



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 09:42 PM EDT

PDB ID : 7SFU
EMDB ID : EMD-25102
Title : CryoEM structure of Venezuelan Equine Encephalitis virus (VEEV) TC-83 strain VLP
Authors : Binshtein, E.; Crowe, J.E.
Deposited on : 2021-10-04
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

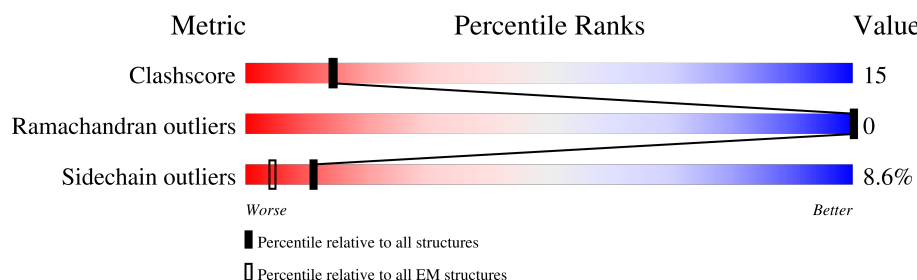
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	442	<div> <div>6%</div> <div>58%</div> <div>39%</div> <div>.</div> </div>
1	D	442	<div> <div>6%</div> <div>63%</div> <div>34%</div> <div>.</div> </div>
1	G	442	<div> <div>12%</div> <div>63%</div> <div>34%</div> <div>.</div> </div>
1	J	442	<div> <div>5%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>
2	B	423	<div> <div>7%</div> <div>63%</div> <div>33%</div> <div>.</div> </div>
2	E	423	<div> <div>6%</div> <div>61%</div> <div>34%</div> <div>.</div> </div>
2	H	423	<div> <div>8%</div> <div>61%</div> <div>35%</div> <div>.</div> </div>
2	K	423	<div> <div>5%</div> <div>61%</div> <div>36%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	162	<div><div></div><div>12%</div><div>68%</div><div>29%</div><div></div></div>
3	F	162	<div><div></div><div>14%</div><div>69%</div><div>27%</div><div></div></div>
3	I	162	<div><div></div><div>15%</div><div>65%</div><div>30%</div><div>5%</div></div>
3	L	162	<div><div></div><div>12%</div><div>67%</div><div>30%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31972 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 Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		
1	D	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		
1	G	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		
1	J	442	Total	C	N	O	S	0	0
			3370	2146	555	648	21		

- Molecule 2 is a protein called Spike glycoprotein E2.

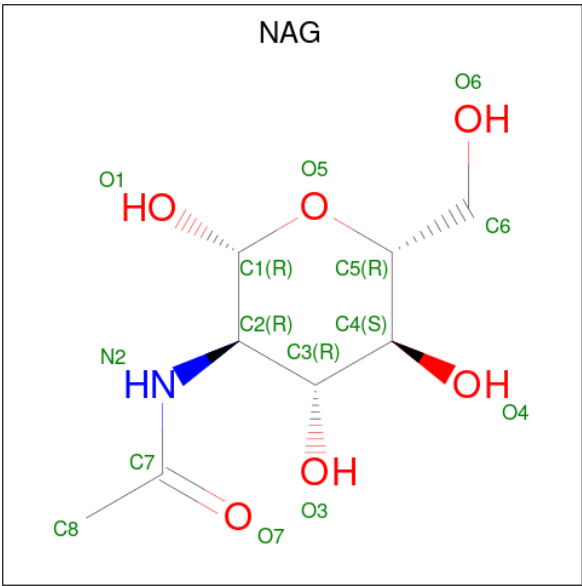
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	423	Total	C	N	O	S	0	0
			3304	2086	586	607	25		
2	E	423	Total	C	N	O	S	0	0
			3304	2086	586	607	25		
2	H	423	Total	C	N	O	S	0	0
			3304	2086	586	607	25		
2	K	423	Total	C	N	O	S	0	0
			3304	2086	586	607	25		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	162	Total	C	N	O	S	0	0
			1277	807	227	235	8		
3	F	162	Total	C	N	O	S	0	0
			1277	807	227	235	8		
3	I	162	Total	C	N	O	S	0	0
			1277	807	227	235	8		
3	L	162	Total	C	N	O	S	0	0
			1277	807	227	235	8		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).

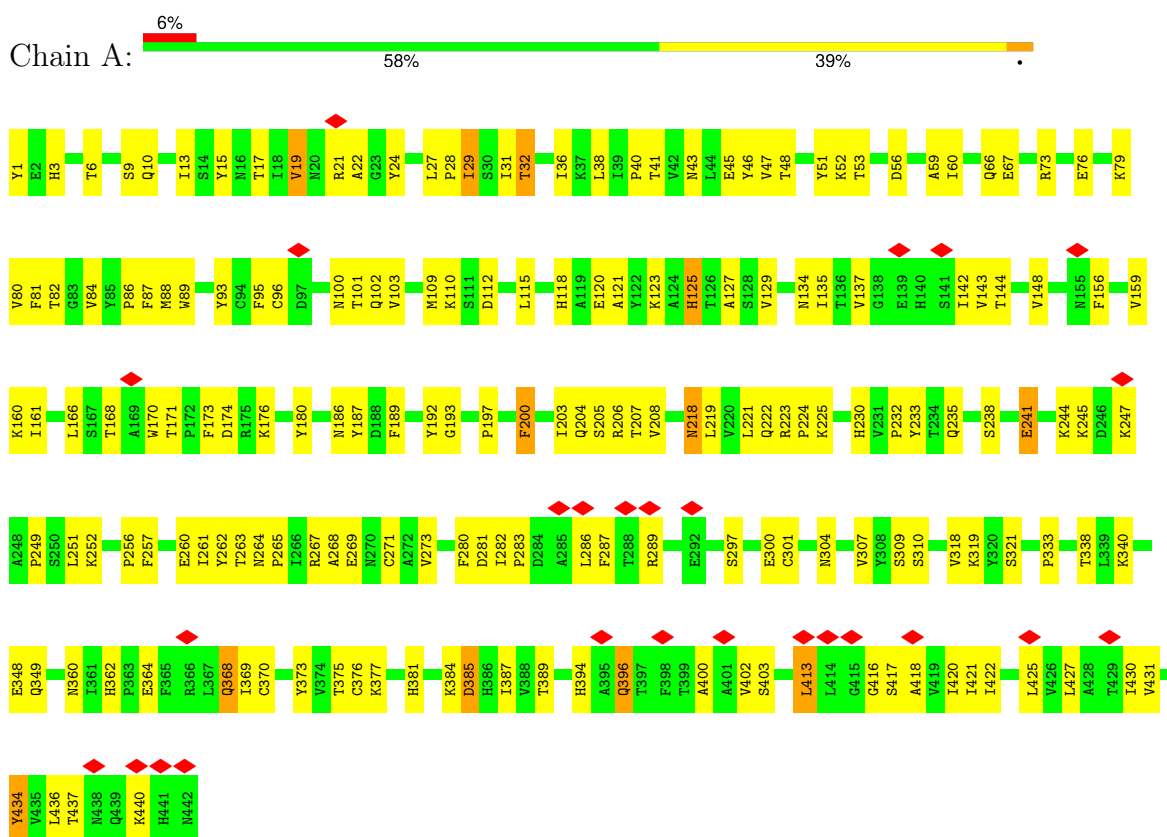


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	

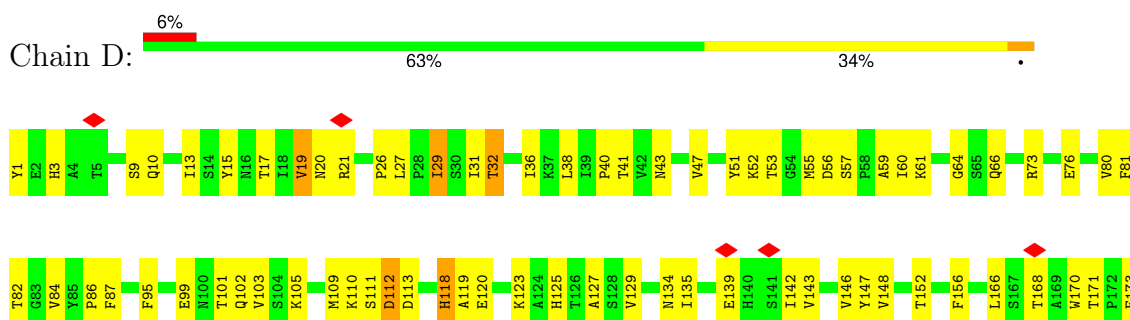
3 Residue-property plots

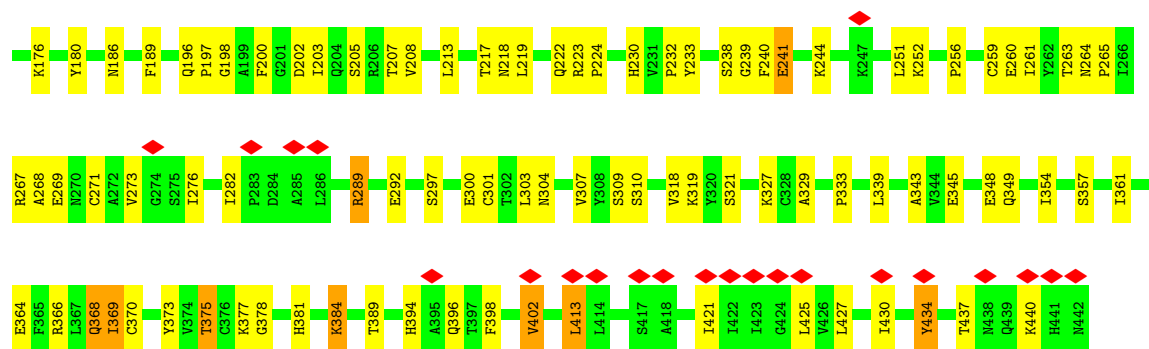
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein E1

