



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:43 PM UTC

PDB ID : 8UIN / pdb\_00008uin  
EMDB ID : EMD-42300  
Title : Structure of the C3bBb-albicin complex  
Authors : Andersen, J.F.; Lei, H.  
Deposited on : 2023-10-10  
Resolution : 3.86 Å (reported)  
Based on initial models : 6XKE, 6RUR

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:

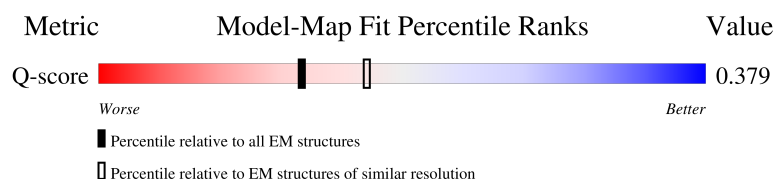
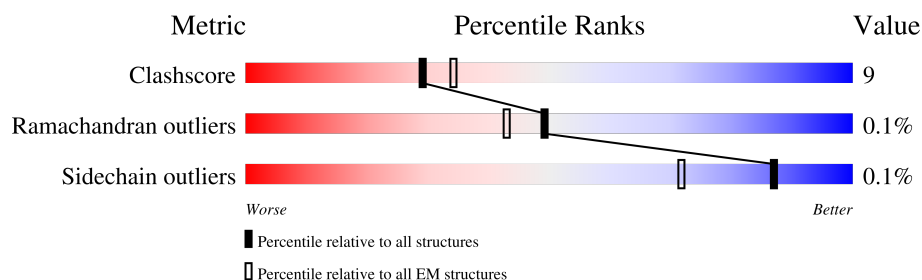
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.86 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	8889 ( 3.36 - 4.35 )

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	C	116	 74% 26%
1	D	116	 75% 25%
2	J	228	 6% 74% 22% .
2	X	228	 7% 76% 21% .

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Mol	Chain	Length	Quality of chain
3	A	642	 79%21%
3	G	642	 80%20%
4	B	915	 20%73%24%.
4	H	915	 18%78%20%.
5	M	2	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28249 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 Albicin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	116	Total	C	N	O	S	0	0
			944	602	154	183	5		
1	D	116	Total	C	N	O	S	0	0
			944	602	154	183	5		

- Molecule 2 is a protein called Complement factor B Bb fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	220	Total	C	N	O	S	0	0
			1513	956	266	285	6		
2	X	221	Total	C	N	O	S	0	0
			1572	1007	270	287	8		

- Molecule 3 is a protein called Complement C3 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	641	Total	C	N	O	S	0	0
			4987	3176	845	951	15		
3	G	640	Total	C	N	O	S	0	0
			4946	3152	837	942	15		

- Molecule 4 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	895	Total	C	N	O	S	0	0
			6695	4274	1124	1261	36		
4	H	897	Total	C	N	O	S	0	0
			6578	4163	1130	1254	31		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

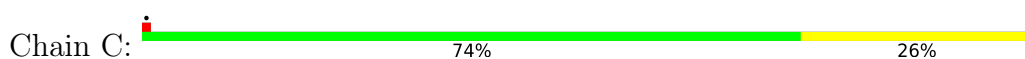


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	G	1	Total	C	N	O	0
			14	8	1	5	
6	H	1	Total	C	N	O	0
			14	8	1	5	

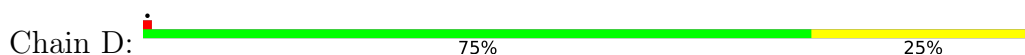
### 3 Residue-property plots

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.

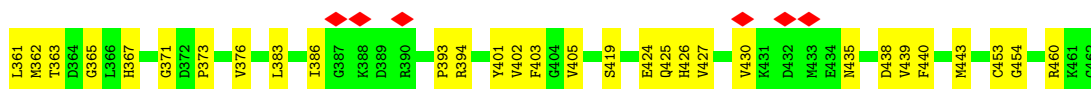
- Molecule 1: Albicin



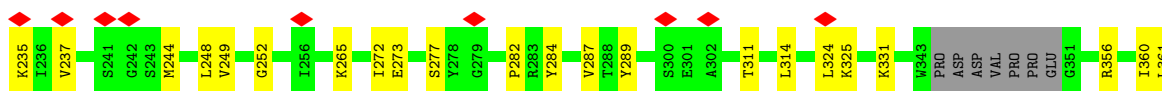
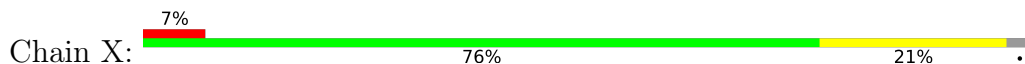
- Molecule 1: Albicin



- Molecule 2: Complement factor B Bb fragment



- Molecule 2: Complement factor B Bb fragment



Chain A:

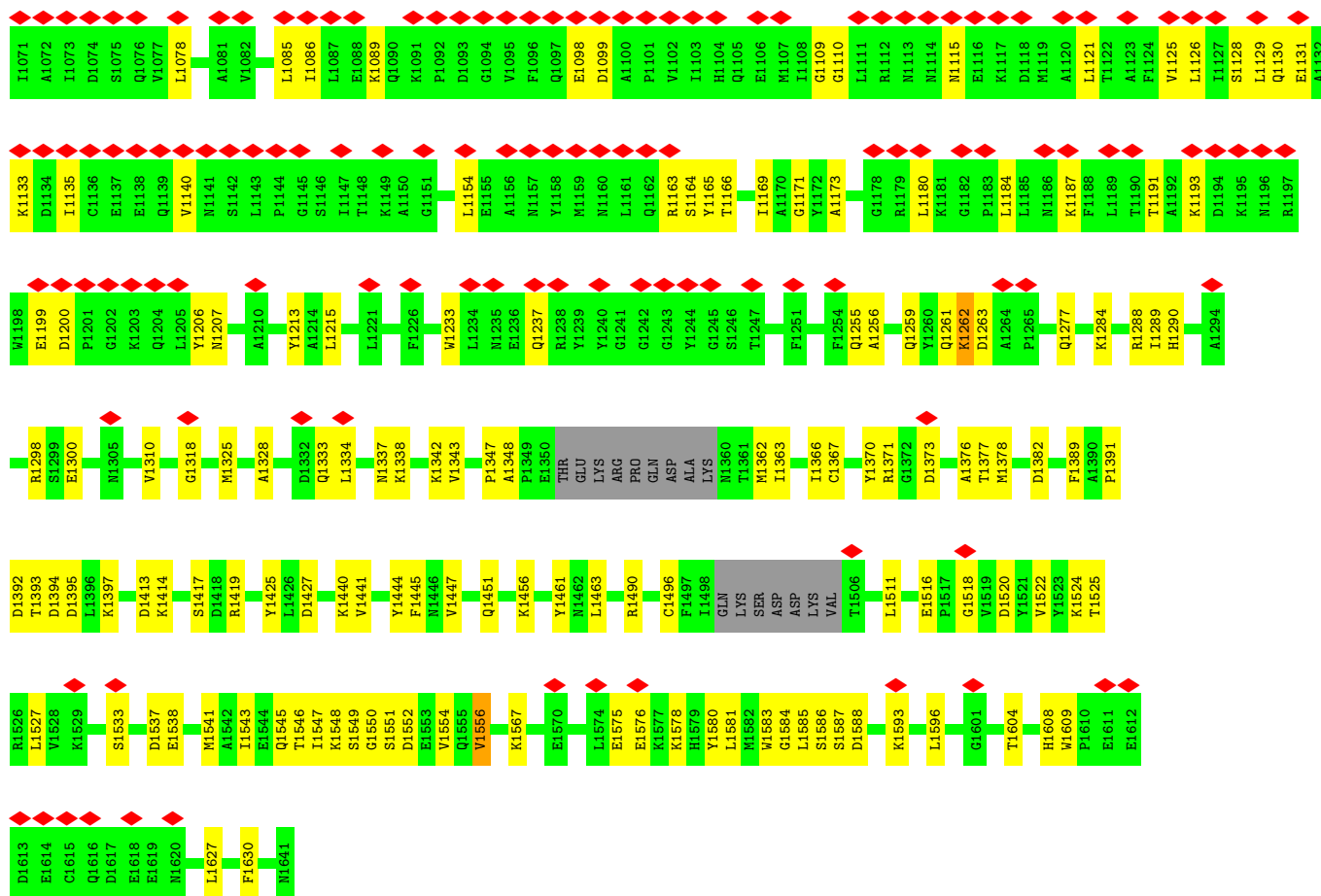
V493	S19	M346	I184	S1
V494	G520	F363	I198	I6
D502	E523	F348	T198	I7
L515	D627	D349	I199	T8
I516	S528	L350	F200	L12
S519	V529	M351	E201	T19
G520	L541	V352	Y205	M20
E523	E549	F353	Y221	E23
D627	D550	R363	Y222	P32
S528	B551	Q370	I223	V37
V529	Q552	V375	I233	F40
L541	P553	K386	R236	P41
E549	M559	I389	Y239	V53
D550	S559	T390	G240	T65
B551	Q552	K241	K242	R72
P553	P553	R403	T404	E73
M559	M559	K405	K406	F74
I563	I563	Q407	F248	K75
E564	E564	E408	V249	S76
G585	G585	L409	Q254	E77
D566	D566	S410	D255	K78
L573	L573	E411	G256	K82
F581	F581	M419	I269	V86
N584	N584	A421	V278	V98
K588	K588	V427	R293	V101
T606	T606	H435	A294	I110
P607	P607	L436	L302	D113
G608	G608	F453	S305	K114
D619	D619	M457	D315	T118
T623	T623	D458	M316	I127
S626	S626	R459	E320	K133
Q630	Q630	E462	I326	R139
G631	G631	N474	V327	N147
T632	T632	R477	T328	I151
P641	P641	L478	S329	S160
GLN	GLN	L479	P330	L167
		R483	H334	
		Q484	F335	
		V485	T338	

Chain G:

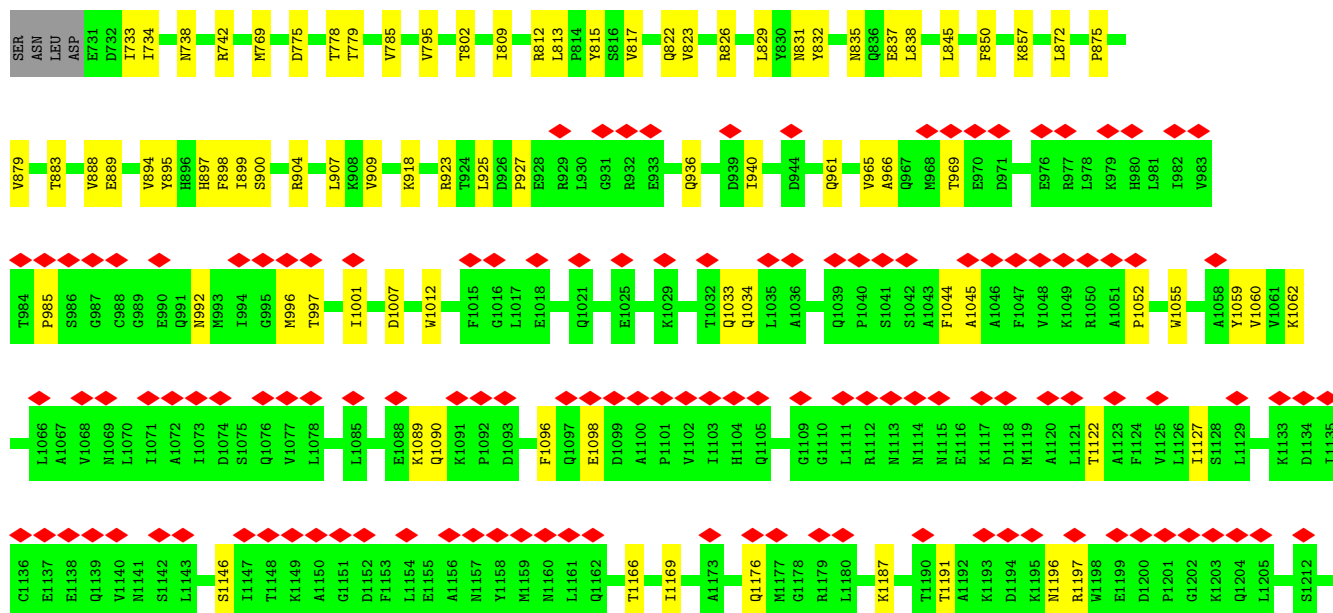
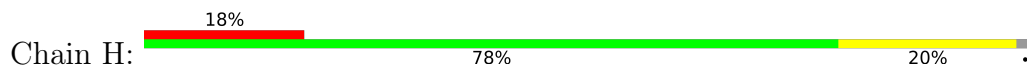
80% 20%

