



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:21 AM UTC

PDB ID : 6WJJ / pdb_00006wjj
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

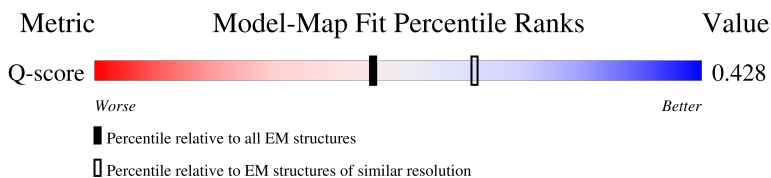
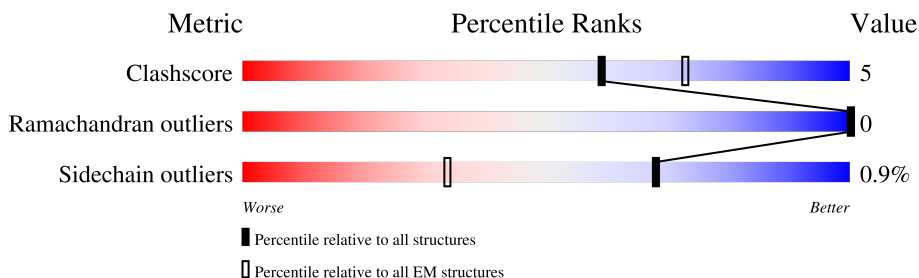
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

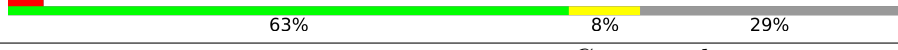
The reported resolution of this entry is 3.80 Å.

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.



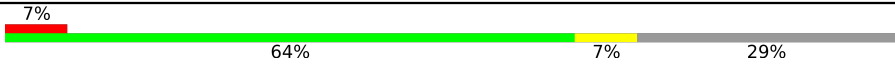
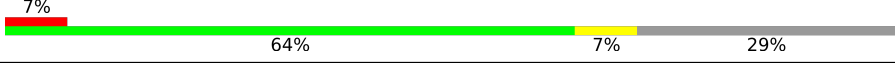
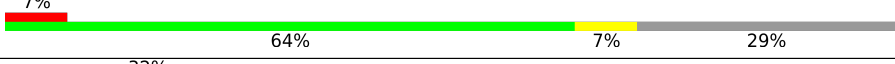
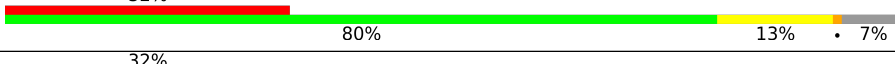
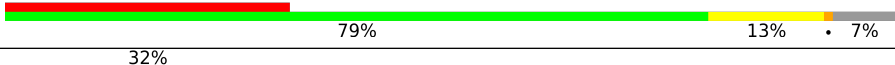
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	

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Mol	Chain	Length	Quality of chain
2	B	735	
2	F	735	
2	G	735	
2	H	735	
3	I	776	
3	J	776	
3	K	776	
3	L	776	

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 (CCD ID: 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

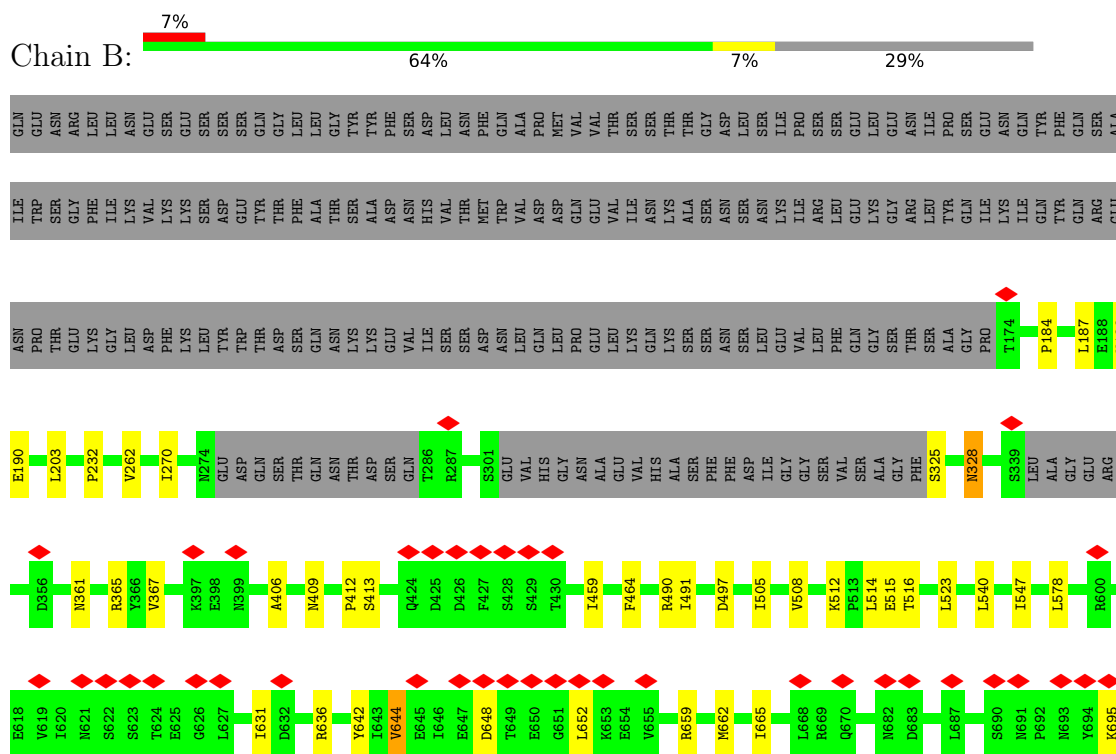
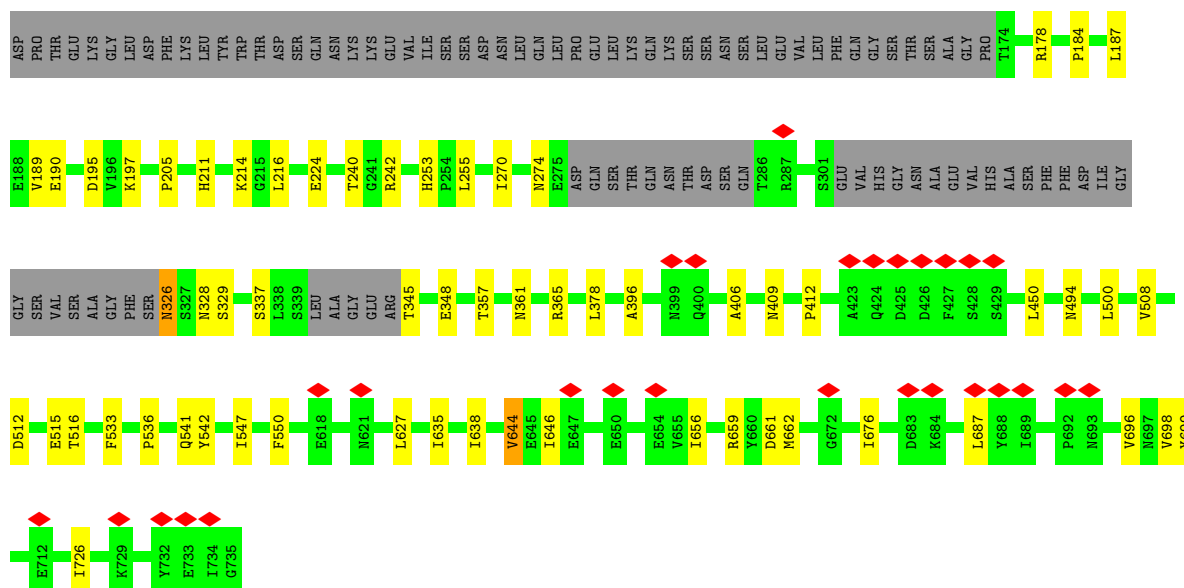
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



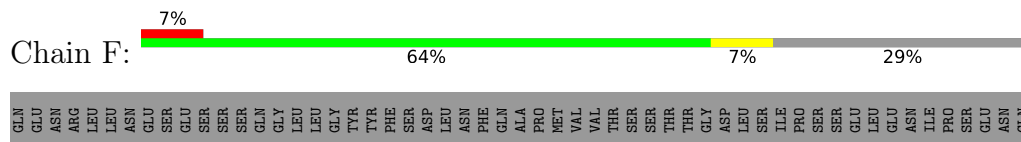
Mol	Chain	Residues	Atoms			AltConf
5	L	1	Total 5	O 4	S 1	0
5	I	1	Total 5	O 4	S 1	0
5	J	1	Total 5	O 4	S 1	0
5	K	1	Total 5	O 4	S 1	0

