:80:LYS:HB3	3:J:82:TYR:CZ	2.48	0.49
1:C:240:THR:HG21	1:C:242:ARG:HH11	1.78	0.48
1:C:270:ILE:HG13	1:C:361:ASN:HB3	1.96	0.48
1:D:635:ILE:HG23	1:D:638:ILE:HD11	1.95	0.48
2:B:730:LYS:H	2:B:734:ILE:HD11	1.79	0.48
3:I:80:LYS:HB3	3:I:82:TYR:CZ	2.48	0.48
1:E:270:ILE:HG13	1:E:361:ASN:HB3	1.96	0.48
1:E:635:ILE:HG23	1:E:638:ILE:HD11	1.95	0.48
3:K:700:LEU:HD11	3:K:708:VAL:HG23	1.95	0.48
3:L:700:LEU:HD11	3:L:708:VAL:HG23	1.95	0.48
3:J:442:ASN:HD21	3:J:444:ASN:HD22	1.61	0.48
3:L:80:LYS:HB3	3:L:82:TYR:CZ	2.48	0.48
3:L:586:ASN:O	3:L:632:THR:OG1	2.24	0.48
3:J:57:GLU:HG2	3:J:61:LYS:HE3	1.94	0.48
1:A:240:THR:HG21	1:A:242:ARG:HH11	1.78	0.48
3:I:57:GLU:HG2	3:I:61:LYS:HE3	1.94	0.48
3:K:327:SER:O	3:K:335:LYS:NZ	2.36	0.48
1:A:270:ILE:HG13	1:A:361:ASN:HB3	1.96	0.48
1:D:270:ILE:HG13	1:D:361:ASN:HB3	1.96	0.48
2:H:497:ASP:OD1	2:H:497:ASP:N	2.46	0.48
1:E:240:THR:HG21	1:E:242:ARG:HH11	1.78	0.48
1:A:547:ILE:HA	1:A:550:PHE:HD2	1.79	0.48
3:I:442:ASN:HD21	3:I:444:ASN:HD22	1.61	0.48
1:D:494:ASN:HB3	1:D:500:LEU:HD23	1.94	0.48
2:G:730:LYS:H	2:G:734:ILE:HD11	1.79	0.48
3:K:442:ASN:HD21	3:K:444:ASN:HD22	1.61	0.48
3:L:442:ASN:HD21	3:L:444:ASN:HD22	1.61	0.47
1:E:494:ASN:HB3	1:E:500:LEU:HD23	1.94	0.47
2:H:365:ARG:NH1	2:H:413:SER:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:VAL:O	2:B:328:ASN:ND2	2.45	0.47
3:L:633:ASP:HB2	3:L:671:PRO:HD3	1.96	0.47
1:C:547:ILE:HA	1:C:550:PHE:HD2	1.79	0.47
3:K:609:ASN:HD22	3:K:685:ILE:HD11	1.79	0.47
3:J:609:ASN:HD22	3:J:685:ILE:HD11	1.79	0.47
2:F:730:LYS:H	2:F:734:ILE:HD11	1.79	0.47
3:I:700:LEU:HD11	3:I:708:VAL:HG23	1.95	0.47
1:D:547:ILE:HA	1:D:550:PHE:HD2	1.79	0.47
3:J:700:LEU:HD11	3:J:708:VAL:HG23	1.95	0.47
2:H:644:VAL:HA	2:H:698:VAL:HA	1.97	0.47
3:L:224:TYR:OH	3:L:245:ASP:OD1	2.29	0.47
2:B:497:ASP:N	2:B:497:ASP:OD1	2.46	0.47
3:I:633:ASP:HB2	3:I:671:PRO:HD3	1.96	0.47
2:H:730:LYS:H	2:H:734:ILE:HD11	1.79	0.47
3:L:300:ILE:HB	3:L:386:TYR:HB3	1.97	0.46
3:K:633:ASP:HB2	3:K:671:PRO:HD3	1.96	0.46
1:D:195:ASP:OD2	1:D:214:LYS:NZ	2.49	0.46
3:L:609:ASN:HD22	3:L:685:ILE:HD11	1.79	0.46
2:G:717:SER:OG	2:G:718:THR:N	2.49	0.46
3:J:633:ASP:HB2	3:J:671:PRO:HD3	1.96	0.46
1:E:547:ILE:HA	1:E:550:PHE:HD2	1.79	0.46
3:K:300:ILE:HB	3:K:386:TYR:HB3	1.97	0.46
1:D:184:PRO:HD2	1:D:187:LEU:HD12	1.97	0.46
1:E:687:LEU:HD21	1:E:696:VAL:HG21	1.98	0.46
3:L:578:LYS:HB3	3:K:81:ILE:HB	1.98	0.46
3:J:224:TYR:OH	3:J:245:ASP:OD1	2.29	0.46
3:K:586:ASN:HD22	3:K:639:ILE:HG23	1.80	0.46
1:A:184:PRO:HD2	1:A:187:LEU:HD12	1.97	0.46
1:A:195:ASP:OD2	1:A:214:LYS:NZ	2.49	0.46
3:L:577:PRO:CB	3:K:80:LYS:HG2	2.26	0.46
2:F:644:VAL:HA	2:F:698:VAL:HA	1.97	0.46
2:G:497:ASP:N	2:G:497:ASP:OD1	2.46	0.46
3:I:486:VAL:N	3:I:519:LEU:O	2.45	0.46
3:K:459:ASP:OD2	3:K:461:THR:OG1	2.27	0.46
3:I:81:ILE:HB	3:J:578:LYS:HB3	1.98	0.46
3:I:609:ASN:HD22	3:I:685:ILE:HD11	1.79	0.46
2:G:365:ARG:NH1	2:G:413:SER:O	2.46	0.46
2:F:497:ASP:OD1	2:F:497:ASP:N	2.46	0.46
2:H:717:SER:OG	2:H:718:THR:N	2.49	0.46
3:I:552:LYS:NZ	3:I:556:ASP:OD2	2.42	0.46
1:D:687:LEU:HD21	1:D:696:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:586:ASN:HD22	3:J:639:ILE:HG23	1.80	0.46
3:K:80:LYS:HB3	3:K:82:TYR:CZ	2.48	0.46
3:L:267:ARG:HH12	3:L:490:GLU:HB3	1.81	0.45
3:L:629:PHE:HE1	3:L:666:ILE:HD12	1.81	0.45
3:I:629:PHE:HE1	3:I:666:ILE:HD12	1.81	0.45
1:D:195:ASP:OD2	3:J:236:TYR:OH	2.28	0.45
2:G:540:LEU:HD22	2:G:547:ILE:HD13	1.98	0.45
3:J:267:ARG:HH12	3:J:490:GLU:HB3	1.81	0.45
3:K:85:ASP:OD1	3:K:133:SER:OG	2.34	0.45
3:J:81:ILE:HB	3:K:578:LYS:HB3	1.98	0.45
1:E:184:PRO:HD2	1:E:187:LEU:HD12	1.97	0.45
3:L:586:ASN:HD22	3:L:639:ILE:HG23	1.80	0.45
1:A:345:THR:HG22	1:A:348:GLU:H	1.82	0.45
2:B:540:LEU:HD22	2:B:547:ILE:HD13	1.98	0.45
3:L:281:TRP:HZ2	3:L:422:LEU:HB3	1.82	0.45
2:F:540:LEU:HD22	2:F:547:ILE:HD13	1.98	0.45
3:I:586:ASN:HD22	3:I:639:ILE:HG23	1.80	0.45
3:K:629:PHE:HE1	3:K:666:ILE:HD12	1.81	0.45
3:K:739:GLU:OE2	3:K:742:ARG:NH2	2.44	0.45
2:B:644:VAL:HA	2:B:698:VAL:HA	1.97	0.45
3:L:406:LEU:HD12	3:L:409:ARG:HH12	1.82	0.45
3:I:267:ARG:HH12	3:I:490:GLU:HB3	1.81	0.45
3:J:629:PHE:HE1	3:J:666:ILE:HD12	1.81	0.45
3:K:281:TRP:HZ2	3:K:422:LEU:HB3	1.82	0.45
3:L:459:ASP:OD2	3:L:461:THR:OG1	2.27	0.45
1:C:184:PRO:HD2	1:C:187:LEU:HD12	1.97	0.45
2:F:717:SER:OG	2:F:718:THR:N	2.49	0.45
2:G:644:VAL:HA	2:G:698:VAL:HA	1.97	0.45
2:H:540:LEU:HD22	2:H:547:ILE:HD13	1.98	0.45
3:I:300:ILE:HB	3:I:386:TYR:HB3	1.97	0.45
3:K:552:LYS:NZ	3:K:556:ASP:OD2	2.42	0.45
1:A:687:LEU:HD21	1:A:696:VAL:HG21	1.98	0.45
2:F:232:PRO:HG3	2:F:459:ILE:HD13	1.99	0.45
3:J:85:ASP:OD1	3:J:133:SER:OG	2.34	0.45
3:J:300:ILE:HB	3:J:386:TYR:HB3	1.97	0.45
1:E:195:ASP:OD2	3:K:236:TYR:OH	2.28	0.45
1:E:345:THR:HG22	1:E:348:GLU:H	1.82	0.45
3:L:505:LEU:HD22	3:L:509:THR:HG21	1.99	0.45
1:C:687:LEU:HD21	1:C:696:VAL:HG21	1.98	0.45
1:D:699:TYR:HA	1:D:726:ILE:HG12	1.99	0.45
3:J:281:TRP:HZ2	3:J:422:LEU:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:586:ASN:O	3:J:632:THR:OG1	2.24	0.45
3:L:81:ILE:HB	3:I:578:LYS:HB3	1.98	0.45
3:L:632:THR:HG21	3:L:639:ILE:HG12	1.99	0.45
3:J:406:LEU:HD12	3:J:409:ARG:HH12	1.82	0.45
1:E:195:ASP:OD2	1:E:214:LYS:NZ	2.49	0.45
2:B:232:PRO:HG3	2:B:459:ILE:HD13	1.99	0.44
3:I:281:TRP:HZ2	3:I:422:LEU:HB3	1.82	0.44
2:G:232:PRO:HG3	2:G:459:ILE:HD13	1.99	0.44
3:J:552:LYS:NZ	3:J:556:ASP:OD2	2.42	0.44
3:J:505:LEU:HD22	3:J:509:THR:HG21	1.99	0.44
3:K:298:ILE:H	3:K:298:ILE:HG13	1.70	0.44
3:L:85:ASP:OD1	3:L:133:SER:OG	2.34	0.44
3:K:267:ARG:HH12	3:K:490:GLU:HB3	1.81	0.44
2:B:717:SER:OG	2:B:718:THR:N	2.49	0.44
3:L:552:LYS:NZ	3:L:556:ASP:OD2	2.42	0.44
2:H:179:ASP:OD1	2:H:179:ASP:N	2.45	0.44
3:K:406:LEU:HD12	3:K:409:ARG:HH12	1.82	0.44
1:C:195:ASP:OD2	1:C:214:LYS:NZ	2.49	0.44
1:C:345:THR:HG22	1:C:348:GLU:H	1.82	0.44
2:F:179:ASP:OD1	2:F:179:ASP:N	2.45	0.44
3:I:85:ASP:OD1	3:I:133:SER:OG	2.34	0.44
1:E:699:TYR:HA	1:E:726:ILE:HG12	1.99	0.44
2:H:232:PRO:HG3	2:H:459:ILE:HD13	1.99	0.44
3:K:632:THR:HG21	3:K:639:ILE:HG12	1.99	0.44
1:A:699:TYR:HA	1:A:726:ILE:HG12	1.99	0.44
3:I:406:LEU:HD12	3:I:409:ARG:HH12	1.82	0.44
3:I:632:THR:HG21	3:I:639:ILE:HG12	1.99	0.44