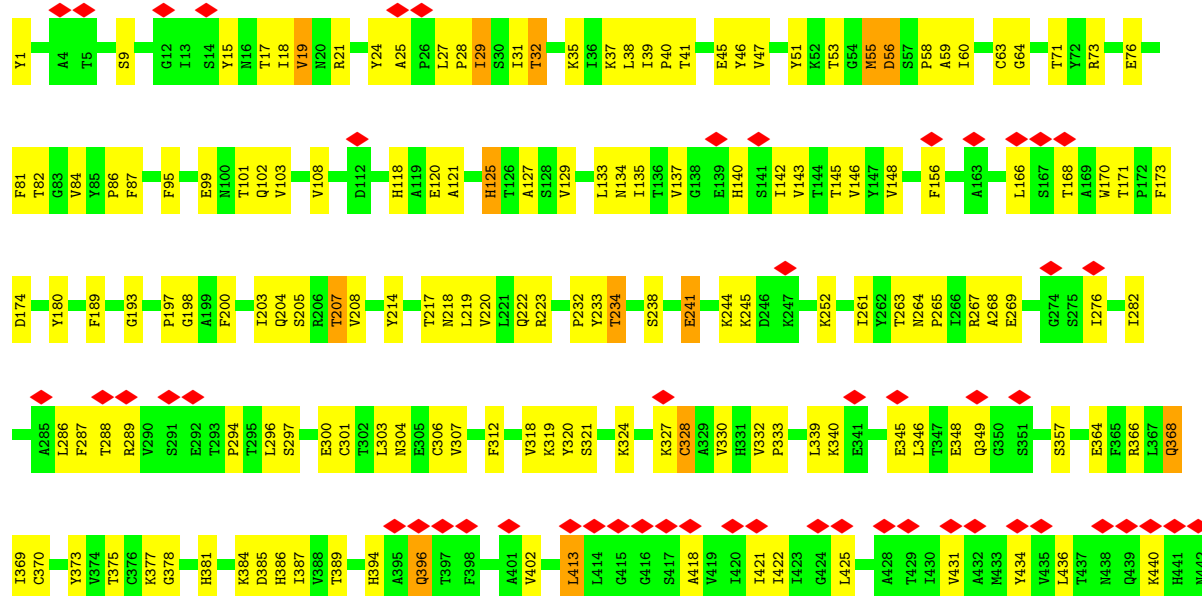


- Molecule 1: Spike glycoprotein E1

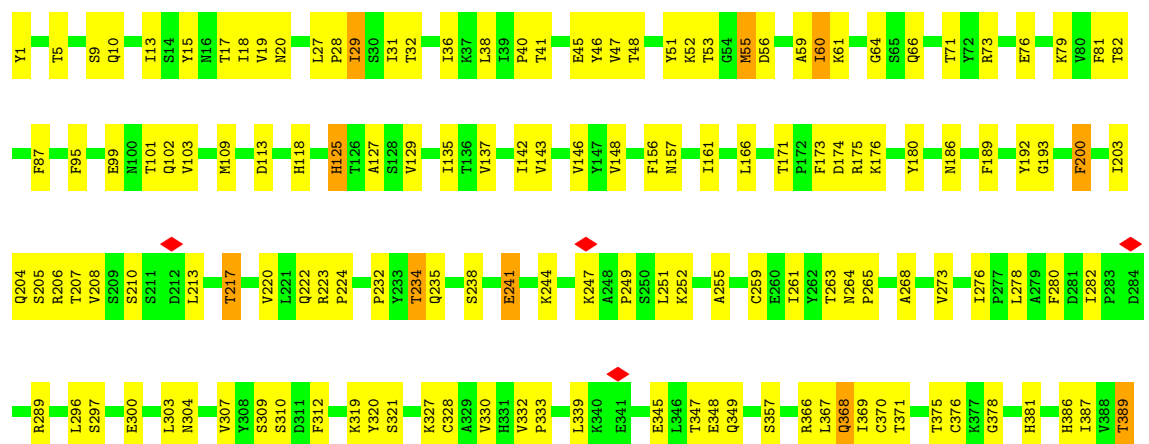


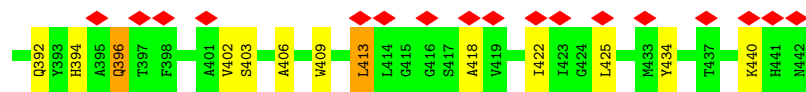


• Molecule 1: Spike glycoprotein E1

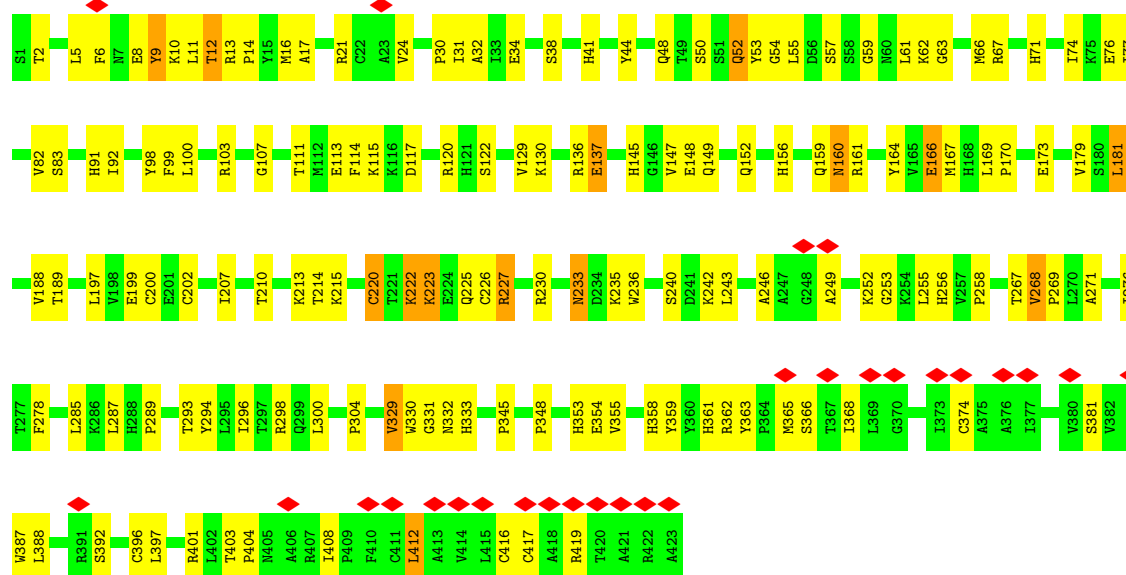


• Molecule 1: Spike glycoprotein E1

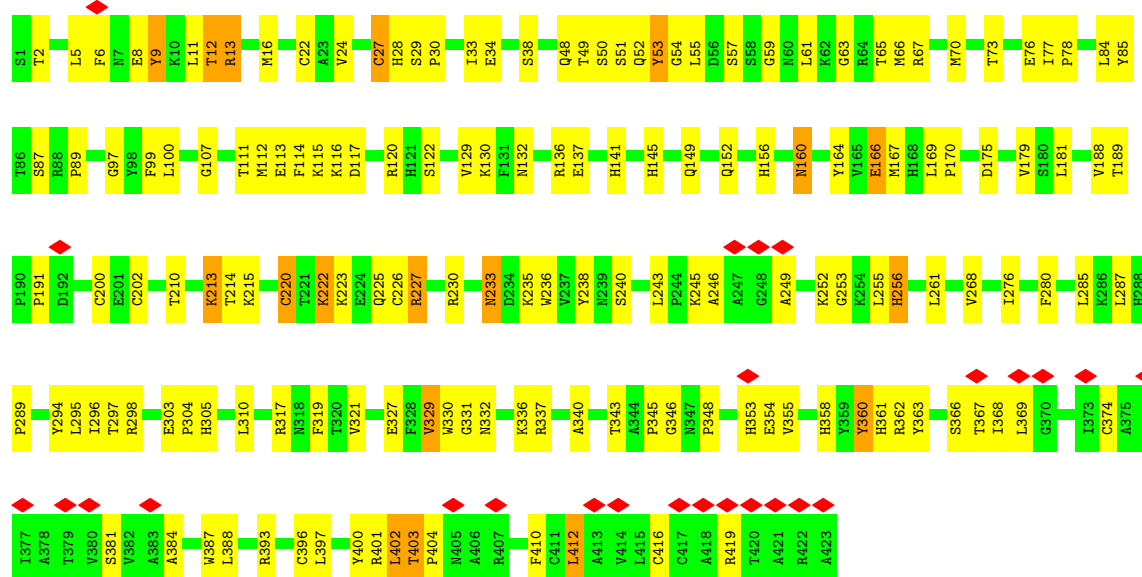




• Molecule 2: Spike glycoprotein E2

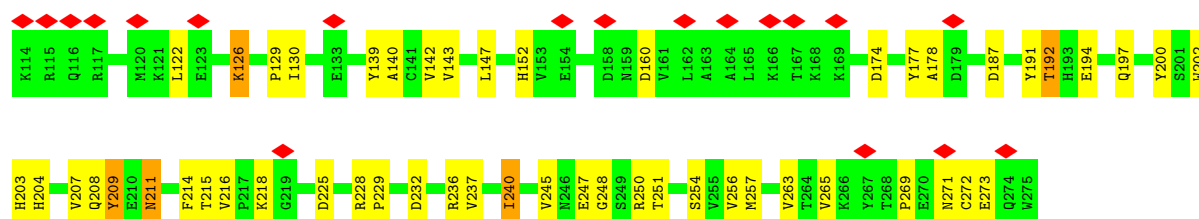


• Molecule 2: Spike glycoprotein E2

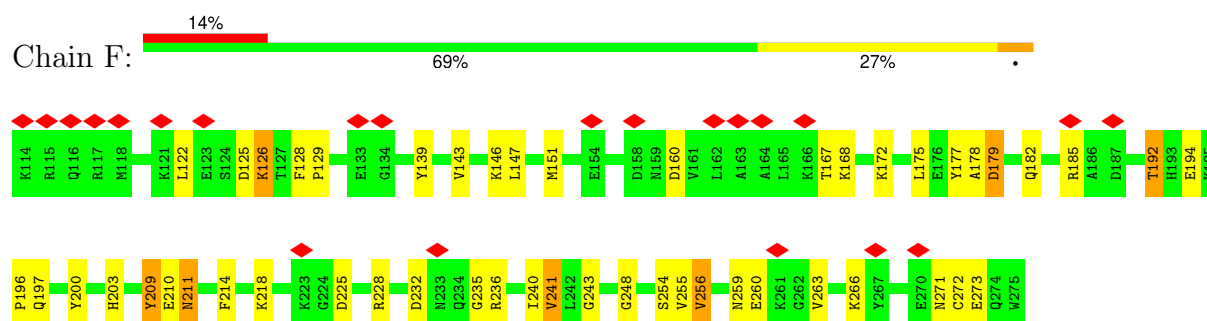


• Molecule 2: Spike glycoprotein E2

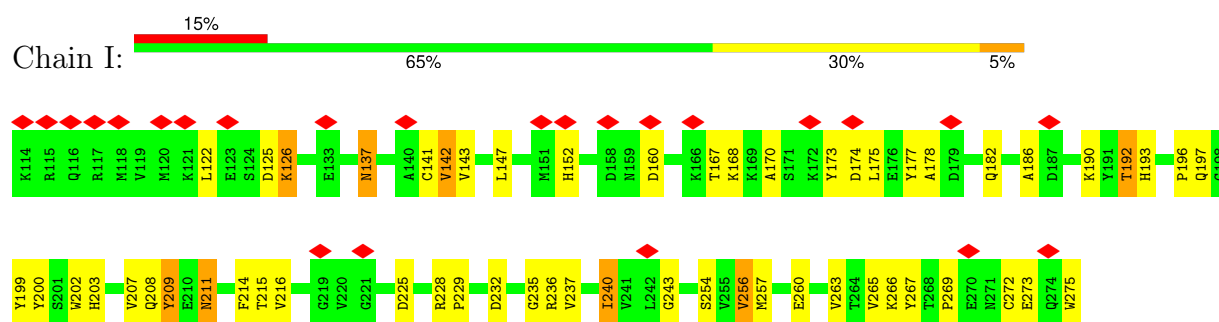




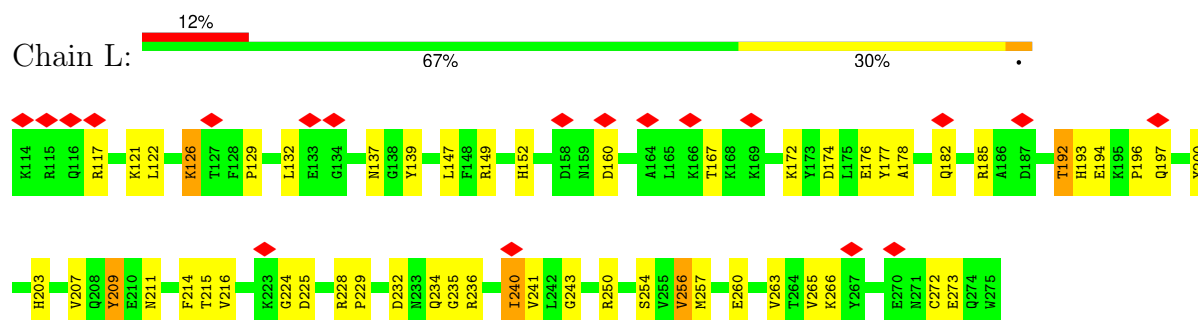
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	7514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.05	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	924.928, 924.928, 924.928	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8065, 1.8065, 1.8065	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	A	0.30	0/3461	0.46	0/4731
1	D	0.29	0/3461	0.46	0/4731
1	G	0.28	0/3461	0.46	0/4731
1	J	0.30	0/3461	0.46	0/4731
2	B	0.29	0/3395	0.49	0/4616
2	E	0.29	0/3395	0.49	0/4616
2	H	0.28	0/3395	0.50	0/4616
2	K	0.29	0/3395	0.50	0/4616
3	C	0.28	0/1305	0.49	0/1757
3	F	0.29	0/1305	0.49	0/1757
3	I	0.29	0/1305	0.49	0/1757
3	L	0.29	0/1305	0.48	0/1757
All	All	0.29	0/32644	0.48	0/44416

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

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	3370	0	3273	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3370	0	3273	104	0
1	G	3370	0	3273	102	0
1	J	3370	0	3273	99	0
2	B	3304	0	3239	110	0
2	E	3304	0	3239	102	0
2	H	3304	0	3239	125	0
2	K	3304	0	3239	123	0
3	C	1277	0	1272	34	0
3	F	1277	0	1272	31	0
3	I	1277	0	1272	38	0
3	L	1277	0	1272	34	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
4	D	14	0	13	0	0
4	E	28	0	26	0	0
4	G	14	0	13	0	0
4	H	28	0	26	1	0
4	J	14	0	13	0	0
4	K	28	0	26	0	0
All	All	31972	0	31292	960	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 15.