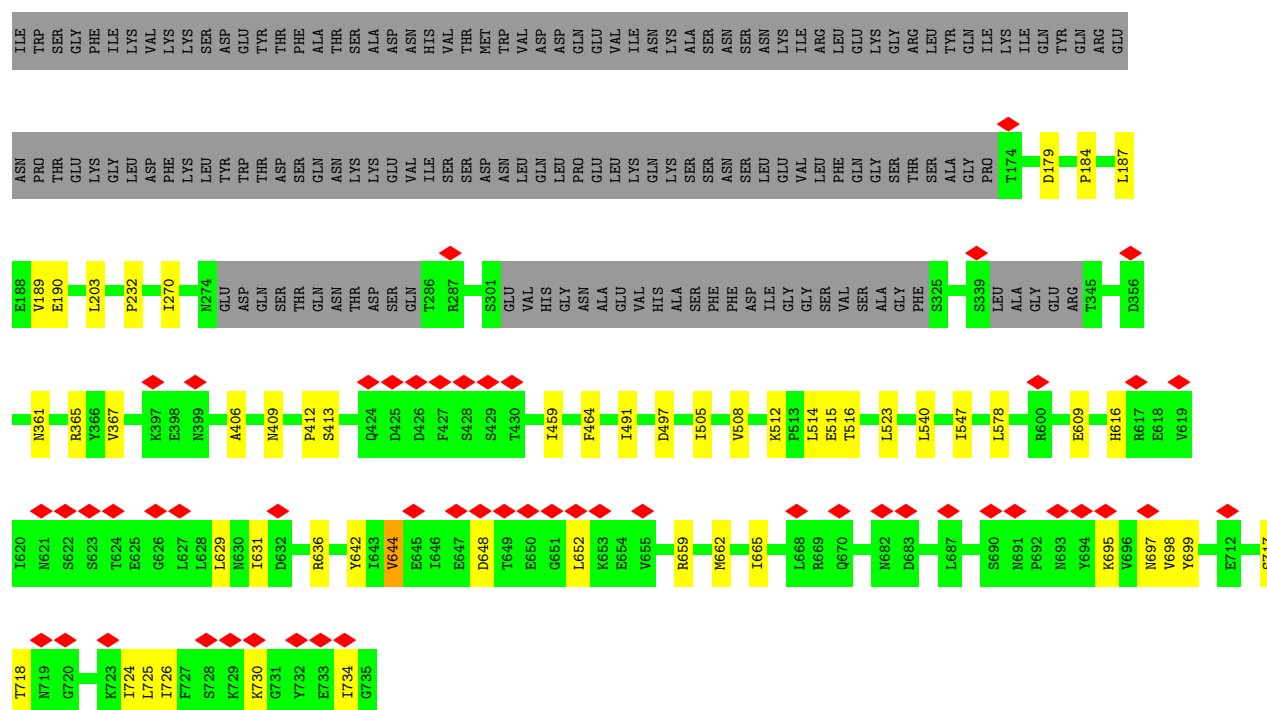
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

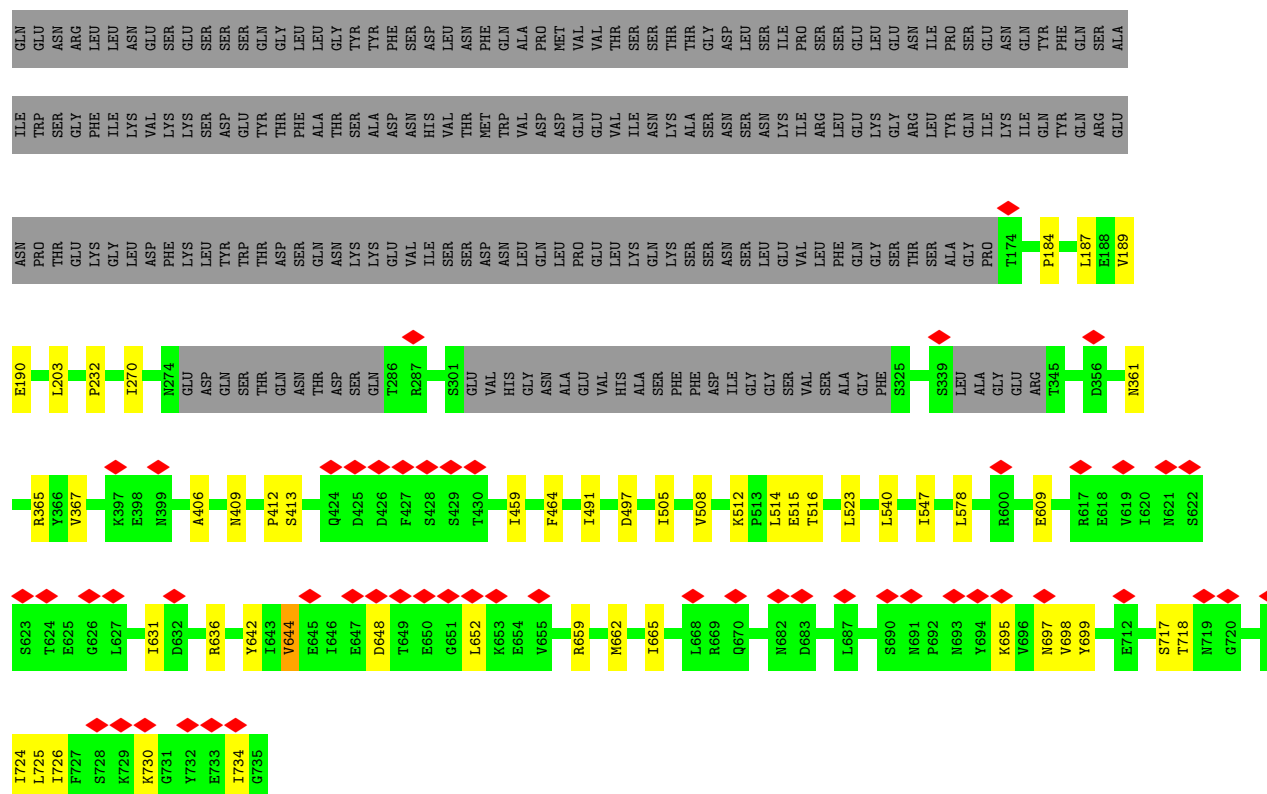


• Molecule 2: Protective antigen





- Molecule 2: Protective antigen



- Molecule 2: Protective antigen



GLN	GLU	ASN	ARG	LEU	ASN	GLU	SER	SER	SER	SER	GLN	GLY	LEU	GLY	THR	THR	PHE	GLN	ASP	ASP	VAL	VAL	THR	SER	SER	THR	THR	GLY	LEU	ILE	PRO	SER	SER	GLU	GLY	GLN	ASN	ILE	PRO	SER	SER	GLU	GLY	ARG	LEU	THR	GLN	THR	PHE	GLN	SER	ALA
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ASN	PRO	THR	GLY	GLY	LEU	ASP	PHE	LEU	SER	SER	THR	THR	GLU	ASP	THR	THR	ALA	ALA	ASP	ASN	ASN	VAL	GLN	THR	THR	GLY	GLN	ASN	GLY	ALA	ALA	THR	THR	ALA	ALA	PRO	GLU	GLU	VAL	ILE	SER	SER	ASN	ASN	LEU	VAL	VAL	THR	THR	GLN	GLY	ARG	GLU
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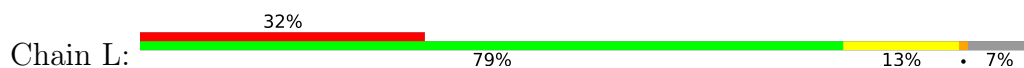
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N361	R365	Y366	V367	K397	E398	N399	A406	M409	P412	S413	Q424	D425	D426	F427	S428	S429	T430	I459	F464	I491	D497	I505	V508	K512	P513	L514	E515	T516	L523	L540	I547	L578	R600	E609	H616	N617	E618	V619
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I620	N621	S622	S623	T624	E625	O626	L627	L628	L629	N630	I631	D632	R636	Y642	I643	V644	E645	I646	E647	D648	T649	E650	G651	L652	K653	E654	V655	R659	M662	I665	L668	R669	O670	N682	D683	L687	S690	N691	P692	N693	V694	K695	V696	N697	V698	V699	E712	S717
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T718	N719	G720	K723	I724	L725	I726	F727	S728	K729	K730	G731	E732	E733	I734	G735
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• Molecule 3: Lethal factor



