



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 07:15 PM JST

PDB ID : 7EVN  
EMDB ID : EMD-31330  
Title : The cryo-EM structure of the DDX42-SF3b complex  
Authors : Zhang, X.; Zhan, X.; Shi, Y.  
Deposited on : 2021-05-21  
Resolution : 2.60 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

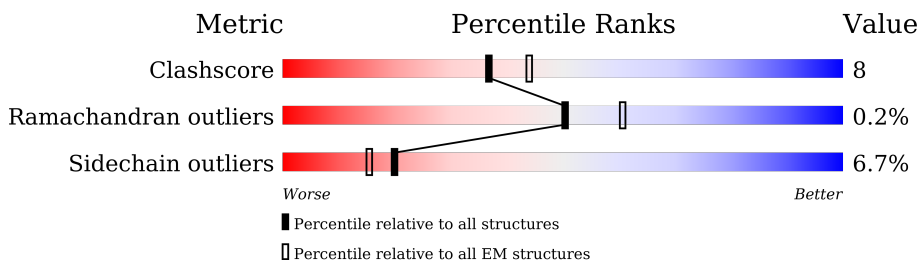
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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  $\geq 3$ , 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	B	86	
2	C	872	
3	D	110	
4	A	1250	
5	E	958	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19668 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 Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	78	Total	C	N	O	S	0	0
			646	409	114	118	5		

- Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	815	Total	C	N	O	S	0	0
			6487	4163	1121	1164	39		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	433	MET	-	initiating methionine	UNP O75533
C	434	ALA	-	expression tag	UNP O75533
C	435	SER	-	expression tag	UNP O75533
C	436	ASP	-	expression tag	UNP O75533
C	437	TYR	-	expression tag	UNP O75533
C	438	LYS	-	expression tag	UNP O75533
C	439	ASP	-	expression tag	UNP O75533
C	440	ASP	-	expression tag	UNP O75533
C	441	ASP	-	expression tag	UNP O75533
C	442	ASP	-	expression tag	UNP O75533
C	443	LYS	-	expression tag	UNP O75533
C	444	ALA	-	expression tag	UNP O75533
C	445	SER	-	expression tag	UNP O75533
C	446	ASP	-	expression tag	UNP O75533
C	447	GLU	-	expression tag	UNP O75533
C	448	VAL	-	expression tag	UNP O75533
C	449	ASP	-	expression tag	UNP O75533
C	450	ALA	-	expression tag	UNP O75533
C	451	GLY	-	expression tag	UNP O75533

- Molecule 3 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			700	429	123	135	13		

- Molecule 4 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1177	Total	C	N	O	S	0	0
			9227	5858	1568	1756	45		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	TRP	-	expression tag	UNP Q15393
A	-31	SER	-	expression tag	UNP Q15393
A	-30	HIS	-	expression tag	UNP Q15393
A	-29	PRO	-	expression tag	UNP Q15393
A	-28	GLN	-	expression tag	UNP Q15393
A	-27	PHE	-	expression tag	UNP Q15393
A	-26	GLU	-	expression tag	UNP Q15393
A	-25	LYS	-	expression tag	UNP Q15393
A	-24	GLY	-	expression tag	UNP Q15393
A	-23	GLY	-	expression tag	UNP Q15393
A	-22	GLY	-	expression tag	UNP Q15393
A	-21	SER	-	expression tag	UNP Q15393
A	-20	GLY	-	expression tag	UNP Q15393
A	-19	GLY	-	expression tag	UNP Q15393
A	-18	GLY	-	expression tag	UNP Q15393
A	-17	SER	-	expression tag	UNP Q15393
A	-16	GLY	-	expression tag	UNP Q15393
A	-15	GLY	-	expression tag	UNP Q15393
A	-14	SER	-	expression tag	UNP Q15393
A	-13	ALA	-	expression tag	UNP Q15393
A	-12	TRP	-	expression tag	UNP Q15393
A	-11	SER	-	expression tag	UNP Q15393
A	-10	HIS	-	expression tag	UNP Q15393
A	-9	PRO	-	expression tag	UNP Q15393
A	-8	GLN	-	expression tag	UNP Q15393
A	-7	PHE	-	expression tag	UNP Q15393
A	-6	GLU	-	expression tag	UNP Q15393
A	-5	LYS	-	expression tag	UNP Q15393
A	-4	GLY	-	expression tag	UNP Q15393
A	-3	SER	-	expression tag	UNP Q15393
A	-2	ALA	-	expression tag	UNP Q15393

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q15393
A	0	ALA	-	expression tag	UNP Q15393

- Molecule 5 is a protein called ATP-dependent RNA helicase DDX42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	486	Total	C	N	O	S	0	0
			2605	1555	505	542	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP Q86XP3
E	-18	ALA	-	expression tag	UNP Q86XP3
E	-17	SER	-	expression tag	UNP Q86XP3
E	-16	ASP	-	expression tag	UNP Q86XP3
E	-15	TYR	-	expression tag	UNP Q86XP3
E	-14	LYS	-	expression tag	UNP Q86XP3
E	-13	ASP	-	expression tag	UNP Q86XP3
E	-12	ASP	-	expression tag	UNP Q86XP3
E	-11	ASP	-	expression tag	UNP Q86XP3
E	-10	ASP	-	expression tag	UNP Q86XP3
E	-9	LYS	-	expression tag	UNP Q86XP3
E	-8	ALA	-	expression tag	UNP Q86XP3
E	-7	SER	-	expression tag	UNP Q86XP3
E	-6	ASP	-	expression tag	UNP Q86XP3
E	-5	GLU	-	expression tag	UNP Q86XP3
E	-4	VAL	-	expression tag	UNP Q86XP3
E	-3	ASP	-	expression tag	UNP Q86XP3
E	-2	ALA	-	expression tag	UNP Q86XP3
E	-1	GLY	-	expression tag	UNP Q86XP3
E	0	THR	-	expression tag	UNP Q86XP3


- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	D	3	Total	Zn	0
			3	3	

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

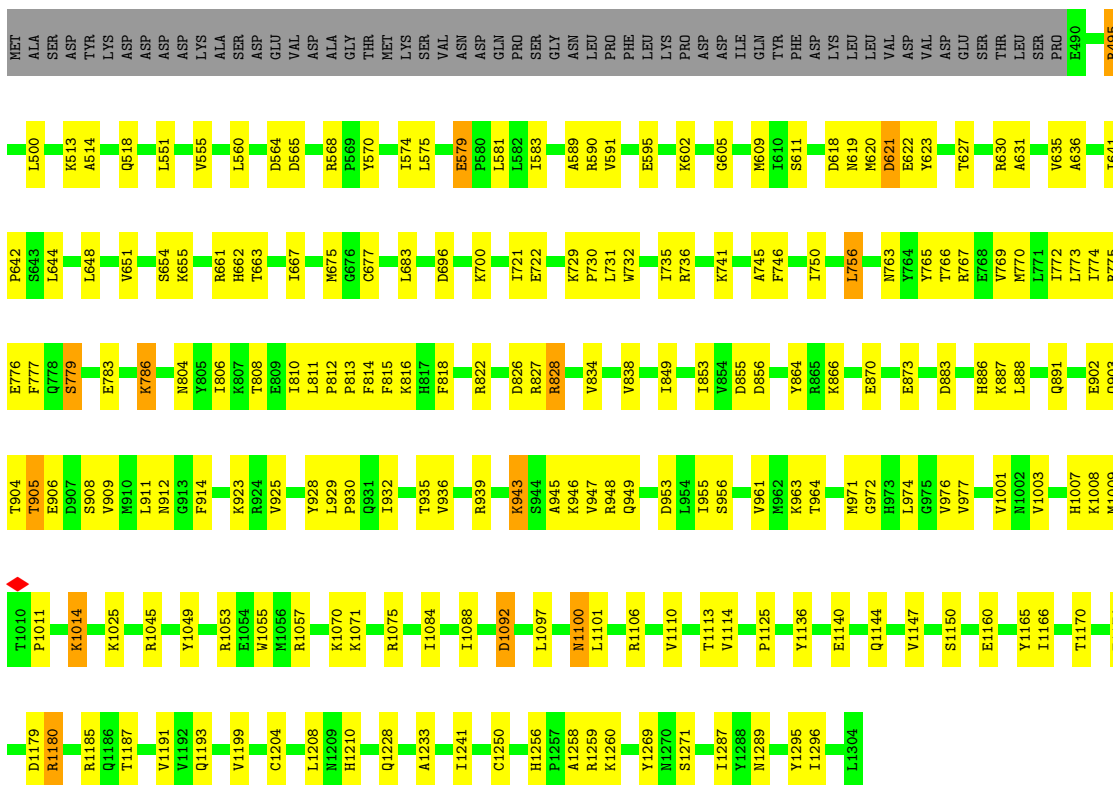
- Molecule 1: Splicing factor 3B subunit 5

Chain B: 