All (960) 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:H:160:ASN:HB2	2:H:256:HIS:HB3	1.54	0.89
2:E:160:ASN:HB2	2:E:256:HIS:HB3	1.56	0.87
2:K:160:ASN:HB2	2:K:256:HIS:HB3	1.58	0.84
2:B:160:ASN:HB2	2:B:256:HIS:HB3	1.59	0.84
2:H:54:GLY:HA2	2:H:63:GLY:HA2	1.61	0.82
2:E:54:GLY:HA2	2:E:63:GLY:HA2	1.62	0.82
1:A:238:SER:HB2	1:A:241:GLU:HB2	1.61	0.81
2:K:11:LEU:HB3	2:K:236:TRP:HB2	1.66	0.78
1:D:43:ASN:HB3	1:D:123:LYS:HB3	1.66	0.78
1:A:333:PRO:HD3	1:A:368:GLN:HB2	1.67	0.77
1:G:222:GLN:HG3	1:G:232:PRO:HB2	1.65	0.76
2:K:416:CYS:O	2:K:419:ARG:NH1	2.19	0.76
1:G:40:PRO:HA	1:G:127:ALA:HA	1.68	0.75
2:H:280:PHE:HE1	2:H:343:THR:H	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:54:GLY:HA2	2:K:63:GLY:HA2	1.68	0.75
2:K:222:LYS:HB2	2:K:225:GLN:HE21	1.52	0.75
1:A:73:ARG:HB2	1:A:76:GLU:HB2	1.68	0.74
2:B:169:LEU:HB3	2:B:249:ALA:HB1	1.69	0.74
1:D:1:TYR:N	1:D:282:ILE:O	2.18	0.74
2:E:169:LEU:HB3	2:E:249:ALA:HB1	1.69	0.73
2:B:149:GLN:OE1	2:B:332:ASN:ND2	2.22	0.72
3:L:197:GLN:HE22	3:L:211:ASN:H	1.37	0.72
1:D:222:GLN:HG3	1:D:232:PRO:HB2	1.72	0.72
1:A:110:LYS:NZ	1:A:208:VAL:O	2.22	0.71
2:B:54:GLY:HA2	2:B:63:GLY:HA2	1.72	0.71
1:D:40:PRO:HA	1:D:127:ALA:HA	1.71	0.71
1:A:1:TYR:N	1:A:282:ILE:O	2.18	0.71
2:H:11:LEU:HB3	2:H:236:TRP:HB2	1.73	0.70
2:K:8:GLU:HG3	2:K:255:LEU:HD21	1.73	0.70
1:G:333:PRO:HD3	1:G:368:GLN:HB2	1.74	0.70
1:G:82:THR:HG22	1:G:101:THR:HG22	1.73	0.70
1:A:180:TYR:OH	1:A:244:LYS:NZ	2.25	0.70
1:J:40:PRO:HA	1:J:127:ALA:HA	1.73	0.70
1:J:297:SER:O	1:J:321:SER:OG	2.08	0.70
1:A:40:PRO:HA	1:A:127:ALA:HA	1.73	0.69
1:D:368:GLN:NE2	1:D:369:ILE:O	2.25	0.69
2:K:149:GLN:OE1	2:K:332:ASN:ND2	2.25	0.69
1:G:303:LEU:HD23	1:G:378:GLY:HA3	1.75	0.69
3:I:152:HIS:NE2	3:I:275:TRP:OXT	2.18	0.69
1:J:307:VAL:HG22	1:J:381:HIS:HB2	1.74	0.69
1:D:238:SER:HB2	1:D:241:GLU:HB2	1.75	0.68
1:J:41:THR:OG1	1:J:125:HIS:O	2.09	0.68
1:A:38:LEU:HB3	1:A:268:ALA:HB3	1.76	0.68
1:G:327:LYS:HA	1:G:345:GLU:HA	1.75	0.68
2:K:169:LEU:HB3	2:K:249:ALA:HB1	1.75	0.68
2:E:11:LEU:HA	2:E:235:LYS:HB3	1.74	0.68
2:E:169:LEU:HD11	2:E:233:ASN:HB3	1.76	0.68
3:F:182:GLN:HG3	3:F:185:ARG:HE	1.59	0.68
2:H:149:GLN:OE1	2:H:332:ASN:ND2	2.27	0.68
1:D:73:ARG:HB2	1:D:76:GLU:HB2	1.76	0.68
1:G:55:MET:SD	1:G:55:MET:N	2.67	0.68
2:B:11:LEU:HA	2:B:235:LYS:HB3	1.75	0.68
2:B:416:CYS:O	2:B:419:ARG:NH1	2.27	0.68
1:G:238:SER:HB2	1:G:241:GLU:HB2	1.74	0.68
1:G:41:THR:OG1	1:G:125:HIS:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:GLN:OE1	2:E:332:ASN:ND2	2.27	0.67
1:J:368:GLN:NE2	1:J:369:ILE:O	2.27	0.67
2:K:179:VAL:HA	2:K:188:VAL:HG22	1.76	0.67
1:A:297:SER:O	1:A:321:SER:OG	2.12	0.67
2:K:175:ASP:OD2	2:K:230:ARG:NH2	2.26	0.67
1:A:17:THR:HG23	1:A:29:ILE:HG23	1.77	0.67
1:J:59:ALA:HB3	1:J:103:VAL:HB	1.75	0.67
2:B:363:TYR:HB3	2:B:366:SER:HB3	1.76	0.67
1:A:300:GLU:O	1:A:319:LYS:N	2.27	0.67
1:A:1:TYR:HE1	1:A:21:ARG:HH11	1.42	0.67
2:K:416:CYS:SG	2:K:419:ARG:NH1	2.67	0.67
2:B:200:CYS:HA	2:B:226:CYS:HA	1.77	0.66
1:G:19:VAL:HG23	1:G:27:LEU:HB3	1.77	0.66
1:J:51:TYR:HB3	1:J:203:ILE:HG13	1.76	0.66
2:K:12:THR:O	2:K:98:TYR:OH	2.14	0.66
1:A:19:VAL:HG23	1:A:27:LEU:HB3	1.77	0.66
3:C:209:TYR:HB2	3:C:214:PHE:HA	1.77	0.66
2:K:152:GLN:HB3	2:K:261:LEU:HD11	1.76	0.66
1:A:41:THR:OG1	1:A:125:HIS:O	2.12	0.66
1:D:333:PRO:HD3	1:D:368:GLN:HB2	1.77	0.66
3:I:209:TYR:HB2	3:I:214:PHE:HA	1.76	0.66
1:A:95:PHE:H	2:B:227:ARG:HH21	1.41	0.66
1:G:38:LEU:HB3	1:G:268:ALA:HB3	1.78	0.66
3:I:167:THR:HG22	3:I:178:ALA:HB2	1.77	0.66
1:D:82:THR:HG22	1:D:101:THR:HG22	1.78	0.66
1:D:180:TYR:OH	1:D:244:LYS:NZ	2.28	0.66
1:D:19:VAL:HG23	1:D:27:LEU:HB3	1.78	0.66
1:G:297:SER:O	1:G:321:SER:OG	2.13	0.66
1:A:252:LYS:O	2:B:298:ARG:NH1	2.30	0.65
3:C:122:LEU:HD11	3:C:203:HIS:HA	1.78	0.65
1:G:307:VAL:HG22	1:G:381:HIS:HB2	1.77	0.65
1:G:180:TYR:OH	1:G:244:LYS:NZ	2.29	0.65
1:J:180:TYR:OH	1:J:244:LYS:NZ	2.29	0.65
1:D:307:VAL:HG22	1:D:381:HIS:HB2	1.78	0.65
3:F:167:THR:HG22	3:F:178:ALA:HB2	1.78	0.65
2:H:2:THR:HA	2:H:61:LEU:HD21	1.77	0.64
1:J:81:PHE:HB2	1:J:102:GLN:HB3	1.79	0.64
2:B:11:LEU:HB3	2:B:236:TRP:HB2	1.79	0.64
2:B:416:CYS:SG	2:B:419:ARG:NH1	2.71	0.64
1:D:230:HIS:HE1	1:D:232:PRO:HB3	1.61	0.64
1:J:95:PHE:HB2	2:K:227:ARG:HE	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:129:PRO:HA	3:F:139:TYR:HA	1.79	0.64
1:G:368:GLN:NE2	1:G:369:ILE:O	2.30	0.64
2:H:11:LEU:HA	2:H:235:LYS:HB3	1.78	0.64
1:G:73:ARG:HB2	1:G:76:GLU:HB2	1.80	0.64
1:D:47:VAL:HG11	1:D:208:VAL:HG22	1.80	0.64
3:F:209:TYR:HB2	3:F:214:PHE:HA	1.80	0.64
1:A:3:HIS:CD2	1:A:19:VAL:HG12	2.33	0.64
1:D:205:SER:OG	1:D:207:THR:O	2.16	0.63
2:H:57:SER:N	2:H:76:GLU:OE1	2.31	0.63
1:D:17:THR:HG23	1:D:29:ILE:HG23	1.80	0.63
3:L:167:THR:HG22	3:L:178:ALA:HB2	1.81	0.63
1:J:82:THR:HG22	1:J:101:THR:HG22	1.78	0.63
2:K:11:LEU:HA	2:K:235:LYS:HB3	1.79	0.63
2:E:11:LEU:HB3	2:E:236:TRP:HB2	1.80	0.63
2:E:166:GLU:HB3	2:E:252:LYS:HG3	1.80	0.62
2:K:169:LEU:HD11	2:K:233:ASN:HB3	1.80	0.62
2:K:171:GLY:HA2	2:K:246:ALA:HB2	1.81	0.62
2:B:55:LEU:HG	2:B:61:LEU:HA	1.80	0.62
1:J:55:MET:N	1:J:55:MET:SD	2.72	0.62
3:F:147:LEU:HB3	3:F:178:ALA:HB3	1.81	0.62
3:F:122:LEU:HD11	3:F:203:HIS:HA	1.81	0.62
2:B:91:HIS:HB2	2:B:103:ARG:HB3	1.81	0.62
2:B:222:LYS:HB2	2:B:225:GLN:HE21	1.63	0.62
2:K:167:MET:HG3	2:K:236:TRP:HE3	1.64	0.62
1:A:10:GLN:HB3	1:A:13:ILE:HD11	1.82	0.62
1:D:31:ILE:HG22	1:D:135:ILE:HG12	1.81	0.62
2:H:169:LEU:HD11	2:H:233:ASN:HB3	1.80	0.62
1:G:402:VAL:HG21	2:H:359:TYR:HE1	1.65	0.62
1:D:260:GLU:HB3	1:D:269:GLU:HG3	1.82	0.61
2:K:200:CYS:HA	2:K:226:CYS:HA	1.81	0.61
3:L:122:LEU:HD11	3:L:203:HIS:HA	1.82	0.61
1:G:32:THR:HG23	1:G:134:ASN:HB3	1.80	0.61
1:D:202:ASP:OD2	1:D:239:GLY:N	2.33	0.61
1:D:252:LYS:O	2:E:298:ARG:NH1	2.33	0.61
2:B:5:LEU:HB3	2:B:55:LEU:HD11	1.82	0.61
2:H:147:VAL:O	2:H:268:VAL:N	2.25	0.61
1:A:283:PRO:HG2	1:A:286:LEU:HD23	1.83	0.61
2:E:70:MET:O	2:E:73:THR:OG1	2.16	0.61
2:H:5:LEU:HB3	2:H:55:LEU:HD11	1.83	0.61
2:H:240:SER:HB2	2:H:243:LEU:HD23	1.81	0.61
1:D:300:GLU:O	1:D:319:LYS:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:GLN:OE1	2:H:286:LYS:NZ	2.34	0.61
2:H:296:ILE:HB	2:H:329:VAL:HG13	1.83	0.61
2:K:22:CYS:SG	2:K:29:SER:OG	2.59	0.61
1:A:47:VAL:HG11	1:A:208:VAL:HG22	1.82	0.60
1:A:168:THR:HG22	1:A:170:TRP:H	1.66	0.60
2:B:169:LEU:HD11	2:B:233:ASN:HB3	1.82	0.60
1:D:10:GLN:HB3	1:D:13:ILE:HD11	1.80	0.60
2:H:297:THR:HG23	2:H:326:TRP:HE1	1.66	0.60
2:H:363:TYR:HB3	2:H:366:SER:HB3	1.83	0.60
1:J:73:ARG:HB2	1:J:76:GLU:HB2	1.82	0.60
3:I:197:GLN:HE22	3:I:211:ASN:H	1.49	0.60
1:G:38:LEU:N	1:G:268:ALA:O	2.34	0.60
1:J:300:GLU:O	1:J:319:LYS:N	2.33	0.60
2:B:167:MET:HG3	2:B:236:TRP:HE3	1.65	0.60
1:D:95:PHE:HD1	2:E:227:ARG:HE	1.48	0.60
3:F:200:TYR:HD2	3:F:232:ASP:HA	1.65	0.60
1:G:15:TYR:HB3	1:G:31:ILE:HG13	1.84	0.60
2:H:175:ASP:OD2	2:H:230:ARG:NH2	2.35	0.60
3:I:272:CYS:SG	3:I:273:GLU:N	2.75	0.60
2:E:345:PRO:HB2	2:E:358:HIS:CE1	2.37	0.59
1:J:413:LEU:HD13	2:K:374:CYS:SG	2.42	0.59
1:A:32:THR:HG23	1:A:134:ASN:HB3	1.84	0.59
1:D:168:THR:HG22	1:D:170:TRP:H	1.66	0.59
2:H:297:THR:HG21	2:H:319:PHE:HE1	1.68	0.59
2:B:91:HIS:O	2:B:103:ARG:N	2.22	0.59
2:H:167:MET:HG3	2:H:236:TRP:HE3	1.67	0.59
1:J:129:VAL:HB	1:J:148:VAL:HB	1.85	0.59
2:K:199:GLU:OE1	2:K:227:ARG:NH1	2.35	0.59
3:I:257:MET:N	3:I:265:VAL:O	2.34	0.59
2:E:240:SER:HB2	2:E:243:LEU:HD23	1.84	0.59
1:J:45:GLU:HG2	1:J:46:TYR:HD1	1.68	0.59
1:D:15:TYR:HB3	1:D:31:ILE:HG13	1.83	0.59
1:G:31:ILE:HG22	1:G:135:ILE:HG12	1.85	0.59
1:A:81:PHE:O	1:A:102:GLN:N	2.35	0.58
1:D:186:ASN:HD21	1:D:251:LEU:HD13	1.67	0.58
2:K:57:SER:N	2:K:76:GLU:OE1	2.35	0.58
3:C:160:ASP:OD1	3:C:160:ASP:N	2.34	0.58
2:E:175:ASP:OD2	2:E:230:ARG:NH2	2.34	0.58
2:E:404:PRO:HA	3:F:146:LYS:HG3	1.86	0.58
1:G:168:THR:HG22	1:G:170:TRP:H	1.67	0.58
1:G:431:VAL:HG21	2:H:392:SER:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:LEU:HB3	3:I:178:ALA:HB3	1.85	0.58
2:K:173:GLU:HG2	2:K:230:ARG:HB3	1.85	0.58
2:B:57:SER:N	2:B:76:GLU:OE1	2.37	0.58
2:B:83:SER:HA	2:B:92:ILE:HD11	1.85	0.58
2:E:200:CYS:HA	2:E:226:CYS:HA	1.85	0.58
2:B:11:LEU:HD22	2:B:236:TRP:H	1.69	0.58
3:F:197:GLN:HE22	3:F:211:ASN:H	1.50	0.58
1:A:51:TYR:HB3	1:A:203:ILE:HG13	1.86	0.57
2:B:9:TYR:CD2	2:B:59:GLY:HA2	2.38	0.57
2:B:200:CYS:HB3	2:B:220:CYS:SG	2.43	0.57
1:D:32:THR:HG23	1:D:134:ASN:HB3	1.85	0.57
1:G:296:LEU:HD11	1:G:320:TYR:HB2	1.84	0.57
1:A:160:LYS:HB3	1:A:281:ASP:HB3	1.86	0.57
2:H:161:ARG:HH21	2:H:260:LEU:HD23	1.68	0.57
1:J:205:SER:OG	1:J:207:THR:O	2.22	0.57
3:I:232:ASP:OD1	3:I:236:ARG:N	2.37	0.57
1:A:24:TYR:CG	1:A:287:PHE:HB3	2.40	0.57
2:B:9:TYR:CE1	2:B:55:LEU:HB2	2.39	0.57
1:D:1:TYR:HE1	1:D:21:ARG:HH11	1.52	0.57
3:I:122:LEU:HD11	3:I:203:HIS:HA	1.86	0.57
2:K:345:PRO:HB2	2:K:358:HIS:CE1	2.39	0.57
1:G:37:LYS:HD3	1:G:267:ARG:HD2	1.86	0.57
1:J:9:SER:OG	1:J:273:VAL:O	2.22	0.57
1:D:230:HIS:CE1	1:D:232:PRO:HB3	2.39	0.57
2:H:297:THR:HB	2:H:307:THR:HB	1.87	0.57
1:A:368:GLN:NE2	1:A:369:ILE:O	2.38	0.57
2:E:363:TYR:HB3	2:E:366:SER:HB3	1.87	0.57
2:B:240:SER:HB2	2:B:243:LEU:HD23	1.87	0.57
2:H:402:LEU:HD13	3:I:175:LEU:HD11	1.87	0.57
1:J:252:LYS:HA	1:J:261:ILE:HD13	1.87	0.57
1:A:38:LEU:N	1:A:268:ALA:O	2.32	0.57
2:B:34:GLU:OE1	2:B:34:GLU:N	2.38	0.57
1:G:220:VAL:HG13	1:G:234:THR:HG23	1.85	0.57
2:K:11:LEU:HD22	2:K:236:TRP:H	1.69	0.57
3:L:149:ARG:NE	3:L:176:GLU:OE1	2.38	0.57
1:G:59:ALA:HB3	1:G:103:VAL:HB	1.87	0.57
1:G:198:GLY:HA3	2:K:288:HIS:CE1	2.40	0.57
1:J:38:LEU:N	1:J:268:ALA:O	2.35	0.57
1:D:41:THR:OG1	1:D:125:HIS:O	2.17	0.56
1:J:15:TYR:HB3	1:J:31:ILE:HG13	1.87	0.56
2:K:151:CYS:SG	2:K:266:CYS:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:TYR:HB3	1:D:203:ILE:HG13	1.86	0.56
2:E:66:MET:N	2:E:77:ILE:O	2.29	0.56
2:E:296:ILE:HB	2:E:329:VAL:HG13	1.88	0.56
1:G:17:THR:HG23	1:G:29:ILE:HG23	1.86	0.56
2:H:200:CYS:HB3	2:H:220:CYS:SG	2.45	0.56
1:J:1:TYR:N	1:J:282:ILE:O	2.33	0.56
1:J:10:GLN:HB3	1:J:13:ILE:HD11	1.87	0.56
2:E:22:CYS:SG	2:E:29:SER:OG	2.64	0.56
1:J:9:SER:HB3	1:J:276:ILE:HG13	1.87	0.56
1:J:174:ASP:OD1	1:J:174:ASP:N	2.37	0.56
3:C:152:HIS:N	3:C:174:ASP:OD1	2.35	0.56
1:J:369:ILE:HG22	1:J:370:CYS:H	1.70	0.56
2:K:12:THR:HG21	2:K:67:ARG:HH22	1.70	0.56
1:A:88:MET:HG2	1:A:93:TYR:HB2	1.87	0.56
1:A:260:GLU:HB3	1:A:269:GLU:HG3	1.88	0.56
2:E:362:ARG:HH11	2:E:363:TYR:H	1.53	0.56
1:G:396:GLN:O	1:G:396:GLN:NE2	2.38	0.56
2:H:87:SER:HA	2:K:88:ARG:HD3	1.88	0.56
2:B:66:MET:N	2:B:77:ILE:O	2.28	0.56
3:C:129:PRO:HA	3:C:139:TYR:HA	1.86	0.56
3:L:211:ASN:O	3:L:211:ASN:ND2	2.39	0.56
2:E:87:SER:HA	2:H:88:ARG:HD3	1.87	0.56
3:I:256:VAL:HA	3:I:266:LYS:HA	1.88	0.56
1:J:396:GLN:NE2	1:J:396:GLN:O	2.39	0.56
2:E:141:HIS:ND1	2:K:126:PRO:HB3	2.21	0.55
2:B:169:LEU:HD12	2:B:170:PRO:HD2	1.88	0.55
2:B:2:THR:HA	2:B:61:LEU:HD21	1.87	0.55
2:E:402:LEU:HD11	3:F:175:LEU:HD11	1.89	0.55
3:I:192:THR:HB	3:I:236:ARG:HH11	1.71	0.55
1:J:64:GLY:N	1:J:99:GLU:O	2.39	0.55
2:K:161:ARG:HH21	2:K:260:LEU:HD23	1.71	0.55
3:C:147:LEU:HB3	3:C:178:ALA:HB3	1.89	0.55
3:C:197:GLN:HE22	3:C:211:ASN:H	1.54	0.55
1:D:95:PHE:CE1	2:E:227:ARG:HB3	2.41	0.55
1:G:47:VAL:HG22	1:G:120:GLU:HG3	1.88	0.55
2:K:166:GLU:HB3	2:K:252:LYS:HG3	1.87	0.55
3:L:147:LEU:HB3	3:L:178:ALA:HB3	1.89	0.55
1:D:59:ALA:HB3	1:D:103:VAL:HB	1.87	0.55
2:H:12:THR:HG21	2:H:67:ARG:HH22	1.71	0.55
2:B:2:THR:HG23	2:B:61:LEU:HD11	1.88	0.55
3:C:272:CYS:SG	3:C:273:GLU:N	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:HIS:CE1	1:G:286:LEU:HD11	2.42	0.55
1:A:22:ALA:HB1	1:G:381:HIS:CD2	2.42	0.55
2:B:179:VAL:HA	2:B:188:VAL:HG22	1.88	0.55
2:E:360:TYR:HA	2:E:368:ILE:HD11	1.89	0.55
2:H:200:CYS:HA	2:H:226:CYS:HA	1.88	0.55
1:J:81:PHE:O	1:J:102:GLN:N	2.37	0.55
2:B:147:VAL:O	2:B:268:VAL:N	2.29	0.55
2:E:11:LEU:HD22	2:E:236:TRP:H	1.71	0.55
1:G:328:CYS:HB2	1:G:346:LEU:HD13	1.89	0.55
1:J:247:LYS:HE3	1:J:249:PRO:HB3	1.89	0.55
1:G:129:VAL:HB	1:G:148:VAL:HB	1.89	0.55
2:H:2:THR:HG23	2:H:61:LEU:HD11	1.89	0.55
3:I:126:LYS:H	3:I:126:LYS:HD3	1.72	0.55
1:A:129:VAL:HB	1:A:148:VAL:HB	1.89	0.54
1:D:38:LEU:HB3	1:D:268:ALA:HB3	1.87	0.54
1:J:392:GLN:OE1	1:J:394:HIS:N	2.24	0.54
3:F:232:ASP:OD1	3:F:236:ARG:N	2.40	0.54
2:K:363:TYR:HB3	2:K:366:SER:HB3	1.87	0.54
3:C:208:GLN:O	3:C:215:THR:OG1	2.22	0.54
1:D:84:VAL:O	1:D:86:PRO:HD3	2.07	0.54
1:J:135:ILE:N	1:J:142:ILE:O	2.40	0.54
2:K:18:ARG:H	2:K:242:LYS:HG2	1.73	0.54
1:G:133:LEU:HB3	1:G:135:ILE:HG13	1.89	0.54
1:J:186:ASN:HD21	1:J:251:LEU:HD13	1.72	0.54
1:D:3:HIS:CD2	1:D:19:VAL:HG12	2.42	0.54
1:D:81:PHE:O	1:D:102:GLN:N	2.39	0.54
1:D:361:ILE:HD12	1:D:402:VAL:HA	1.88	0.54
2:K:9:TYR:CZ	2:K:55:LEU:HB2	2.41	0.54
2:K:240:SER:HB2	2:K:243:LEU:HD23	1.89	0.54
2:K:9:TYR:CD2	2:K:59:GLY:HA2	2.43	0.54
2:K:52:GLN:N	2:K:67:ARG:O	2.39	0.54
1:A:43:ASN:HB3	1:A:123:LYS:HB3	1.89	0.54
1:G:45:GLU:HG2	1:G:46:TYR:HD1	1.72	0.54
1:G:95:PHE:CE1	2:H:227:ARG:HB3	2.43	0.54
2:K:5:LEU:HB3	2:K:55:LEU:HD11	1.90	0.54
2:K:11:LEU:HD13	2:K:236:TRP:CD2	2.42	0.54
1:G:387:ILE:HD12	2:H:278:PHE:HD1	1.73	0.54
3:L:256:VAL:HA	3:L:266:LYS:HA	1.89	0.54
3:C:215:THR:HB	3:C:250:ARG:HB3	1.90	0.54
2:K:199:GLU:HB3	2:K:227:ARG:HG2	1.90	0.54
2:H:9:TYR:CZ	2:H:55:LEU:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:ASP:HA	2:K:239:ASN:HD21	1.73	0.53
3:L:272:CYS:SG	3:L:273:GLU:N	2.81	0.53
2:E:289:PRO:HG3	2:E:330:TRP:HH2	1.72	0.53
1:G:348:GLU:O	1:G:349:GLN:NE2	2.41	0.53
1:J:38:LEU:HB3	1:J:268:ALA:HB3	1.90	0.53
2:E:136:ARG:HB2	2:E:294:TYR:HB2	1.91	0.53
2:E:400:TYR:O	2:E:403:THR:OG1	2.25	0.53
1:G:140:HIS:HE1	1:G:286:LEU:HD11	1.73	0.53
2:B:397:LEU:O	2:B:401:ARG:N	2.39	0.53
1:D:129:VAL:HB	1:D:148:VAL:HB	1.91	0.53
1:G:63:CYS:SG	2:H:227:ARG:NH2	2.77	0.53
1:A:174:ASP:OD1	1:A:174:ASP:N	2.41	0.53
1:A:413:LEU:HD13	2:B:374:CYS:SG	2.49	0.53
1:D:219:LEU:HD11	1:D:233:TYR:HB2	1.90	0.53
2:E:222:LYS:HB2	2:E:225:GLN:HE21	1.72	0.53
2:E:280:PHE:HE1	2:E:343:THR:H	1.57	0.53
1:G:142:ILE:HG13	1:G:156:PHE:CD2	2.43	0.53
3:L:232:ASP:OD1	3:L:236:ARG:N	2.42	0.53
1:A:396:GLN:O	1:A:396:GLN:NE2	2.42	0.53
2:H:136:ARG:HD2	2:H:331:GLY:O	2.09	0.53
1:A:86:PRO:HB2	1:A:93:TYR:HB3	1.90	0.53
1:A:224:PRO:HA	1:A:232:PRO:HG3	1.91	0.53
2:K:191:PRO:HG3	2:K:230:ARG:HH12	1.74	0.53
2:B:8:GLU:HG3	2:B:255:LEU:HD21	1.91	0.53
1:G:264:ASN:HB2	1:G:265:PRO:HD3	1.91	0.53
2:H:348:PRO:HD2	2:H:355:VAL:HA	1.89	0.53
3:L:132:LEU:HD23	3:L:137:ASN:HD21	1.74	0.53
1:A:1:TYR:OH	1:A:21:ARG:HD3	2.09	0.53
2:E:33:ILE:HG12	2:E:49:THR:HG22	1.91	0.53
1:G:25:ALA:N	1:G:288:THR:O	2.26	0.53
1:J:394:HIS:HB3	1:J:396:GLN:OE1	2.09	0.53
2:K:326:TRP:CH2	2:K:328:PHE:HB3	2.44	0.53
1:D:297:SER:O	1:D:321:SER:OG	2.24	0.52
1:J:193:GLY:N	1:J:204:GLN:OE1	2.41	0.52
1:A:307:VAL:HG22	1:A:381:HIS:HB2	1.91	0.52
2:K:296:ILE:HB	2:K:329:VAL:HG13	1.91	0.52
1:D:259:CYS:SG	1:D:268:ALA:HB1	2.49	0.52
1:A:66:GLN:NE2	1:A:67:GLU:O	2.41	0.52
2:B:412:LEU:HD23	2:B:416:CYS:HA	1.92	0.52
2:H:169:LEU:HB3	2:H:249:ALA:HB1	1.91	0.52
2:K:70:MET:O	2:K:73:THR:OG1	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:137:GLU:OE2	2:K:332:ASN:ND2	2.42	0.52
2:B:67:ARG:HD3	2:B:74:ILE:HG23	1.92	0.52
1:D:95:PHE:H	2:E:227:ARG:HH21	1.58	0.52
1:G:369:ILE:HG22	1:G:370:CYS:H	1.74	0.52
2:H:22:CYS:SG	2:H:29:SER:OG	2.67	0.52
1:J:222:GLN:HG3	1:J:232:PRO:HB2	1.90	0.52
1:A:252:LYS:HA	1:A:261:ILE:HD13	1.91	0.52
2:K:2:THR:HA	2:K:61:LEU:HD21	1.92	0.52
2:K:222:LYS:HB2	2:K:225:GLN:NE2	2.24	0.52
1:A:84:VAL:O	1:A:86:PRO:HD3	2.10	0.52
1:A:89:TRP:CZ3	2:B:71:HIS:HA	2.45	0.52
3:I:269:PRO:HG2	3:I:272:CYS:HB2	1.91	0.52
1:A:142:ILE:HG13	1:A:156:PHE:CD2	2.45	0.52
1:D:142:ILE:HG13	1:D:156:PHE:CD2	2.44	0.52
1:D:366:ARG:HG2	1:D:375:THR:HB	1.91	0.52
2:H:317:ARG:HB3	2:H:319:PHE:HE2	1.75	0.52
3:I:243:GLY:O	3:I:254:SER:N	2.37	0.52
1:D:309:SER:OG	1:D:310:SER:N	2.43	0.52
1:D:348:GLU:O	1:D:349:GLN:NE2	2.43	0.52
2:E:34:GLU:N	2:E:34:GLU:OE1	2.42	0.52
2:H:148:GLU:HA	2:H:267:THR:HA	1.92	0.52
1:A:96:CYS:O	1:A:100:ASN:ND2	2.36	0.52
2:E:2:THR:HG23	2:E:61:LEU:HD11	1.91	0.51
1:G:300:GLU:O	1:G:319:LYS:N	2.39	0.51
3:L:152:HIS:N	3:L:174:ASP:OD1	2.43	0.51
2:B:115:LYS:HA	2:B:120:ARG:HA	1.92	0.51
2:B:117:ASP:OD1	2:B:117:ASP:N	2.41	0.51
2:B:276:ILE:HG22	2:B:285:LEU:HG	1.92	0.51
2:E:84:LEU:HA	2:E:112:MET:HA	1.91	0.51
2:B:113:GLU:HA	2:B:122:SER:HB2	1.92	0.51
2:E:412:LEU:HD23	2:E:416:CYS:HA	1.92	0.51
1:G:294:PRO:HB3	1:G:324:LYS:HB3	1.92	0.51
1:A:95:PHE:H	2:B:227:ARG:NH2	2.07	0.51
1:A:192:TYR:CD2	1:A:206:ARG:HD3	2.45	0.51
1:J:5:THR:O	1:J:278:LEU:N	2.32	0.51
1:J:238:SER:HB2	1:J:241:GLU:HB2	1.92	0.51
1:J:348:GLU:O	1:J:349:GLN:NE2	2.43	0.51
1:A:15:TYR:HB3	1:A:31:ILE:HG13	1.92	0.51
1:A:247:LYS:HG3	1:A:249:PRO:HD3	1.92	0.51
1:D:256:PRO:HG3	2:E:304:PRO:HD3	1.91	0.51
1:G:1:TYR:N	1:G:282:ILE:O	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:TYR:CE1	2:H:55:LEU:HB2	2.45	0.51
2:H:11:LEU:HD22	2:H:236:TRP:H	1.75	0.51
1:A:59:ALA:HB3	1:A:103:VAL:HB	1.91	0.51
1:D:327:LYS:HA	1:D:345:GLU:HA	1.93	0.51
2:E:11:LEU:HD13	2:E:236:TRP:CD2	2.45	0.51
3:I:257:MET:HG3	3:I:265:VAL:HB	1.93	0.51
1:J:17:THR:HG23	1:J:29:ILE:HG23	1.93	0.51
1:D:171:THR:HG22	1:D:173:PHE:H	1.75	0.51
1:D:224:PRO:HA	1:D:232:PRO:HG3	1.93	0.51
2:E:117:ASP:OD1	2:E:117:ASP:N	2.41	0.51
2:H:151:CYS:SG	2:H:266:CYS:N	2.84	0.51
1:D:264:ASN:HB2	1:D:265:PRO:HD3	1.93	0.51
2:E:9:TYR:CD2	2:E:59:GLY:HA2	2.46	0.51
1:G:84:VAL:O	1:G:86:PRO:HD3	2.11	0.51
1:J:171:THR:HG22	1:J:173:PHE:H	1.75	0.51
1:J:224:PRO:HA	1:J:232:PRO:HG3	1.92	0.51
1:A:82:THR:HG22	1:A:101:THR:HG22	1.93	0.50
3:C:142:VAL:HG12	3:C:147:LEU:HA	1.93	0.50
2:E:113:GLU:HA	2:E:122:SER:HB2	1.93	0.50
3:F:160:ASP:OD1	3:F:160:ASP:N	2.44	0.50
1:J:142:ILE:HG13	1:J:156:PHE:CE2	2.47	0.50
2:H:38:SER:OG	2:H:130:LYS:N	2.39	0.50
2:H:164:TYR:HB3	2:H:256:HIS:ND1	2.26	0.50
3:I:207:VAL:HG22	3:I:216:VAL:HG12	1.91	0.50
2:K:160:ASN:O	2:K:160:ASN:ND2	2.40	0.50
1:D:111:SER:OG	1:D:113:ASP:OD1	2.25	0.50
3:F:272:CYS:SG	3:F:273:GLU:N	2.84	0.50
1:G:218:ASN:ND2	1:G:218:ASN:O	2.45	0.50
2:K:2:THR:HG23	2:K:61:LEU:HD11	1.94	0.50
1:A:224:PRO:CA	1:A:232:PRO:HG3	2.41	0.50
1:D:252:LYS:HA	1:D:261:ILE:HD13	1.92	0.50
1:D:384:LYS:H	1:D:384:LYS:HD2	1.76	0.50
1:A:159:VAL:HG22	1:A:283:PRO:HD2	1.93	0.50
2:B:14:PRO:HG3	2:B:67:ARG:NE	2.27	0.50
3:C:257:MET:HG3	3:C:265:VAL:HB	1.94	0.50
1:D:9:SER:OG	1:D:273:VAL:O	2.30	0.50
2:K:236:TRP:HZ3	2:K:253:GLY:HA3	1.76	0.50
1:A:171:THR:HG22	1:A:173:PHE:H	1.75	0.50
1:G:366:ARG:HG2	1:G:375:THR:HB	1.92	0.50
1:J:418:ALA:O	1:J:422:ILE:HG12	2.11	0.50
2:K:397:LEU:HD21	2:K:401:ARG:HH21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:PHE:H	2:H:227:ARG:HH21	1.58	0.50
2:H:167:MET:HG2	2:H:253:GLY:O	2.12	0.50
2:H:345:PRO:HG2	2:H:358:HIS:HA	1.93	0.50
2:K:186:VAL:HB	2:K:217:PHE:HD2	1.76	0.50
1:A:219:LEU:HD11	1:A:233:TYR:HB2	1.94	0.50
1:A:427:LEU:HD23	1:A:430:ILE:HD11	1.94	0.50
2:B:107:GLY:O	2:B:129:VAL:N	2.39	0.50
1:G:418:ALA:O	1:G:422:ILE:HG12	2.11	0.50
2:K:53:TYR:CE2	2:K:100:LEU:HB2	2.47	0.50
2:K:345:PRO:HB2	2:K:358:HIS:ND1	2.27	0.50
1:A:264:ASN:HB2	1:A:265:PRO:HD3	1.93	0.49
1:A:348:GLU:O	1:A:349:GLN:NE2	2.45	0.49
1:G:171:THR:HG22	1:G:173:PHE:H	1.77	0.49
2:K:66:MET:N	2:K:77:ILE:O	2.33	0.49
1:A:47:VAL:HG13	1:A:120:GLU:HG3	1.93	0.49
3:F:197:GLN:HE22	3:F:211:ASN:N	2.10	0.49
2:H:70:MET:O	2:H:73:THR:OG1	2.20	0.49
2:H:317:ARG:HB3	2:H:319:PHE:CE2	2.47	0.49
1:A:218:ASN:O	1:A:218:ASN:ND2	2.40	0.49
1:D:38:LEU:N	1:D:268:ALA:O	2.40	0.49
1:A:225:LYS:H	1:A:230:HIS:CE1	2.31	0.49
2:E:321:VAL:HG12	2:E:340:ALA:HB2	1.94	0.49
2:H:291:ASN:O	2:H:293:THR:HG23	2.12	0.49
2:B:199:GLU:O	2:B:227:ARG:N	2.33	0.49
2:E:169:LEU:HD12	2:E:170:PRO:HD2	1.93	0.49
2:H:53:TYR:CE2	2:H:100:LEU:HB2	2.48	0.49
2:H:411:CYS:HA	2:H:414:VAL:HG22	1.93	0.49
1:J:247:LYS:HG3	1:J:249:PRO:HD3	1.95	0.49
1:A:402:VAL:HG21	2:B:359:TYR:CE1	2.46	0.49
2:H:345:PRO:HB2	2:H:358:HIS:CG	2.47	0.49
1:J:61:LYS:HB2	1:J:66:GLN:HB2	1.93	0.49
1:A:29:ILE:HG13	1:A:137:VAL:HG22	1.92	0.49
2:B:181:LEU:HD23	2:B:223:LYS:HB3	1.94	0.49
3:I:211:ASN:O	3:I:211:ASN:ND2	2.44	0.49
1:J:95:PHE:HB2	2:K:227:ARG:HH21	1.77	0.49
1:A:51:TYR:HE2	1:A:238:SER:HA	1.77	0.49
1:A:80:VAL:HA	1:A:102:GLN:O	2.11	0.49
1:D:364:GLU:HB3	1:D:377:LYS:HG3	1.93	0.49
2:E:346:GLY:O	2:E:358:HIS:HB3	2.12	0.49
3:F:192:THR:HB	3:F:236:ARG:HH11	1.76	0.49
2:H:397:LEU:HD21	2:H:401:ARG:HE	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:200:CYS:HB3	2:K:220:CYS:SG	2.52	0.49
1:A:121:ALA:HB1	1:A:189:PHE:CZ	2.47	0.49
2:H:126:PRO:HB3	2:K:141:HIS:ND1	2.28	0.49
2:H:136:ARG:HH11	2:H:332:ASN:HA	1.78	0.49
2:K:136:ARG:HB2	2:K:294:TYR:HD2	1.77	0.49
2:K:215:LYS:HZ3	2:K:215:LYS:HB2	1.76	0.49
1:D:413:LEU:HD13	2:E:374:CYS:SG	2.53	0.49
2:H:298:ARG:NH2	2:H:327:GLU:OE1	2.42	0.49
1:J:18:ILE:HG22	1:J:28:PRO:HA	1.95	0.49
1:J:402:VAL:HG21	2:K:359:TYR:CE1	2.47	0.49
2:K:113:GLU:HA	2:K:122:SER:HB2	1.95	0.49
2:H:84:LEU:HA	2:H:112:MET:HA	1.94	0.48
2:K:48:GLN:HA	2:K:99:PHE:HA	1.95	0.48
2:B:397:LEU:HG	2:B:401:ARG:HB2	1.95	0.48
2:H:345:PRO:HB2	2:H:358:HIS:CE1	2.47	0.48
1:J:296:LEU:HD11	1:J:320:TYR:HB2	1.95	0.48
2:K:348:PRO:HD2	2:K:355:VAL:HA	1.95	0.48
2:B:268:VAL:HG22	2:B:269:PRO:HD2	1.95	0.48
1:J:60:ILE:HD11	2:K:244:PRO:HB3	1.94	0.48
1:J:192:TYR:CD2	1:J:206:ARG:HD3	2.48	0.48
1:J:217:THR:O	1:J:217:THR:OG1	2.30	0.48
2:K:9:TYR:CE1	2:K:55:LEU:HB2	2.49	0.48
3:C:211:ASN:O	3:C:211:ASN:ND2	2.44	0.48
1:D:304:ASN:OD1	1:D:304:ASN:N	2.41	0.48
2:H:360:TYR:CD1	2:H:368:ILE:HD11	2.49	0.48
2:H:397:LEU:HG	2:H:401:ARG:HB2	1.94	0.48
2:H:397:LEU:O	2:H:401:ARG:N	2.41	0.48
1:J:71:THR:OG1	1:J:76:GLU:OE2	2.30	0.48
2:K:55:LEU:HG	2:K:61:LEU:HA	1.94	0.48
2:K:84:LEU:HA	2:K:112:MET:HA	1.95	0.48