1:D:345:THR:HG22	1:D:348:GLU:H	1.82	0.44
3:K:224:TYR:OH	3:K:245:ASP:OD1	2.29	0.44
3:J:271:TRP:HZ3	3:J:517:GLY:HA2	1.83	0.43
3:J:632:THR:HG21	3:J:639:ILE:HG12	1.99	0.43
2:B:491:ILE:HD12	2:B:505:ILE:HD13	2.01	0.43
3:L:754:LYS:HA	3:L:757:LYS:HG2	2.01	0.43
3:I:459:ASP:OD2	3:I:461:THR:OG1	2.27	0.43
3:I:505:LEU:HD22	3:I:509:THR:HG21	1.99	0.43
3:I:754:LYS:HA	3:I:757:LYS:HG2	2.01	0.43
3:K:271:TRP:HZ3	3:K:517:GLY:HA2	1.83	0.43
1:C:699:TYR:HA	1:C:726:ILE:HG12	1.99	0.43
3:J:298:ILE:H	3:J:298:ILE:HG13	1.70	0.43
2:B:270:ILE:HG13	2:B:361:ASN:HB3	2.00	0.43
1:C:253:HIS:HE1	1:C:255:LEU:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:LYS:HA	3:I:40:MET:HG2	2.01	0.43
1:D:253:HIS:HE1	1:D:255:LEU:HD12	1.84	0.43
2:H:491:ILE:HD12	2:H:505:ILE:HD13	2.01	0.43
1:A:253:HIS:HE1	1:A:255:LEU:HD12	1.84	0.43
3:J:459:ASP:OD2	3:J:461:THR:OG1	2.27	0.43
3:J:754:LYS:HA	3:J:757:LYS:HG2	2.01	0.43
2:H:270:ILE:HG13	2:H:361:ASN:HB3	2.00	0.43
3:L:271:TRP:HZ3	3:L:517:GLY:HA2	1.83	0.43
2:G:491:ILE:HD12	2:G:505:ILE:HD13	2.01	0.43
3:J:37:LYS:HA	3:J:40:MET:HG2	2.01	0.43
3:K:505:LEU:HD22	3:K:509:THR:HG21	1.99	0.43
2:F:491:ILE:HD12	2:F:505:ILE:HD13	2.01	0.43
3:I:271:TRP:CZ3	3:I:517:GLY:HA2	2.54	0.43
3:K:754:LYS:HA	3:K:757:LYS:HG2	2.01	0.43
3:I:271:TRP:HZ3	3:I:517:GLY:HA2	1.83	0.43
1:D:213:LYS:NZ	3:J:187:ASP:OD1	2.48	0.42
1:E:197:LYS:NZ	3:K:184:ASP:OD2	2.46	0.42
3:K:271:TRP:CZ3	3:K:517:GLY:HA2	2.54	0.42
2:G:270:ILE:HG13	2:G:361:ASN:HB3	2.00	0.42
3:J:271:TRP:CZ3	3:J:517:GLY:HA2	2.54	0.42
1:E:253:HIS:HE1	1:E:255:LEU:HD12	1.84	0.42
3:K:37:LYS:HA	3:K:40:MET:HG2	2.01	0.42
3:K:586:ASN:O	3:K:632:THR:OG1	2.24	0.42
3:L:252:ILE:HD12	3:L:252:ILE:HA	1.94	0.42
1:C:179:ASP:OD1	1:C:179:ASP:N	2.50	0.42
3:K:57:GLU:HA	3:K:60:GLU:HG2	2.01	0.42
2:G:512:LYS:HB3	2:G:515:GLU:HB2	2.02	0.42
3:L:37:LYS:HA	3:L:40:MET:HG2	2.01	0.42
1:D:536:PRO:HG2	1:D:541:GLN:HE21	1.85	0.42
1:C:536:PRO:HG2	1:C:541:GLN:HE21	1.85	0.42
2:F:270:ILE:HG13	2:F:361:ASN:HB3	2.00	0.42
3:I:739:GLU:OE2	3:I:742:ARG:NH2	2.44	0.42
3:J:739:GLU:OE2	3:J:742:ARG:NH2	2.44	0.42
3:L:307:ILE:O	3:L:310:SER:OG	2.30	0.42
2:F:512:LYS:HB3	2:F:515:GLU:HB2	2.02	0.42
3:I:669:HIS:CE1	3:I:671:PRO:HD2	2.55	0.42
3:L:57:GLU:HA	3:L:60:GLU:HG2	2.01	0.42
1:C:627:LEU:O	1:C:676:ILE:N	2.52	0.42
1:D:644:VAL:HG23	1:D:698:VAL:HG22	2.02	0.42
3:J:57:GLU:HA	3:J:60:GLU:HG2	2.01	0.42
1:E:644:VAL:HG23	1:E:698:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:512:LYS:HB3	2:H:515:GLU:HB2	2.02	0.42
2:B:512:LYS:HB3	2:B:515:GLU:HB2	2.02	0.41
3:I:82:TYR:CD2	3:I:128:VAL:HG13	2.55	0.41
1:E:378:LEU:HB2	1:E:396:ALA:HB2	2.02	0.41
1:E:536:PRO:HG2	1:E:541:GLN:HE21	1.85	0.41
1:E:627:LEU:O	1:E:676:ILE:N	2.52	0.41
3:J:82:TYR:CD2	3:J:128:VAL:HG13	2.55	0.41
1:A:378:LEU:HB2	1:A:396:ALA:HB2	2.02	0.41
3:L:271:TRP:CZ3	3:L:517:GLY:HA2	2.54	0.41
3:L:669:HIS:CE1	3:L:671:PRO:HD2	2.55	0.41
3:J:384:GLN:HA	3:J:385:PRO:HD3	1.92	0.41
3:K:668:LEU:HD12	3:K:668:LEU:HA	1.93	0.41
1:A:536:PRO:HG2	1:A:541:GLN:HE21	1.85	0.41
3:L:82:TYR:CD2	3:L:128:VAL:HG13	2.55	0.41
3:J:669:HIS:CE1	3:J:671:PRO:HD2	2.55	0.41
3:K:440:ASN:HD21	3:K:500:LYS:NZ	2.19	0.41
3:L:440:ASN:HD21	3:L:500:LYS:NZ	2.19	0.41
3:K:82:TYR:CD2	3:K:128:VAL:HG13	2.55	0.41
3:I:524:ASN:HB3	3:I:552:LYS:HD2	2.03	0.41
3:I:586:ASN:O	3:I:632:THR:OG1	2.24	0.41
1:D:378:LEU:HB2	1:D:396:ALA:HB2	2.02	0.41
1:A:533:PHE:CE2	1:A:542:TYR:HB2	2.56	0.41
2:F:464:PHE:HD2	3:I:32:GLN:HE21	1.68	0.41
3:I:39:ILE:HD12	3:I:39:ILE:HA	1.96	0.41
3:J:440:ASN:HD21	3:J:500:LYS:NZ	2.19	0.41
3:K:669:HIS:CE1	3:K:671:PRO:HD2	2.55	0.41
1:C:378:LEU:HB2	1:C:396:ALA:HB2	2.02	0.41
3:I:307:ILE:O	3:I:310:SER:OG	2.30	0.41
3:I:322:ILE:HD11	3:I:376:LEU:HD11	2.03	0.41
1:D:533:PHE:CE2	1:D:542:TYR:HB2	2.56	0.41
3:J:524:ASN:HB3	3:J:552:LYS:HD2	2.03	0.41
1:C:533:PHE:CE2	1:C:542:TYR:HB2	2.56	0.41
3:K:87:ASP:OD2	3:K:89:THR:OG1	2.31	0.41
3:K:399:ILE:H	3:K:399:ILE:HG13	1.56	0.41
3:L:668:LEU:HD12	3:L:668:LEU:HA	1.93	0.40
3:I:298:ILE:H	3:I:298:ILE:HG13	1.70	0.40
1:E:644:VAL:HG13	1:E:656:ILE:HG22	2.03	0.40
3:I:57:GLU:HA	3:I:60:GLU:HG2	2.01	0.40
2:G:464:PHE:HD2	3:J:32:GLN:HE21	1.68	0.40
3:J:56:LYS:HB2	3:K:572:LYS:HZ1	1.86	0.40
3:K:252:ILE:HD12	3:K:252:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:322:ILE:HD11	3:L:376:LEU:HD11	2.03	0.40
1:C:329:SER:HB2	1:C:450:LEU:O	2.22	0.40
2:F:616:HIS:CD2	2:F:629:LEU:HD11	2.56	0.40
3:I:56:LYS:HB2	3:J:572:LYS:HZ2	1.86	0.40
1:E:533:PHE:CE2	1:E:542:TYR:HB2	2.56	0.40
2:H:616:HIS:CD2	2:H:629:LEU:HD11	2.56	0.40
3:K:322:ILE:HD11	3:K:376:LEU:HD11	2.03	0.40
1:A:266:MET:H	1:A:295:THR:HG21	1.87	0.40
2:B:464:PHE:HD2	3:L:32:GLN:HE21	1.68	0.40
3:L:524:ASN:HB3	3:L:552:LYS:HD2	2.03	0.40
1:D:298:THR:HG22	1:D:603:ILE:HD11	2.04	0.40
1:E:329:SER:HB2	1:E:450:LEU:O	2.22	0.40
2:H:464:PHE:HD2	3:K:32:GLN:HE21	1.68	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	515/735 (70%)	490 (95%)	25 (5%)	0	100	100
1	C	515/735 (70%)	490 (95%)	25 (5%)	0	100	100
1	D	515/735 (70%)	490 (95%)	25 (5%)	0	100	100
1	E	515/735 (70%)	490 (95%)	25 (5%)	0	100	100
2	B	515/735 (70%)	481 (93%)	34 (7%)	0	100	100
2	F	515/735 (70%)	481 (93%)	34 (7%)	0	100	100
2	G	515/735 (70%)	481 (93%)	34 (7%)	0	100	100
2	H	515/735 (70%)	481 (93%)	34 (7%)	0	100	100
3	I	719/776 (93%)	676 (94%)	43 (6%)	0	100	100
3	J	719/776 (93%)	676 (94%)	43 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	719/776 (93%)	676 (94%)	43 (6%)	0	100	100
3	L	719/776 (93%)	676 (94%)	43 (6%)	0	100	100
All	All	6996/8984 (78%)	6588 (94%)	408 (6%)	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	470/659 (71%)	467 (99%)	3 (1%)	86	92
1	C	470/659 (71%)	467 (99%)	3 (1%)	86	92
1	D	470/659 (71%)	467 (99%)	3 (1%)	86	92
1	E	470/659 (71%)	467 (99%)	3 (1%)	86	92
2	B	471/660 (71%)	468 (99%)	3 (1%)	86	92
2	F	471/660 (71%)	470 (100%)	1 (0%)	93	97
2	G	471/660 (71%)	470 (100%)	1 (0%)	93	97
2	H	471/660 (71%)	470 (100%)	1 (0%)	93	97
3	I	657/710 (92%)	650 (99%)	7 (1%)	73	85
3	J	657/710 (92%)	650 (99%)	7 (1%)	73	85
3	K	657/710 (92%)	650 (99%)	7 (1%)	73	85
3	L	657/710 (92%)	650 (99%)	7 (1%)	73	85
All	All	6392/8116 (79%)	6346 (99%)	46 (1%)	84	91