- Molecule 2: Splicing factor 3B subunit 1

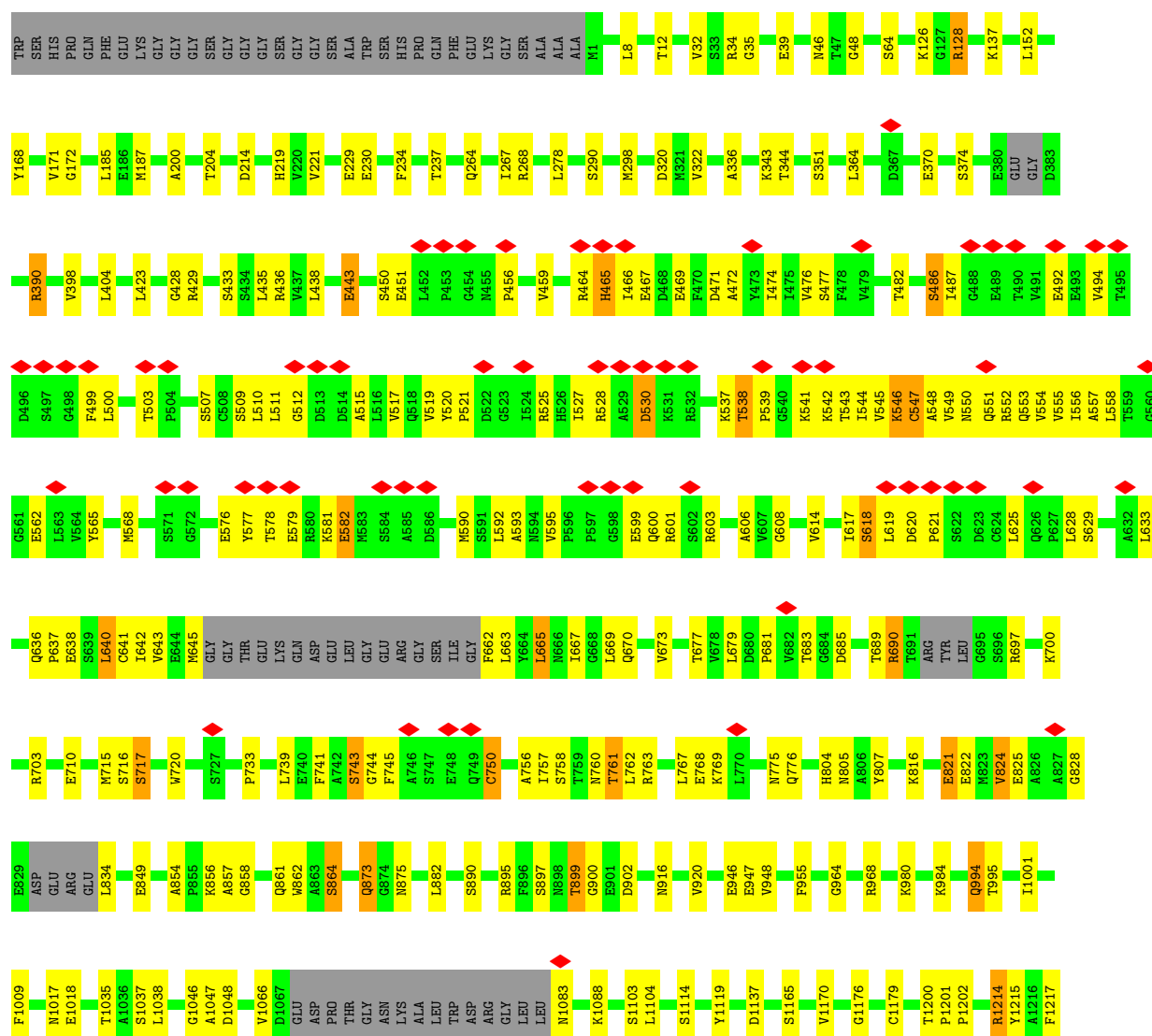
Chain C: 



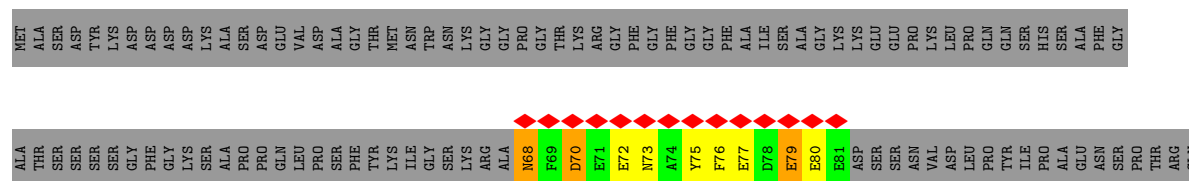
- Molecule 3: PHD finger-like domain-containing protein 5A

Chain D: 





- Molecule 5: ATP-dependent RNA helicase DDX42



PRO	GLY	THR	ASN	LEU	N538	L478	E418	V358	K298	K238	GLU	GLN
LYS	ARG	TYR	GLN	GLY	K539	H479	Y419	A359	T299	L239	ASP	PHE
MET	HIS	PRO	LYS	TYR	K540	H480	Q420	V360	G300	N240	ASN	HIS
ASP	GLY	ALA	ALA	ARG	K541	G481	Y421	Y361	S301	L241	LEU	LYS
VAL	GLY	ALA	SER	ARG	S542	P482	R422	G363	G302	R242	TYR	PRO
ASP	ARG	ALA	SER	PRO	D543	S483	S423	G364	K303	V243	ASP	VAL
LYS	GLY	GLN	ALA	GLY	F544	K484	I424	G364	T304	S244	ASP	VAL
VAL	GLY	VAL	GLY	GLY	K545	V485	A425	S365	A305	G245	ASP	ASP
ASP	GLY	ASN	ALA	GLY	K546	M486	S426	M366	A306	G246	ASP	ASP
ASP	GLY	ASN	GLY	ASN	K547	V487	H427	V367	F307	A247	ASP	ASP
LYS	SER	ALA	TRP	MET	D548	L488	V428	E368	I308	P248	ASP	ASP
VAL	ARG	SER	THR	ASP	I549	T489	R429	Q369	W309	P249	ALA	D114
ASP	HIS	GLY	THR	ARG	P550	R490	D430	A370	P310	R250	PRO	P115
SER	THR	ASN	ALA	GLY	K551	R491	D431	K371	M311	P251	THR	L116
THR	ASP	ASN	GLY	ASN	L552	L492	R432	A372	L312	G252	LYS	E117
ASP	HIS	ARG	LEU	ASN	V553	V493	Q433	L373	I313	S253	ILE	M120
THR	GLY	GLY	LEU	ASN	A554	E494	T434	Q374	H314	S254	ASP	Q126
GLY	GLY	THR	VAL	SER	T555	F495	L435	E375	I315	F255	PRO	D130
ASP	ASN	GLY	PRO	ASN	D556	T496	L436	G376	M316	A256	PRO	M131
PHE	ARG	SER	THR	TYR	V557	S497	F437	A377	D317	H257	ILE	K132
ALA	HIS	ASN	ALA	ALA	A558	S498	S438	E378	Q318	F258	ASP	R133
VAL	GLY	TYR	ALA	TYR	A559	G499	A439	I379	K319	G259	ASP	L134
PRO	GLY	LYS	GLN	LYS	R560	S500	T440	V380	E320	F260	SER	E135
GLU	ALA	GLY	GLY	SER	G561	V501	F441	V381	L321	D261	GLU	K145
PRO	ALA	ARG	GLY	THR	L562	L502	R442	C382	E322	I262	ASP	G146
LYS	GLY	TYR	ASN	GLY	D563	L503	K443	T383	P223	Q263	LYS	L147
ARG	HIS	THR	SER	ALA	I564	F504	K444	P384	G324	L264	GLU	R148
GLY	GLY	GLY	PRO	MET	P565	V505	I445	G385	D325	M265	ARG	D149
ASP	ASN	ARG	ASP	GLY	S566	T506	E446	R386	G326	H266	LYS	K145
TRP	ARG	GLY	PRO	ARG	I567	K507	K447	L387	P327	Q267	ASN	G146
ASP	ALA	SER	THR	LEU	K568	K508	L448	I388	I328	I268	VAL	E155
GLY	ALA	ARG	ALA	ALA	T569	A509	A449	D389	A329	R269	GLU	E158
ASP	LYS	HIS	LYS	LYS	V570	N510	R450	H390	V330	K270	ASP	R162
ARG	GLY	HIS	LYS	ALA	I571	A511	D451	V391	I331	S271	PRO	N167
ASN	ALA	GLY	GLY	ALA	N572	E512	I452	K392	V332	E272	THR	PRO
GLY	ILE	GLU	ILE	PHE	V573	E513	L453	K393	C333	Y273	ALA	ALA
THR	PRO	THR	PRO	GLN	D574	L514	I454	K394	P334	T274	GLY	GLY
SER	GLY	GLY	GLY	SER	V575	A515	D455	A395	T335	Q275	VAL	VAL
ASN	PHE	ASN	PHE	GLN	A576	N516	P456	T396	R336	P276	GLU	GLU
ARG	GLY	ARG	GLY	TYR	R577	N517	I457	N397	E337	T277	GLU	GLU
GLY	ASN	HIS	ASN	LYS	D578	L518	R458	L398	L338	P278	GLU	GLU
ASP	THR	ASP	GLY	SER	I579	K519	V459	Q399	C339	I279	ALA	ALA
PRO	ILE	PRO	ILE	VAL	D580	Q520	V460	R400	Q340	Q280	GLY	GLY
ALA	ALA	ARG	ALA	ALA	T581	E521	Q461	V401	Q341	C281	VAL	VAL
SER	GLY	ALA	GLY	ALA	H582	G522	G462	S402	I342	Q282	GLN	GLN
PRO	ALA	SER	PRO	LEU	T583	H523	D463	Y403	H343	G283	GLU	GLU
MET	ASP	ASP	ASP	SER	H584	N524	I464	L404	A344	V284	GLU	GLU
GLY	GLY	GLY	GLY	SER	R585	L525	G465	V405	E345	P285	GLU	GLU
					I586	G526	E466	F406	C346	V286		
					G587	L527	ALA	D407	K347	A287		
					R588	L528	ASN	E408	R348	L288		
					T589	H529	GLU	A409	F349	S289		
					G590	G530	D470	D410	G350	G290		
					ALA	D531	V471	R411	K351	R291		
					GLY	M532	T472	M412	A352	D292		
						D533	Q473	F413	Y353	M293		
					E594	Q534	I474	D414	N354	I294		
					K595	Q535	V475	M415	L355	G295		
					G596	E536	E476	G416	R356	I296		
					V597	R537	I477	F417	S357	A297		



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.087, 1.087, 1.087	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	B	0.36	0/665	0.47	0/899
2	C	0.33	0/6609	0.48	1/8946 (0.0%)
3	D	0.36	0/709	0.49	0/952
4	A	0.34	0/9415	0.51	0/12775
5	E	0.40	0/2607	0.56	1/3593 (0.0%)
All	All	0.35	0/20005	0.51	2/27165 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	564	ASP	O-C-N	-5.13	114.49	122.70
5	E	271	SER	C-N-CA	5.03	134.27	121.70

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	B	646	0	608	6	0
2	C	6487	0	6700	148	0
3	D	700	0	682	6	0
4	A	9227	0	9154	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2605	0	1378	63	0
6	D	3	0	0	0	0
All	All	19668	0	18522	317	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 8.