2:K:246:ALA:HB3	2:K:249:ALA:HB3	1.94	0.48
2:B:384:ALA:O	2:B:388:LEU:HG	2.13	0.48
1:J:304:ASN:OD1	1:J:304:ASN:N	2.47	0.48
2:K:169:LEU:HD12	2:K:170:PRO:HD2	1.94	0.48
1:A:362:HIS:CE1	1:A:403:SER:HA	2.48	0.48
2:E:200:CYS:HB3	2:E:220:CYS:SG	2.53	0.48
1:J:310:SER:HA	1:J:392:GLN:HE22	1.79	0.48
2:K:276:ILE:HG22	2:K:285:LEU:HG	1.96	0.48
2:K:303:GLU:HB2	2:K:305:HIS:HD2	1.77	0.48
2:B:353:HIS:CE1	2:B:354:GLU:HG2	2.49	0.48
1:D:368:GLN:HG2	1:D:373:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ILE:N	1:G:142:ILE:O	2.45	0.48
1:G:303:LEU:HD11	1:G:306:CYS:HB2	1.95	0.48
1:G:394:HIS:HB3	1:G:396:GLN:OE1	2.13	0.48
3:I:137:ASN:OD1	3:I:137:ASN:N	2.46	0.48
2:B:9:TYR:CZ	2:B:55:LEU:HB2	2.49	0.48
2:B:345:PRO:HG2	2:B:358:HIS:HA	1.96	0.48
2:E:303:GLU:OE1	2:E:305:HIS:HE1	1.97	0.48
2:H:268:VAL:HG22	2:H:269:PRO:HD2	1.96	0.48
1:A:197:PRO:HG3	1:A:218:ASN:HB2	1.95	0.48
2:E:8:GLU:HG3	2:E:255:LEU:HD21	1.94	0.48
2:E:167:MET:HG3	2:E:236:TRP:HE3	1.77	0.48
2:K:166:GLU:HG2	2:K:252:LYS:HE3	1.95	0.48
1:G:364:GLU:HB3	1:G:377:LYS:HG3	1.96	0.47
2:H:113:GLU:HA	2:H:122:SER:HB2	1.94	0.47
1:J:312:PHE:HA	1:J:357:SER:HB2	1.96	0.47
2:E:164:TYR:HB3	2:E:256:HIS:ND1	2.28	0.47
2:E:295:LEU:HD13	2:E:330:TRP:HE3	1.78	0.47
3:F:179:ASP:OD1	3:F:179:ASP:N	2.47	0.47
1:J:320:TYR:OH	1:J:347:THR:N	2.42	0.47
1:A:171:THR:HG22	1:A:173:PHE:N	2.29	0.47
2:B:61:LEU:HD12	2:B:61:LEU:H	1.78	0.47
2:B:348:PRO:HD2	2:B:355:VAL:HA	1.96	0.47
1:G:197:PRO:HB3	1:G:217:THR:HA	1.96	0.47
2:H:8:GLU:HG3	2:H:255:LEU:HD21	1.95	0.47
2:H:136:ARG:NH1	2:H:332:ASN:HA	2.29	0.47
2:H:283:VAL:HG23	2:H:321:VAL:HG21	1.95	0.47
2:H:345:PRO:HB2	2:H:358:HIS:ND1	2.29	0.47
1:J:386:HIS:HA	2:K:343:THR:HG21	1.97	0.47
3:L:196:PRO:O	3:L:200:TYR:OH	2.20	0.47
2:B:12:THR:O	2:B:98:TYR:OH	2.30	0.47
1:D:1:TYR:OH	1:D:21:ARG:HD3	2.13	0.47
3:F:241:VAL:HB	3:F:255:VAL:HG12	1.96	0.47
1:G:205:SER:OG	1:G:207:THR:O	2.28	0.47
2:H:288:HIS:ND1	2:H:314:PRO:HB3	2.28	0.47
2:B:246:ALA:HB3	2:B:249:ALA:HB3	1.97	0.47
2:E:276:ILE:HG22	2:E:285:LEU:HG	1.95	0.47
3:F:243:GLY:O	3:F:254:SER:N	2.40	0.47
1:G:47:VAL:HG11	1:G:208:VAL:HG22	1.96	0.47
2:H:53:TYR:O	2:H:97:GLY:N	2.35	0.47
2:H:115:LYS:HA	2:H:120:ARG:HA	1.95	0.47
2:H:289:PRO:HG3	2:H:330:TRP:HH2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:THR:O	1:J:210:SER:OG	2.30	0.47
2:K:167:MET:HG2	2:K:253:GLY:O	2.14	0.47
1:A:416:GLY:O	1:A:420:ILE:HG13	2.13	0.47
2:E:53:TYR:CE2	2:E:100:LEU:HB2	2.50	0.47
2:E:189:THR:HA	2:E:214:THR:HB	1.97	0.47
2:H:152:GLN:NE2	2:H:263:ASP:OD2	2.47	0.47
1:J:259:CYS:SG	1:J:268:ALA:HB1	2.54	0.47
2:B:164:TYR:HB3	2:B:256:HIS:ND1	2.30	0.47
2:B:233:ASN:OD1	2:B:233:ASN:N	2.48	0.47
2:B:365:MET:HA	2:B:368:ILE:HD12	1.96	0.47
3:C:207:VAL:HG22	3:C:216:VAL:HG12	1.96	0.47
1:D:81:PHE:HB2	1:D:102:GLN:HB3	1.97	0.47
1:D:289:ARG:HB2	1:D:292:GLU:HG2	1.95	0.47
2:E:5:LEU:HB3	2:E:55:LEU:HD11	1.97	0.47
2:E:393:ARG:HH22	2:E:419:ARG:CZ	2.28	0.47
2:H:173:GLU:HG2	2:H:230:ARG:HB3	1.96	0.47
3:L:137:ASN:O	3:L:224:GLY:HA2	2.14	0.47
2:B:17:ALA:HB3	2:B:32:ALA:HB3	1.96	0.47
2:B:55:LEU:HA	2:B:62:LYS:H	1.80	0.47
2:H:160:ASN:O	2:H:160:ASN:ND2	2.46	0.47
1:G:193:GLY:HA2	1:G:214:TYR:CG	2.49	0.47
2:K:151:CYS:O	2:K:264:GLY:N	2.47	0.47
2:B:11:LEU:HD13	2:B:236:TRP:CD2	2.49	0.47
1:G:18:ILE:HG22	1:G:28:PRO:HA	1.97	0.47
1:G:252:LYS:HA	1:G:261:ILE:HD13	1.97	0.47
2:H:17:ALA:HB3	2:H:32:ALA:HB3	1.96	0.47
2:H:246:ALA:HB3	2:H:249:ALA:HB3	1.97	0.47
1:A:394:HIS:HB3	1:A:396:GLN:OE1	2.15	0.46
2:H:9:TYR:CD2	2:H:59:GLY:HA2	2.49	0.46
2:B:136:ARG:HB2	2:B:294:TYR:HB2	1.97	0.46
1:D:369:ILE:HG22	1:D:370:CYS:H	1.80	0.46
2:E:238:TYR:HD2	2:E:240:SER:HG	1.59	0.46
1:A:369:ILE:HG22	1:A:370:CYS:H	1.80	0.46
2:B:137:GLU:HA	2:B:293:THR:HG22	1.97	0.46
2:B:167:MET:HG2	2:B:253:GLY:O	2.15	0.46
1:D:9:SER:HB3	1:D:276:ILE:HG13	1.96	0.46
2:E:107:GLY:H	2:E:129:VAL:HB	1.80	0.46
2:H:34:GLU:N	2:H:34:GLU:OE1	2.48	0.46
1:J:387:ILE:HB	2:K:278:PHE:CD1	2.51	0.46
1:A:161:ILE:HG22	1:A:280:PHE:HD1	1.80	0.46
2:B:53:TYR:CE2	2:B:100:LEU:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:LEU:HD23	1:D:378:GLY:HA3	1.97	0.46
1:G:193:GLY:N	1:G:204:GLN:OE1	2.48	0.46
1:G:330:VAL:HG12	1:G:369:ILE:HG23	1.97	0.46
2:H:215:LYS:HB2	2:H:215:LYS:HZ2	1.78	0.46
3:I:225:ASP:O	3:I:228:ARG:HG3	2.15	0.46
1:J:19:VAL:HG23	1:J:27:LEU:HB3	1.98	0.46
3:L:243:GLY:O	3:L:254:SER:N	2.43	0.46
1:A:192:TYR:CE2	1:A:206:ARG:HD3	2.51	0.46
2:E:9:TYR:CE1	2:E:55:LEU:HB2	2.50	0.46
3:F:196:PRO:O	3:F:200:TYR:OH	2.19	0.46
1:A:27:LEU:HD12	1:A:28:PRO:HD2	1.98	0.46
1:D:56:ASP:HB2	1:D:105:LYS:HG3	1.98	0.46
2:E:52:GLN:N	2:E:67:ARG:O	2.48	0.46
2:E:297:THR:HG21	2:E:319:PHE:CE1	2.51	0.46
2:H:67:ARG:HD3	2:H:74:ILE:HG23	1.98	0.46
2:H:181:LEU:HD23	2:H:223:LYS:HB3	1.97	0.46
1:J:220:VAL:HG13	1:J:234:THR:HG23	1.97	0.46
3:L:229:PRO:HA	3:L:240:ILE:HG22	1.98	0.46
1:A:219:LEU:HD13	1:A:235:GLN:HB3	1.97	0.46
2:H:210:THR:HG22	2:H:215:LYS:HZ2	1.81	0.46
2:H:400:TYR:O	2:H:406:ALA:HA	2.16	0.46
1:D:55:MET:SD	1:D:55:MET:N	2.89	0.46
2:E:9:TYR:CZ	2:E:55:LEU:HB2	2.50	0.46
2:E:27:CYS:SG	2:E:28:HIS:N	2.89	0.46
1:G:39:ILE:HG12	1:G:267:ARG:HB3	1.98	0.46
1:D:198:GLY:HA3	2:H:288:HIS:CE1	2.51	0.46
3:F:197:GLN:OE1	3:F:210:GLU:HA	2.16	0.46
1:G:413:LEU:HD13	2:H:374:CYS:SG	2.56	0.46
2:H:416:CYS:O	2:H:419:ARG:NH1	2.49	0.46
3:C:229:PRO:HA	3:C:240:ILE:HG22	1.98	0.46
2:E:50:SER:O	2:E:52:GLN:NE2	2.47	0.46
1:G:51:TYR:HB3	1:G:203:ILE:HG13	1.97	0.46
2:B:82:VAL:HG13	2:B:113:GLU:O	2.17	0.45
1:D:301:CYS:HA	1:D:318:VAL:HA	1.98	0.45
3:F:225:ASP:O	3:F:228:ARG:HG3	2.16	0.45
3:L:160:ASP:OD1	3:L:160:ASP:N	2.49	0.45
1:A:52:LYS:N	1:A:109:MET:O	2.45	0.45
2:B:12:THR:HG21	2:B:67:ARG:HH22	1.80	0.45
2:B:12:THR:HG23	2:B:13:ARG:H	1.81	0.45
2:B:44:TYR:CE1	2:B:103:ARG:HD3	2.51	0.45
1:A:417:SER:HA	1:A:420:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:386:HIS:HA	2:H:343:THR:OG1	2.15	0.45
2:K:12:THR:HG23	2:K:13:ARG:H	1.82	0.45
1:A:418:ALA:O	1:A:422:ILE:HG12	2.17	0.45
1:D:232:PRO:HA	2:H:145:HIS:ND1	2.31	0.45
1:J:251:LEU:O	1:J:255:ALA:N	2.50	0.45
1:J:387:ILE:HG23	2:K:339:TRP:O	2.17	0.45
3:L:126:LYS:HD3	3:L:126:LYS:H	1.80	0.45
1:A:135:ILE:N	1:A:142:ILE:O	2.47	0.45
1:A:309:SER:OG	1:A:310:SER:N	2.50	0.45
1:A:360:ASN:ND2	1:A:400:ALA:HA	2.32	0.45
3:C:130:ILE:HD11	3:C:140:ALA:HB2	1.98	0.45
2:K:85:TYR:HB2	2:K:89:PRO:HA	1.98	0.45
1:A:9:SER:OG	1:A:273:VAL:O	2.31	0.45
1:A:222:GLN:O	1:A:232:PRO:HG2	2.16	0.45
1:D:421:ILE:HD11	2:E:381:SER:HA	1.98	0.45
1:G:56:ASP:HA	2:H:239:ASN:HD21	1.82	0.45
2:K:210:THR:HG22	2:K:215:LYS:HZ3	1.80	0.45
1:A:431:VAL:HG21	2:B:392:SER:HA	1.98	0.45
3:C:271:ASN:OD1	3:I:182:GLN:NE2	2.48	0.45
1:D:339:LEU:HD22	1:D:354:ILE:HD12	1.98	0.45
2:E:132:ASN:OD1	2:E:132:ASN:N	2.38	0.45
1:J:47:VAL:HG11	1:J:208:VAL:HG22	1.99	0.45
2:K:164:TYR:HB3	2:K:256:HIS:ND1	2.32	0.45
1:A:193:GLY:N	1:A:204:GLN:OE1	2.49	0.45
1:D:170:TRP:HZ3	1:D:271:CYS:SG	2.40	0.45
3:I:160:ASP:N	3:I:160:ASP:OD1	2.50	0.45
2:B:17:ALA:HB1	2:B:242:LYS:HG2	1.99	0.45
2:B:199:GLU:HB3	2:B:227:ARG:HG2	1.98	0.45
3:C:147:LEU:O	3:C:177:TYR:HA	2.17	0.45
1:G:64:GLY:N	1:G:99:GLU:O	2.48	0.45
1:A:81:PHE:HB2	1:A:102:GLN:HB3	1.98	0.45
3:C:126:LYS:H	3:C:126:LYS:HD3	1.82	0.45
2:H:202:CYS:HB3	2:H:225:GLN:OE1	2.16	0.45
3:L:192:THR:OG1	3:L:194:GLU:OE2	2.31	0.45
1:A:368:GLN:HG2	1:A:373:TYR:CE2	2.52	0.44
3:C:202:TRP:CZ3	3:C:204:HIS:HB2	2.53	0.44
1:D:64:GLY:N	1:D:99:GLU:O	2.48	0.44
1:D:110:LYS:NZ	1:D:208:VAL:O	2.48	0.44
1:D:224:PRO:CA	1:D:232:PRO:HG3	2.46	0.44
1:G:219:LEU:HD11	1:G:233:TYR:HB2	1.98	0.44
1:G:421:ILE:HD11	2:H:381:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:TYR:CD1	2:H:55:LEU:HD13	2.52	0.44
1:J:113:ASP:HA	2:K:260:LEU:HD11	1.98	0.44
1:A:304:ASN:OD1	1:A:304:ASN:N	2.49	0.44
3:C:257:MET:N	3:C:265:VAL:O	2.41	0.44
1:G:197:PRO:HG3	1:G:218:ASN:HB2	1.99	0.44
2:H:300:LEU:HD11	2:H:327:GLU:HB2	1.99	0.44
1:A:170:TRP:HZ3	1:A:271:CYS:SG	2.41	0.44
2:E:327:GLU:HB2	2:E:337:ARG:HG2	2.00	0.44
2:H:190:PRO:HG3	2:H:210:THR:O	2.16	0.44
2:K:160:ASN:CB	2:K:256:HIS:HB3	2.40	0.44
1:A:186:ASN:HD21	1:A:251:LEU:HD22	1.82	0.44
2:B:210:THR:HG22	2:B:215:LYS:HZ2	1.82	0.44
1:D:329:ALA:HA	1:D:343:ALA:HA	1.99	0.44
1:G:368:GLN:HG2	1:G:373:TYR:CE2	2.52	0.44
2:H:11:LEU:HD13	2:H:236:TRP:CD2	2.52	0.44
3:I:197:GLN:HE22	3:I:211:ASN:N	2.14	0.44
2:K:115:LYS:HA	2:K:120:ARG:HA	1.99	0.44
2:K:201:GLU:O	2:K:225:GLN:HB3	2.18	0.44
3:C:232:ASP:OD1	3:C:236:ARG:N	2.50	0.44
1:G:21:ARG:HB3	1:G:24:TYR:HD2	1.82	0.44
1:G:301:CYS:HA	1:G:318:VAL:HA	1.98	0.44
2:H:233:ASN:N	2:H:233:ASN:OD1	2.50	0.44
1:J:200:PHE:HD1	1:J:200:PHE:HA	1.69	0.44
2:K:17:ALA:HB3	2:K:32:ALA:HB3	1.99	0.44
1:A:222:GLN:HG3	1:A:232:PRO:HB2	1.99	0.44
1:A:340:LYS:HB3	1:A:340:LYS:HE2	1.84	0.44
2:B:202:CYS:HB3	2:B:225:GLN:OE1	2.18	0.44
2:E:115:LYS:HA	2:E:120:ARG:HA	1.99	0.44
2:E:215:LYS:HB2	2:E:215:LYS:HZ3	1.83	0.44
3:I:168:LYS:HB2	3:I:177:TYR:CZ	2.53	0.44
1:J:333:PRO:HD3	1:J:368:GLN:HB2	2.00	0.44
3:L:257:MET:N	3:L:265:VAL:O	2.45	0.44
1:A:45:GLU:HG2	1:A:46:TYR:HD1	1.83	0.44
2:H:133:PRO:HG2	2:H:138:LEU:HD22	2.00	0.44
1:J:161:ILE:HG22	1:J:280:PHE:HD1	1.83	0.44
1:J:440:LYS:HA	1:J:440:LYS:HD3	1.72	0.44
2:K:83:SER:HA	2:K:92:ILE:HD11	2.00	0.44
1:G:265:PRO:HG2	1:G:267:ARG:CZ	2.48	0.44
2:B:77:ILE:HD12	2:B:77:ILE:HA	1.91	0.44
2:E:12:THR:HG23	2:E:13:ARG:H	1.83	0.44
2:E:116:LYS:HD3	2:E:116:LYS:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:PRO:HB2	2:E:358:HIS:ND1	2.33	0.44
2:E:353:HIS:CE1	2:E:354:GLU:HG2	2.53	0.44
1:J:52:LYS:N	1:J:109:MET:O	2.42	0.44
1:J:403:SER:OG	1:J:406:ALA:N	2.40	0.44
1:A:421:ILE:HD11	2:B:381:SER:HA	2.00	0.43
2:E:397:LEU:HD11	2:E:401:ARG:NH2	2.33	0.43
2:K:55:LEU:HA	2:K:62:LYS:H	1.81	0.43
3:L:207:VAL:HG22	3:L:216:VAL:HG12	2.00	0.43
1:A:384:LYS:H	1:A:384:LYS:HD2	1.83	0.43
2:B:41:HIS:CE1	2:B:152:GLN:HB2	2.53	0.43
2:B:197:LEU:HB3	2:B:207:ILE:HD11	2.00	0.43
3:C:200:TYR:HD2	3:C:232:ASP:HA	1.83	0.43
1:D:119:ALA:HB2	1:D:240:PHE:HE1	1.83	0.43
2:K:408:ILE:HG13	2:K:411:CYS:HB2	1.99	0.43
3:L:209:TYR:HB2	3:L:214:PHE:HA	2.00	0.43
1:A:434:TYR:HA	1:A:437:THR:HG22	2.00	0.43
2:B:52:GLN:N	2:B:67:ARG:O	2.48	0.43
3:F:256:VAL:HA	3:F:266:LYS:HA	2.01	0.43
2:K:48:GLN:HB3	2:K:99:PHE:CD2	2.54	0.43
2:K:287:LEU:HD22	2:K:330:TRP:CZ3	2.54	0.43
3:L:192:THR:HB	3:L:236:ARG:HH11	1.83	0.43
2:E:85:TYR:HB2	2:E:89:PRO:HA	2.00	0.43
2:E:210:THR:HG22	2:E:215:LYS:HZ3	1.83	0.43
2:E:348:PRO:HD2	2:E:355:VAL:HA	2.00	0.43
3:C:216:VAL:O	3:C:251:THR:N	2.51	0.43
1:G:340:LYS:HE2	1:G:340:LYS:HB3	1.77	0.43
2:H:55:LEU:HA	2:H:62:LYS:H	1.82	0.43
2:H:360:TYR:HD1	2:H:368:ILE:HD11	1.83	0.43
3:I:202:TRP:HE1	3:I:228:ARG:HB2	1.84	0.43
1:A:262:TYR:HB2	1:A:267:ARG:HE	1.82	0.43
2:B:12:THR:OG1	2:B:52:GLN:OE1	2.35	0.43
1:D:80:VAL:HA	1:D:102:GLN:O	2.17	0.43
1:D:366:ARG:HA	1:D:375:THR:HA	2.01	0.43
1:G:9:SER:HB3	1:G:276:ILE:HG13	2.00	0.43
2:H:157:ASP:OD1	2:H:158:ALA:N	2.52	0.43
2:H:318:ASN:HD21	4:H:502:NAG:H62	1.84	0.43
1:J:366:ARG:HG2	1:J:375:THR:HB	2.00	0.43
2:K:67:ARG:HD3	2:K:74:ILE:HG23	2.00	0.43
2:K:303:GLU:OE1	2:K:305:HIS:NE2	2.48	0.43
3:L:234:GLN:CD	3:L:236:ARG:HH21	2.21	0.43
2:B:48:GLN:HB3	2:B:99:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:HB3	1:D:217:THR:HA	1.99	0.43
2:E:160:ASN:O	2:E:160:ASN:ND2	2.51	0.43
1:J:303:LEU:HD23	1:J:378:GLY:HA3	2.01	0.43
3:L:197:GLN:HE22	3:L:211:ASN:N	2.10	0.43
2:B:159:GLN:HB3	2:B:161:ARG:HD2	2.01	0.43
2:B:166:GLU:HB3	2:B:252:LYS:HG3	2.01	0.43
2:B:189:THR:HA	2:B:214:THR:HB	2.01	0.43
2:E:191:PRO:HG3	2:E:230:ARG:HH12	1.84	0.43
2:E:233:ASN:N	2:E:233:ASN:OD1	2.51	0.43
2:E:246:ALA:HB3	2:E:249:ALA:HB3	2.00	0.43
2:K:34:GLU:N	2:K:34:GLU:OE1	2.52	0.43
1:A:221:LEU:HA	1:A:233:TYR:HA	2.01	0.43
1:D:112:ASP:N	1:D:112:ASP:OD1	2.52	0.43
1:D:222:GLN:O	1:D:232:PRO:HG2	2.19	0.43
1:G:312:PHE:HA	1:G:357:SER:HB2	2.00	0.43
1:J:31:ILE:HG22	1:J:135:ILE:HG23	2.00	0.43
2:K:345:PRO:HB2	2:K:358:HIS:CG	2.54	0.43
3:L:117:ARG:O	3:L:121:LYS:HG2	2.19	0.43
1:D:265:PRO:O	1:D:267:ARG:HG2	2.19	0.43
1:D:357:SER:O	1:D:394:HIS:NE2	2.51	0.43
2:H:12:THR:OG1	2:H:52:GLN:OE1	2.36	0.43
2:H:44:TYR:CE1	2:H:103:ARG:HD3	2.54	0.43
1:J:175:ARG:HA	1:J:175:ARG:HD3	1.85	0.43
1:A:387:ILE:HB	2:B:278:PHE:CD1	2.54	0.42
2:B:289:PRO:HG3	2:B:330:TRP:HH2	1.83	0.42
1:G:332:VAL:HG23	1:G:339:LEU:HG	2.00	0.42
2:H:66:MET:N	2:H:77:ILE:O	2.34	0.42
2:K:189:THR:HA	2:K:214:THR:HB	2.01	0.42
2:K:419:ARG:HD2	2:K:419:ARG:N	2.33	0.42
1:A:51:TYR:CE2	1:A:238:SER:HA	2.54	0.42
1:D:176:LYS:HB3	1:D:189:PHE:CE2	2.54	0.42
2:E:384:ALA:O	2:E:388:LEU:HG	2.19	0.42
1:G:174:ASP:OD1	1:G:174:ASP:N	2.44	0.42
3:I:197:GLN:HA	3:I:209:TYR:CE1	2.54	0.42
2:K:52:GLN:HE21	2:K:98:TYR:HA	1.84	0.42
3:L:232:ASP:OD1	3:L:235:GLY:N	2.52	0.42
1:A:89:TRP:CH2	2:B:71:HIS:HA	2.54	0.42
1:A:364:GLU:HB3	1:A:377:LYS:HG3	2.02	0.42
1:A:385:ASP:OD1	1:A:385:ASP:N	2.52	0.42
3:C:192:THR:OG1	3:C:194:GLU:OE2	2.31	0.42
2:E:179:VAL:HA	2:E:188:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:126:LYS:HZ1	3:F:128:PHE:HE1	1.64	0.42
2:H:302:ASP:OD1	2:H:303:GLU:N	2.52	0.42
1:J:409:TRP:O	1:J:413:LEU:HG	2.19	0.42
2:K:9:TYR:CD1	2:K:55:LEU:HD13	2.54	0.42
3:L:129:PRO:HA	3:L:139:TYR:HA	1.99	0.42
3:L:147:LEU:O	3:L:177:TYR:HA	2.18	0.42
2:E:167:MET:HG2	2:E:253:GLY:O	2.20	0.42
3:F:147:LEU:O	3:F:177:TYR:HA	2.19	0.42
2:H:161:ARG:HE	2:H:260:LEU:HD23	1.84	0.42
1:A:417:SER:HB2	2:B:381:SER:CB	2.49	0.42
1:D:61:LYS:HB2	1:D:66:GLN:HB2	2.02	0.42
1:D:427:LEU:HA	1:D:430:ILE:HG12	2.00	0.42
2:E:152:GLN:HB3	2:E:261:LEU:HD11	2.02	0.42
3:F:194:GLU:H	3:F:194:GLU:HG3	1.63	0.42
3:I:152:HIS:N	3:I:174:ASP:OD1	2.52	0.42
1:J:29:ILE:HG13	1:J:137:VAL:HG22	2.02	0.42
1:J:264:ASN:HB2	1:J:265:PRO:HD3	2.01	0.42
2:K:362:ARG:HD2	2:K:362:ARG:HA	1.79	0.42
3:L:193:HIS:CG	3:L:260:GLU:HA	2.54	0.42
1:D:52:LYS:N	1:D:109:MET:O	2.50	0.42
2:E:38:SER:OG	2:E:130:LYS:N	2.52	0.42
2:E:289:PRO:HG3	2:E:330:TRP:CH2	2.53	0.42
3:F:271:ASN:ND2	3:F:271:ASN:O	2.53	0.42
2:K:33:ILE:HG12	2:K:49:THR:HG22	2.01	0.42
2:B:10:LYS:HG3	2:B:11:LEU:HG	2.01	0.42
2:E:51:SER:OG	2:E:67:ARG:O	2.30	0.42
2:E:160:ASN:CB	2:E:256:HIS:HB3	2.40	0.42
1:G:95:PHE:HE1	2:H:227:ARG:HB3	1.82	0.42
1:J:296:LEU:H	1:J:371:THR:HG21	1.83	0.42
2:K:157:ASP:OD1	2:K:158:ALA:N	2.53	0.42
1:A:187:TYR:CE2	1:A:200:PHE:HD2	2.38	0.42
2:B:30:PRO:O	2:B:50:SER:OG	2.26	0.42
3:C:248:GLY:HA3	3:I:186:ALA:HB3	2.01	0.42
3:C:254:SER:HA	3:C:269:PRO:HD2	2.02	0.42
1:D:57:SER:O	2:E:245:LYS:HB2	2.20	0.42
1:G:108:VAL:HG11	1:G:203:ILE:HD11	2.02	0.42
1:J:332:VAL:HG23	1:J:339:LEU:HG	2.01	0.42
3:L:182:GLN:HG3	3:L:185:ARG:HE	1.84	0.42
1:A:257:PHE:HA	2:B:300:LEU:O	2.20	0.42
2:E:136:ARG:HD2	2:E:331:GLY:O	2.19	0.42
1:J:309:SER:OG	1:J:310:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:397:LEU:O	2:K:401:ARG:N	2.52	0.42
1:A:440:LYS:HD3	1:A:440:LYS:HA	1.66	0.42
2:B:38:SER:OG	2:B:130:LYS:N	2.52	0.42
3:C:197:GLN:HE22	3:C:211:ASN:N	2.17	0.42
1:D:197:PRO:HG3	1:D:218:ASN:HB2	2.01	0.42
1:G:81:PHE:O	1:G:102:GLN:N	2.43	0.42
1:G:222:GLN:O	1:G:232:PRO:HG2	2.20	0.42
1:G:304:ASN:OD1	1:G:304:ASN:N	2.51	0.42
2:H:169:LEU:HD12	2:H:170:PRO:HD2	2.02	0.42
3:I:208:GLN:O	3:I:215:THR:OG1	2.29	0.42
1:J:176:LYS:HB3	1:J:189:PHE:CE2	2.54	0.42
3:L:215:THR:HB	3:L:250:ARG:HB3	2.02	0.42
2:B:9:TYR:CD1	2:B:55:LEU:HD13	2.55	0.41
2:B:362:ARG:HD2	2:B:362:ARG:HA	1.80	0.41
3:C:218:LYS:HD3	3:C:248:GLY:O	2.20	0.41
2:E:30:PRO:O	2:E:50:SER:OG	2.37	0.41
2:E:317:ARG:HB3	2:E:319:PHE:CE2	2.54	0.41
1:G:24:TYR:CG	1:G:287:PHE:HB3	2.55	0.41
1:G:121:ALA:HB1	1:G:189:PHE:CZ	2.55	0.41
1:G:245:LYS:HE2	1:G:245:LYS:HB3	1.88	0.41
2:H:53:TYR:HE1	2:H:66:MET:HE2	1.84	0.41
2:B:31:ILE:HD12	2:B:31:ILE:HA	1.96	0.41
2:B:136:ARG:HD2	2:B:331:GLY:O	2.21	0.41
1:D:139:GLU:OE2	1:D:327:LYS:NZ	2.53	0.41
2:E:53:TYR:O	2:E:97:GLY:N	2.41	0.41
3:F:168:LYS:HB2	3:F:177:TYR:CZ	2.56	0.41
1:G:29:ILE:HG13	1:G:137:VAL:HG22	2.02	0.41
2:H:85:TYR:HE1	2:H:113:GLU:HG3	1.85	0.41
1:A:360:ASN:HD21	1:A:400:ALA:HA	1.84	0.41
2:B:173:GLU:HG2	2:B:230:ARG:HB3	2.02	0.41
2:B:236:TRP:HZ3	2:B:253:GLY:HA3	1.85	0.41
3:C:216:VAL:HG23	3:C:251:THR:HB	2.02	0.41
1:G:133:LEU:HD12	1:G:146:VAL:HG11	2.01	0.41
2:H:12:THR:HG23	2:H:13:ARG:H	1.85	0.41
2:H:179:VAL:HA	2:H:188:VAL:HG22	2.02	0.41
1:J:357:SER:O	1:J:394:HIS:NE2	2.52	0.41
2:K:147:VAL:O	2:K:268:VAL:N	2.37	0.41
1:A:256:PRO:HG3	2:B:304:PRO:HD3	2.03	0.41
1:D:222:GLN:HE22	2:H:146:GLY:HA2	1.86	0.41
2:E:213:LYS:HD2	2:E:214:THR:N	2.36	0.41
2:H:14:PRO:HG3	2:H:67:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:231:LEU:HD22	2:K:231:LEU:HA	1.92	0.41
2:B:99:PHE:CD1	2:B:258:PRO:HD2	2.55	0.41
2:B:404:PRO:HG3	3:C:191:TYR:CE1	2.56	0.41
1:D:20:ASN:HB3	1:D:26:PRO:HB3	2.02	0.41
3:I:193:HIS:HB2	3:I:260:GLU:HA	2.02	0.41
3:I:232:ASP:OD1	3:I:235:GLY:N	2.54	0.41
1:J:203:ILE:HG23	1:J:213:LEU:HD12	2.02	0.41
1:A:338:THR:HB	1:A:394:HIS:NE2	2.36	0.41
2:B:148:GLU:HA	2:B:267:THR:HA	2.02	0.41
2:E:57:SER:N	2:E:76:GLU:OE1	2.47	0.41
1:G:71:THR:OG1	1:G:76:GLU:OE2	2.38	0.41
1:G:217:THR:O	1:G:217:THR:OG1	2.39	0.41
1:G:421:ILE:HD13	1:G:421:ILE:HA	1.92	0.41
1:J:222:GLN:CG	1:J:232:PRO:HB2	2.50	0.41
2:K:169:LEU:HD21	2:K:233:ASN:HD22	1.85	0.41
2:K:199:GLU:O	2:K:227:ARG:N	2.35	0.41
3:L:193:HIS:ND1	3:L:260:GLU:HG2	2.36	0.41
1:A:173:PHE:CE2	1:A:268:ALA:HB2	2.55	0.41
1:A:245:LYS:HE2	1:A:245:LYS:HB3	1.87	0.41
1:D:203:ILE:HG23	1:D:213:LEU:HD12	2.03	0.41
2:H:86:THR:OG1	2:H:88:ARG:O	2.26	0.41
1:J:192:TYR:CE2	1:J:206:ARG:HD3	2.56	0.41
2:K:303:GLU:HB2	2:K:305:HIS:CD2	2.55	0.41
1:A:176:LYS:HB3	1:A:189:PHE:CE2	2.56	0.41
1:A:301:CYS:HA	1:A:318:VAL:HA	2.02	0.41
1:D:61:LYS:HB3	1:D:101:THR:OG1	2.21	0.41
1:J:51:TYR:HE1	1:J:235:GLN:NE2	2.19	0.41
1:J:206:ARG:HA	1:J:206:ARG:HD2	1.92	0.41
1:J:327:LYS:HA	1:J:345:GLU:HA	2.03	0.41
1:J:389:THR:O	1:J:389:THR:OG1	2.30	0.41
2:K:291:ASN:O	2:K:293:THR:HG23	2.21	0.41
2:B:296:ILE:HB	2:B:329:VAL:HG13	2.03	0.41
1:D:440:LYS:HA	1:D:440:LYS:HD3	1.85	0.41
2:E:48:GLN:HB3	2:E:99:PHE:CE2	2.56	0.41
3:F:232:ASP:OD1	3:F:235:GLY:N	2.54	0.41
3:F:259:ASN:OD1	3:F:260:GLU:N	2.54	0.41
1:G:35:LYS:NZ	1:G:269:GLU:OE1	2.48	0.41
2:H:236:TRP:HZ3	2:H:253:GLY:HA3	1.85	0.41
2:H:297:THR:HG21	2:H:319:PHE:CE1	2.51	0.41
2:H:415:LEU:HD23	2:H:417:CYS:SG	2.61	0.41
3:I:141:CYS:SG	3:I:142:VAL:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:196:PRO:O	3:I:200:TYR:OH	2.28	0.41
3:I:199:TYR:HB3	3:I:208:GLN:OE1	2.21	0.41
1:J:20:ASN:OD1	1:J:20:ASN:N	2.54	0.41
1:J:255:ALA:HB1	1:J:259:CYS:HB3	2.02	0.41
2:K:14:PRO:HG3	2:K:67:ARG:NE	2.36	0.41
2:K:48:GLN:HB3	2:K:99:PHE:CE2	2.56	0.41
2:K:180:SER:HB3	2:K:187:THR:O	2.21	0.41
2:K:345:PRO:HG2	2:K:358:HIS:HA	2.03	0.41
3:L:172:LYS:HE3	3:L:172:LYS:HB2	1.89	0.41
3:L:225:ASP:O	3:L:228:ARG:HG3	2.21	0.41
3:C:191:TYR:HA	3:C:237:VAL:HG13	2.02	0.41
1:G:440:LYS:HA	1:G:440:LYS:HD3	1.81	0.41
2:K:154:TYR:HA	2:K:261:LEU:HA	2.03	0.41
1:A:205:SER:OG	1:A:207:THR:O	2.32	0.40
1:D:118:HIS:ND1	1:D:120:GLU:OE2	2.54	0.40
3:F:218:LYS:HD3	3:F:248:GLY:O	2.21	0.40
2:H:31:ILE:HD12	2:H:31:ILE:HA	1.92	0.40
2:H:297:THR:HG23	2:H:326:TRP:NE1	2.35	0.40
2:B:21:ARG:HE	2:B:21:ARG:HA	1.85	0.40
2:B:215:LYS:HZ2	2:B:215:LYS:HB2	1.86	0.40
2:B:271:ALA:O	2:B:333:HIS:NE2	2.36	0.40
1:D:434:TYR:HA	1:D:437:THR:HG22	2.03	0.40
1:G:402:VAL:HG21	2:H:359:TYR:CE1	2.50	0.40
3:I:190:LYS:O	3:I:237:VAL:HG12	2.22	0.40
2:K:78:PRO:HG2	2:K:81:GLN:HB2	2.03	0.40
3:C:225:ASP:O	3:C:228:ARG:HG3	2.21	0.40
1:D:396:GLN:H	1:D:396:GLN:CD	2.25	0.40
2:E:294:TYR:HE1	2:E:310:LEU:HB2	1.85	0.40
3:F:151:MET:N	3:F:175:LEU:HA	2.37	0.40
1:G:58:PRO:HB3	1:G:102:GLN:HE22	1.85	0.40
2:H:137:GLU:OE2	2:H:332:ASN:HB2	2.21	0.40
3:I:200:TYR:HD2	3:I:232:ASP:HA	1.87	0.40
3:I:229:PRO:HA	3:I:240:ILE:HG22	2.02	0.40
1:J:205:SER:OG	1:J:210:SER:OG	2.40	0.40
2:K:327:GLU:HB2	2:K:337:ARG:HG2	2.02	0.40
1:A:262:TYR:CB	1:A:267:ARG:HE	2.35	0.40
1:D:147:TYR:CD1	1:D:152:THR:HG21	2.56	0.40
3:I:170:ALA:HB1	3:I:173:TYR:HB2	2.02	0.40
3:C:192:THR:HB	3:C:236:ARG:HH11	1.87	0.40
2:E:65:THR:HA	2:E:78:PRO:HA	2.04	0.40
2:E:141:HIS:HD1	2:K:126:PRO:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:LYS:HE2	2:H:115:LYS:HB3	1.83	0.40
2:K:93:VAL:HB	2:K:101:LEU:HG	2.04	0.40
2:K:292:PRO:HB3	2:K:312:SER: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	440/442 (100%)	417 (95%)	23 (5%)	0	100	100
1	D	440/442 (100%)	418 (95%)	22 (5%)	0	100	100
1	G	440/442 (100%)	417 (95%)	23 (5%)	0	100	100
1	J	440/442 (100%)	416 (94%)	24 (6%)	0	100	100
2	B	421/423 (100%)	388 (92%)	33 (8%)	0	100	100
2	E	421/423 (100%)	393 (93%)	28 (7%)	0	100	100
2	H	421/423 (100%)	390 (93%)	31 (7%)	0	100	100
2	K	421/423 (100%)	389 (92%)	32 (8%)	0	100	100
3	C	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
3	F	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
3	I	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
3	L	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
All	All	4084/4108 (99%)	3859 (94%)	225 (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	368/368 (100%)	334 (91%)	34 (9%)	7	26
1	D	368/368 (100%)	341 (93%)	27 (7%)	11	34
1	G	368/368 (100%)	338 (92%)	30 (8%)	9	30
1	J	368/368 (100%)	336 (91%)	32 (9%)	8	28
2	B	364/364 (100%)	334 (92%)	30 (8%)	9	30
2	E	364/364 (100%)	326 (90%)	38 (10%)	5	22
2	H	364/364 (100%)	331 (91%)	33 (9%)	7	26
2	K	364/364 (100%)	332 (91%)	32 (9%)	8	28
3	C	135/135 (100%)	124 (92%)	11 (8%)	9	31
3	F	135/135 (100%)	123 (91%)	12 (9%)	8	27
3	I	135/135 (100%)	123 (91%)	12 (9%)	8	27
3	L	135/135 (100%)	128 (95%)	7 (5%)	19	43
All	All	3468/3468 (100%)	3170 (91%)	298 (9%)	11	29