ALA	GLY	HIS	GLY	ASP	VAL	GLY	MET	HIS	VAL	LYS	LYS	GLU	LYS	LYS	ASN	ASP	GLU	ASN	ARG	N29	Q32	K37	M40	V44	E51	K55	K56	E57	E60	K61	L62	K75	K80	I81	Y82	D85	E95	E99
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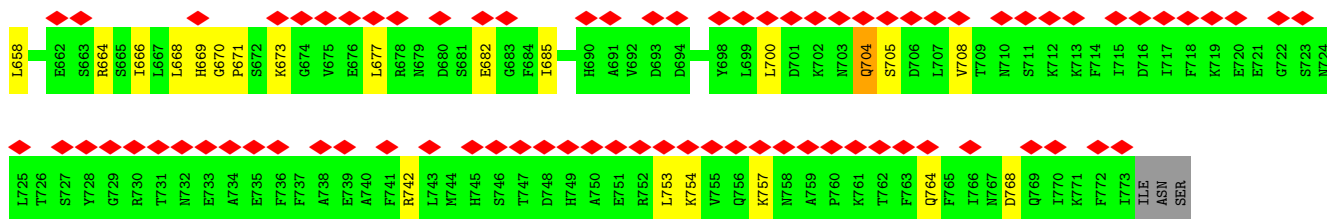
V119	Y125	V128	S133	T141	L145	M146	V147	D184	Y224	V232	D245	I252	R267	Y268	E269	K270	W271	L274	K275	Q276	H277	Y278	Q279	H280	W281	S282	D283	S284	L285	S286	E287	E288	G289	R290	G291	L292	L293	K294	K295	L296	Q297	I298	P299	I300	E301	P302	K303
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K304	D305	D306	I307	I308	H309	S310	L311	S312	Q313	E314	E315	K316	E317	L318	L319	K320	R321	I322	Q323	I324	D325	S326	S327	D328	F329	L330	S331	T332	E333	E334	K335	E336	F337	L338	K339	K340	L341	Q342	I343	D344	I345	ARG	ASP	SER	LEU	SER	GLU	GLU	GLY	LYS	GLU	LEU	ASN	ARG	THR	GLN	VAL	ASP
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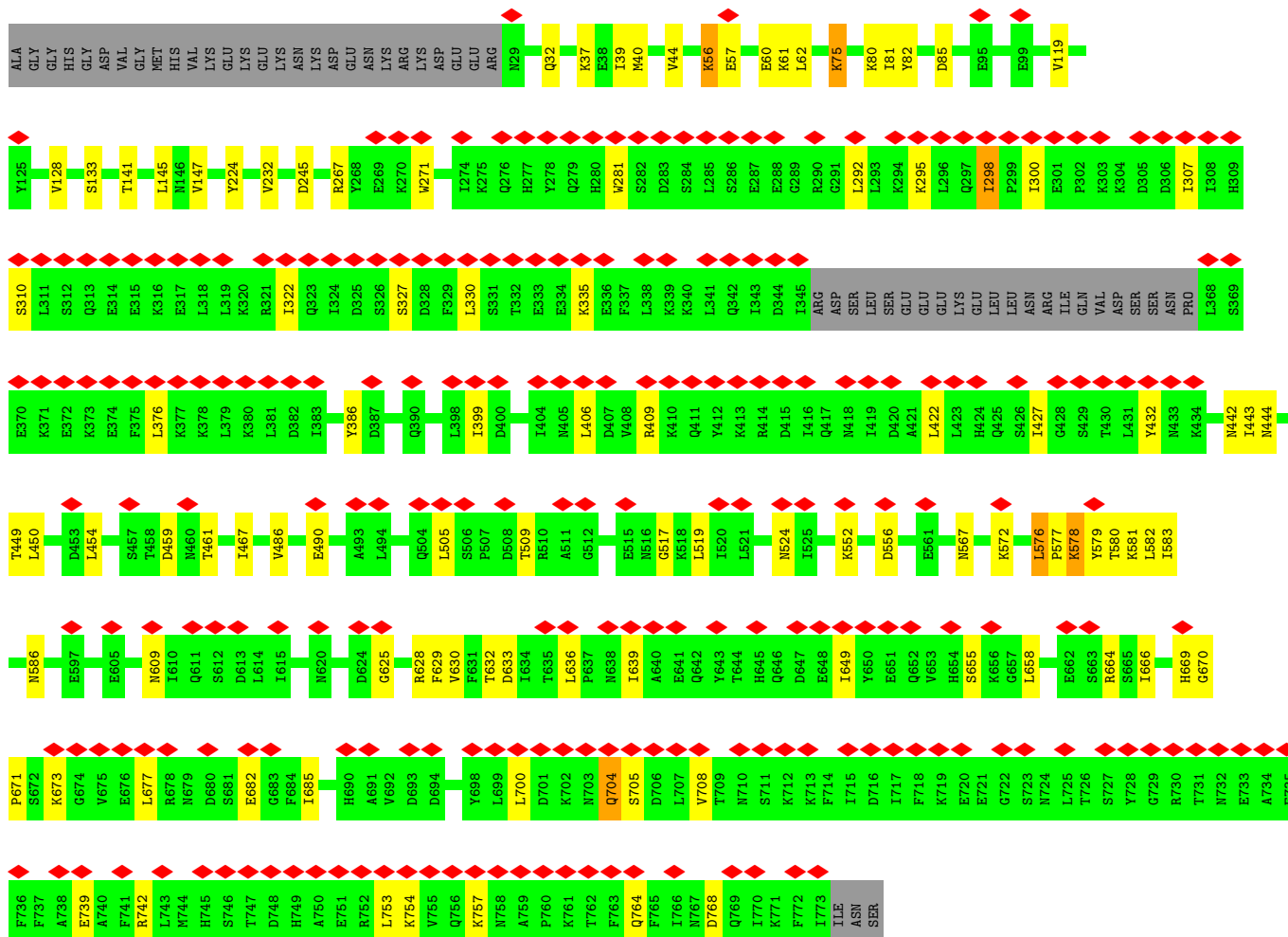
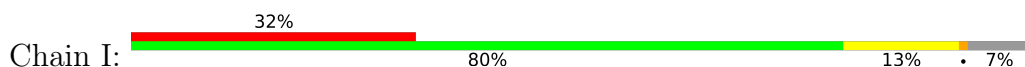
SER	SER	ASN	PRD	L368	S369	E370	K371	E372	K373	E374	F375	L376	K377	K378	K380	L381	D382	I383	Y386	D387	Q390	L398	I399	D400	I404	N405	L406	D407	V408	R409	K410	Q411	Y412	K413	R414	D415	T416	Q417	N418	I419	D420	A421	L422	L423	H424	Q425	S426	I427	G428	S429	T430	L431	Y432	N433
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K434	N440	N441	N442	N443	N444	T449	L450	D453	L454	S457	T458	D459	N460	T461	I467	Y468	E490	A493	L494	K500	D504	L505	S506	P507	P508	D509	R510	A511	G512	E515	N516	G517	K518	L519	I520	T521	N524	T525	K552	D556	E561	N567
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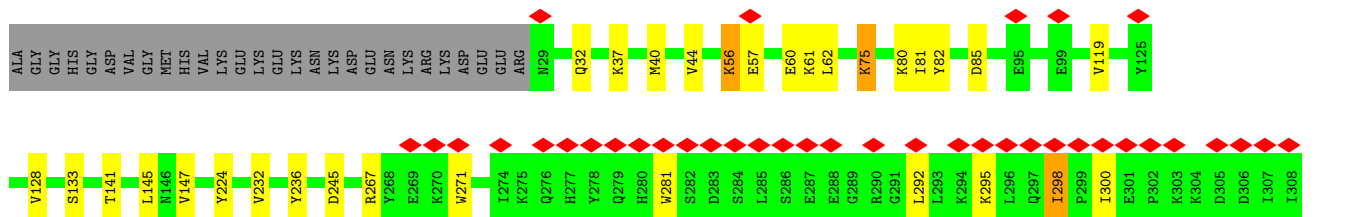
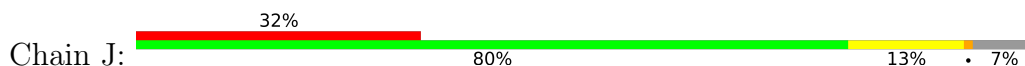
K572	L576	P577	K578	Y579	T580	K581	L582	L583	N586	E597	E605	N609	I610	Q611	S612	D613	L614	I615	N620	D624	G625	R628	P629	V630	F631	T632	D633	T634	T635	L636	P637	N638	I639	A640	E641	Q642	Y643	T644	H645	Q646	D647	E648	I649	V650	E651	Q652	V653	H654	S655	K656	G657
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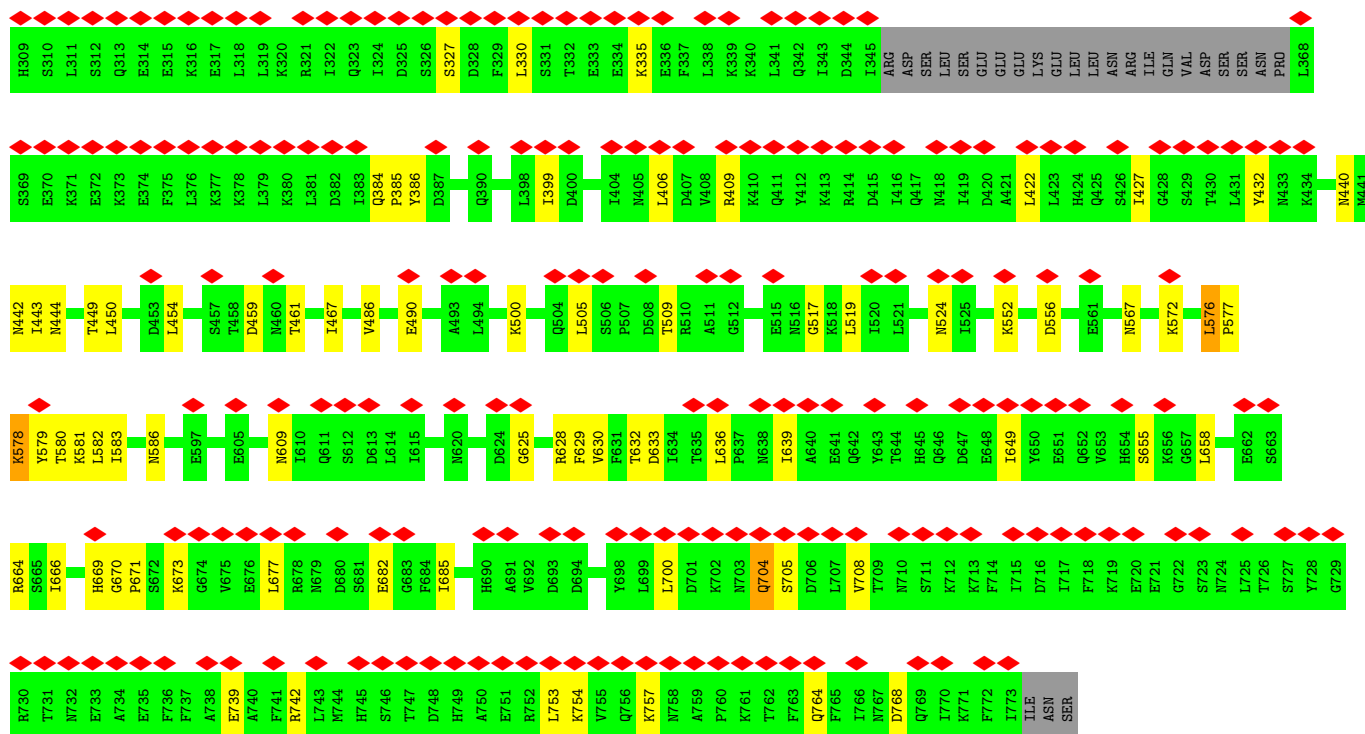