Residue	State
S1	80%
T8	80%
P9	80%
N10	80%
L14	80%
M20	80%
V21	80%
L22	80%
V35	80%
T36	80%
V37	80%
F40	80%
P41	80%
K44	80%
L47	80%
S48	80%
S49	80%
T55	80%
P56	80%
A57	80%
G62	80%
M63	80%
V64	80%
E73	80%
F74	80%
K75	80%
S76	80%
K82	80%
T85	80%
E86	80%
K87	80%
V98	80%
S102	80%
L103	80%
Q104	80%
L108	80%
Q111	80%
T112	80%
D113	80%
K114	80%
R139	80%
N147	80%
I151	80%
S160	80%
K351	80%
L167	80%
K183	80%
Y188	80%
E199	80%
E204	80%
Y222	80%
I223	80%
Y224	80%
N225	80%
I233	80%
V249	80%
G252	80%
R268	80%
I269	80%
V278	80%
V279	80%
L280	80%
L285	80%
Q290	80%
N291	80%
D296	80%
L302	80%
Y303	80%
D315	80%
M316	80%
I326	80%
S327	80%
S328	80%
S329	80%
I333	80%
H334	80%
F335	80%
F342	80%
K343	80%
P344	80%
G345	80%
M346	80%
P347	80%
F348	80%
D349	80%
L350	80%
V352	80%
F353	80%
V354	80%
T355	80%
P361	80%
A362	80%
V363	80%
R364	80%
V367	80%
D373	80%
T379	80%
A385	80%
K386	80%
L387	80%
S388	80%
R403	80%
E411	80%
M419	80%
Q420	80%
A421	80%
Y424	80%
Y433	80%
V438	80%
L439	80%
R440	80%
T441	80%
V451	80%
R456	80%
M457	80%
E462	80%
T469	80%
V470	80%
L471	80%
N474	80%
L478	80%
Q484	80%
V485	80%
R486	20%
P496	20%
L497	20%
D502	20%
A511	20%
L515	20%
I516	20%
S519	20%
G520	20%
V530	20%
V531	20%
D532	20%
V543	20%
S548	20%
E549	20%
D550	20%
R551	20%
L561	20%
K562	20%
I563	20%
V576	20%
D577	20%
K578	20%
G579	20%
V582	20%
L589	20%
T606	20%
P607	20%
G608	20%
D612	20%
D619	20%
R635	20%
G640	20%
P60	20%
GLN	20%

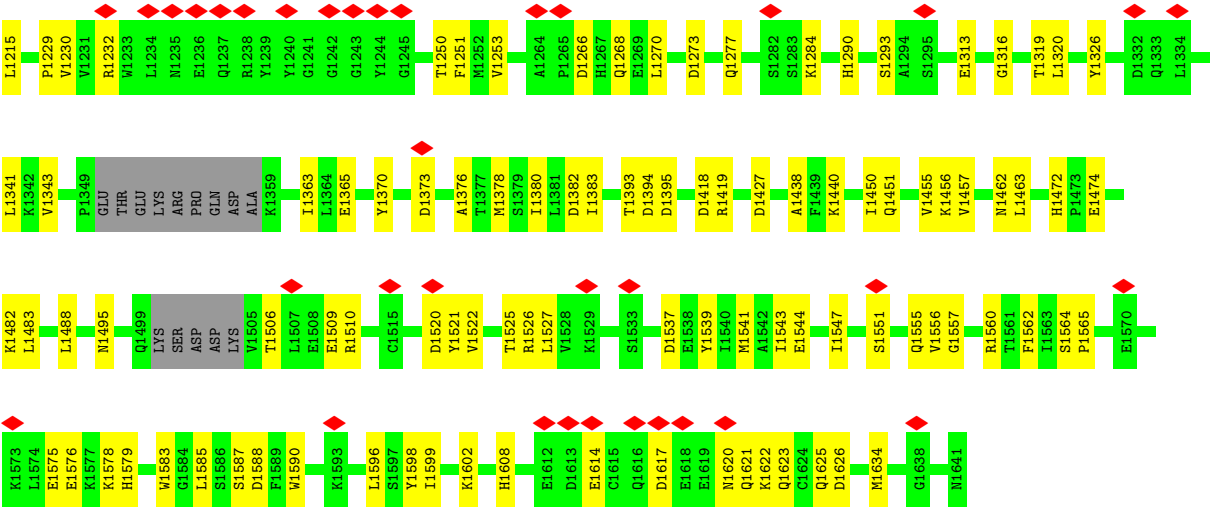
[illegible]



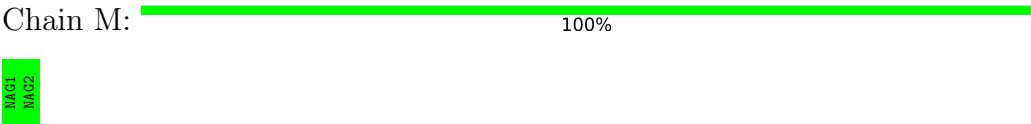
• Molecule 4: Complement C3b alpha' chain







● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	65862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66.7	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.717	Depositor
Minimum map value	-0.391	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.087	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	C	0.18	0/961	0.36	0/1295
1	D	0.18	0/961	0.39	0/1295
2	J	0.14	0/1541	0.31	0/2115
2	X	0.12	0/1603	0.28	0/2191
3	A	0.16	0/5088	0.28	0/6915
3	G	0.16	0/5046	0.29	0/6862
4	B	0.13	0/6829	0.29	1/9305 (0.0%)
4	H	0.13	0/6697	0.27	0/9131
All	All	0.15	0/28726	0.29	1/39109 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	967	GLN	CB-CA-C	-5.29	110.49	116.63

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	C	944	0	937	22	0
1	D	944	0	937	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1513	0	1302	34	0
2	X	1572	0	1436	32	0
3	A	4987	0	5042	97	0
3	G	4946	0	4979	79	0
4	B	6695	0	6355	152	0
4	H	6578	0	6148	112	0
5	M	28	0	25	0	0
6	B	14	0	13	0	0
6	G	14	0	13	0	0
6	H	14	0	13	0	0
All	All	28249	0	27200	514	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 9.