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	A	328	ASN
1	A	644	VAL
2	B	325	SER

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Mol	Chain	Res	Type
2	B	328	ASN
2	B	512	LYS
3	L	56	LYS
3	L	253	ASN
3	L	373	LYS
3	L	523	ARG
3	L	578	LYS
3	L	594	ASN
3	L	704	GLN
1	C	326	ASN
1	C	328	ASN
1	C	644	VAL
2	F	512	LYS
3	I	56	LYS
3	I	253	ASN
3	I	373	LYS
3	I	523	ARG
3	I	578	LYS
3	I	594	ASN
3	I	704	GLN
1	D	326	ASN
1	D	328	ASN
1	D	644	VAL
2	G	512	LYS
3	J	56	LYS
3	J	253	ASN
3	J	373	LYS
3	J	523	ARG
3	J	578	LYS
3	J	594	ASN
3	J	704	GLN
1	E	326	ASN
1	E	328	ASN
1	E	644	VAL
2	H	512	LYS
3	K	56	LYS
3	K	253	ASN
3	K	373	LYS
3	K	523	ARG
3	K	578	LYS
3	K	594	ASN
3	K	704	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	326	ASN
1	A	363	ASN
1	A	409	ASN
1	A	541	GLN
2	B	363	ASN
2	B	409	ASN
2	B	422	ASN
2	B	616	HIS
2	B	697	ASN
3	L	32	GLN
3	L	117	HIS
3	L	253	ASN
3	L	393	GLN
3	L	440	ASN
3	L	444	ASN
3	L	445	ASN
3	L	567	ASN
3	L	571	ASN
3	L	586	ASN
3	L	609	ASN
3	L	704	GLN
3	L	769	GLN
1	C	263	HIS
1	C	326	ASN
1	C	363	ASN
1	C	409	ASN
1	C	541	GLN
2	F	363	ASN
2	F	409	ASN
2	F	422	ASN
2	F	616	HIS
2	F	697	ASN
3	I	32	GLN
3	I	117	HIS
3	I	253	ASN
3	I	393	GLN
3	I	440	ASN
3	I	444	ASN
3	I	445	ASN
3	I	567	ASN

