



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 9GG2 / pdb_00009gg2
EMDB ID : EMD-51321
Title : Structure of IPNV L5 capsid
Authors : Munke, A.; Gamil, A.; Mikalsen, A.; Wang, H.; Evensen, O.; Okamoto, K.
Deposited on : 2024-08-13
Resolution : 2.75 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

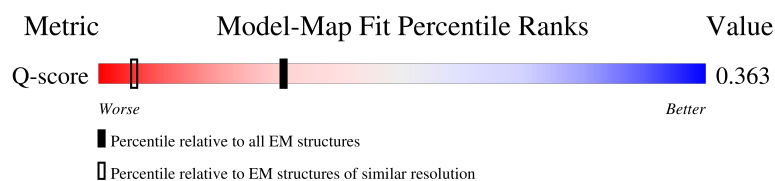
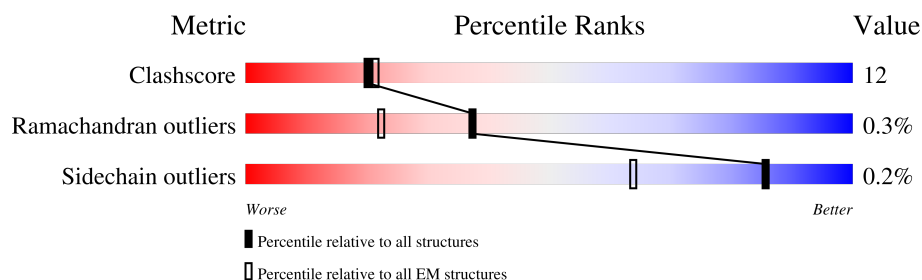
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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	508	
1	B	508	
1	C	508	
1	D	508	

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Mol	Chain	Length	Quality of chain
1	E	508	
1	F	508	
1	G	508	
1	H	508	
1	I	508	
1	J	508	
1	K	508	
1	L	508	
1	M	508	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42492 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.

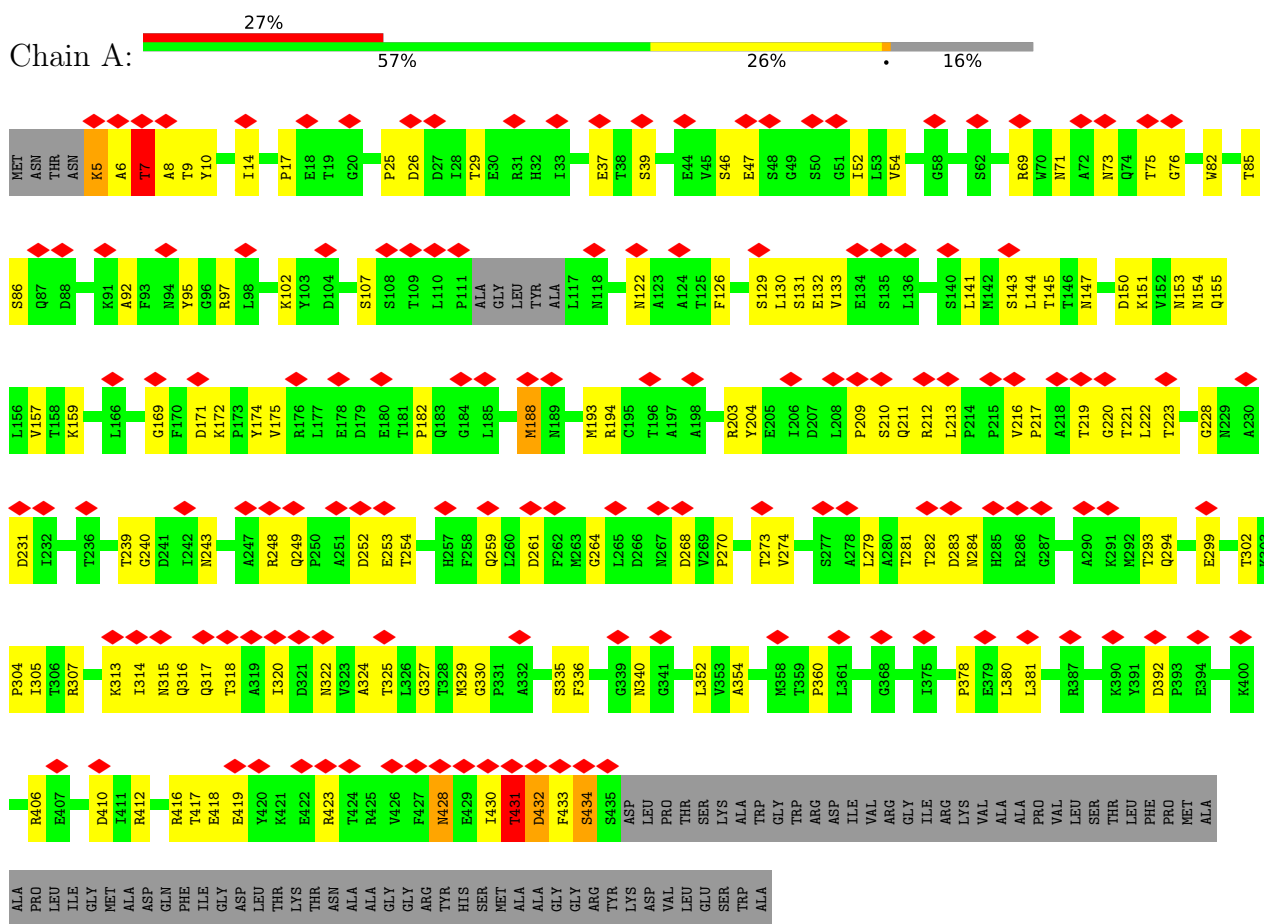
- Molecule 1 is a protein called Structural polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	426	Total	C	N	O	S	0	0
			3292	2065	560	655	12		
1	B	424	Total	C	N	O	S	0	0
			3277	2059	557	649	12		
1	C	430	Total	C	N	O	S	0	0
			3323	2088	564	659	12		
1	D	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	E	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	F	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	G	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	H	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	I	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	J	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	K	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	L	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		
1	M	422	Total	C	N	O	S	0	0
			3260	2048	555	645	12		

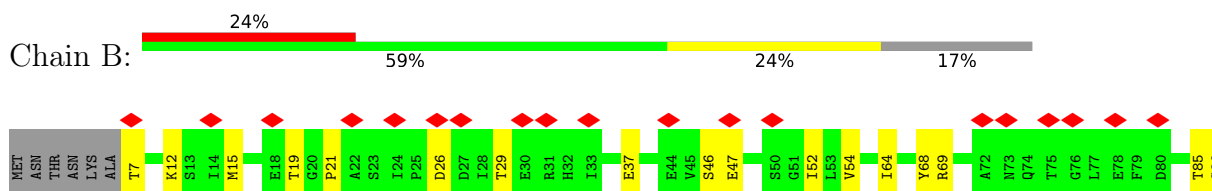
3 Residue-property plots

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.