All (514) 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)
4:B:997:THR:HG23	4:B:998:PRO:HD3	1.49	0.95
4:B:997:THR:CG2	4:B:998:PRO:HD3	2.01	0.90
4:B:997:THR:HG23	4:B:998:PRO:CD	2.11	0.81
4:B:997:THR:CG2	4:B:998:PRO:CD	2.60	0.80
4:B:1255:GLN:HG2	4:B:1259:GLN:HE22	1.45	0.79
2:J:309:TRP:HD1	2:J:312:LYS:HE3	1.47	0.79
3:A:559:MET:HE3	4:B:773:LEU:HD21	1.63	0.78
4:B:1363:ILE:HG12	4:B:1440:LYS:HG2	1.63	0.78
3:A:527:ASP:OD1	3:A:528:SER:N	2.18	0.76
3:A:327:VAL:HG12	3:A:329:SER:H	1.52	0.73
2:J:363:THR:HG22	2:J:365:GLY:H	1.55	0.71
3:G:327:VAL:HG12	3:G:329:SER:H	1.55	0.71
4:H:1393:THR:HG22	4:H:1419:ARG:HH22	1.55	0.70
1:C:49:LEU:HD22	4:B:837:GLU:HG2	1.72	0.70
2:X:331:LYS:HE3	2:X:371:GLY:H	1.56	0.69
2:J:405:VAL:HA	2:J:430:VAL:HG22	1.74	0.68
4:H:1007:ASP:OD1	4:H:1012:TRP:NE1	2.22	0.68
4:H:1215:LEU:HD21	4:H:1230:VAL:HG21	1.75	0.68
3:A:201:GLU:OE1	3:A:584:ASN:ND2	2.26	0.68
2:X:244:MET:HE1	2:X:356:ARG:HB2	1.74	0.68
3:G:457:MET:HE1	3:G:515:LEU:HD11	1.76	0.68
3:A:474:ASN:ND2	3:A:502:ASP:O	2.27	0.67
3:A:349:ASP:HB3	3:A:351:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:244:MET:HB3	2:X:282:PRO:HB3	1.77	0.67
4:B:1078:LEU:HD23	4:B:1135:ILE:HG21	1.75	0.67
2:X:324:LEU:HG	2:X:325:LYS:HG3	1.78	0.66
4:B:973:VAL:HG12	4:B:975:ALA:H	1.61	0.66
4:B:975:ALA:HA	4:B:978:LEU:HD13	1.77	0.66
1:D:83:ASP:OD1	1:D:84:HIS:N	2.27	0.65
1:D:22:LYS:NZ	2:X:425:GLN:OE1	2.25	0.65
3:G:268:ARG:HH11	4:H:1378:MET:HE1	1.61	0.65
2:J:252:GLY:N	2:J:289:TYR:O	2.30	0.64
4:H:1608:HIS:O	4:H:1623:GLN:NE2	2.30	0.64
2:J:362:MET:HG3	2:J:403:PHE:HB2	1.79	0.64
3:A:246:THR:HG21	4:B:1425:TYR:HE2	1.61	0.64
3:A:370:GLN:OE1	3:A:403:ARG:NH1	2.30	0.64
3:G:147:ASN:HD21	3:G:151:ILE:HB	1.63	0.64
4:B:1391:PRO:HA	4:B:1441:VAL:HG12	1.80	0.64
4:H:826:ARG:NH2	4:H:1382:ASP:OD2	2.27	0.64
2:X:405:VAL:HA	2:X:430:VAL:HG22	1.80	0.63
4:B:833:ARG:HD2	4:B:838:LEU:HD11	1.78	0.63
3:G:183:LYS:HG3	3:G:199:GLU:HG2	1.79	0.63
4:H:785:VAL:HG22	4:H:795:VAL:HG22	1.80	0.63
4:H:1614:GLU:O	4:H:1620:ASN:ND2	2.31	0.63
1:D:62:MET:HE2	1:D:110:THR:HG21	1.80	0.63
4:B:992:ASN:ND2	4:B:1033:GLN:OE1	2.32	0.63
3:A:419:MET:HE1	3:A:421:ALA:HB2	1.81	0.63
4:B:1262:LYS:HG3	4:B:1263:ASP:H	1.62	0.62
4:B:1007:ASP:OD1	4:B:1012:TRP:NE1	2.31	0.62
4:B:1581:LEU:HG	4:B:1609:TRP:HB2	1.81	0.62
4:B:785:VAL:HG22	4:B:795:VAL:HG22	1.81	0.62
4:H:1541:MET:HB2	4:H:1560:ARG:HB2	1.82	0.62
4:B:1333:GLN:NE2	4:B:1334:LEU:O	2.33	0.62
3:G:55:THR:HG22	3:G:57:ALA:H	1.64	0.61
4:B:1255:GLN:O	4:B:1259:GLN:NE2	2.32	0.61
1:D:1:ALA:N	1:D:46:GLY:O	2.32	0.61
3:A:457:MET:HE1	3:A:515:LEU:HD11	1.81	0.61
3:G:419:MET:HE1	3:G:421:ALA:HB2	1.83	0.61
4:B:1062:LYS:HZ3	4:B:1128:SER:HA	1.65	0.61
4:H:1341:LEU:HD21	4:H:1343:VAL:HG23	1.83	0.61
3:A:315:ASP:OD2	4:B:812:ARG:NH2	2.34	0.60
4:B:1045:ALA:HB2	4:B:1052:PRO:HA	1.83	0.60
4:H:1588:ASP:HA	4:H:1599:ILE:HG22	1.83	0.60
3:A:375:VAL:HG12	3:G:496:PRO:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:997:THR:HG22	4:B:998:PRO:CD	2.31	0.60
3:A:160:SER:HA	3:A:167:LEU:HD21	1.83	0.60
3:A:541:LEU:HD22	4:B:796:ALA:HB2	1.83	0.60
4:B:1551:SER:HA	2:X:371:GLY:HA3	1.84	0.60
4:H:992:ASN:ND2	4:H:1034:GLN:OE1	2.35	0.60
3:G:474:ASN:ND2	3:G:502:ASP:O	2.34	0.60
3:A:335:PHE:HE1	3:A:352:VAL:HG12	1.67	0.59
2:X:248:LEU:HG	2:X:360:ILE:HD11	1.82	0.59
3:A:236:ARG:HH12	3:A:242:LYS:HG2	1.67	0.59
3:G:280:LEU:HD21	3:G:285:LEU:HB2	1.85	0.59
4:B:997:THR:HG22	4:B:998:PRO:HD3	1.82	0.59
1:D:15:ILE:HG13	1:D:67:TYR:HE1	1.67	0.59
3:A:459:ARG:NH1	3:A:462:GLU:OE1	2.35	0.59
2:J:289:TYR:OH	2:J:363:THR:OG1	2.20	0.59
4:B:813:LEU:HD23	4:B:907:LEU:HB3	1.84	0.59
3:G:363:TYR:OH	3:G:364:ARG:NH2	2.33	0.59
3:A:269:ILE:HD13	3:A:278:VAL:HB	1.85	0.58
2:J:334:LEU:HB3	2:J:376:VAL:HG11	1.85	0.58
3:A:249:VAL:HG21	3:A:278:VAL:HG11	1.85	0.58
4:B:1525:THR:HB	4:B:1541:MET:HB3	1.83	0.58
3:A:346:MET:HE2	3:A:435:HIS:HB3	1.85	0.58
3:G:8:THR:OG1	3:G:20:MET:SD	2.57	0.58
3:G:63:ASN:OD1	3:G:63:ASN:N	2.34	0.58
3:G:350:LEU:C	3:G:351:MET:HE2	2.29	0.58
1:D:69:ILE:HG12	1:D:102:GLN:OE1	2.03	0.57
3:G:160:SER:HA	3:G:167:LEU:HD21	1.85	0.57
2:X:438:ASP:HB2	2:X:460:ARG:HH12	1.69	0.57
1:D:76:LYS:HA	1:D:80:ALA:HB3	1.86	0.57
4:B:949:VAL:O	4:B:952:THR:OG1	2.21	0.57
3:G:471:LEU:HD23	3:G:478:LEU:HD11	1.87	0.57
2:X:252:GLY:N	2:X:289:TYR:O	2.35	0.57
3:A:12:LEU:HB2	3:A:101:VAL:HG22	1.85	0.57
4:B:1343:VAL:HG13	4:B:1366:ILE:HG22	1.86	0.57
4:H:1617:ASP:O	4:H:1621:GLN:N	2.31	0.57
1:C:62:MET:HE2	1:C:110:THR:HG21	1.84	0.57
1:D:107:PHE:HA	1:D:110:THR:HG22	1.87	0.57
2:J:272:ILE:HG13	2:J:284:TYR:HE2	1.69	0.57
3:A:241:LYS:HG3	4:B:832:TYR:CE2	2.39	0.57
4:B:1164:SER:OG	4:B:1193:LYS:NZ	2.37	0.57
3:A:133:LYS:HG2	3:A:477:ARG:HE	1.68	0.57
4:H:992:ASN:OD1	4:H:1033:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:LEU:HG	3:A:326:ILE:HD11	1.86	0.56
3:G:355:THR:HG22	3:G:361:PRO:HA	1.87	0.56
4:H:1543:ILE:HB	4:H:1557:GLY:HA2	1.88	0.56
3:A:19:THR:HG22	3:A:65:THR:HG22	1.87	0.56
4:H:1483:LEU:HD21	4:H:1565:PRO:HA	1.86	0.56
3:G:113:ASP:OD1	3:G:114:LYS:N	2.38	0.56
3:G:579:GLY:HA2	3:G:582:VAL:HG12	1.88	0.56
3:G:606:THR:HB	3:G:619:ASP:HB3	1.88	0.56
2:X:407:PRO:HD2	2:X:408:LEU:H	1.70	0.56
4:H:817:VAL:HG11	4:H:823:VAL:HG21	1.88	0.56
1:C:21:LYS:HD3	1:C:25:TYR:HE2	1.70	0.55
4:B:1548:LYS:NZ	2:X:368:ASN:O	2.39	0.55
3:G:355:THR:HA	3:G:362:ALA:H	1.72	0.55
4:H:1001:ILE:HD13	4:H:1251:PHE:HA	1.88	0.55
4:B:926:ASP:N	4:B:936:GLN:OE1	2.39	0.55
3:A:254:GLN:NE2	3:A:256:GLY:O	2.40	0.55
4:B:1062:LYS:HZ3	4:B:1131:GLU:HG2	1.71	0.55
3:G:335:PHE:HE1	3:G:352:VAL:HG12	1.70	0.55
4:B:1522:VAL:HG12	4:B:1547:ILE:HD12	1.87	0.55
1:C:21:LYS:HD3	1:C:25:TYR:CE2	2.42	0.55
3:A:98:VAL:HG21	4:B:1017:LEU:HB3	1.87	0.55
4:B:1130:GLN:O	4:B:1133:LYS:NZ	2.38	0.55
4:H:734:ILE:HD12	4:H:900:SER:HB3	1.87	0.55
4:H:1522:VAL:HB	4:H:1547:ILE:HB	1.89	0.55
3:G:379:THR:HG22	3:G:385:ALA:HB2	1.89	0.55
4:B:1261:GLN:O	4:B:1263:ASP:N	2.40	0.54
4:B:1342:LYS:HB3	4:B:1367:CYS:HB2	1.89	0.54
4:B:1533:SER:OG	4:B:1538:GLU:OE2	2.23	0.54
4:B:1584:GLY:HA2	4:B:1604:THR:HG22	1.88	0.54
1:C:2:ASN:HB3	1:C:6:ARG:HH12	1.72	0.54
3:A:139:ARG:N	3:A:160:SER:OG	2.31	0.54
2:J:435:ASN:ND2	2:J:460:ARG:HE	2.05	0.54
1:D:83:ASP:OD1	1:D:84:HIS:ND1	2.39	0.54
2:J:256:ILE:O	2:J:260:ASN:ND2	2.38	0.54
2:J:311:THR:HA	2:J:314:LEU:HD12	1.89	0.54
4:H:992:ASN:O	4:H:996:MET:HG2	2.08	0.54
4:H:1229:PRO:O	4:H:1232:ARG:HD3	2.08	0.54
4:B:1382:ASP:HB3	4:B:1456:LYS:HG2	1.89	0.54
3:A:564:GLU:HG2	4:B:766:THR:HG22	1.90	0.54
2:X:272:ILE:HD12	2:X:314:LEU:HD11	1.90	0.54
2:X:389:ASP:OD2	2:X:392:ASN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:SER:HB2	2:X:427:VAL:HG23	1.89	0.54
4:H:1634:MET:O	4:H:1634:MET:HE3	2.08	0.54
4:B:734:ILE:HD12	4:B:900:SER:HB3	1.90	0.54
4:B:1419:ARG:CZ	4:B:1419:ARG:HA	2.37	0.54
4:B:1546:THR:HG21	4:B:1554:VAL:HB	1.90	0.54
4:H:813:LEU:HD13	4:H:907:LEU:HB3	1.89	0.54
4:H:918:LYS:HG2	4:H:1326:TYR:HE1	1.73	0.54
4:B:875:PRO:O	4:B:1451:GLN:NE2	2.29	0.54
2:X:272:ILE:HG23	2:X:284:TYR:HE2	1.73	0.54
3:A:566:ASP:OD1	3:A:566:ASP:N	2.41	0.53
4:H:850:PHE:HE2	4:H:888:VAL:HB	1.74	0.53
4:H:985:PRO:HB2	4:H:1033:GLN:HE22	1.72	0.53
4:B:1347:PRO:HA	4:B:1362:MET:HG3	1.90	0.53
3:A:351:MET:HE1	3:A:386:LYS:HD2	1.90	0.53
4:B:1378:MET:HE2	4:B:1427:ASP:HA	1.89	0.53
4:B:1525:THR:O	4:B:1580:TYR:N	2.40	0.53
3:G:233:ILE:HD12	3:G:269:ILE:HD11	1.89	0.53
1:C:96:ARG:HG2	1:C:100:LEU:HD23	1.91	0.53
1:D:65:GLU:O	1:D:68:GLU:HG3	2.08	0.53
3:A:477:ARG:HH12	3:A:479:LEU:HD13	1.74	0.53
2:X:265:LYS:NZ	2:X:314:LEU:O	2.41	0.53
4:H:822:GLN:HB3	4:H:879:VAL:HG22	1.90	0.53
4:H:1585:LEU:HG	4:H:1587:SER:H	1.73	0.53
1:C:78:SER:HB3	1:C:87:TYR:CE1	2.44	0.53
4:B:1277:GLN:HA	4:B:1284:LYS:HD2	1.90	0.53
2:X:311:THR:HA	2:X:314:LEU:HD12	1.91	0.53
1:D:66:VAL:HA	1:D:69:ILE:HG22	1.90	0.53
3:G:139:ARG:H	3:G:160:SER:HG	1.55	0.53
4:H:779:THR:HG22	4:H:802:THR:HA	1.90	0.53
2:J:360:ILE:HG22	2:J:401:TYR:HB2	1.89	0.52
3:A:239:TYR:HE2	4:B:832:TYR:HE2	1.57	0.52
3:A:6:ILE:HD11	3:A:20:MET:HE2	1.92	0.52
4:B:985:PRO:HD2	4:B:1029:LYS:HZ1	1.74	0.52
3:G:268:ARG:HD3	4:H:1378:MET:HE1	1.92	0.52
4:B:742:ARG:HB3	4:B:775:ASP:HB3	1.90	0.52
3:G:333:ILE:HG12	3:G:354:VAL:HG12	1.90	0.52
4:B:735:ALA:HB3	4:B:738:ASN:HB2	1.92	0.52
4:H:879:VAL:HG11	4:H:1482:LYS:HE2	1.92	0.52
3:A:147:ASN:HD21	3:A:151:ILE:HB	1.75	0.52
4:B:993:MET:HA	4:B:996:MET:HG3	1.91	0.52
2:X:235:LYS:HD2	2:X:445:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:THR:HG21	4:B:1425:TYR:CE2	2.43	0.51
3:G:543:VAL:HG22	3:G:563:ILE:HG22	1.91	0.51
4:H:838:LEU:HD22	4:H:894:VAL:HG21	1.92	0.51
3:A:338:THR:OG1	3:A:351:MET:O	2.28	0.51
4:B:1554:VAL:O	4:B:1556:VAL:N	2.42	0.51
3:G:344:PRO:HD2	3:G:433:TYR:CE2	2.46	0.51
4:H:1462:ASN:OD1	4:H:1463:LEU:N	2.42	0.51
3:A:8:THR:HG21	3:A:20:MET:HE3	1.92	0.51
3:A:32:PRO:HB3	3:A:53:VAL:HG12	1.92	0.51
4:H:1045:ALA:HB2	4:H:1052:PRO:HA	1.93	0.51
2:J:334:LEU:HD12	2:J:373:PRO:HB3	1.93	0.51
3:A:606:THR:HB	3:A:619:ASP:HB3	1.93	0.51
3:A:427:VAL:HG21	3:A:523:GLU:HB2	1.92	0.51
4:B:797:ASP:OD1	4:B:797:ASP:N	2.43	0.51
4:B:1126:LEU:HD23	4:B:1173:ALA:HB1	1.93	0.51
3:G:302:LEU:HG	3:G:326:ILE:HD11	1.93	0.51
2:X:365:GLY:O	2:X:413:ASN:ND2	2.43	0.51
4:B:1545:GLN:HE22	4:B:1547:ILE:HG12	1.76	0.51
4:H:1365:GLU:HG3	4:H:1438:ALA:HB2	1.93	0.51
4:B:1496:CYS:SG	4:B:1567:LYS:NZ	2.84	0.51
4:H:845:LEU:HB2	4:H:889:GLU:OE1	2.11	0.51
4:B:1215:LEU:HD23	4:B:1256:ALA:HB1	1.91	0.51
4:H:742:ARG:HB3	4:H:775:ASP:HB3	1.92	0.51
1:D:36:GLN:HG3	1:D:100:LEU:HD12	1.92	0.51
4:B:1064:PHE:O	4:B:1068:VAL:HG13	2.11	0.51
3:A:32:PRO:HA	3:A:53:VAL:HA	1.93	0.51
3:G:403:ARG:HH21	3:G:411:GLU:HG3	1.76	0.51
3:G:74:PHE:HD1	3:G:82:LYS:HZ3	1.59	0.50
3:G:484:GLN:NE2	3:G:485:VAL:O	2.30	0.50
4:B:1038:ARG:NH2	4:B:1042:SER:OG	2.44	0.50
3:A:223:ILE:HD11	3:A:294:ALA:HB1	1.93	0.50
3:A:453:PHE:HB2	3:A:493:VAL:HG23	1.92	0.50
4:B:1348:ALA:HB2	4:B:1363:ILE:HG13	1.92	0.50
4:B:1370:TYR:CG	4:B:1376:ALA:HB2	2.46	0.50
4:B:1578:LYS:HD3	4:B:1608:HIS:CE1	2.47	0.50
4:B:1593:LYS:HG2	4:B:1596:LEU:HD21	1.94	0.50
1:D:96:ARG:HG2	1:D:100:LEU:HD23	1.93	0.50
4:H:1625:GLN:NE2	4:H:1626:ASP:OD1	2.45	0.50
2:J:273:GLU:O	2:J:277:SER:OG	2.27	0.50
3:A:516:ILE:HD11	3:A:520:GLY:HA2	1.92	0.50
4:B:867:PRO:O	4:B:870:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:291:ASN:ND2	3:G:296:ASP:OD2	2.45	0.50
3:A:293:ARG:HE	3:A:294:ALA:H	1.59	0.50
2:J:440:PHE:HA	2:J:443:MET:HB2	1.93	0.50
3:A:334:HIS:HB2	3:A:353:PHE:HB3	1.93	0.50
4:B:845:LEU:HB2	4:B:889:GLU:OE2	2.12	0.50
3:G:35:VAL:HG11	3:G:64:VAL:HG21	1.92	0.50
4:H:1363:ILE:HG12	4:H:1440:LYS:HG2	1.92	0.50
2:X:273:GLU:O	2:X:277:SER:OG	2.28	0.50
1:C:18:ASP:OD2	1:C:21:LYS:NZ	2.45	0.49
4:H:925:LEU:HD11	4:H:1320:LEU:HD22	1.93	0.49
3:A:114:LYS:HD3	4:B:747:GLU:HB3	1.92	0.49
4:H:875:PRO:O	4:H:1451:GLN:NE2	2.35	0.49
4:H:1196:ASN:OD1	4:H:1197:ARG:N	2.45	0.49
3:A:351:MET:HE2	3:A:351:MET:N	2.27	0.49
4:B:1115:ASN:O	4:B:1163:ARG:NH1	2.45	0.49
2:J:393:PRO:HD2	2:J:394:ARG:H	1.77	0.49
3:A:348:PHE:HD2	3:A:389:ILE:HD11	1.76	0.49
3:G:111:GLN:HE21	3:G:589:LEU:HD23	1.78	0.49
4:B:831:ASN:ND2	4:B:838:LEU:HD13	2.27	0.49
3:G:85:THR:HG23	3:G:96:GLU:OE2	2.13	0.49
3:G:222:TYR:HB3	3:G:225:ASN:HB2	1.95	0.49
1:C:38:ARG:HH12	4:H:738:ASN:HB3	1.76	0.49
2:J:338:TYR:HE1	2:J:383:LEU:HD12	1.78	0.49
4:B:1015:PHE:O	4:B:1019:LYS:NZ	2.39	0.49
3:A:316:MET:HE3	4:B:1463:LEU:HD12	1.93	0.49
3:A:350:LEU:C	3:A:351:MET:HE2	2.37	0.49
4:B:813:LEU:HG	4:B:825:ILE:HD11	1.93	0.49
4:B:1550:GLY:O	4:B:1552:ASP:N	2.46	0.49
4:B:1392:ASP:OD2	4:B:1440:LYS:HB2	2.13	0.49
3:A:40:PHE:CE2	4:B:1020:ARG:HD2	2.48	0.48
3:G:316:MET:HE2	4:H:1463:LEU:HB3	1.95	0.48
4:H:883:THR:HA	4:H:909:VAL:HG23	1.94	0.48
3:A:233:ILE:HD12	3:A:269:ILE:HD11	1.95	0.48
4:B:938:GLU:HB3	4:B:1310:VAL:HB	1.95	0.48
4:H:1166:THR:HA	4:H:1169:ILE:HG22	1.94	0.48
