



Preliminary Full wwPDB EM Validation Report ⓘ

Oct 8, 2021 – 01:08 PM JST

Deposition ID : D_1300024911

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

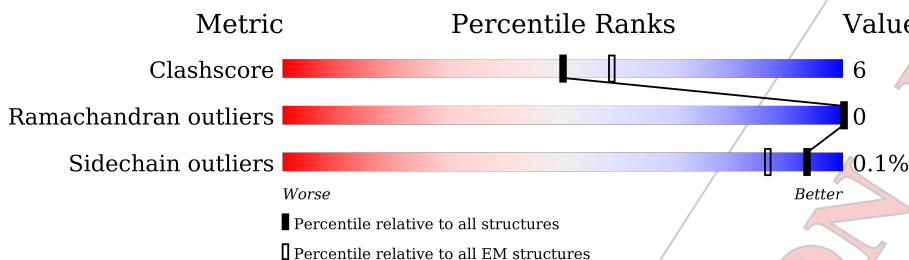
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 unknown.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	7% 86% 14%
1	B	494	9% 87% 13%
1	C	494	9% 86% 14%
1	E	494	8% 85% 15%
1	F	494	10% 81% 19%
1	G	494	10% 86% 14%
2	D	497	9% 86% 14%
3	H	395	32% 85% 15%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30682 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	494	Total	C	N	O	S	12	0
			3942	2462	641	833	6		
1	B	494	Total	C	N	O	S	11	0
			3935	2458	640	831	6		
1	C	494	Total	C	N	O	S	1	0
			3867	2418	627	816	6		
1	E	494	Total	C	N	O	S	12	0
			3942	2462	641	833	6		
1	F	494	Total	C	N	O	S	1	0
			3867	2418	627	816	6		
1	G	494	Total	C	N	O	S	21	0
			3935	2458	640	831	6		

- Molecule 2 is a protein called CALCIUM ION.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	497	Total	C	N	O	S	12	0
			3973	2482	645	840	6		

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	395	Total	C	N	O	S	0	0
			3200	2038	534	623	5		

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

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			3	3	
4	A	1	Total	Ca	0
			3	3	

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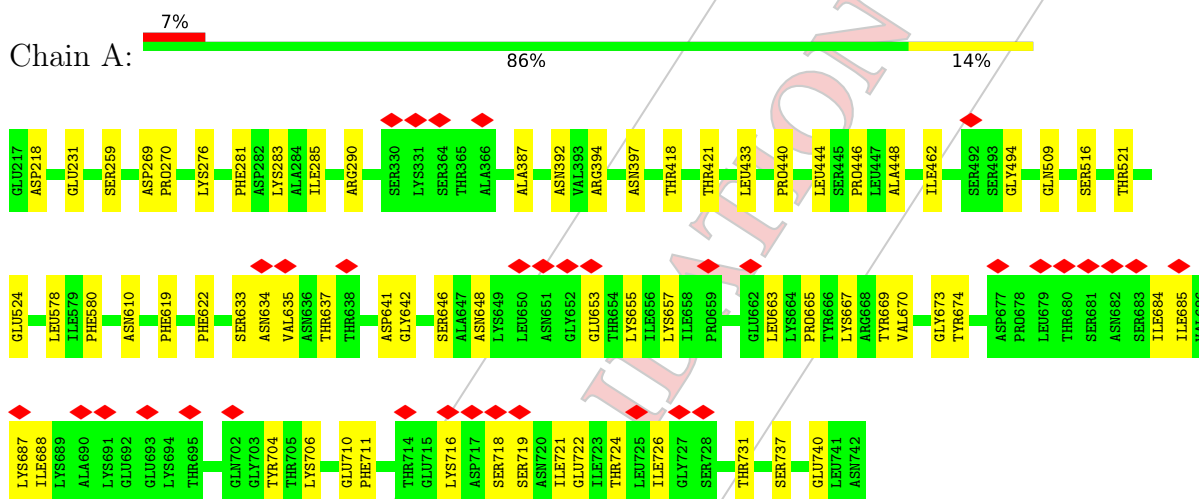
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Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 3	Ca 3	0
4	B	1	Total 3	Ca 3	0
4	B	1	Total 3	Ca 3	0
4	B	1	Total 3	Ca 3	0
4	C	1	Total 3	Ca 3	0
4	C	1	Total 3	Ca 3	0
4	C	1	Total 3	Ca 3	0
4	D	1	Total 3	Ca 3	0
4	D	1	Total 3	Ca 3	0
4	D	1	Total 3	Ca 3	0
4	E	1	Total 3	Ca 3	0
4	E	1	Total 3	Ca 3	0
4	E	1	Total 3	Ca 3	0
4	F	1	Total 3	Ca 3	0
4	F	1	Total 3	Ca 3	0
4	F	1	Total 3	Ca 3	0
4	G	1	Total 3	Ca 3	0
4	G	1	Total 3	Ca 3	0
4	G	1	Total 3	Ca 3	0

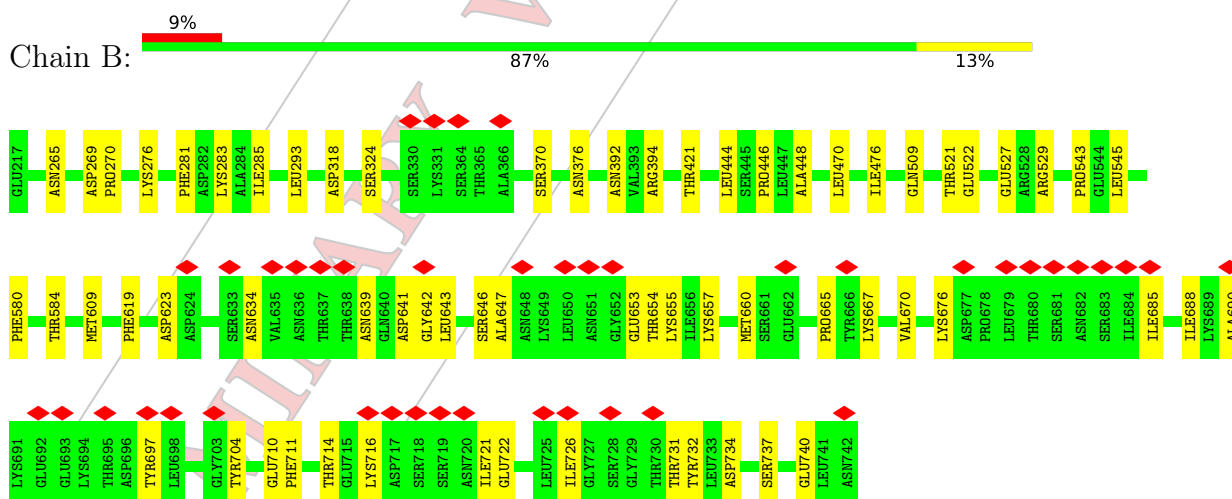
3 Residue-property plots

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.

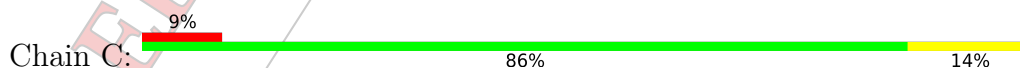
• Molecule 1:

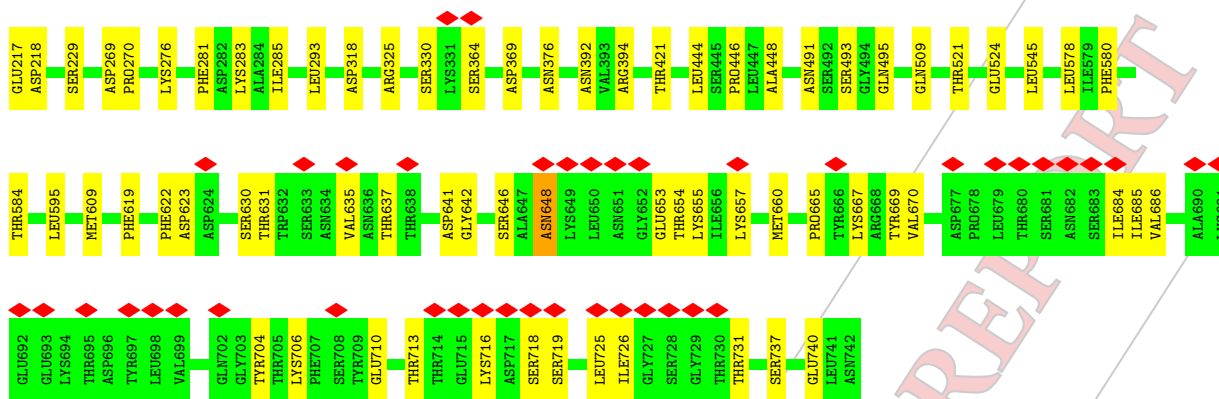


• Molecule 1:

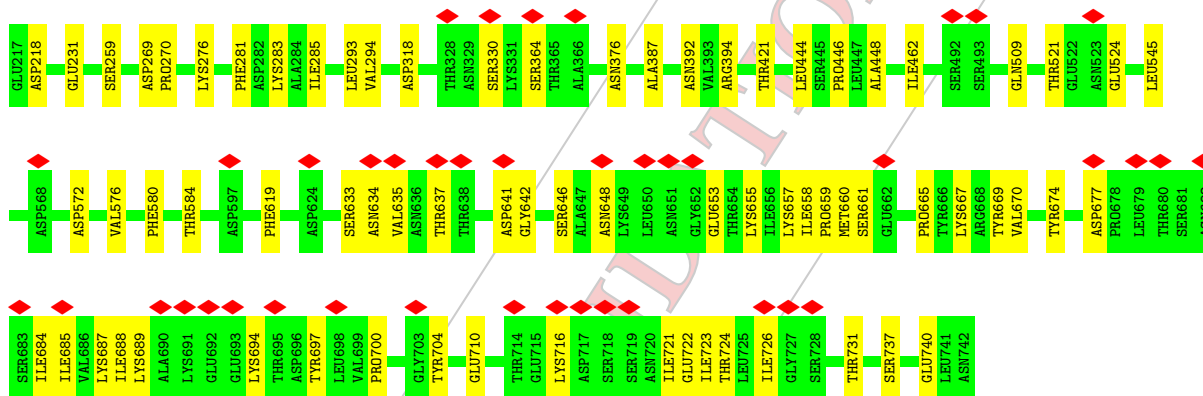
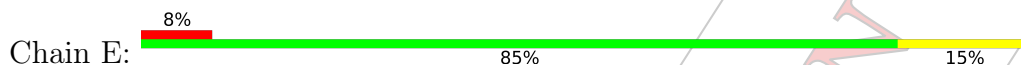


• Molecule 1:

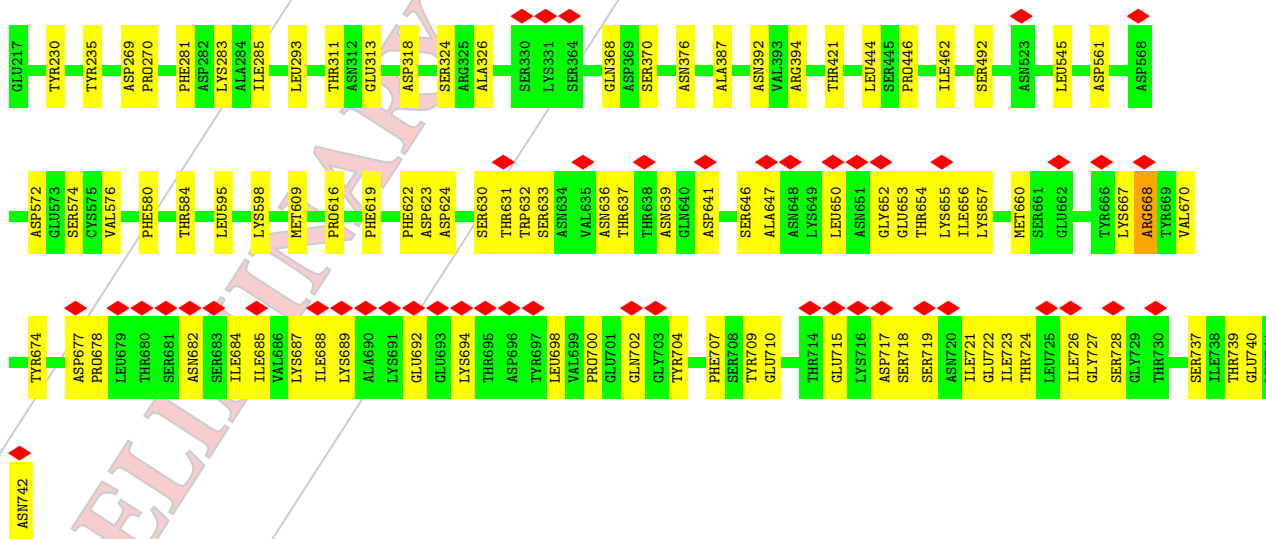
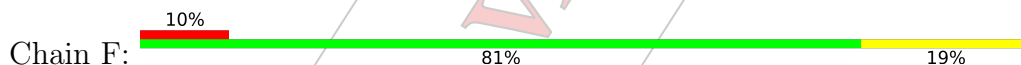




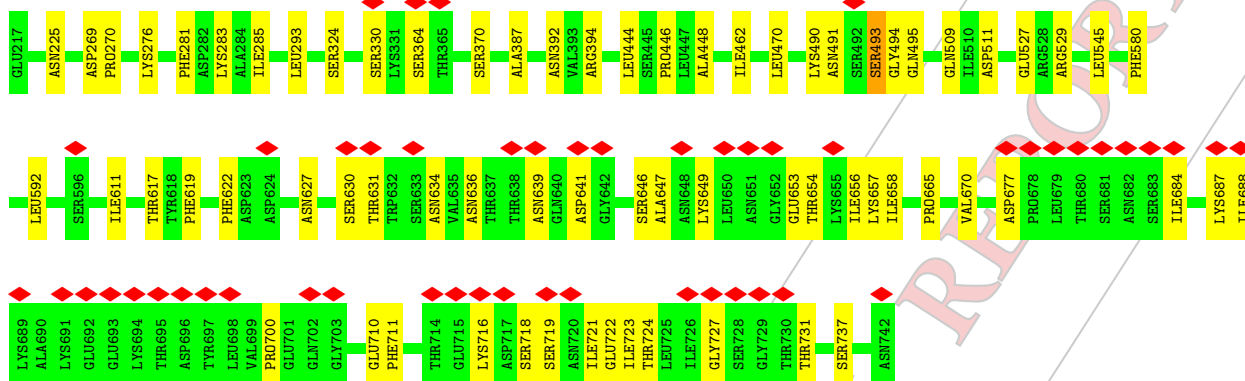
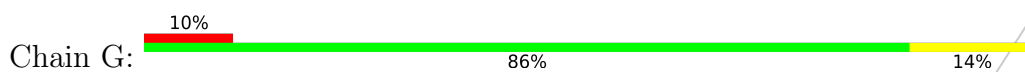
• Molecule 1:



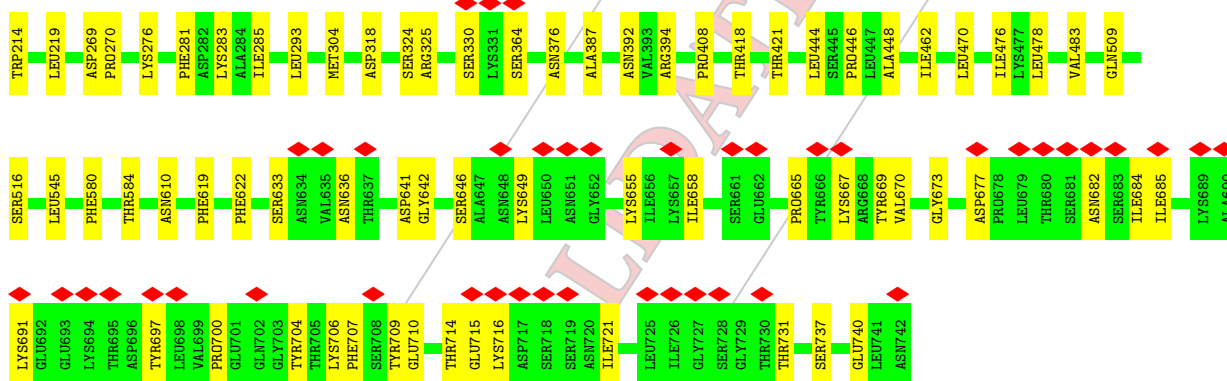
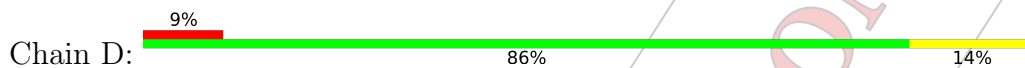
• Molecule 1:



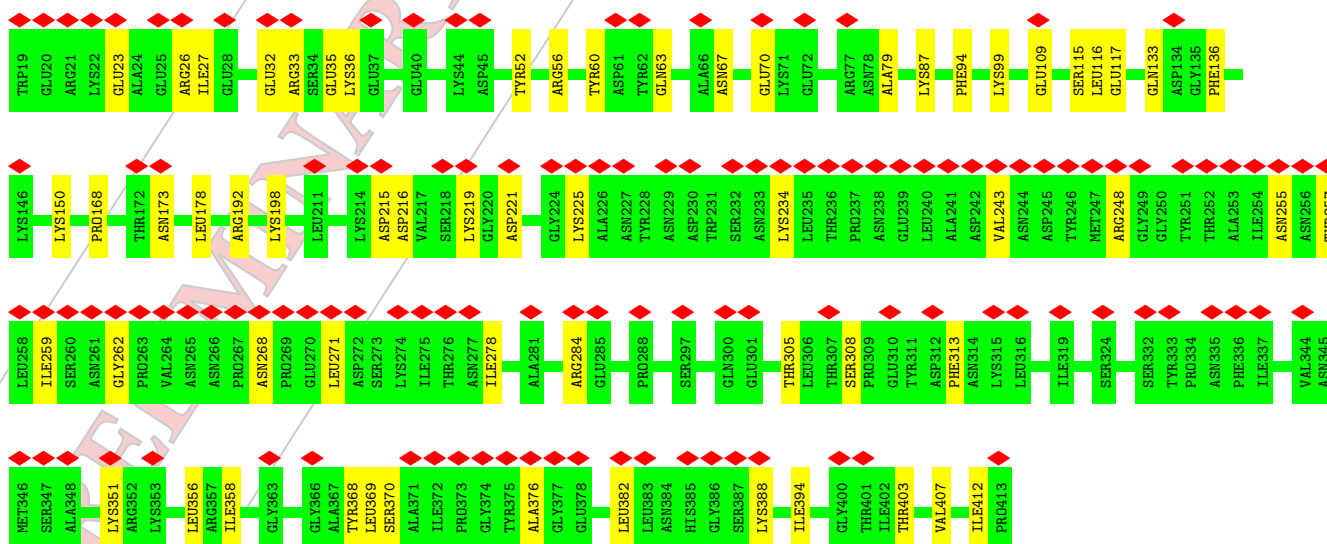
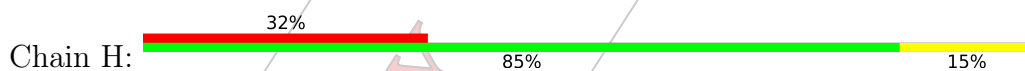
• Molecule 1:



• Molecule 2: CALCIUM ION



• Molecule 3:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	0.161	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0156	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/4008	0.47	0/5433
1	B	0.26	0/4001	0.47	0/5423
1	C	0.26	0/3933	0.47	0/5332
1	E	0.26	0/4008	0.47	0/5433
1	F	0.26	0/3933	0.48	0/5332
1	G	0.26	0/4001	0.48	0/5423
2	D	0.26	0/4041	0.47	0/5479
3	H	0.25	0/3269	0.45	0/4414
All	All	0.26	0/31194	0.47	0/42269