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Mol	Chain	Res	Type
3	I	571	ASN
3	I	586	ASN
3	I	609	ASN
3	I	704	GLN
3	I	769	GLN
1	D	263	HIS
1	D	326	ASN
1	D	363	ASN
1	D	409	ASN
1	D	541	GLN
2	G	363	ASN
2	G	409	ASN
2	G	422	ASN
2	G	616	HIS
2	G	697	ASN
3	J	32	GLN
3	J	117	HIS
3	J	253	ASN
3	J	393	GLN
3	J	440	ASN
3	J	444	ASN
3	J	445	ASN
3	J	567	ASN
3	J	571	ASN
3	J	586	ASN
3	J	609	ASN
3	J	704	GLN
3	J	769	GLN
1	E	263	HIS
1	E	326	ASN
1	E	363	ASN
1	E	409	ASN
1	E	541	GLN
2	H	363	ASN
2	H	409	ASN
2	H	422	ASN
2	H	616	HIS
2	H	697	ASN
3	K	32	GLN
3	K	117	HIS
3	K	253	ASN
3	K	393	GLN

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Mol	Chain	Res	Type
3	K	440	ASN
3	K	444	ASN
3	K	445	ASN
3	K	567	ASN
3	K	571	ASN
3	K	586	ASN
3	K	609	ASN
3	K	704	GLN
3	K	769	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 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	$\# Z > 2$
5	SO4	I	801	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	J	801	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	L	801	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	K	801	-	4,4,4	0.13	0	6,6,6	0.09	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

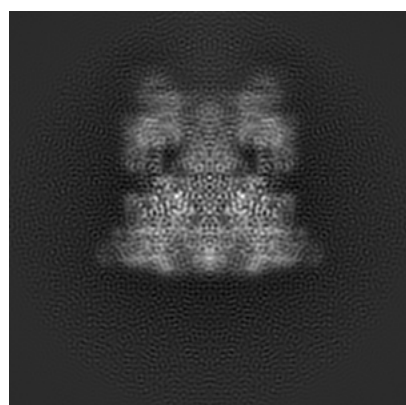
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21694. These allow visual inspection of the internal detail of the map and identification of artifacts.