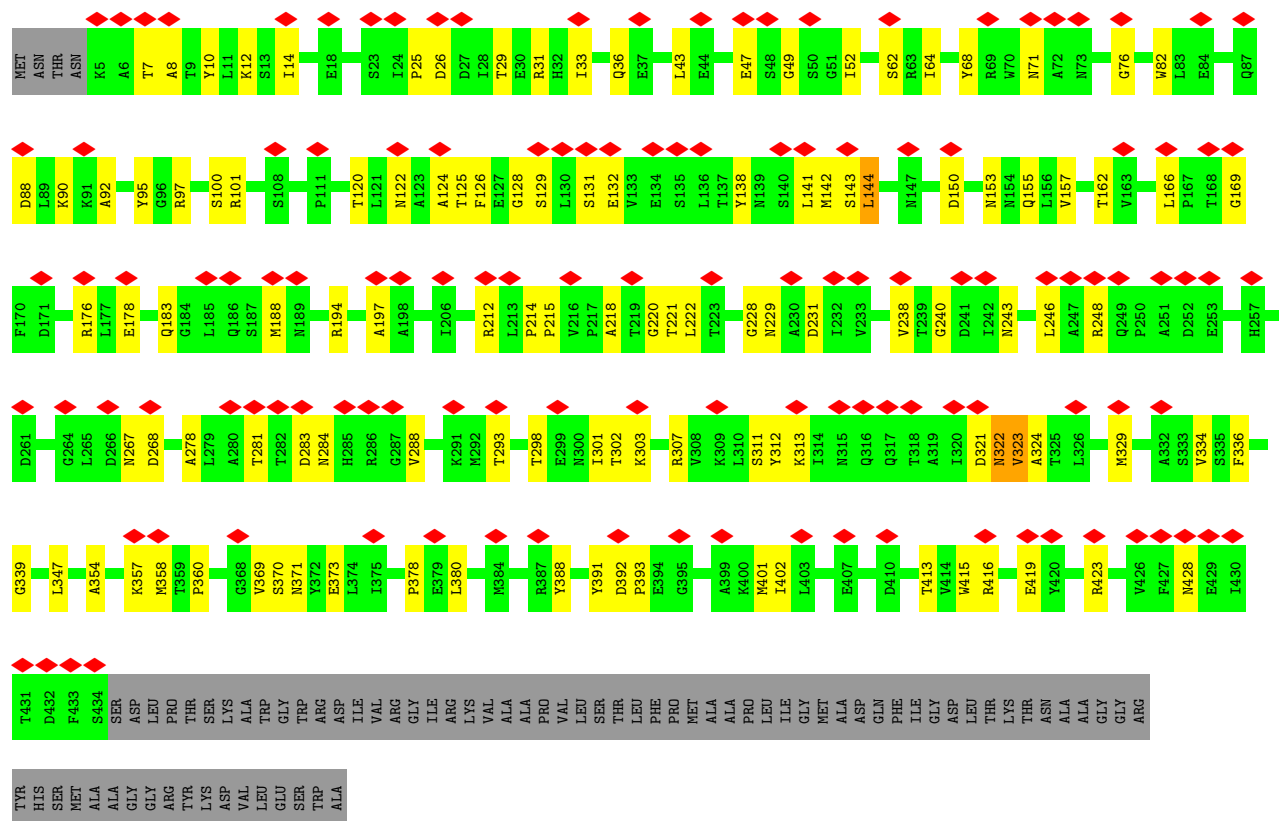
• Molecule 1: Structural polyprotein



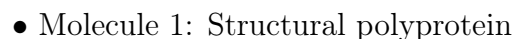
• Molecule 1: Structural polyprotein



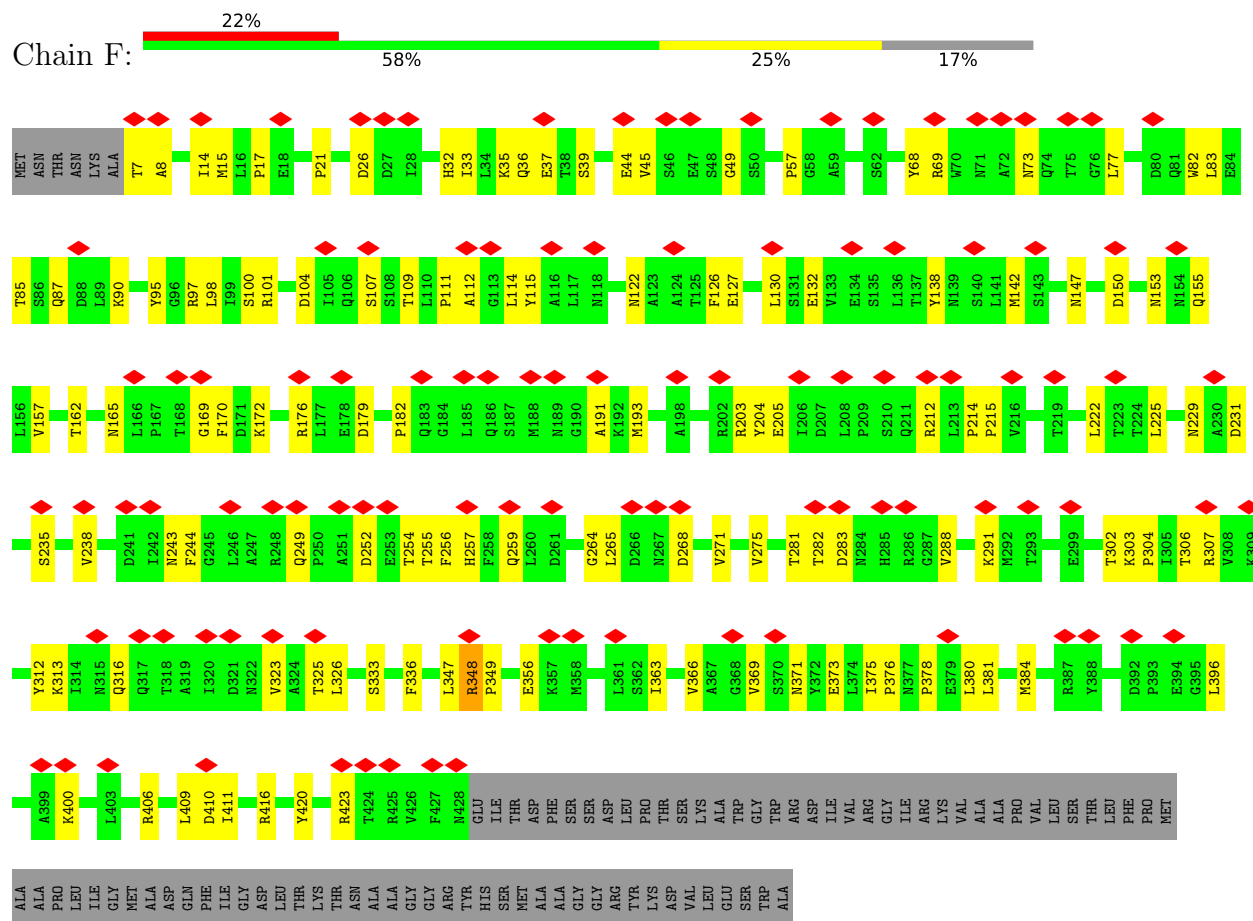
- Molecule 1: Structural polypeptide



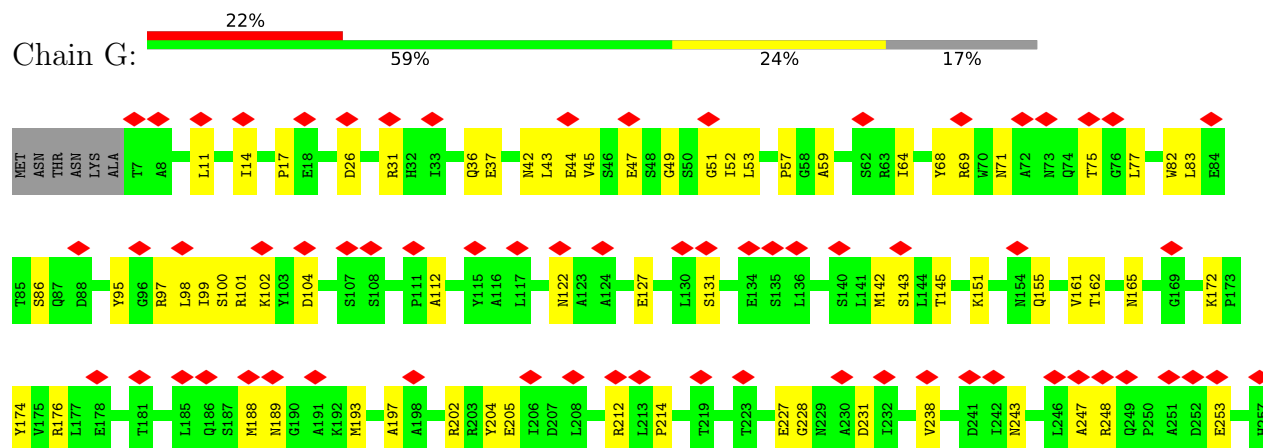
- Molecule 1: Structural polyprotein

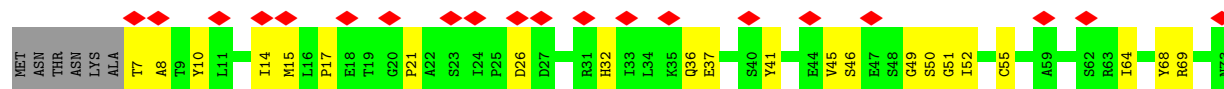


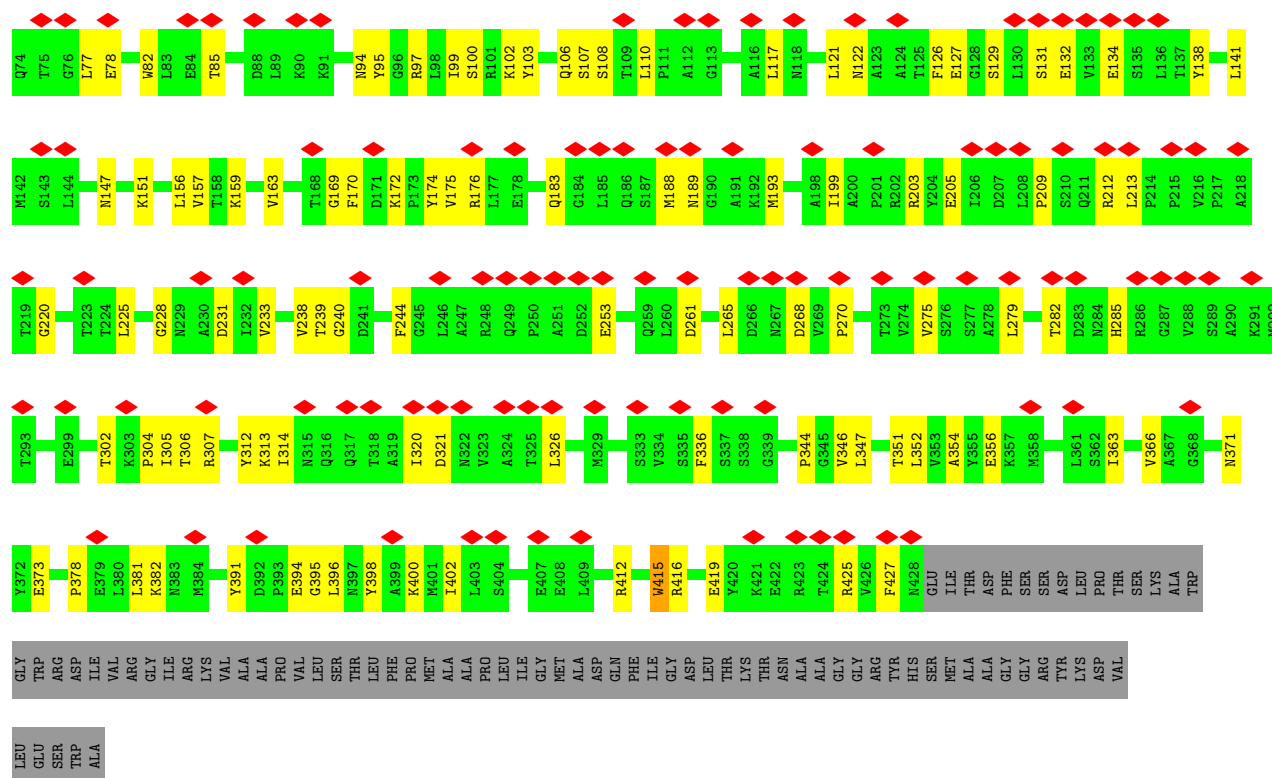
- Molecule 1: Structural polyprotein



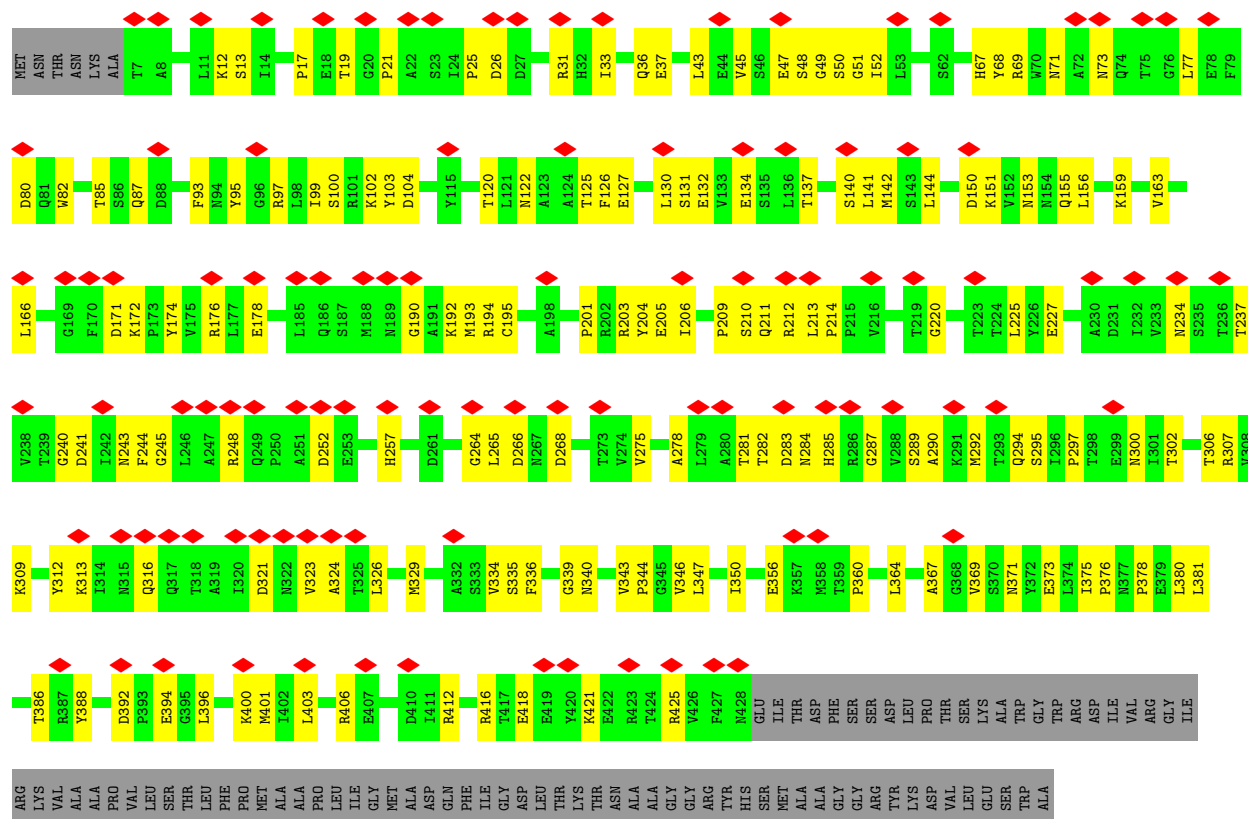
- Molecule 1: Structural polypeptide



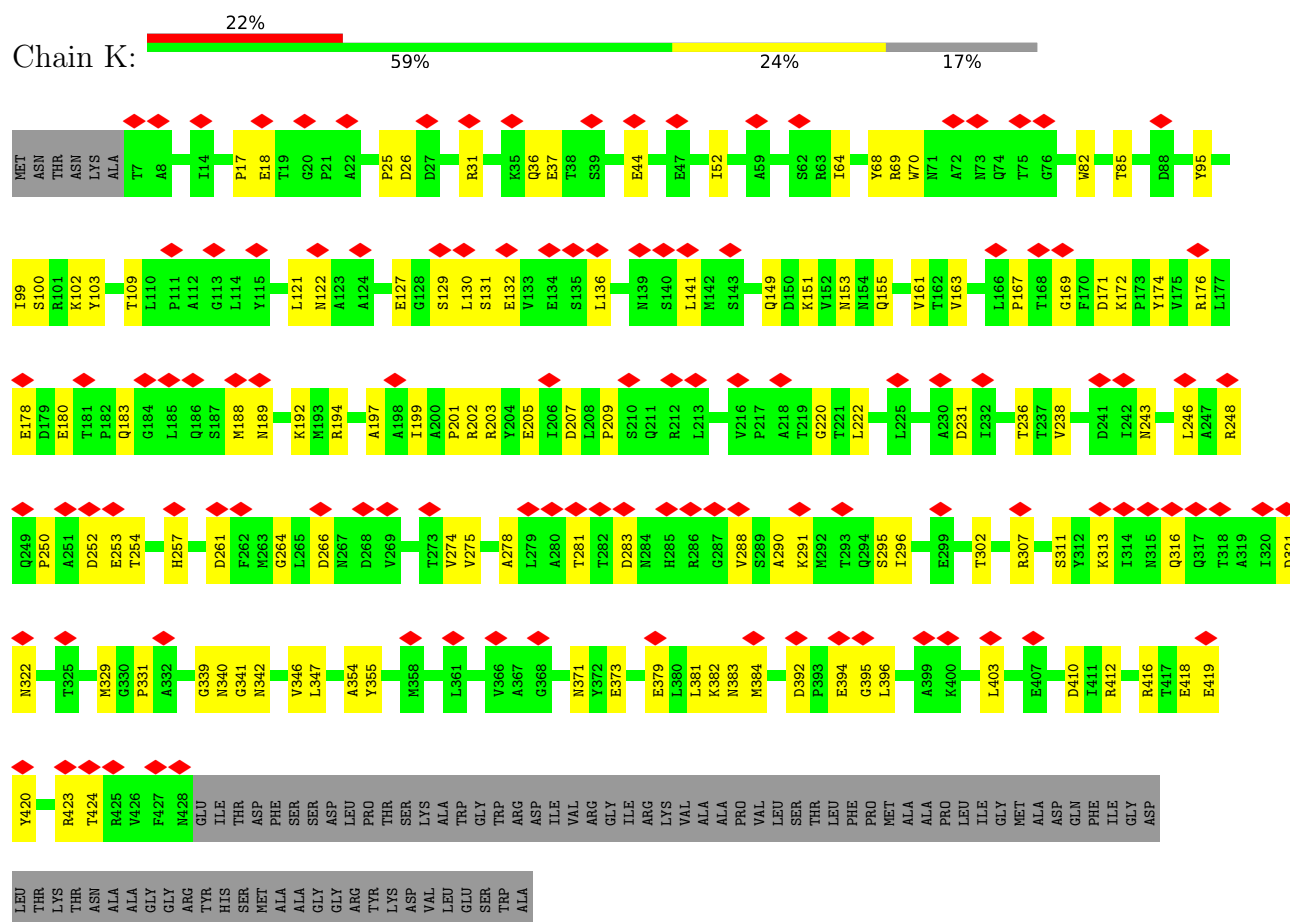




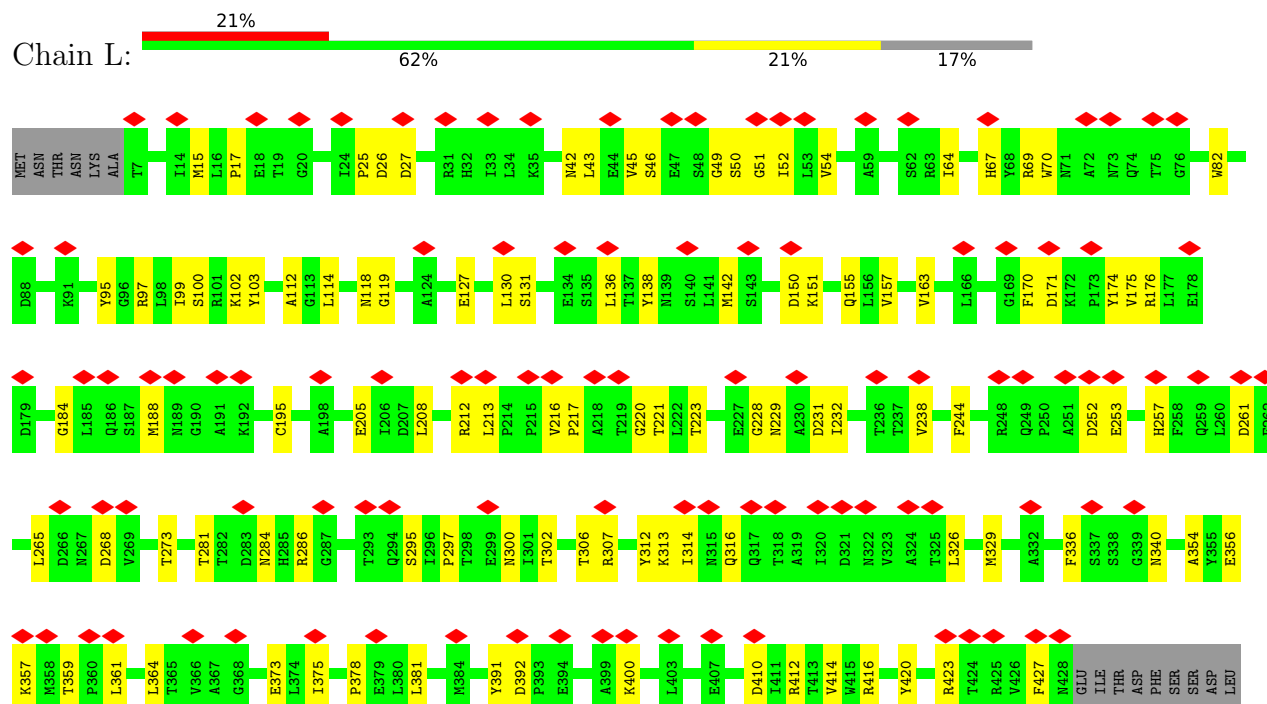
• Molecule 1: Structural polyprotein



Chain K:



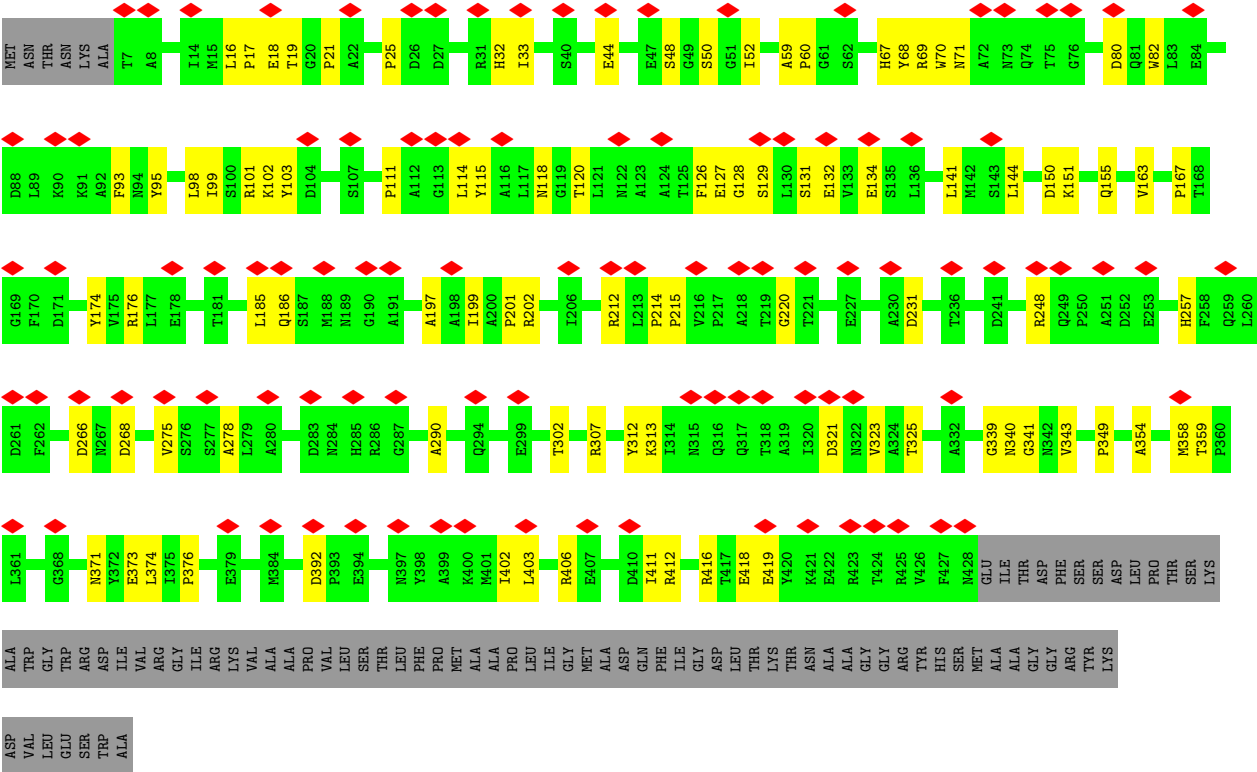
Chain L:



PRO THR
THR SER
LYS LYS
ALA TRP
GLY TRP
ARG ASP
ASP ILE
VAL ARG
VAL ARG
GLY ILE
ILE ARG
LYS VAL
ALA VAL
ALA PRO
VAL VAL
LEU SER
THR THR
LEU PHE
PHE PRO
MET MET
ALA ALA
ALA PRO
LEU LEU
ILE GLY
MET MET
ALA MET
ASP ASP
GLN PHE
ILE ILE
GLY GLY
ASP LEU
THR THR
LYS THR
ASN ASN
ALA ALA
ALA GLY
GLY GLY

GLY ARG
TYR LYS
ASP ASP
VAL VAL
LEU LEU
SER SER
TRP TRP
ALA ALA

● Molecule 1: Structural polyprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	35498	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 ($e^-/\text{\AA}^2$)	26.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.983	Depositor
Minimum map value	-1.911	Depositor
Average map value	0.038	Depositor
Map value standard deviation	0.231	Depositor
Recommended contour level	0.92	Depositor
Map size (Å)	898.80005, 898.80005, 898.80005	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.284, 1.284, 1.284	Depositor

5 Model quality

5.1 Standard geometry

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	0.35	0/3355	0.61	3/4568 (0.1%)
1	B	0.30	0/3341	0.52	0/4552
1	C	0.31	0/3388	0.52	1/4615 (0.0%)
1	D	0.30	0/3324	0.53	0/4529
1	E	0.31	0/3324	0.51	0/4529
1	F	0.31	0/3324	0.54	2/4529 (0.0%)
1	G	0.30	0/3324	0.53	0/4529
1	H	0.30	0/3324	0.56	2/4529 (0.0%)
1	I	0.29	0/3324	0.54	1/4529 (0.0%)
1	J	0.30	0/3324	0.53	1/4529 (0.0%)
1	K	0.29	0/3324	0.54	1/4529 (0.0%)
1	L	0.30	0/3324	0.53	0/4529
1	M	0.29	0/3324	0.50	0/4529
All	All	0.30	0/43324	0.54	11/59025 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	2
1	F	0	1
1	H	0	1
All	All	0	7

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	THR	CA-C-N	-10.50	106.54	125.02
1	A	7	THR	C-N-CA	-10.50	106.54	125.02
1	A	431	THR	N-CA-C	-6.78	96.36	110.80
1	J	425	ARG	N-CA-C	-6.36	107.37	114.62
1	C	144	LEU	N-CA-C	-5.97	107.23	114.75
1	K	18	GLU	N-CA-C	-5.22	108.18	114.75
1	H	347	LEU	CA-C-N	-5.18	109.16	121.80
1	H	347	LEU	C-N-CA	-5.18	109.16	121.80
1	F	347	LEU	CA-C-N	-5.02	109.54	121.80
1	F	347	LEU	C-N-CA	-5.02	109.54	121.80
1	I	425	ARG	N-CA-C	-5.02	107.54	113.97

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	428	ASN	Peptide
1	B	322	ASN	Peptide
1	C	322	ASN	Peptide
1	E	322	ASN	Peptide
1	E	424	THR	Peptide
1	F	348	ARG	Peptide
1	H	348	ARG	Peptide

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	3292	0	3268	102	0
1	B	3277	0	3263	97	0
1	C	3323	0	3306	82	0
1	D	3260	0	3246	85	0
1	E	3260	0	3246	79	0
1	F	3260	0	3246	92	0
1	G	3260	0	3246	84	0
1	H	3260	0	3246	88	0
1	I	3260	0	3246	91	0
1	J	3260	0	3246	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3260	0	3246	88	0
1	L	3260	0	3246	83	0
1	M	3260	0	3246	65	0
All	All	42492	0	42297	1043	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 12.