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3942	0	3842	45	0
1	B	3935	0	3835	48	0
1	C	3867	0	3766	47	0
1	E	3942	0	3842	47	0
1	F	3867	0	3766	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3935	0	3833	50	0
2	D	3973	0	3862	45	0
3	H	3200	0	3179	40	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
All	All	30682	0	29925	366	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (366) 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:D:677:ASP:HB2	2:D:700:PRO:HB2	1.64	0.78
1:E:670:VAL:HG22	1:E:710:GLU:HG2	1.67	0.77
1:C:685:ILE:HB	1:C:726:ILE:HG13	1.68	0.75
2:D:658:ILE:HB	2:D:721:ILE:HB	1.69	0.75
1:C:670:VAL:HG22	1:C:710:GLU:HG2	1.69	0.74
1:E:685:ILE:HB	1:E:726:ILE:HG13	1.69	0.74
1:B:670:VAL:HG22	1:B:710:GLU:HG2	1.68	0.74
1:F:650:LEU:HD12	1:F:652:GLY:H	1.54	0.73
3:H:305:THR:HG1	3:H:308:SER:HG	1.35	0.73
2:D:394:ARG:NH2	2:D:444:LEU:O	2.22	0.71
1:B:665:PRO:HD3	1:B:716:LYS:HD3	1.71	0.71
1:A:685:ILE:HB	1:A:726:ILE:HG13	1.72	0.70
1:F:394:ARG:NH2	1:F:444:LEU:O	2.23	0.70
1:B:394:ARG:NH2	1:B:444:LEU:O	2.23	0.70
1:A:684:ILE:HD11	1:A:731:THR:HG21	1.74	0.69
2:D:684:ILE:HD11	2:D:731:THR:HG21	1.74	0.69
1:B:521:THR:HG22	1:B:522:GLU:H	1.55	0.69
1:A:634:ASN:ND2	1:A:653:GLU:O	2.26	0.69
1:E:634:ASN:ND2	1:E:653:GLU:O	2.27	0.67
1:A:670:VAL:HG22	1:A:710:GLU:HG2	1.77	0.67
1:E:688:ILE:HG22	1:E:723:ILE:HD12	1.75	0.67
1:C:684:ILE:HD11	1:C:731:THR:HG21	1.77	0.66
1:G:677:ASP:HB2	1:G:700:PRO:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:NH2	1:A:444:LEU:O	2.29	0.66
1:B:584:THR:HG23	1:B:609:MET:HG2	1.77	0.66
1:C:330:SER:HB2	1:C:364:SER:HB2	1.77	0.65
1:G:634:ASN:ND2	1:G:653:GLU:O	2.30	0.65
1:A:667:LYS:NZ	1:A:740:GLU:OE1	2.31	0.63
2:D:691:LYS:HE2	2:D:714:THR:HG22	1.81	0.63
3:H:313:PHE:O	3:H:403:THR:OG1	2.17	0.63
2:D:670:VAL:HG22	2:D:710:GLU:HG2	1.81	0.63
1:G:658:ILE:HB	1:G:721:ILE:HB	1.82	0.62
1:F:678:PRO:O	1:F:702:GLN:NE2	2.32	0.62
3:H:216:ASP:HB3	3:H:219:LYS:HB2	1.81	0.62
3:H:56:ARG:NH1	3:H:215:ASP:OD2	2.33	0.61
1:G:324:SER:HB3	1:G:370:SER:HB2	1.81	0.61
3:H:35:GLU:HG2	3:H:79:ALA:HB2	1.82	0.61
1:C:641:ASP:O	1:C:646:SER:N	2.34	0.61
1:B:653:GLU:HG3	1:B:726:ILE:HG22	1.81	0.61
2:D:665:PRO:HG3	2:D:716:LYS:HB2	1.81	0.61
1:E:633:SER:HB3	1:E:655:LYS:HB2	1.83	0.61
1:E:658:ILE:HB	1:E:721:ILE:HB	1.83	0.61
1:F:622:PHE:HB2	1:F:646:SER:HB2	1.81	0.61
2:D:619:PHE:HD1	2:D:737:SER:HB3	1.65	0.61
1:E:394:ARG:NH2	1:E:444:LEU:O	2.27	0.61
1:C:394:ARG:NH2	1:C:444:LEU:O	2.24	0.60
1:F:668:ARG:NH2	1:F:742:ASN:O	2.34	0.60
1:A:641:ASP:O	1:A:646:SER:N	2.35	0.60
2:D:636:ASN:HD21	2:D:649:LYS:H	1.48	0.60
2:D:667:LYS:NZ	2:D:740:GLU:OE1	2.35	0.60
1:E:641:ASP:O	1:E:646:SER:N	2.35	0.60
3:H:248:ARG:HH12	3:H:376:ALA:HA	1.65	0.60
1:B:641:ASP:O	1:B:646:SER:N	2.35	0.59
2:D:283:LYS:HB2	1:E:509:GLN:HG3	1.85	0.59
1:B:667:LYS:NZ	1:B:740:GLU:OE1	2.35	0.59
3:H:370:SER:HA	3:H:376:ALA:HB3	1.84	0.59
1:F:318:ASP:HB3	1:F:376:ASN:HB2	1.85	0.58
1:F:698:LEU:HD12	1:F:700:PRO:HD3	1.85	0.58
1:F:667:LYS:HE3	1:F:740:GLU:HB3	1.86	0.58
3:H:388:LYS:HG3	3:H:412:ILE:HG13	1.84	0.58
1:B:324:SER:HB3	1:B:370:SER:HB2	1.86	0.58
1:E:684:ILE:HD11	1:E:731:THR:HG21	1.86	0.58
1:E:667:LYS:NZ	1:E:740:GLU:OE1	2.37	0.58
3:H:60:TYR:HB2	3:H:63:GLN:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:PHE:HB2	1:C:646:SER:HB2	1.87	0.57
1:E:619:PHE:HD1	1:E:737:SER:HB3	1.69	0.57
1:E:635:VAL:HG13	1:E:637:THR:HG23	1.87	0.57
1:E:637:THR:HG22	1:E:648:ASN:HB2	1.85	0.57
1:A:509:GLN:HG3	1:G:283:LYS:HB2	1.86	0.57
1:G:491[A]:ASN:HD21	1:G:495[A]:GLN:HB2	1.70	0.57
1:A:635:VAL:HG13	1:A:637:THR:HG23	1.86	0.56
1:F:619:PHE:HD1	1:F:737:SER:HB3	1.70	0.56
1:F:655:LYS:HD3	1:F:724:THR:HG22	1.86	0.56
1:E:318:ASP:HB2	1:E:376:ASN:HB2	1.88	0.56
3:H:243:VAL:HG22	3:H:278:ILE:HD13	1.87	0.56
1:G:684:ILE:HG23	1:G:727:GLY:HA3	1.87	0.56
1:F:639:ASN:ND2	1:F:641:ASP:OD2	2.39	0.56
1:C:655:LYS:HE2	1:C:657:LYS:HD3	1.87	0.56
1:C:635:VAL:HG13	1:C:637:THR:HG23	1.88	0.56
1:A:657:LYS:HD3	1:A:722:GLU:HB3	1.87	0.55
1:G:293:LEU:HD13	1:G:545:LEU:HD11	1.89	0.55
1:F:584:THR:HG23	1:F:609:MET:HG2	1.87	0.55
2:D:281:PHE:HE2	2:D:285:ILE:HB	1.70	0.55
1:F:692:GLU:HB3	1:F:694:LYS:NZ	2.22	0.55
1:G:649:LYS:HE3	1:G:731:THR:HG23	1.89	0.55
1:G:657:LYS:HG2	1:G:722:GLU:HG2	1.88	0.55
1:C:283:LYS:HB2	2:D:509:GLN:HG3	1.88	0.54
3:H:394:ILE:HG12	3:H:407:VAL:HG22	1.89	0.54
1:A:516:SER:OG	1:A:610:ASN:OD1	2.26	0.54
1:B:527:GLU:OE2	1:B:529:ARG:NH2	2.41	0.54
1:F:281:PHE:HE2	1:F:285:ILE:HB	1.71	0.54
1:G:656:ILE:HG22	1:G:723:ILE:HB	1.89	0.54
3:H:369:LEU:HD11	3:H:382:LEU:HG	1.89	0.54
1:F:633:SER:OG	1:F:655:LYS:N	2.39	0.54
1:G:281:PHE:HE2	1:G:285:ILE:HB	1.73	0.54
1:F:688:ILE:HG12	1:F:723:ILE:HG12	1.90	0.53
1:F:650:LEU:HD12	1:F:652:GLY:N	2.23	0.53
1:G:622:PHE:HB2	1:G:646:SER:HB2	1.89	0.53
1:A:619:PHE:HD1	1:A:737:SER:HB3	1.73	0.53
1:F:293:LEU:HD13	1:F:545:LEU:HD11	1.90	0.53
1:F:682:ASN:HD21	1:F:728:SER:H	1.56	0.53
1:F:595:LEU:O	1:F:598:LYS:NZ	2.41	0.53
1:B:685:ILE:HG12	1:B:697:TYR:CE1	2.43	0.53
1:F:653:GLU:HG3	1:F:726:ILE:HD13	1.90	0.53
1:G:653:GLU:OE1	1:G:727:GLY:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LYS:HB3	1:A:724:THR:OG1	2.08	0.52
1:F:689:LYS:HE3	1:F:722:GLU:HB2	1.91	0.52
1:G:634:ASN:HB2	1:G:654:THR:HG22	1.92	0.52
1:F:674:TYR:HB3	1:F:704:TYR:HB3	1.90	0.52
3:H:94:PHE:CZ	3:H:150:LYS:HG3	2.45	0.52
1:C:584:THR:HG23	1:C:609:MET:HG2	1.91	0.52
1:F:653:GLU:HG3	1:F:726:ILE:HA	1.91	0.52
1:G:687:LYS:HB2	1:G:724:THR:OG1	2.10	0.52
1:G:641:ASP:HB2	1:G:647:ALA:HB2	1.92	0.52
1:E:688:ILE:HD11	1:E:694:LYS:HB2	1.91	0.52
1:G:225:ASN:OD1	3:H:33:ARG:NH2	2.42	0.52
1:G:619:PHE:HD1	1:G:737:SER:HB3	1.75	0.51
2:D:318:ASP:HB2	2:D:376:ASN:HB2	1.91	0.51
1:E:330:SER:HB2	1:E:364:SER:HB2	1.92	0.51
1:E:687:LYS:HB2	1:E:724:THR:OG1	2.10	0.51
1:C:392:ASN:HB3	1:C:446:PRO:HB2	1.92	0.51
2:D:214:TRP:CG	3:H:116:LEU:HD13	2.46	0.51
1:G:665:PRO:HB3	1:G:716:LYS:HB2	1.92	0.51
1:A:394:ARG:HD3	1:A:440:PRO:HD2	1.93	0.51
1:G:330:SER:HB2	1:G:364:SER:HB3	1.93	0.51
1:A:663:LEU:HD12	1:A:721:ILE:HD12	1.92	0.51
2:D:669:TYR:CE2	2:D:740:GLU:HG2	2.46	0.51
1:C:521:THR:OG1	1:C:524:GLU:O	2.27	0.51
1:A:283:LYS:HB2	1:B:509:GLN:HG3	1.92	0.51
1:C:293:LEU:HD13	1:C:545:LEU:HD11	1.92	0.51
3:H:109:GLU:O	3:H:198:LYS:NZ	2.41	0.51
1:B:685:ILE:HG12	1:B:697:TYR:HE1	1.76	0.50
1:F:632:TRP:HE3	1:F:654:THR:HG22	1.76	0.50
1:G:670:VAL:HG22	1:G:710:GLU:HG2	1.93	0.50
1:A:218:ASP:OD1	1:A:218:ASP:N	2.42	0.50
1:A:231:GLU:OE1	1:A:259:SER:OG	2.26	0.50
1:C:619:PHE:HD1	1:C:737:SER:HB3	1.77	0.50
2:D:685:ILE:HG12	2:D:697:TYR:CD2	2.47	0.50
1:E:677:ASP:HB2	1:E:700:PRO:HB2	1.92	0.50
1:G:641:ASP:O	1:G:646:SER:N	2.35	0.50
2:D:580:PHE:HB3	2:D:584:THR:HB	1.93	0.50
1:E:293:LEU:HD13	1:E:545:LEU:HD11	1.93	0.50
1:F:324:SER:HB3	1:F:370:SER:HB2	1.93	0.50
1:F:580:PHE:HB3	1:F:584:THR:HB	1.94	0.50
1:B:580:PHE:HB3	1:B:584:THR:HB	1.94	0.50
1:G:630:SER:OG	1:G:631:THR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LYS:HB2	1:C:509:GLN:HG3	1.93	0.50
1:C:281:PHE:HE2	1:C:285:ILE:HB	1.75	0.50
1:G:658:ILE:N	1:G:721:ILE:O	2.37	0.50
3:H:32:GLU:HG2	3:H:35:GLU:OE1	2.12	0.50
1:C:648:ASN:O	1:C:648:ASN:ND2	2.42	0.49
2:D:281:PHE:CD2	2:D:285:ILE:HD12	2.47	0.49
1:F:630:SER:OG	1:F:631:THR:N	2.43	0.49
2:D:392:ASN:HB3	2:D:446:PRO:HB2	1.94	0.49
1:C:281:PHE:CD2	1:C:285:ILE:HD12	2.46	0.49
1:G:617:THR:O	1:G:627:ASN:ND2	2.44	0.49
1:G:665:PRO:HG3	1:G:716:LYS:HD3	1.94	0.49
1:C:217:GLU:N	1:C:229:SER:HG	2.10	0.49
1:F:572:ASP:OD2	1:F:574:SER:OG	2.30	0.49
3:H:356:LEU:HD23	3:H:358:ILE:HD11	1.95	0.49
2:D:622:PHE:HB2	2:D:646:SER:HB2	1.92	0.49
1:E:392:ASN:HB3	1:E:446:PRO:HB2	1.94	0.49
1:G:269:ASP:HB2	1:G:270:PRO:HD2	1.95	0.49
1:G:281:PHE:CD2	1:G:285:ILE:HD12	2.48	0.49
1:G:394:ARG:NH2	1:G:444:LEU:O	2.30	0.49
1:F:636:ASN:ND2	1:F:650:LEU:HB3	2.27	0.49
3:H:255:ASN:O	3:H:259:ILE:HG12	2.12	0.49
1:B:269:ASP:HB2	1:B:270:PRO:HD2	1.94	0.49
1:B:619:PHE:HD1	1:B:737:SER:HB3	1.78	0.49
1:F:715:GLU:HG2	1:F:717:ASP:H	1.77	0.49
3:H:52:TYR:OH	3:H:70:GLU:OE1	2.30	0.49
1:B:318:ASP:HB2	1:B:376:ASN:HB2	1.95	0.48
1:E:657:LYS:HD3	1:E:722:GLU:HB3	1.94	0.48
1:G:527:GLU:OE2	1:G:529:ARG:NH2	2.46	0.48
1:F:283:LYS:HB2	1:G:509:GLN:HG3	1.96	0.48
1:G:511:ASP:OD1	1:G:529:ARG:NH1	2.46	0.48
3:H:136:PHE:HB3	3:H:178:LEU:HD11	1.94	0.48
1:C:665:PRO:HG3	1:C:716:LYS:HB2	1.94	0.48
1:G:493[B]:SER:OG	1:G:495[B]:GLN:NE2	2.46	0.48
1:C:318:ASP:HB2	1:C:376:ASN:HB2	1.95	0.48
1:F:269:ASP:HB2	1:F:270:PRO:HD2	1.96	0.48
1:B:634:ASN:HB2	1:B:654:THR:HG22	1.95	0.48
1:E:665:PRO:HG3	1:E:716:LYS:HB2	1.95	0.48
1:F:616:PRO:HA	1:F:739:THR:HG22	1.95	0.48
1:F:492:SER:OG	3:H:32:GLU:HB3	2.14	0.48
3:H:225:LYS:NZ	3:H:370:SER:O	2.30	0.48
1:E:276:LYS:HA	1:E:281:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:516:SER:OG	2:D:610:ASN:OD1	2.32	0.48
1:G:718:SER:OG	1:G:719:SER:N	2.47	0.48
1:B:660:MET:HE1	1:B:714:THR:H	1.79	0.48
1:C:392:ASN:HD21	2:D:418:THR:H	1.61	0.48
2:D:685:ILE:HG12	2:D:697:TYR:HD2	1.79	0.48
1:A:276:LYS:HA	1:A:281:PHE:CE1	2.49	0.47
1:E:218:ASP:N	1:E:218:ASP:OD1	2.45	0.47
1:A:269:ASP:HB2	1:A:270:PRO:HD2	1.96	0.47
1:E:642:GLY:HA2	1:E:704:TYR:OH	2.15	0.47
1:G:580:PHE:HE1	1:G:611:ILE:HG12	1.79	0.47
3:H:33:ARG:O	3:H:36:LYS:HB2	2.14	0.47
1:F:622:PHE:HB3	1:F:637:THR:HG21	1.96	0.47
1:G:387:ALA:HB3	1:G:462:ILE:HD11	1.97	0.47
2:D:269:ASP:HB2	2:D:270:PRO:HD2	1.97	0.47
2:D:330:SER:HB2	2:D:364:SER:HB2	1.96	0.47
1:C:491:ASN:OD1	1:C:493:SER:OG	2.24	0.47
2:D:293:LEU:HD13	2:D:545:LEU:HD11	1.96	0.47
1:E:580:PHE:HB3	1:E:584:THR:HB	1.96	0.47
1:F:326:ALA:HB3	1:F:368:GLN:HB3	1.96	0.47
1:F:660:MET:SD	1:F:721:ILE:HD11	2.54	0.47
1:E:281:PHE:CD2	1:E:285:ILE:HD12	2.50	0.47
2:D:304:MET:HB2	2:D:478:LEU:HD13	1.97	0.47
2:D:642:GLY:HA2	2:D:704:TYR:CE2	2.50	0.47
1:F:670:VAL:HG22	1:F:710:GLU:HG2	1.96	0.47
1:E:269:ASP:HB2	1:E:270:PRO:HD2	1.97	0.46
1:F:281:PHE:CE2	1:F:285:ILE:HB	2.50	0.46
1:G:639:ASN:ND2	1:G:641:ASP:OD2	2.48	0.46
2:D:281:PHE:CE2	2:D:285:ILE:HB	2.50	0.46
3:H:23:GLU:HG3	3:H:26:ARG:HH21	1.80	0.46
1:E:653:GLU:HG3	1:E:726:ILE:HG22	1.96	0.46
1:A:448:ALA:H	1:B:421:THR:HG23	1.80	0.46
1:A:642:GLY:HA2	1:A:704:TYR:OH	2.16	0.46
2:D:641:ASP:O	2:D:646:SER:N	2.48	0.46
1:F:692:GLU:HB3	1:F:694:LYS:HZ1	1.80	0.46
1:A:688:ILE:HG21	1:A:711:PHE:HB3	1.98	0.46
1:E:660:MET:HE2	1:E:716:LYS:H	1.79	0.46
1:C:281:PHE:CE2	1:C:285:ILE:HB	2.51	0.46
1:B:639:ASN:HD21	1:B:647:ALA:HB3	1.81	0.46
1:C:669:TYR:CE2	1:C:740:GLU:HG2	2.51	0.45
2:D:470:LEU:HD21	2:D:476:ILE:HG13	1.99	0.45
1:A:276:LYS:HA	1:A:281:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASN:HB3	1:A:446:PRO:HB2	1.98	0.45
1:B:448:ALA:H	1:C:421:THR:HG23	1.79	0.45
1:F:677:ASP:HB2	1:F:700:PRO:HG2	1.99	0.45
1:C:218:ASP:N	1:C:218:ASP:OD1	2.48	0.45
1:F:623:ASP:OD1	1:F:646:SER:HB3	2.16	0.45
1:A:421:THR:HG23	1:G:448:ALA:H	1.82	0.45
1:A:521:THR:OG1	1:A:524:GLU:O	2.33	0.45
1:E:655:LYS:HD2	1:E:724:THR:HG22	1.98	0.45
1:E:276:LYS:NZ	1:E:294:VAL:O	2.31	0.45
1:F:639:ASN:HD21	1:F:647:ALA:HB2	1.82	0.45
2:D:633:SER:OG	2:D:655:LYS:N	2.49	0.45
1:E:448:ALA:H	1:F:421:THR:HG23	1.82	0.45
1:F:281:PHE:CD2	1:F:285:ILE:HD12	2.52	0.45
1:A:622:PHE:HB3	1:A:637:THR:HG21	1.99	0.44
1:C:448:ALA:H	2:D:421:THR:HG23	1.82	0.44
1:A:494[B]:GLY:HA3	1:B:265:ASN:ND2	2.31	0.44
1:B:392:ASN:HB3	1:B:446:PRO:HB2	1.99	0.44
1:B:521:THR:HG22	1:B:522:GLU:N	2.29	0.44
1:C:269:ASP:HB2	1:C:270:PRO:HD2	1.98	0.44
1:G:392:ASN:HB3	1:G:446:PRO:HB2	1.99	0.44
1:B:448:ALA:H	1:C:421:THR:CG2	2.31	0.44
1:B:676:LYS:HB2	1:B:704:TYR:HD1	1.82	0.44
2:D:707:PHE:HB2	2:D:709:TYR:CZ	2.53	0.44
1:G:276:LYS:HA	1:G:281:PHE:CE1	2.53	0.44
2:D:682:ASN:N	2:D:682:ASN:OD1	2.51	0.44
3:H:33:ARG:O	3:H:36:LYS:N	2.49	0.44
3:H:87:LYS:HB2	3:H:87:LYS:HE2	1.81	0.44
1:A:281:PHE:HZ	1:A:290:ARG:HG3	1.82	0.44
1:B:281:PHE:CD2	1:B:285:ILE:HD12	2.53	0.44
1:E:521:THR:OG1	1:E:524:GLU:O	2.35	0.44
1:B:688:ILE:HG21	1:B:711:PHE:HB3	1.99	0.44
2:D:387:ALA:HB3	2:D:462:ILE:HD11	2.00	0.44
1:F:707:PHE:HB2	1:F:709:TYR:CZ	2.53	0.44
3:H:268:ASN:HD21	3:H:271:LEU:HD12	1.83	0.44
1:A:281:PHE:CE2	1:A:285:ILE:HB	2.53	0.44
1:B:623:ASP:OD1	1:B:646:SER:OG	2.36	0.44
1:E:669:TYR:CE2	1:E:740:GLU:HG2	2.52	0.44
3:H:63:GLN:O	3:H:67:ASN:N	2.51	0.43
3:H:257:TYR:CE1	3:H:262:GLY:HA3	2.53	0.43
1:B:281:PHE:CE2	1:B:285:ILE:HB	2.53	0.43
1:C:578:LEU:HD23	1:C:580:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:673:GLY:O	2:D:706:LYS:HA	2.18	0.43
1:E:276:LYS:HA	1:E:281:PHE:HE1	1.82	0.43
1:A:281:PHE:CD2	1:A:285:ILE:HD12	2.53	0.43
1:C:276:LYS:HA	1:C:281:PHE:CE1	2.53	0.43
1:E:659:PRO:O	1:E:661:SER:N	2.52	0.43
1:A:718:SER:OG	1:A:719:SER:N	2.52	0.43
1:B:657:LYS:HG2	1:B:722:GLU:HG2	1.99	0.43
2:D:214:TRP:CZ3	3:H:192:ARG:HD3	2.53	0.43
1:E:689:LYS:HD3	1:E:722:GLU:OE2	2.18	0.43
1:F:311:THR:HG22	1:F:313:GLU:HG3	2.00	0.43
1:A:674:TYR:HB3	1:A:704:TYR:CD1	2.53	0.43
3:H:234:LYS:O	3:H:284:ARG:NH1	2.51	0.43
1:E:231:GLU:OE1	1:E:259:SER:OG	2.24	0.43
1:B:690:ALA:HA	1:B:721:ILE:HG12	2.00	0.43
1:C:491:ASN:HB3	1:C:495:GLN:HB2	2.00	0.43
1:C:660:MET:HE1	1:C:713:THR:HB	2.01	0.43
1:F:230:TYR:HB3	1:F:235:TYR:HB3	2.01	0.43
1:A:665:PRO:HG3	1:A:716:LYS:HB2	2.01	0.42
1:F:387:ALA:HB3	1:F:462:ILE:HD11	2.02	0.42
1:G:653:GLU:CD	1:G:727:GLY:H	2.21	0.42
1:B:281:PHE:HE2	1:B:285:ILE:HB	1.83	0.42
2:D:448:ALA:H	1:E:421:THR:HG23	1.84	0.42
1:A:669:TYR:CE2	1:A:740:GLU:HG2	2.54	0.42
1:B:470:LEU:HD21	1:B:476:ILE:HG13	2.00	0.42
1:C:642:GLY:HA2	1:C:704:TYR:OH	2.20	0.42
1:C:667:LYS:NZ	1:C:740:GLU:OE1	2.52	0.42
3:H:369:LEU:HD21	3:H:382:LEU:HD12	2.00	0.42
1:C:653:GLU:HG3	1:C:726:ILE:HG22	2.02	0.42
1:F:687:LYS:HB2	1:F:724:THR:OG1	2.20	0.42
1:A:387:ALA:HB3	1:A:462:ILE:HD11	2.01	0.42
1:E:283:LYS:HA	1:E:283:LYS:HD3	1.91	0.42
1:C:283:LYS:HA	1:C:283:LYS:HD3	1.88	0.42
1:F:657:LYS:HD3	1:F:722:GLU:OE1	2.20	0.42
1:F:718:SER:OG	1:F:719:SER:N	2.52	0.42
1:G:281:PHE:CE2	1:G:285:ILE:HB	2.52	0.42
1:A:653:GLU:HG3	1:A:726:ILE:HG22	2.01	0.42
1:E:572:ASP:O	1:E:576:VAL:HG22	2.20	0.42
1:B:293:LEU:HD21	1:B:543:PRO:HD2	2.01	0.42
1:B:676:LYS:HB2	1:B:704:TYR:CD1	2.55	0.42
1:C:630:SER:OG	1:C:631:THR:N	2.53	0.42
1:A:673:GLY:O	1:A:706:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:PRO:HB3	2:D:483:VAL:HG22	2.01	0.41
1:F:572:ASP:O	1:F:576:VAL:HG22	2.20	0.41
1:G:592:LEU:HD23	1:G:592:LEU:HA	1.94	0.41
1:B:660:MET:HE2	1:B:716:LYS:H	1.85	0.41
1:B:685:ILE:HB	1:B:726:ILE:HG13	2.02	0.41
1:E:674:TYR:HB3	1:E:704:TYR:CD1	2.56	0.41
1:F:694:LYS:HA	1:F:694:LYS:HD3	1.89	0.41
1:B:276:LYS:HA	1:B:281:PHE:CE1	2.55	0.41
1:B:643:LEU:N	1:B:734:ASP:OD2	2.53	0.41
1:C:325:ARG:NH1	1:C:369:ASP:OD1	2.53	0.41
1:G:639:ASN:OD1	1:G:639:ASN:N	2.53	0.41
3:H:368:TYR:CZ	3:H:370:SER:HB3	2.56	0.41
1:B:641:ASP:HB3	1:B:647:ALA:HB2	2.02	0.41
1:B:655:LYS:NZ	1:B:722:GLU:OE1	2.49	0.41
1:E:387:ALA:HB3	1:E:462:ILE:HD11	2.01	0.41
1:F:684:ILE:HG23	1:F:727:GLY:HA3	2.01	0.41
2:D:214:TRP:N	2:D:219:LEU:HD11	2.34	0.41
3:H:221:ASP:O	3:H:225:LYS:HG2	2.20	0.41
1:C:654:THR:OG1	1:C:725:LEU:HB2	2.20	0.41
1:E:685:ILE:HG12	1:E:697:TYR:CE2	2.56	0.41
3:H:115:SER:OG	3:H:117:GLU:OE1	2.38	0.41
1:A:578:LEU:HD23	1:A:580:PHE:HZ	1.86	0.41
1:B:731:THR:OG1	1:B:732:TYR:N	2.53	0.41
1:C:686:VAL:HG22	1:C:725:LEU:HD13	2.02	0.41
2:D:714:THR:OG1	2:D:715:GLU:N	2.54	0.41
1:F:636:ASN:HD21	1:F:650:LEU:HB3	1.85	0.41
1:F:677:ASP:N	1:F:700:PRO:HB2	2.35	0.41
3:H:99:LYS:HE2	3:H:133:GLN:HG3	2.03	0.41
3:H:173:ASN:OD1	3:H:173:ASN:N	2.54	0.41
2:D:276:LYS:HA	2:D:281:PHE:CE1	2.55	0.41
1:F:561:ASP:OD1	1:F:561:ASP:N	2.51	0.41
1:F:684:ILE:HD12	1:F:698:LEU:HD11	2.02	0.41
1:G:470:LEU:HD23	1:G:470:LEU:HA	1.90	0.41
1:A:418:THR:H	1:G:392:ASN:HD21	1.69	0.40
1:C:595:LEU:HD12	1:C:595:LEU:HA	1.96	0.40
1:E:448:ALA:H	1:F:421:THR:CG2	2.35	0.40
1:F:624:ASP:OD1	1:F:624:ASP:N	2.53	0.40
1:F:685:ILE:HG22	1:F:687:LYS:HE3	2.03	0.40
3:H:27:ILE:HG21	3:H:168:PRO:HG2	2.02	0.40
1:A:397:ASN:HB2	1:A:433:LEU:HG	2.03	0.40
1:G:636:ASN:OD1	1:G:649:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:HA	1:A:283:LYS:HD3	1.90	0.40
1:B:647:ALA:HB1	1:B:732:TYR:HD1	1.85	0.40
1:C:623:ASP:OD1	1:C:646:SER:HB3	2.20	0.40
1:G:490[B]:LYS:HD3	1:G:494[B]:GLY:HA2	2.04	0.40
1:A:635:VAL:HA	1:A:648:ASN:OD1	2.21	0.40
1:C:706:LYS:HB2	1:C:706:LYS:HE3	1.88	0.40
1:C:718:SER:OG	1:C:719:SER:N	2.53	0.40
1:F:632:TRP:CE3	1:F:656:ILE:HB	2.56	0.40
1:G:688:ILE:HG21	1:G:711:PHE:HB3	2.03	0.40
3:H:268:ASN:OD1	3:H:268:ASN:N	2.54	0.40
1:A:633:SER:HB3	1:A:655:LYS:HB3	2.03	0.40
1:B:293:LEU:HD13	1:B:545:LEU:HD11	2.04	0.40
1:B:642:GLY:HA3	1:B:646:SER:O	2.21	0.40
2:D:324:SER:OG	2:D:325:ARG:N	2.54	0.40
1:F:392:ASN:HB3	1:F:446:PRO:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/494 (101%)	474 (95%)	27 (5%)	0	100	100
1	B	500/494 (101%)	477 (95%)	23 (5%)	0	100	100
1	C	490/494 (99%)	464 (95%)	26 (5%)	0	100	100
1	E	501/494 (101%)	475 (95%)	26 (5%)	0	100	100
1	F	490/494 (99%)	466 (95%)	24 (5%)	0	100	100
1	G	500/494 (101%)	479 (96%)	21 (4%)	0	100	100
2	D	504/497 (101%)	479 (95%)	25 (5%)	0	100	100
3	H	393/395 (100%)	381 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3879/3856 (101%)	3695 (95%)	184 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/438 (102%)	447 (100%)	0	100	100
1	B	446/438 (102%)	446 (100%)	0	100	100
1	C	438/438 (100%)	437 (100%)	1 (0%)	93	93
1	E	447/438 (102%)	447 (100%)	0	100	100
1	F	438/438 (100%)	437 (100%)	1 (0%)	93	93
1	G	446/438 (102%)	444 (100%)	2 (0%)	91	91
2	D	450/441 (102%)	450 (100%)	0	100	100
3	H	355/355 (100%)	354 (100%)	1 (0%)	92	92
All	All	3467/3424 (101%)	3462 (100%)	5 (0%)	93	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	648	ASN
1	F	668	ARG
1	G	493[A]	SER
1	G	493[B]	SER
3	H	351	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	634	ASN
1	E	634	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 21 ligands modelled in this entry, 21 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	C	1
1	B	1
2	D	1
1	A	1
1	F	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	331:LYS	C	364:SER	N	6.54
1	C	331:LYS	C	364:SER	N	6.49
1	B	331:LYS	C	364:SER	N	6.41
1	D	331:LYS	C	364:SER	N	6.37
1	A	331:LYS	C	364:SER	N	6.33
1	F	331:LYS	C	364:SER	N	6.14
1	E	331:LYS	C	364:SER	N	5.91