• Molecule 3: Lethal factor

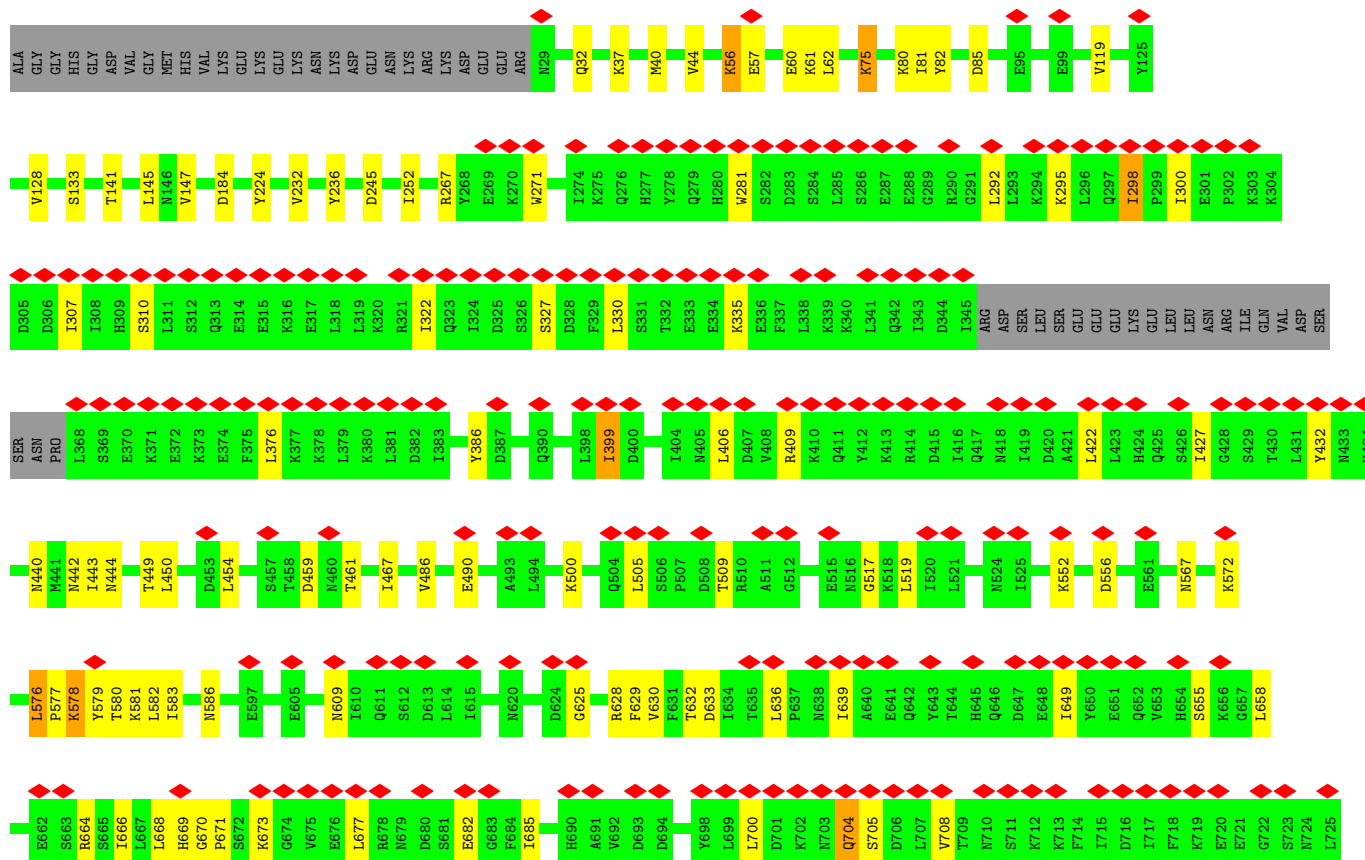
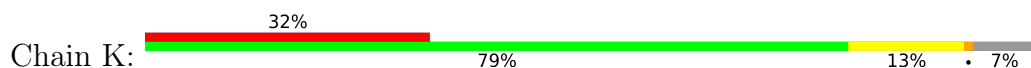


• Molecule 3: Lethal factor





• Molecule 3: Lethal factor



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	ASN	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 (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA, ZN

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	0.40	0/4213	0.65	0/5715
1	C	0.40	0/4213	0.65	0/5715
1	D	0.40	0/4213	0.65	0/5715
1	E	0.40	0/4213	0.65	0/5715
2	B	0.39	0/4219	0.68	1/5720 (0.0%)
2	F	0.39	0/4219	0.68	1/5720 (0.0%)
2	G	0.39	0/4219	0.68	1/5720 (0.0%)
2	H	0.39	0/4219	0.68	1/5720 (0.0%)
3	I	0.30	1/6029 (0.0%)	0.62	0/8122
3	J	0.30	1/6029 (0.0%)	0.62	0/8122
3	K	0.30	1/6029 (0.0%)	0.62	0/8122
3	L	0.30	1/6029 (0.0%)	0.62	0/8122
All	All	0.36	4/57844 (0.0%)	0.65	4/78228 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	576	LEU	N-CA	5.21	1.49	1.46
3	I	576	LEU	N-CA	5.21	1.49	1.46
3	J	576	LEU	N-CA	5.21	1.49	1.46
3	K	576	LEU	N-CA	5.21	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	726	ILE	N-CA-C	-6.13	106.35	112.17
2	F	726	ILE	N-CA-C	-6.13	106.35	112.17
2	G	726	ILE	N-CA-C	-6.13	106.35	112.17
2	H	726	ILE	N-CA-C	-6.13	106.35	112.17

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	31	0
1	C	4144	0	4110	32	0
1	D	4144	0	4110	32	0
1	E	4144	0	4110	34	0
2	B	4150	0	4135	28	0
2	F	4150	0	4135	28	0
2	G	4150	0	4135	26	0
2	H	4150	0	4135	28	0
3	I	5923	0	5915	83	0
3	J	5923	0	5915	84	0
3	K	5923	0	5915	86	0
3	L	5923	0	5915	83	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	525	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (525) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:327:SER:O	3:K:335:LYS:NZ	2.36	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
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:L:327:SER:O	3:L:335:LYS:NZ	2.36	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:327:SER:O	3:I:335:LYS:NZ	2.36	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:586:ASN:O	3:J:632:THR:OG1	2.24	0.55
3:J:764:GLN:NE2	3:J:768:ASP:OD2	2.40	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:56:LYS:HB2	3:K:572:LYS:NZ	2.24	0.53
3:K:581:LYS:O	3:K:628:ARG:NH1	2.42	0.53
3:L:579:TYR:CG	3:L:579:TYR:O	2.62	0.52
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:459:ASP:OD2	3:J:461:THR:OG1	2.27	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
3:K:586:ASN:O	3:K:632:THR:OG1	2.24	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:459:ASP:OD2	3:L:461:THR:OG1	2.27	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
3:I:552:LYS:NZ	3:I:556:ASP:OD2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:224:TYR:OH	3:I:245:ASP:OD1	2.29	0.49
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
3:I:459:ASP:OD2	3:I:461:THR:OG1	2.27	0.48
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:J:56:LYS:HB2	3:K:572:LYS:HZ1	1.79	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
3:K:552:LYS:NZ	3:K:556:ASP:OD2	2.42	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
1:A:270:ILE:HG13	1:A:361:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:51:GLU:OE2	3:L:55:LYS:NZ	2.42	0.46
3:I:486:VAL:N	3:I:519:LEU:O	2.45	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
1:C:195:ASP:OD2	1:C:214:LYS:NZ	2.49	0.46
1:D:687:LEU:HD21	1:D:696:VAL:HG21	1.98	0.46
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:K:459:ASP:OD2	3:K: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:56:LYS:HB2	3:J:572:LYS:HZ1	1.82	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: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
1:A:197:LYS:NZ	3:L:184:ASP:OD2	2.46	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
3:J:552:LYS:NZ	3:J: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:J:704:GLN:CD	3:J:705:SER:H	2.27	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
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:K:704:GLN:CD	3:K:705:SER:H	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: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
3:I:704:GLN:CD	3:I:705:SER:H	2.27	0.42
2:G:270:ILE:HG13	2:G:361:ASN:HB3	2.00	0.42
2:G:659:ARG:HD3	2:G:662:MET:HE2	2.01	0.42
3:J:271:TRP:CZ3	3:J:517:GLY:HA2	2.54	0.42
3:L:704:GLN:CD	3:L:705:SER:H	2.27	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
2:H:659:ARG:HD3	2:H:662:MET:HE2	2.01	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:J:56:LYS:HD2	3:J:56:LYS:C	2.45	0.42
3:K:57:GLU:HA	3:K:60:GLU:HG2	2.01	0.42
3:K:307:ILE:O	3:K:310:SER:OG	2.30	0.42
2:G:512:LYS:HB3	2:G:515:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:512:LYS:HB3	2:F:515:GLU:HB2	2.02	0.42
3:I:56:LYS:HD2	3:I:56:LYS:C	2.45	0.42
3:I:669:HIS:CE1	3:I:671:PRO:HD2	2.55	0.42
2:B:659:ARG:HD3	2:B:662:MET:HE2	2.01	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
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
2:F:659:ARG:HD3	2:F:662:MET:HE2	2.01	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
1:D:255:LEU:HD13	1:D:521:MET:HE1	2.03	0.41
3:K:82:TYR:CD2	3:K:128:VAL:HG13	2.55	0.41
3:L:56:LYS:HD2	3:L:56:LYS:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:659:ARG:HG3	1:A:662:MET:HE2	2.03	0.41
1:C:255:LEU:HD13	1:C:521:MET:HE1	2.03	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
1:D:659:ARG:HG3	1:D:662:MET:HE2	2.03	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: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
1:C:659:ARG:HG3	1:C:662:MET:HE2	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:K:252:ILE:HD12	3:K:252:ILE:HA	1.94	0.40
1:A:255:LEU:HD13	1:A:521:MET:HE1	2.03	0.40
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
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
1:E:659:ARG:HG3	1:E:662:MET:HE2	2.03	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
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%)	78	79
1	C	470/659 (71%)	467 (99%)	3 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	470/659 (71%)	467 (99%)	3 (1%)	78	79
1	E	470/659 (71%)	467 (99%)	3 (1%)	78	79
2	B	471/660 (71%)	468 (99%)	3 (1%)	78	79
2	F	471/660 (71%)	469 (100%)	2 (0%)	84	83
2	G	471/660 (71%)	469 (100%)	2 (0%)	84	83
2	H	471/660 (71%)	469 (100%)	2 (0%)	84	83
3	I	657/710 (92%)	648 (99%)	9 (1%)	59	70
3	J	657/710 (92%)	648 (99%)	9 (1%)	59	70
3	K	657/710 (92%)	648 (99%)	9 (1%)	59	70
3	L	657/710 (92%)	648 (99%)	9 (1%)	59	70
All	All	6392/8116 (79%)	6335 (99%)	57 (1%)	68	74