All (1043) 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:J:212:ARG:HG3	1:J:323:VAL:HG13	1.56	0.88
1:A:430:ILE:O	1:A:431:THR:O	1.91	0.88
1:A:7:THR:O	1:A:8:ALA:HB3	1.74	0.87
1:E:419:GLU:O	1:E:423:ARG:HB2	1.73	0.87
1:L:17:PRO:HB3	1:L:100:SER:HB3	1.56	0.87
1:L:50:SER:HA	1:L:356:GLU:HA	1.54	0.85
1:G:127:GLU:HB2	1:I:381:LEU:HD21	1.59	0.84
1:K:381:LEU:HD21	1:L:127:GLU:HB2	1.56	0.84
1:L:17:PRO:HG2	1:L:102:LYS:HB2	1.59	0.84
1:I:82:TRP:NE1	1:I:302:THR:O	2.10	0.84
1:A:7:THR:OG1	1:A:8:ALA:N	2.10	0.82
1:K:394:GLU:HG2	1:K:395:GLY:H	1.42	0.82
1:A:317:GLN:HB3	1:A:320:ILE:HB	1.61	0.82
1:K:17:PRO:HG2	1:K:102:LYS:HB2	1.61	0.81
1:A:150:ASP:OD1	1:A:406:ARG:NH2	2.16	0.79
1:A:46:SER:HB3	1:A:69:ARG:HD3	1.65	0.78
1:J:275:VAL:HB	1:K:329:MET:HB2	1.66	0.78
1:M:99:ILE:HD11	1:M:373:GLU:HG3	1.67	0.77
1:I:46:SER:HB3	1:I:69:ARG:HD3	1.67	0.76
1:F:214:PRO:O	1:F:312:TYR:OH	2.04	0.76
1:C:26:ASP:OD1	1:C:97:ARG:NH2	2.18	0.76
1:J:150:ASP:OD1	1:J:406:ARG:NH2	2.19	0.76
1:J:21:PRO:HB3	1:J:371:ASN:HB3	1.66	0.76
1:C:82:TRP:NE1	1:C:302:THR:O	2.19	0.76
1:D:141:LEU:HA	1:D:144:LEU:HD13	1.68	0.75
1:I:37:GLU:HG2	1:I:85:THR:HB	1.68	0.74
1:J:82:TRP:NE1	1:J:302:THR:O	2.18	0.74
1:K:17:PRO:HB3	1:K:100:SER:HB3	1.68	0.74
1:L:114:LEU:O	1:M:115:TYR:OH	2.06	0.74
1:M:214:PRO:O	1:M:312:TYR:OH	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HE2	1:A:6:ALA:HB2	1.69	0.74
1:A:217:PRO:HG2	1:A:221:THR:HG21	1.70	0.74
1:I:122:ASN:ND2	1:I:138:TYR:O	2.21	0.74
1:L:130:LEU:HD22	1:L:306:THR:HG21	1.69	0.74
1:M:33:ILE:HD11	1:M:93:PHE:HE1	1.52	0.74
1:L:82:TRP:NE1	1:L:302:THR:O	2.17	0.74
1:G:51:GLY:HA2	1:G:69:ARG:HA	1.70	0.73
1:J:151:LYS:O	1:J:412:ARG:NH2	2.22	0.73
1:B:394:GLU:HG3	1:B:395:GLY:H	1.54	0.72
1:K:64:ILE:O	1:K:103:TYR:OH	2.07	0.72
1:I:169:GLY:O	1:I:172:LYS:NZ	2.22	0.72
1:M:48:SER:OG	1:M:71:ASN:O	2.07	0.72
1:G:212:ARG:HA	1:G:325:THR:HA	1.69	0.72
1:E:31:ARG:NH1	1:F:127:GLU:OE2	2.20	0.72
1:I:151:LYS:O	1:I:412:ARG:NH2	2.22	0.72
1:B:212:ARG:HH12	1:B:215:PRO:HD3	1.56	0.71
1:F:82:TRP:NE1	1:F:302:THR:O	2.20	0.71
1:K:169:GLY:O	1:K:172:LYS:NZ	2.23	0.71
1:F:26:ASP:OD1	1:F:97:ARG:NH2	2.22	0.71
1:I:17:PRO:HG2	1:I:102:LYS:HB2	1.71	0.71
1:J:26:ASP:OD1	1:J:97:ARG:NH2	2.21	0.71
1:A:264:GLY:O	1:A:307:ARG:NH1	2.24	0.70
1:H:409:LEU:O	1:H:423:ARG:NH2	2.23	0.70
1:B:150:ASP:OD1	1:B:406:ARG:NH2	2.24	0.70
1:K:151:LYS:O	1:K:412:ARG:NH2	2.25	0.70
1:A:122:ASN:HD22	1:A:153:ASN:HA	1.57	0.70
1:J:241:ASP:OD2	1:J:289:SER:OG	2.09	0.70
1:K:82:TRP:NE1	1:K:302:THR:O	2.17	0.70
1:J:51:GLY:HA2	1:J:69:ARG:HA	1.74	0.70
1:H:129:SER:O	1:H:131:SER:N	2.24	0.69
1:A:155:GLN:OE1	1:A:416:ARG:NH1	2.23	0.69
1:C:141:LEU:HA	1:C:144:LEU:HD13	1.74	0.69
1:C:419:GLU:O	1:C:423:ARG:HB2	1.91	0.69
1:F:268:ASP:OD1	1:F:307:ARG:NH2	2.26	0.69
1:H:82:TRP:NE1	1:H:302:THR:O	2.21	0.69
1:J:103:TYR:HB2	1:J:163:VAL:HB	1.73	0.69
1:B:212:ARG:HA	1:B:325:THR:HA	1.75	0.69
1:A:95:TYR:HB3	1:A:174:TYR:HB3	1.75	0.69
1:J:127:GLU:HB2	1:L:381:LEU:HD21	1.75	0.69
1:A:17:PRO:HG2	1:A:102:LYS:HB2	1.73	0.69
1:B:12:LYS:HE2	1:B:19:THR:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:HB2	1:D:341:GLY:HA3	1.75	0.69
1:M:82:TRP:NE1	1:M:302:THR:O	2.23	0.69
1:M:167:PRO:HD2	1:M:403:LEU:HD11	1.73	0.68
1:B:275:VAL:HB	1:C:329:MET:HB3	1.76	0.68
1:J:268:ASP:OD1	1:J:307:ARG:NH2	2.27	0.68
1:I:394:GLU:O	1:I:396:LEU:N	2.26	0.68
1:K:254:THR:HG22	1:K:316:GLN:HB2	1.76	0.68
1:B:141:LEU:HA	1:B:144:LEU:HD13	1.75	0.68
1:E:378:PRO:HG2	1:F:132:GLU:HB3	1.74	0.68
1:L:176:ARG:NE	1:L:195:CYS:SG	2.63	0.68
1:E:82:TRP:NE1	1:E:302:THR:O	2.25	0.68
1:H:244:PHE:HB3	1:H:326:LEU:HD12	1.76	0.68
1:D:71:ASN:ND2	1:D:75:THR:OG1	2.27	0.68
1:M:129:SER:OG	1:M:231:ASP:OD2	2.12	0.68
1:I:64:ILE:O	1:I:103:TYR:OH	2.10	0.67
1:K:243:ASN:ND2	1:K:329:MET:O	2.27	0.67
1:H:55:CYS:HB2	1:H:351:THR:HG23	1.77	0.67
1:M:278:ALA:HB2	1:M:290:ALA:HB2	1.76	0.67
1:F:35:LYS:NZ	1:F:87:GLN:OE1	2.27	0.67
1:C:7:THR:HG22	1:C:8:ALA:H	1.60	0.67
1:I:239:THR:HG22	1:I:240:GLY:H	1.60	0.67
1:F:130:LEU:HD22	1:F:306:THR:HG21	1.77	0.67
1:J:234:ASN:HD21	1:J:339:GLY:HA3	1.60	0.67
1:A:378:PRO:HG3	1:B:132:GLU:HB3	1.75	0.67
1:G:295:SER:OG	1:H:205:GLU:OE2	2.13	0.67
1:D:151:LYS:O	1:D:412:ARG:NH2	2.28	0.66
1:A:314:ILE:HD12	1:A:320:ILE:HG22	1.77	0.66
1:G:99:ILE:HD11	1:G:373:GLU:HG3	1.77	0.66
1:I:50:SER:HA	1:I:356:GLU:HA	1.77	0.66
1:I:261:ASP:HB2	1:I:270:PRO:HB3	1.78	0.66
1:G:281:THR:HG23	1:G:283:ASP:H	1.61	0.66
1:H:254:THR:HG22	1:H:316:GLN:HG3	1.77	0.65
1:K:155:GLN:OE1	1:K:416:ARG:NH1	2.27	0.65
1:L:151:LYS:O	1:L:412:ARG:NH2	2.29	0.65
1:E:122:ASN:ND2	1:E:138:TYR:O	2.27	0.65
1:G:205:GLU:OE2	1:G:333:SER:OG	2.08	0.65
1:G:275:VAL:HB	1:H:329:MET:HB2	1.78	0.65
1:M:150:ASP:OD1	1:M:406:ARG:NH2	2.27	0.65
1:I:203:ARG:NH2	1:I:205:GLU:OE2	2.29	0.65
1:J:205:GLU:HG3	1:J:335:SER:HB3	1.79	0.65
1:M:151:LYS:O	1:M:412:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:GLY:HA2	1:D:69:ARG:HA	1.78	0.64
1:L:54:VAL:HG11	1:L:130:LEU:HD12	1.77	0.64
1:A:243:ASN:HD22	1:A:329:MET:HB2	1.62	0.64
1:G:410:ASP:HB3	1:G:423:ARG:HH22	1.60	0.64
1:K:129:SER:O	1:K:131:SER:N	2.30	0.64
1:M:98:LEU:HD13	1:M:101:ARG:HH21	1.63	0.64
1:L:155:GLN:OE1	1:L:416:ARG:NH1	2.31	0.64
1:I:99:ILE:HD11	1:I:373:GLU:HG3	1.77	0.64
1:A:169:GLY:O	1:A:172:LYS:NZ	2.31	0.64
1:A:150:ASP:OD2	1:C:31:ARG:NH1	2.30	0.64
1:A:175:VAL:HG13	1:A:340:ASN:HD21	1.63	0.64
1:A:410:ASP:O	1:A:423:ARG:NH2	2.29	0.64
1:F:409:LEU:O	1:F:423:ARG:NH2	2.31	0.64
1:C:178:GLU:O	1:C:194:ARG:NH1	2.31	0.63
1:K:95:TYR:HB3	1:K:174:TYR:HB3	1.80	0.63
1:C:322:ASN:O	1:C:324:ALA:N	2.31	0.63
1:A:220:GLY:HA2	1:A:313:LYS:HD2	1.81	0.63
1:B:265:LEU:HD23	1:B:306:THR:HG21	1.81	0.63
1:F:14:ILE:HD13	1:F:100:SER:HB3	1.80	0.63
1:G:31:ARG:NH1	1:H:127:GLU:OE2	2.31	0.63
1:K:420:TYR:O	1:K:424:THR:OG1	2.16	0.63
1:D:127:GLU:HB2	1:F:381:LEU:HD21	1.80	0.63
1:G:37:GLU:OE2	1:G:86:SER:OG	2.17	0.63
1:A:212:ARG:NH1	1:A:213:LEU:O	2.31	0.63
1:D:278:ALA:HB2	1:D:290:ALA:HB2	1.81	0.63
1:H:145:THR:OG1	1:H:147:ASN:OD1	2.17	0.63
1:F:95:TYR:HB2	1:F:375:ILE:HB	1.79	0.63
1:J:33:ILE:HD11	1:J:386:THR:HG22	1.80	0.63
1:F:44:GLU:O	1:F:69:ARG:NH2	2.26	0.62
1:J:141:LEU:HA	1:J:144:LEU:HD13	1.81	0.62
1:F:169:GLY:O	1:F:172:LYS:NZ	2.31	0.62
1:L:359:THR:HG22	1:L:361:LEU:H	1.63	0.62
1:M:111:PRO:HG2	1:M:114:LEU:HD12	1.81	0.62
1:G:68:TYR:HB3	1:G:77:LEU:HD22	1.80	0.62
1:G:297:PRO:HD2	1:G:300:ASN:HD22	1.64	0.62
1:J:93:PHE:HA	1:J:376:PRO:HA	1.82	0.62
1:M:268:ASP:OD1	1:M:307:ARG:NH2	2.21	0.62
1:B:328:THR:HG23	1:B:329:MET:HG3	1.81	0.62
1:B:394:GLU:O	1:B:396:LEU:N	2.31	0.62
1:E:45:VAL:HG13	1:E:49:GLY:HA2	1.80	0.62
1:M:17:PRO:HG2	1:M:102:LYS:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:ASP:OD1	1:G:307:ARG:NH2	2.33	0.62
1:M:212:ARG:HE	1:M:323:VAL:HG13	1.63	0.62
1:J:122:ASN:HD22	1:J:153:ASN:HA	1.65	0.61
1:K:346:VAL:HG12	1:K:347:LEU:HG	1.81	0.61
1:B:264:GLY:O	1:B:307:ARG:NH1	2.33	0.61
1:D:99:ILE:HD11	1:D:373:GLU:HG3	1.81	0.61
1:D:169:GLY:O	1:D:172:LYS:NZ	2.33	0.61
1:J:155:GLN:NE2	1:J:418:GLU:OE2	2.31	0.61
1:B:52:ILE:HD11	1:B:352:LEU:HB3	1.82	0.61
1:D:82:TRP:NE1	1:D:302:THR:O	2.29	0.61
1:F:122:ASN:HD22	1:F:153:ASN:HA	1.65	0.61
1:J:95:TYR:HB3	1:J:174:TYR:HB3	1.82	0.61
1:K:222:LEU:HD22	1:K:313:LYS:HD3	1.82	0.61
1:M:59:ALA:O	1:M:101:ARG:NH2	2.33	0.61
1:H:57:PRO:O	1:H:165:ASN:ND2	2.33	0.61
1:J:155:GLN:OE1	1:J:416:ARG:NH1	2.32	0.61
1:L:95:TYR:HB3	1:L:174:TYR:HB3	1.82	0.61
1:A:7:THR:O	1:A:8:ALA:CB	2.34	0.61
1:H:348:ARG:HD2	1:H:348:ARG:O	2.01	0.61
1:K:220:GLY:HA2	1:K:313:LYS:HD2	1.81	0.61
1:M:95:TYR:HB3	1:M:174:TYR:HB3	1.82	0.61
1:B:145:THR:HG22	1:B:147:ASN:H	1.63	0.61
1:E:99:ILE:HD11	1:E:373:GLU:HG3	1.81	0.61
1:A:52:ILE:HD11	1:A:352:LEU:HD12	1.83	0.61
1:D:248:ARG:HG3	1:D:249:GLN:H	1.66	0.61
1:E:237:THR:OG1	1:F:203:ARG:NH1	2.34	0.61
1:H:261:ASP:HB2	1:H:270:PRO:HB3	1.83	0.61
1:A:82:TRP:NE1	1:A:302:THR:O	2.25	0.60
1:C:126:PHE:HB2	1:C:144:LEU:HD23	1.82	0.60
1:G:155:GLN:OE1	1:G:416:ARG:NH1	2.34	0.60
1:G:248:ARG:NH2	1:G:321:ASP:OD2	2.34	0.60
1:M:220:GLY:HA2	1:M:313:LYS:HD2	1.83	0.60
1:E:214:PRO:O	1:E:312:TYR:OH	2.19	0.60
1:F:281:THR:HG23	1:F:283:ASP:H	1.65	0.60
1:A:107:SER:HB2	1:A:157:VAL:HG22	1.83	0.60
1:E:138:TYR:OH	1:E:154:ASN:OD1	2.19	0.60
1:C:214:PRO:O	1:C:312:TYR:OH	2.20	0.60
1:J:214:PRO:O	1:J:312:TYR:OH	2.20	0.60
1:F:111:PRO:HG2	1:F:114:LEU:HD13	1.84	0.60
1:K:31:ARG:NH1	1:L:150:ASP:OD2	2.35	0.60
1:K:264:GLY:O	1:K:307:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:GLU:HA	1:H:360:PRO:HB3	1.83	0.60
1:I:106:GLN:HG2	1:I:107:SER:H	1.67	0.60
1:L:410:ASP:O	1:L:423:ARG:NH2	2.29	0.60
1:B:95:TYR:HB3	1:B:174:TYR:HB3	1.82	0.60
1:C:129:SER:HB3	1:C:231:ASP:OD2	2.01	0.60
1:D:189:ASN:OD1	1:D:190:GLY:N	2.34	0.59
1:K:394:GLU:HG2	1:K:395:GLY:N	2.15	0.59
1:B:248:ARG:NH2	1:B:321:ASP:OD1	2.27	0.59
1:I:141:LEU:HD11	1:I:352:LEU:HB3	1.82	0.59
1:B:252:ASP:N	1:B:252:ASP:OD1	2.36	0.59
1:J:31:ARG:NH1	1:K:127:GLU:OE2	2.35	0.59
1:M:212:ARG:HA	1:M:325:THR:HA	1.84	0.59
1:A:294:GLN:NE2	1:B:241:ASP:OD2	2.35	0.59
1:F:150:ASP:OD1	1:F:406:ARG:NH2	2.28	0.59
1:F:212:ARG:HA	1:F:325:THR:HA	1.83	0.59
1:A:194:ARG:NE	1:A:299:GLU:OE2	2.35	0.59
1:K:394:GLU:O	1:K:396:LEU:N	2.35	0.59
1:I:131:SER:OG	1:I:231:ASP:OD1	2.17	0.59
1:J:37:GLU:HG2	1:J:85:THR:HB	1.83	0.59
1:J:257:HIS:HB3	1:J:313:LYS:HG2	1.83	0.59
1:C:12:LYS:NZ	1:C:428:ASN:O	2.35	0.59
1:C:47:GLU:HA	1:C:360:PRO:HB3	1.85	0.59
1:C:97:ARG:NH1	1:C:373:GLU:OE2	2.35	0.59
1:M:50:SER:HG	1:M:70:TRP:CD1	2.20	0.59
1:A:430:ILE:C	1:A:431:THR:O	2.45	0.59
1:B:122:ASN:ND2	1:B:153:ASN:HA	2.17	0.59
1:F:244:PHE:HB3	1:F:326:LEU:HD23	1.85	0.58
1:H:265:LEU:HD23	1:H:265:LEU:H	1.67	0.58
1:C:246:LEU:HD12	1:C:322:ASN:HB3	1.84	0.58
1:E:17:PRO:HG2	1:E:102:LYS:HB2	1.86	0.58
1:B:419:GLU:O	1:B:423:ARG:HB2	2.03	0.58
1:K:281:THR:OG1	1:K:283:ASP:OD1	2.21	0.58
1:M:185:LEU:O	1:M:186:GLN:NE2	2.37	0.58
1:B:212:ARG:HE	1:B:323:VAL:HB	1.69	0.58
1:H:306:THR:HG23	1:H:307:ARG:HG3	1.84	0.58
1:J:126:PHE:HB3	1:J:350:ILE:HG22	1.86	0.58
1:K:141:LEU:HD21	1:K:354:ALA:HB2	1.85	0.58
1:G:57:PRO:O	1:G:165:ASN:ND2	2.37	0.58
1:L:119:GLY:HA2	1:L:157:VAL:HG12	1.85	0.58
1:A:73:ASN:HB2	1:A:75:THR:HG23	1.86	0.58
1:I:15:MET:HG3	1:I:427:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:ILE:HD13	1:M:354:ALA:HB2	1.86	0.58
1:C:220:GLY:HA2	1:C:313:LYS:HD2	1.85	0.58
1:J:45:VAL:HG13	1:J:49:GLY:HA2	1.86	0.58
1:F:264:GLY:O	1:F:307:ARG:NH1	2.37	0.58
1:B:188:MET:HG3	1:B:189:ASN:H	1.69	0.57
1:I:346:VAL:HG12	1:I:347:LEU:HG	1.85	0.57
1:L:42:ASN:HD21	1:M:120:THR:HG22	1.69	0.57
1:E:376:PRO:HB3	1:E:380:LEU:HD23	1.85	0.57
1:J:50:SER:OG	1:J:356:GLU:OE1	2.20	0.57
1:E:37:GLU:HG2	1:E:85:THR:HB	1.86	0.57
1:A:151:LYS:O	1:A:412:ARG:NH2	2.37	0.57
1:I:52:ILE:HG23	1:I:68:TYR:HB2	1.86	0.57
1:J:190:GLY:HA3	1:K:209:PRO:HG3	1.86	0.57
1:L:46:SER:HB3	1:L:69:ARG:HD3	1.86	0.57
1:B:7:THR:OG1	1:B:394:GLU:OE2	2.21	0.57
1:E:142:MET:SD	1:E:153:ASN:HB3	2.45	0.57
1:H:44:GLU:O	1:H:69:ARG:NH2	2.38	0.57
1:J:378:PRO:HG2	1:K:132:GLU:HB3	1.85	0.57
1:L:268:ASP:OD2	1:L:307:ARG:NH2	2.37	0.57
1:A:39:SER:HB3	1:A:85:THR:HA	1.87	0.57
1:B:37:GLU:OE2	1:B:86:SER:OG	2.21	0.57
1:D:17:PRO:HG2	1:D:102:LYS:HB2	1.87	0.57
1:D:372:TYR:HB2	1:D:374:LEU:HD11	1.86	0.57
1:J:48:SER:OG	1:J:71:ASN:O	2.20	0.57
1:I:103:TYR:HB2	1:I:163:VAL:HB	1.86	0.57
1:A:259:GLN:NE2	1:A:273:THR:OG1	2.38	0.57
1:C:155:GLN:OE1	1:C:416:ARG:NH1	2.32	0.57
1:F:155:GLN:OE1	1:F:416:ARG:NH1	2.32	0.56
1:A:141:LEU:HD21	1:A:354:ALA:HB2	1.86	0.56
1:A:219:THR:HB	1:A:315:ASN:HA	1.87	0.56