PRELIMINARY VALIDATION REPORT

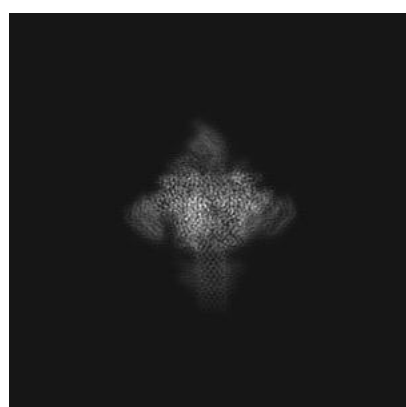
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D_1300024911. These allow visual inspection of the internal detail of the map and identification of artifacts.

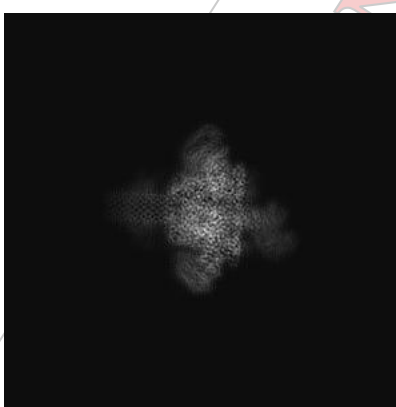
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

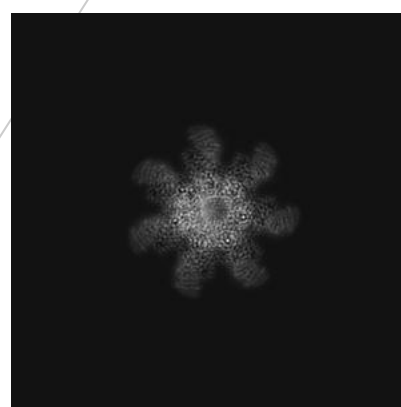
6.1.1 Primary map



X



Y

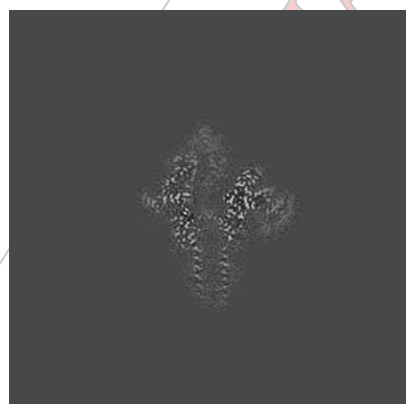


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 216



Y Index: 216

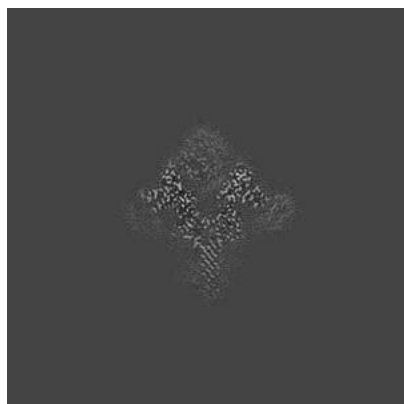


Z Index: 216

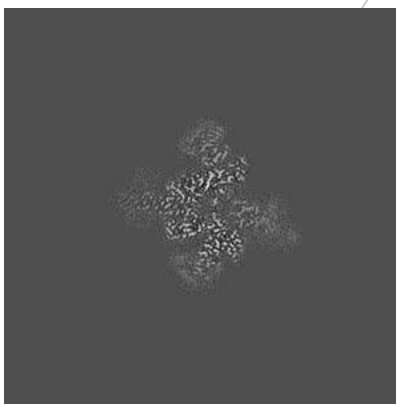
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

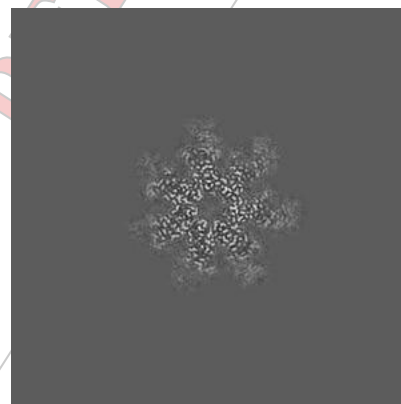
6.3.1 Primary map



X Index: 205



Y Index: 201



Z Index: 227

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 0.0156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation [i](#)

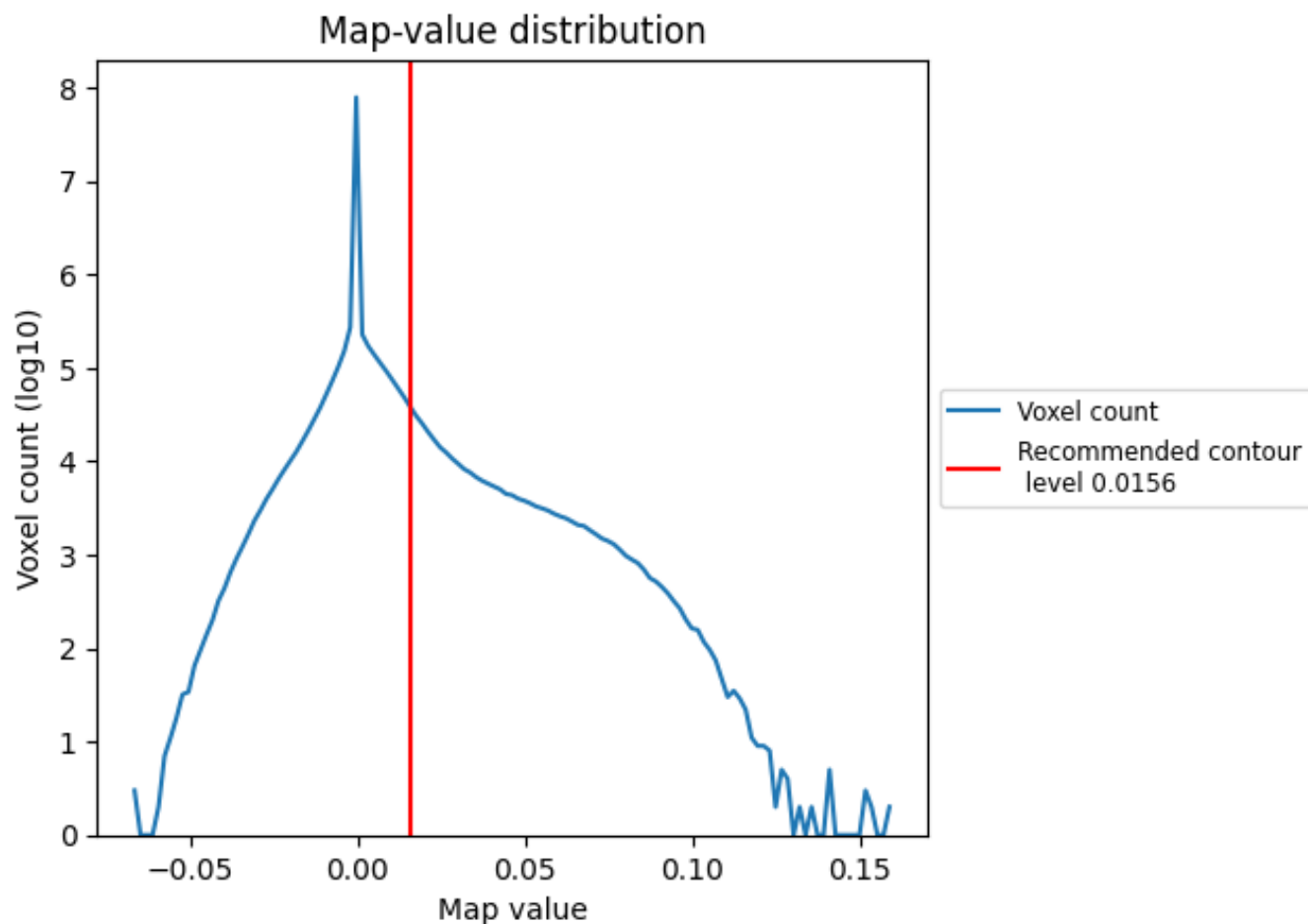
This section was not generated. No masks/segmentation were deposited.