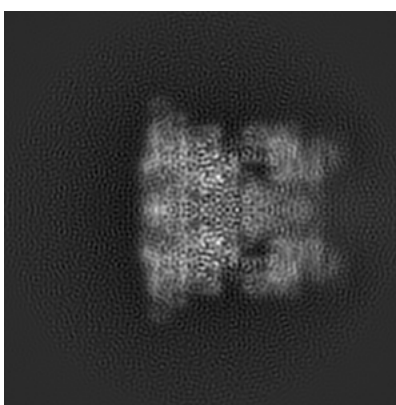
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

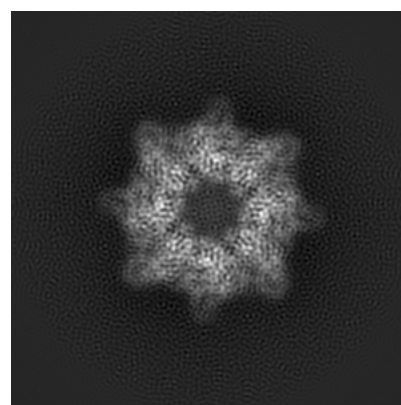
6.1.1 Primary map



X



Y

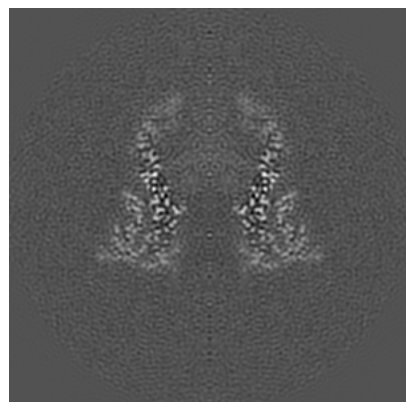


Z

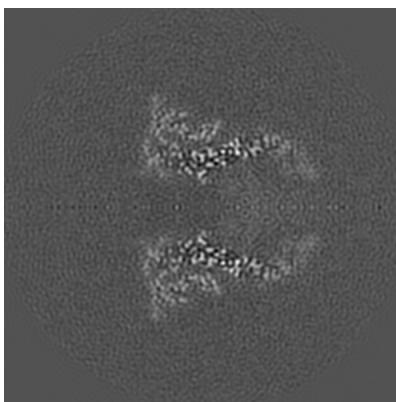
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

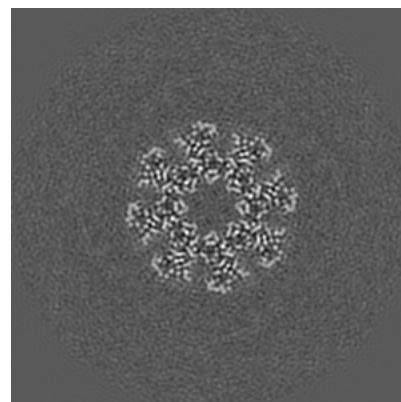
6.2.1 Primary map



X Index: 150



Y Index: 150

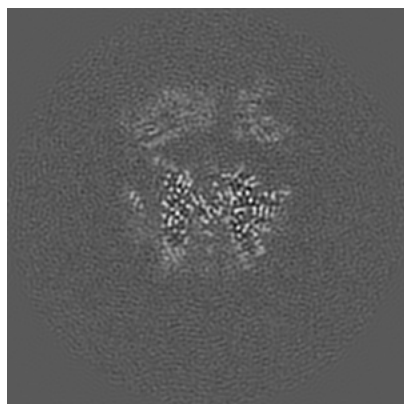


Z Index: 150

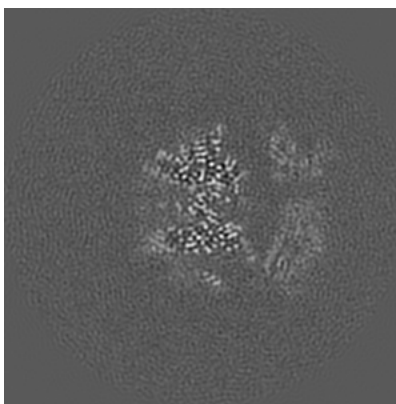
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

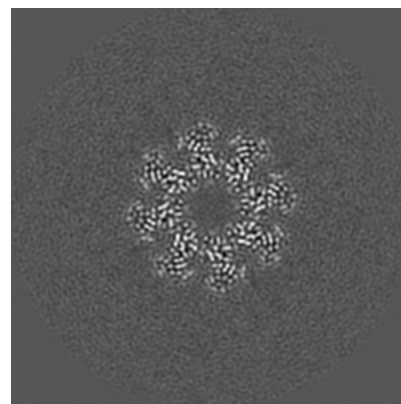
6.3.1 Primary map



X Index: 176



Y Index: 124

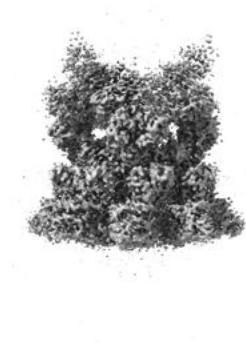


Z Index: 148

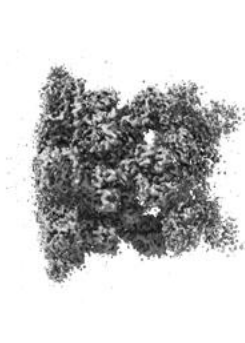
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

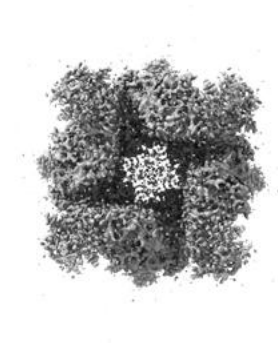
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