1:B:151:LYS:O	1:B:412:ARG:NH2	2.38	0.56
1:C:268:ASP:OD1	1:C:307:ARG:NH2	2.28	0.56
1:D:110:LEU:HD23	1:D:117:LEU:HD12	1.87	0.56
1:E:141:LEU:HA	1:E:144:LEU:HD13	1.86	0.56
1:A:47:GLU:HA	1:A:360:PRO:HB3	1.87	0.56
1:E:42:ASN:HD21	1:H:120:THR:HG22	1.68	0.56
1:C:240:GLY:HA3	1:C:334:VAL:HA	1.86	0.56
1:E:87:GLN:HE22	1:G:383:ASN:HD21	1.54	0.56
1:G:394:GLU:O	1:G:396:LEU:N	2.38	0.56
1:J:21:PRO:HD3	1:J:36:GLN:HB2	1.87	0.56
1:D:44:GLU:O	1:D:69:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:ILE:O	1:H:103:TYR:OH	2.22	0.56
1:J:206:ILE:HD12	1:J:334:VAL:HG23	1.87	0.56
1:L:130:LEU:HD21	1:L:265:LEU:HD12	1.86	0.56
1:I:314:ILE:HD11	1:I:320:ILE:HD13	1.86	0.56
1:J:126:PHE:HB2	1:J:144:LEU:HD23	1.87	0.56
1:L:238:VAL:HG22	1:L:336:PHE:HB3	1.87	0.56
1:M:44:GLU:O	1:M:69:ARG:NH2	2.38	0.56
1:B:47:GLU:HA	1:B:360:PRO:HB3	1.87	0.56
1:B:246:LEU:HD13	1:B:324:ALA:HB2	1.87	0.56
1:H:129:SER:OG	1:H:231:ASP:OD2	2.24	0.56
1:H:240:GLY:HA3	1:H:334:VAL:HA	1.88	0.56
1:J:43:LEU:N	1:J:364:LEU:O	2.38	0.56
1:B:46:SER:HB3	1:B:69:ARG:HD3	1.87	0.56
1:G:419:GLU:O	1:G:423:ARG:HB2	2.06	0.56
1:H:35:LYS:NZ	1:H:87:GLN:OE1	2.38	0.56
1:D:386:THR:OG1	1:E:127:GLU:OE2	2.23	0.56
1:H:376:PRO:HB2	1:H:381:LEU:HD22	1.87	0.56
1:I:170:PHE:CG	1:I:396:LEU:HD11	2.41	0.56
1:H:247:ALA:HB2	1:H:323:VAL:HG22	1.86	0.55
1:K:275:VAL:HB	1:L:329:MET:HB3	1.87	0.55
1:F:212:ARG:HH12	1:F:215:PRO:HD3	1.71	0.55
1:I:46:SER:CB	1:I:69:ARG:HD3	2.37	0.55
1:H:17:PRO:HG2	1:H:102:LYS:HB3	1.89	0.55
1:L:64:ILE:O	1:L:103:TYR:OH	2.22	0.55
1:A:252:ASP:OD1	1:A:252:ASP:N	2.39	0.55
1:C:122:ASN:ND2	1:C:138:TYR:O	2.40	0.55
1:D:132:GLU:HB3	1:F:378:PRO:HG3	1.87	0.55
1:E:212:ARG:HH12	1:E:215:PRO:HD3	1.70	0.55
1:F:112:ALA:HA	1:L:359:THR:HG23	1.89	0.55
1:I:17:PRO:HD2	1:I:102:LYS:HD3	1.89	0.55
1:C:142:MET:SD	1:C:153:ASN:HB3	2.47	0.55
1:E:212:ARG:HA	1:E:325:THR:HA	1.89	0.55
1:G:214:PRO:O	1:G:312:TYR:OH	2.24	0.55
1:H:96:GLY:HA3	1:H:374:LEU:HD23	1.89	0.55
1:A:261:ASP:HB2	1:A:270:PRO:HB3	1.89	0.55
1:C:122:ASN:HB3	1:C:141:LEU:HD11	1.88	0.55
1:G:52:ILE:HG23	1:G:68:TYR:HB2	1.89	0.55
1:H:59:ALA:O	1:H:101:ARG:NH2	2.38	0.55
1:A:416:ARG:O	1:A:417:THR:HG22	2.06	0.55
1:C:131:SER:HB2	1:C:229:ASN:HB3	1.89	0.55
1:H:50:SER:OG	1:H:74:GLN:NE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG23	1:A:223:THR:OG1	2.07	0.55
1:B:21:PRO:HB3	1:B:371:ASN:HB3	1.87	0.54
1:C:95:TYR:OH	1:C:176:ARG:NH1	2.40	0.54
1:F:222:LEU:HD12	1:F:313:LYS:HD3	1.87	0.54
1:G:122:ASN:HB3	1:G:142:MET:HE3	1.89	0.54
1:J:52:ILE:HG23	1:J:68:TYR:HB2	1.88	0.54
1:G:309:LYS:NZ	1:G:311:SER:OG	2.39	0.54
1:H:95:TYR:OH	1:H:176:ARG:NH1	2.41	0.54
1:H:419:GLU:O	1:H:423:ARG:HB2	2.06	0.54
1:J:248:ARG:NH2	1:J:321:ASP:OD1	2.40	0.54
1:A:141:LEU:HA	1:A:144:LEU:HD13	1.88	0.54
1:A:222:LEU:HD11	1:A:259:GLN:HB2	1.89	0.54
1:E:220:GLY:HA2	1:E:313:LYS:HD2	1.88	0.54
1:B:412:ARG:O	1:B:415:TRP:NE1	2.41	0.54
1:D:229:ASN:HD22	1:F:182:PRO:HG2	1.73	0.54
1:K:167:PRO:HG2	1:K:403:LEU:HD11	1.90	0.54
1:K:248:ARG:O	1:K:322:ASN:ND2	2.38	0.54
1:I:95:TYR:HB3	1:I:174:TYR:HB3	1.88	0.54
1:C:243:ASN:HD22	1:C:329:MET:HB2	1.73	0.54
1:J:203:ARG:NH2	1:L:295:SER:OG	2.41	0.54
1:J:212:ARG:NH1	1:J:213:LEU:O	2.37	0.54
1:L:212:ARG:NH1	1:L:213:LEU:O	2.40	0.54
1:M:95:TYR:OH	1:M:176:ARG:NH2	2.41	0.54
1:A:268:ASP:OD1	1:A:307:ARG:NH2	2.41	0.54
1:E:295:SER:O	1:F:333:SER:OG	2.25	0.54
1:C:36:GLN:HE21	1:C:369:VAL:HG21	1.73	0.54
1:D:268:ASP:OD1	1:D:307:ARG:NH2	2.28	0.54
1:H:378:PRO:HB3	1:I:126:PHE:HZ	1.73	0.54
1:I:147:ASN:O	1:I:151:LYS:NZ	2.41	0.54
1:K:410:ASP:HB3	1:K:423:ARG:HH22	1.73	0.54
1:M:141:LEU:HA	1:M:144:LEU:HD13	1.89	0.54
1:A:293:THR:HG22	1:B:291:LYS:HD2	1.90	0.53
1:F:249:GLN:NE2	1:F:282:THR:OG1	2.42	0.53
1:K:178:GLU:O	1:K:194:ARG:NH1	2.41	0.53
1:K:295:SER:OG	1:L:205:GLU:OE1	2.22	0.53
1:L:15:MET:HG3	1:L:427:PHE:CE2	2.43	0.53
1:L:220:GLY:HA2	1:L:313:LYS:HD2	1.88	0.53
1:L:252:ASP:OD1	1:L:252:ASP:N	2.41	0.53
1:L:261:ASP:HB2	1:L:273:THR:HG22	1.91	0.53
1:E:170:PHE:HE2	1:E:400:LYS:HG3	1.73	0.53
1:H:410:ASP:HB3	1:H:423:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:HIS:CD2	1:F:373:GLU:HG2	2.43	0.53
1:H:227:GLU:HB3	1:H:309:LYS:HG3	1.90	0.53
1:I:220:GLY:HA2	1:I:313:LYS:HG3	1.91	0.53
1:M:52:ILE:HG23	1:M:68:TYR:HB2	1.89	0.53
1:A:37:GLU:OE2	1:A:86:SER:OG	2.26	0.53
1:D:252:ASP:OD2	1:D:316:GLN:NE2	2.41	0.53
1:G:11:LEU:HD12	1:G:399:ALA:HA	1.91	0.53
1:L:138:TYR:CG	1:L:356:GLU:HG2	2.43	0.53
1:A:228:GLY:HA2	1:C:183:GLN:HA	1.90	0.53
1:C:126:PHE:CE2	1:C:128:GLY:HA3	2.44	0.53
1:D:118:ASN:HB3	1:K:109:THR:HA	1.89	0.53
1:B:294:GLN:N	1:B:294:GLN:OE1	2.42	0.53
1:F:21:PRO:HB3	1:F:371:ASN:HB3	1.91	0.53
1:G:205:GLU:O	1:I:193:MET:HA	2.08	0.53
1:J:12:LYS:HE2	1:J:19:THR:HG21	1.91	0.53
1:L:163:VAL:HG22	1:L:414:VAL:HG12	1.91	0.53
1:A:274:VAL:HG13	1:A:294:GLN:HG3	1.90	0.53
1:C:238:VAL:HG22	1:C:336:PHE:HB3	1.91	0.53
1:E:37:GLU:OE2	1:E:87:GLN:HG2	2.08	0.53
1:A:248:ARG:HB2	1:A:322:ASN:ND2	2.24	0.53
1:D:378:PRO:HG3	1:E:132:GLU:HB3	1.91	0.53
1:I:26:ASP:OD1	1:I:97:ARG:NH2	2.42	0.53
1:E:182:PRO:HB2	1:F:229:ASN:HD22	1.74	0.53
1:I:129:SER:OG	1:I:132:GLU:OE1	2.27	0.53
1:K:99:ILE:HD11	1:K:373:GLU:HG3	1.91	0.53
1:D:247:ALA:N	1:D:322:ASN:OD1	2.40	0.52
1:H:125:THR:HB	1:H:150:ASP:HB3	1.91	0.52
1:J:99:ILE:HD11	1:J:373:GLU:HG3	1.91	0.52
1:G:238:VAL:HG22	1:G:336:PHE:HB3	1.90	0.52
1:M:129:SER:C	1:M:131:SER:H	2.17	0.52
1:K:129:SER:C	1:K:131:SER:H	2.16	0.52
1:K:246:LEU:HD23	1:K:250:PRO:HG3	1.91	0.52
1:D:329:MET:HB3	1:F:275:VAL:HB	1.91	0.52
1:G:143:SER:O	1:I:382:LYS:HG2	2.10	0.52
1:G:17:PRO:HG2	1:G:102:LYS:HB2	1.91	0.52
1:I:110:LEU:HD23	1:I:117:LEU:HD23	1.91	0.52
1:D:155:GLN:OE1	1:D:416:ARG:NH1	2.40	0.52
1:H:31:ARG:NH1	1:I:127:GLU:OE2	2.40	0.52
1:L:392:ASP:OD2	1:L:392:ASP:N	2.40	0.52
1:C:416:ARG:HB2	1:C:419:GLU:HG2	1.91	0.52
1:H:203:ARG:NH2	1:H:205:GLU:OE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:VAL:HG22	1:I:336:PHE:HB3	1.92	0.52
1:J:227:GLU:OE2	1:L:184:GLY:HA3	2.10	0.52
1:G:162:THR:HG23	1:G:415:TRP:HB2	1.90	0.52
1:I:107:SER:O	1:I:108:SER:OG	2.24	0.52
1:K:201:PRO:O	1:K:342:ASN:ND2	2.43	0.52
1:D:193:MET:HA	1:E:205:GLU:O	2.09	0.52
1:F:410:ASP:HB3	1:F:423:ARG:HH22	1.75	0.52
1:M:103:TYR:HB2	1:M:163:VAL:HB	1.92	0.52
1:A:381:LEU:HD21	1:B:127:GLU:HB2	1.91	0.52
1:E:87:GLN:HE22	1:G:383:ASN:ND2	2.08	0.52
1:F:238:VAL:HG22	1:F:336:PHE:HB3	1.93	0.51
1:L:131:SER:O	1:L:229:ASN:ND2	2.43	0.51
1:C:212:ARG:HG3	1:C:323:VAL:HB	1.91	0.51
1:G:45:VAL:HB	1:G:49:GLY:HA2	1.92	0.51
1:I:244:PHE:HB3	1:I:326:LEU:HD23	1.90	0.51
1:C:125:THR:HB	1:C:150:ASP:HB3	1.93	0.51
1:G:36:GLN:HG2	1:G:371:ASN:ND2	2.26	0.51
1:I:225:LEU:HD11	1:I:312:TYR:HB3	1.93	0.51
1:L:99:ILE:HD11	1:L:373:GLU:HG3	1.91	0.51
1:A:213:LEU:HD12	1:A:324:ALA:HB3	1.93	0.51
1:I:7:THR:OG1	1:I:8:ALA:N	2.44	0.51
1:L:45:VAL:CG1	1:L:49:GLY:HA2	2.41	0.51
1:A:182:PRO:HG2	1:B:229:ASN:HB2	1.93	0.51
1:F:37:GLU:HG2	1:F:85:THR:HB	1.91	0.51
1:J:400:LYS:NZ	1:L:27:ASP:OD2	2.40	0.51
1:A:54:VAL:HG11	1:A:130:LEU:HD22	1.92	0.51
1:B:134:GLU:HG2	1:B:135:SER:N	2.26	0.51
1:C:293:THR:O	1:C:293:THR:OG1	2.29	0.51
1:J:132:GLU:HB3	1:L:378:PRO:HG2	1.92	0.51
1:A:249:GLN:HE22	1:A:282:THR:HA	1.76	0.51
1:D:46:SER:OG	1:D:47:GLU:OE1	2.27	0.51
1:D:243:ASN:HD22	1:D:329:MET:HB2	1.75	0.51
1:G:228:GLY:HA2	1:I:183:GLN:HA	1.93	0.51
1:I:265:LEU:HD23	1:I:306:THR:HG21	1.91	0.51
1:E:80:ASP:OD2	1:E:81:GLN:HG2	2.11	0.51
1:F:142:MET:HE3	1:F:153:ASN:HB3	1.93	0.51
1:G:82:TRP:CH2	1:G:304:PRO:HG3	2.45	0.51
1:A:7:THR:O	1:A:8:ALA:C	2.50	0.50
1:B:297:PRO:HD2	1:B:300:ASN:HD22	1.76	0.50
1:G:394:GLU:CD	1:G:395:GLY:H	2.18	0.50
1:J:394:GLU:O	1:J:396:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLN:HE21	1:A:159:LYS:HB2	1.76	0.50
1:A:416:ARG:HB2	1:A:419:GLU:HG2	1.92	0.50
1:E:45:VAL:CG1	1:E:49:GLY:HA2	2.41	0.50
1:G:52:ILE:HD13	1:G:354:ALA:HB2	1.92	0.50
1:A:129:SER:HB3	1:A:231:ASP:OD2	2.12	0.50
1:B:64:ILE:O	1:B:103:TYR:OH	2.18	0.50
1:B:391:TYR:CZ	1:C:401:MET:HB3	2.46	0.50
1:E:127:GLU:HA	1:E:349:PRO:HB3	1.93	0.50
1:H:193:MET:HA	1:I:205:GLU:O	2.12	0.50
1:J:142:MET:SD	1:J:153:ASN:HB3	2.51	0.50
1:D:21:PRO:HB3	1:D:371:ASN:HB3	1.92	0.50
1:G:64:ILE:HG12	1:G:83:LEU:O	2.12	0.50
1:G:145:THR:HG23	1:G:151:LYS:HD3	1.92	0.50
1:G:172:LYS:HD3	1:G:344:PRO:HG2	1.94	0.50
1:J:376:PRO:HG2	1:J:381:LEU:HD22	1.94	0.50
1:D:71:ASN:HD21	1:D:75:THR:HG1	1.58	0.50
1:B:29:THR:H	1:C:169:GLY:HA2	1.76	0.50
1:D:55:CYS:HB2	1:D:351:THR:HB	1.93	0.50
1:D:314:ILE:HD11	1:D:320:ILE:HD13	1.94	0.50
1:J:281:THR:OG1	1:J:282:THR:N	2.44	0.50
1:D:113:GLY:O	1:D:114:LEU:HD12	2.12	0.50
1:E:131:SER:OG	1:E:231:ASP:OD2	2.28	0.50
1:F:57:PRO:O	1:F:165:ASN:ND2	2.45	0.50
1:B:94:ASN:ND2	1:B:377:ASN:HA	2.27	0.50
1:D:132:GLU:HB3	1:F:378:PRO:CG	2.42	0.50
1:F:212:ARG:HE	1:F:323:VAL:HB	1.77	0.50
1:K:103:TYR:HB2	1:K:163:VAL:HB	1.92	0.50
1:I:172:LYS:HE3	1:I:344:PRO:HG2	1.92	0.49
1:J:283:ASP:OD1	1:J:284:ASN:N	2.45	0.49
1:F:15:MET:HE1	1:F:411:ILE:HG23	1.94	0.49
1:L:43:LEU:N	1:L:364:LEU:O	2.38	0.49
1:G:275:VAL:HG12	1:H:329:MET:HE3	1.93	0.49
1:L:244:PHE:HB3	1:L:326:LEU:HD23	1.93	0.49
1:A:29:THR:H	1:B:169:GLY:HA2	1.78	0.49
1:D:57:PRO:O	1:D:165:ASN:ND2	2.46	0.49
1:H:142:MET:SD	1:H:153:ASN:HB3	2.53	0.49
1:J:47:GLU:HA	1:J:360:PRO:HB3	1.94	0.49
1:L:253:GLU:OE1	1:L:281:THR:HA	2.12	0.49
1:A:145:THR:OG1	1:A:147:ASN:ND2	2.42	0.49
1:E:217:PRO:HG2	1:E:221:THR:HG21	1.94	0.49
1:M:32:HIS:CD2	1:M:373:GLU:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:GLU:N	1:M:134:GLU:OE1	2.46	0.49
1:F:83:LEU:HD21	1:F:366:VAL:HG11	1.93	0.49
1:G:14:ILE:HD13	1:G:100:SER:HB3	1.93	0.49
1:I:77:LEU:HD11	1:I:265:LEU:HD12	1.94	0.49
1:J:77:LEU:HD11	1:J:265:LEU:HD11	1.93	0.49
1:J:130:LEU:HD21	1:J:265:LEU:HD22	1.94	0.49
1:M:127:GLU:HA	1:M:349:PRO:HB3	1.95	0.49
1:A:10:TYR:CZ	1:A:14:ILE:HD11	2.48	0.49
1:D:134:GLU:N	1:D:134:GLU:OE1	2.44	0.49
1:C:283:ASP:OD1	1:C:284:ASN:N	2.46	0.49
1:A:126:PHE:HB2	1:A:144:LEU:HD23	1.95	0.49
1:B:52:ILE:HG23	1:B:68:TYR:HB2	1.95	0.49
1:C:321:ASP:OD1	1:C:321:ASP:N	2.46	0.49
1:D:107:SER:OG	1:D:108:SER:N	2.45	0.49
1:F:252:ASP:OD1	1:F:252:ASP:N	2.44	0.49
1:G:227:GLU:HG2	1:G:309:LYS:HB2	1.95	0.49
1:H:253:GLU:HB3	1:H:279:LEU:HD11	1.95	0.49
1:K:248:ARG:NH2	1:K:321:ASP:OD1	2.45	0.49
1:M:21:PRO:HB3	1:M:371:ASN:HB3	1.95	0.49
1:A:283:ASP:OD1	1:A:284:ASN:N	2.46	0.48
1:B:392:ASP:OD1	1:B:392:ASP:N	2.44	0.48
1:J:237:THR:OG1	1:K:203:ARG:NH1	2.46	0.48
1:L:252:ASP:OD2	1:L:316:GLN:NE2	2.46	0.48
1:E:197:ALA:HB1	1:E:340:ASN:ND2	2.27	0.48
1:F:7:THR:OG1	1:F:8:ALA:N	2.47	0.48
1:I:15:MET:O	1:I:17:PRO:HD3	2.13	0.48
1:L:97:ARG:HD2	1:L:174:TYR:CZ	2.49	0.48
1:A:145:THR:HG1	1:A:147:ASN:HD22	1.58	0.48
1:A:182:PRO:HB2	1:B:229:ASN:HD22	1.78	0.48
1:A:316:GLN:C	1:A:318:THR:H	2.20	0.48
1:C:391:TYR:CZ	1:C:393:PRO:HG3	2.48	0.48
1:J:178:GLU:HG3	1:J:194:ARG:HD3	1.95	0.48
1:A:131:SER:HB3	1:A:231:ASP:HB3	1.95	0.48
1:H:10:TYR:CE2	1:H:14:ILE:HD11	2.48	0.48
1:J:104:ASP:HB2	1:J:367:ALA:HB3	1.94	0.48
1:J:297:PRO:HD2	1:J:300:ASN:HD22	1.78	0.48
1:A:209:PRO:HG2	1:C:188:MET:HE2	1.96	0.48
1:D:95:TYR:HB3	1:D:174:TYR:HB3	1.96	0.48
1:F:107:SER:HB2	1:F:157:VAL:HG22	1.95	0.48
1:F:170:PHE:HE2	1:F:400:LYS:HG2	1.78	0.48
1:G:378:PRO:CG	1:H:132:GLU:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:45:VAL:CG1	1:J:49:GLY:HA2	2.43	0.48
1:J:68:TYR:HB3	1:J:77:LEU:HD13	1.94	0.48
1:L:297:PRO:HD2	1:L:300:ASN:HD22	1.79	0.48
1:C:129:SER:C	1:C:131:SER:H	2.22	0.48
1:C:281:THR:OG1	1:C:284:ASN:OD1	2.18	0.48
1:D:45:VAL:CG1	1:D:49:GLY:HA2	2.43	0.48
1:E:64:ILE:HG12	1:E:83:LEU:O	2.14	0.48
1:L:15:MET:O	1:L:420:TYR:OH	2.25	0.48