All (317) 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)
2:C:786:LYS:NZ	5:E:72:GLU:HG3	1.52	1.22
2:C:741:LYS:HE3	5:E:79:GLU:HB2	1.19	1.15
4:A:221:VAL:CG1	5:E:146:GLY:HA3	1.82	1.10
2:C:741:LYS:CE	5:E:79:GLU:HB2	1.87	1.04
2:C:786:LYS:HZ1	5:E:72:GLU:HG3	0.87	1.01
2:C:662:HIS:CE1	2:C:700:LYS:HD2	1.95	1.00
2:C:630:ARG:NH2	5:E:68:ASN:HB2	1.79	0.97
5:E:162:ARG:HH11	5:E:162:ARG:HB3	1.27	0.96
5:E:162:ARG:HB3	5:E:162:ARG:NH1	1.82	0.94
5:E:120:MET:HA	5:E:120:MET:CE	2.00	0.91
2:C:786:LYS:NZ	5:E:72:GLU:CG	2.33	0.90
2:C:786:LYS:HZ1	5:E:72:GLU:CG	1.80	0.89
2:C:662:HIS:HE1	2:C:700:LYS:HD2	1.40	0.87
2:C:783:GLU:CG	5:E:75:TYR:CD2	2.56	0.87
2:C:783:GLU:HG3	5:E:75:TYR:CD2	2.14	0.82
5:E:145:LYS:HB2	5:E:145:LYS:NZ	1.95	0.80
4:A:221:VAL:HG12	5:E:146:GLY:HA3	1.63	0.79
5:E:120:MET:HA	5:E:120:MET:HE1	1.63	0.79
2:C:1180:ARG:CZ	5:E:442:ARG:HA	2.13	0.79
4:A:459:VAL:HG11	4:A:757:ILE:HD13	1.65	0.78
5:E:70:ASP:HB2	5:E:73:ASN:ND2	1.99	0.77
4:A:221:VAL:HG11	5:E:146:GLY:HA3	1.64	0.77
4:A:264:GLN:HE22	4:A:322:VAL:H	1.31	0.77
2:C:783:GLU:HG2	5:E:75:TYR:CD2	2.20	0.76
4:A:486:SER:HB2	4:A:494:VAL:HB	1.68	0.76
2:C:1208:LEU:HB2	2:C:1241:ILE:HD11	1.66	0.76
4:A:221:VAL:CG1	5:E:146:GLY:CA	2.63	0.74
4:A:804:HIS:HD2	4:A:862:TRP:CZ2	2.06	0.74
5:E:149:ASP:N	5:E:149:ASP:OD1	2.20	0.74
4:A:547:CYS:SG	4:A:548:ALA:N	2.61	0.73
4:A:528:ARG:HG3	4:A:530:ASP:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:961:VAL:HA	2:C:964:THR:HG22	1.72	0.71
4:A:1200:THR:HG22	4:A:1202:PRO:HD2	1.73	0.71
4:A:552:ARG:NH1	4:A:600:GLN:O	2.24	0.70
2:C:655:LYS:NZ	5:E:114:ASP:HB2	2.05	0.70
2:C:963:LYS:HD3	2:C:1003:VAL:HG22	1.73	0.70
4:A:828:GLY:O	4:A:834:LEU:N	2.24	0.70
2:C:568:ARG:NH1	5:E:130:ASP:OD1	2.24	0.69
2:C:783:GLU:OE2	5:E:72:GLU:HG2	1.91	0.69
4:A:507:SER:HB2	4:A:519:VAL:HB	1.73	0.69
2:C:1180:ARG:NH2	5:E:443:LYS:H	1.90	0.69
4:A:1001:ILE:HG13	4:A:1038:LEU:HD21	1.74	0.68
5:E:300:GLY:O	5:E:302:GLY:N	2.21	0.68
2:C:1289:ASN:ND2	2:C:1295:TYR:H	1.93	0.67
4:A:603:ARG:HA	4:A:619:LEU:HB2	1.77	0.66
2:C:662:HIS:HE1	2:C:700:LYS:CD	2.09	0.66
4:A:499:PHE:O	4:A:525:ARG:NH1	2.30	0.65
2:C:622:GLU:OE2	2:C:622:GLU:HA	1.97	0.65
5:E:145:LYS:HB2	5:E:145:LYS:HZ2	1.58	0.65
4:A:550:ASN:ND2	4:A:593:ALA:O	2.30	0.64
4:A:637:PRO:HA	4:A:669:LEU:HA	1.78	0.64
4:A:558:LEU:HD23	4:A:558:LEU:H	1.63	0.63
2:C:731:LEU:HB3	2:C:750:ILE:HD11	1.80	0.63
2:C:1097:LEU:O	2:C:1100:ASN:ND2	2.32	0.62
2:C:618:ASP:OD1	2:C:618:ASP:N	2.33	0.62
2:C:621:ASP:OD2	2:C:621:ASP:N	2.30	0.62
5:E:68:ASN:O	5:E:68:ASN:ND2	2.32	0.62
4:A:947:GLU:HG3	4:A:948:VAL:H	1.65	0.61
2:C:655:LYS:HZ2	5:E:114:ASP:HB2	1.65	0.61
2:C:769:VAL:O	2:C:773:LEU:HB2	2.00	0.61
4:A:549:VAL:HG13	4:A:554:VAL:HG22	1.83	0.61
4:A:465:HIS:CE1	4:A:467:GLU:HB2	2.36	0.60
4:A:720:TRP:HA	4:A:733:PRO:HA	1.84	0.60
2:C:581:LEU:HD22	2:C:589:ALA:HB1	1.84	0.60
2:C:974:LEU:HA	2:C:977:VAL:HG12	1.83	0.60
2:C:1001:VAL:O	2:C:1045:ARG:NH2	2.34	0.60
2:C:630:ARG:HH21	5:E:68:ASN:HB2	1.67	0.60
4:A:554:VAL:HG12	4:A:556:ILE:HD11	1.84	0.60
4:A:603:ARG:O	4:A:619:LEU:N	2.34	0.60
4:A:1083:ASN:N	4:A:1088:LYS:HZ1	2.01	0.59
4:A:221:VAL:HG13	5:E:146:GLY:C	2.23	0.59
4:A:614:VAL:HG13	4:A:633:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:320:ASP:N	4:A:320:ASP:OD1	2.36	0.58
4:A:553:GLN:HE21	4:A:601:ARG:HB2	1.67	0.58
4:A:511:LEU:HD22	4:A:517:VAL:HG21	1.84	0.58
4:A:466:ILE:HA	4:A:510:LEU:HD21	1.85	0.57
2:C:972:GLY:O	2:C:976:VAL:HG23	2.04	0.57
5:E:117:GLU:OE1	5:E:117:GLU:HA	2.04	0.57
2:C:513:LYS:HE2	5:E:158:GLU:HG3	1.87	0.57
2:C:570:TYR:O	2:C:574:ILE:HG12	2.04	0.57
2:C:786:LYS:HZ2	5:E:72:GLU:CG	2.17	0.57
4:A:126:LYS:HB2	4:A:128:ARG:HE	1.69	0.57
4:A:946:GLU:OE2	4:A:968:ARG:NH2	2.34	0.57
1:B:25:ASP:OD1	2:C:1259:ARG:NH2	2.30	0.56
2:C:903:GLN:HE21	2:C:906:GLU:HA	1.69	0.56
2:C:1113:THR:HG23	2:C:1150:SER:HA	1.87	0.56
2:C:786:LYS:HZ2	5:E:72:GLU:CD	2.09	0.56
4:A:545:VAL:HG22	4:A:546:LYS:HE2	1.87	0.56
4:A:617:ILE:HG21	4:A:625:LEU:HD13	1.86	0.56
4:A:464:ARG:HE	4:A:472:ALA:HB1	1.71	0.56
2:C:783:GLU:HG2	5:E:75:TYR:CG	2.41	0.55
4:A:562:GLU:HG2	4:A:582:GLU:HG2	1.88	0.55
2:C:1174:GLU:OE1	2:C:1210:HIS:NE2	2.36	0.55
4:A:640:LEU:HD12	4:A:667:ILE:HD12	1.87	0.55
2:C:1289:ASN:HD22	2:C:1295:TYR:H	1.52	0.55
4:A:278:LEU:HD21	4:A:816:LYS:HG3	1.88	0.54
4:A:739:LEU:HG	4:A:756:ALA:HB1	1.89	0.54
4:A:565:TYR:HD2	4:A:577:TYR:HB2	1.72	0.54
4:A:428:GLY:HA3	4:A:433:SER:HA	1.89	0.54
2:C:581:LEU:O	2:C:590:ARG:HA	2.07	0.54
4:A:200:ALA:O	4:A:204:THR:OG1	2.22	0.54
2:C:1166:ILE:O	2:C:1170:THR:HG23	2.08	0.54
4:A:456:PRO:HB2	4:A:757:ILE:HG21	1.90	0.54
4:A:544:ILE:HA	4:A:558:LEU:HA	1.89	0.54
2:C:741:LYS:HD3	5:E:76:PHE:HA	1.90	0.54
2:C:834:VAL:O	2:C:838:VAL:HG23	2.08	0.54
2:C:655:LYS:NZ	5:E:115:PRO:HD3	2.22	0.53
4:A:955:PHE:HD1	4:A:995:THR:HG21	1.73	0.53
2:C:729:LYS:HB3	2:C:730:PRO:HD3	1.90	0.53
2:C:932:ILE:O	2:C:936:VAL:HG23	2.07	0.53
4:A:438:LEU:HD22	4:A:776:GLN:HB3	1.90	0.53
4:A:474:ILE:HG22	4:A:476:VAL:HG23	1.90	0.53
2:C:565:ASP:O	2:C:568:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:555:VAL:HG13	4:A:565:TYR:HA	1.89	0.53
4:A:955:PHE:CD1	4:A:995:THR:HG21	2.43	0.53
5:E:132:LYS:HG3	5:E:132:LYS:O	2.08	0.53
2:C:655:LYS:HZ1	5:E:115:PRO:HD3	1.73	0.53
1:B:47:PHE:CZ	4:A:35:GLY:HA3	2.44	0.53
4:A:436:ARG:HH11	4:A:776:GLN:HE22	1.56	0.52
5:E:145:LYS:HB2	5:E:145:LYS:HZ3	1.73	0.52
2:C:1199:VAL:HG11	2:C:1204:CYS:SG	2.49	0.52
2:C:971:MET:HA	2:C:974:LEU:HG	1.91	0.52
4:A:539:PRO:O	4:A:542:LYS:NZ	2.42	0.52
4:A:550:ASN:HB2	4:A:592:LEU:HD11	1.92	0.52
1:B:58:ASN:O	4:A:856:LYS:NZ	2.37	0.51
2:C:1179:ASP:O	2:C:1185:ARG:NH1	2.41	0.51
4:A:899:THR:OG1	4:A:900:GLY:N	2.43	0.51
2:C:883:ASP:OD1	2:C:883:ASP:N	2.43	0.51
2:C:722:GLU:CD	2:C:722:GLU:H	2.15	0.50
4:A:1176:GLY:HA2	4:A:1179:CYS:HB2	1.92	0.50
4:A:636:GLN:HG2	4:A:670:GLN:HG2	1.94	0.50
2:C:770:MET:O	2:C:774:ILE:HG12	2.11	0.50
2:C:826:ASP:OD1	2:C:827:ARG:N	2.44	0.50
2:C:746:PHE:O	2:C:750:ILE:HG12	2.12	0.50
2:C:513:LYS:CE	5:E:158:GLU:HG3	2.42	0.50
4:A:343:LYS:O	4:A:344:THR:OG1	2.17	0.50
4:A:553:GLN:HE21	4:A:601:ARG:HD2	1.76	0.49
2:C:812:PRO:HB2	2:C:813:PRO:HD3	1.94	0.49
2:C:1180:ARG:NH1	5:E:442:ARG:HA	2.28	0.49
4:A:512:GLY:H	4:A:515:ALA:HB3	1.77	0.49
2:C:662:HIS:CE1	2:C:700:LYS:CD	2.82	0.49
2:C:741:LYS:HE2	5:E:79:GLU:HB2	1.84	0.49
2:C:1084:ILE:O	2:C:1088:ILE:HG12	2.12	0.49
2:C:700:LYS:HG3	5:E:80:GLU:HG3	1.94	0.49
2:C:903:GLN:NE2	2:C:906:GLU:HA	2.27	0.49
4:A:525:ARG:HG2	4:A:527:ILE:HD11	1.94	0.49
4:A:673:VAL:HA	4:A:690:ARG:HA	1.95	0.49
2:C:622:GLU:OE1	5:E:77:GLU:OE2	2.30	0.49
2:C:661:ARG:NH1	2:C:696:ASP:OD2	2.46	0.48
4:A:404:LEU:HD11	4:A:438:LEU:HD11	1.95	0.48
4:A:849:GLU:HG2	4:A:854:ALA:HA	1.94	0.48
5:E:300:GLY:C	5:E:302:GLY:H	2.13	0.48
4:A:608:GLY:HA2	4:A:614:VAL:HA	1.96	0.48
4:A:864:SER:HB3	4:A:882:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:550:ASN:ND2	4:A:595:VAL:HG13	2.29	0.48
4:A:716:SER:OG	4:A:717:SER:N	2.46	0.48
2:C:1071:LYS:O	2:C:1075:ARG:HG2	2.14	0.48
4:A:471:ASP:O	4:A:487:ILE:HG21	2.13	0.48
4:A:807:TYR:CE2	4:A:857:ALA:HB3	2.48	0.48
2:C:732:TRP:CZ2	2:C:765:TYR:HB3	2.48	0.48
2:C:810:ILE:O	2:C:813:PRO:HD2	2.14	0.48
4:A:606:ALA:HB3	4:A:642:ILE:HD11	1.95	0.48
4:A:665:LEU:HD21	4:A:667:ILE:HD11	1.96	0.48