1:C:36:GLN:HG3	1:C:100:LEU:HD12	1.95	0.48
4:H:1555:GLN:C	4:H:1557:GLY:H	2.20	0.48
4:B:1187:LYS:O	4:B:1191:THR:OG1	2.30	0.48
4:B:1490:ARG:NH2	4:B:1587:SER:O	2.47	0.48
3:G:22:LEU:HB2	3:G:62:GLY:O	2.14	0.48
2:X:356:ARG:HG2	2:X:397:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1393:THR:O	4:B:1397:LYS:HG2	2.14	0.48
4:H:1370:TYR:CG	4:H:1376:ALA:HB2	2.48	0.48
2:J:453:CYS:SG	2:J:454:GLY:N	2.86	0.48
1:D:18:ASP:HB3	1:D:21:LYS:HG3	1.95	0.48
4:B:1527:LEU:HG	4:B:1576:GLU:HG2	1.95	0.48
3:G:44:LYS:HE3	3:G:73:GLU:HG3	1.95	0.48
1:C:12:PHE:CZ	1:C:41:ILE:HD11	2.47	0.48
3:A:221:TYR:HE1	3:A:228:GLY:HA2	1.79	0.48
4:B:958:ILE:HB	4:B:1300:GLU:HB2	1.96	0.48
4:B:985:PRO:HB3	4:B:992:ASN:OD1	2.14	0.48
4:B:1520:ASP:OD2	4:B:1586:SER:N	2.47	0.48
3:A:110:ILE:HG12	3:A:127:ILE:HD13	1.95	0.48
4:B:732:ASP:OD1	4:B:732:ASP:N	2.42	0.48
4:B:1171:GLY:HA2	4:B:1180:LEU:HD13	1.95	0.48
3:G:577:ASP:OD1	3:G:578:LYS:N	2.47	0.48
1:C:5:ILE:HG21	4:H:898:PHE:CD1	2.49	0.47
4:B:994:ILE:O	4:B:997:THR:HG22	2.14	0.47
4:B:997:THR:HG23	4:B:998:PRO:N	2.28	0.47
4:H:1127:ILE:HG23	4:H:1176:GLN:HE22	1.79	0.47
4:H:809:ILE:HG12	4:H:829:LEU:HD23	1.95	0.47
3:A:346:MET:SD	3:A:347:PRO:HD2	2.54	0.47
4:B:1549:SER:OG	2:X:370:GLY:N	2.40	0.47
3:G:252:GLY:HA3	3:G:303:TYR:CZ	2.50	0.47
2:J:361:LEU:HB3	2:J:402:VAL:HG12	1.97	0.47
4:B:930:LEU:HD22	4:B:936:GLN:HG3	1.97	0.47
4:B:1085:LEU:HA	4:B:1089:LYS:HB2	1.96	0.47
4:H:1290:HIS:H	4:H:1293:SER:HG	1.60	0.47
2:J:439:VAL:HG13	2:J:440:PHE:HD1	1.79	0.47
2:X:361:LEU:HB3	2:X:402:VAL:HG12	1.97	0.47
4:B:1233:TRP:NE1	4:B:1237:GLN:HE22	2.13	0.47
4:B:1524:LYS:HB2	4:B:1547:ILE:HD11	1.97	0.47
4:H:1560:ARG:NH2	4:H:1596:LEU:O	2.48	0.47
3:A:410:SER:OG	3:A:411:GLU:N	2.48	0.47
3:G:108:LEU:HD11	3:G:188:TYR:CE1	2.50	0.47
4:H:1488:LEU:HD22	4:H:1590:TRP:HE1	1.80	0.47
4:H:1450:ILE:HG13	4:H:1472:HIS:HE2	1.79	0.46
4:B:1338:LYS:HA	4:B:1371:ARG:HB2	1.97	0.46
3:G:530:TRP:HZ3	3:G:532:ASP:HB2	1.80	0.46
2:X:249:VAL:HG12	2:X:287:VAL:HB	1.96	0.46
2:X:440:PHE:HA	2:X:443:MET:HB2	1.97	0.46
2:J:425:GLN:HE21	2:J:427:VAL:HG22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1377:THR:HG21	4:B:1461:TYR:HE2	1.79	0.46
4:B:1288:ARG:HB3	4:B:1290:HIS:CE1	2.50	0.46
4:B:1581:LEU:HD12	4:B:1627:LEU:HD13	1.97	0.46
3:G:346:MET:CE	3:G:456:ARG:HB2	2.45	0.46
4:H:997:THR:O	4:H:1001:ILE:HG12	2.16	0.46
4:H:1270:LEU:HD23	4:H:1316:GLY:HA3	1.96	0.46
4:B:825:ILE:HG22	4:B:876:TYR:HB2	1.97	0.46
4:B:1193:LYS:HD3	4:B:1199:GLU:H	1.80	0.46
1:C:20:SER:HB2	2:J:427:VAL:HG23	1.98	0.46
2:J:435:ASN:HD22	2:J:460:ARG:HH21	1.63	0.46
3:G:102:SER:OG	3:G:104:GLN:OE1	2.33	0.46
4:H:1382:ASP:HB3	4:H:1456:LYS:HB3	1.98	0.46
3:A:114:LYS:NZ	4:B:747:GLU:OE1	2.32	0.46
4:B:809:ILE:HG12	4:B:829:LEU:HD23	1.97	0.46
3:A:458:ASP:OD1	3:A:458:ASP:N	2.49	0.46
3:A:74:PHE:HD1	3:A:82:LYS:HD3	1.81	0.46
4:B:920:VAL:HG22	4:B:943:ALA:HB2	1.97	0.46
4:B:1126:LEU:HD12	4:B:1129:LEU:HD11	1.98	0.45
4:H:1250:THR:HA	4:H:1253:VAL:HG12	1.97	0.45
4:H:1277:GLN:HA	4:H:1284:LYS:HD2	1.98	0.45
1:D:5:ILE:HG21	4:B:898:PHE:CD1	2.52	0.45
2:J:371:GLY:HA3	4:H:1551:SER:HA	1.98	0.45
3:A:113:ASP:N	3:A:113:ASP:OD1	2.48	0.45
4:B:976:GLU:O	4:B:979:LYS:NZ	2.42	0.45
3:G:37:VAL:N	3:G:47:LEU:O	2.46	0.45
3:G:439:LEU:HD21	3:G:441:THR:HG22	1.99	0.45
4:H:894:VAL:HG12	4:H:899:ILE:O	2.15	0.45
1:D:47:GLY:HA3	4:H:835:ASN:O	2.16	0.45
4:H:1522:VAL:HG13	4:H:1583:TRP:HB3	1.98	0.45
1:C:69:ILE:HG23	1:C:102:GLN:NE2	2.31	0.45
4:H:1187:LYS:O	4:H:1191:THR:OG1	2.27	0.45
2:X:367:HIS:HE1	2:X:413:ASN:HD22	1.63	0.45
2:J:258:ALA:O	2:J:262:THR:HG23	2.16	0.45
3:A:73:GLU:O	3:A:76:SER:OG	2.32	0.45
3:A:407:GLN:O	3:A:408:GLU:HG2	2.16	0.45
3:G:10:ASN:OD1	3:G:635:ARG:HD3	2.17	0.45
3:G:352:VAL:HG21	3:G:367:VAL:HG21	1.99	0.45
3:G:438:VAL:HG22	3:G:451:VAL:HG12	1.99	0.45
4:H:969:THR:HG22	4:H:1266:ASP:HB3	1.99	0.45
4:H:1622:LYS:O	4:H:1625:GLN:HG3	2.16	0.45
1:D:49:LEU:HG	4:H:837:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:895:TYR:C	4:H:897:HIS:H	2.23	0.45
4:H:1059:TYR:HA	4:H:1062:LYS:HG2	1.98	0.45
4:B:1053:SER:OG	4:B:1098:GLU:OE2	2.33	0.45
4:B:1525:THR:HG22	4:B:1543:ILE:HA	1.98	0.45
1:C:43:ARG:O	4:B:835:ASN:ND2	2.49	0.45
3:G:14:LEU:HD11	3:G:103:LEU:HD13	1.98	0.45
3:G:351:MET:HE1	3:G:386:LYS:HE3	1.98	0.45
4:H:1089:LYS:HA	4:H:1089:LYS:HD3	1.74	0.45
4:B:925:LEU:N	4:B:1318:GLY:O	2.46	0.45
4:B:1511:LEU:HD12	4:B:1630:PHE:CE2	2.51	0.45
3:G:268:ARG:NH1	4:H:1427:ASP:OD2	2.50	0.45
4:H:778:THR:OG1	4:H:779:THR:N	2.49	0.45
1:C:65:GLU:OE1	1:C:106:LEU:HD22	2.16	0.44
4:H:966:ALA:HB2	4:H:1268:GLN:HG2	1.98	0.44
3:A:118:THR:HG23	3:A:205:TYR:CZ	2.52	0.44
4:B:1024:LEU:HD13	4:B:1027:ILE:HD11	1.99	0.44
3:A:403:ARG:HH21	3:A:405:LYS:HE2	1.81	0.44
4:B:1166:THR:HA	4:B:1169:ILE:HG22	1.99	0.44
1:D:63:ILE:HA	1:D:66:VAL:HG12	2.00	0.44
4:H:1537:ASP:OD1	4:H:1564:SER:HB3	2.17	0.44
3:A:184:ILE:HB	3:A:198:THR:HG22	1.98	0.44
4:B:895:TYR:C	4:B:897:HIS:H	2.26	0.44
4:B:1164:SER:HB2	4:B:1200:ASP:OD1	2.17	0.44
4:B:1527:LEU:HD23	4:B:1575:GLU:C	2.42	0.44
3:G:73:GLU:O	3:G:76:SER:OG	2.32	0.44
4:H:1055:TRP:N	4:H:1098:GLU:OE1	2.49	0.44
1:D:34:GLN:HE21	1:D:38:ARG:NH2	2.15	0.44
4:B:1419:ARG:HA	4:B:1419:ARG:NE	2.32	0.44
4:H:1472:HIS:HE1	4:H:1474:GLU:HB2	1.83	0.44
4:H:1541:MET:HE2	4:H:1541:MET:HA	1.98	0.44
3:G:249:VAL:HG21	3:G:278:VAL:HG21	1.99	0.44
4:H:1273:ASP:HB3	4:H:1313:GLU:HG2	1.99	0.44
4:H:1472:HIS:CE1	4:H:1474:GLU:HB2	2.53	0.44
4:H:1575:GLU:HB3	4:H:1578:LYS:HD2	1.99	0.44
3:A:335:PHE:CE1	3:A:352:VAL:HG12	2.49	0.44
3:A:552:GLN:H	3:A:552:GLN:HE21	1.64	0.44
4:B:916:MET:N	4:B:916:MET:SD	2.91	0.44
1:C:11:LEU:O	1:C:14:THR:OG1	2.25	0.44
2:J:308:ASP:HA	2:J:311:THR:HG22	2.00	0.44
2:J:424:GLU:OE2	2:J:424:GLU:HA	2.18	0.44
3:A:484:GLN:NE2	3:A:485:VAL:O	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:386:LYS:HD2	3:G:386:LYS:HA	1.81	0.44
3:G:516:ILE:HD11	3:G:520:GLY:HA2	2.00	0.44
3:G:612:ASP:N	3:G:612:ASP:OD1	2.50	0.44
4:H:1539:TYR:HB2	4:H:1562:PHE:HB2	1.99	0.44
1:D:63:ILE:HA	1:D:63:ILE:HD13	1.87	0.43
3:A:23:GLU:OE2	3:A:483:ARG:NE	2.52	0.43
3:A:201:GLU:OE2	3:A:201:GLU:N	2.51	0.43
4:B:1417:SER:HB2	4:B:1444:TYR:CZ	2.53	0.43
4:H:1495:ASN:O	4:H:1602:LYS:N	2.51	0.43
2:X:409:VAL:HG11	2:X:429:LYS:NZ	2.33	0.43
4:B:917:ASN:HB3	4:B:1325:MET:SD	2.58	0.43
4:B:1522:VAL:HA	4:B:1583:TRP:HB3	1.99	0.43
3:A:246:THR:HG22	3:A:247:ALA:N	2.33	0.43
3:G:222:TYR:CE2	3:G:224:TYR:HB2	2.54	0.43
1:C:63:ILE:HA	1:C:66:VAL:HG12	2.00	0.43
3:A:346:MET:O	3:A:391:THR:OG1	2.33	0.43
3:A:335:PHE:CE2	3:A:419:MET:HB2	2.53	0.43
4:B:916:MET:HE2	4:B:1328:ALA:HB3	2.01	0.43
3:G:561:LEU:HB2	4:H:769:MET:SD	2.59	0.43
4:H:1506:THR:OG1	4:H:1509:GLU:OE1	2.29	0.43
3:A:563:ILE:HD11	3:A:573:LEU:HD11	2.00	0.43
3:G:47:LEU:HD23	3:G:49:SER:H	1.84	0.43
3:G:113:ASP:O	3:G:576:VAL:HG11	2.18	0.43
3:A:37:VAL:HG22	3:A:86:VAL:HG12	2.00	0.43
3:A:184:ILE:HG13	3:A:200:PHE:HE1	1.84	0.43
4:B:1394:ASP:OD1	4:B:1395:ASP:N	2.51	0.43
3:A:581:PHE:CZ	3:A:588:LYS:HD2	2.54	0.43
1:C:25:TYR:HA	1:C:92:LEU:HD11	1.99	0.42
3:A:606:THR:O	3:A:608:GLY:N	2.50	0.42
4:B:1086:ILE:HD12	4:B:1140:VAL:HG11	2.01	0.42
4:H:1527:LEU:HG	4:H:1576:GLU:HA	2.00	0.42
4:H:1562:PHE:CE1	4:H:1598:TYR:HB2	2.53	0.42
2:J:419:SER:O	2:J:426:HIS:HD2	2.02	0.42
4:B:1537:ASP:OD1	4:B:1537:ASP:N	2.50	0.42
4:B:1200:ASP:N	4:B:1207:ASN:OD1	2.46	0.42
3:G:462:GLU:OE2	3:G:486:ARG:NH2	2.52	0.42
3:G:40:PHE:HA	3:G:41:PRO:HA	1.80	0.42
2:X:402:VAL:HG22	2:X:418:ALA:HB2	2.01	0.42
3:A:623:THR:HA	3:A:632:THR:HG21	2.01	0.42
4:B:809:ILE:HD11	4:B:892:ALA:HB2	2.00	0.42
4:B:1154:LEU:HD23	4:B:1154:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1413:ASP:OD1	4:B:1414:LYS:N	2.52	0.42
4:B:1516:GLU:HG2	4:B:1518:GLY:H	1.84	0.42
3:A:305:SER:HA	3:A:320:GLU:HG2	2.00	0.42
3:G:183:LYS:HB2	3:G:183:LYS:HE3	1.78	0.42
3:G:204:GLU:HG2	4:H:815:TYR:CD2	2.54	0.42
3:G:315:ASP:OD2	4:H:812:ARG:NH2	2.52	0.42
3:G:342:PHE:HB2	3:G:348:PHE:HB2	2.01	0.42
2:X:237:VAL:HG21	2:X:356:ARG:HE	1.85	0.42
4:H:733:ILE:HD12	4:H:733:ILE:HA	1.90	0.42
4:H:872:LEU:HD13	4:H:1418:ASP:HB2	2.02	0.42
2:J:328:THR:HB	2:J:367:HIS:HA	2.02	0.42
3:A:552:GLN:HE21	3:A:552:GLN:N	2.18	0.42
4:B:1289:ILE:HD11	4:B:1298:ARG:HH12	1.84	0.42
1:C:78:SER:HB3	1:C:87:TYR:HE1	1.81	0.42
3:A:549:GLU:HA	3:A:551:ARG:NH1	2.34	0.42
4:B:1169:ILE:HB	4:B:1213:TYR:CE2	2.55	0.42
4:B:1337:ASN:O	4:B:1338:LYS:HG2	2.20	0.42
4:B:1373:ASP:OD1	4:B:1373:ASP:N	2.53	0.42
4:H:889:GLU:HB3	4:H:904:ARG:HG3	2.01	0.42
3:A:494:VAL:HG11	3:G:388:SER:HB3	2.02	0.41
2:J:309:TRP:CD1	2:J:312:LYS:HE3	2.37	0.41
2:J:394:ARG:O	2:J:394:ARG:HG3	2.21	0.41
3:A:329:SER:HA	3:A:330:PRO:HD3	1.93	0.41
3:G:343:LYS:HE3	3:G:424:TYR:CD2	2.55	0.41
1:D:18:ASP:OD1	1:D:20:SER:N	2.37	0.41
4:B:1550:GLY:HA3	4:B:1554:VAL:HG12	2.02	0.41
4:H:1380:ILE:O	4:H:1457:VAL:HA	2.20	0.41
3:A:72:ARG:HA	3:A:72:ARG:HD3	1.86	0.41
4:B:1546:THR:HG23	4:B:1556:VAL:HG22	2.02	0.41
4:H:1520:ASP:OD1	4:H:1521:TYR:N	2.53	0.41
2:J:435:ASN:ND2	2:J:438:ASP:OD2	2.54	0.41
4:B:1362:MET:HE1	4:B:1389:PHE:CE2	2.55	0.41
4:B:1522:VAL:HB	4:B:1547:ILE:HB	2.02	0.41
4:H:1383:ILE:HG12	4:H:1455:VAL:HG23	2.02	0.41
4:H:1526:ARG:HB2	4:H:1579:HIS:NE2	2.36	0.41
3:A:223:ILE:HG21	3:A:328:THR:HG22	2.03	0.41
3:A:553:PRO:HG2	3:A:559:MET:HE2	2.02	0.41
4:H:961:GLN:O	4:H:1319:THR:N	2.49	0.41
4:H:1127:ILE:HA	4:H:1176:GLN:OE1	2.19	0.41
4:B:999:THR:HG21	4:B:1026:LEU:HD23	2.03	0.41
4:B:1180:LEU:HD12	4:B:1184:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1445:PHE:CE2	4:B:1447:VAL:HB	2.56	0.41
3:G:606:THR:O	3:G:608:GLY:N	2.50	0.41
2:J:286:LEU:H	2:J:297:VAL:HB	1.85	0.41
2:J:386:ILE:HD12	2:J:394:ARG:O	2.20	0.41
3:A:335:PHE:CD2	3:A:419:MET:HB2	2.56	0.41
3:G:497:LEU:HD12	3:G:497:LEU:HA	1.86	0.41
4:H:927:PRO:HA	4:H:936:GLN:HB2	2.03	0.41
4:H:1526:ARG:NH2	4:H:1544:GLU:OE2	2.54	0.41
3:A:338:THR:HG21	3:A:350:LEU:HD23	2.03	0.41
3:A:363:TYR:CE2	3:A:364:ARG:HG3	2.56	0.41
4:H:923:ARG:HH22	4:H:940:ILE:HD11	1.86	0.41
2:X:244:MET:HA	2:X:244:MET:HE2	2.02	0.41
3:A:139:ARG:H	3:A:160:SER:HG	1.59	0.40
3:A:436:LEU:HD22	3:A:529:VAL:HG11	2.04	0.40
4:B:1110:GLY:HA3	4:B:1165:TYR:CZ	2.56	0.40
4:B:1121:LEU:O	4:B:1125:VAL:HG23	2.21	0.40
3:G:562:LYS:HE2	3:G:562:LYS:HB2	1.84	0.40
4:H:831:ASN:OD1	4:H:832:TYR:N	2.54	0.40
4:H:965:VAL:HG22	4:H:1270:LEU:HG	2.03	0.40
4:H:1373:ASP:OD1	4:H:1373:ASP:N	2.53	0.40
4:B:1089:LYS:NZ	4:B:1099:ASP:OD2	2.33	0.40
4:H:1090:GLN:HE22	4:H:1146:SER:HB2	1.87	0.40
3:G:85:THR:HA	3:G:98:VAL:HG12	2.03	0.40
3:G:346:MET:HB3	3:G:347:PRO:HD2	2.01	0.40
4:H:1044:PHE:CE2	4:H:1060:VAL:HG11	2.56	0.40
4:H:1525:THR:OG1	4:H:1541:MET:SD	2.78	0.40
2:X:439:VAL:HG13	2:X:440:PHE:HD1	1.85	0.40
1:C:22:LYS:HB2	1:C:25:TYR:HB3	2.02	0.40
3:A:40:PHE:HA	3:A:41:PRO:HA	1.93	0.40
3:A:147:ASN:OD1	3:A:151:ILE:N	2.39	0.40
4:B:1585:LEU:H	4:B:1588:ASP:HB2	1.86	0.40
4:H:857:LYS:HD2	4:H:857:LYS:HA	1.88	0.40
1:C:107:PHE:HA	1:C:110:THR:HG22	2.03	0.40
3:A:626:SER:HG	3:A:630:GLN:N	2.19	0.40
4:B:1109:GLY:O	4:B:1206:TYR:OH	2.32	0.40
3:G:290:GLN:H	3:G:290:GLN:CD	2.28	0.40
3:G:469:THR:O	3:G:511:ALA:HA	2.21	0.40
4:H:1096:PHE:HB2	4:H:1122:THR:HA	2.02	0.40
4:H:1394:ASP:OD1	4:H:1395:ASP:N	2.55	0.40
4:H:1510:ARG:HD3	4:H:1510:ARG:HA	1.72	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	C	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
1	D	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
2	J	216/228 (95%)	209 (97%)	7 (3%)	0	100	100
2	X	217/228 (95%)	207 (95%)	10 (5%)	0	100	100
3	A	639/642 (100%)	616 (96%)	23 (4%)	0	100	100
3	G	638/642 (99%)	616 (97%)	22 (3%)	0	100	100
4	B	889/915 (97%)	852 (96%)	35 (4%)	2 (0%)	43	74
4	H	891/915 (97%)	857 (96%)	33 (4%)	1 (0%)	48	80
All	All	3718/3802 (98%)	3578 (96%)	137 (4%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	1262	LYS
4	B	1556	VAL
4	H	1556	VAL