1:M:118:ASN:OD1	1:M:359:THR:OG1	2.27	0.48
1:B:183:GLN:HA	1:C:228:GLY:HA2	1.94	0.48
1:D:209:PRO:HB2	1:D:211:GLN:OE1	2.14	0.48
1:K:266:ASP:OD1	1:K:266:ASP:N	2.43	0.48
1:M:199:ILE:HD12	1:M:199:ILE:H	1.79	0.48
1:A:203:ARG:NH1	1:A:335:SER:OG	2.47	0.48
1:H:249:GLN:HE21	1:H:282:THR:HB	1.79	0.48
1:K:253:GLU:HG3	1:K:281:THR:HA	1.96	0.48
1:A:430:ILE:O	1:A:431:THR:HG22	2.13	0.48
1:D:238:VAL:HG22	1:D:336:PHE:HB3	1.95	0.48
1:K:121:LEU:HD13	1:K:161:VAL:HG22	1.96	0.48
1:A:71:ASN:HD21	1:A:76:GLY:H	1.62	0.48
1:F:204:TYR:OH	1:F:231:ASP:OD1	2.28	0.48
1:G:193:MET:HA	1:H:205:GLU:O	2.14	0.48
1:H:25:PRO:HB3	1:H:392:ASP:HB3	1.96	0.48
1:B:111:PRO:HD2	1:B:114:LEU:HD12	1.96	0.47
1:B:247:ALA:HB2	1:B:323:VAL:HG22	1.96	0.47
1:H:212:ARG:CZ	1:H:215:PRO:HG3	2.44	0.47
1:I:68:TYR:HB3	1:I:77:LEU:HD13	1.95	0.47
1:K:392:ASP:OD1	1:K:392:ASP:N	2.35	0.47
1:A:239:THR:HG22	1:A:240:GLY:H	1.79	0.47
1:A:327:GLY:HA2	1:A:330:GLY:O	2.13	0.47
1:B:209:PRO:HB2	1:B:211:GLN:NE2	2.29	0.47
1:B:268:ASP:HB3	1:B:307:ARG:HH22	1.79	0.47
1:B:268:ASP:OD1	1:B:268:ASP:N	2.47	0.47
1:C:101:ARG:NE	1:C:370:SER:OG	2.48	0.47
1:D:212:ARG:HD3	1:D:213:LEU:O	2.14	0.47
1:F:36:GLN:HE21	1:F:369:VAL:HG21	1.79	0.47
1:H:52:ILE:HG22	1:H:68:TYR:HB2	1.97	0.47
1:M:257:HIS:CE1	1:M:275:VAL:HG22	2.49	0.47
1:B:122:ASN:HD22	1:B:153:ASN:HA	1.78	0.47
1:D:141:LEU:HD21	1:D:354:ALA:HB2	1.95	0.47
1:D:198:ALA:HB2	1:E:203:ARG:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:GLN:OE1	1:E:273:THR:OG1	2.32	0.47
1:H:68:TYR:HB3	1:H:77:LEU:HD13	1.96	0.47
1:I:212:ARG:HD2	1:I:213:LEU:O	2.15	0.47
1:K:44:GLU:O	1:K:69:ARG:NH2	2.47	0.47
1:L:131:SER:HB2	1:L:229:ASN:OD1	2.13	0.47
1:B:129:SER:HB2	1:B:231:ASP:OD2	2.14	0.47
1:E:57:PRO:O	1:E:165:ASN:ND2	2.47	0.47
1:J:244:PHE:HB3	1:J:326:LEU:HD23	1.97	0.47
1:K:416:ARG:HB2	1:K:419:GLU:HG2	1.96	0.47
1:L:136:LEU:O	1:L:136:LEU:HD12	2.13	0.47
1:A:431:THR:C	1:A:432:ASP:O	2.55	0.47
1:D:199:ILE:HD12	1:D:199:ILE:H	1.79	0.47
1:I:10:TYR:O	1:I:14:ILE:HG12	2.14	0.47
1:J:193:MET:HA	1:K:205:GLU:O	2.14	0.47
1:E:243:ASN:HA	1:E:288:VAL:O	2.14	0.47
1:G:59:ALA:O	1:G:101:ARG:NH2	2.48	0.47
1:B:410:ASP:O	1:B:423:ARG:NH2	2.42	0.47
1:C:162:THR:HB	1:C:415:TRP:HB2	1.95	0.47
1:C:212:ARG:HH12	1:C:215:PRO:HD3	1.80	0.47
1:D:230:ALA:HB2	1:F:193:MET:HE1	1.97	0.47
1:D:281:THR:HG22	1:D:284:ASN:OD1	2.15	0.47
1:G:44:GLU:O	1:G:69:ARG:NH2	2.43	0.47
1:G:188:MET:HG3	1:G:189:ASN:H	1.80	0.47
1:J:26:ASP:CG	1:J:97:ARG:HH22	2.20	0.47
1:K:197:ALA:O	1:K:339:GLY:HA2	2.15	0.47
1:K:252:ASP:OD1	1:K:252:ASP:N	2.46	0.47
1:M:266:ASP:OD1	1:M:266:ASP:N	2.47	0.47
1:M:340:ASN:O	1:M:343:VAL:HG12	2.15	0.47
1:C:49:GLY:O	1:C:358:MET:N	2.47	0.47
1:D:376:PRO:HB2	1:D:381:LEU:HD22	1.96	0.47
1:E:293:THR:HG21	1:F:291:LYS:HB3	1.96	0.47
1:B:396:LEU:O	1:B:400:LYS:N	2.37	0.47
1:C:88:ASP:OD2	1:C:90:LYS:NZ	2.36	0.47
1:D:266:ASP:OD1	1:D:266:ASP:N	2.45	0.47
1:F:82:TRP:CH2	1:F:304:PRO:HG3	2.50	0.47
1:K:149:GLN:HB3	1:K:412:ARG:HA	1.97	0.47
1:E:322:ASN:O	1:E:324:ALA:N	2.48	0.47
1:F:176:ARG:NH2	1:F:179:ASP:OD2	2.46	0.47
1:F:384:MET:HE2	1:K:384:MET:HG2	1.97	0.47
1:G:151:LYS:O	1:G:412:ARG:NH2	2.47	0.47
1:G:420:TYR:O	1:G:424:THR:OG1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:ASP:OD2	1:H:303:LYS:HD2	2.15	0.47
1:I:17:PRO:HB3	1:I:100:SER:HB3	1.96	0.47
1:J:77:LEU:HD11	1:J:265:LEU:CD1	2.45	0.47
1:J:287:GLY:HA3	1:J:329:MET:HE3	1.97	0.47
1:C:10:TYR:CZ	1:C:14:ILE:HD11	2.50	0.46
1:C:120:THR:HB	1:D:42:ASN:HD21	1.79	0.46
1:D:95:TYR:CE2	1:D:176:ARG:HG2	2.50	0.46
1:B:133:VAL:HG21	1:B:136:LEU:HD12	1.95	0.46
1:B:257:HIS:HB3	1:B:313:LYS:HG2	1.98	0.46
1:C:92:ALA:HB1	1:C:380:LEU:HD21	1.97	0.46
1:I:95:TYR:CE2	1:I:176:ARG:HG2	2.51	0.46
1:L:42:ASN:HD21	1:M:120:THR:CG2	2.27	0.46
1:E:88:ASP:OD2	1:E:90:LYS:NZ	2.38	0.46
1:E:232:ILE:HD13	1:E:236:THR:HG21	1.97	0.46
1:J:137:THR:HG1	1:J:140:SER:HG	1.62	0.46
1:J:401:MET:HB2	1:L:391:TYR:CZ	2.51	0.46
1:A:26:ASP:OD1	1:A:97:ARG:NH2	2.49	0.46
1:B:130:LEU:O	1:B:130:LEU:HD23	2.15	0.46
1:C:298:THR:HA	1:C:301:ILE:HD13	1.97	0.46
1:H:129:SER:C	1:H:131:SER:H	2.13	0.46
1:A:132:GLU:HB3	1:C:378:PRO:HG2	1.96	0.46
1:B:209:PRO:HB2	1:B:211:GLN:HE22	1.81	0.46
1:D:403:LEU:HD23	1:D:403:LEU:HA	1.80	0.46
1:L:136:LEU:HD21	1:L:265:LEU:HD11	1.97	0.46
1:E:193:MET:HA	1:F:205:GLU:O	2.16	0.46
1:F:68:TYR:HB3	1:F:77:LEU:HD22	1.96	0.46
1:F:252:ASP:OD2	1:F:316:GLN:NE2	2.49	0.46
1:F:356:GLU:HG2	1:G:42:ASN:HD22	1.81	0.46
1:H:191:ALA:HB2	1:I:209:PRO:HD3	1.96	0.46
1:J:220:GLY:HA2	1:J:313:LYS:HD2	1.98	0.46
1:J:282:THR:O	1:J:285:HIS:HD2	1.98	0.46
1:K:236:THR:HG22	1:K:296:ILE:HB	1.98	0.46
1:M:418:GLU:CD	1:M:418:GLU:H	2.23	0.46
1:A:122:ASN:ND2	1:A:154:ASN:H	2.12	0.46
1:B:118:ASN:OD1	1:B:118:ASN:N	2.47	0.46
1:C:129:SER:HA	1:C:347:LEU:O	2.15	0.46
1:F:87:GLN:HE22	1:K:383:ASN:HD21	1.63	0.46
1:G:231:ASP:OD1	1:G:231:ASP:N	2.45	0.46
1:E:378:PRO:HB3	1:F:126:PHE:HZ	1.81	0.46
1:J:156:LEU:HD12	1:J:159:LYS:NZ	2.31	0.46
1:K:257:HIS:HB2	1:K:313:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:THR:O	1:A:279:LEU:HD12	2.15	0.46
1:B:249:GLN:NE2	1:B:282:THR:OG1	2.49	0.46
1:D:111:PRO:HB2	1:D:114:LEU:HD13	1.98	0.46
1:G:95:TYR:OH	1:G:176:ARG:NH1	2.49	0.46
1:G:102:LYS:NZ	1:G:104:ASP:OD2	2.49	0.46
1:J:243:ASN:HB3	1:J:289:SER:HB2	1.97	0.46
1:A:145:THR:HG1	1:A:147:ASN:ND2	2.14	0.46
1:C:25:PRO:HB3	1:C:392:ASP:OD1	2.16	0.46
1:D:46:SER:OG	1:D:47:GLU:N	2.49	0.46
1:G:47:GLU:O	1:G:360:PRO:HB3	2.16	0.46
1:I:51:GLY:HA2	1:I:69:ARG:HA	1.98	0.46
1:A:211:GLN:HA	1:A:325:THR:HG23	1.99	0.45
1:B:248:ARG:N	1:B:322:ASN:OD1	2.44	0.45
1:B:406:ARG:HH21	1:B:413:THR:HG23	1.80	0.45
1:C:157:VAL:HG21	1:C:358:MET:SD	2.56	0.45
1:C:281:THR:OG1	1:C:283:ASP:OD1	2.35	0.45
1:D:346:VAL:HG12	1:D:347:LEU:HG	1.98	0.45
1:E:222:LEU:HD11	1:E:259:GLN:HB2	1.98	0.45
1:L:25:PRO:HB3	1:L:392:ASP:OD2	2.15	0.45
1:E:10:TYR:CZ	1:E:14:ILE:HD11	2.52	0.45
1:H:265:LEU:HB3	1:H:306:THR:HG21	1.97	0.45
1:K:52:ILE:HG22	1:K:68:TYR:HB2	1.98	0.45
1:K:202:ARG:HB2	1:K:341:GLY:HA3	1.98	0.45
1:A:71:ASN:ND2	1:A:76:GLY:O	2.49	0.45
1:F:130:LEU:HD21	1:F:265:LEU:HD23	1.99	0.45
1:H:163:VAL:HG11	1:H:351:THR:HG21	1.97	0.45
1:H:261:ASP:HA	1:H:273:THR:HA	1.97	0.45
1:I:21:PRO:HG3	1:I:36:GLN:HB2	1.97	0.45
1:J:210:SER:OG	1:J:326:LEU:O	2.30	0.45
1:J:264:GLY:O	1:J:307:ARG:NH1	2.48	0.45
1:C:197:ALA:O	1:C:339:GLY:HA2	2.16	0.45
1:C:278:ALA:HB1	1:C:288:VAL:HG12	1.98	0.45
1:G:95:TYR:HB2	1:G:375:ILE:HB	1.99	0.45
1:M:402:ILE:HG23	1:M:411:ILE:HD13	1.97	0.45
1:H:418:GLU:HG2	1:H:419:GLU:N	2.32	0.45
1:L:103:TYR:HB2	1:L:163:VAL:HB	1.98	0.45
1:C:52:ILE:CG2	1:C:68:TYR:HB2	2.46	0.45
1:D:203:ARG:HH21	1:F:235:SER:HB2	1.81	0.45
1:E:197:ALA:O	1:E:339:GLY:HA2	2.16	0.45
1:F:243:ASN:HA	1:F:288:VAL:O	2.17	0.45
1:G:247:ALA:N	1:G:322:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASN:N	1:G:340:ASN:OD1	2.50	0.45
1:J:134:GLU:OE1	1:J:134:GLU:N	2.35	0.45
1:M:120:THR:HG1	1:M:155:GLN:C	2.22	0.45
1:A:248:ARG:HB2	1:A:322:ASN:HD22	1.81	0.45
1:D:134:GLU:HG2	1:D:135:SER:N	2.32	0.45
1:D:217:PRO:HG2	1:D:221:THR:HG21	1.97	0.45
1:I:94:ASN:HD21	1:I:378:PRO:HD3	1.82	0.45
1:I:134:GLU:OE1	1:I:134:GLU:N	2.48	0.45
1:I:415:TRP:CD1	1:I:415:TRP:N	2.85	0.45
1:J:212:ARG:HG2	1:J:213:LEU:O	2.17	0.45
1:K:278:ALA:HB2	1:K:290:ALA:HB2	1.98	0.45
1:L:138:TYR:CD1	1:L:356:GLU:HG2	2.52	0.45
1:L:216:VAL:HA	1:L:223:THR:HG21	1.98	0.45
1:C:141:LEU:HD21	1:C:354:ALA:HB2	1.99	0.45
1:G:329:MET:HB3	1:I:275:VAL:HB	1.97	0.45
1:H:46:SER:HB3	1:H:69:ARG:HD3	1.99	0.45
1:H:183:GLN:HA	1:I:228:GLY:HA2	1.97	0.45
1:J:13:SER:O	1:J:100:SER:OG	2.30	0.45
1:J:252:ASP:OD2	1:J:316:GLN:NE2	2.49	0.45
1:J:292:MET:HE3	1:J:294:GLN:HE22	1.82	0.45
1:K:180:GLU:OE1	1:K:192:LYS:HB2	2.16	0.45
1:L:175:VAL:HG13	1:L:340:ASN:HD21	1.81	0.45
1:M:118:ASN:OD1	1:M:118:ASN:N	2.49	0.45
1:A:25:PRO:HB3	1:A:392:ASP:HB3	1.99	0.45
1:B:178:GLU:O	1:B:194:ARG:NH1	2.49	0.45
1:D:274:VAL:HG11	1:D:296:ILE:HD11	1.99	0.45
1:D:406:ARG:O	1:D:410:ASP:N	2.49	0.45
1:E:157:VAL:HG21	1:E:358:MET:SD	2.57	0.45
1:F:254:THR:HG22	1:F:255:THR:H	1.82	0.45
1:G:82:TRP:NE1	1:G:302:THR:O	2.46	0.45
1:G:292:MET:HE3	1:G:292:MET:HB3	1.82	0.45
1:H:126:PHE:N	1:H:350:ILE:O	2.43	0.45
1:F:15:MET:O	1:F:17:PRO:HD3	2.16	0.45
1:J:166:LEU:HD22	1:J:403:LEU:HD21	1.98	0.45
1:K:25:PRO:HB3	1:K:392:ASP:OD1	2.17	0.45
1:B:134:GLU:HG2	1:B:135:SER:H	1.82	0.44
1:D:236:THR:OG1	1:D:337:SER:O	2.23	0.44
1:E:212:ARG:HE	1:E:323:VAL:HB	1.81	0.44
1:F:162:THR:HG21	1:F:420:TYR:CD2	2.53	0.44
1:G:43:LEU:HD11	1:G:364:LEU:HD23	1.99	0.44
1:G:95:TYR:HB3	1:G:174:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:TYR:HB3	1:H:174:TYR:HB3	1.97	0.44
1:I:363:ILE:HD13	1:I:363:ILE:HA	1.83	0.44
1:K:253:GLU:HG2	1:K:281:THR:HG22	1.97	0.44
1:L:51:GLY:H	1:L:70:TRP:HB2	1.82	0.44
1:L:297:PRO:HD2	1:L:300:ASN:ND2	2.32	0.44
1:L:312:TYR:HE2	1:L:314:ILE:HD11	1.81	0.44
1:D:222:LEU:HD13	1:D:313:LYS:HD3	1.99	0.44
1:E:263:MET:HE3	1:E:263:MET:HB2	1.86	0.44
1:J:297:PRO:HD2	1:J:300:ASN:ND2	2.33	0.44
1:A:418:GLU:HG2	1:A:419:GLU:H	1.83	0.44
1:D:252:ASP:OD1	1:D:252:ASP:N	2.48	0.44
1:E:188:MET:HE1	1:F:326:LEU:HD12	2.00	0.44
1:H:50:SER:HB3	1:H:357:LYS:H	1.82	0.44
1:K:36:GLN:HG3	1:K:371:ASN:ND2	2.32	0.44
1:J:52:ILE:N	1:J:68:TYR:O	2.49	0.44
1:K:129:SER:OG	1:K:231:ASP:OD1	2.36	0.44
1:M:257:HIS:O	1:M:312:TYR:HB2	2.17	0.44
1:B:216:VAL:HG11	1:B:314:ILE:HG12	1.99	0.44
1:F:73:ASN:OD1	1:F:73:ASN:N	2.49	0.44
1:I:21:PRO:HB3	1:I:371:ASN:HB3	1.99	0.44
1:I:416:ARG:HB2	1:I:419:GLU:HG2	2.00	0.44
1:J:17:PRO:HG2	1:J:102:LYS:HB2	1.99	0.44
1:K:188:MET:HG3	1:K:189:ASN:H	1.82	0.44
1:K:203:ARG:NH2	1:K:205:GLU:OE1	2.51	0.44
1:K:379:GLU:O	1:K:382:LYS:HG2	2.18	0.44
1:M:126:PHE:CE2	1:M:128:GLY:HA3	2.53	0.44
1:M:201:PRO:HA	1:M:339:GLY:O	2.16	0.44
1:B:54:VAL:HG11	1:B:130:LEU:CD1	2.47	0.44
1:E:264:GLY:O	1:E:307:ARG:NH1	2.48	0.44
1:I:156:LEU:HB2	1:I:159:LYS:HZ3	1.83	0.44
1:D:410:ASP:HB3	1:D:423:ARG:HH22	1.82	0.44
1:E:417:THR:O	1:E:421:LYS:HB2	2.17	0.44
1:F:15:MET:C	1:F:17:PRO:HD3	2.43	0.44
1:F:33:ILE:HD12	1:F:376:PRO:HG3	1.99	0.44
1:F:222:LEU:HD21	1:F:259:GLN:HG3	1.99	0.44
1:I:398:TYR:O	1:I:402:ILE:HG12	2.18	0.44
1:K:419:GLU:O	1:K:423:ARG:HB2	2.18	0.44
1:L:52:ILE:HD12	1:L:354:ALA:HB2	1.99	0.44
1:L:359:THR:C	1:L:361:LEU:H	2.26	0.44
1:D:209:PRO:HD3	1:F:191:ALA:HA	1.99	0.44
1:H:73:ASN:HB2	1:H:75:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:ASN:HA	1:H:288:VAL:O	2.17	0.44
1:J:240:GLY:HA3	1:J:334:VAL:HA	2.00	0.44
1:J:346:VAL:HG12	1:J:347:LEU:HG	1.99	0.44
1:K:183:GLN:HA	1:L:228:GLY:HA2	2.00	0.44
1:L:26:ASP:OD1	1:L:97:ARG:NH2	2.32	0.44
1:M:16:LEU:O	1:M:19:THR:HG22	2.17	0.44
1:A:253:GLU:OE1	1:A:281:THR:HA	2.17	0.43
1:B:231:ASP:HA	1:B:305:ILE:O	2.18	0.43
1:B:283:ASP:OD1	1:B:284:ASN:N	2.51	0.43
1:G:297:PRO:HD2	1:G:300:ASN:ND2	2.31	0.43
1:K:122:ASN:HD22	1:K:122:ASN:HA	1.64	0.43
1:L:97:ARG:HG2	1:L:373:GLU:HB2	1.99	0.43
1:M:257:HIS:HB3	1:M:313:LYS:HG2	2.00	0.43
1:G:161:VAL:HG23	1:G:415:TRP:O	2.19	0.43
1:H:274:VAL:HG13	1:H:274:VAL:O	2.18	0.43
1:A:210:SER:HB2	1:A:327:GLY:HA3	2.00	0.43
1:D:26:ASP:CG	1:D:97:ARG:HH22	2.25	0.43
1:D:164:LEU:HD12	1:D:164:LEU:HA	1.81	0.43
1:E:52:ILE:HD11	1:E:352:LEU:HD12	1.99	0.43
1:H:391:TYR:O	1:H:393:PRO:HD3	2.18	0.43
1:J:201:PRO:HA	1:J:339:GLY:O	2.18	0.43
1:C:36:GLN:HE21	1:C:369:VAL:CG2	2.31	0.43
1:D:129:SER:HB2	1:D:231:ASP:OD2	2.17	0.43
1:E:149:GLN:HB3	1:E:412:ARG:HB3	2.01	0.43
1:J:100:SER:HB2	1:J:371:ASN:OD1	2.17	0.43
1:B:394:GLU:HG3	1:B:395:GLY:N	2.29	0.43
1:G:204:TYR:HB2	1:G:336:PHE:CE2	2.54	0.43