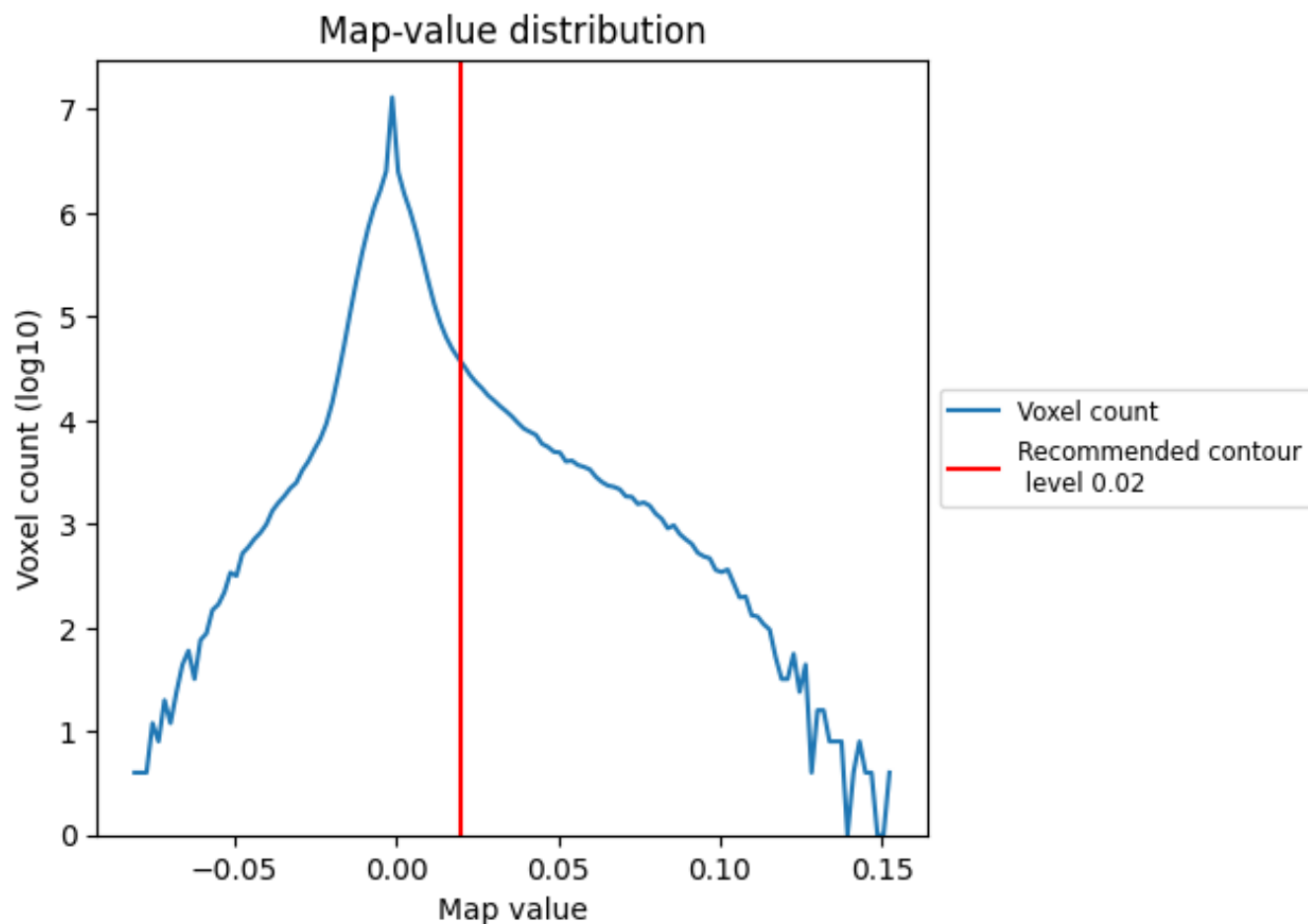
6.5 Mask visualisation

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

7 Map analysis [i](#)

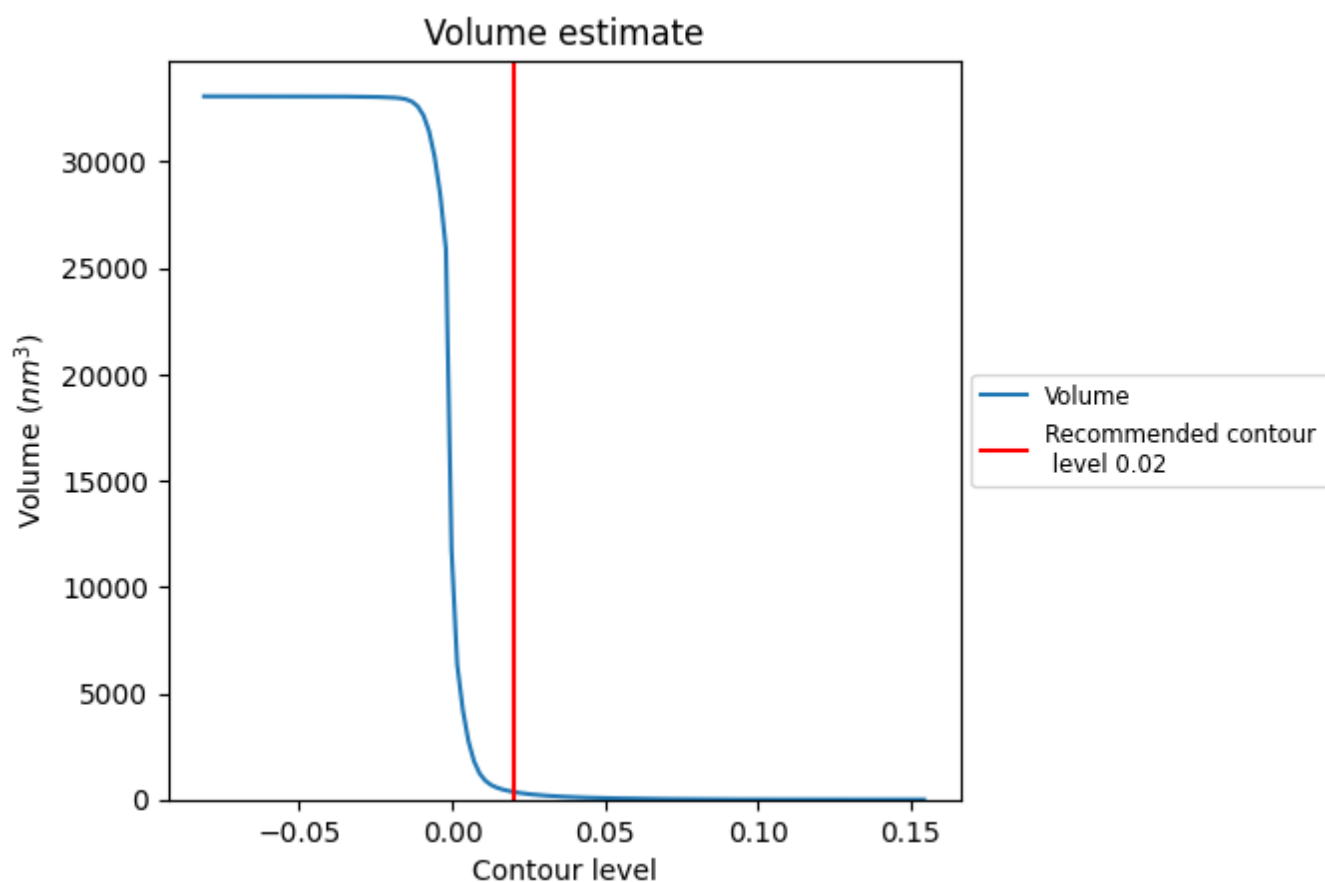
This section contains the results of statistical analysis of the map.

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.