4:A:994:GLN:HG2	4:A:1038:LEU:HG	1.96	0.48
2:C:591:VAL:O	2:C:595:GLU:HG3	2.13	0.47
2:C:605:GLY:O	2:C:609:MET:HG2	2.14	0.47
4:A:500:LEU:HB2	4:A:525:ARG:HH22	1.79	0.47
4:A:443:GLU:H	4:A:443:GLU:CD	2.17	0.47
2:C:935:THR:O	2:C:939:ARG:HG2	2.14	0.47
4:A:1201:PRO:HB2	4:A:1202:PRO:HD3	1.96	0.47
5:E:114:ASP:N	5:E:115:PRO:HD2	2.29	0.47
2:C:945:ALA:HA	2:C:948:ARG:HB2	1.95	0.47
4:A:822:GLU:HA	4:A:825:GLU:HG2	1.95	0.47
2:C:648:LEU:HA	2:C:651:VAL:HG12	1.96	0.47
4:A:515:ALA:HA	4:A:528:ARG:HA	1.95	0.47
4:A:642:ILE:HG13	4:A:665:LEU:HD12	1.95	0.47
3:D:26:CYS:HB3	3:D:29:LYS:HE2	1.95	0.47
4:A:137:LYS:O	4:A:137:LYS:HG2	2.15	0.47
4:A:697:ARG:HB2	4:A:717:SER:H	1.80	0.47
2:C:946:LYS:HB3	2:C:946:LYS:HE3	1.68	0.46
4:A:48:GLY:HA3	4:A:398:VAL:HG11	1.97	0.46
2:C:495:ARG:O	2:C:495:ARG:NH2	2.43	0.46
2:C:1007:HIS:ND1	2:C:1049:TYR:OH	2.46	0.46
2:C:1187:THR:O	2:C:1191:VAL:HG23	2.14	0.46
4:A:336:ALA:HA	4:A:351:SER:HA	1.97	0.46
2:C:908:SER:OG	2:C:912:ASN:ND2	2.49	0.46
2:C:786:LYS:HE2	2:C:828:ARG:HH12	1.81	0.46
5:E:590:GLY:O	5:E:594:GLU:HA	2.16	0.46
2:C:630:ARG:NH2	5:E:68:ASN:CB	2.67	0.46
4:A:581:LYS:HD2	4:A:625:LEU:HD12	1.98	0.46
2:C:575:LEU:O	2:C:579:GLU:HB2	2.16	0.46
2:C:663:THR:O	2:C:667:ILE:HG13	2.16	0.46
4:A:530:ASP:OD2	4:A:530:ASP:N	2.49	0.46
2:C:636:ALA:HB2	2:C:644:LEU:HD22	1.97	0.45
2:C:763:ASN:O	2:C:767:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:735:ILE:HD12	2:C:772:ILE:HD13	1.97	0.45
2:C:1140:GLU:O	2:C:1144:GLN:HG3	2.16	0.45
4:A:477:SER:HA	4:A:482:THR:HA	1.99	0.45
4:A:550:ASN:OD1	4:A:551:GLN:N	2.41	0.45
2:C:911:LEU:HD21	2:C:953:ASP:HB2	1.97	0.45
2:C:925:VAL:HG23	2:C:928:TYR:HB2	1.99	0.45
4:A:579:GLU:OE1	4:A:625:LEU:HG	2.16	0.45
4:A:873:GLN:HG3	4:A:875:ASN:HD22	1.82	0.45
4:A:556:ILE:HG22	4:A:557:ALA:H	1.80	0.45
5:E:120:MET:CE	5:E:120:MET:CA	2.86	0.45
3:D:29:LYS:HG2	3:D:36:TYR:CZ	2.52	0.45
2:C:1092:ASP:OD2	2:C:1092:ASP:N	2.49	0.45
2:C:1136:TYR:HB2	2:C:1147:VAL:HG11	1.97	0.45
4:A:465:HIS:CE1	4:A:467:GLU:H	2.35	0.45
5:E:133:ARG:CD	5:E:133:ARG:C	2.85	0.45
4:A:1009:PHE:HZ	4:A:1046:GLY:HA3	1.81	0.44
2:C:925:VAL:HG23	2:C:928:TYR:HD2	1.81	0.44
2:C:1256:HIS:HD2	2:C:1258:ALA:H	1.65	0.44
2:C:766:THR:O	2:C:770:MET:HB2	2.17	0.44
5:E:133:ARG:CZ	5:E:134:LEU:HB2	2.47	0.44
2:C:630:ARG:CZ	5:E:68:ASN:HB2	2.44	0.44
2:C:783:GLU:HG3	5:E:75:TYR:HD2	1.78	0.44
2:C:855:ASP:OD1	2:C:891:GLN:NE2	2.50	0.44
4:A:663:LEU:HD23	4:A:679:LEU:HB3	1.99	0.44
4:A:643:VAL:HG12	4:A:703:ARG:HD3	2.00	0.44
2:C:866:LYS:HG3	2:C:909:VAL:HG11	1.99	0.44
4:A:538:THR:HG21	4:A:558:LEU:HD13	1.98	0.44
4:A:620:ASP:OD1	4:A:621:PRO:HD2	2.16	0.44
4:A:1165:SER:OG	4:A:1170:VAL:HG23	2.18	0.44
5:E:145:LYS:O	5:E:145:LYS:HG2	2.17	0.44
4:A:219:HIS:CD2	5:E:148:ARG:HD3	2.52	0.44
4:A:509:SER:HB2	4:A:549:VAL:HG11	2.00	0.44
5:E:299:THR:HA	5:E:300:GLY:HA2	1.71	0.44
2:C:1053:ARG:HH22	2:C:1057:ARG:HD2	1.83	0.44
2:C:721:ILE:HD13	2:C:756:LEU:HB3	2.01	0.43
2:C:804:ASN:O	2:C:808:THR:HG22	2.17	0.43
2:C:623:TYR:O	2:C:627:THR:HG23	2.18	0.43
4:A:745:PHE:HD2	4:A:750:CYS:HB2	1.84	0.43
4:A:1114:SER:HB2	4:A:1215:TYR:CE1	2.53	0.43
2:C:886:HIS:O	2:C:887:LYS:HB3	2.18	0.43
4:A:537:LYS:HE3	4:A:537:LYS:HB2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1104:LEU:HD23	4:A:1119:TYR:HB3	2.01	0.43
2:C:1125:PRO:HG2	2:C:1165:TYR:CE2	2.53	0.43
2:C:904:THR:OG1	2:C:905:THR:N	2.52	0.43
4:A:618:SER:OG	4:A:628:LEU:HD21	2.19	0.43
4:A:873:GLN:HG3	4:A:875:ASN:ND2	2.33	0.43
4:A:230:GLU:OE1	4:A:268:ARG:NH2	2.52	0.42
4:A:947:GLU:HG2	4:A:964:GLY:HA3	2.02	0.42
4:A:697:ARG:HH11	4:A:717:SER:HA	1.84	0.42
4:A:710:GLU:OE2	4:A:710:GLU:HA	2.19	0.42
2:C:873:GLU:OE1	2:C:912:ASN:HB3	2.20	0.42
2:C:886:HIS:C	2:C:888:LEU:H	2.23	0.42
4:A:758:SER:HB2	4:A:763:ARG:HE	1.84	0.42
4:A:980:LYS:HD2	4:A:980:LYS:HA	1.75	0.42
1:B:7:ILE:HG13	3:D:8:LEU:O	2.19	0.42
2:C:806:ILE:HG12	2:C:810:ILE:HD12	2.00	0.42
2:C:1025:LYS:HA	2:C:1025:LYS:HD2	1.82	0.42
4:A:32:VAL:HG22	4:A:39:GLU:HB3	2.00	0.42
2:C:1053:ARG:CZ	2:C:1053:ARG:HB3	2.49	0.42
4:A:715:MET:HE3	4:A:715:MET:HB3	1.86	0.42
4:A:1035:THR:HG22	4:A:1047:ALA:HB3	2.00	0.42
4:A:370:GLU:OE2	4:A:390:ARG:HD3	2.18	0.42
2:C:641:ILE:HD11	2:C:675:MET:SD	2.60	0.42
2:C:1260:LYS:HA	2:C:1260:LYS:HD3	1.84	0.42
2:C:568:ARG:NH2	5:E:130:ASP:OD1	2.53	0.42
2:C:774:ILE:O	2:C:777:PHE:HB2	2.19	0.42
2:C:1009:MET:HG2	2:C:1011:PRO:HD2	2.02	0.42
2:C:1289:ASN:HD21	2:C:1296:ILE:H	1.68	0.42
4:A:267:ILE:HD13	4:A:322:VAL:HG12	2.01	0.42
4:A:1214:ARG:HG2	4:A:1215:TYR:CE2	2.55	0.42
4:A:743:SER:OG	4:A:744:GLY:O	2.38	0.41
2:C:732:TRP:O	2:C:735:ILE:HG13	2.19	0.41
2:C:811:LEU:HD22	2:C:815:PHE:HE2	1.84	0.41
2:C:929:LEU:N	2:C:930:PRO:HD2	2.35	0.41
2:C:1110:VAL:O	2:C:1114:VAL:HG23	2.19	0.41
4:A:629:SER:OG	4:A:681:PRO:O	2.38	0.41
4:A:821:GLU:O	4:A:824:VAL:HG12	2.19	0.41
4:A:858:GLY:HA3	4:A:861:GLN:HG3	2.03	0.41
1:B:32:LEU:HD11	2:C:1287:ILE:HG21	2.02	0.41
2:C:631:ALA:O	2:C:635:VAL:HG12	2.20	0.41
2:C:814:PHE:O	2:C:818:PHE:HB2	2.20	0.41
2:C:1070:LYS:NZ	2:C:1070:LYS:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:947:GLU:HG3	4:A:948:VAL:N	2.33	0.41
4:A:1018:GLU:N	4:A:1018:GLU:OE2	2.52	0.41
4:A:638:GLU:HG3	4:A:670:GLN:HB3	2.02	0.41
2:C:1180:ARG:NH2	5:E:442:ARG:HA	2.35	0.41
2:C:1250:CYS:SG	2:C:1269:TYR:HB2	2.60	0.41
4:A:172:GLY:O	4:A:237:THR:OG1	2.30	0.41
4:A:187:MET:HE2	4:A:204:THR:HG22	2.01	0.41
4:A:472:ALA:O	4:A:487:ILE:HG22	2.20	0.41
2:C:551:LEU:O	2:C:555:VAL:HG23	2.20	0.41
4:A:895:ARG:HG2	4:A:902:ASP:O	2.21	0.41
1:B:57:GLU:O	1:B:59:GLU:N	2.53	0.41
2:C:641:ILE:N	2:C:642:PRO:HD2	2.35	0.41
2:C:745:ALA:HB2	5:E:76:PHE:CE1	2.55	0.41
2:C:776:GLU:O	2:C:779:SER:HB3	2.21	0.41
2:C:1014:LYS:H	2:C:1014:LYS:HE2	1.84	0.41
4:A:451:GLU:HG3	4:A:760:ASN:O	2.21	0.41
5:E:134:LEU:HD12	5:E:134:LEU:HA	1.90	0.41
2:C:1193:GLN:HB2	2:C:1233:ALA:HA	2.02	0.41
4:A:761:THR:HG22	4:A:762:LEU:H	1.85	0.41
3:D:22:LEU:HG	3:D:69:ALA:HB2	2.03	0.41
4:A:168:TYR:HB2	4:A:185:LEU:HB2	2.03	0.41
3:D:59:VAL:HG13	3:D:87:LYS:HA	2.02	0.41
4:A:423:LEU:HB2	4:A:438:LEU:HB2	2.03	0.40
2:C:856:ASP:HB3	2:C:864:TYR:CE2	2.57	0.40
2:C:925:VAL:HG23	2:C:928:TYR:CD2	2.56	0.40
2:C:943:LYS:HB3	2:C:947:VAL:HG21	2.02	0.40
2:C:955:ILE:HD13	2:C:974:LEU:HD13	2.03	0.40
4:A:521:PRO:HA	4:A:544:ILE:HB	2.02	0.40
4:A:683:THR:O	4:A:683:THR:OG1	2.38	0.40
2:C:514:ALA:O	2:C:518:GLN:HG3	2.21	0.40
2:C:583:ILE:HD13	2:C:627:THR:HG22	2.02	0.40
2:C:772:ILE:HG23	2:C:775:ARG:HH21	1.86	0.40
2:C:849:ILE:O	2:C:853:ILE:HG12	2.21	0.40
2:C:1055:TRP:CE3	2:C:1055:TRP:HA	2.56	0.40
3:D:49:CYS:HB3	3:D:87:LYS:HD3	2.02	0.40
4:A:618:SER:CB	4:A:628:LEU:HD21	2.51	0.40
2:C:766:THR:HA	2:C:769:VAL:HG12	2.03	0.40
2:C:783:GLU:OE2	2:C:786:LYS:HE3	2.21	0.40
4:A:34:ARG:H	4:A:34:ARG:HG2	1.75	0.40
4:A:492:GLU:N	4:A:492:GLU:OE1	2.55	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	B	76/86 (88%)	75 (99%)	1 (1%)	0	100	100
2	C	813/872 (93%)	784 (96%)	29 (4%)	0	100	100
3	D	91/110 (83%)	86 (94%)	5 (6%)	0	100	100
4	A	1165/1250 (93%)	1088 (93%)	76 (6%)	1 (0%)	51	75
5	E	474/958 (50%)	459 (97%)	12 (2%)	3 (1%)	25	47
All	All	2619/3276 (80%)	2492 (95%)	123 (5%)	4 (0%)	50	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	301	SER
5	E	595	LYS
5	E	275	GLN
4	A	234	PHE