1:G:401:MET:HB2	1:I:391:TYR:CZ	2.54	0.43
1:H:220:GLY:HA2	1:H:313:LYS:HD2	1.99	0.43
1:K:36:GLN:HG3	1:K:371:ASN:HD21	1.84	0.43
1:B:100:SER:HB2	1:B:371:ASN:HD22	1.84	0.43
1:B:137:THR:OG1	1:B:140:SER:OG	2.35	0.43
1:E:37:GLU:CD	1:E:86:SER:HG	2.25	0.43
1:F:39:SER:OG	1:F:85:THR:HA	2.19	0.43
1:A:26:ASP:HB2	1:A:171:ASP:OD1	2.18	0.43
1:A:92:ALA:HB1	1:A:380:LEU:HD13	2.00	0.43
1:B:268:ASP:HB3	1:B:307:ARG:NH2	2.34	0.43
1:C:222:LEU:HG	1:C:311:SER:OG	2.18	0.43
1:D:409:LEU:HB3	1:D:411:ILE:HG12	1.99	0.43
1:G:253:GLU:HB3	1:G:279:LEU:HD11	2.00	0.43
1:H:102:LYS:HG2	1:H:369:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:HIS:CD2	1:I:373:GLU:HG2	2.53	0.43
1:I:69:ARG:O	1:I:78:GLU:HG3	2.18	0.43
1:L:257:HIS:HB3	1:L:313:LYS:HG2	2.01	0.43
1:M:248:ARG:HH21	1:M:321:ASP:CG	2.27	0.43
1:B:207:ASP:H	1:B:333:SER:HB2	1.83	0.43
1:J:227:GLU:HB3	1:J:309:LYS:HG3	2.01	0.43
1:K:238:VAL:HG11	1:K:274:VAL:HG11	2.01	0.43
1:M:118:ASN:O	1:M:358:MET:HA	2.18	0.43
1:A:231:ASP:HA	1:A:305:ILE:O	2.19	0.43
1:B:246:LEU:HD12	1:B:322:ASN:ND2	2.33	0.43
1:B:253:GLU:HG2	1:B:281:THR:HA	2.01	0.43
1:E:125:THR:HB	1:E:150:ASP:HB3	2.01	0.43
1:M:95:TYR:CE2	1:M:176:ARG:HG2	2.53	0.43
1:A:428:ASN:HB3	1:A:430:ILE:HG12	2.00	0.43
1:D:236:THR:HG22	1:D:296:ILE:HB	2.00	0.43
1:D:255:THR:OG1	1:D:315:ASN:ND2	2.52	0.43
1:G:71:ASN:ND2	1:G:75:THR:OG1	2.48	0.43
1:G:378:PRO:HG2	1:H:132:GLU:HB3	2.01	0.43
1:J:176:ARG:HE	1:J:195:CYS:HB3	1.83	0.43
1:L:170:PHE:HE2	1:L:400:LYS:HG3	1.84	0.43
1:A:193:MET:HA	1:B:205:GLU:O	2.19	0.42
1:H:17:PRO:HD2	1:H:102:LYS:HD2	2.01	0.42
1:J:204:TYR:HB2	1:J:336:PHE:CE2	2.54	0.42
1:J:278:ALA:HB2	1:J:290:ALA:HB2	2.01	0.42
1:L:131:SER:HB3	1:L:231:ASP:HB3	2.00	0.42
1:A:7:THR:C	1:A:9:THR:N	2.76	0.42
1:B:37:GLU:HG2	1:B:85:THR:HB	2.00	0.42
1:F:376:PRO:HB3	1:F:380:LEU:HD23	2.01	0.42
1:H:75:THR:OG1	1:H:76:GLY:N	2.52	0.42
1:J:67:HIS:HD2	1:J:80:ASP:HB3	1.84	0.42
1:J:130:LEU:HD21	1:J:265:LEU:CD2	2.48	0.42
1:A:143:SER:O	1:A:144:LEU:HD12	2.18	0.42
1:B:182:PRO:HB2	1:C:229:ASN:HD22	1.84	0.42
1:I:141:LEU:O	1:I:141:LEU:HD23	2.20	0.42
1:J:340:ASN:HB2	1:J:343:VAL:CG2	2.50	0.42
1:L:26:ASP:HB2	1:L:171:ASP:OD1	2.19	0.42
1:M:202:ARG:HB2	1:M:341:GLY:HA3	2.02	0.42
1:B:378:PRO:HG2	1:C:132:GLU:HB3	2.01	0.42
1:D:108:SER:O	1:D:108:SER:OG	2.35	0.42
1:D:188:MET:HG3	1:D:189:ASN:H	1.82	0.42
1:E:35:LYS:HB3	1:E:374:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:LEU:HD12	1:F:396:LEU:HA	1.86	0.42
1:I:199:ILE:H	1:I:199:ILE:HD12	1.83	0.42
1:C:166:LEU:HG	1:C:413:THR:HG22	2.01	0.42
1:D:247:ALA:HB2	1:D:323:VAL:HG22	2.01	0.42
1:H:196:THR:HG21	1:I:205:GLU:HG3	2.00	0.42
1:I:156:LEU:HB2	1:I:159:LYS:NZ	2.35	0.42
1:J:376:PRO:HB3	1:J:380:LEU:HD22	2.02	0.42
1:L:208:LEU:HD13	1:L:326:LEU:HD13	2.01	0.42
1:A:82:TRP:CH2	1:A:304:PRO:HG3	2.55	0.42
1:A:130:LEU:O	1:A:133:VAL:HG22	2.19	0.42
1:A:188:MET:SD	1:B:214:PRO:HD3	2.60	0.42
1:C:218:ALA:H	1:C:221:THR:HG21	1.84	0.42
1:E:167:PRO:HG2	1:E:403:LEU:HD11	2.02	0.42
1:I:231:ASP:HA	1:I:305:ILE:O	2.20	0.42
1:I:233:VAL:HB	1:I:347:LEU:HD21	2.01	0.42
1:J:25:PRO:HB3	1:J:392:ASP:OD1	2.20	0.42
1:J:36:GLN:HE21	1:J:369:VAL:HG21	1.85	0.42
1:L:142:MET:HA	1:L:151:LYS:HD2	2.02	0.42
1:L:217:PRO:HG2	1:L:221:THR:HG21	2.00	0.42
1:B:363:ILE:HG12	1:E:118:ASN:HD22	1.85	0.42
1:G:53:LEU:HD23	1:G:53:LEU:HA	1.83	0.42
1:G:98:LEU:HD13	1:G:101:ARG:HH21	1.84	0.42
1:H:238:VAL:HB	1:H:294:GLN:HB2	2.01	0.42
1:H:254:THR:O	1:H:279:LEU:HD12	2.20	0.42
1:I:268:ASP:CG	1:I:307:ARG:HH22	2.28	0.42
1:L:45:VAL:HG13	1:L:49:GLY:HA2	2.00	0.42
1:A:419:GLU:O	1:A:423:ARG:HB2	2.20	0.42
1:B:15:MET:HE2	1:B:15:MET:HA	2.01	0.42
1:C:124:ALA:HA	1:C:150:ASP:O	2.20	0.42
1:C:143:SER:O	1:C:143:SER:OG	2.29	0.42
1:D:118:ASN:OD1	1:D:118:ASN:N	2.52	0.42
1:E:222:LEU:H	1:E:313:LYS:HB3	1.84	0.42
1:E:257:HIS:HB3	1:E:313:LYS:HG2	2.00	0.42
1:F:138:TYR:CD1	1:F:356:GLU:HB2	2.55	0.42
1:G:26:ASP:OD1	1:G:97:ARG:NH2	2.50	0.42
1:H:52:ILE:CG2	1:H:68:TYR:HB2	2.49	0.42
1:I:253:GLU:HB3	1:I:279:LEU:HD11	2.01	0.42
1:G:131:SER:HB3	1:G:231:ASP:HB3	2.02	0.42
1:H:27:ASP:OD2	1:I:400:LYS:NZ	2.48	0.42
1:I:41:TYR:HB2	1:I:366:VAL:CG2	2.50	0.42
1:G:197:ALA:O	1:G:339:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:LYS:HD3	1:C:357:LYS:HA	1.81	0.41
1:J:95:TYR:HB2	1:J:375:ILE:HD12	2.01	0.41
1:J:120:THR:O	1:J:356:GLU:N	2.47	0.41
1:M:93:PHE:CD1	1:M:374:LEU:HB3	2.54	0.41
1:A:254:THR:HG22	1:A:316:GLN:HG3	2.02	0.41
1:A:299:GLU:OE1	1:A:299:GLU:N	2.54	0.41
1:C:100:SER:OG	1:C:371:ASN:OD1	2.37	0.41
1:D:50:SER:OG	1:D:74:GLN:NE2	2.53	0.41
1:E:250:PRO:HB2	1:E:252:ASP:O	2.20	0.41
1:I:52:ILE:HD13	1:I:354:ALA:HB2	2.02	0.41
1:J:418:GLU:H	1:J:418:GLU:CD	2.28	0.41
1:A:431:THR:O	1:A:431:THR:HG23	2.20	0.41
1:B:166:LEU:HG	1:B:413:THR:HG22	2.02	0.41
1:C:391:TYR:CE1	1:C:393:PRO:HG3	2.55	0.41
1:E:164:LEU:HD12	1:E:164:LEU:HA	1.89	0.41
1:E:188:MET:N	1:F:225:LEU:O	2.53	0.41
1:G:346:VAL:O	1:G:347:LEU:HB2	2.20	0.41
1:I:121:LEU:HD23	1:I:157:VAL:HA	2.02	0.41
1:I:193:MET:HE2	1:I:193:MET:HB3	1.88	0.41
1:L:119:GLY:HA2	1:L:157:VAL:CG1	2.50	0.41
1:M:67:HIS:HD2	1:M:80:ASP:CB	2.33	0.41
1:B:52:ILE:HG12	1:B:136:LEU:HD21	2.03	0.41
1:D:222:LEU:HD11	1:D:259:GLN:HB2	2.02	0.41
1:D:257:HIS:NE2	1:D:275:VAL:HG11	2.35	0.41
1:E:255:THR:OG1	1:E:315:ASN:ND2	2.53	0.41
1:F:109:THR:OG1	1:L:118:ASN:ND2	2.52	0.41
1:F:115:TYR:O	1:G:112:ALA:HB3	2.19	0.41
1:G:202:ARG:HH12	1:I:176:ARG:HH11	1.69	0.41
1:I:55:CYS:HB2	1:I:351:THR:HB	2.01	0.41
1:J:172:LYS:HD3	1:J:344:PRO:O	2.19	0.41
1:J:266:ASP:OD1	1:J:266:ASP:N	2.53	0.41
1:L:112:ALA:N	1:M:115:TYR:O	2.45	0.41
1:B:26:ASP:CG	1:B:97:ARG:HH22	2.29	0.41
1:C:62:SER:O	1:C:64:ILE:HG23	2.21	0.41
1:E:18:GLU:HA	1:E:369:VAL:HG11	2.01	0.41
1:F:256:PHE:HA	1:F:313:LYS:O	2.20	0.41
1:I:41:TYR:HB2	1:I:366:VAL:HG22	2.03	0.41
1:J:26:ASP:HB2	1:J:171:ASP:OD1	2.21	0.41
1:J:131:SER:HA	1:J:306:THR:HG23	2.03	0.41
1:A:219:THR:CG2	1:A:318:THR:HA	2.51	0.41
1:F:363:ILE:HD12	1:L:357:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:CYS:HB2	1:H:351:THR:CG2	2.48	0.41
1:J:37:GLU:OE2	1:J:87:GLN:HB3	2.20	0.41
1:J:295:SER:HB2	1:K:203:ARG:HH22	1.85	0.41
1:K:122:ASN:ND2	1:K:153:ASN:HA	2.35	0.41
1:L:43:LEU:HD13	1:L:67:HIS:ND1	2.35	0.41
1:M:18:GLU:OE1	1:M:18:GLU:N	2.49	0.41
1:B:188:MET:HE3	1:B:188:MET:HB2	1.97	0.41
1:B:257:HIS:O	1:B:312:TYR:HA	2.20	0.41
1:B:346:VAL:HG12	1:B:347:LEU:HG	2.03	0.41
1:C:71:ASN:HD21	1:C:76:GLY:H	1.69	0.41
1:E:46:SER:HB3	1:E:69:ARG:HD3	2.01	0.41
1:E:123:ALA:HA	1:E:352:LEU:O	2.21	0.41
1:F:212:ARG:NH1	1:F:215:PRO:HD3	2.35	0.41
1:H:189:ASN:C	1:H:191:ALA:N	2.78	0.41
1:H:202:ARG:HG3	1:H:341:GLY:HA3	2.03	0.41
1:I:82:TRP:CH2	1:I:304:PRO:HG3	2.55	0.41
1:J:225:LEU:HD21	1:J:312:TYR:CE1	2.55	0.41
1:K:291:LYS:H	1:K:291:LYS:HG2	1.72	0.41
1:L:95:TYR:HB2	1:L:375:ILE:HD12	2.02	0.41
1:M:132:GLU:O	1:M:132:GLU:HG3	2.20	0.41
1:B:378:PRO:CG	1:C:132:GLU:HB3	2.51	0.41
1:F:45:VAL:CG1	1:F:49:GLY:HA2	2.51	0.41
1:F:90:LYS:HG3	1:F:179:ASP:HA	2.03	0.41
1:F:104:ASP:O	1:F:366:VAL:HA	2.21	0.41
1:G:243:ASN:HA	1:G:288:VAL:O	2.21	0.41
1:H:197:ALA:O	1:H:339:GLY:HA2	2.21	0.41
1:J:125:THR:HB	1:J:150:ASP:HB3	2.02	0.41
1:K:70:TRP:HZ2	1:K:136:LEU:O	2.04	0.41
1:K:222:LEU:HD12	1:K:311:SER:HB2	2.02	0.41
1:M:197:ALA:O	1:M:339:GLY:HA2	2.21	0.41
1:A:204:TYR:HB2	1:A:336:PHE:CE2	2.56	0.41
1:B:87:GLN:HB2	1:E:143:SER:HB2	2.03	0.41
1:B:112:ALA:HB2	1:E:359:THR:CG2	2.50	0.41
1:B:170:PHE:CD1	1:B:396:LEU:HD11	2.56	0.41
1:B:243:ASN:OD1	1:B:332:ALA:HB2	2.21	0.41
1:C:248:ARG:HD3	1:C:322:ASN:OD1	2.21	0.41
1:D:73:ASN:OD1	1:D:73:ASN:N	2.54	0.41
1:D:201:PRO:HB2	1:D:337:SER:OG	2.21	0.41
1:D:410:ASP:HB3	1:D:423:ARG:NH2	2.35	0.41
1:E:274:VAL:HG21	1:E:296:ILE:HD11	2.02	0.41
1:F:21:PRO:HD3	1:F:36:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:VAL:HG22	1:F:303:LYS:HE2	2.03	0.41
1:G:278:ALA:HB2	1:G:290:ALA:HB2	2.02	0.41
1:J:52:ILE:CG2	1:J:68:TYR:HB2	2.51	0.41
1:J:192:LYS:O	1:K:207:ASP:HB3	2.20	0.41
1:J:225:LEU:O	1:L:188:MET:N	2.54	0.41
1:J:265:LEU:HB3	1:J:306:THR:OG1	2.20	0.41
1:J:421:LYS:HB2	1:J:421:LYS:HE3	1.90	0.41
1:K:278:ALA:HB1	1:K:288:VAL:HG12	2.03	0.41
1:M:114:LEU:HD23	1:M:114:LEU:HA	1.81	0.41
1:B:29:THR:O	1:C:169:GLY:N	2.53	0.41
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.85	0.41
1:E:326:LEU:HD12	1:E:332:ALA:HB1	2.03	0.41
1:F:98:LEU:HD13	1:F:101:ARG:NH2	2.35	0.41
1:F:98:LEU:HD13	1:F:101:ARG:HH21	1.86	0.41
1:F:257:HIS:NE2	1:F:275:VAL:HG11	2.35	0.41
1:H:36:GLN:HE21	1:H:369:VAL:HG21	1.86	0.41
1:H:95:TYR:HB2	1:H:375:ILE:HD12	2.02	0.41
1:H:385:VAL:HG13	1:I:147:ASN:OD1	2.21	0.41
1:J:245:GLY:O	1:J:324:ALA:HA	2.21	0.41
1:J:388:TYR:CZ	1:K:403:LEU:HD22	2.56	0.41
1:K:261:ASP:OD1	1:K:261:ASP:N	2.40	0.41
1:L:231:ASP:O	1:L:232:ILE:HG13	2.21	0.41
1:D:118:ASN:O	1:D:358:MET:HA	2.21	0.40
1:F:231:ASP:OD1	1:F:231:ASP:N	2.54	0.40
1:H:79:PHE:HB2	1:H:266:ASP:OD2	2.21	0.40
1:H:92:ALA:HB1	1:H:380:LEU:HD21	2.02	0.40
1:I:188:MET:HG3	1:I:189:ASN:H	1.86	0.40
1:J:126:PHE:HB3	1:J:350:ILE:CG2	2.51	0.40
1:K:95:TYR:CE2	1:K:176:ARG:HG2	2.56	0.40
1:B:293:THR:N	1:B:294:GLN:OE1	2.54	0.40
1:E:363:ILE:HG13	1:H:357:LYS:HB3	2.03	0.40
1:G:376:PRO:HB3	1:G:380:LEU:HD23	2.02	0.40
1:H:391:TYR:CE1	1:H:393:PRO:HG3	2.56	0.40
1:M:212:ARG:HH12	1:M:215:PRO:HD3	1.86	0.40
1:M:416:ARG:O	1:M:419:GLU:N	2.54	0.40
1:B:297:PRO:HD2	1:B:300:ASN:ND2	2.35	0.40
1:C:29:THR:HG22	1:C:388:TYR:CD1	2.56	0.40
1:C:402:ILE:HD13	1:C:402:ILE:HA	1.89	0.40
1:E:390:LYS:HD2	1:E:390:LYS:O	2.22	0.40
1:E:418:GLU:HG2	1:E:419:GLU:N	2.35	0.40
1:G:11:LEU:HD11	1:G:402:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:VAL:O	1:H:347:LEU:HB2	2.20	0.40
1:H:419:GLU:O	1:H:423:ARG:CB	2.70	0.40
1:I:282:THR:O	1:I:285:HIS:HD2	2.04	0.40
1:J:73:ASN:OD1	1:J:73:ASN:N	2.54	0.40
1:K:26:ASP:HB2	1:K:171:ASP:OD1	2.22	0.40
1:K:418:GLU:HG2	1:K:419:GLU:N	2.36	0.40
1:A:274:VAL:CG1	1:A:294:GLN:HG3	2.51	0.40
1:B:129:SER:C	1:B:131:SER:H	2.28	0.40
1:C:43:LEU:HD23	1:C:43:LEU:HA	1.87	0.40
1:C:267:ASN:OD1	1:C:303:LYS:NZ	2.55	0.40
1:G:292:MET:HE3	1:G:294:GLN:HE22	1.86	0.40
1:H:281:THR:OG1	1:H:282:THR:N	2.54	0.40
1:I:321:ASP:OD1	1:I:321:ASP:N	2.55	0.40
1:K:121:LEU:HD23	1:K:355:TYR:HB3	2.04	0.40
1:K:199:ILE:HD13	1:K:340:ASN:HD21	1.86	0.40
1:M:33:ILE:HD13	1:M:376:PRO:HG3	2.04	0.40
1:M:60:PRO:HA	1:M:98:LEU:HB2	2.04	0.40
1:D:370:SER:O	1:D:371:ASN:ND2	2.54	0.40
1:D:378:PRO:HB3	1:E:126:PHE:HZ	1.86	0.40
1:E:385:VAL:HG13	1:F:147:ASN:ND2	2.37	0.40
1:G:11:LEU:HD13	1:G:398:TYR:HD2	1.87	0.40
1:I:45:VAL:CG1	1:I:49:GLY:HA2	2.51	0.40
1:I:95:TYR:HA	1:I:175:VAL:O	2.22	0.40
1:J:209:PRO:HB2	1:J:211:GLN:OE1	2.21	0.40
1:J:300:ASN:ND2	1:K:331:PRO:HB3	2.37	0.40
1:J:378:PRO:CG	1:K:132:GLU:HB3	2.51	0.40
1:K:37:GLU:HG2	1:K:85:THR:HB	2.04	0.40
1:L:284:ASN:C	1:L:286:ARG:H	2.29	0.40
1:M:25:PRO:HB3	1:M:392:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/508 (83%)	369 (87%)	48 (11%)	5 (1%)	10	20
1	B	422/508 (83%)	379 (90%)	42 (10%)	1 (0%)	43	64
1	C	428/508 (84%)	381 (89%)	46 (11%)	1 (0%)	43	64
1	D	420/508 (83%)	371 (88%)	49 (12%)	0	100	100
1	E	420/508 (83%)	380 (90%)	38 (9%)	2 (0%)	24	43
1	F	420/508 (83%)	367 (87%)	51 (12%)	2 (0%)	24	43
1	G	420/508 (83%)	375 (89%)	45 (11%)	0	100	100
1	H	420/508 (83%)	380 (90%)	37 (9%)	3 (1%)	18	34
1	I	420/508 (83%)	374 (89%)	45 (11%)	1 (0%)	43	64
1	J	420/508 (83%)	359 (86%)	61 (14%)	0	100	100
1	K	420/508 (83%)	376 (90%)	43 (10%)	1 (0%)	43	64
1	L	420/508 (83%)	365 (87%)	55 (13%)	0	100	100
1	M	420/508 (83%)	363 (86%)	57 (14%)	0	100	100
All	All	5472/6604 (83%)	4839 (88%)	617 (11%)	16 (0%)	37	56