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	19	VAL
1	A	29	ILE
1	A	32	THR
1	A	36	ILE
1	A	48	THR
1	A	53	THR
1	A	56	ASP
1	A	60	ILE
1	A	79	LYS
1	A	87	PHE
1	A	112	ASP
1	A	115	LEU
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	125	HIS
1	A	143	VAL
1	A	144	THR
1	A	166	LEU
1	A	200	PHE
1	A	218	ASN
1	A	223	ARG
1	A	241	GLU
1	A	263	THR
1	A	289	ARG
1	A	368	GLN
1	A	375	THR
1	A	376	CYS
1	A	385	ASP
1	A	389	THR
1	A	396	GLN
1	A	413	LEU
1	A	425	LEU
1	A	434	TYR
1	A	436	LEU
2	B	6	PHE
2	B	9	TYR
2	B	12	THR
2	B	16	MET
2	B	24	VAL
2	B	52	GLN
2	B	111	THR
2	B	114	PHE
2	B	137	GLU
2	B	145	HIS
2	B	156	HIS
2	B	160	ASN
2	B	166	GLU
2	B	181	LEU
2	B	213	LYS
2	B	220	CYS
2	B	222	LYS
2	B	223	LYS
2	B	227	ARG
2	B	233	ASN
2	B	268	VAL
2	B	287	LEU