### 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	B	69/77 (90%)	68 (99%)	1 (1%)	67	85
2	C	701/753 (93%)	664 (95%)	37 (5%)	22	45
3	D	80/95 (84%)	76 (95%)	4 (5%)	24	47
4	A	1020/1071 (95%)	945 (93%)	75 (7%)	13	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	51/787 (6%)	40 (78%)	11 (22%)	1	1
All	All	1921/2783 (69%)	1793 (93%)	128 (7%)	20	33

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	THR
2	C	495	ARG
2	C	500	LEU
2	C	560	LEU
2	C	579	GLU
2	C	602	LYS
2	C	611	SER
2	C	619	ASN
2	C	620	MET
2	C	621	ASP
2	C	654	SER
2	C	677	CYS
2	C	683	LEU
2	C	736	ARG
2	C	756	LEU
2	C	779	SER
2	C	786	LYS
2	C	816	LYS
2	C	822	ARG
2	C	828	ARG
2	C	870	GLU
2	C	902	GLU
2	C	905	THR
2	C	914	PHE
2	C	923	LYS
2	C	943	LYS
2	C	949	GLN
2	C	956	SER
2	C	1008	LYS
2	C	1014	LYS
2	C	1092	ASP
2	C	1100	ASN
2	C	1101	LEU
2	C	1106	ARG
2	C	1160	GLU
2	C	1180	ARG