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	THR
1	A	432	ASP
1	A	433	PHE
1	C	323	VAL
1	H	130	LEU
1	K	130	LEU
1	A	188	MET
1	A	434	SER
1	E	188	MET
1	B	395	GLY
1	E	323	VAL
1	F	348	ARG
1	I	395	GLY
1	F	349	PRO
1	H	349	PRO
1	H	190	GLY

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	371/432 (86%)	368 (99%)	3 (1%)	73	84
1	B	368/432 (85%)	368 (100%)	0	100	100
1	C	373/432 (86%)	373 (100%)	0	100	100
1	D	366/432 (85%)	364 (100%)	2 (0%)	81	89
1	E	366/432 (85%)	365 (100%)	1 (0%)	86	93
1	F	366/432 (85%)	366 (100%)	0	100	100
1	G	366/432 (85%)	366 (100%)	0	100	100
1	H	366/432 (85%)	365 (100%)	1 (0%)	86	93
1	I	366/432 (85%)	365 (100%)	1 (0%)	86	93
1	J	366/432 (85%)	366 (100%)	0	100	100
1	K	366/432 (85%)	366 (100%)	0	100	100
1	L	366/432 (85%)	366 (100%)	0	100	100
1	M	366/432 (85%)	366 (100%)	0	100	100
All	All	4772/5616 (85%)	4764 (100%)	8 (0%)	85	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	7	THR
1	A	434	SER
1	D	114	LEU
1	D	402	ILE
1	E	45	VAL
1	H	118	ASN
1	I	415	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	71	ASN
1	A	94	ASN
1	A	122	ASN
1	A	147	ASN
1	A	249	GLN
1	A	259	GLN
1	A	322	ASN
1	A	371	ASN
1	A	377	ASN
1	B	32	HIS
1	B	67	HIS
1	B	94	ASN
1	B	122	ASN
1	B	211	GLN
1	B	229	ASN
1	B	249	GLN
1	B	285	HIS
1	B	300	ASN
1	B	316	GLN
1	B	317	GLN
1	B	342	ASN
1	B	371	ASN
1	B	383	ASN
1	C	36	GLN
1	C	67	HIS
1	C	229	ASN
1	C	285	HIS
1	C	428	ASN
1	D	67	HIS
1	D	139	ASN
1	D	229	ASN
1	D	294	GLN
1	D	316	GLN
1	D	317	GLN
1	D	342	ASN
1	D	371	ASN
1	E	42	ASN
1	E	67	HIS
1	E	147	ASN
1	E	165	ASN
1	E	211	GLN
1	E	317	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	E	322	ASN
1	E	383	ASN
1	F	36	GLN
1	F	42	ASN
1	F	67	HIS
1	F	122	ASN
1	F	147	ASN
1	F	229	ASN
1	F	249	GLN
1	F	257	HIS
1	F	285	HIS
1	F	316	GLN
1	F	342	ASN
1	F	383	ASN
1	G	42	ASN
1	G	67	HIS
1	G	74	GLN
1	G	94	ASN
1	G	153	ASN
1	G	229	ASN
1	G	294	GLN
1	G	300	ASN
1	G	316	GLN
1	G	371	ASN
1	G	383	ASN
1	H	36	GLN
1	H	74	GLN
1	H	243	ASN
1	H	285	HIS
1	H	371	ASN
1	I	36	GLN
1	I	81	GLN
1	I	94	ASN
1	I	211	GLN
1	I	229	ASN
1	I	285	HIS
1	I	294	GLN
1	I	315	ASN
1	I	317	GLN
1	I	383	ASN
1	J	32	HIS
1	J	36	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	J	67	HIS
1	J	118	ASN
1	J	122	ASN
1	J	186	GLN
1	J	234	ASN
1	J	285	HIS
1	J	294	GLN
1	J	300	ASN
1	J	316	GLN
1	K	32	HIS
1	K	67	HIS
1	K	122	ASN
1	K	317	GLN
1	K	371	ASN
1	K	383	ASN
1	L	36	GLN
1	L	42	ASN
1	L	67	HIS
1	L	118	ASN
1	L	211	GLN
1	L	300	ASN
1	L	316	GLN
1	L	317	GLN
1	M	32	HIS
1	M	36	GLN
1	M	186	GLN
1	M	249	GLN
1	M	257	HIS
1	M	285	HIS
1	M	317	GLN
1	M	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