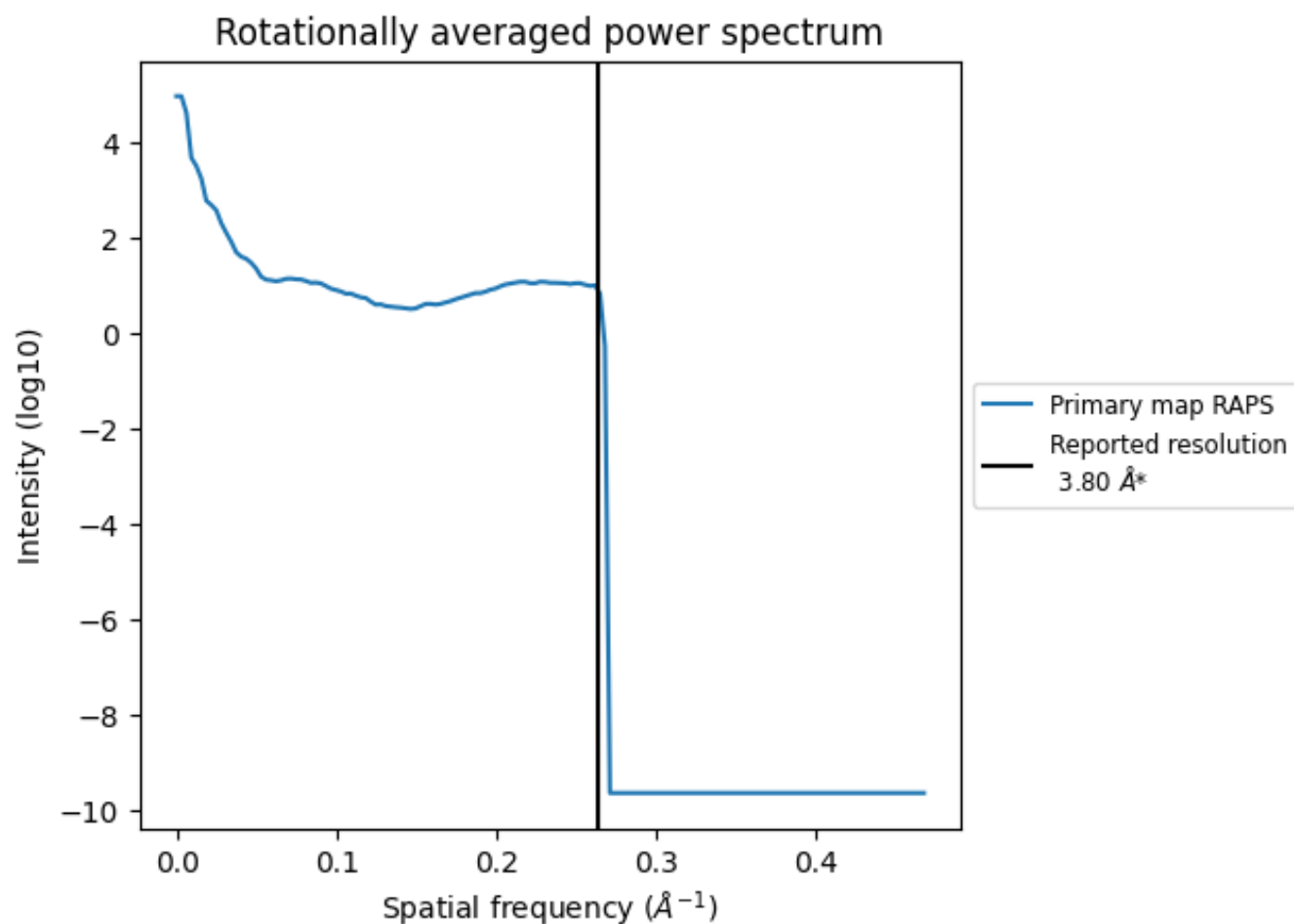
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm³; this corresponds to an approximate mass of 328 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 0.263 Å⁻¹

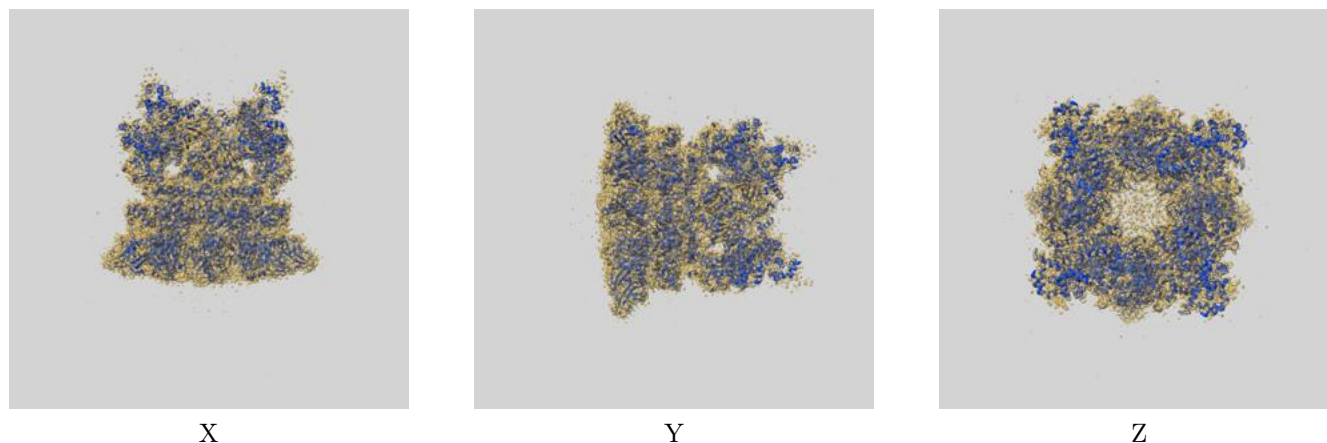
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

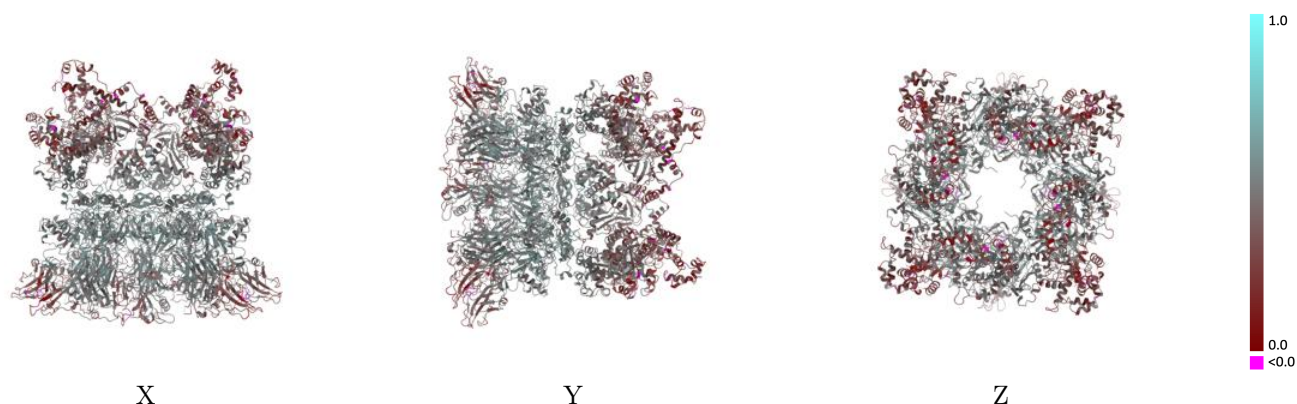
This section contains information regarding the fit between EMDB map EMD-21694 and PDB model 6WJJ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