All (57) 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	328	ASN
2	B	367	VAL
2	B	644	VAL
3	L	56	LYS
3	L	75	LYS
3	L	298	ILE
3	L	399	ILE
3	L	578	LYS
3	L	649	ILE
3	L	658	LEU
3	L	704	GLN
3	L	753	LEU
1	C	326	ASN
1	C	328	ASN
1	C	644	VAL
2	F	367	VAL
2	F	644	VAL
3	I	56	LYS
3	I	75	LYS
3	I	298	ILE

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Mol	Chain	Res	Type
3	I	399	ILE
3	I	578	LYS
3	I	649	ILE
3	I	658	LEU
3	I	704	GLN
3	I	753	LEU
1	D	326	ASN
1	D	328	ASN
1	D	644	VAL
2	G	367	VAL
2	G	644	VAL
3	J	56	LYS
3	J	75	LYS
3	J	298	ILE
3	J	399	ILE
3	J	578	LYS
3	J	649	ILE
3	J	658	LEU
3	J	704	GLN
3	J	753	LEU
1	E	326	ASN
1	E	328	ASN
1	E	644	VAL
2	H	367	VAL
2	H	644	VAL
3	K	56	LYS
3	K	75	LYS
3	K	298	ILE
3	K	399	ILE
3	K	578	LYS
3	K	649	ILE
3	K	658	LEU
3	K	704	GLN
3	K	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	HIS
1	A	263	HIS
1	A	326	ASN
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	409	ASN
1	A	541	GLN
1	A	709	ASN
2	B	326	ASN
2	B	409	ASN
2	B	541	GLN
2	B	565	GLN
2	B	697	ASN
3	L	32	GLN
3	L	117	HIS
3	L	228	GLN
3	L	242	ASN
3	L	253	ASN
3	L	279	GLN
3	L	390	GLN
3	L	393	GLN
3	L	411	GLN
3	L	440	ASN
3	L	444	ASN
3	L	474	ASN
3	L	489	ASN
3	L	567	ASN
3	L	571	ASN
3	L	586	ASN
3	L	588	HIS
3	L	609	ASN
3	L	620	ASN
3	L	642	GLN
3	L	758	ASN
3	L	767	ASN
3	L	769	GLN
1	C	253	HIS
1	C	263	HIS
1	C	326	ASN
1	C	328	ASN
1	C	409	ASN
1	C	541	GLN
2	F	263	HIS
2	F	326	ASN
2	F	409	ASN
2	F	541	GLN
2	F	565	GLN

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Mol	Chain	Res	Type
2	F	682	ASN
2	F	697	ASN
3	I	32	GLN
3	I	117	HIS
3	I	214	GLN
3	I	228	GLN
3	I	242	ASN
3	I	253	ASN
3	I	279	GLN
3	I	390	GLN
3	I	393	GLN
3	I	411	GLN
3	I	440	ASN
3	I	444	ASN
3	I	474	ASN
3	I	489	ASN
3	I	567	ASN
3	I	571	ASN
3	I	586	ASN
3	I	588	HIS
3	I	609	ASN
3	I	620	ASN
3	I	642	GLN
3	I	767	ASN
3	I	769	GLN
1	D	253	HIS
1	D	263	HIS
1	D	326	ASN
1	D	328	ASN
1	D	409	ASN
1	D	541	GLN
1	D	709	ASN
2	G	263	HIS
2	G	409	ASN
2	G	541	GLN
2	G	565	GLN
2	G	682	ASN
2	G	697	ASN
3	J	32	GLN
3	J	117	HIS
3	J	214	GLN
3	J	228	GLN

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Mol	Chain	Res	Type
3	J	242	ASN
3	J	253	ASN
3	J	279	GLN
3	J	390	GLN
3	J	393	GLN
3	J	411	GLN
3	J	440	ASN
3	J	444	ASN
3	J	474	ASN
3	J	489	ASN
3	J	567	ASN
3	J	571	ASN
3	J	586	ASN
3	J	588	HIS
3	J	609	ASN
3	J	620	ASN
3	J	642	GLN
3	J	758	ASN
3	J	767	ASN
3	J	769	GLN
1	E	253	HIS
1	E	263	HIS
1	E	326	ASN
1	E	328	ASN
1	E	409	ASN
1	E	709	ASN
2	H	263	HIS
2	H	409	ASN
2	H	541	GLN
2	H	565	GLN
2	H	697	ASN
3	K	32	GLN
3	K	117	HIS
3	K	193	GLN
3	K	214	GLN
3	K	228	GLN
3	K	242	ASN
3	K	253	ASN
3	K	279	GLN
3	K	390	GLN
3	K	393	GLN
3	K	411	GLN

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Mol	Chain	Res	Type
3	K	440	ASN
3	K	444	ASN
3	K	474	ASN
3	K	489	ASN
3	K	567	ASN
3	K	571	ASN
3	K	586	ASN
3	K	588	HIS
3	K	609	ASN
3	K	620	ASN
3	K	642	GLN
3	K	704	GLN
3	K	767	ASN
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 oligosaccharides 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	K	801	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	I	801	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	J	801	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	L	801	-	4,4,4	0.22	0	6,6,6	0.11	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.

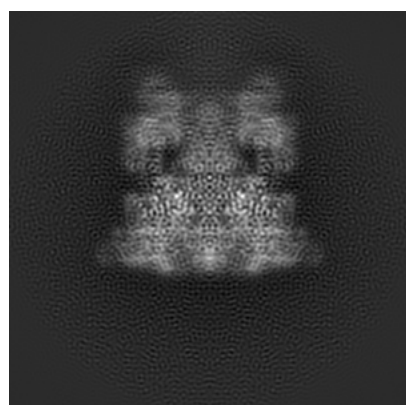
6 Map visualisation [i](#)

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.