### 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	C	105/105 (100%)	105 (100%)	0	100	100
1	D	105/105 (100%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	130/202 (64%)	130 (100%)	0	100	100
2	X	145/202 (72%)	145 (100%)	0	100	100
3	A	562/566 (99%)	561 (100%)	1 (0%)	87	87
3	G	553/566 (98%)	552 (100%)	1 (0%)	87	87
4	B	676/810 (84%)	676 (100%)	0	100	100
4	H	646/810 (80%)	646 (100%)	0	100	100
All	All	2922/3366 (87%)	2920 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	552	GLN
3	G	63	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	270	ASN
2	J	322	HIS
2	J	411	GLN
2	J	415	ASN
2	J	435	ASN
3	A	71	ASN
3	A	390	ASN
3	A	552	GLN
4	B	805	GLN
4	B	831	ASN
4	B	835	ASN
4	B	1011	GLN
4	B	1176	GLN
4	B	1237	GLN
4	B	1248	GLN
4	B	1259	GLN
4	B	1261	GLN
3	G	10	ASN
3	G	25	HIS
3	G	132	HIS
3	G	258	GLN
3	G	334	HIS

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Mol	Chain	Res	Type
3	G	390	ASN
3	G	552	GLN
3	G	557	GLN
3	G	631	GLN
4	H	770	ASN
4	H	822	GLN
4	H	992	ASN
4	H	1033	GLN
4	H	1034	GLN
4	H	1097	GLN
4	H	1186	ASN
4	H	1287	HIS
4	H	1545	GLN
2	X	245	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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	NAG	M	1	3,5	14,14,15	0.20	0	17,19,21	0.46	0
5	NAG	M	2	5	14,14,15	0.20	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

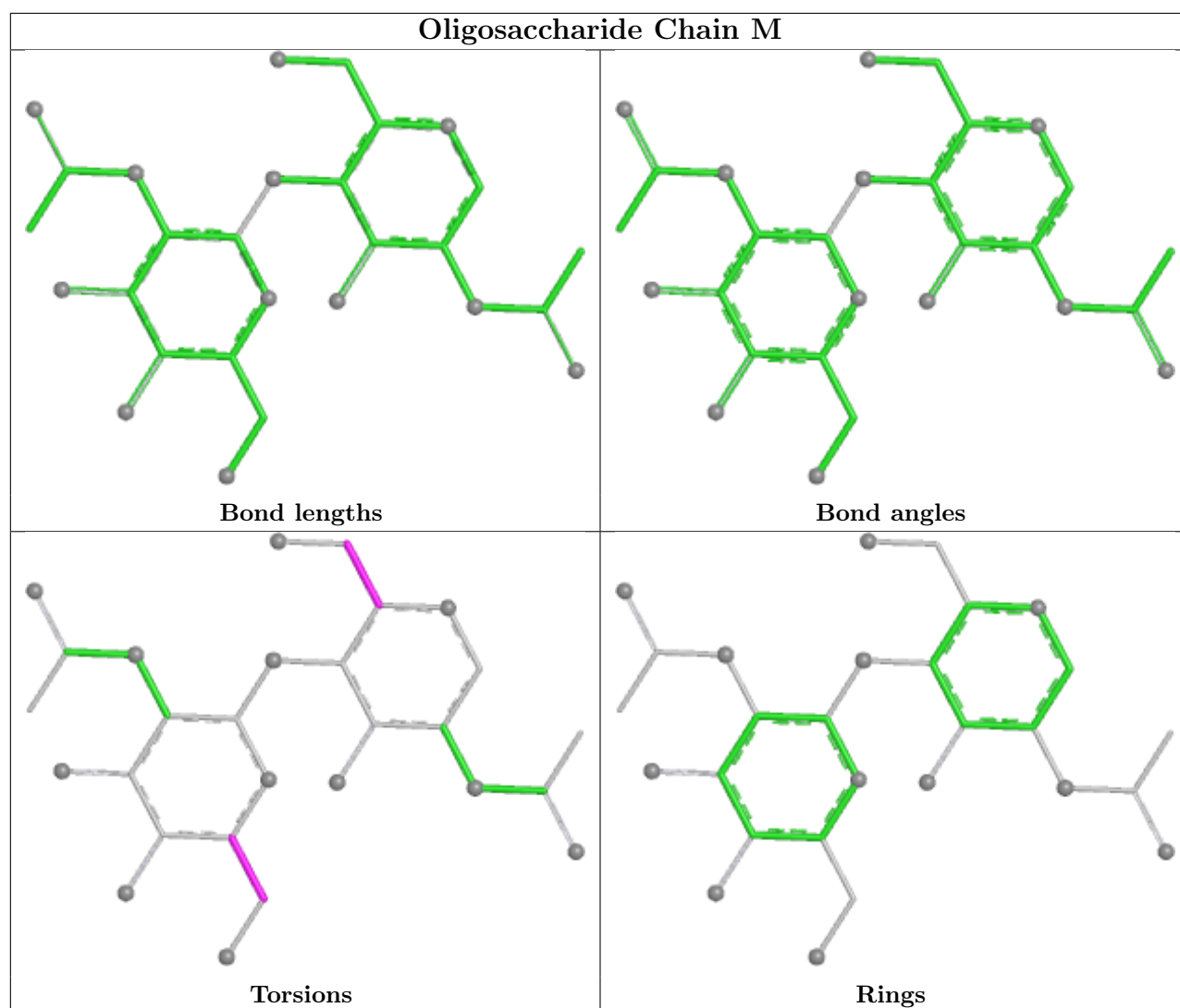
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z  > 2$
6	NAG	B	1701	4	14,14,15	0.41	0	17,19,21	0.35	0
6	NAG	G	701	3	14,14,15	0.28	0	17,19,21	0.72	0
6	NAG	H	1701	4	14,14,15	0.50	0	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1701	4	-	0/6/23/26	0/1/1/1
6	NAG	G	701	3	-	3/6/23/26	0/1/1/1
6	NAG	H	1701	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	701	NAG	C1-C2-N2-C7
6	H	1701	NAG	O5-C5-C6-O6
6	H	1701	NAG	C4-C5-C6-O6
6	G	701	NAG	O5-C5-C6-O6
6	H	1701	NAG	C3-C2-N2-C7
6	H	1701	NAG	C1-C2-N2-C7
6	G	701	NAG	C3-C2-N2-C7

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.