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Mol	Chain	Res	Type
2	B	329	VAL
2	B	361	HIS
2	B	387	TRP
2	B	396	CYS
2	B	403	THR
2	B	408	ILE
2	B	412	LEU
2	B	417	CYS
3	C	126	LYS
3	C	143	VAL
3	C	187	ASP
3	C	192	THR
3	C	209	TYR
3	C	211	ASN
3	C	240	ILE
3	C	245	VAL
3	C	247	GLU
3	C	256	VAL
3	C	263	VAL
1	D	19	VAL
1	D	29	ILE
1	D	32	THR
1	D	36	ILE
1	D	53	THR
1	D	60	ILE
1	D	87	PHE
1	D	112	ASP
1	D	118	HIS
1	D	143	VAL
1	D	146	VAL
1	D	166	LEU
1	D	200	PHE
1	D	223	ARG
1	D	241	GLU
1	D	263	THR
1	D	289	ARG
1	D	368	GLN
1	D	369	ILE
1	D	375	THR
1	D	384	LYS
1	D	389	THR
1	D	398	PHE

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Mol	Chain	Res	Type
1	D	402	VAL
1	D	413	LEU
1	D	425	LEU
1	D	434	TYR
2	E	6	PHE
2	E	9	TYR
2	E	12	THR
2	E	13	ARG
2	E	16	MET
2	E	24	VAL
2	E	27	CYS
2	E	53	TYR
2	E	111	THR
2	E	114	PHE
2	E	137	GLU
2	E	145	HIS
2	E	156	HIS
2	E	160	ASN
2	E	166	GLU
2	E	181	LEU
2	E	202	CYS
2	E	213	LYS
2	E	220	CYS
2	E	222	LYS
2	E	223	LYS
2	E	227	ARG
2	E	233	ASN
2	E	256	HIS
2	E	268	VAL
2	E	287	LEU
2	E	329	VAL
2	E	336	LYS
2	E	360	TYR
2	E	361	HIS
2	E	367	THR
2	E	369	LEU
2	E	387	TRP
2	E	396	CYS
2	E	402	LEU
2	E	403	THR
2	E	410	PHE
2	E	412	LEU

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Mol	Chain	Res	Type
3	F	125	ASP
3	F	126	LYS
3	F	143	VAL
3	F	172	LYS
3	F	179	ASP
3	F	192	THR
3	F	209	TYR
3	F	211	ASN
3	F	240	ILE
3	F	241	VAL
3	F	256	VAL
3	F	263	VAL
1	G	19	VAL
1	G	29	ILE
1	G	32	THR
1	G	53	THR
1	G	55	MET
1	G	56	ASP
1	G	60	ILE
1	G	87	PHE
1	G	118	HIS
1	G	125	HIS
1	G	143	VAL
1	G	145	THR
1	G	166	LEU
1	G	200	PHE
1	G	207	THR
1	G	223	ARG
1	G	234	THR
1	G	241	GLU
1	G	263	THR
1	G	289	ARG
1	G	328	CYS
1	G	368	GLN
1	G	384	LYS
1	G	385	ASP
1	G	389	THR
1	G	396	GLN
1	G	413	LEU
1	G	425	LEU
1	G	434	TYR
1	G	436	LEU

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Mol	Chain	Res	Type
2	H	6	PHE
2	H	9	TYR
2	H	12	THR
2	H	13	ARG
2	H	16	MET
2	H	52	GLN
2	H	111	THR
2	H	114	PHE
2	H	137	GLU
2	H	145	HIS
2	H	156	HIS
2	H	160	ASN
2	H	166	GLU
2	H	181	LEU
2	H	202	CYS
2	H	211	ILE
2	H	213	LYS
2	H	220	CYS
2	H	222	LYS
2	H	223	LYS
2	H	227	ARG
2	H	233	ASN
2	H	268	VAL
2	H	287	LEU
2	H	329	VAL
2	H	360	TYR
2	H	361	HIS
2	H	387	TRP
2	H	396	CYS
2	H	403	THR
2	H	408	ILE
2	H	410	PHE
2	H	412	LEU
3	I	125	ASP
3	I	126	LYS
3	I	137	ASN
3	I	142	VAL
3	I	143	VAL
3	I	192	THR
3	I	209	TYR
3	I	211	ASN
3	I	240	ILE

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Mol	Chain	Res	Type
3	I	256	VAL
3	I	263	VAL
3	I	267	TYR
1	J	29	ILE
1	J	32	THR
1	J	36	ILE
1	J	48	THR
1	J	53	THR
1	J	55	MET
1	J	60	ILE
1	J	79	LYS
1	J	87	PHE
1	J	118	HIS
1	J	125	HIS
1	J	143	VAL
1	J	146	VAL
1	J	157	ASN
1	J	166	LEU
1	J	200	PHE
1	J	217	THR
1	J	223	ARG
1	J	234	THR
1	J	241	GLU
1	J	263	THR
1	J	289	ARG
1	J	328	CYS
1	J	330	VAL
1	J	367	LEU
1	J	368	GLN
1	J	376	CYS
1	J	389	THR
1	J	396	GLN
1	J	413	LEU
1	J	425	LEU
1	J	434	TYR
2	K	6	PHE
2	K	9	TYR
2	K	12	THR
2	K	13	ARG
2	K	16	MET
2	K	52	GLN
2	K	111	THR

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Mol	Chain	Res	Type
2	K	114	PHE
2	K	137	GLU
2	K	144	GLU
2	K	145	HIS
2	K	156	HIS
2	K	160	ASN
2	K	166	GLU
2	K	181	LEU
2	K	198	VAL
2	K	213	LYS
2	K	220	CYS
2	K	222	LYS
2	K	227	ARG
2	K	268	VAL
2	K	287	LEU
2	K	329	VAL
2	K	360	TYR
2	K	361	HIS
2	K	387	TRP
2	K	396	CYS
2	K	403	THR
2	K	408	ILE
2	K	412	LEU
2	K	419	ARG
2	K	420	THR
3	L	126	LYS
3	L	192	THR
3	L	209	TYR
3	L	240	ILE
3	L	241	VAL
3	L	256	VAL
3	L	263	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	349	GLN
2	B	332	ASN
1	D	349	GLN
2	E	305	HIS
2	E	332	ASN

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Mol	Chain	Res	Type
1	G	349	GLN
2	H	332	ASN
1	J	349	GLN
2	K	288	HIS
2	K	332	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
4	NAG	A	501	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	E	502	-	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	D	501	1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	H	501	2	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	K	502	-	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	B	501	2	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	E	501	2	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	K	501	2	14,14,15	0.19	0	17,19,21	0.39	0
4	NAG	H	502	-	14,14,15	0.18	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	501	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	G	501	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	B	502	-	14,14,15	0.21	0	17,19,21	0.46	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
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	E	502	-	-	3/6/23/26	0/1/1/1
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1
4	NAG	H	501	2	-	0/6/23/26	0/1/1/1
4	NAG	K	502	-	-	4/6/23/26	0/1/1/1
4	NAG	B	501	2	-	0/6/23/26	0/1/1/1
4	NAG	E	501	2	-	2/6/23/26	0/1/1/1
4	NAG	K	501	2	-	2/6/23/26	0/1/1/1
4	NAG	H	502	-	-	2/6/23/26	0/1/1/1
4	NAG	J	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	502	-	-	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 (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	501	NAG	C4-C5-C6-O6
4	D	501	NAG	O5-C5-C6-O6
4	B	502	NAG	C8-C7-N2-C2
4	B	502	NAG	O7-C7-N2-C2
4	E	502	NAG	C8-C7-N2-C2
4	E	502	NAG	O7-C7-N2-C2
4	H	502	NAG	C8-C7-N2-C2
4	H	502	NAG	O7-C7-N2-C2
4	K	502	NAG	C8-C7-N2-C2
4	K	502	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	501	NAG	C4-C5-C6-O6
4	E	501	NAG	O5-C5-C6-O6
4	K	502	NAG	C4-C5-C6-O6
4	K	501	NAG	C4-C5-C6-O6
4	K	502	NAG	O5-C5-C6-O6
4	K	501	NAG	O5-C5-C6-O6
4	G	501	NAG	C4-C5-C6-O6
4	G	501	NAG	O5-C5-C6-O6
4	E	502	NAG	C4-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	502	NAG	1	0

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.

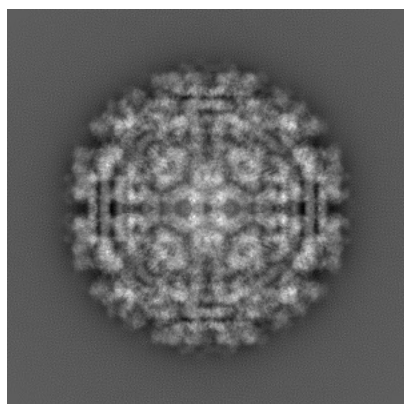
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25102. These allow visual inspection of the internal detail of the map and identification of artifacts.