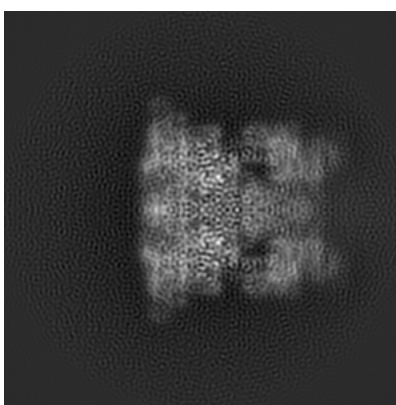
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

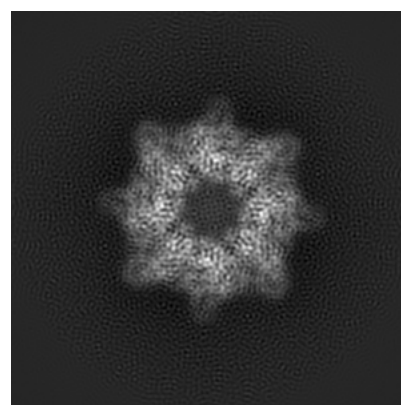
6.1.1 Primary map



X



Y

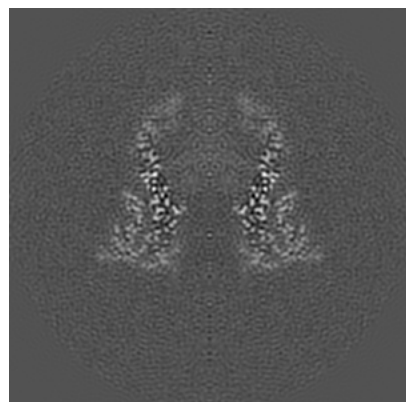


Z

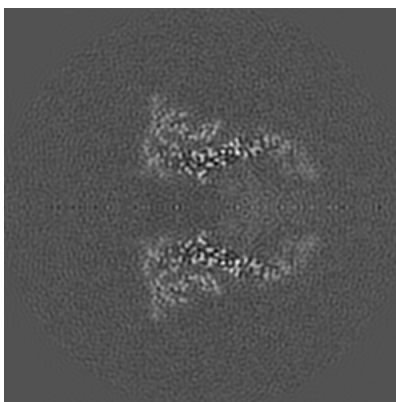
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

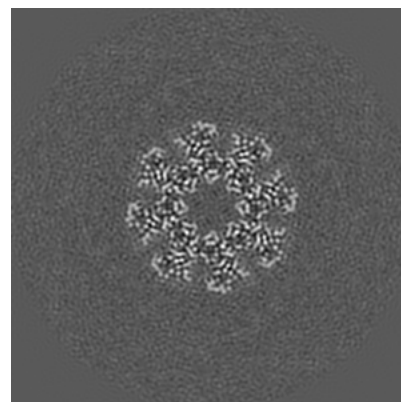
6.2.1 Primary map



X Index: 150



Y Index: 150

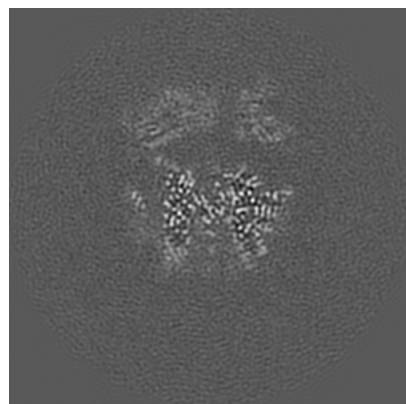


Z Index: 150

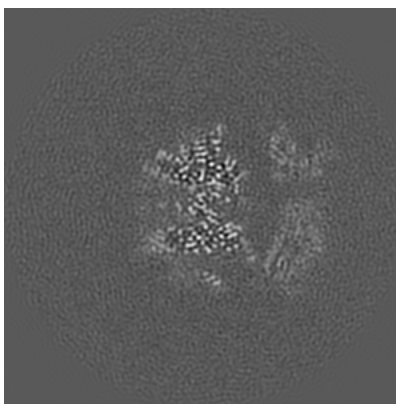
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

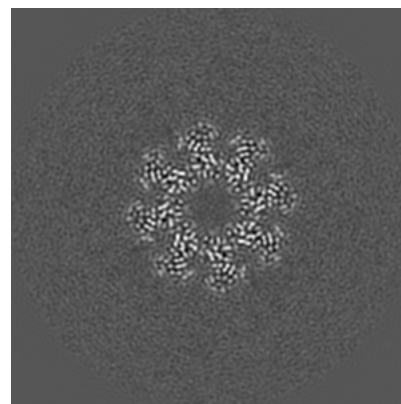
6.3.1 Primary map



X Index: 176



Y Index: 124

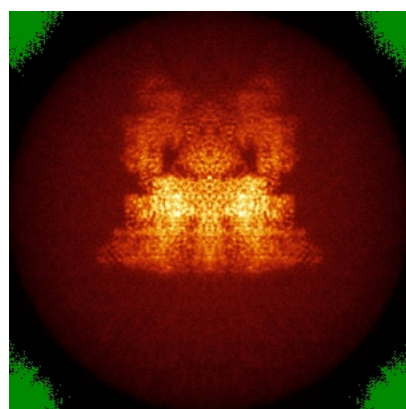


Z Index: 148

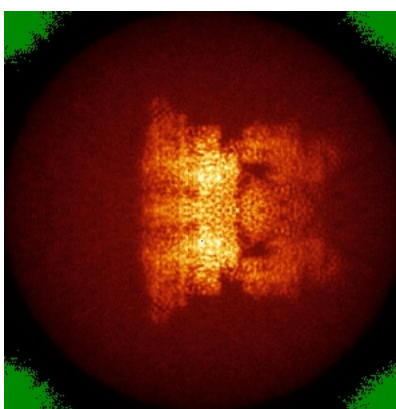
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

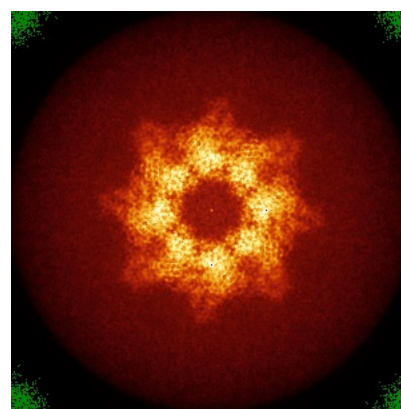
6.4.1 Primary map



X



Y

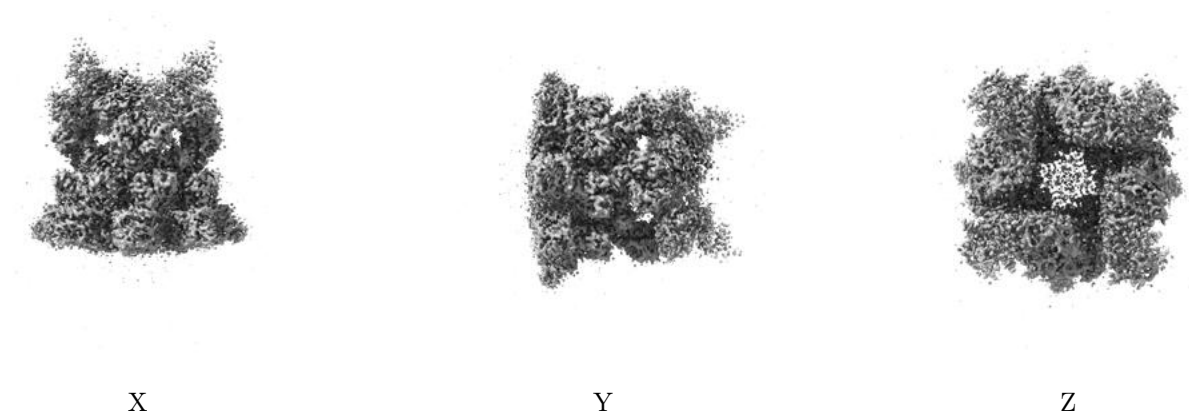


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

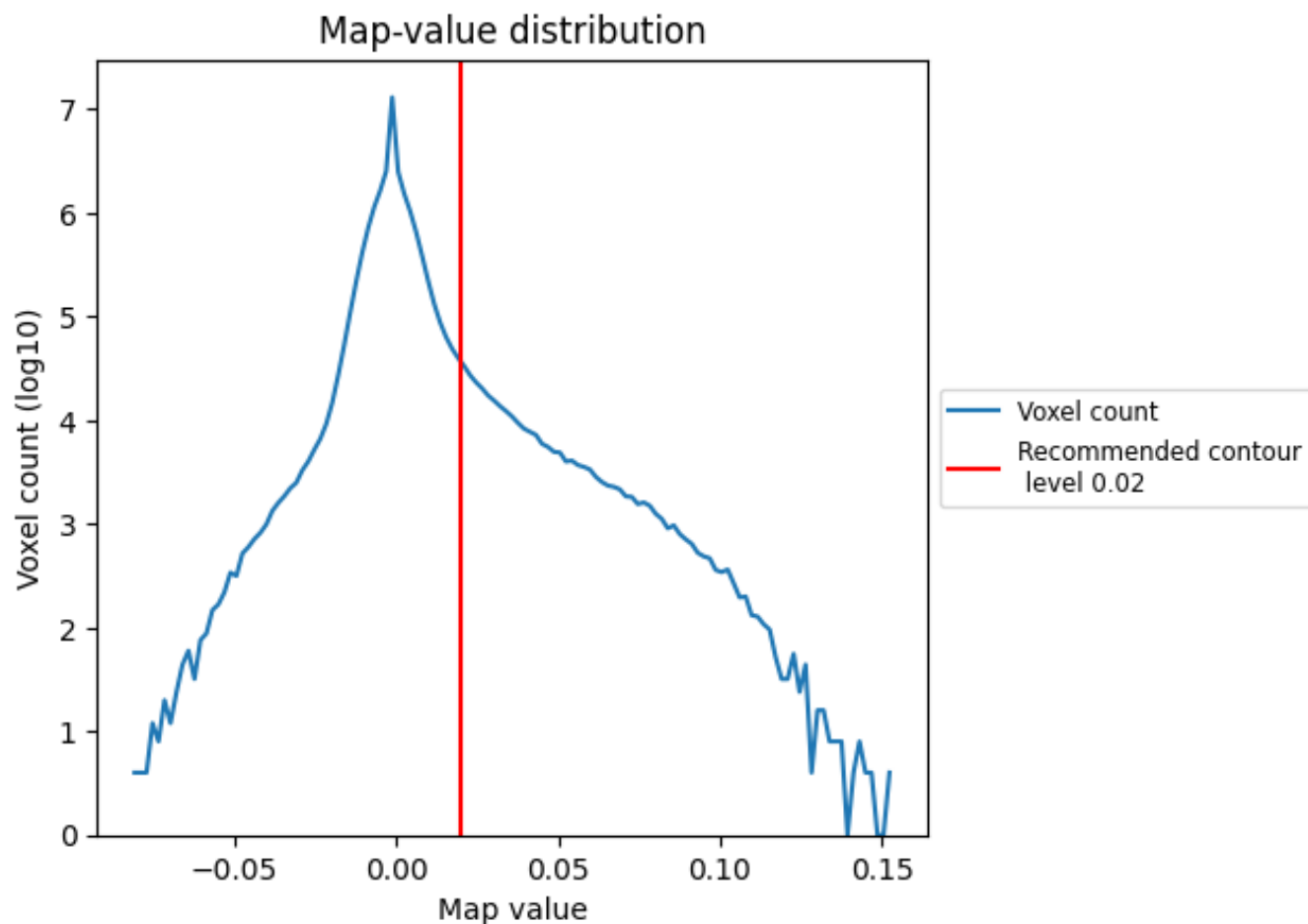
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