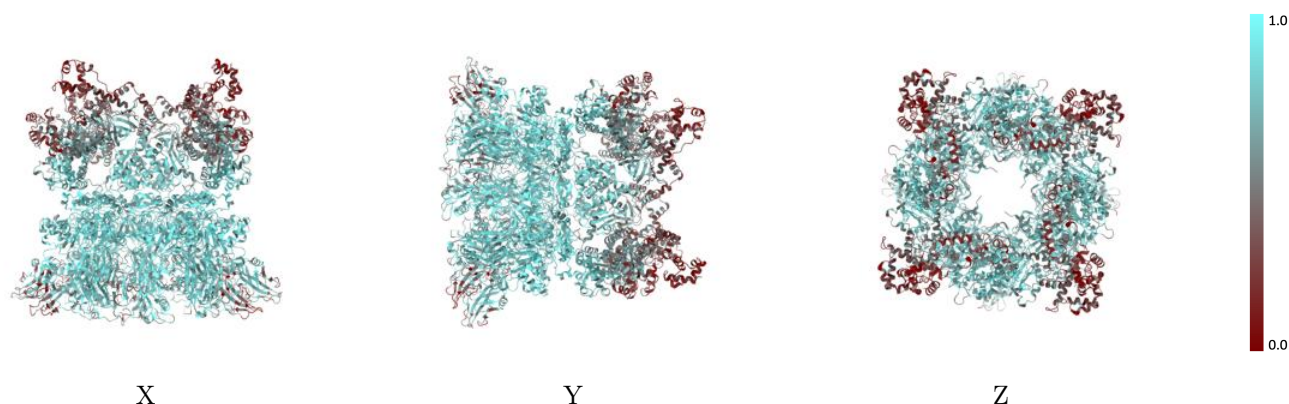
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



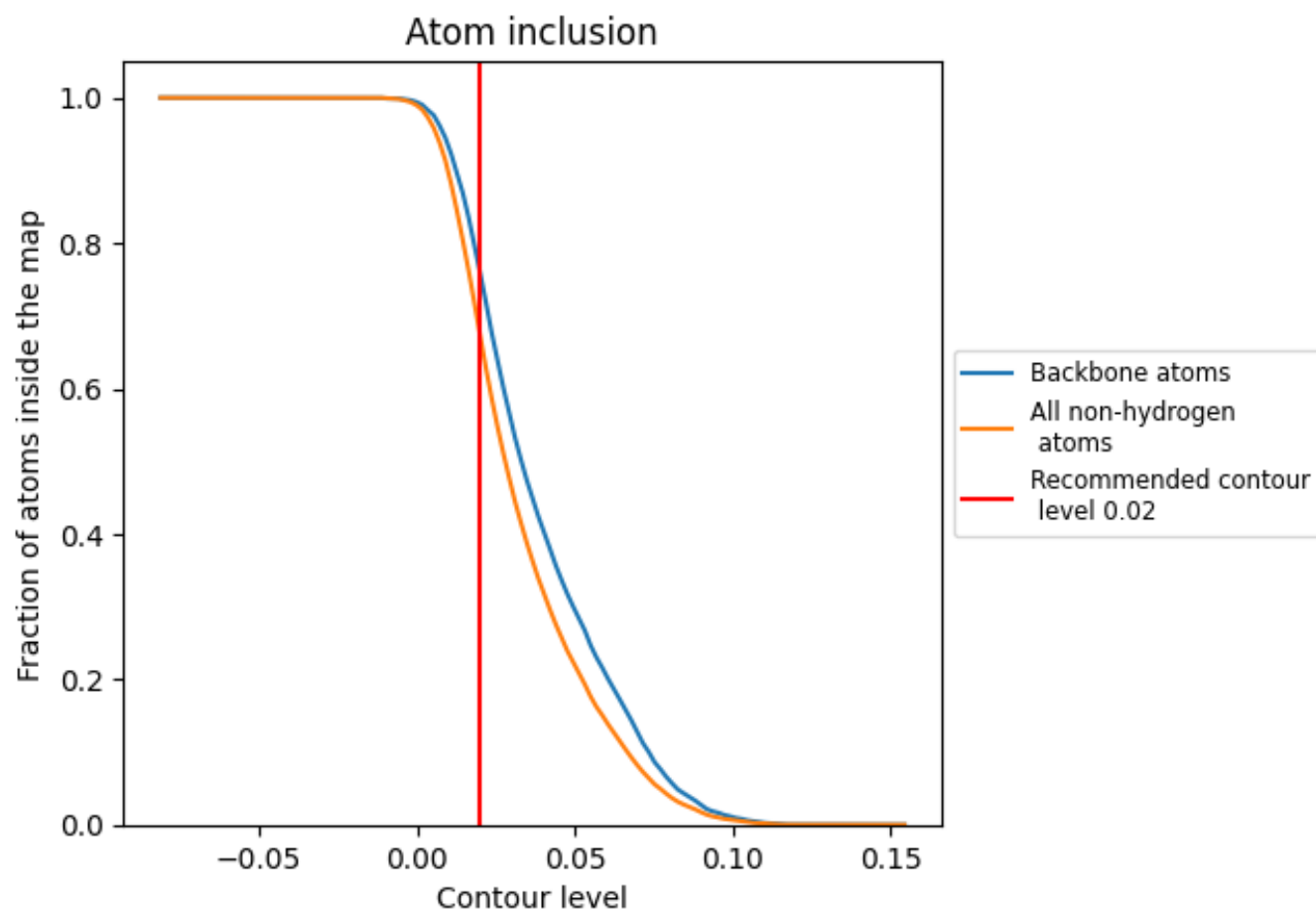
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6736	<div></div> 0.4280
A	<div></div> 0.7917	<div></div> 0.4770
B	<div></div> 0.7635	<div></div> 0.4580
C	<div></div> 0.7917	<div></div> 0.4770
D	<div></div> 0.7917	<div></div> 0.4750
E	<div></div> 0.7917	<div></div> 0.4770
F	<div></div> 0.7633	<div></div> 0.4570
G	<div></div> 0.7633	<div></div> 0.4570
H	<div></div> 0.7633	<div></div> 0.4560
I	<div></div> 0.5286	<div></div> 0.3740
J	<div></div> 0.5284	<div></div> 0.3730
K	<div></div> 0.5284	<div></div> 0.3720
L	<div></div> 0.5284	<div></div> 0.3730