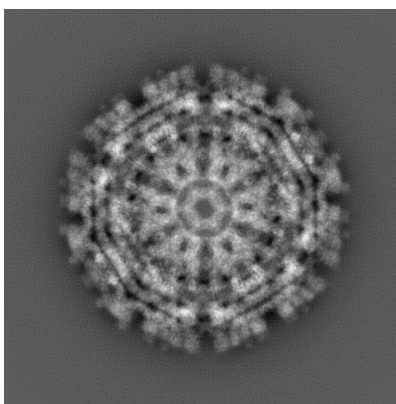
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

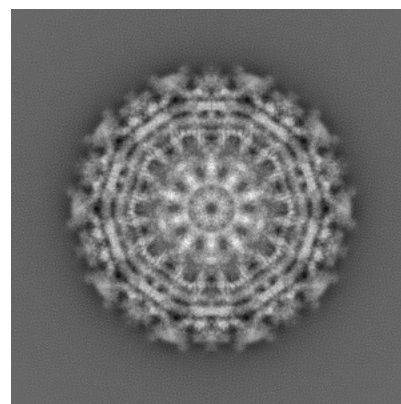
6.1.1 Primary map



X

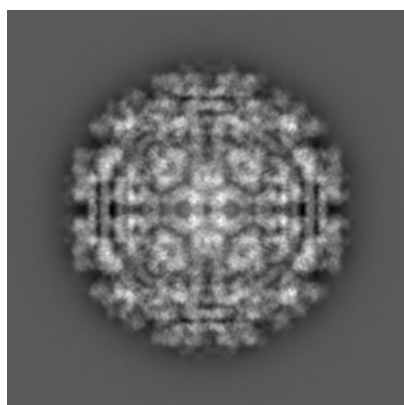


Y

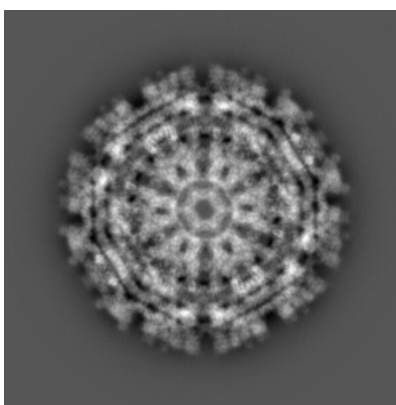


Z

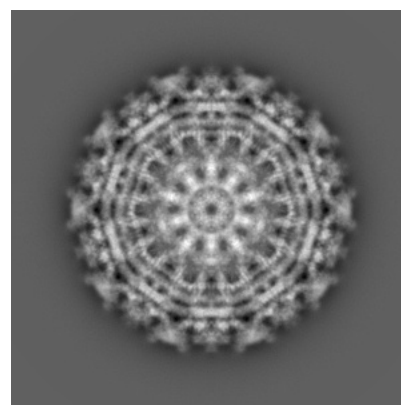
6.1.2 Raw map



X



Y

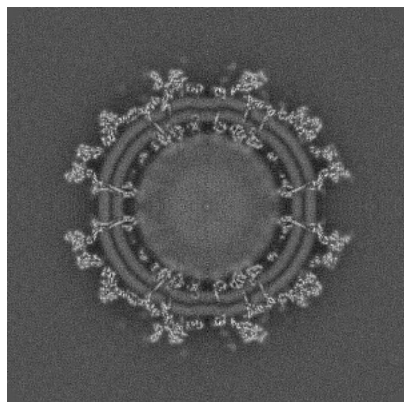


Z

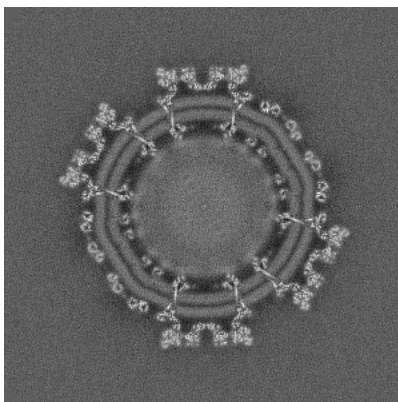
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

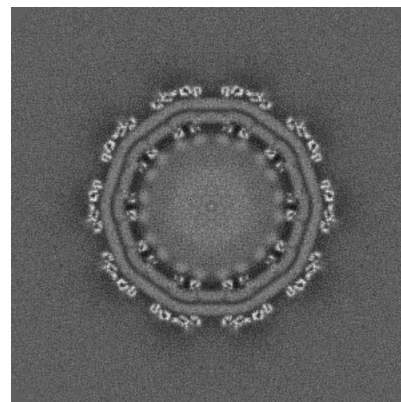
6.2.1 Primary map



X Index: 256

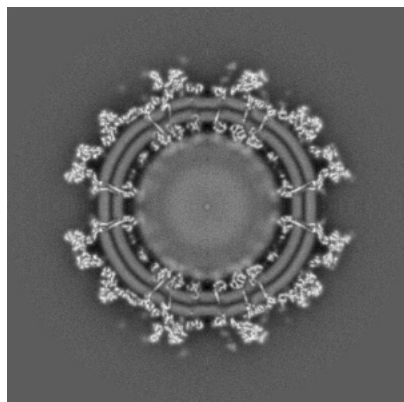


Y Index: 256

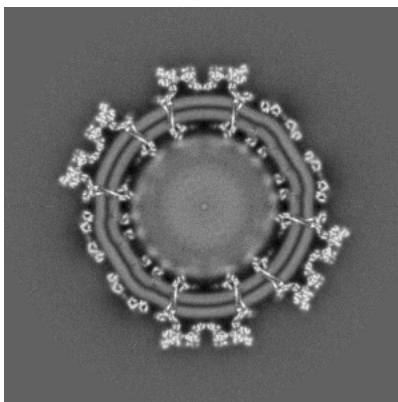


Z Index: 256

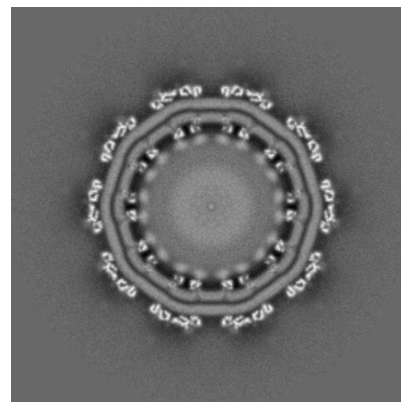
6.2.2 Raw map



X Index: 256



Y Index: 256

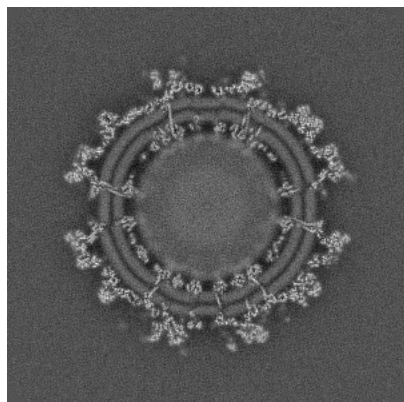


Z Index: 256

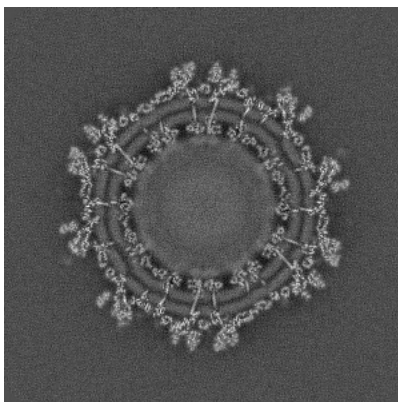
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

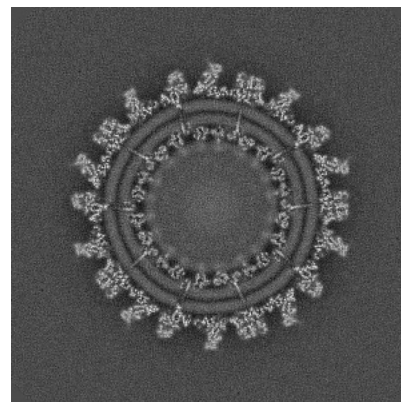
6.3.1 Primary map



X Index: 258

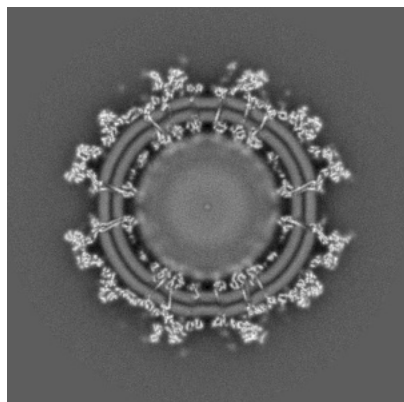


Y Index: 272

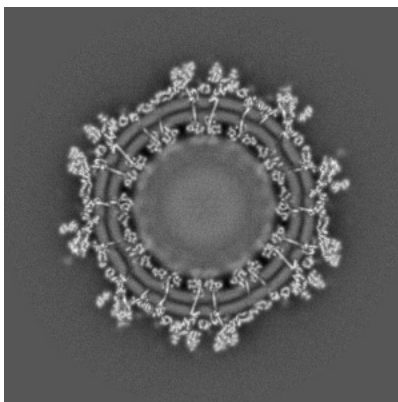


Z Index: 216

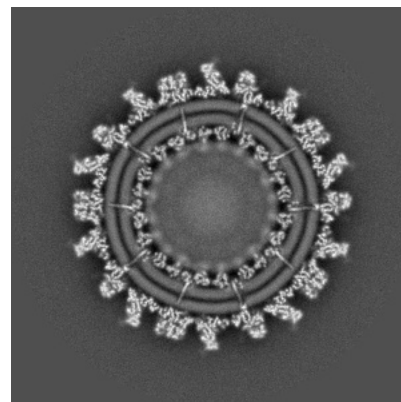
6.3.2 Raw map



X Index: 255



Y Index: 272

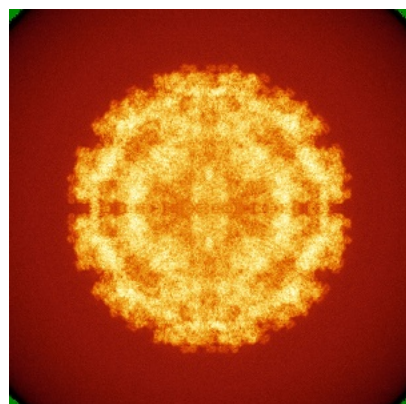


Z Index: 296

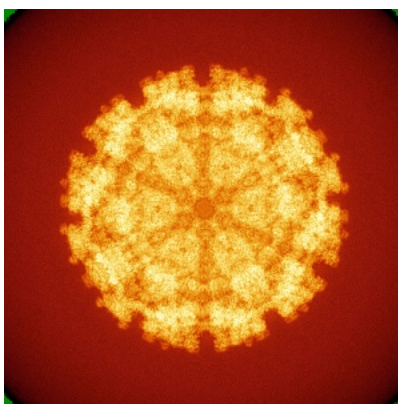
The images above show the largest variance slices of the map in three orthogonal directions.

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

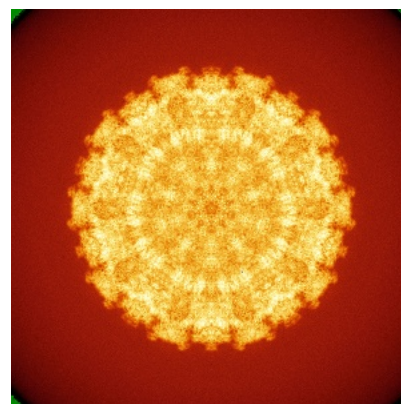
6.4.1 Primary map



X

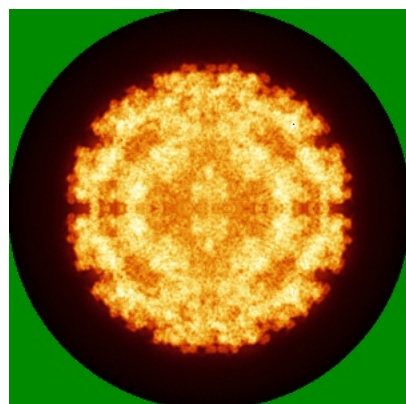


Y

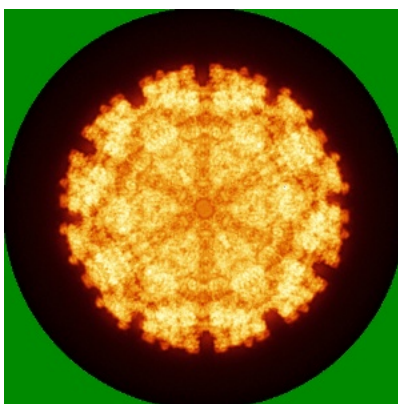


Z

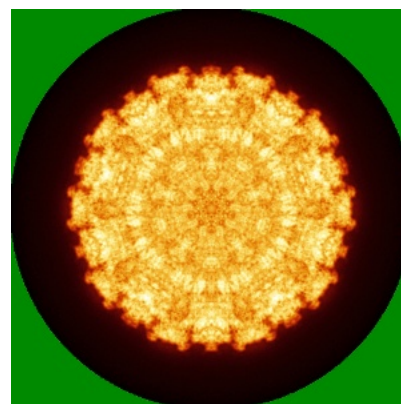
6.4.2 Raw map



X



Y



Z

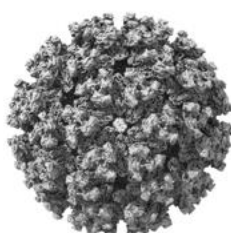
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

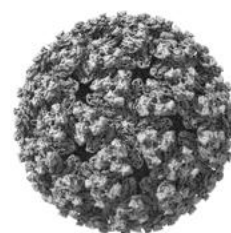
6.5.1 Primary map



X



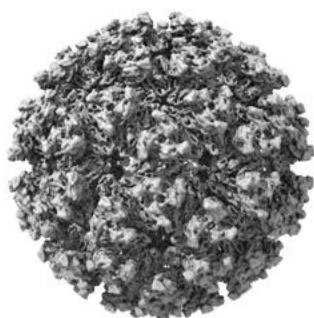
Y



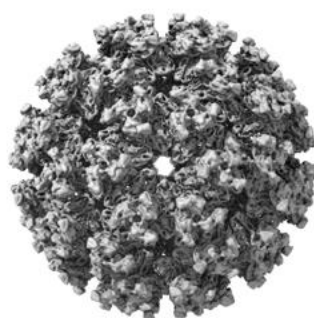
Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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



X



Y



Z

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.

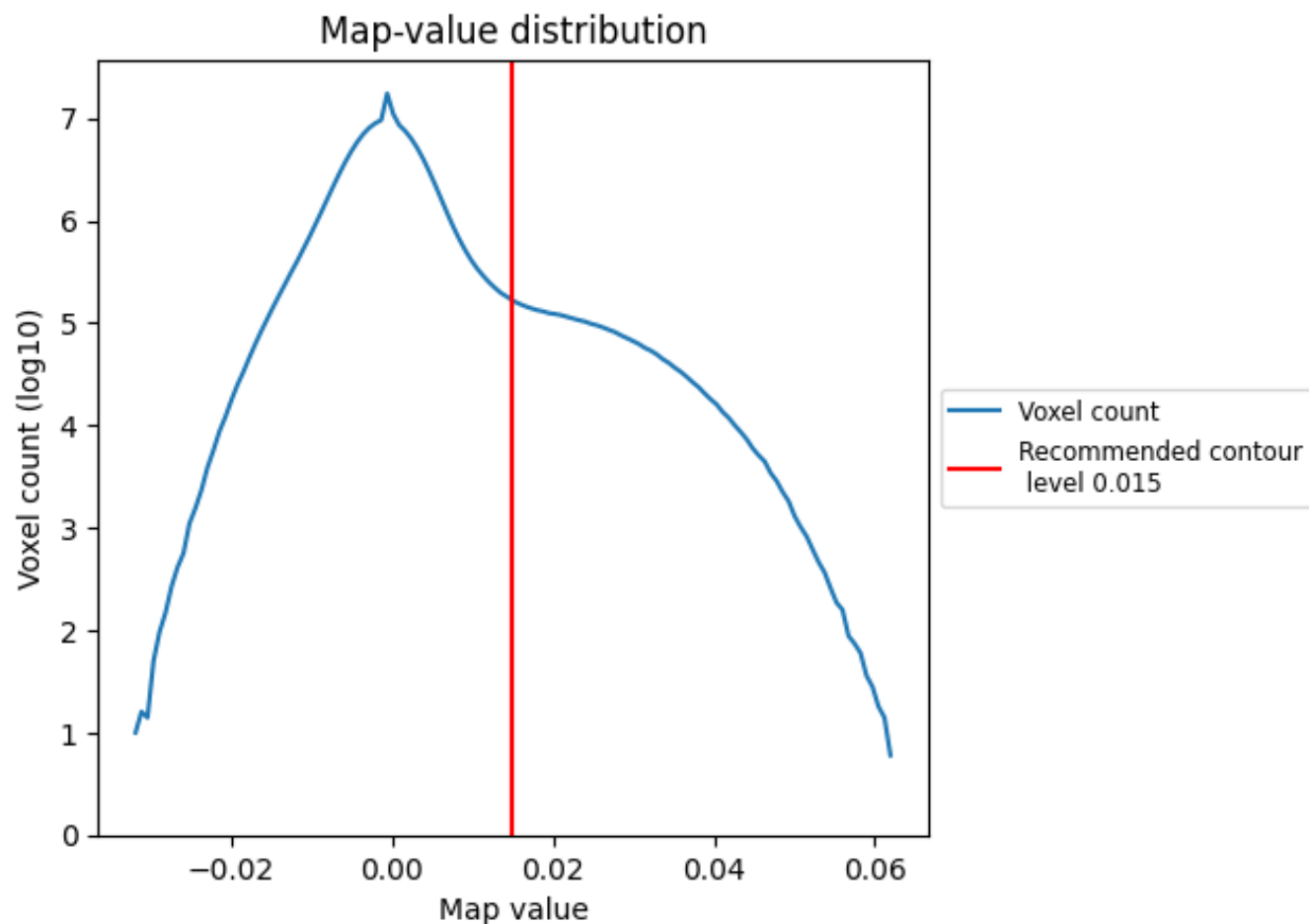
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

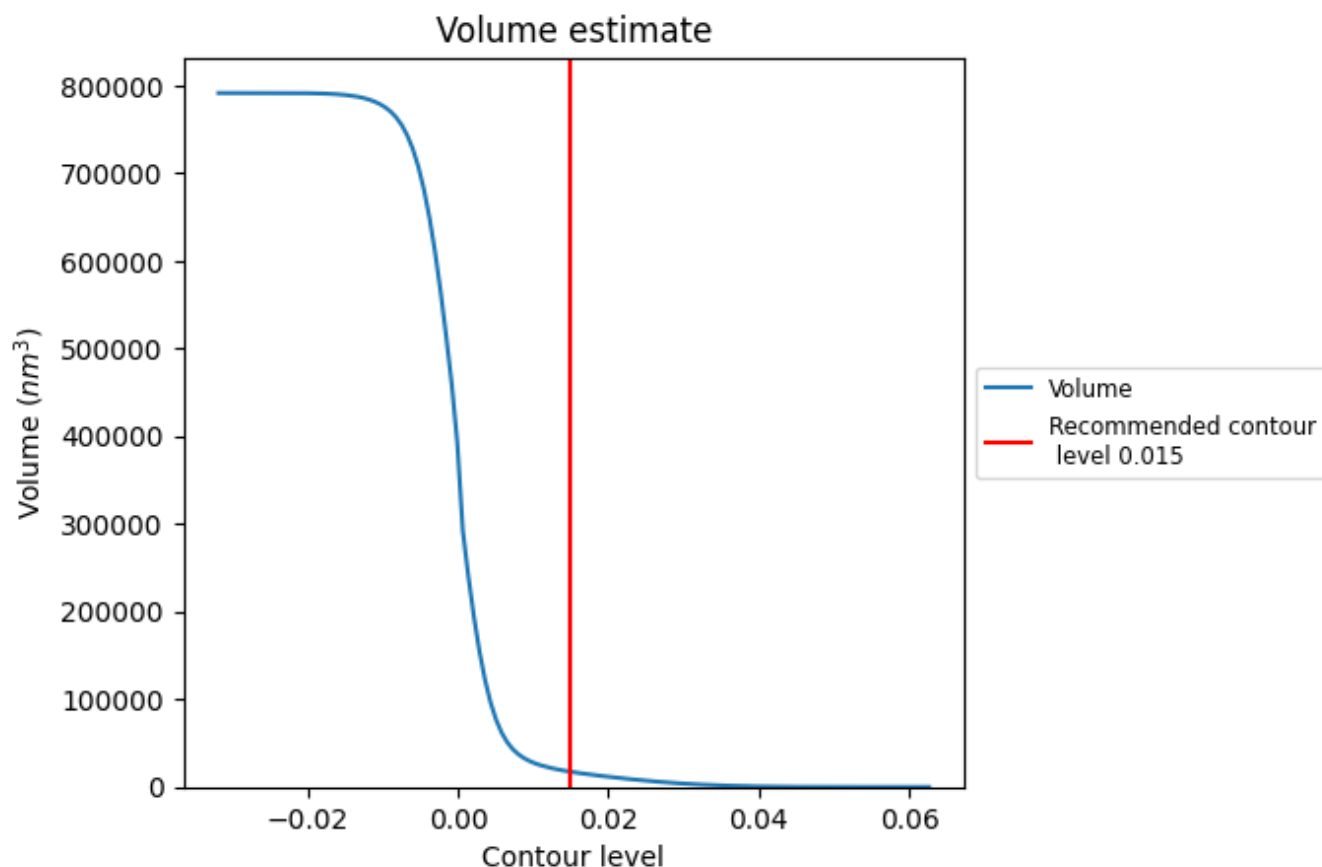
This section contains the results of statistical analysis of the map.