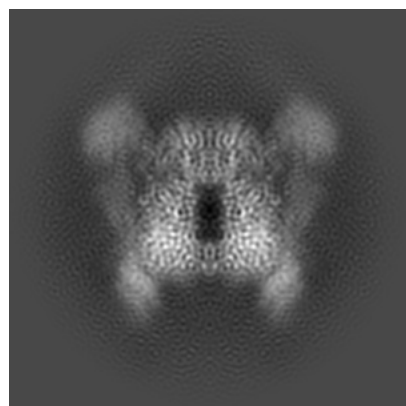
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42300. These allow visual inspection of the internal detail of the map and identification of artifacts.

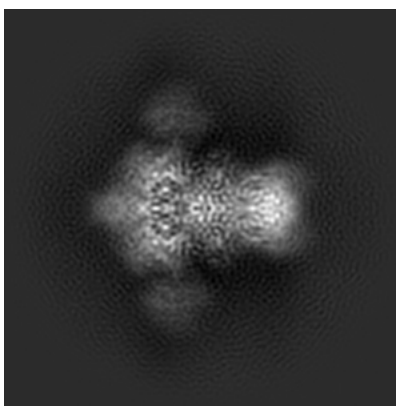
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

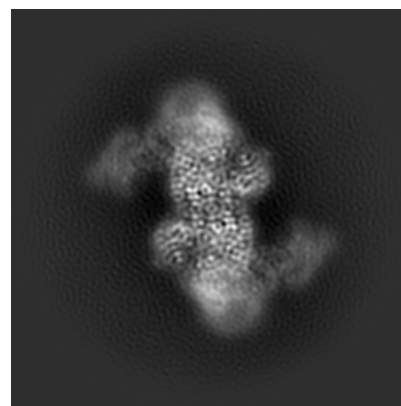
#### 6.1.1 Primary map



X

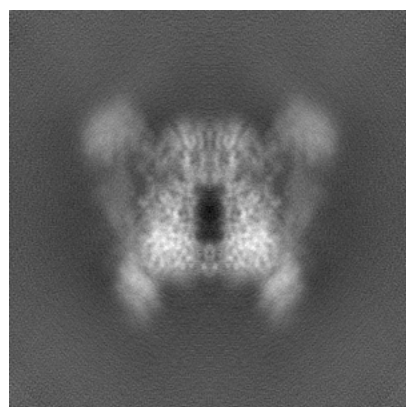


Y

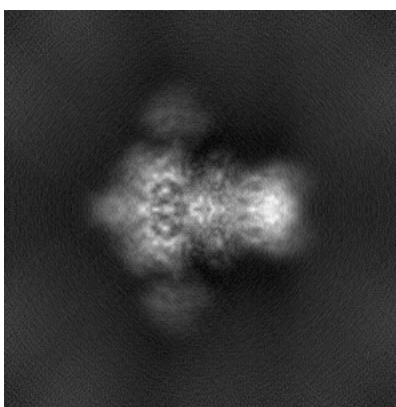


Z

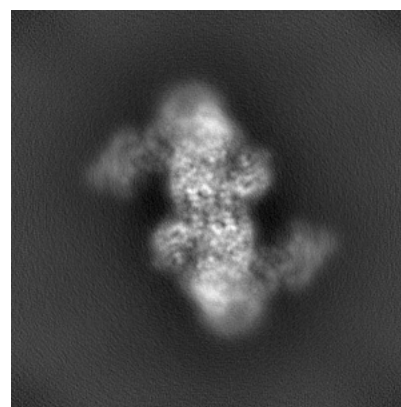
#### 6.1.2 Raw map



X



Y

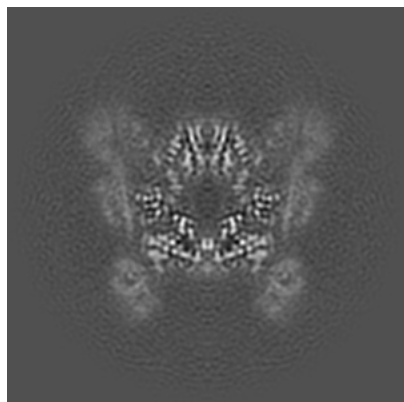


Z

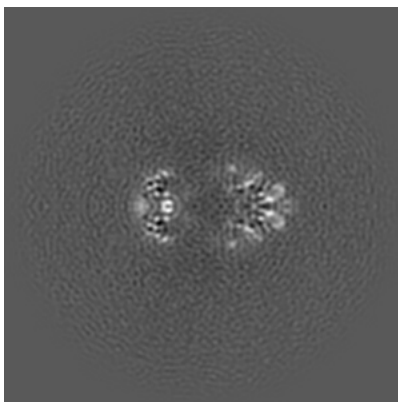
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

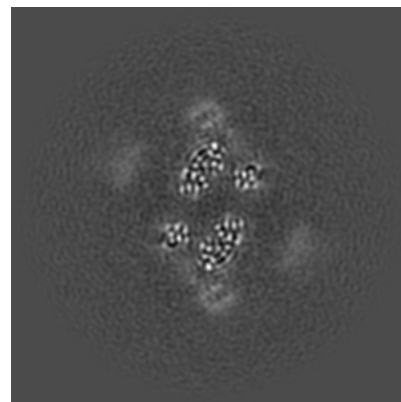
### 6.2.1 Primary map



X Index: 160

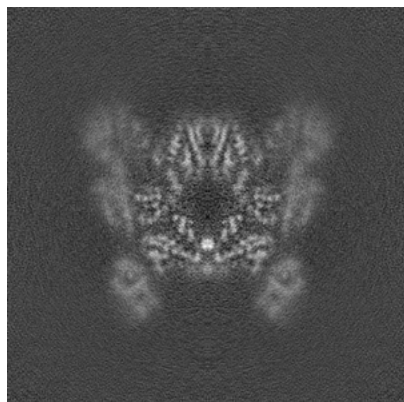


Y Index: 160

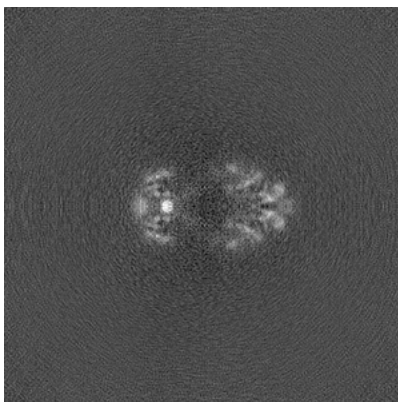


Z Index: 160

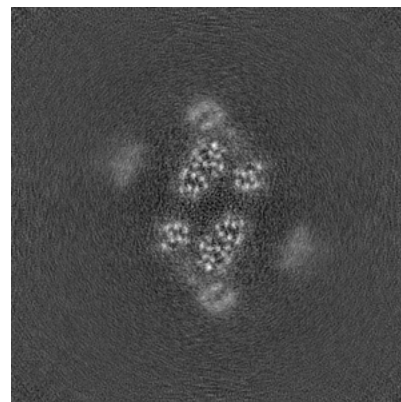
### 6.2.2 Raw map



X Index: 160



Y Index: 160



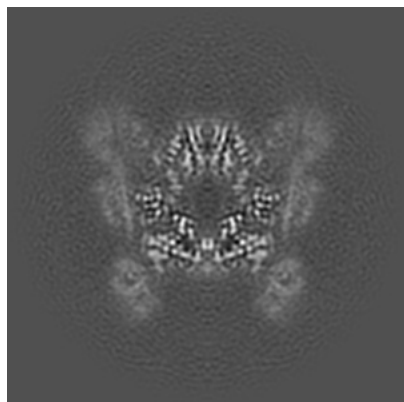
Z Index: 160

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

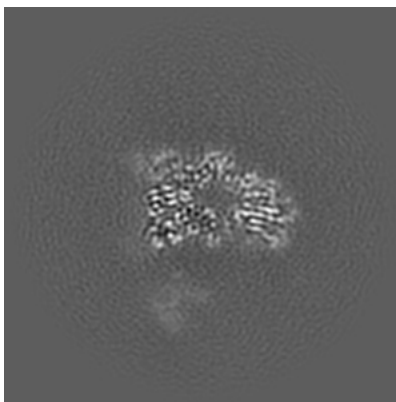


## 6.3 Largest variance slices [i](#)

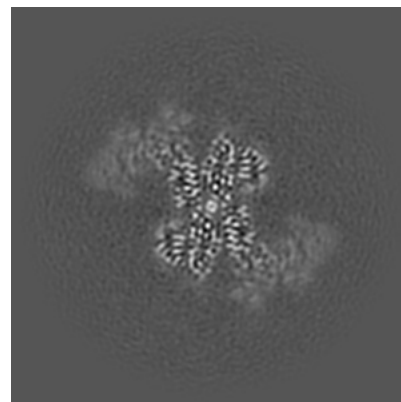
### 6.3.1 Primary map



X Index: 160

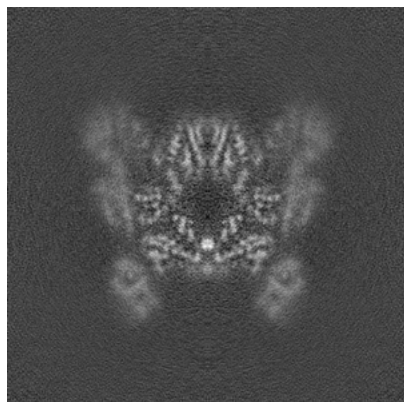


Y Index: 178

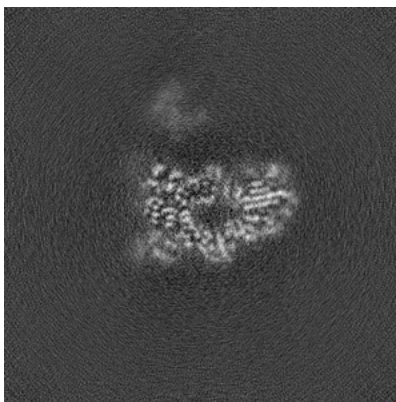


Z Index: 129

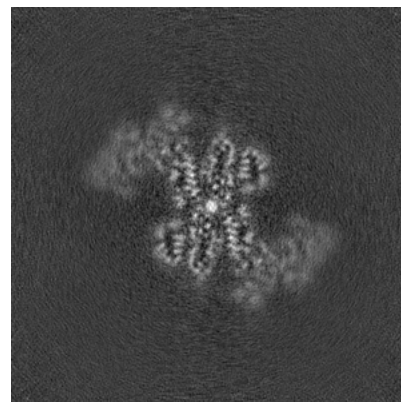
### 6.3.2 Raw map



X Index: 160



Y Index: 143

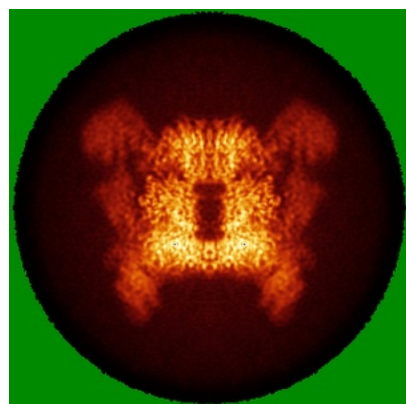


Z Index: 129

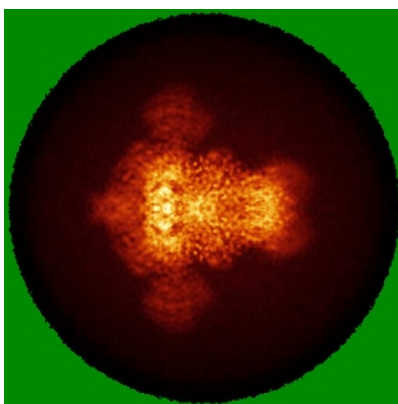
The images above show the largest variance slices of the map in three orthogonal directions.