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Mol	Chain	Res	Type
2	C	1228	GLN
2	C	1271	SER
3	D	26	CYS
3	D	35	SER
3	D	97	ASP
3	D	98	LEU
4	A	8	LEU
4	A	12	THR
4	A	46	ASN
4	A	64	SER
4	A	128	ARG
4	A	152	LEU
4	A	171	VAL
4	A	214	ASP
4	A	229	GLU
4	A	290	SER
4	A	298	MET
4	A	364	LEU
4	A	374	SER
4	A	390	ARG
4	A	429	ARG
4	A	435	LEU
4	A	443	GLU
4	A	450	SER
4	A	465	HIS
4	A	469	GLU
4	A	486	SER
4	A	503	THR
4	A	520	TYR
4	A	530	ASP
4	A	538	THR
4	A	541	LYS
4	A	543	THR
4	A	546	LYS
4	A	547	CYS
4	A	568	MET
4	A	576	GLU
4	A	578	THR
4	A	582	GLU
4	A	590	MET
4	A	599	GLU
4	A	618	SER

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Mol	Chain	Res	Type
4	A	640	LEU
4	A	641	CYS
4	A	645	MET
4	A	662	PHE
4	A	665	LEU
4	A	677	THR
4	A	685	ASP
4	A	689	THR
4	A	690	ARG
4	A	700	LYS
4	A	717	SER
4	A	741	PHE
4	A	743	SER
4	A	750	CYS
4	A	761	THR
4	A	767	LEU
4	A	768	GLU
4	A	769	LYS
4	A	775	ASN
4	A	805	ASN
4	A	821	GLU
4	A	824	VAL
4	A	864	SER
4	A	873	GLN
4	A	890	SER
4	A	897	SER
4	A	899	THR
4	A	916	ASN
4	A	920	VAL
4	A	984	LYS
4	A	994	GLN
4	A	1017	ASN
4	A	1037	SER
4	A	1048	ASP
4	A	1066	VAL
4	A	1103	SER
4	A	1137	ASP
4	A	1214	ARG
4	A	1217	PHE
5	E	68	ASN
5	E	70	ASP
5	E	79	GLU

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Mol	Chain	Res	Type
5	E	116	LEU
5	E	126	GLN
5	E	130	ASP
5	E	133	ARG
5	E	148	ARG
5	E	149	ASP
5	E	155	ASP
5	E	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	35	GLN
2	C	547	GLN
2	C	662	HIS
2	C	737	GLN
2	C	804	ASN
2	C	829	ASN
2	C	863	GLN
2	C	891	GLN
2	C	903	GLN
2	C	941	ASN
2	C	1100	ASN
2	C	1104	GLN
2	C	1108	ASN
2	C	1134	ASN
2	C	1144	GLN
2	C	1184	HIS
2	C	1194	HIS
2	C	1256	HIS
2	C	1289	ASN
2	C	1293	ASN
4	A	104	GLN
4	A	138	GLN
4	A	203	ASN
4	A	219	HIS
4	A	264	GLN
4	A	417	ASN
4	A	465	HIS
4	A	553	GLN
4	A	776	GLN

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Mol	Chain	Res	Type
4	A	796	ASN
4	A	804	HIS
4	A	870	ASN
4	A	875	ASN
4	A	916	ASN
4	A	1017	ASN
4	A	1052	ASN
4	A	1083	ASN
5	E	68	ASN

### 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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

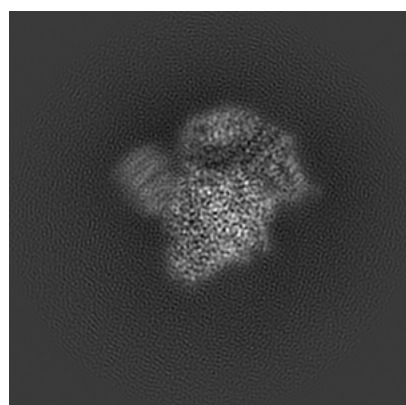
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31330. These allow visual inspection of the internal detail of the map and identification of artifacts.

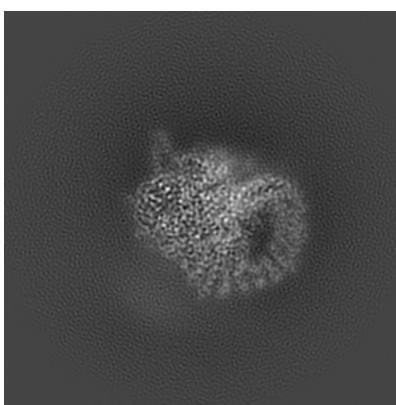
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

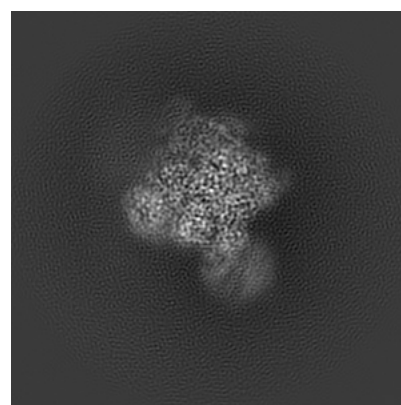
#### 6.1.1 Primary map



X



Y

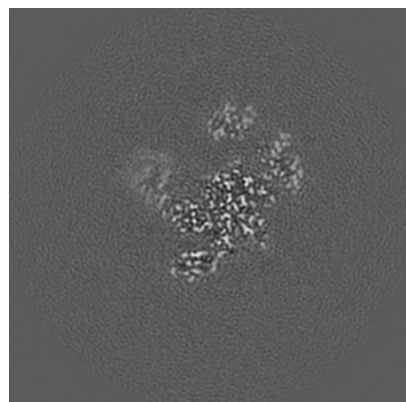


Z

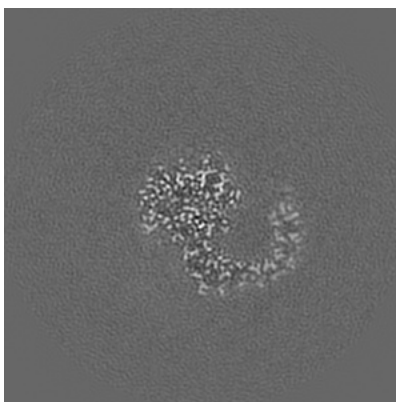
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

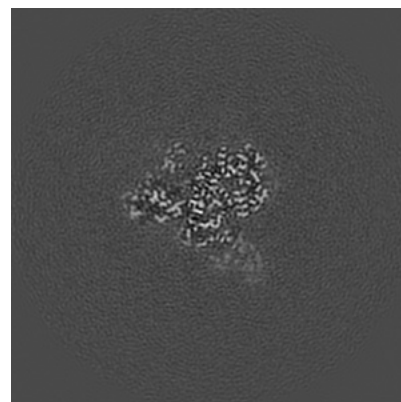
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

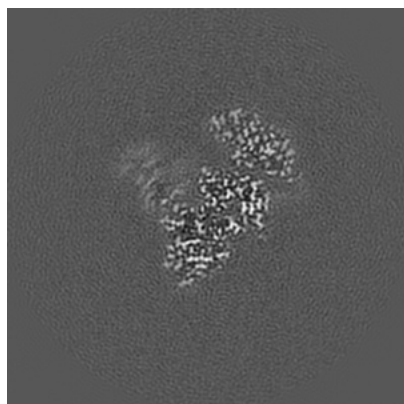


Z Index: 120

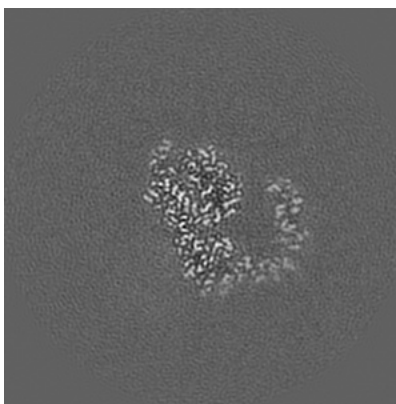
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

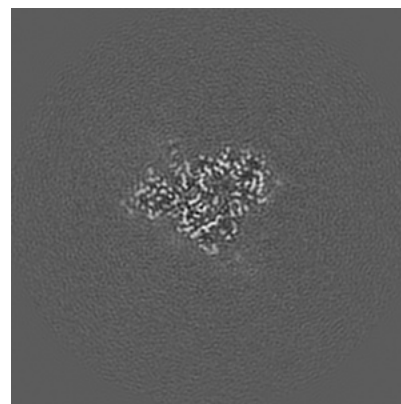
### 6.3.1 Primary map



X Index: 127



Y Index: 127

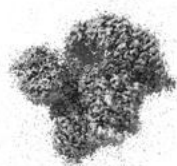


Z Index: 116

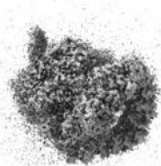
The images above show the largest variance slices of the map in three orthogonal directions.