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.

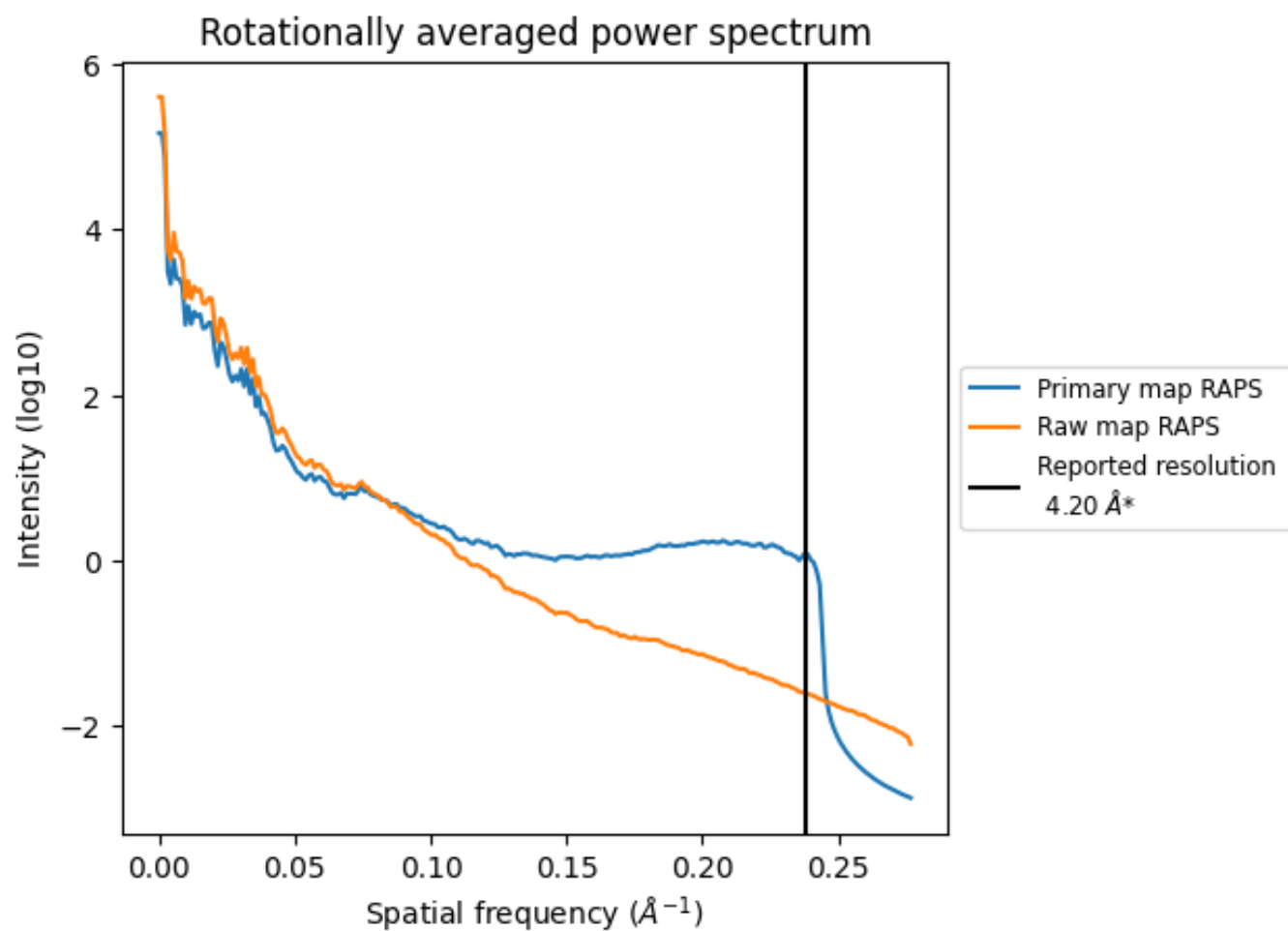
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 17314 nm^3 ; this corresponds to an approximate mass of 15641 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 ⓘ

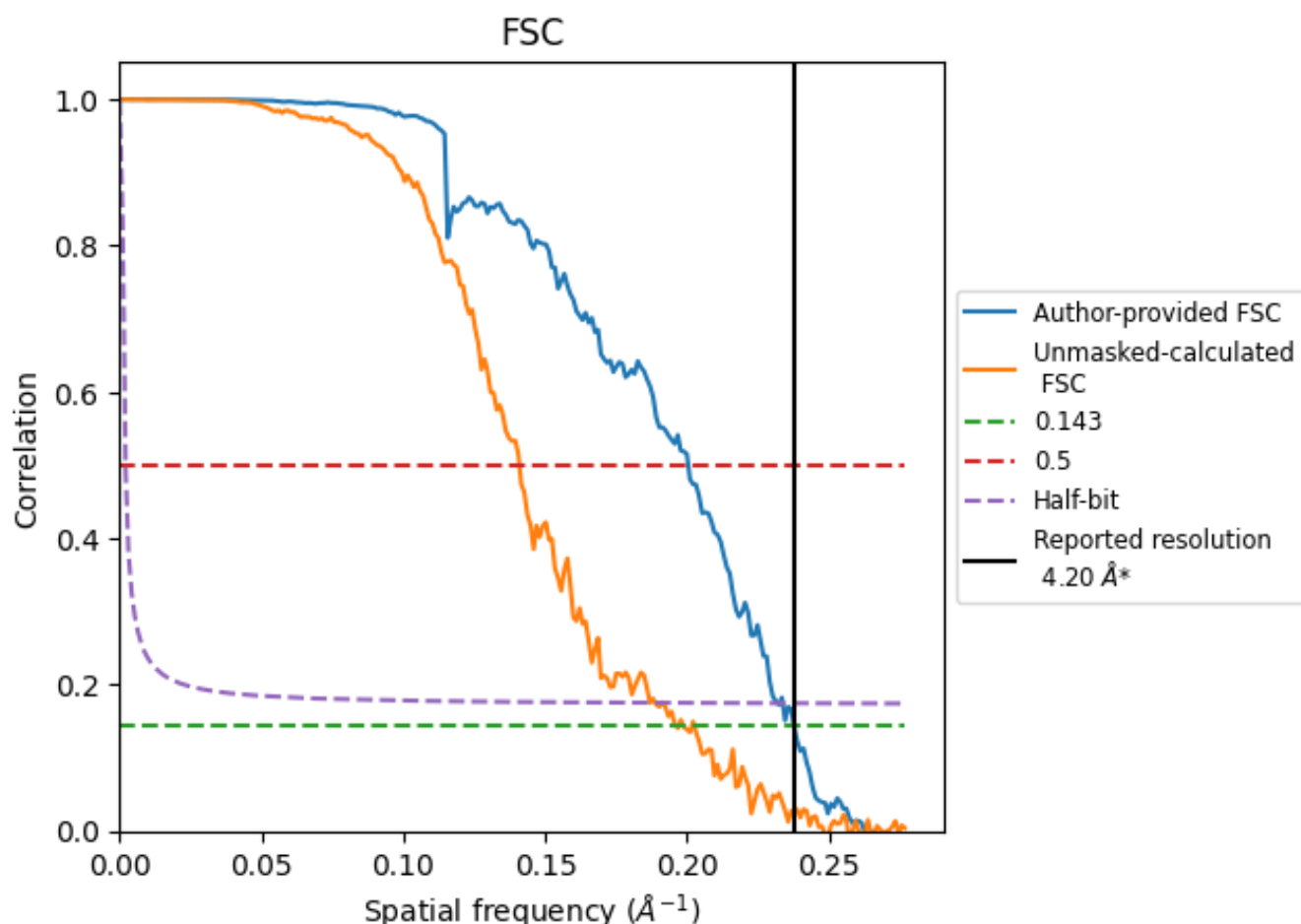


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.21	4.99	4.31
Unmasked-calculated*	5.10	7.10	5.35

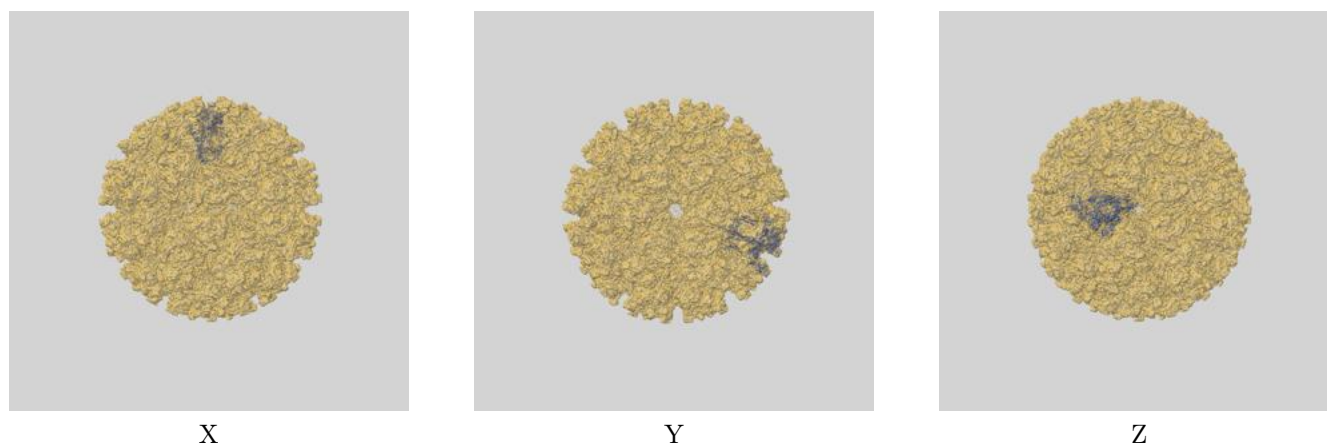
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.10 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

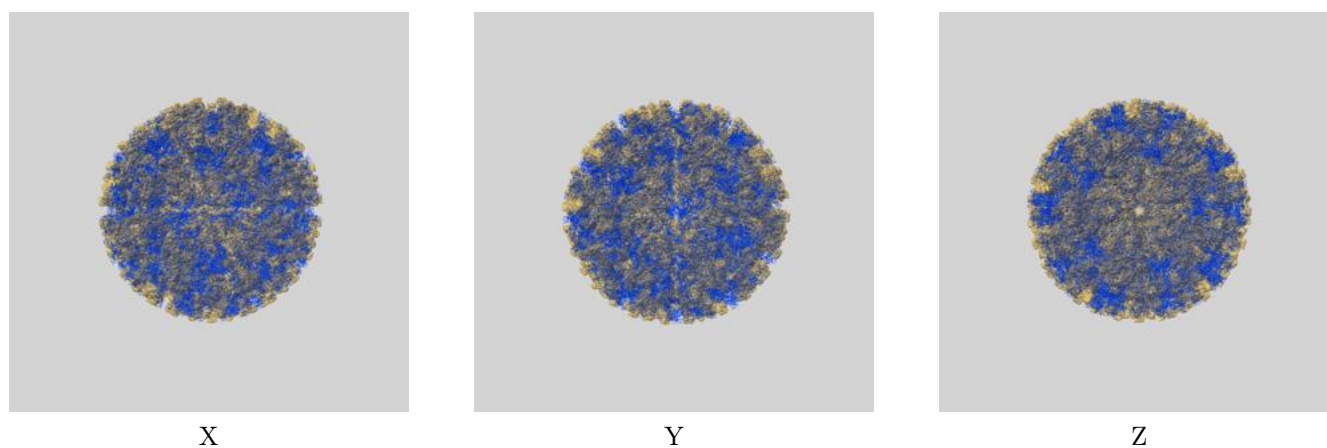
This section contains information regarding the fit between EMDB map EMD-25102 and PDB model 7SFU. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

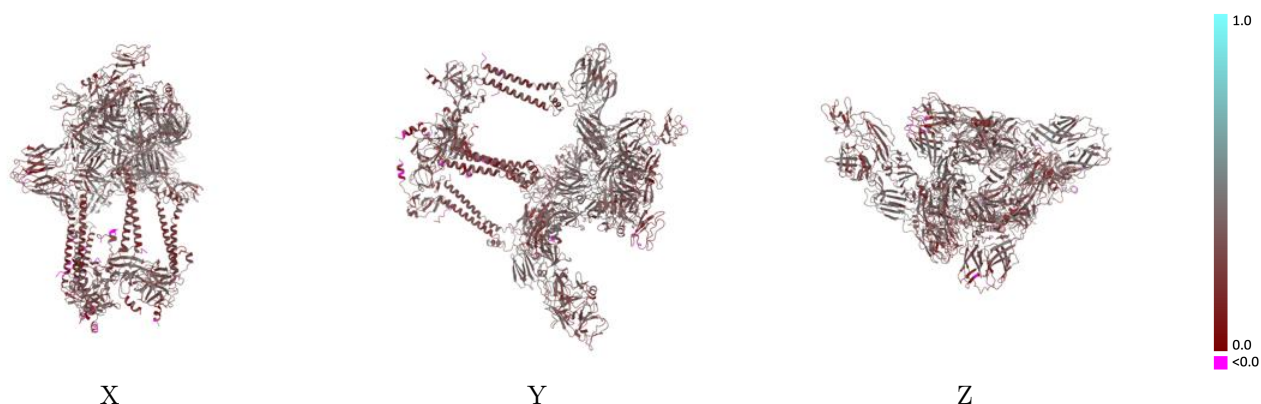


9.1.2 Map-model assembly overlay [i](#)



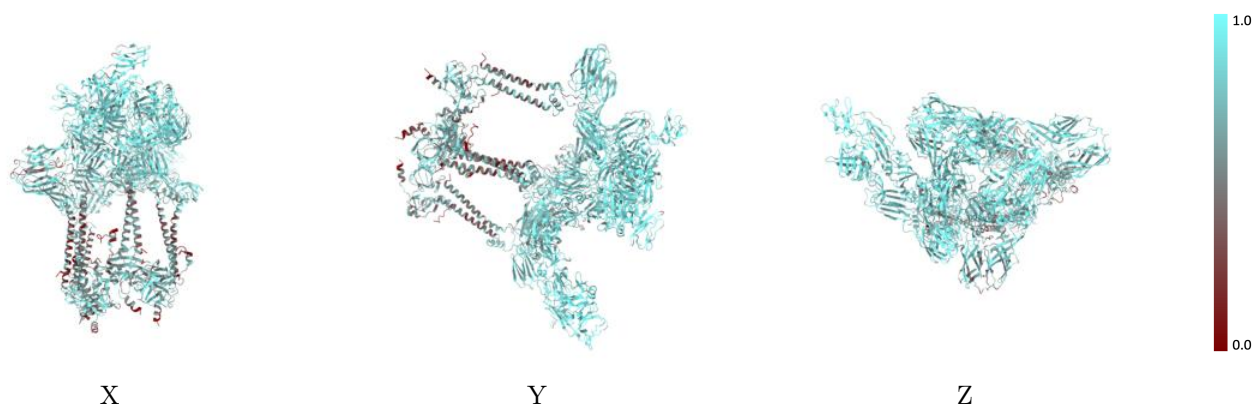
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



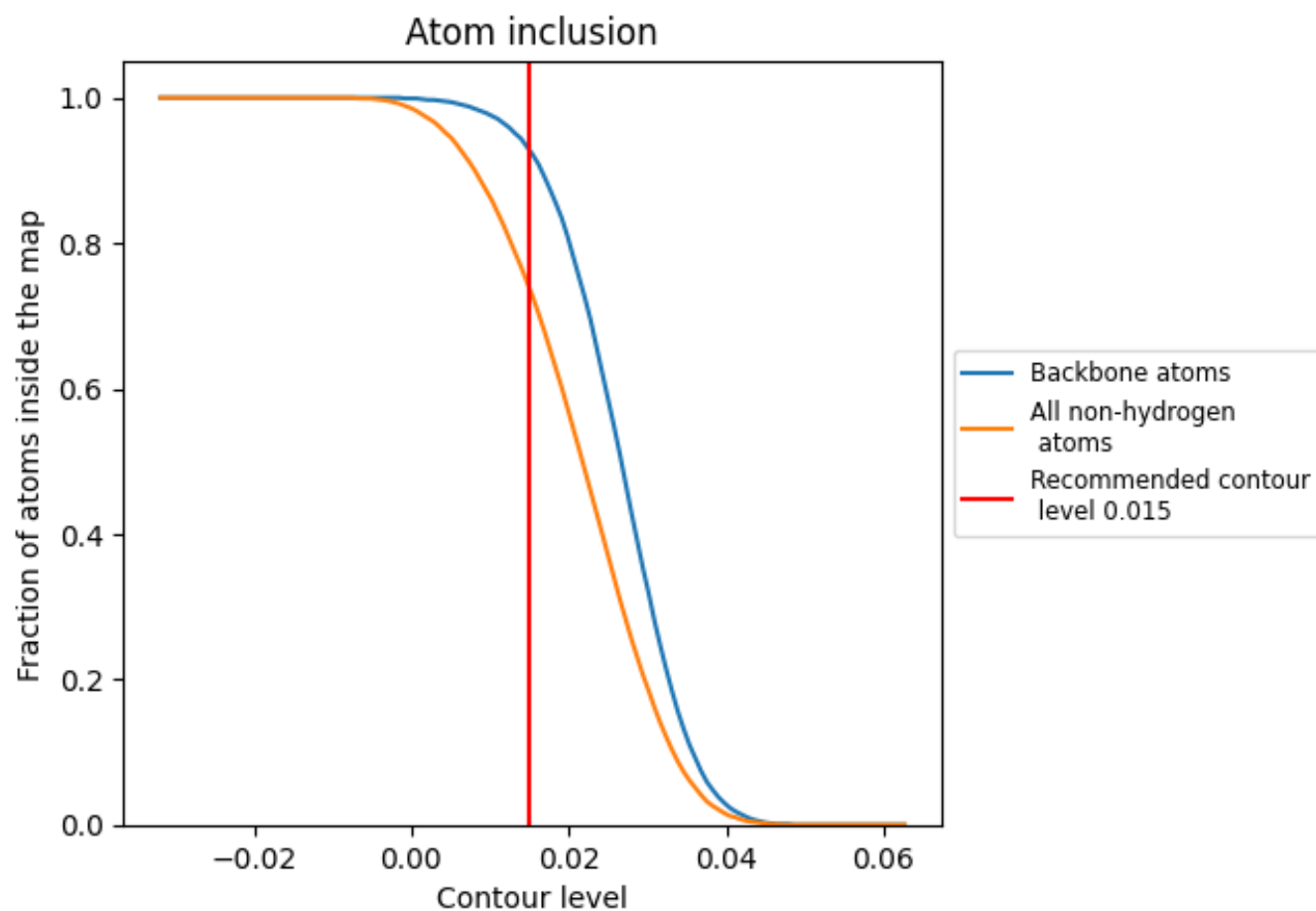
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 74% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7380	<div></div> 0.3320
A	<div></div> 0.7440	<div></div> 0.3270
B	<div></div> 0.7860	<div></div> 0.3350
C	<div></div> 0.6150	<div></div> 0.3100
D	<div></div> 0.7410	<div></div> 0.3360
E	<div></div> 0.7930	<div></div> 0.3480
F	<div></div> 0.6130	<div></div> 0.3100
G	<div></div> 0.7050	<div></div> 0.3050
H	<div></div> 0.7590	<div></div> 0.3110
I	<div></div> 0.6160	<div></div> 0.3180
J	<div></div> 0.7770	<div></div> 0.3790
K	<div></div> 0.7850	<div></div> 0.3260
L	<div></div> 0.6220	<div></div> 0.3540

1.0

0.0

<0.0