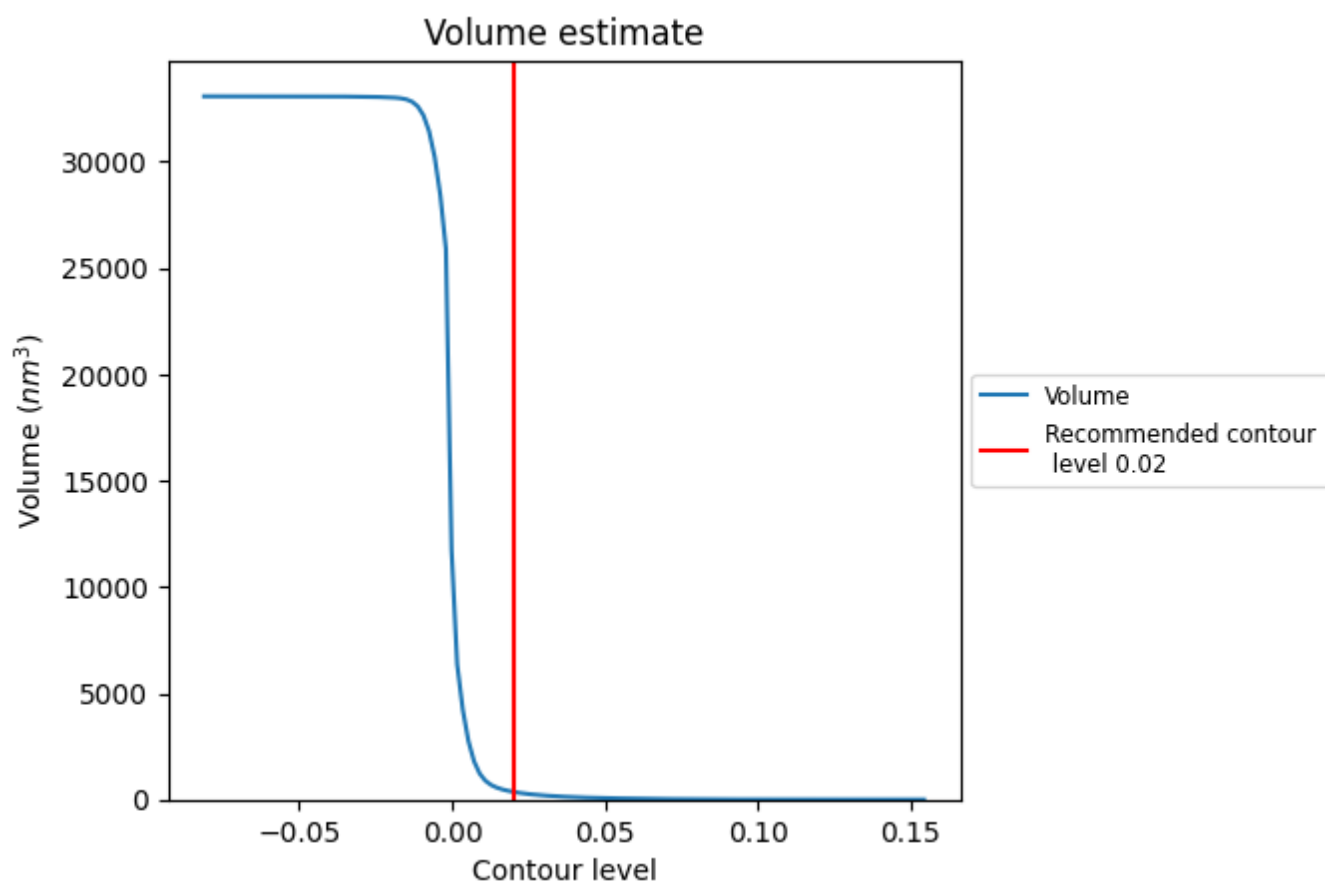
This section contains the results of statistical analysis of the map.

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.

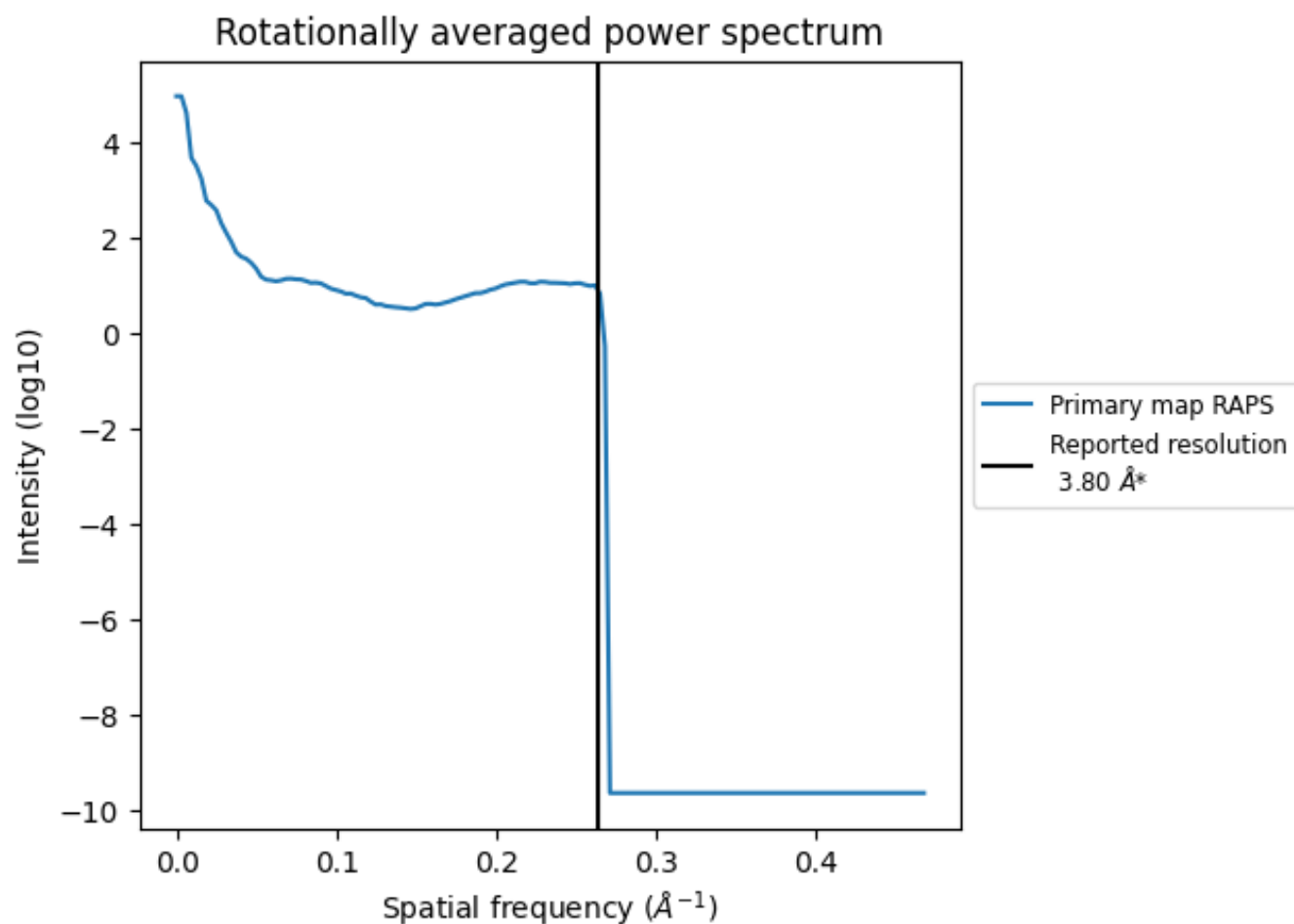
7.2 Volume estimate [i](#)