## 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.

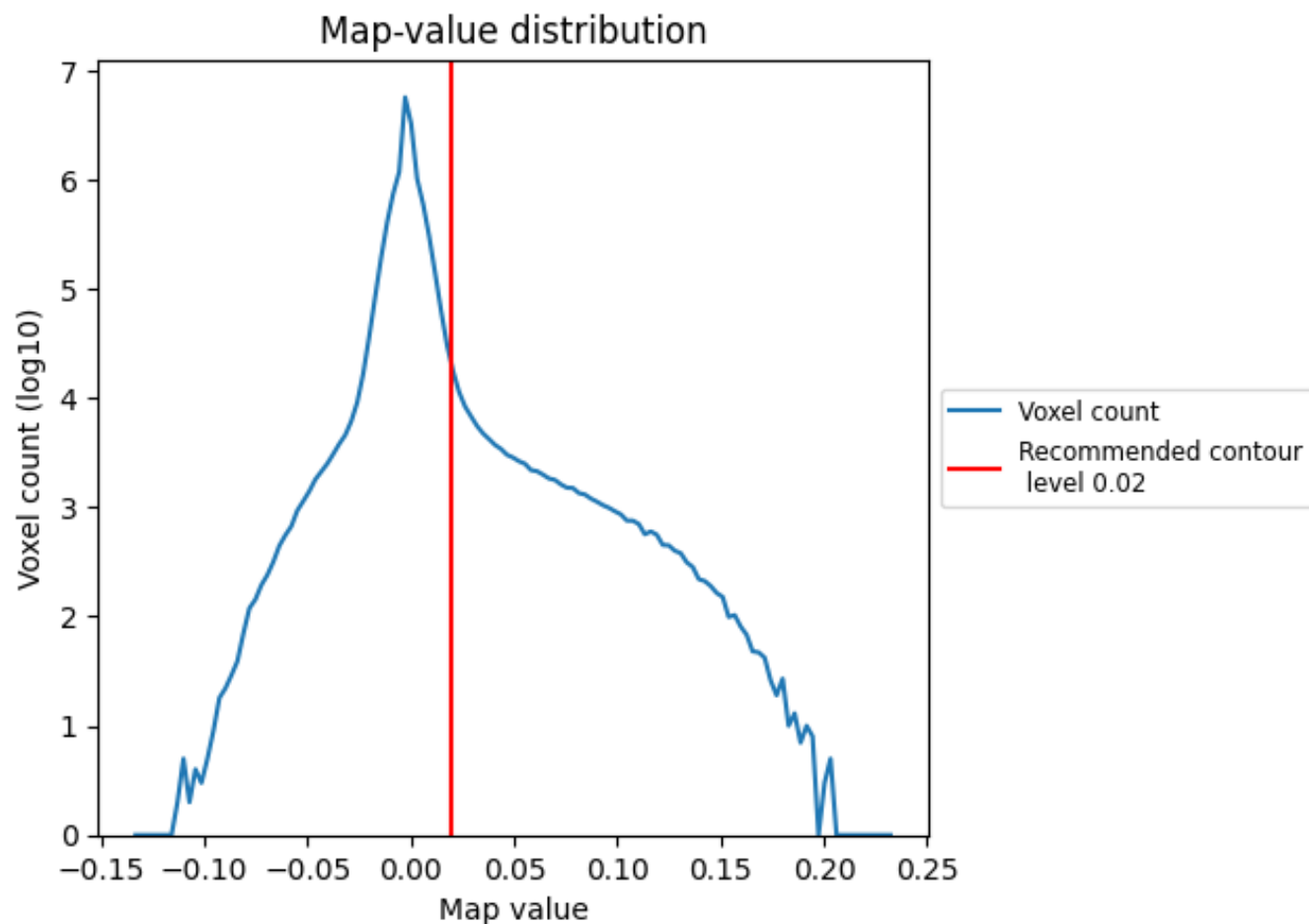
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

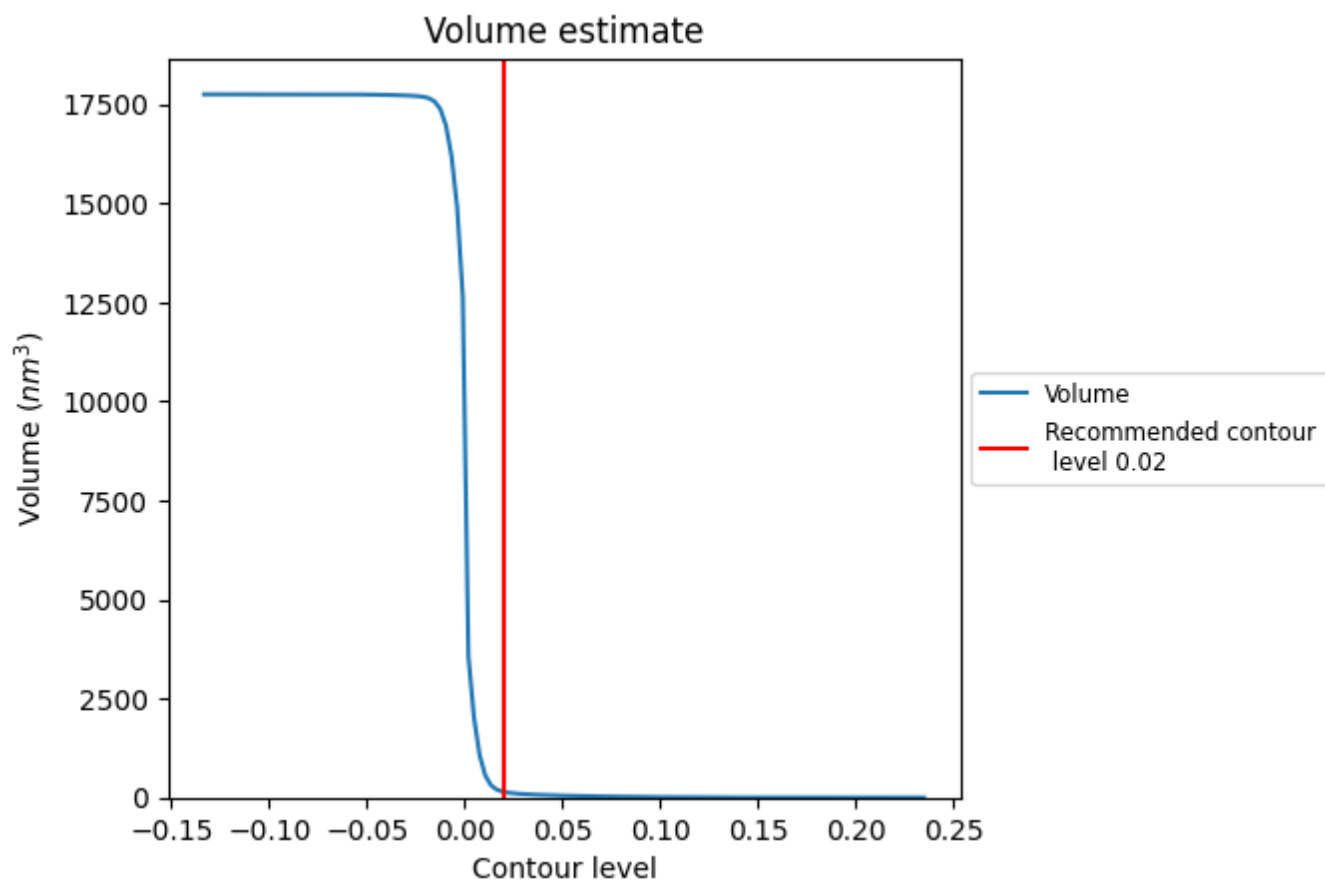
This section contains the results of statistical analysis of the map.

### 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.

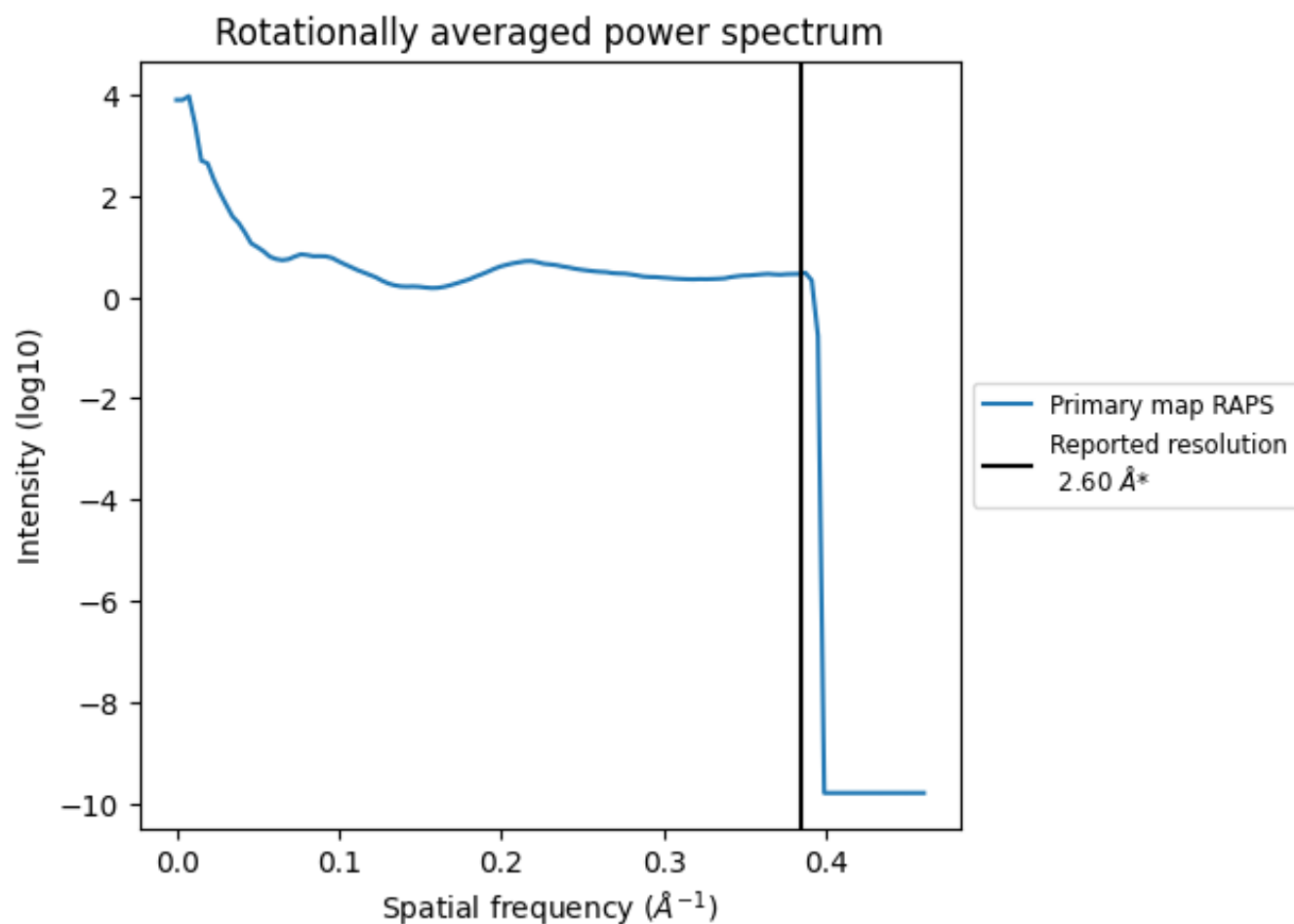
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm<sup>3</sup>; this corresponds to an approximate mass of 131 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 0.385 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