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

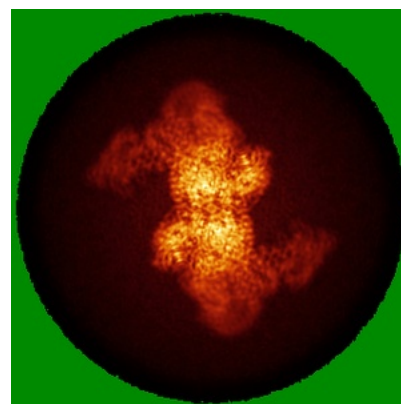
### 6.4.1 Primary map



X

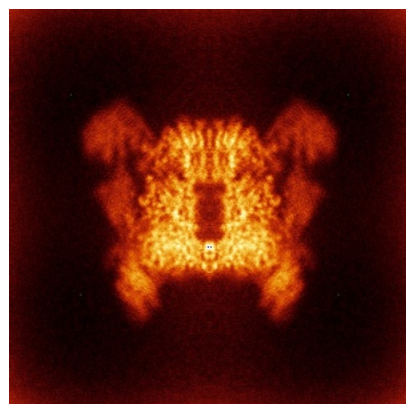


Y

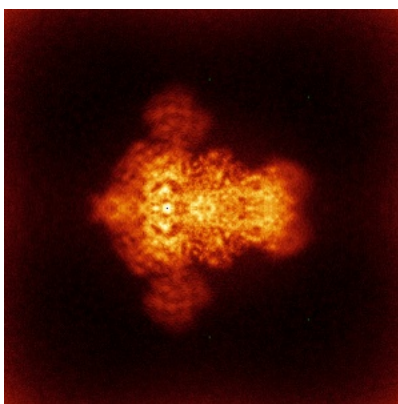


Z

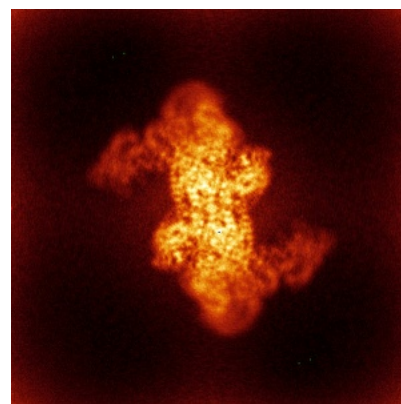
### 6.4.2 Raw map



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.

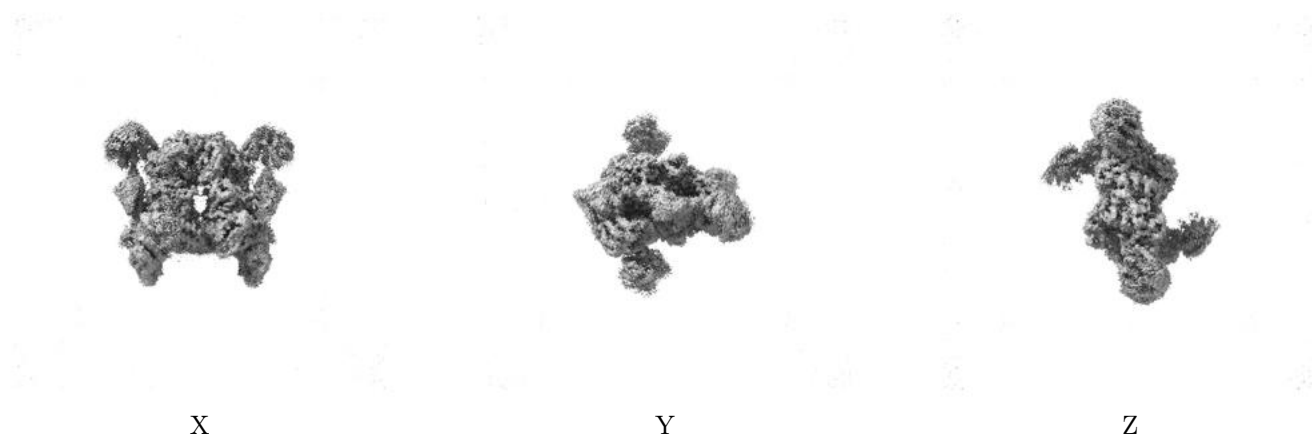
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.087. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

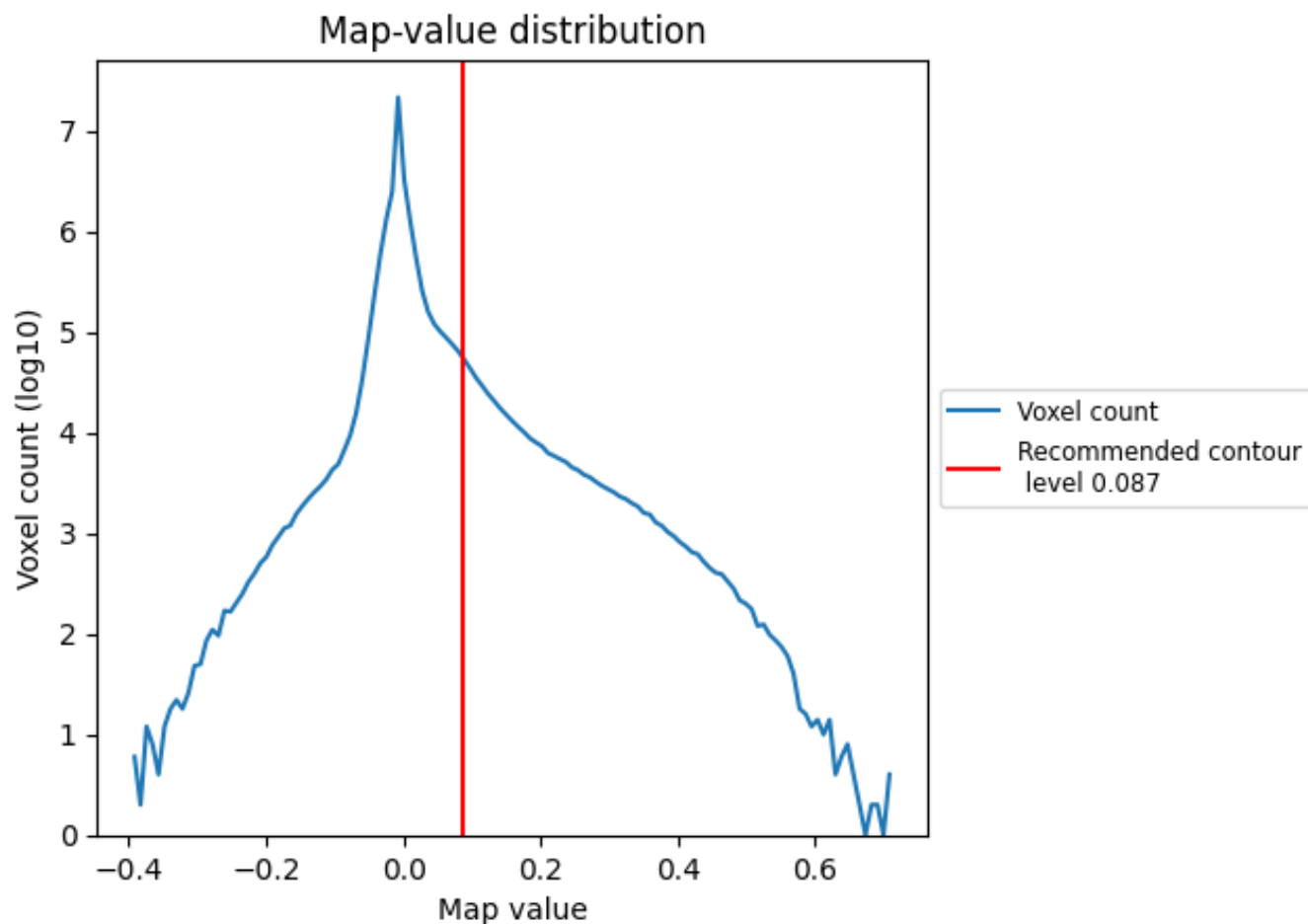
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

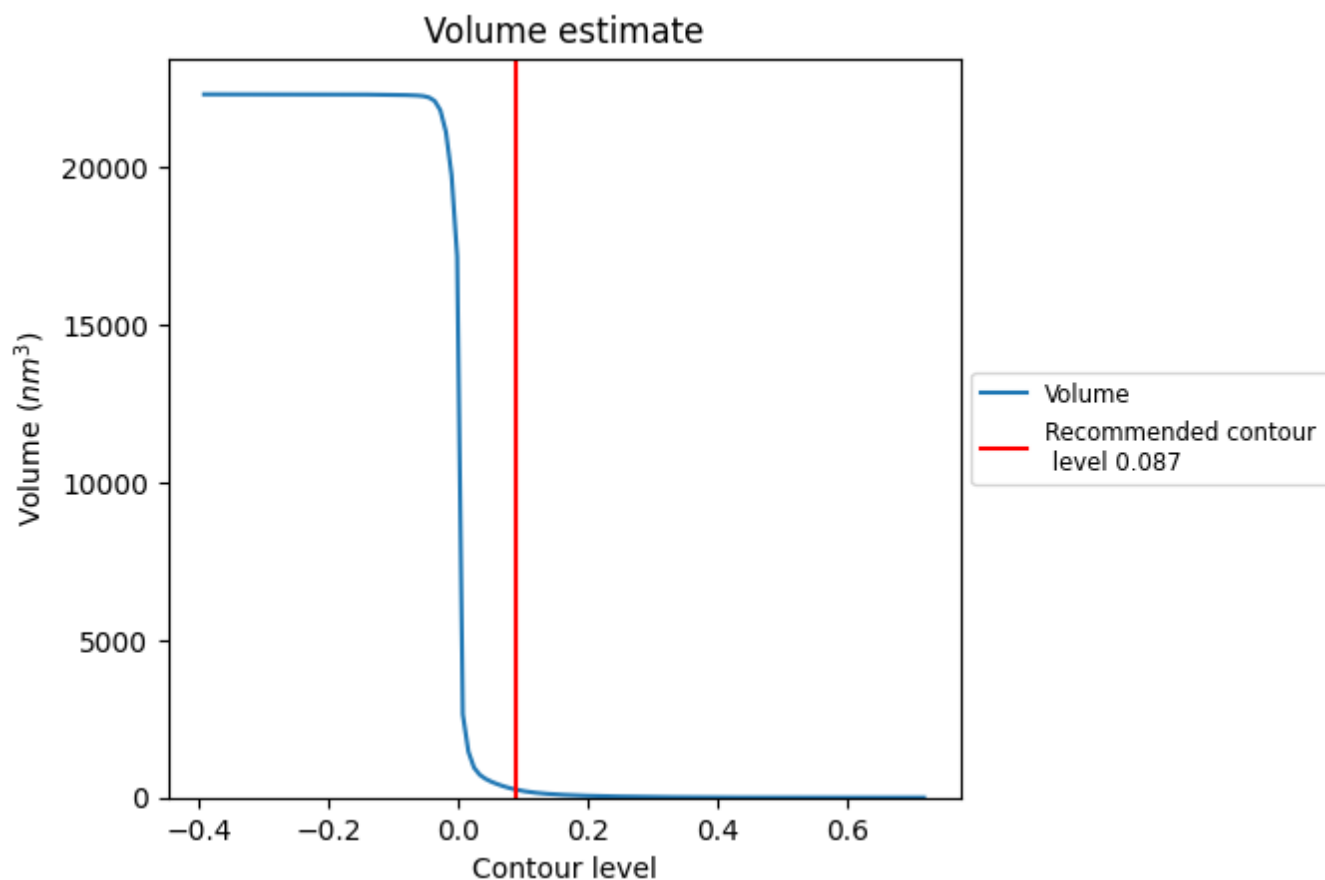
This section contains the results of statistical analysis of the map.

### 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.

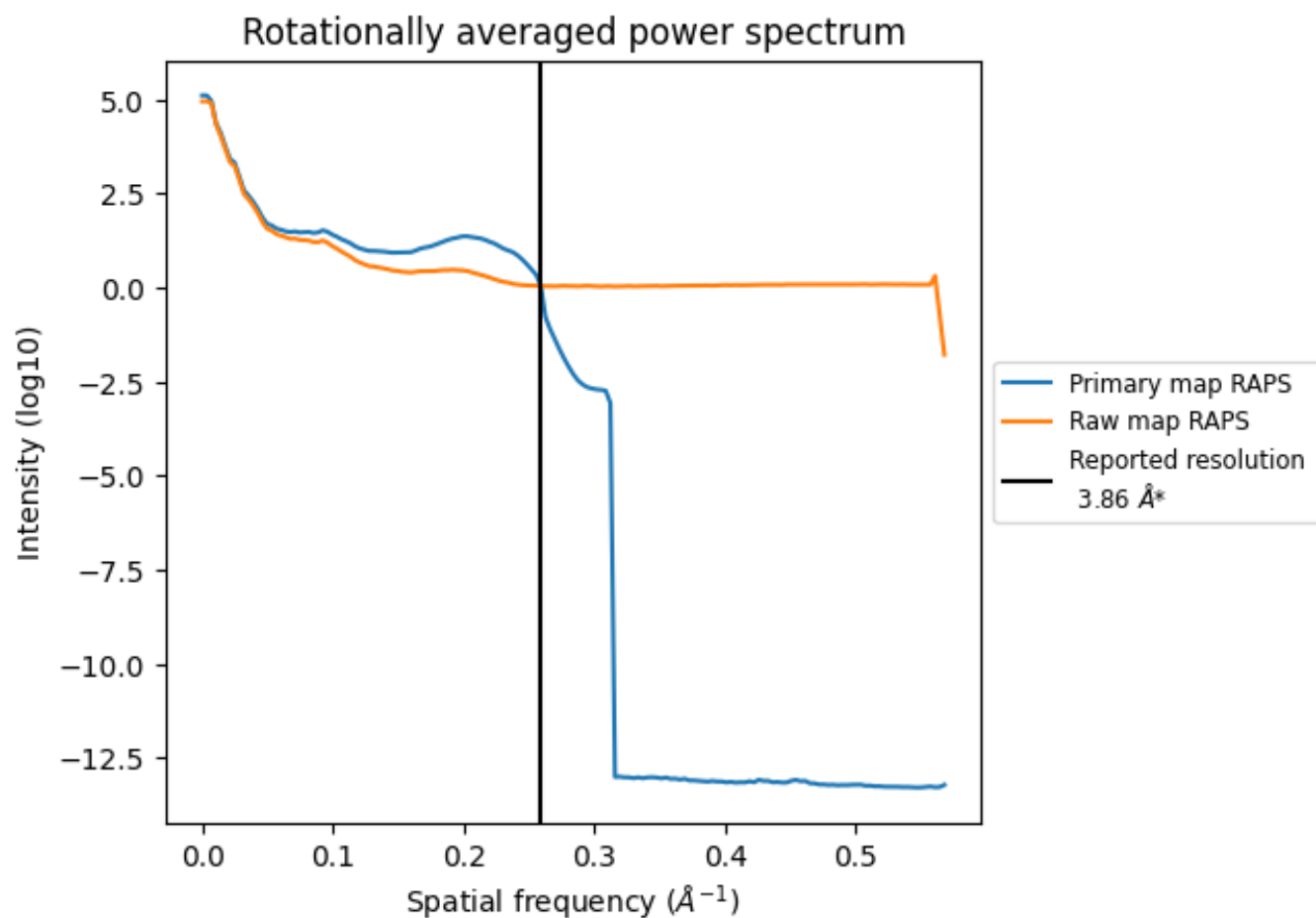
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm<sup>3</sup>; this corresponds to an approximate mass of 236 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 ⓘ