PRELIMINARY VALIDATION REPORT

7 Map analysis [i](#)

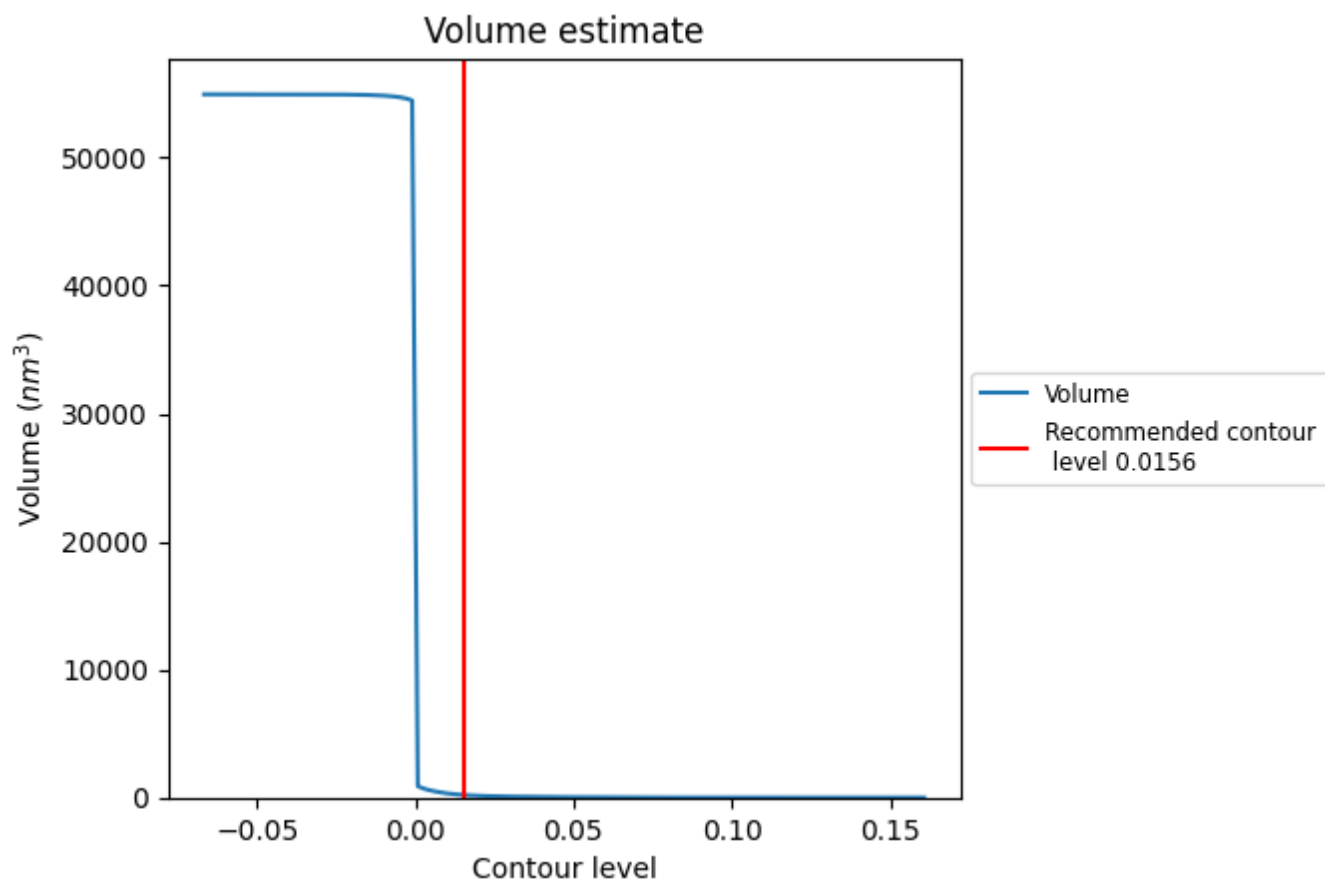
This section contains the results of statistical analysis of the map.

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.

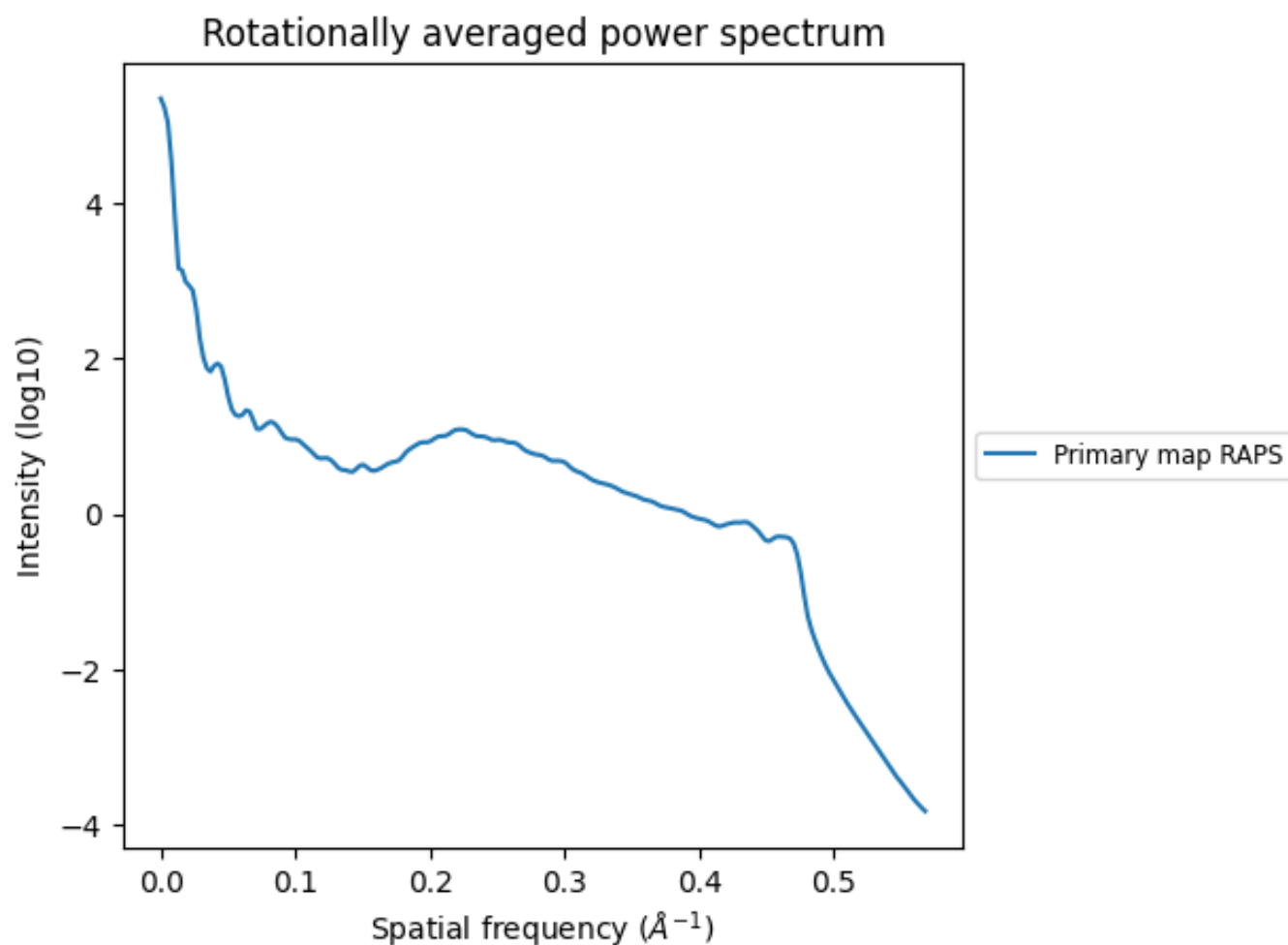
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm^3 ; this corresponds to an approximate mass of 177 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 ⓘ

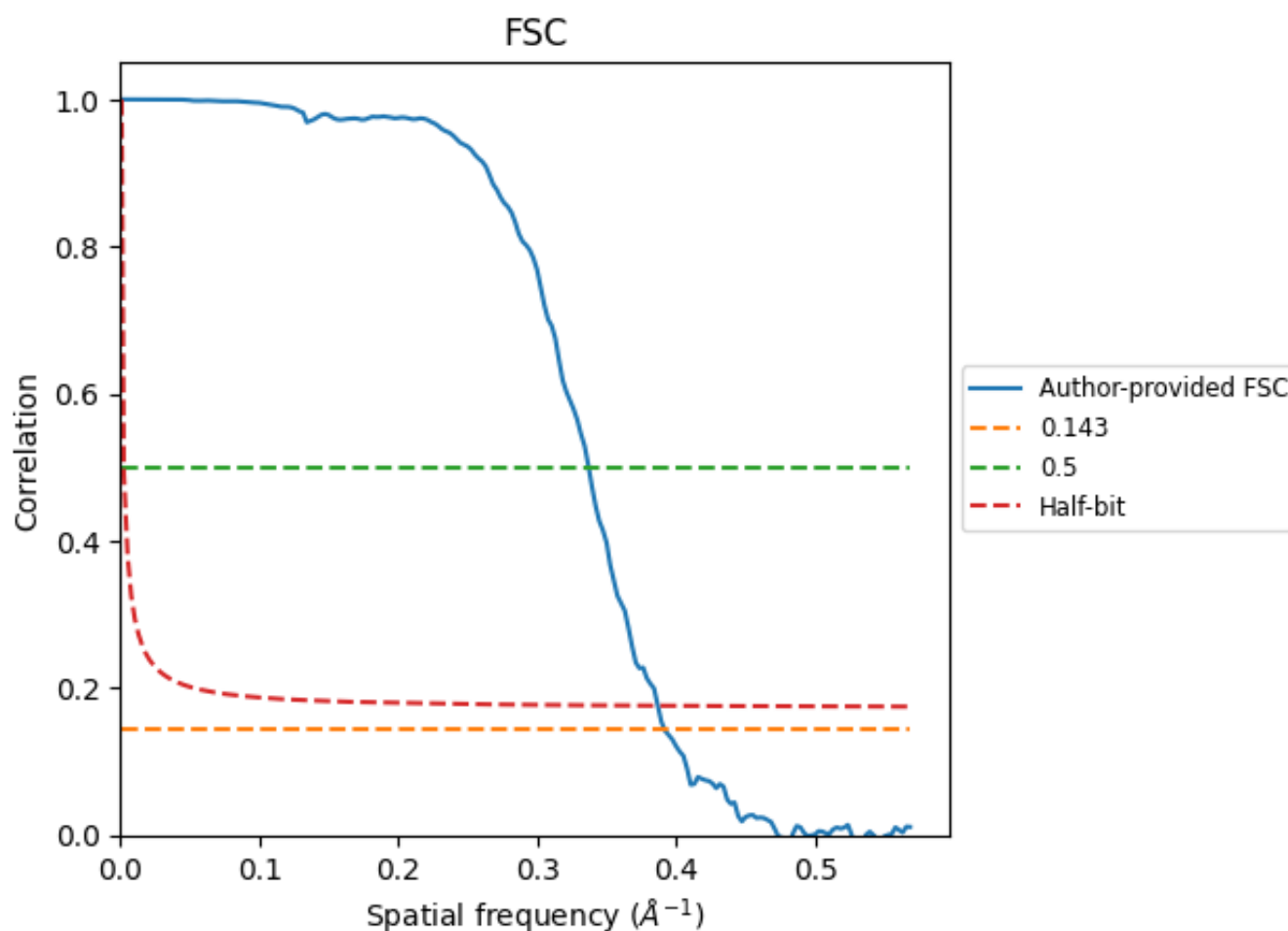


PRELIMINARY

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](#)



8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.55	2.97	2.59
Unmasked-calculated*	-	-	-

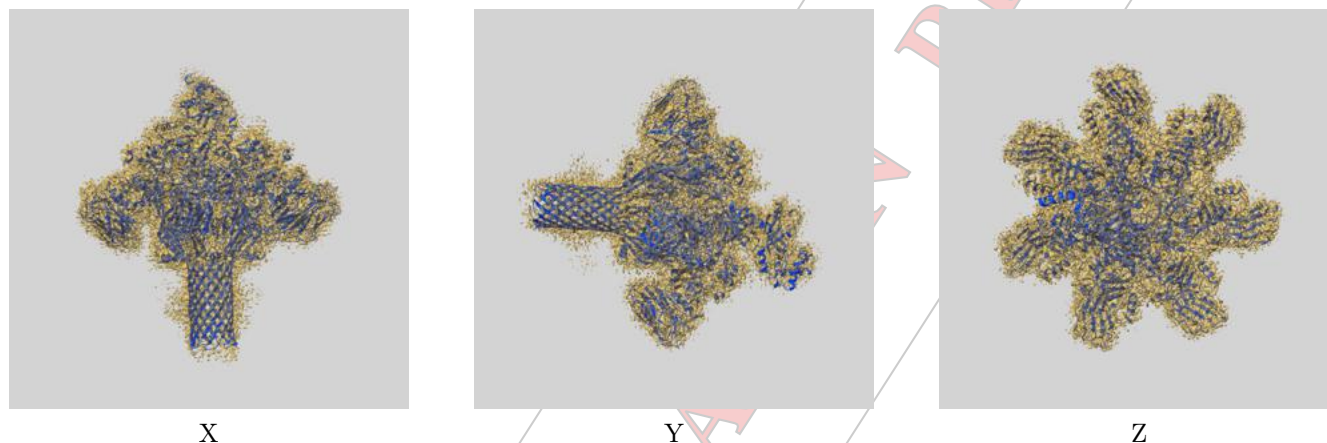
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

PRELIMINARY VALIDATION REPORT

9 Map-model fit ⓘ

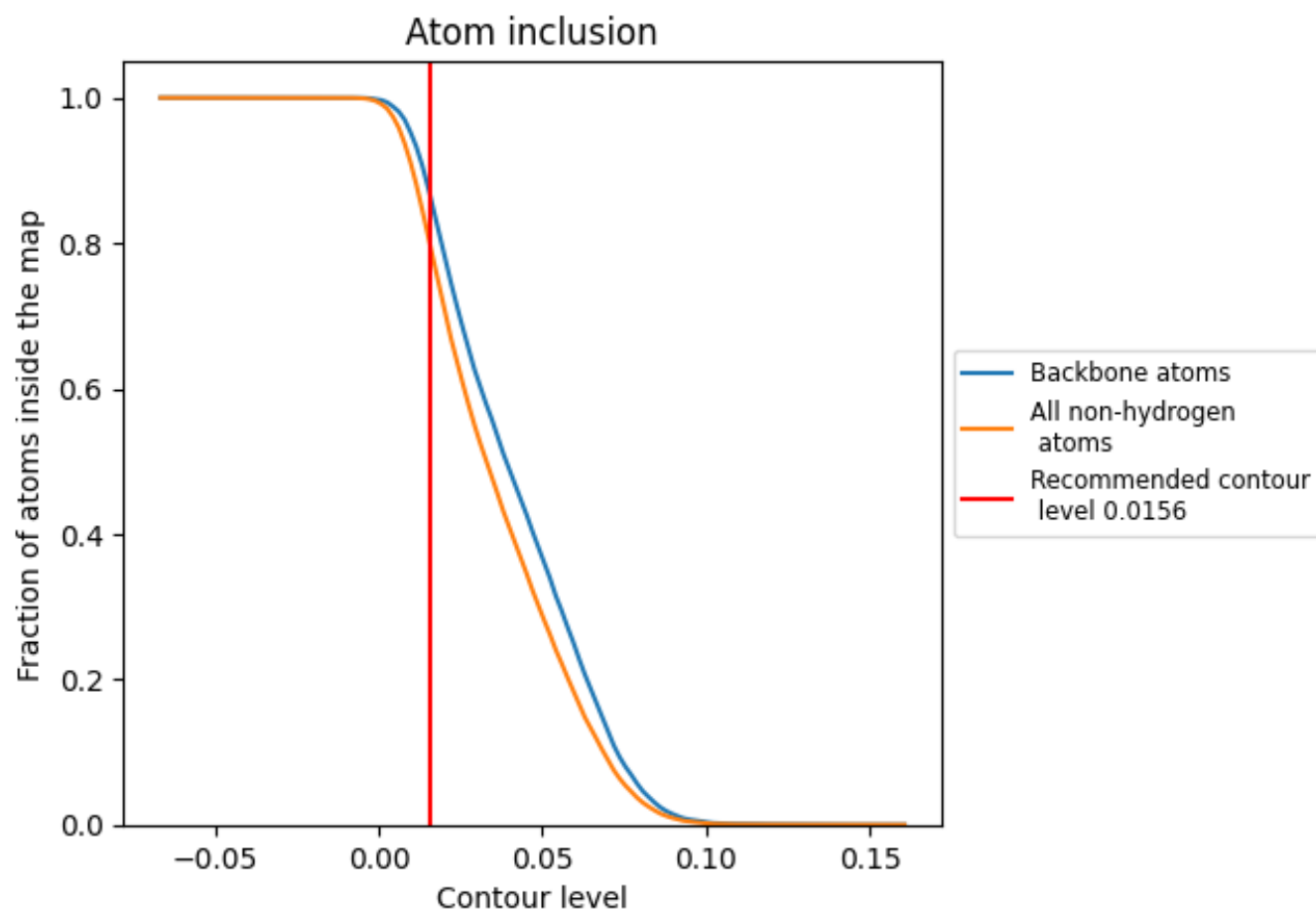
This section contains information regarding the fit between EMDB map D_1300024911 and PDB model D_1300024911. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ



The images above show the 3D surface view of the map at the recommended contour level 0.0156 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 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

PRELIMINARY



Preliminary Full wwPDB EM Validation Report ⓘ

Oct 11, 2021 – 04:33 PM JST

Deposition ID : D_1300025005

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

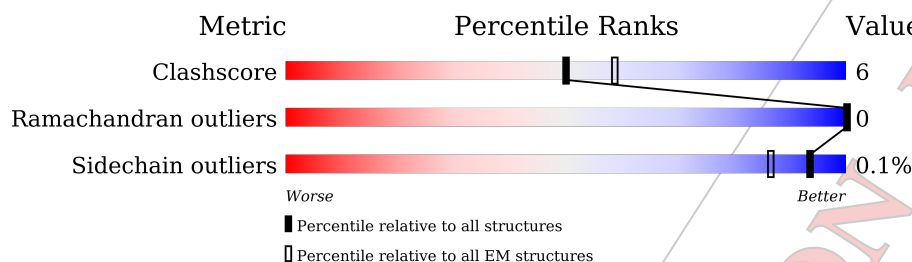
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

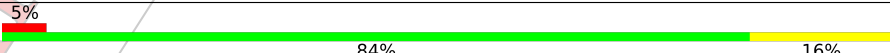
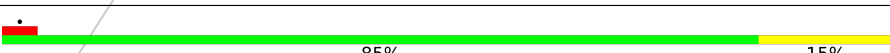
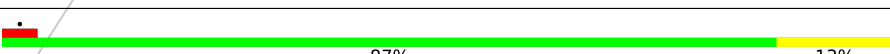
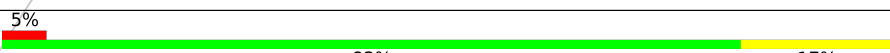
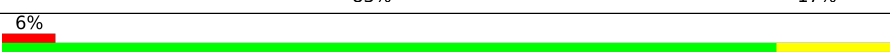
The reported resolution of this entry is unknown.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	638	
1	B	638	
1	C	638	
1	E	638	
1	F	638	
1	G	638	
2	D	641	
3	H	394	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 38842 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	638	Total	C	N	O	S	11	0
			5110	3198	831	1071	10		
1	B	638	Total	C	N	O	S	10	0
			5103	3194	830	1069	10		
1	C	638	Total	C	N	O	S	0	0
			5035	3154	817	1054	10		
1	E	638	Total	C	N	O	S	11	0
			5110	3198	831	1071	10		
1	F	638	Total	C	N	O	S	0	0
			5035	3154	817	1054	10		
1	G	638	Total	C	N	O	S	18	0
			5102	3194	829	1069	10		

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	641	Total	C	N	O	S	11	0
			5140	3218	834	1078	10		

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	394	Total	C	N	O	S	0	0
			3186	2027	532	622	5		

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

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			3	3	
4	A	1	Total	Ca	0
			3	3	

Continued on next page...