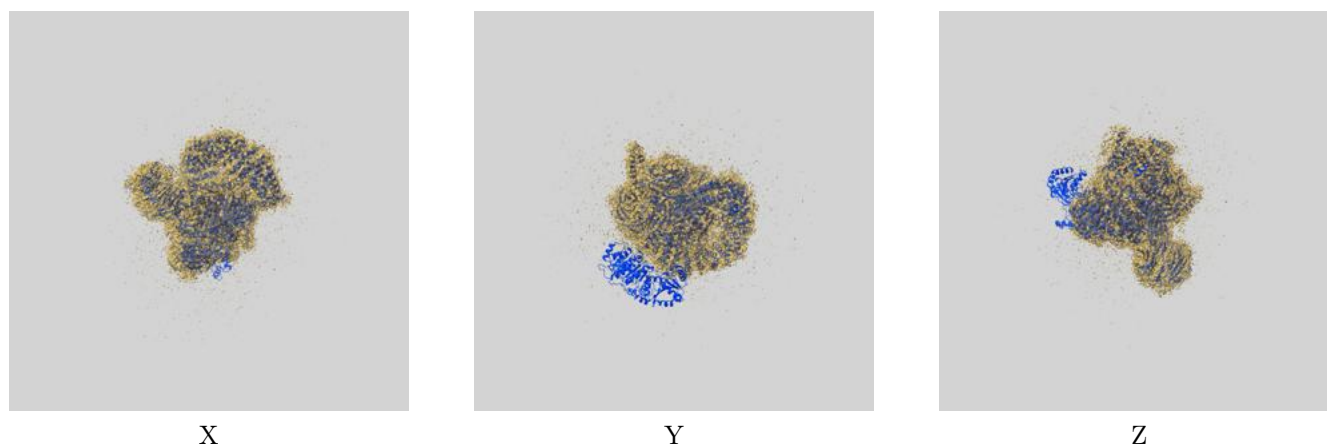
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31330 and PDB model 7EVN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



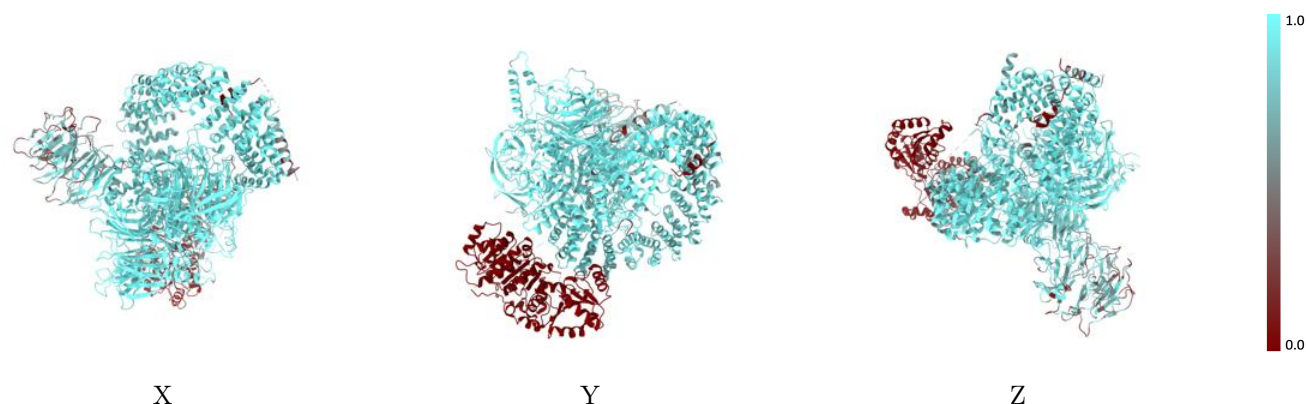
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



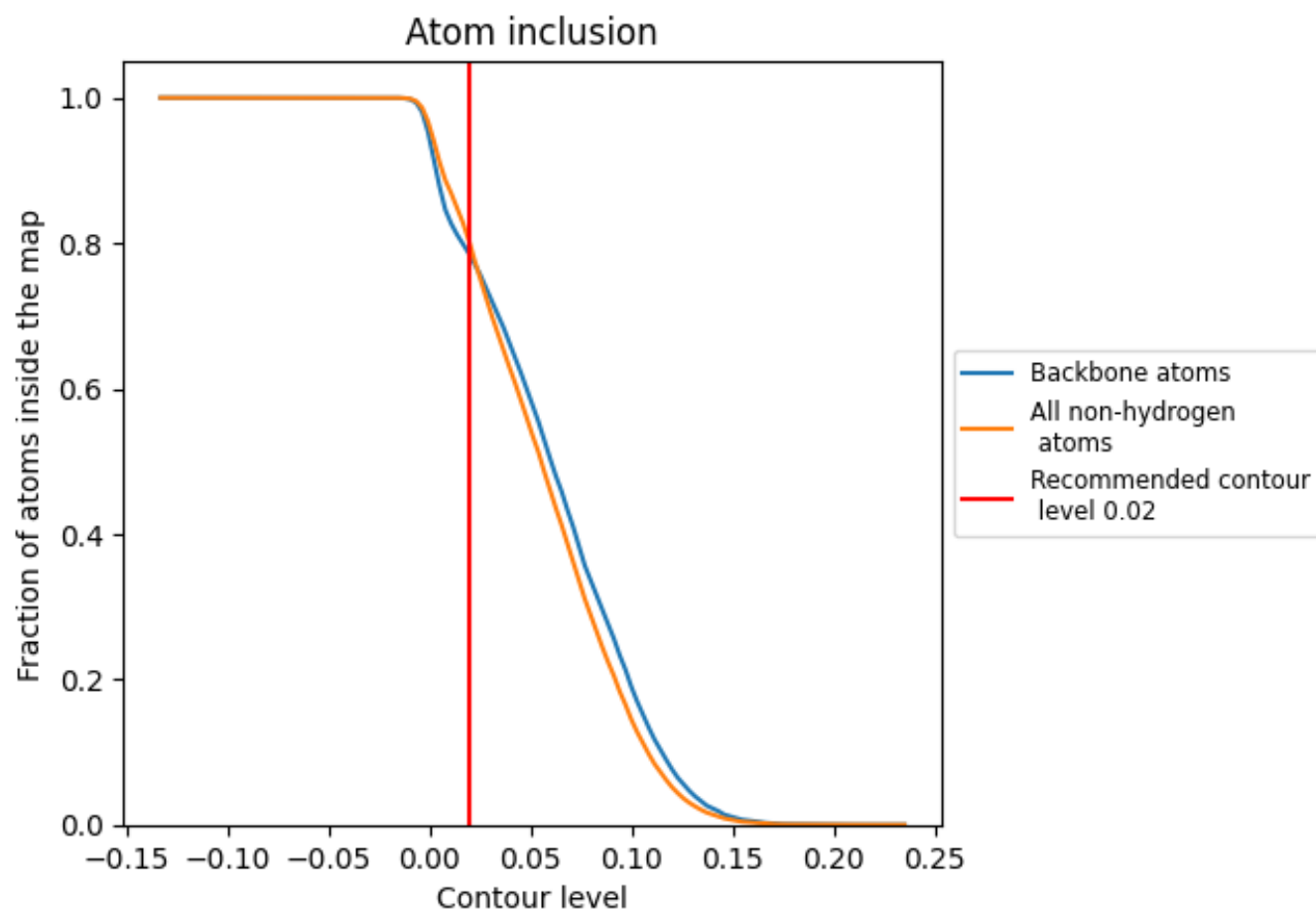
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 80% 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> 0.7993	<div></div> 0.5400
A	<div></div> 0.8871	<div></div> 0.6040
B	<div></div> 0.9842	<div></div> 0.6760
C	<div></div> 0.9296	<div></div> 0.6110
D	<div></div> 0.9242	<div></div> 0.6470
E	<div></div> 0.0952	<div></div> 0.0770