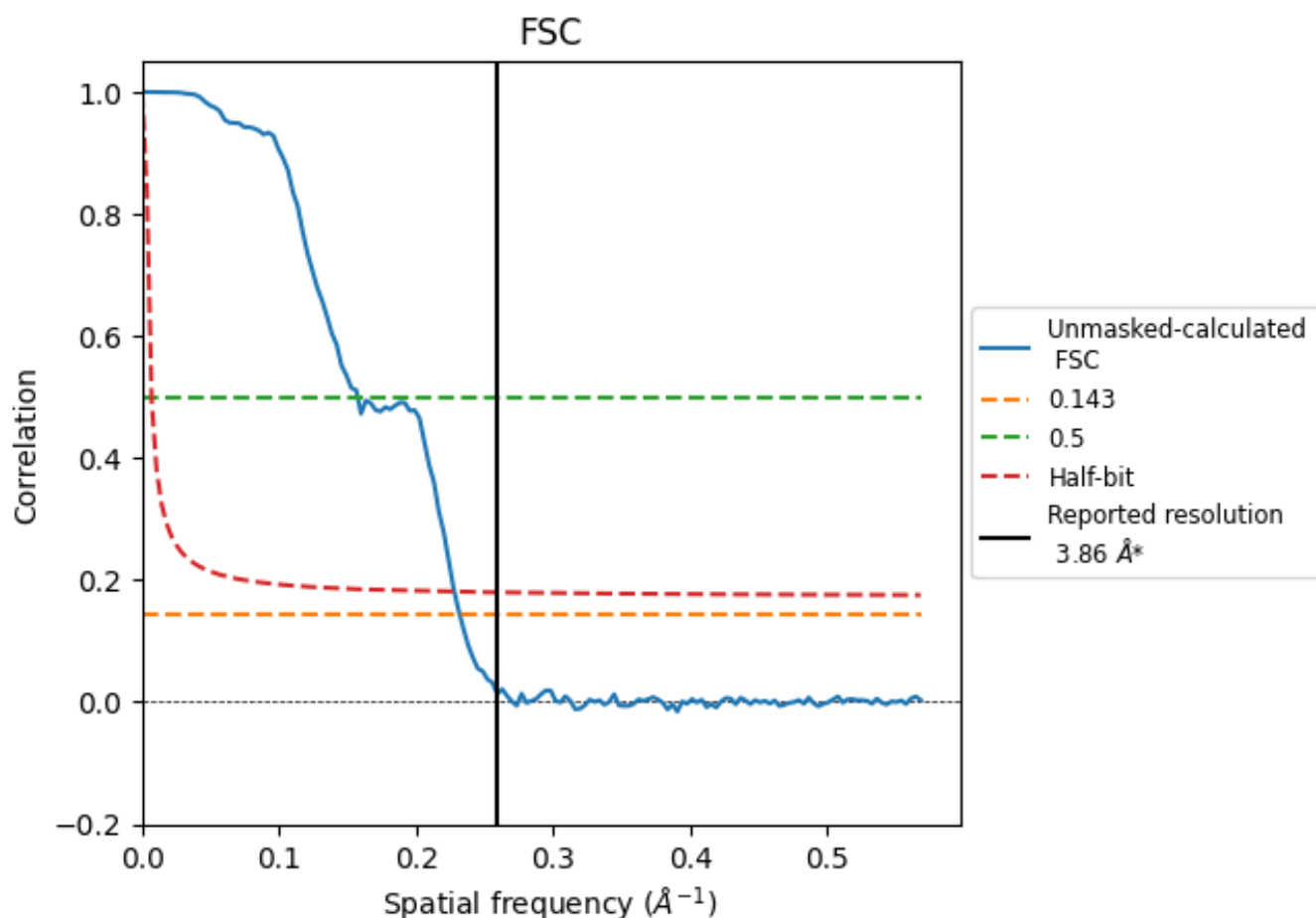


\*Reported resolution corresponds to spatial frequency of 0.259 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.259  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	6.36	4.39

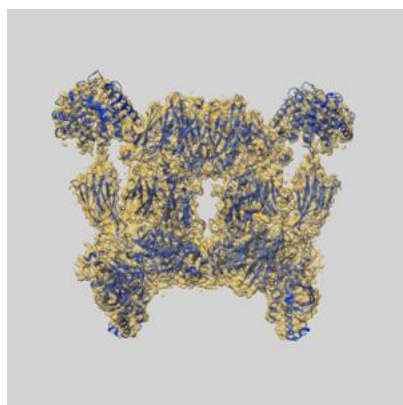
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.86 by more than 10 %



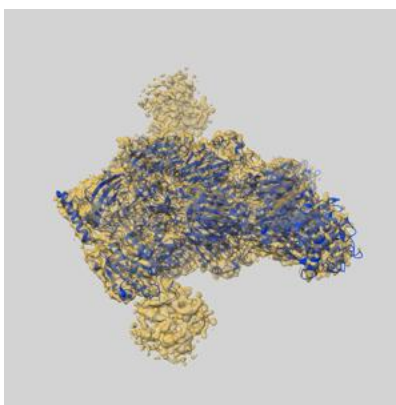
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42300 and PDB model 8UIN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

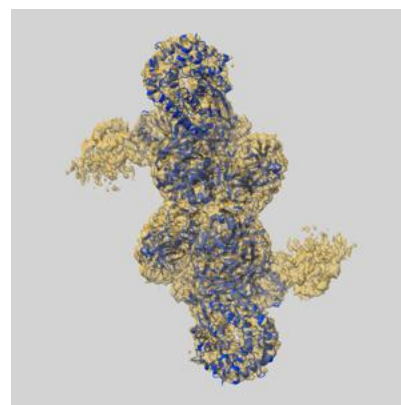
### 9.1 Map-model overlay [i](#)



X



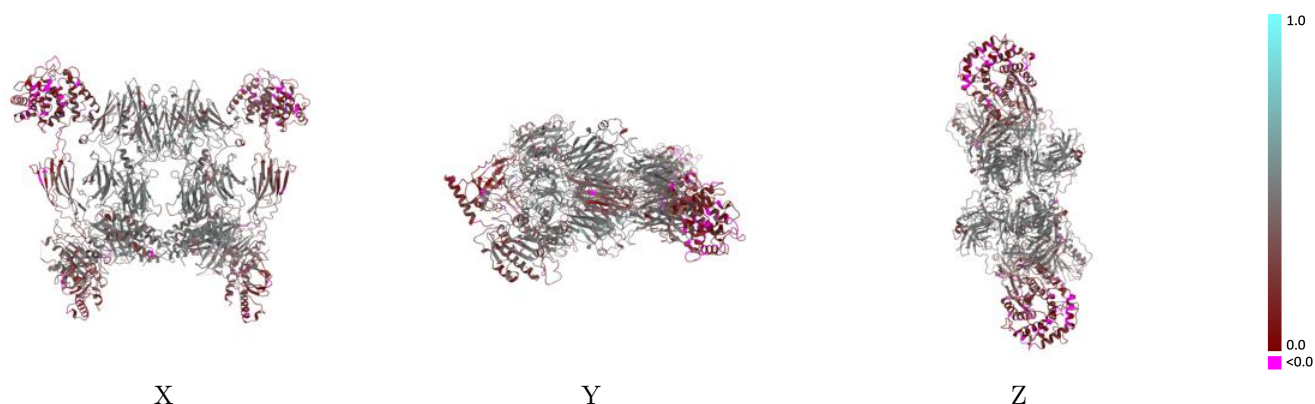
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.087 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](#)

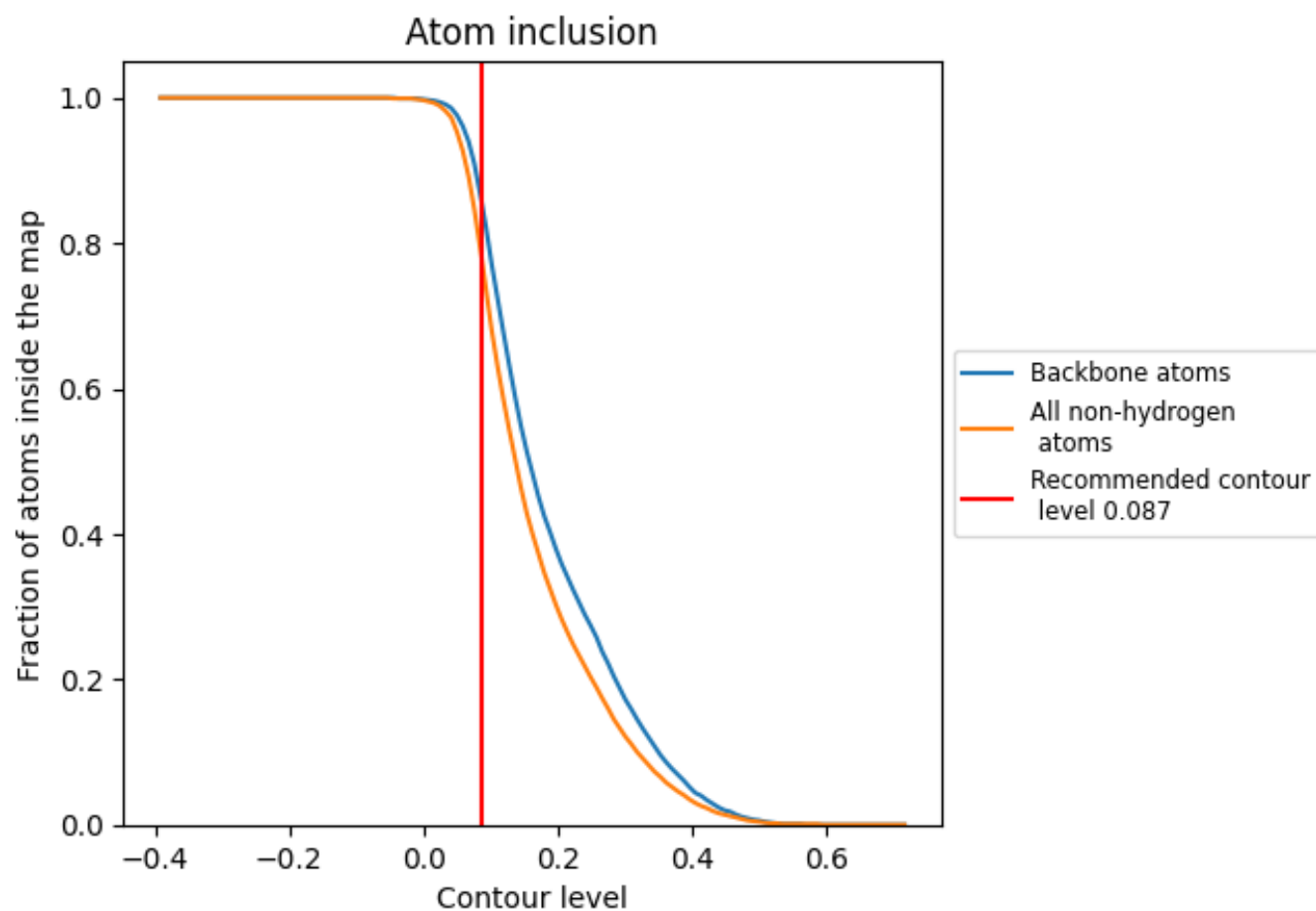


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.087) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7790</div>	<div><div></div>0.3790</div>
A	<div><div></div>0.8640</div>	<div><div></div>0.4490</div>
B	<div><div></div>0.6980</div>	<div><div></div>0.3160</div>
C	<div><div></div>0.8460</div>	<div><div></div>0.4290</div>
D	<div><div></div>0.8530</div>	<div><div></div>0.4140</div>
G	<div><div></div>0.8660</div>	<div><div></div>0.4490</div>
H	<div><div></div>0.7170</div>	<div><div></div>0.3300</div>
J	<div><div></div>0.7700</div>	<div><div></div>0.3650</div>
M	<div><div></div>0.6430</div>	<div><div></div>0.3240</div>
X	<div><div></div>0.7660</div>	<div><div></div>0.3710</div>

1.0

0.0

<0.0