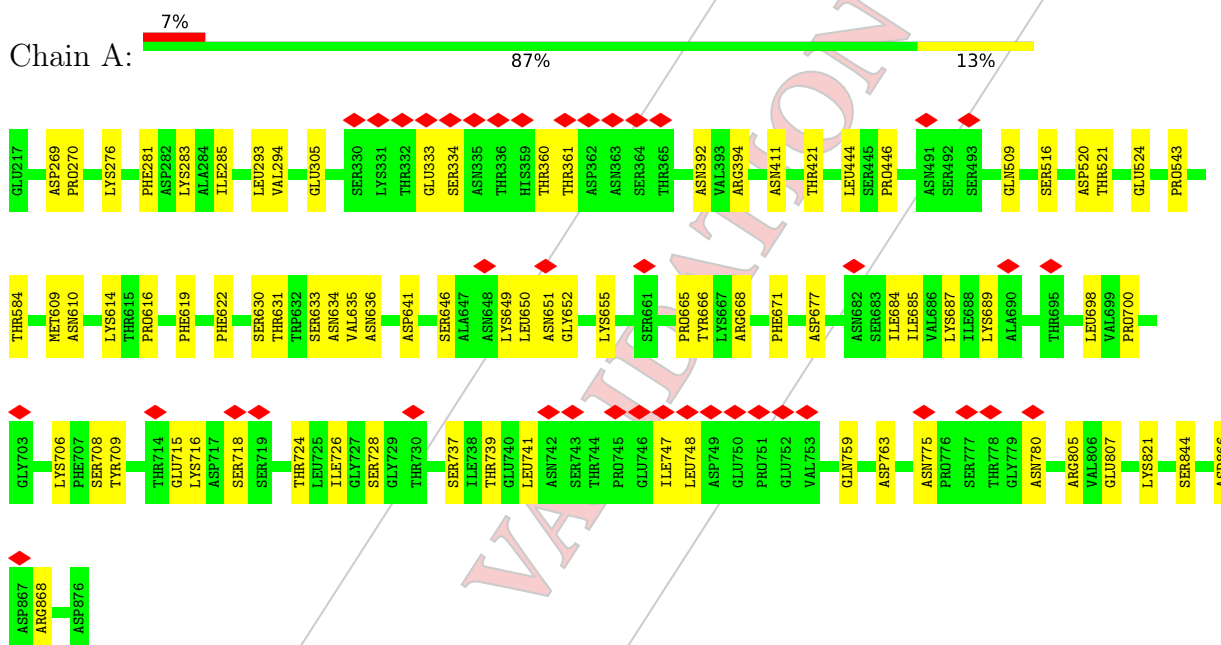
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 3	Ca 3	0
4	B	1	Total 3	Ca 3	0
4	B	1	Total 3	Ca 3	0
4	B	1	Total 3	Ca 3	0
4	C	1	Total 3	Ca 3	0
4	C	1	Total 3	Ca 3	0
4	C	1	Total 3	Ca 3	0
4	D	1	Total 3	Ca 3	0
4	D	1	Total 3	Ca 3	0
4	D	1	Total 3	Ca 3	0
4	E	1	Total 3	Ca 3	0
4	E	1	Total 3	Ca 3	0
4	E	1	Total 3	Ca 3	0
4	F	1	Total 3	Ca 3	0
4	F	1	Total 3	Ca 3	0
4	F	1	Total 3	Ca 3	0
4	G	1	Total 3	Ca 3	0
4	G	1	Total 3	Ca 3	0
4	G	1	Total 3	Ca 3	0

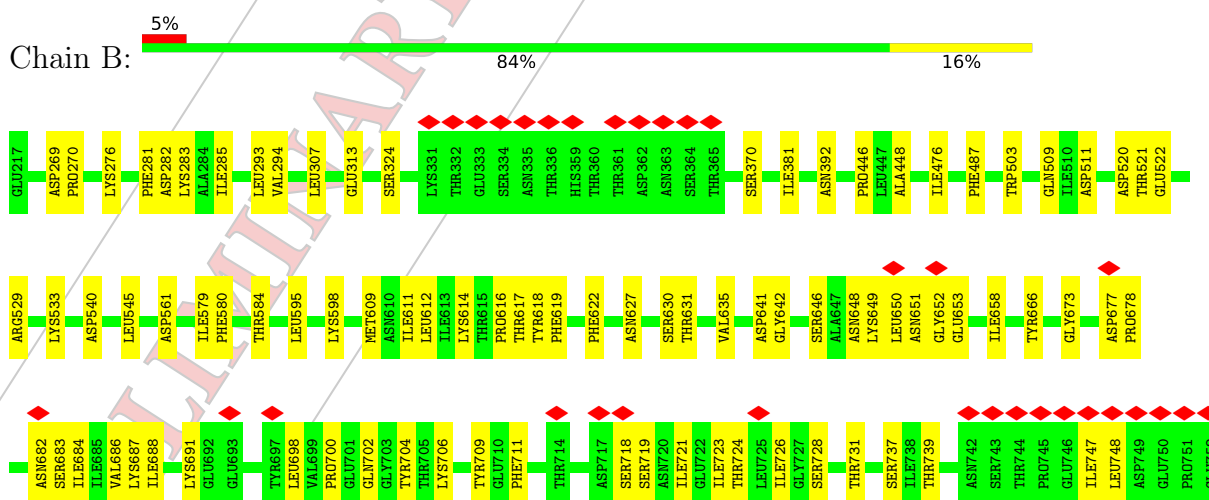
3 Residue-property plots

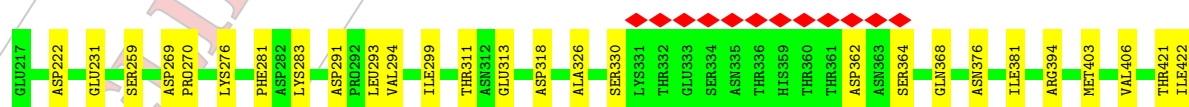
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

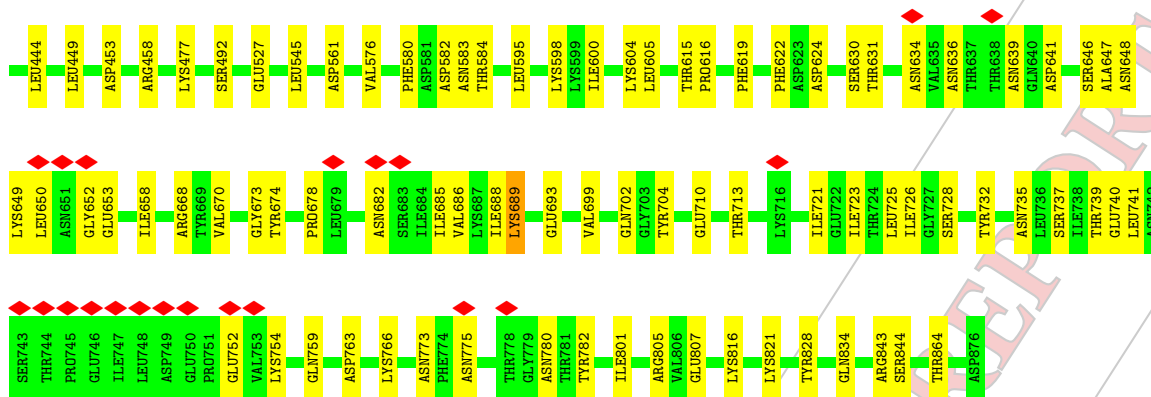
• Molecule 1:



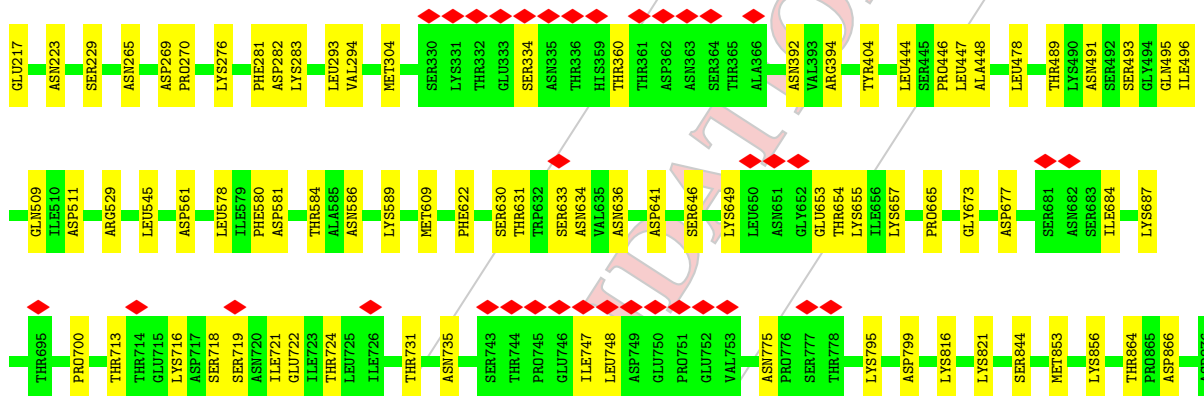
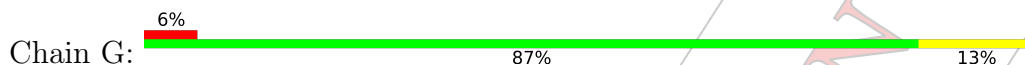
• Molecule 1:



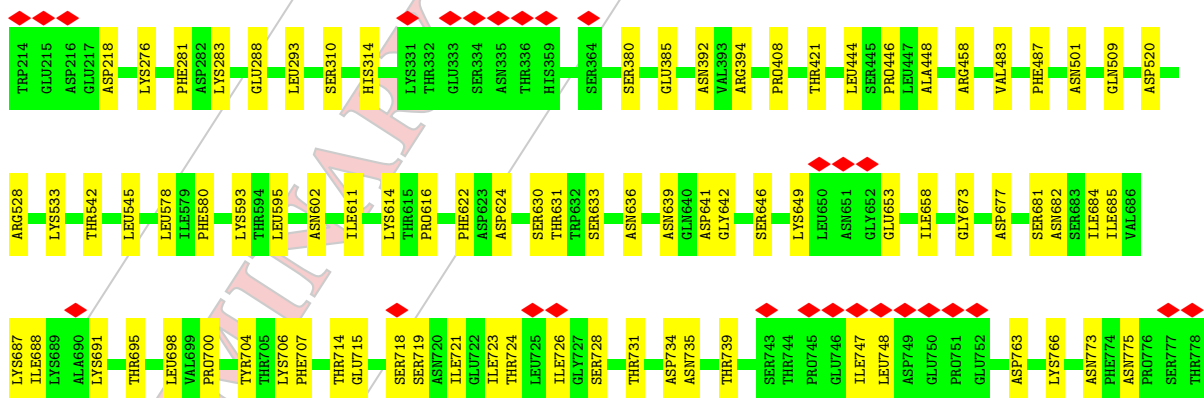
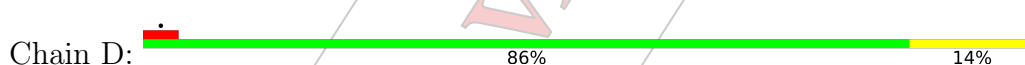




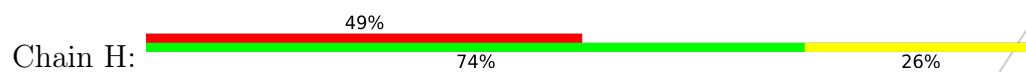
- Molecule 1:



- Molecule 2:



- Molecule 3:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	0.120	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0154	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/5202	0.47	0/7056
1	B	0.27	0/5195	0.47	0/7046
1	C	0.27	0/5127	0.47	0/6955
1	E	0.27	0/5202	0.47	0/7056
1	F	0.27	0/5127	0.47	0/6955
1	G	0.27	0/5193	0.47	0/7041
2	D	0.27	0/5233	0.48	0/7097
3	H	0.25	0/3253	0.47	0/4391
All	All	0.27	0/39532	0.47	0/53597