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

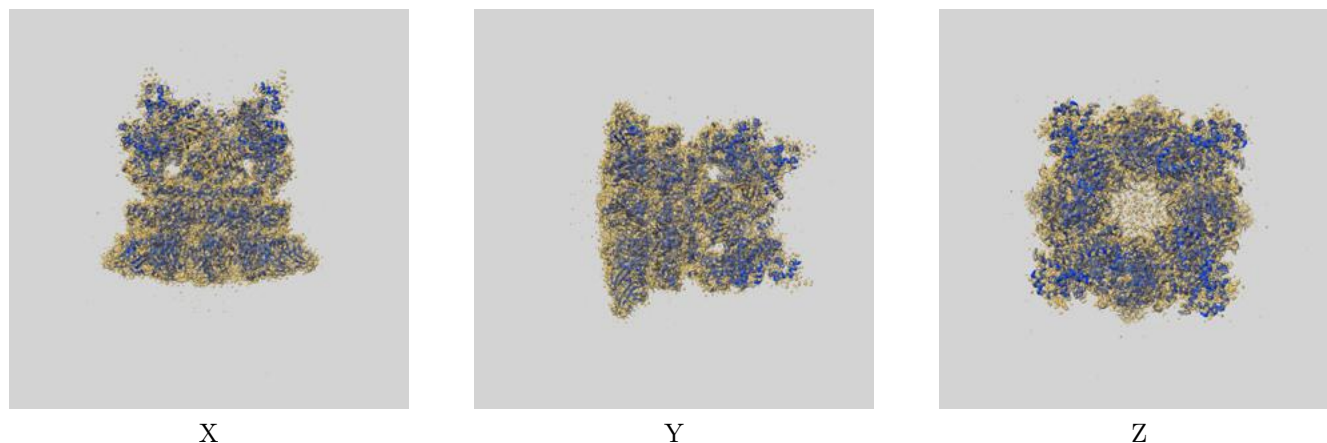
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

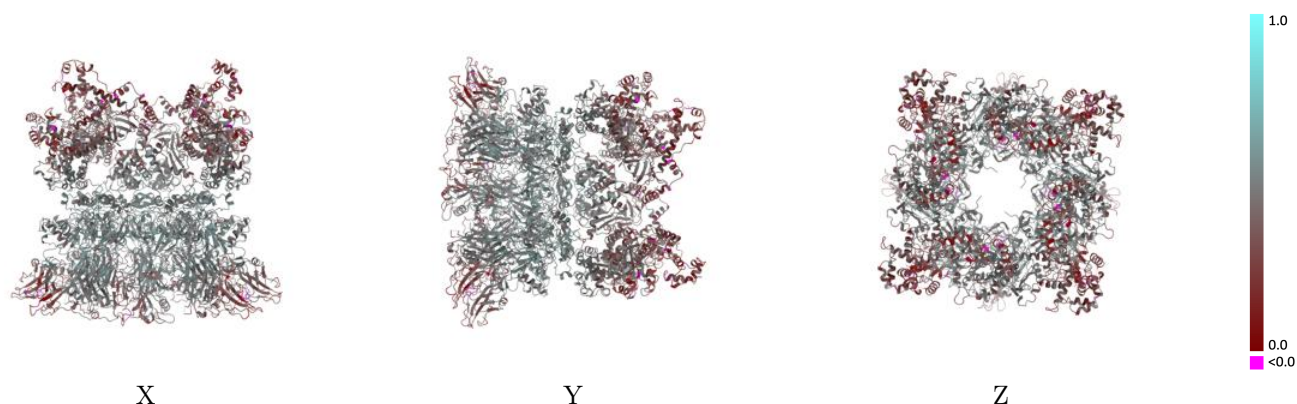
This section contains information regarding the fit between EMDB map EMD-21694 and PDB model 6WJJ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



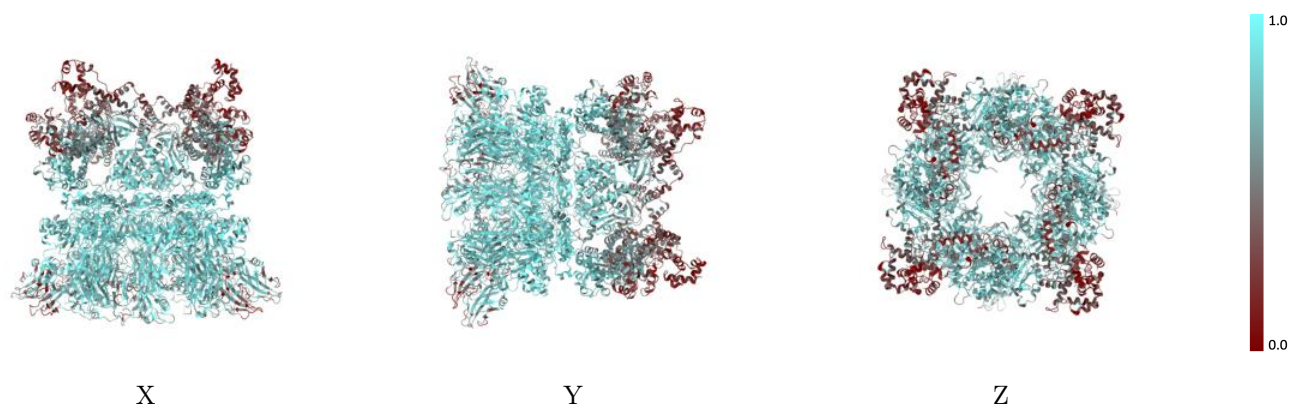
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



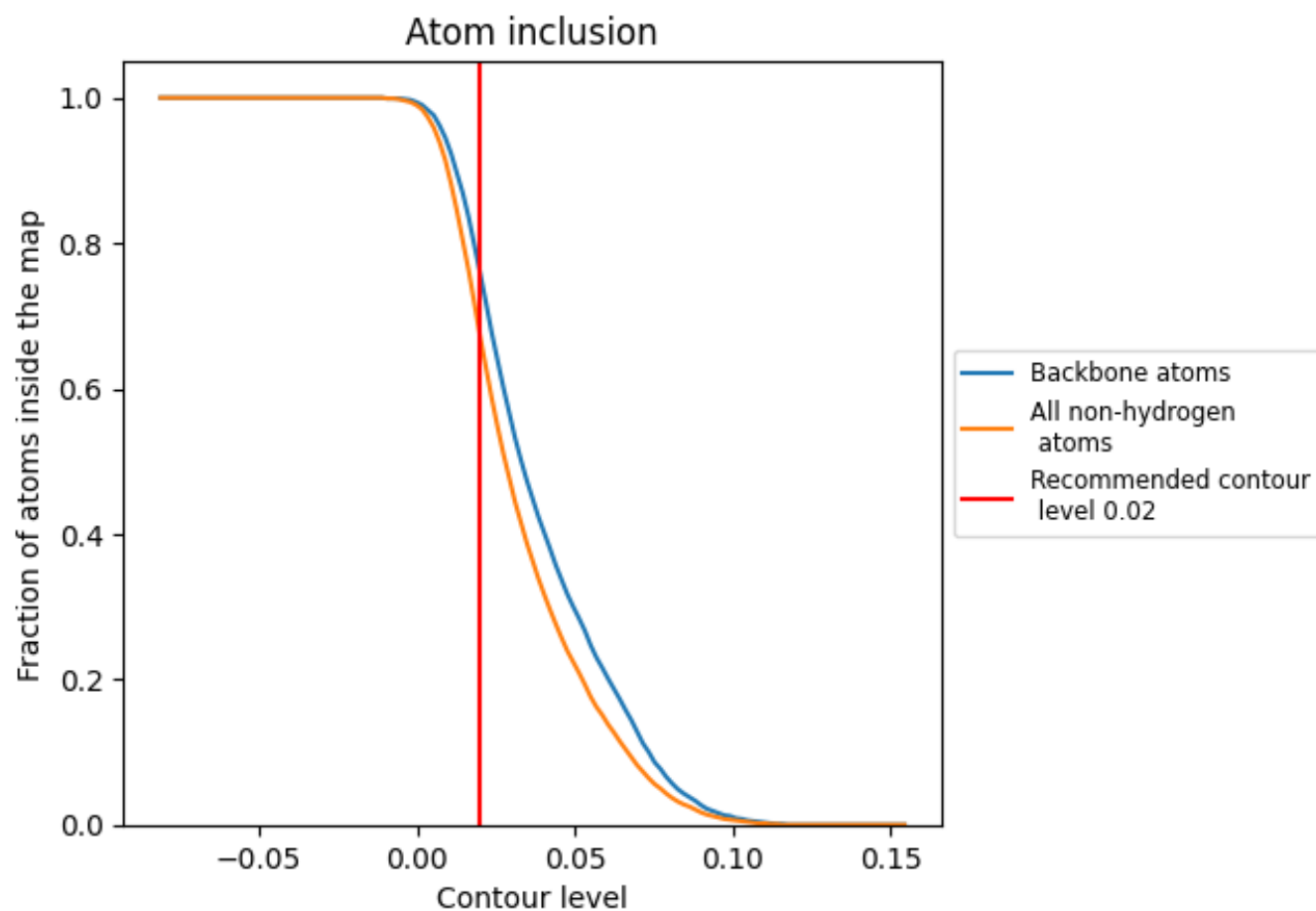
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.6740	0.4280
A	0.7920	0.4770
B	0.7630	0.4580
C	0.7920	0.4770
D	0.7920	0.4750
E	0.7920	0.4770
F	0.7630	0.4570
G	0.7630	0.4570
H	0.7630	0.4560
I	0.5290	0.3740
J	0.5280	0.3730
K	0.5280	0.3720
L	0.5280	0.3730

1.0

0.0

<0.0