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5110	0	4966	53	0
1	B	5103	0	4959	66	0
1	C	5035	0	4890	61	0
1	E	5110	0	4966	58	0
1	F	5035	0	4890	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	5102	0	4955	51	0
2	D	5140	0	4984	63	0
3	H	3186	0	3169	60	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
All	All	38842	0	37779	459	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:GLU:N	1:G:229:SER:HG	1.68	0.91
1:B:521:THR:HG22	1:B:522:GLU:H	1.43	0.84
1:G:677:ASP:HB2	1:G:700:PRO:HB2	1.63	0.80
1:F:775:ASN:OD1	1:F:780:ASN:ND2	2.17	0.77
1:E:775:ASN:O	1:E:780:ASN:ND2	2.19	0.75
2:D:775:ASN:O	2:D:780:ASN:ND2	2.19	0.75
1:F:330:SER:HB2	1:F:364:SER:HB2	1.67	0.75
1:C:225:ASN:ND2	3:H:196:ASP:O	2.21	0.74
1:A:684:ILE:HB	1:A:698:LEU:HB3	1.71	0.73
2:D:276:LYS:HA	2:D:281:PHE:HE2	1.55	0.72
2:D:677:ASP:HB2	2:D:700:PRO:HB2	1.70	0.72
1:E:635:VAL:HG13	1:E:648:ASN:HD21	1.55	0.71
1:E:394:ARG:NH2	1:E:444:LEU:O	2.22	0.71
1:E:716:LYS:NZ	1:F:752:GLU:OE2	2.23	0.71
3:H:128:ASN:HA	3:H:186:LYS:HE2	1.74	0.70
3:H:216:ASP:HB3	3:H:219:LYS:HB2	1.74	0.69
1:F:394:ARG:NH2	1:F:444:LEU:O	2.23	0.69
1:C:775:ASN:O	1:C:780:ASN:ND2	2.25	0.68
1:B:650:LEU:HG	1:B:652:GLY:H	1.57	0.68
3:H:251:TYR:O	3:H:255:ASN:ND2	2.27	0.68
1:E:334:SER:HB3	1:E:360:THR:HB	1.74	0.68
1:C:667:LYS:NZ	1:C:740:GLU:OE1	2.27	0.67
2:D:394:ARG:NH2	2:D:444:LEU:O	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:PHE:HB2	1:B:646:SER:HB2	1.77	0.67
1:G:276:LYS:HA	1:G:281:PHE:HE2	1.60	0.66
1:C:688:ILE:HD12	1:C:711:PHE:HB3	1.76	0.66
1:E:685:ILE:HB	1:E:726:ILE:HG13	1.78	0.66
1:G:622:PHE:HB2	1:G:646:SER:HB2	1.77	0.66
1:F:650:LEU:HD12	1:F:652:GLY:H	1.61	0.66
1:A:715:GLU:HG3	1:A:718:SER:HB3	1.78	0.66
1:F:641:ASP:O	1:F:646:SER:N	2.29	0.66
1:F:682:ASN:HD21	1:F:728:SER:HB2	1.61	0.66
1:B:584:THR:HG23	1:B:609:MET:HG2	1.77	0.65
1:B:775:ASN:OD1	1:B:780:ASN:ND2	2.30	0.65
3:H:331:LEU:HB3	3:H:389:PHE:HB2	1.78	0.65
1:E:619:PHE:HD1	1:E:737:SER:HB3	1.62	0.64
1:B:520:ASP:OD2	1:B:614:LYS:NZ	2.29	0.64
1:A:650:LEU:HG	1:A:652:GLY:H	1.63	0.64
1:G:586:ASN:HA	1:G:589:LYS:HE3	1.79	0.64
1:F:775:ASN:O	1:F:780:ASN:ND2	2.32	0.63
1:E:641:ASP:HB2	1:E:647:ALA:HB2	1.78	0.63
3:H:309:PRO:O	3:H:318:ASN:ND2	2.32	0.63
1:F:276:LYS:HA	1:F:281:PHE:HE1	1.63	0.63
2:D:684:ILE:HD11	2:D:731:THR:HG21	1.81	0.62
3:H:257:TYR:HE2	3:H:275:ILE:HD11	1.63	0.62
1:F:634:ASN:ND2	1:F:653:GLU:O	2.33	0.62
1:A:334:SER:HB3	1:A:360:THR:HB	1.80	0.62
1:A:775:ASN:O	1:A:780:ASN:ND2	2.32	0.62
1:B:533:LYS:NZ	1:B:540:ASP:O	2.33	0.62
3:H:132:LYS:HE2	3:H:292:THR:HG21	1.82	0.62
1:C:334:SER:HB3	1:C:360:THR:HB	1.82	0.62
1:C:639:ASN:ND2	1:C:641:ASP:OD2	2.33	0.62
1:G:491[A]:ASN:HD21	1:G:495[A]:GLN:HB2	1.65	0.62
3:H:212:ASP:OD2	3:H:292:THR:OG1	2.18	0.61
3:H:295:ARG:NH2	3:H:301:GLU:OE2	2.33	0.61
1:C:655:LYS:HG3	1:C:724:THR:HG22	1.83	0.61
1:F:759:GLN:NE2	1:F:763:ASP:OD1	2.34	0.60
1:F:622:PHE:HB2	1:F:646:SER:HB2	1.83	0.60
2:D:276:LYS:HA	2:D:281:PHE:CE2	2.37	0.60
1:G:511:ASP:OD1	1:G:529:ARG:NH1	2.35	0.60
2:D:682:ASN:ND2	2:D:728:SER:OG	2.34	0.60
1:B:805:ARG:NH1	1:B:807:GLU:OE2	2.32	0.60
1:A:633:SER:HB3	1:A:655:LYS:HB2	1.84	0.60
1:C:640:GLN:HA	1:C:645:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:658:ILE:HB	1:F:721:ILE:HB	1.82	0.60
1:E:641:ASP:O	1:E:646:SER:N	2.26	0.59
1:F:636:ASN:HD21	1:F:649:LYS:H	1.51	0.59
1:G:217:GLU:N	1:G:229:SER:OG	2.36	0.59
1:A:516:SER:OG	1:A:610:ASN:OD1	2.20	0.58
1:E:653:GLU:HG3	1:E:726:ILE:HG22	1.86	0.58
1:G:276:LYS:NZ	1:G:294:VAL:O	2.28	0.58
2:D:622:PHE:HB2	2:D:646:SER:HB2	1.86	0.58
1:B:580:PHE:HE1	1:B:611:ILE:HG12	1.68	0.58
1:B:684:ILE:HB	1:B:698:LEU:HB3	1.85	0.58
1:G:795:LYS:NZ	1:G:799:ASP:OD2	2.37	0.58
1:C:650:LEU:HG	1:C:652:GLY:H	1.67	0.58
1:F:453:ASP:OD1	1:F:458:ARG:N	2.36	0.58
1:G:282:ASP:OD2	1:G:404:TYR:OH	2.22	0.58
3:H:252:THR:O	3:H:256:ASN:ND2	2.36	0.57
2:D:805:ARG:NH1	2:D:807:GLU:OE2	2.33	0.57
1:G:665:PRO:HB3	1:G:716:LYS:HB2	1.85	0.57
1:B:595:LEU:O	1:B:598:LYS:NZ	2.37	0.57
2:D:283:LYS:HB2	1:E:509:GLN:HG3	1.85	0.57
1:F:299:ILE:HG13	1:F:527:GLU:HB3	1.87	0.57
1:F:313:GLU:HG2	1:F:381:ILE:HD13	1.85	0.57
3:H:50:SER:O	3:H:54:GLN:NE2	2.38	0.57
1:G:821:LYS:NZ	1:G:844:SER:O	2.37	0.57
1:C:580:PHE:HB3	1:C:584:THR:HB	1.86	0.57
1:C:718:SER:OG	1:C:719:SER:N	2.38	0.56
1:F:293:LEU:HD13	1:F:545:LEU:HD11	1.87	0.56
1:B:641:ASP:O	1:B:646:SER:N	2.33	0.56
1:C:491:ASN:OD1	1:C:492:SER:N	2.38	0.56
1:C:795:LYS:NZ	1:C:799:ASP:OD2	2.38	0.56
1:B:860:ILE:HD12	1:B:873:LEU:HD23	1.88	0.56
1:C:584:THR:HG23	1:C:609:MET:HG2	1.87	0.56
2:D:639:ASN:ND2	2:D:641:ASP:OD2	2.38	0.56
1:E:493[A]:SER:H	3:H:26:ARG:HH22	1.54	0.56
1:E:668:ARG:HE	1:E:741:LEU:HD12	1.69	0.56
1:F:821:LYS:NZ	1:F:844:SER:O	2.38	0.56
1:F:619:PHE:HD1	1:F:737:SER:HB3	1.70	0.56
1:A:394:ARG:NH2	1:A:444:LEU:O	2.32	0.56
1:A:821:LYS:NZ	1:A:844:SER:O	2.38	0.56
1:B:653:GLU:OE2	1:B:728:SER:OG	2.22	0.56
1:F:752:GLU:OE1	1:F:754:LYS:NZ	2.39	0.56
1:E:231:GLU:OE1	1:E:259:SER:OG	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:516:SER:OG	1:E:610:ASN:OD1	2.23	0.56
1:E:670:VAL:HG22	1:E:710:GLU:HG2	1.88	0.56
1:F:647:ALA:HB1	1:F:732:TYR:HD1	1.71	0.56
1:C:276:LYS:HA	1:C:281:PHE:HE1	1.71	0.55
1:A:630:SER:OG	1:A:631:THR:N	2.38	0.55
1:A:521:THR:OG1	1:A:524:GLU:O	2.23	0.55
1:B:619:PHE:HD1	1:B:737:SER:HB3	1.72	0.55
1:B:653:GLU:HG3	1:B:726:ILE:HD13	1.87	0.55
1:G:394:ARG:NH2	1:G:444:LEU:O	2.30	0.55
1:A:276:LYS:HA	1:A:281:PHE:CE2	2.42	0.55
1:B:324:SER:HB3	1:B:370:SER:HB3	1.88	0.55
1:F:689:LYS:HB2	1:F:693:GLU:HG2	1.88	0.55
3:H:168:PRO:HB3	3:H:177:THR:HG22	1.89	0.55
1:C:408:PRO:HB3	1:C:483:VAL:HG22	1.89	0.55
1:F:685:ILE:HB	1:F:726:ILE:HB	1.89	0.55
1:E:859:ARG:NH2	1:E:876:ASP:OD1	2.37	0.54
2:D:834:GLN:NE2	1:E:843:ARG:O	2.39	0.54
1:B:392:ASN:HB3	1:B:446:PRO:HB2	1.89	0.54
3:H:123:LYS:HB2	3:H:190:ILE:HD11	1.89	0.54
3:H:132:LYS:NZ	3:H:359:THR:OG1	2.33	0.54
1:E:276:LYS:HA	1:E:281:PHE:CE1	2.43	0.54
1:F:276:LYS:HA	1:F:281:PHE:CE1	2.42	0.54
1:F:685:ILE:N	1:F:726:ILE:O	2.29	0.54
1:G:276:LYS:HA	1:G:281:PHE:CE2	2.40	0.54
1:B:658:ILE:HB	1:B:721:ILE:HB	1.89	0.54
1:E:276:LYS:HA	1:E:281:PHE:HE1	1.73	0.54
1:G:864:THR:OG1	1:G:866:ASP:OD1	2.17	0.53
1:C:276:LYS:NZ	1:C:294:VAL:O	2.28	0.53
1:C:690:ALA:HB1	1:C:713:THR:HG22	1.89	0.53
1:E:394:ARG:NH1	1:E:440:PRO:O	2.41	0.53
1:G:392:ASN:HB3	1:G:446:PRO:HB2	1.89	0.53
1:A:665:PRO:HB3	1:A:716:LYS:HB2	1.89	0.53
1:E:747:ILE:HG13	1:E:748:LEU:H	1.74	0.53
1:C:511:ASP:OD1	1:C:529:ARG:NH1	2.40	0.53
1:C:630:SER:OG	1:C:631:THR:N	2.41	0.53
1:F:648:ASN:O	1:F:648:ASN:ND2	2.42	0.53
3:H:368:TYR:HA	3:H:381:VAL:HG22	1.90	0.53
1:A:584:THR:HG23	1:A:609:MET:HG2	1.91	0.53
1:B:642:GLY:HA2	1:B:704:TYR:OH	2.09	0.53
1:C:753:VAL:HG23	1:C:754:LYS:H	1.73	0.52
1:E:775:ASN:OD1	1:E:780:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD21	1:A:543:PRO:HD2	1.92	0.52
1:B:521:THR:HG22	1:B:522:GLU:N	2.21	0.52
3:H:225:LYS:O	3:H:229:ASN:ND2	2.37	0.52
1:A:276:LYS:HA	1:A:281:PHE:HE2	1.74	0.52
2:D:715:GLU:O	1:E:754:LYS:NZ	2.41	0.52
3:H:160:LEU:HD23	3:H:164:THR:HG21	1.90	0.52
1:B:276:LYS:HA	1:B:281:PHE:CE2	2.44	0.52
1:F:650:LEU:HD12	1:F:652:GLY:N	2.24	0.52
1:G:747:ILE:HG13	1:G:748:LEU:H	1.75	0.52
3:H:290:ASN:OD1	3:H:362:LYS:N	2.43	0.52
1:C:425:GLN:OE1	1:C:451:THR:OG1	2.24	0.52
1:A:687:LYS:HB2	1:A:724:THR:OG1	2.10	0.52
1:C:283:LYS:HB2	2:D:509:GLN:HG3	1.91	0.52
1:G:223:ASN:O	3:H:33:ARG:NH1	2.42	0.52
2:D:624:ASP:OD1	2:D:624:ASP:N	2.43	0.52
1:F:283:LYS:HB2	1:G:509:GLN:HG3	1.92	0.52
1:A:641:ASP:O	1:A:646:SER:N	2.27	0.52
1:A:805:ARG:NH1	1:A:807:GLU:OE2	2.40	0.51
1:C:276:LYS:HA	1:C:281:PHE:CE1	2.45	0.51
2:D:633:SER:OG	2:D:653:GLU:O	2.26	0.51
1:G:684:ILE:HD11	1:G:731:THR:HG21	1.91	0.51
1:A:651:ASN:O	1:A:728:SER:OG	2.25	0.51
1:A:671:PHE:O	1:A:709:TYR:N	2.43	0.51
1:C:535:LEU:HD21	1:C:604:LYS:HE3	1.92	0.51
3:H:353:LYS:HE2	3:H:402:ILE:HD12	1.91	0.51
1:B:561:ASP:OD1	1:B:561:ASP:N	2.43	0.51
3:H:388:LYS:HG3	3:H:412:ILE:HB	1.93	0.51
1:F:636:ASN:ND2	1:F:649:LYS:O	2.43	0.51
1:A:655:LYS:HD2	1:A:724:THR:HG22	1.91	0.51
3:H:136:PHE:HB3	3:H:178:LEU:HD11	1.92	0.51
2:D:578:LEU:HD23	2:D:580:PHE:HZ	1.76	0.51
2:D:408:PRO:HB3	2:D:483:VAL:HG22	1.93	0.51
1:E:834:GLN:NE2	1:F:843:ARG:O	2.44	0.51
1:G:687:LYS:HB2	1:G:724:THR:OG1	2.11	0.51
3:H:334:PRO:HA	3:H:386:GLY:HA2	1.93	0.51
1:E:665:PRO:HB3	1:E:716:LYS:HB2	1.93	0.51
1:F:670:VAL:HG22	1:F:710:GLU:HG2	1.93	0.51
1:G:718:SER:OG	1:G:719:SER:N	2.44	0.51
1:E:533:LYS:NZ	1:E:540:ASP:O	2.43	0.50
1:F:311:THR:HG22	1:F:313:GLU:HG3	1.91	0.50
3:H:90:TYR:HE1	3:H:159:LYS:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:327:GLU:HG3	3:H:393:LYS:HA	1.93	0.50
1:B:307:LEU:HD21	1:B:476:ILE:HD12	1.94	0.50
1:C:331:LYS:NZ	1:C:333:GLU:OE2	2.34	0.50
1:G:657:LYS:HG2	1:G:722:GLU:HG3	1.92	0.50
1:B:688:ILE:HG21	1:B:711:PHE:HB3	1.94	0.50
1:F:639:ASN:HD21	1:F:647:ALA:HB2	1.76	0.50
1:A:668:ARG:HE	1:A:741:LEU:HB2	1.77	0.50
1:C:653:GLU:OE2	1:C:728:SER:OG	2.29	0.50
2:D:288:GLU:OE2	2:D:528:ARG:NH2	2.44	0.50
1:E:281:PHE:CD2	1:E:285:ILE:HD12	2.47	0.50
1:E:658:ILE:HB	1:E:721:ILE:HB	1.94	0.50
1:A:276:LYS:NZ	1:A:294:VAL:O	2.31	0.50
2:D:616:PRO:HA	2:D:739:THR:HG22	1.93	0.50
1:F:582:ASP:OD2	1:F:583:ASN:N	2.45	0.50
2:D:448:ALA:H	1:E:421:THR:HG23	1.77	0.49
1:A:392:ASN:HB3	1:A:446:PRO:HB2	1.94	0.49
1:G:580:PHE:HB3	1:G:584:THR:HB	1.94	0.49
1:B:666:TYR:CE2	1:C:755:ILE:HD12	2.47	0.49
2:D:392:ASN:HB3	2:D:446:PRO:HB2	1.93	0.49
2:D:747:ILE:HG13	2:D:748:LEU:N	2.27	0.49
1:E:568:ASP:OD2	1:E:568:ASP:N	2.45	0.49
1:B:630:SER:OG	1:B:631:THR:N	2.45	0.49
1:E:330:SER:HB3	1:E:364:SER:HB2	1.95	0.49
1:B:283:LYS:HB2	1:C:509:GLN:HG3	1.95	0.49
1:E:227:PRO:HD2	1:E:230:TYR:CD2	2.48	0.49
1:G:293:LEU:HD13	1:G:545:LEU:HD11	1.93	0.49
1:C:330:SER:HB3	1:C:364:SER:HB2	1.95	0.49
3:H:38:ALA:HB2	3:H:75:GLU:HG3	1.94	0.49
2:D:580:PHE:HE1	2:D:611:ILE:HG12	1.78	0.49
2:D:688:ILE:HG12	2:D:723:ILE:HG12	1.94	0.49
1:F:403:MET:HG2	1:F:406:VAL:HG22	1.94	0.49
1:A:759:GLN:NE2	1:A:763:ASP:OD1	2.47	0.48
1:B:649:LYS:HG2	1:B:731:THR:HG23	1.95	0.48
1:B:788:PHE:O	1:B:837:THR:OG1	2.20	0.48
1:F:773:ASN:N	1:F:782:TYR:O	2.45	0.48
1:C:616:PRO:HA	1:C:739:THR:HG22	1.95	0.48
1:F:805:ARG:NH1	1:F:807:GLU:OE2	2.41	0.48
1:C:394:ARG:NH2	1:C:444:LEU:O	2.31	0.48
1:B:511:ASP:OD1	1:B:529:ARG:NH1	2.47	0.48
2:D:763:ASP:HA	2:D:766:LYS:HE2	1.95	0.48
1:E:281:PHE:HE2	1:E:285:ILE:HB	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:636:ASN:ND2	1:F:649:LYS:H	2.11	0.48
1:G:630:SER:OG	1:G:631:THR:N	2.46	0.48
2:D:747:ILE:HG13	2:D:748:LEU:H	1.79	0.48
1:A:421:THR:HG23	1:G:448:ALA:H	1.79	0.48
2:D:385:GLU:OE2	2:D:458:ARG:NH2	2.41	0.48
1:E:447:LEU:HB2	1:F:421:THR:HG21	1.96	0.48
1:G:655:LYS:HG3	1:G:724:THR:HG22	1.95	0.48
1:A:684:ILE:HD12	1:A:698:LEU:HD23	1.94	0.48
2:D:636:ASN:OD1	2:D:649:LYS:N	2.46	0.48
1:B:293:LEU:HD13	1:B:545:LEU:HD11	1.96	0.48
1:B:688:ILE:HG12	1:B:723:ILE:HG13	1.95	0.48
1:C:684:ILE:HB	1:C:698:LEU:HB3	1.96	0.48
2:D:595:LEU:HD21	2:D:602:ASN:HB2	1.96	0.48
1:E:653:GLU:OE1	1:E:727:GLY:N	2.40	0.48
1:C:677:ASP:OD1	1:C:700:PRO:HB2	2.14	0.47
1:C:222:ASP:N	1:C:222:ASP:OD1	2.47	0.47
1:F:231:GLU:OE1	1:F:259:SER:OG	2.25	0.47
1:G:636:ASN:ND2	1:G:649:LYS:O	2.34	0.47
1:B:617:THR:O	1:B:627:ASN:ND2	2.47	0.47
1:G:713:THR:HG22	1:G:721:ILE:HD11	1.96	0.47
1:C:639:ASN:HD21	1:C:647:ALA:HB2	1.79	0.47
1:F:276:LYS:NZ	1:F:294:VAL:O	2.30	0.47
3:H:268:ASN:HB2	3:H:270:GLU:OE1	2.14	0.47
1:B:718:SER:OG	1:B:719:SER:N	2.48	0.47
1:C:860:ILE:HD12	1:C:873:LEU:HD23	1.96	0.47
2:D:773:ASN:HB2	2:D:784:ASN:OD1	2.14	0.47
2:D:691:LYS:HD2	2:D:714:THR:HG22	1.97	0.47
1:E:674:TYR:CZ	1:E:706:LYS:HG3	2.49	0.47
1:A:715:GLU:HG2	1:A:716:LYS:H	1.80	0.47
1:C:747:ILE:HG13	1:C:748:LEU:H	1.80	0.47
3:H:390:LYS:HB2	3:H:412:ILE:HD11	1.96	0.47
1:B:618:TYR:HA	1:B:627:ASN:HD22	1.79	0.47
3:H:21:ARG:O	3:H:25:GLU:HG2	2.15	0.47
3:H:91:VAL:HG11	3:H:139:ILE:HD12	1.97	0.47
3:H:313:PHE:O	3:H:403:THR:OG1	2.33	0.47
1:G:304:MET:HB2	1:G:478:LEU:HD13	1.96	0.46
3:H:121:GLU:O	3:H:125:THR:OG1	2.22	0.46
1:A:283:LYS:HB2	1:B:509:GLN:HG3	1.96	0.46
1:B:392:ASN:HD21	1:C:418:THR:H	1.62	0.46
2:D:773:ASN:N	2:D:782:TYR:O	2.44	0.46
1:A:333:GLU:OE1	1:A:361:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:834:GLN:NE2	2:D:843:ARG:O	2.48	0.46
1:F:678:PRO:O	1:F:702:GLN:NE2	2.49	0.46
1:F:688:ILE:HG23	1:F:723:ILE:HG12	1.98	0.46
1:B:276:LYS:HA	1:B:281:PHE:HE2	1.81	0.46
1:C:715:GLU:HG2	1:C:716:LYS:H	1.81	0.46
3:H:92:TYR:HD1	3:H:157:HIS:ND1	2.14	0.46
3:H:312:ASP:O	3:H:318:ASN:ND2	2.31	0.46
1:F:624:ASP:OD1	1:F:624:ASP:N	2.48	0.46
3:H:279:GLU:OE1	3:H:385:HIS:NE2	2.43	0.46
1:A:619:PHE:HD1	1:A:737:SER:HB3	1.80	0.45
1:B:682:ASN:OD1	1:B:682:ASN:N	2.49	0.45
2:D:658:ILE:HB	2:D:721:ILE:HB	1.97	0.45
2:D:687:LYS:NZ	2:D:695:THR:HB	2.31	0.45
1:E:580:PHE:HB3	1:E:584:THR:HB	1.98	0.45
3:H:294:TYR:O	3:H:340:SER:OG	2.31	0.45
1:E:687:LYS:HB3	1:E:724:THR:OG1	2.16	0.45
1:F:595:LEU:O	1:F:598:LYS:NZ	2.38	0.45
3:H:250:GLY:O	3:H:254:ILE:HG12	2.17	0.45
1:A:685:ILE:HB	1:A:726:ILE:HG13	1.98	0.45
1:C:633:SER:HB3	1:C:655:LYS:HB2	1.97	0.45
1:C:687:LYS:HB2	1:C:724:THR:OG1	2.17	0.45
1:C:788:PHE:O	1:C:837:THR:OG1	2.29	0.45
2:D:314:HIS:HB2	2:D:380:SER:HB2	1.98	0.45
1:E:470:LEU:HD21	1:E:476:ILE:HG13	1.98	0.45
3:H:56:ARG:NH2	3:H:57:ASN:HB3	2.31	0.45
1:C:395:TYR:O	1:C:438:THR:HG23	2.17	0.45
1:C:714:THR:N	1:C:715:GLU:OE2	2.46	0.45
3:H:272:ASP:HA	3:H:275:ILE:HD12	1.99	0.45
1:F:580:PHE:HB3	1:F:584:THR:HB	1.99	0.45
1:G:265:ASN:ND2	1:G:269:ASP:O	2.48	0.45
1:G:649:LYS:HG2	1:G:731:THR:O	2.16	0.45
2:D:218:ASP:OD1	2:D:218:ASP:N	2.49	0.45
2:D:641:ASP:O	2:D:646:SER:N	2.40	0.45
1:E:694:LYS:HD2	1:E:694:LYS:HA	1.72	0.45
1:G:584:THR:HG23	1:G:609:MET:HG2	1.99	0.45
1:F:816:LYS:HB2	1:F:816:LYS:HE3	1.77	0.45
1:A:671:PHE:N	1:A:709:TYR:O	2.44	0.44
1:F:604:LYS:NZ	1:F:605:LEU:O	2.47	0.44
1:G:561:ASP:OD1	1:G:561:ASP:N	2.49	0.44
1:G:269:ASP:HB2	1:G:270:PRO:HD2	2.00	0.44
1:B:757:THR:OG1	1:B:760:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:310:SER:HA	1:E:463:ASN:HD21	1.82	0.44
2:D:622:PHE:HB2	2:D:646:SER:CB	2.47	0.44
1:B:281:PHE:HE1	1:B:285:ILE:HB	1.82	0.44
1:B:683:SER:OG	1:B:684:ILE:N	2.51	0.44
1:B:747:ILE:HG13	1:B:748:LEU:N	2.33	0.44
2:D:630:SER:OG	2:D:631:THR:N	2.50	0.44
1:E:816:LYS:HE3	1:E:816:LYS:HB2	1.71	0.44
1:C:448:ALA:H	2:D:421:THR:HG23	1.82	0.44
1:E:334:SER:HA	1:F:362:ASP:HB3	1.99	0.44
3:H:60:TYR:CD1	3:H:345:ASN:HB3	2.53	0.44
1:B:580:PHE:CE1	1:B:611:ILE:HG12	2.50	0.44
3:H:354:ILE:HG12	3:H:405:LEU:HB3	2.00	0.44
1:B:805:ARG:HH21	1:B:869:GLU:CD	2.21	0.44
1:F:699:VAL:HG23	1:F:699:VAL:O	2.18	0.44
1:A:269:ASP:HB2	1:A:270:PRO:HD2	2.00	0.44
1:A:635:VAL:O	1:A:636:ASN:ND2	2.50	0.44
1:C:773:ASN:N	1:C:782:TYR:O	2.42	0.43
1:E:397:ASN:HB2	1:E:433:LEU:HG	2.00	0.43
1:F:291:ASP:OD1	1:F:291:ASP:N	2.51	0.43
1:B:616:PRO:HA	1:B:739:THR:HG22	2.00	0.43
2:D:520:ASP:OD2	2:D:614:LYS:NZ	2.44	0.43
1:F:674:TYR:HB3	1:F:704:TYR:CD1	2.53	0.43
3:H:391:ILE:HG23	3:H:407:VAL:HG13	1.99	0.43
1:A:866:ASP:HB2	1:A:868:ARG:HE	1.83	0.43
1:F:318:ASP:HB2	1:F:376:ASN:HB2	2.00	0.43
1:F:668:ARG:HD2	1:F:741:LEU:HD12	2.01	0.43
1:G:334:SER:HB3	1:G:360:THR:HB	2.01	0.43
3:H:31:LEU:O	3:H:36:LYS:HE3	2.17	0.43
1:E:448:ALA:H	1:F:421:THR:CG2	2.32	0.43
1:F:561:ASP:OD1	1:F:561:ASP:N	2.50	0.43
3:H:323:LYS:HA	3:H:394:ILE:HD12	1.99	0.43
1:A:509:GLN:HG3	1:G:283:LYS:HB2	2.00	0.43
1:B:448:ALA:H	1:C:421:THR:HG23	1.83	0.43
1:E:798:LEU:HD23	1:E:798:LEU:HA	1.90	0.43
3:H:70:GLU:O	3:H:74:LYS:HG2	2.18	0.43
1:A:520:ASP:OD2	1:A:614:LYS:HE2	2.18	0.43
2:D:687:LYS:HZ3	2:D:695:THR:HB	1.84	0.43
3:H:358:ILE:HG13	3:H:409:ALA:HB3	2.00	0.43
1:F:763:ASP:HA	1:F:766:LYS:HG3	2.01	0.43
1:A:706:LYS:HE2	1:A:708:SER:HB3	2.00	0.43
3:H:34:SER:O	3:H:37:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:GLY:HA2	1:C:735:ASN:O	2.19	0.43
2:D:578:LEU:HD23	2:D:580:PHE:CZ	2.54	0.43
2:D:687:LYS:HB2	2:D:724:THR:OG1	2.19	0.43
1:E:448:ALA:H	1:F:421:THR:HG23	1.84	0.43
3:H:236:THR:HG23	3:H:239:GLU:H	1.83	0.43
1:A:305:GLU:OE2	1:A:394:ARG:HD2	2.19	0.42
1:B:282:ASP:OD1	1:B:283:LYS:N	2.52	0.42
1:B:677:ASP:OD1	1:B:700:PRO:HB2	2.19	0.42
1:B:686:VAL:HG11	1:B:709:TYR:HD2	1.84	0.42
2:D:658:ILE:N	2:D:721:ILE:O	2.46	0.42
2:D:698:LEU:HD13	2:D:707:PHE:HB3	2.01	0.42
1:F:492:SER:OG	3:H:32:GLU:HB3	2.19	0.42
1:A:684:ILE:O	1:A:698:LEU:N	2.46	0.42
2:D:816:LYS:HB2	2:D:816:LYS:HE3	1.85	0.42
3:H:99:LYS:HE2	3:H:133:GLN:HG3	2.01	0.42
2:D:673:GLY:O	2:D:706:LYS:HA	2.18	0.42
1:F:283:LYS:HD3	1:F:283:LYS:HA	1.86	0.42
1:G:489[A]:THR:O	1:G:496[A]:ILE:HA	2.19	0.42
1:C:741:LEU:HD23	1:C:741:LEU:HA	1.83	0.42
2:D:677:ASP:OD2	2:D:681:SER:HB2	2.19	0.42
1:G:578:LEU:HD23	1:G:578:LEU:HA	1.85	0.42
1:G:581:ASP:OD1	1:G:581:ASP:N	2.45	0.42
2:D:533:LYS:HB2	2:D:542:THR:HG23	2.00	0.42
1:E:618:TYR:OH	1:E:662:GLU:HB3	2.19	0.42
1:F:477:LYS:HA	1:F:477:LYS:HD3	1.90	0.42
1:F:828:TYR:HB3	1:F:834:GLN:HB3	2.02	0.42
1:A:411:ASN:OD1	1:A:421:THR:HG22	2.19	0.42
1:F:713:THR:HG22	1:F:721:ILE:HD11	2.01	0.42
2:D:685:ILE:HB	2:D:726:ILE:HB	2.02	0.42
3:H:336:PHE:CE1	3:H:385:HIS:HB3	2.54	0.42
1:B:635:VAL:HA	1:B:648:ASN:OD1	2.19	0.42
1:C:572:ASP:O	1:C:576:VAL:HG22	2.20	0.42
1:F:673:GLY:HA2	1:F:735:ASN:O	2.20	0.42
1:A:616:PRO:HA	1:A:739:THR:HG22	2.01	0.42
1:B:758:ASP:O	1:B:762:MET:HG3	2.19	0.42
2:D:718:SER:OG	2:D:719:SER:N	2.52	0.42
1:G:775:ASN:OD1	1:G:775:ASN:O	2.38	0.42
1:B:616:PRO:HB3	1:B:739:THR:HG22	2.02	0.41
1:E:544:GLU:HG3	1:E:604:LYS:HE2	2.02	0.41
1:A:666:TYR:OH	1:B:755:ILE:HG12	2.20	0.41
1:B:281:PHE:CD1	1:B:285:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:828:TYR:HB3	2:D:834:GLN:HB3	2.02	0.41
1:E:238:LYS:HE2	1:E:238:LYS:HB3	1.85	0.41
1:F:630:SER:OG	1:F:631:THR:N	2.52	0.41
1:F:686:VAL:HG22	1:F:725:LEU:HD13	2.01	0.41
1:A:622:PHE:HB2	1:A:646:SER:CB	2.50	0.41
1:B:651:ASN:O	1:B:728:SER:OG	2.38	0.41
1:C:668:ARG:HB2	1:C:710:GLU:OE2	2.20	0.41
1:G:634:ASN:ND2	1:G:653:GLU:O	2.53	0.41
1:A:281:PHE:CD1	1:A:285:ILE:HD12	2.55	0.41
1:A:634:ASN:ND2	1:A:650:LEU:HD21	2.35	0.41
1:B:487:PHE:HB3	1:B:503:TRP:CE2	2.56	0.41
1:B:618:TYR:HA	1:B:627:ASN:ND2	2.34	0.41
1:G:747:ILE:HG13	1:G:748:LEU:N	2.34	0.41
1:B:579:ILE:HD12	1:B:612:LEU:HD23	2.03	0.41
1:E:310:SER:HB2	1:E:388:TYR:HB2	2.03	0.41
2:D:593:LYS:HB3	2:D:593:LYS:HE2	1.80	0.41
2:D:798:LEU:HD23	2:D:798:LEU:HA	1.85	0.41
1:E:686:VAL:HG11	1:E:709:TYR:CD2	2.56	0.41
1:F:576:VAL:HG12	1:F:615:THR:HA	2.03	0.41
1:G:641:ASP:O	1:G:646:SER:N	2.36	0.41
1:G:673:GLY:HA2	1:G:735:ASN:O	2.21	0.41
3:H:294:TYR:CE1	3:H:343:SER:HB3	2.55	0.41
1:A:649:LYS:HA	1:A:649:LYS:HD3	1.92	0.41
2:D:642:GLY:HA2	2:D:704:TYR:CE2	2.56	0.41
1:F:422:ILE:HG21	1:F:449:LEU:HD11	2.03	0.41
1:G:816:LYS:HE3	1:G:816:LYS:HB2	1.75	0.41
3:H:63:GLN:O	3:H:67:ASN:ND2	2.54	0.41
1:C:749:ASP:OD1	1:C:750:GLU:N	2.53	0.41
2:D:487:PHE:CZ	2:D:501:ASN:HB3	2.55	0.41
1:F:269:ASP:HB2	1:F:270:PRO:HD2	2.02	0.41
1:F:326:ALA:HB3	1:F:368:GLN:HB3	2.02	0.41
3:H:76:LEU:HD12	3:H:76:LEU:HA	1.93	0.41
3:H:127:GLN:OE1	3:H:128:ASN:ND2	2.54	0.41
1:B:313:GLU:HG3	1:B:381:ILE:HD13	2.03	0.41
1:B:673:GLY:O	1:B:706:LYS:HA	2.21	0.41
1:C:324:SER:OG	1:C:325:ARG:N	2.53	0.41
2:D:734:ASP:OD1	2:D:735:ASN:N	2.54	0.41
1:E:230:TYR:CE1	1:E:244:LYS:HG2	2.56	0.41
1:E:387:ALA:HB3	1:E:462:ILE:HD11	2.03	0.41
3:H:368:TYR:CZ	3:H:370:SER:HB3	2.56	0.41
1:A:747:ILE:HG13	1:A:748:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:673:GLY:HA2	1:E:735:ASN:O	2.20	0.41
1:F:222:ASP:OD1	1:F:222:ASP:N	2.52	0.41
1:F:740:GLU:O	1:F:741:LEU:HD23	2.21	0.41
1:F:801:ILE:HD11	1:F:864:THR:HG22	2.02	0.41
1:B:269:ASP:HB2	1:B:270:PRO:HD2	2.03	0.40
1:B:687:LYS:HB3	1:B:724:THR:OG1	2.21	0.40
1:C:330:SER:OG	1:C:331:LYS:N	2.54	0.40
1:C:448:ALA:H	2:D:421:THR:CG2	2.33	0.40
1:E:283:LYS:HA	1:E:283:LYS:HD3	1.97	0.40
1:F:600:ILE:H	1:F:600:ILE:HD12	1.87	0.40
1:F:616:PRO:HB3	1:F:739:THR:HG22	2.02	0.40
1:G:853:MET:HB2	1:G:856:LYS:HG3	2.02	0.40
1:C:801:ILE:HG21	1:C:862:ALA:HB1	2.04	0.40
1:E:470:LEU:HD23	1:E:470:LEU:HA	1.93	0.40
3:H:323:LYS:HG2	3:H:394:ILE:HB	2.03	0.40
1:A:421:THR:HG21	1:G:447:LEU:HB2	2.04	0.40
1:A:689:LYS:HE3	1:A:689:LYS:HB3	1.94	0.40
1:B:678:PRO:O	1:B:702:GLN:NE2	2.41	0.40
1:C:318:ASP:HB2	1:C:376:ASN:HB2	2.02	0.40
2:D:293:LEU:HD13	2:D:545:LEU:HD11	2.03	0.40
1:G:633:SER:OG	1:G:654:THR:HA	2.20	0.40
3:H:251:TYR:CD2	3:H:252:THR:HG23	2.56	0.40
1:A:677:ASP:OD2	1:A:700:PRO:HB2	2.22	0.40
1:B:276:LYS:NZ	1:B:294:VAL:O	2.35	0.40
1:C:676:LYS:HD3	1:C:704:TYR:CZ	2.57	0.40
1:C:860:ILE:HB	1:C:873:LEU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	645/638 (101%)	605 (94%)	40 (6%)	0	100	100
1	B	644/638 (101%)	599 (93%)	45 (7%)	0	100	100
1	C	634/638 (99%)	594 (94%)	40 (6%)	0	100	100
1	E	645/638 (101%)	603 (94%)	42 (6%)	0	100	100
1	F	634/638 (99%)	594 (94%)	40 (6%)	0	100	100
1	G	642/638 (101%)	605 (94%)	37 (6%)	0	100	100
2	D	646/641 (101%)	607 (94%)	39 (6%)	0	100	100
3	H	392/394 (100%)	379 (97%)	13 (3%)	0	100	100
All	All	4882/4863 (100%)	4586 (94%)	296 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	578/569 (102%)	578 (100%)	0	100	100
1	B	577/569 (101%)	576 (100%)	1 (0%)	93	93
1	C	569/569 (100%)	569 (100%)	0	100	100
1	E	578/569 (102%)	578 (100%)	0	100	100
1	F	569/569 (100%)	568 (100%)	1 (0%)	93	93
1	G	576/569 (101%)	574 (100%)	2 (0%)	92	92
2	D	580/572 (101%)	580 (100%)	0	100	100
3	H	354/354 (100%)	353 (100%)	1 (0%)	92	92
All	All	4381/4340 (101%)	4376 (100%)	5 (0%)	93	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	691	LYS
1	F	689	LYS

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Mol	Chain	Res	Type
1	G	493[A]	SER
1	G	493[B]	SER
3	H	351	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	627	ASN
1	E	780	ASN
3	H	54	GLN
3	H	128	ASN
3	H	256	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 21 ligands modelled in this entry, 21 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	G	1
1	B	1
1	F	1
2	D	1
1	A	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	336:THR	C	359:HIS	N	6.84
1	G	336:THR	C	359:HIS	N	6.48
1	B	336:THR	C	359:HIS	N	6.29
1	F	336:THR	C	359:HIS	N	5.96
1	D	336:THR	C	359:HIS	N	5.89
1	A	336:THR	C	359:HIS	N	5.72
1	E	336:THR	C	359:HIS	N	5.57

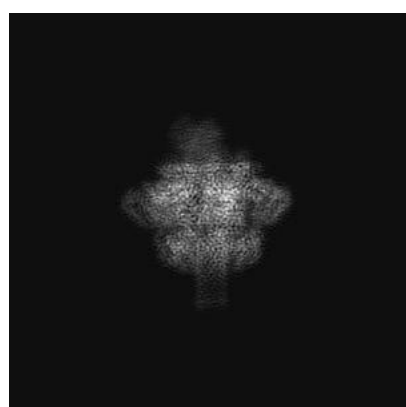
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D_1300025005. These allow visual inspection of the internal detail of the map and identification of artifacts.

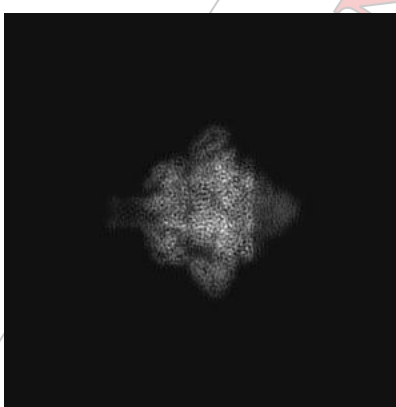
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

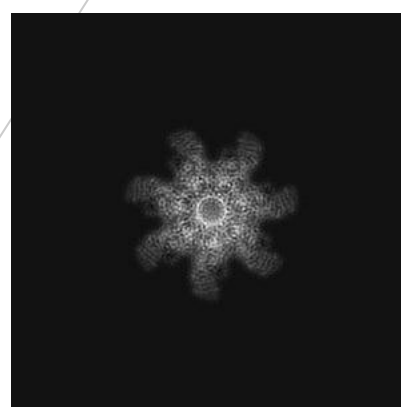
6.1.1 Primary map



X



Y

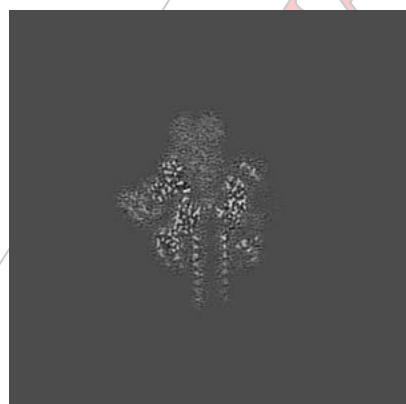


Z

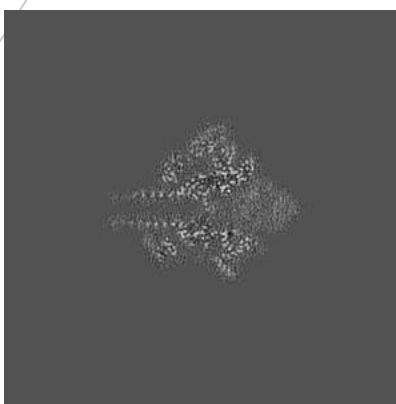
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

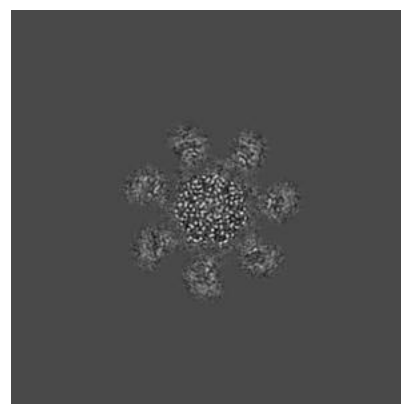
6.2.1 Primary map



X Index: 216



Y Index: 216

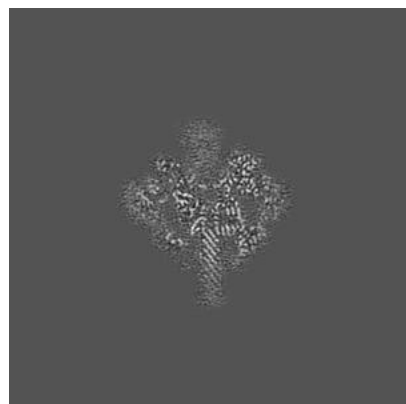


Z Index: 216

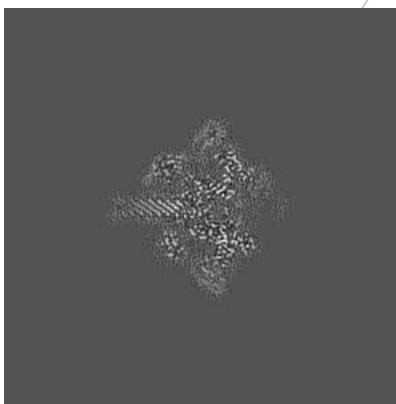
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

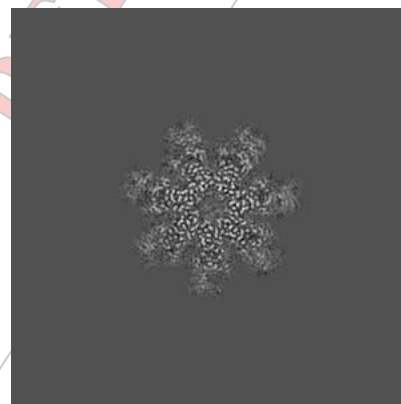
6.3.1 Primary map



X Index: 201



Y Index: 232

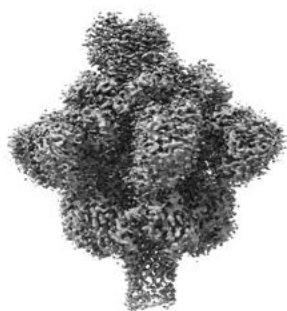


Z Index: 238

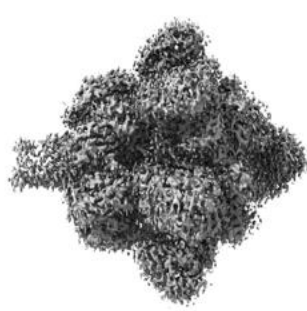
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

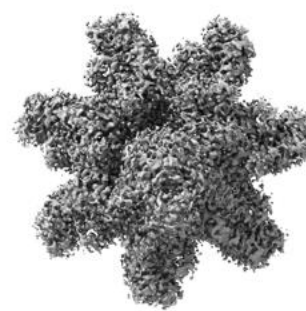
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation [i](#)

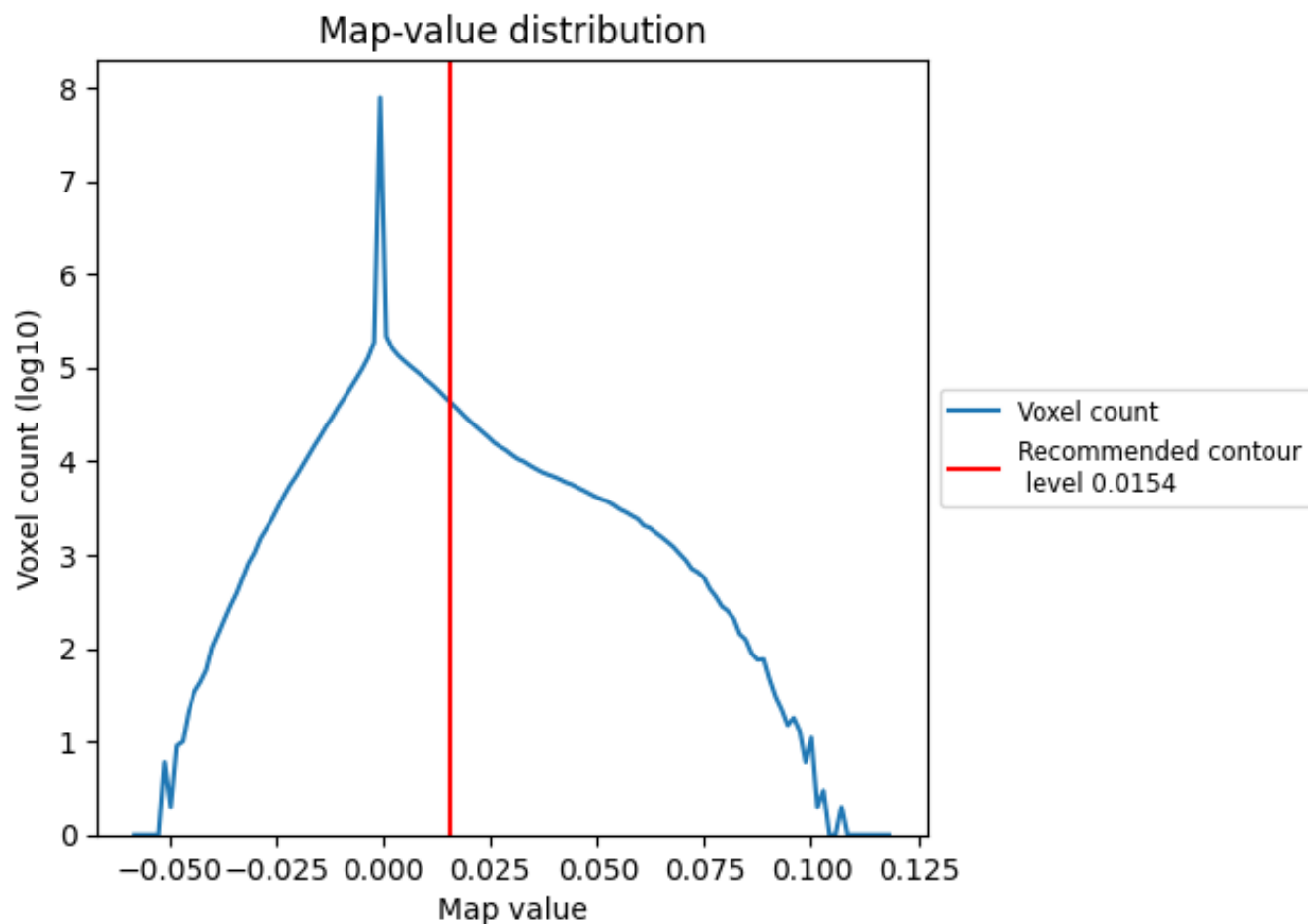
This section was not generated. No masks/segmentation were deposited.

PRELIMINARY VALIDATION REPORT

7 Map analysis [i](#)

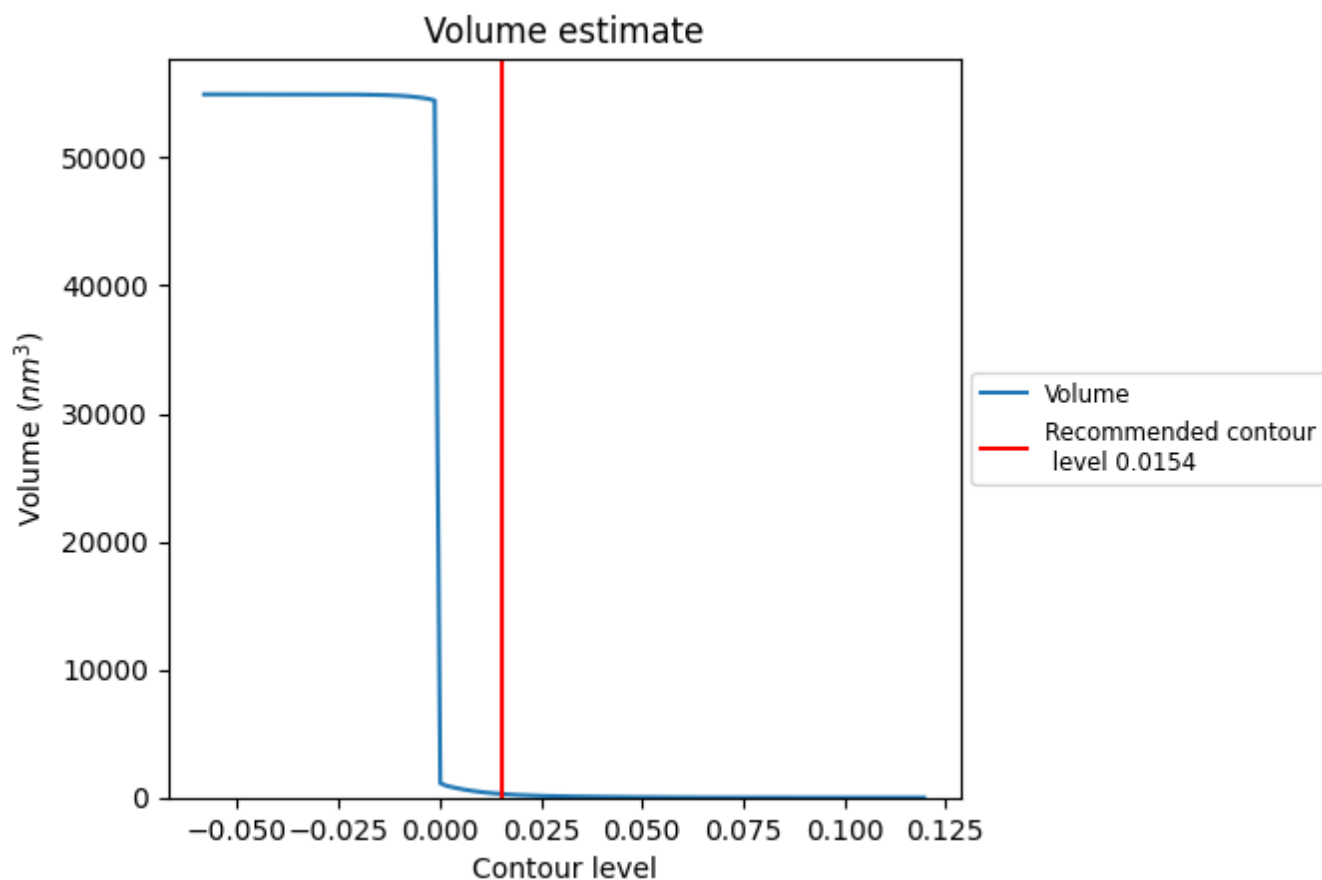
This section contains the results of statistical analysis of the map.

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.

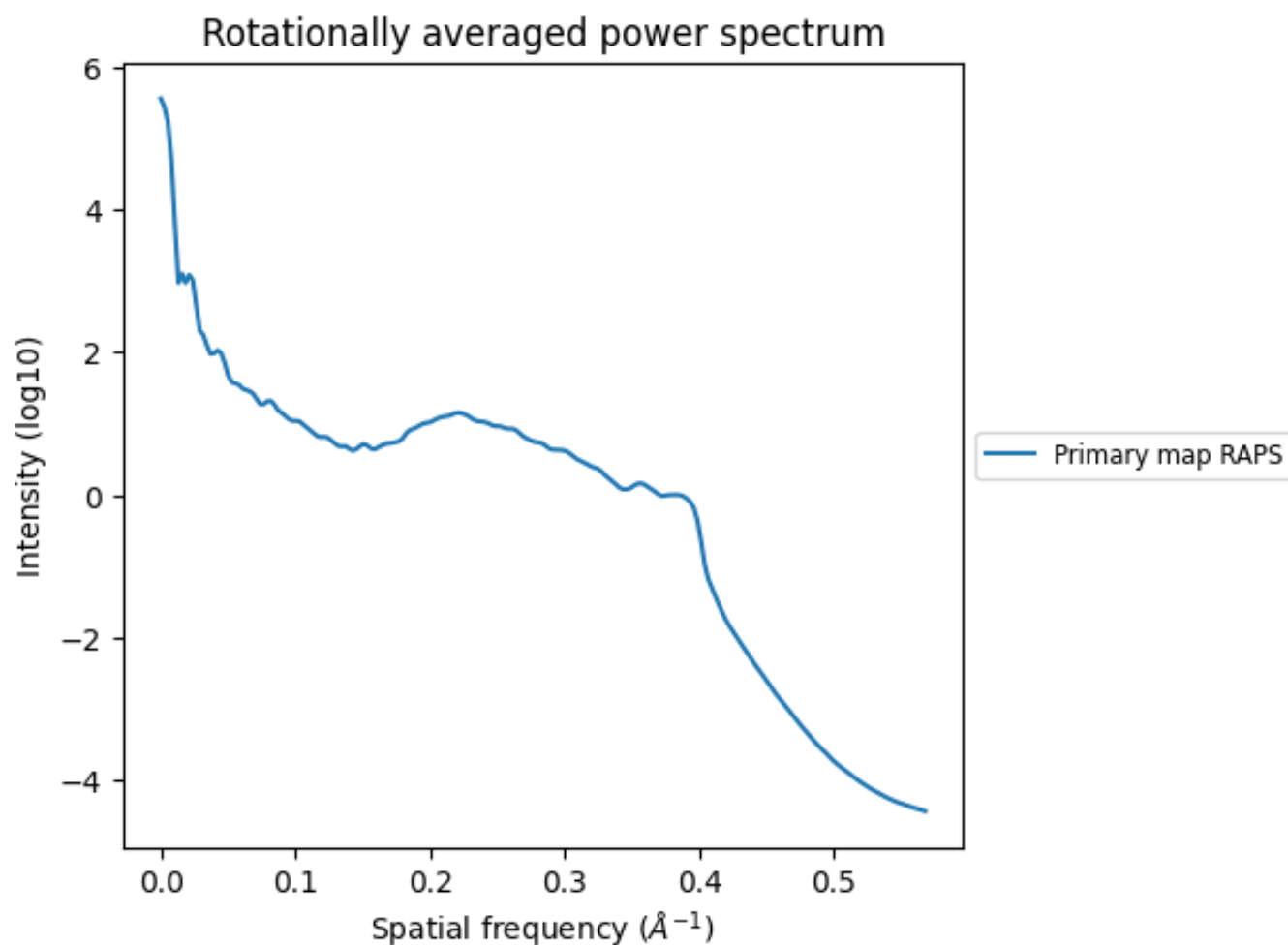
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 250 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 ⓘ

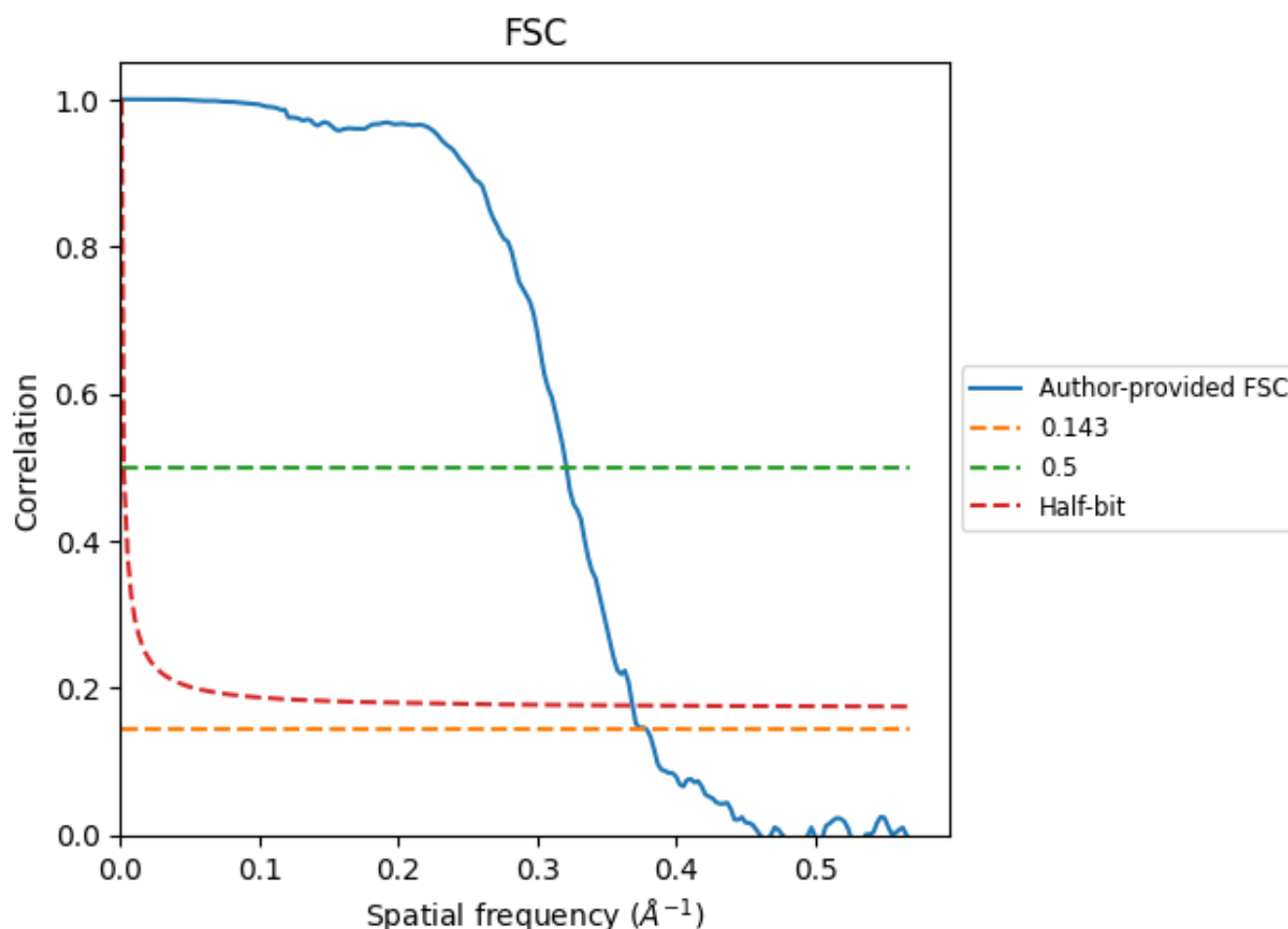


PRELIMINARY

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](#)



8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.64	3.12	2.71
Unmasked-calculated*	-	-	-

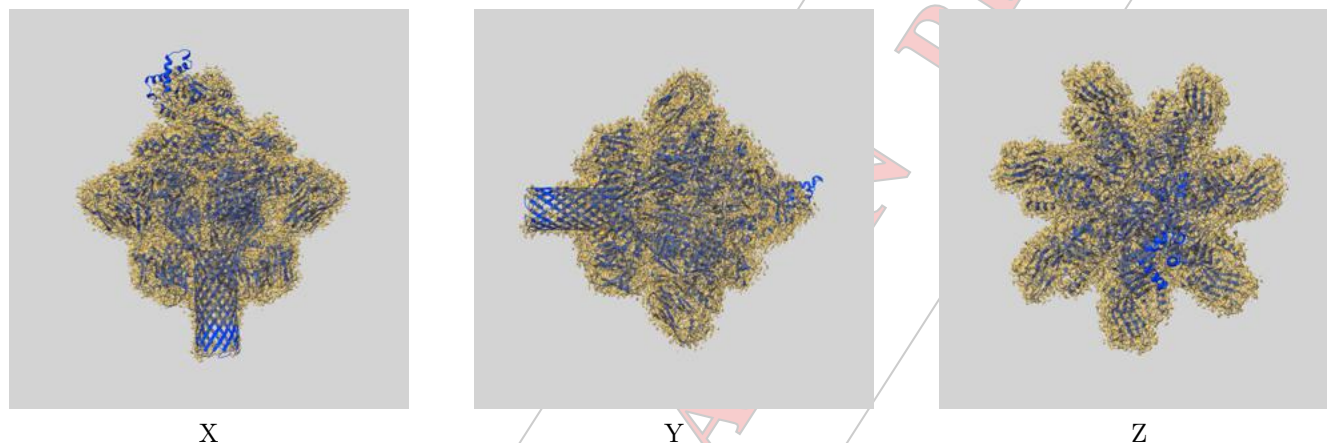
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

PRELIMINARY VALIDATION REPORT

9 Map-model fit ⓘ

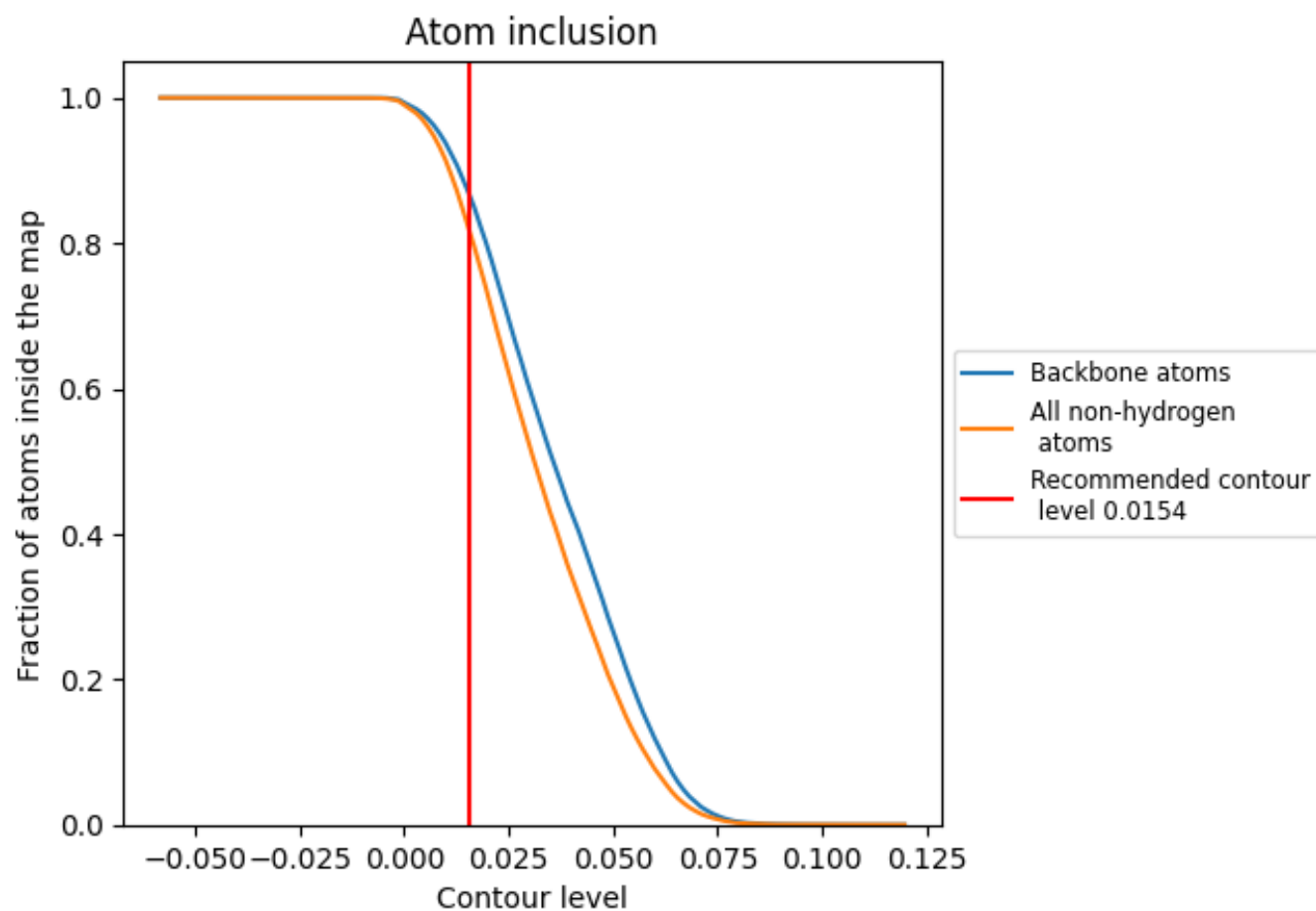
This section contains information regarding the fit between EMDB map D_1300025005 and PDB model D_1300025005. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ



The images above show the 3D surface view of the map at the recommended contour level 0.0154 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 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

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