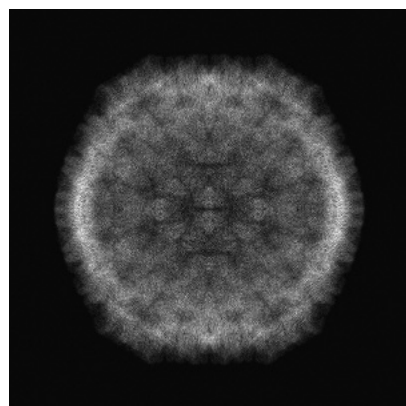
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51321. These allow visual inspection of the internal detail of the map and identification of artifacts.

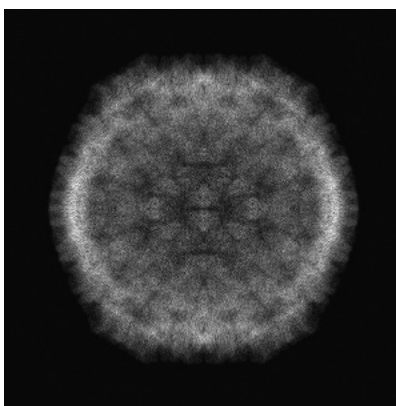
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

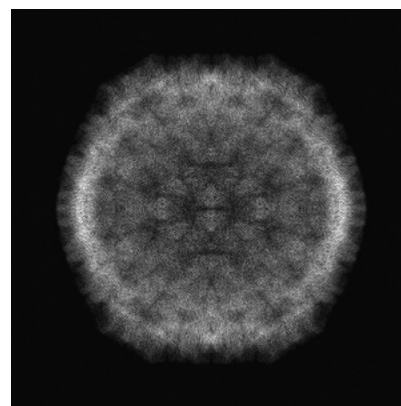
6.1.1 Primary map



X

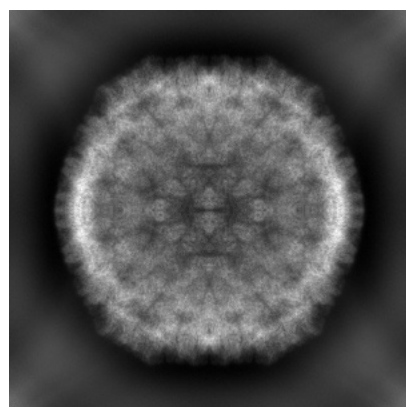


Y

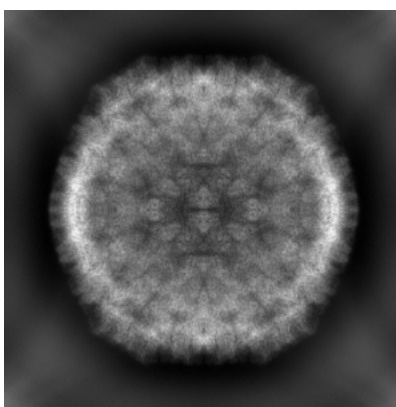


Z

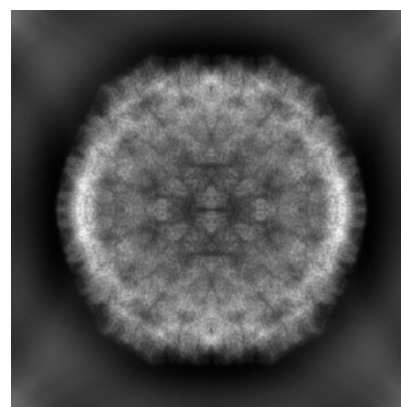
6.1.2 Raw map



X



Y

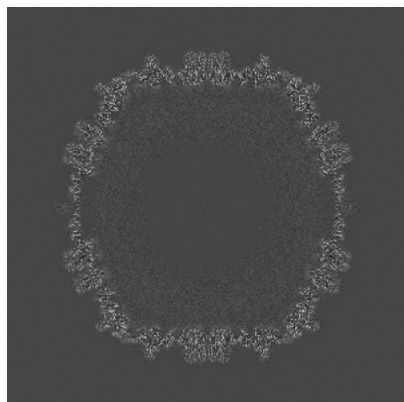


Z

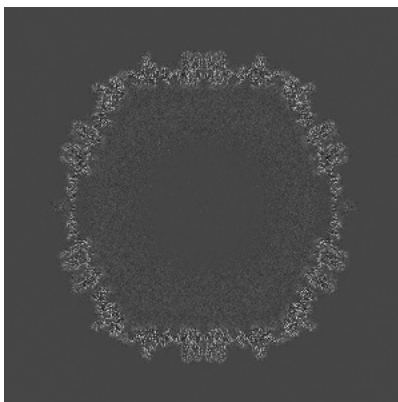
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

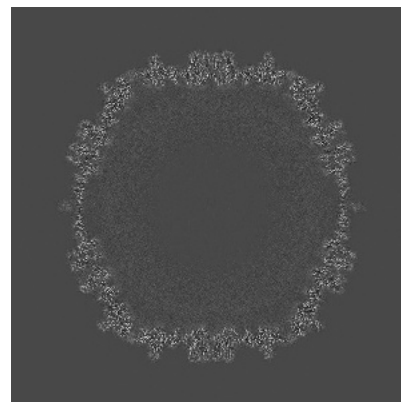
6.2.1 Primary map



X Index: 350

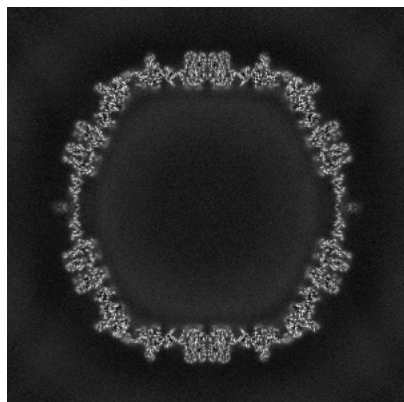


Y Index: 350

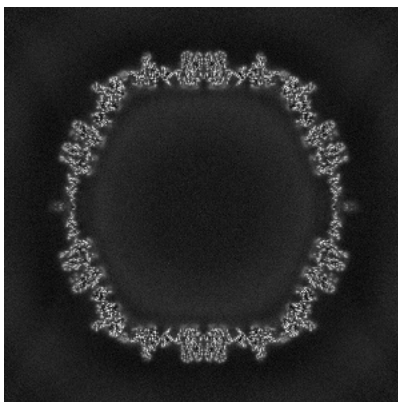


Z Index: 350

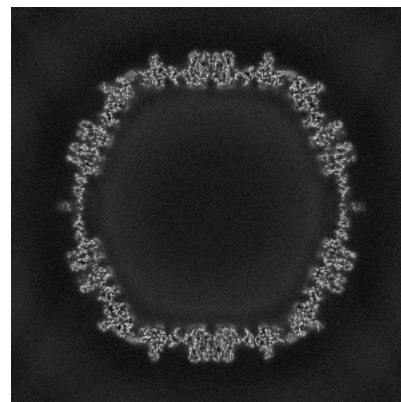
6.2.2 Raw map



X Index: 350



Y Index: 350

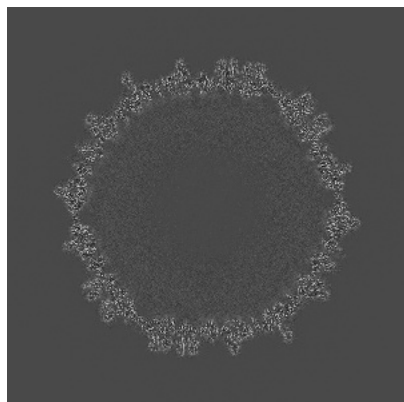


Z Index: 350

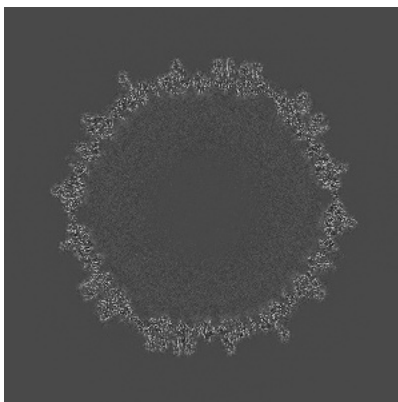
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

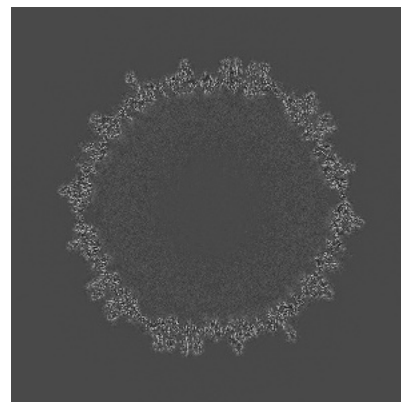
6.3.1 Primary map



X Index: 283

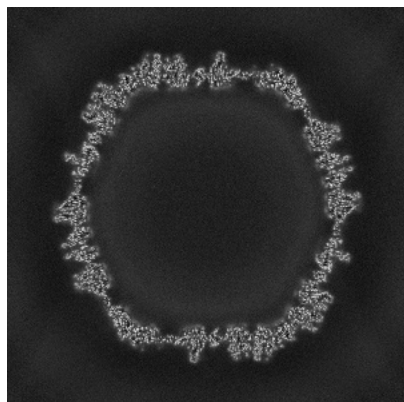


Y Index: 283

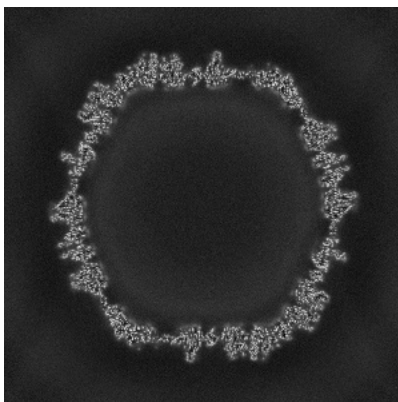


Z Index: 282

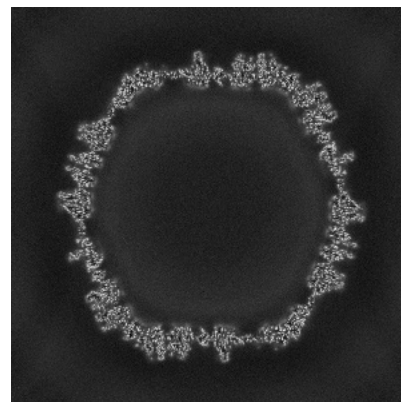
6.3.2 Raw map



X Index: 333



Y Index: 333

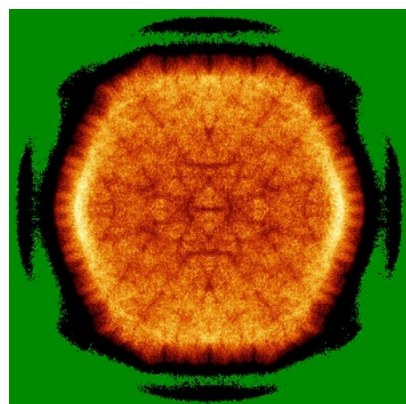


Z Index: 366

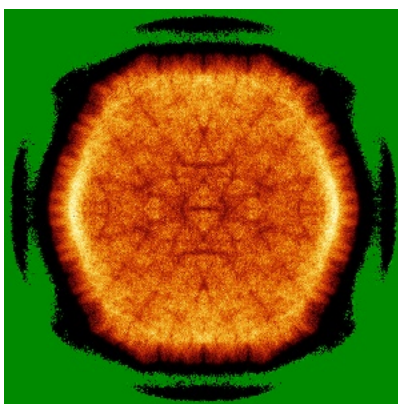
The images above show the largest variance slices of the map in three orthogonal directions.

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

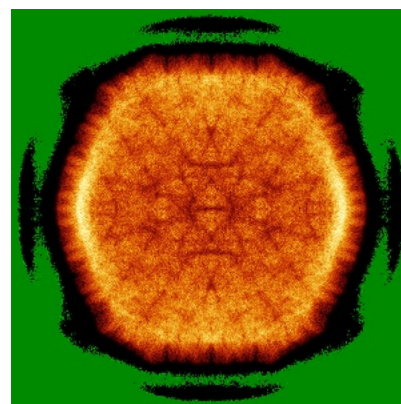
6.4.1 Primary map



X

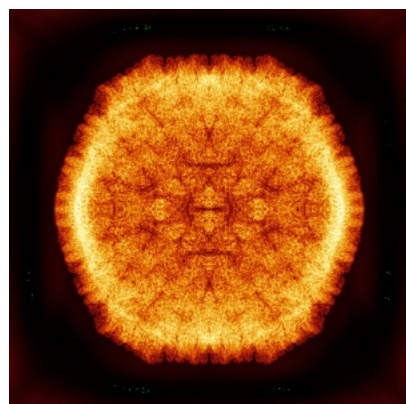


Y

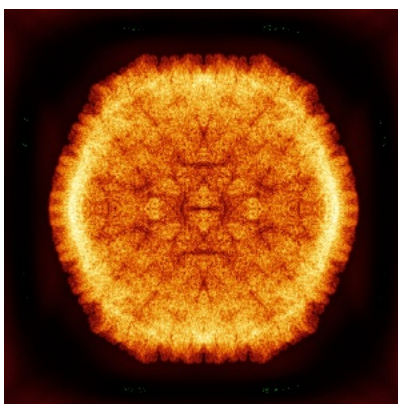


Z

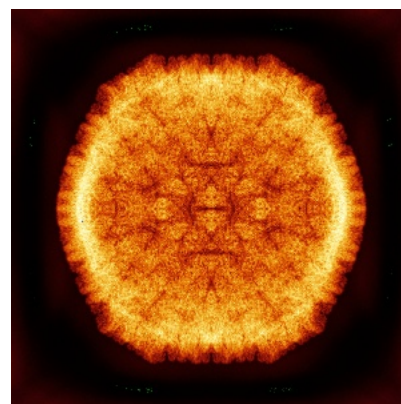
6.4.2 Raw map



X



Y

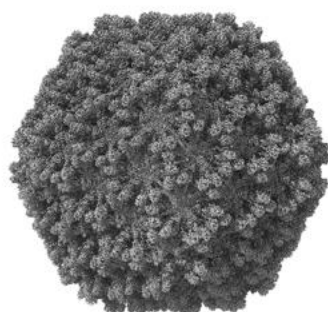


Z

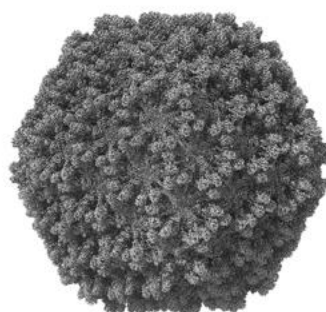
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

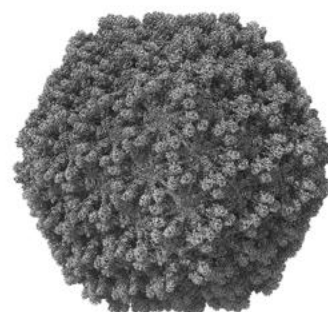
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.92. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

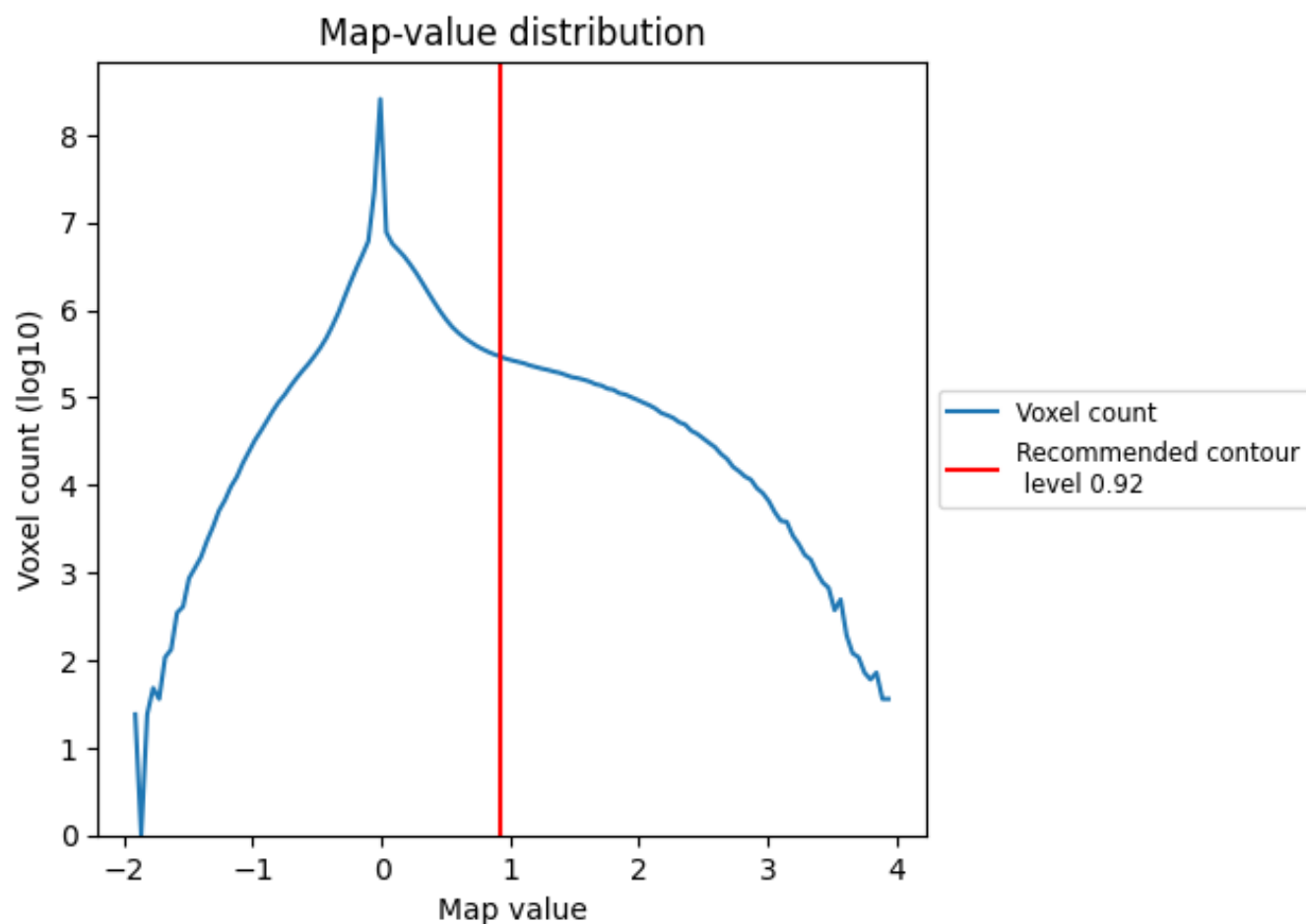
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

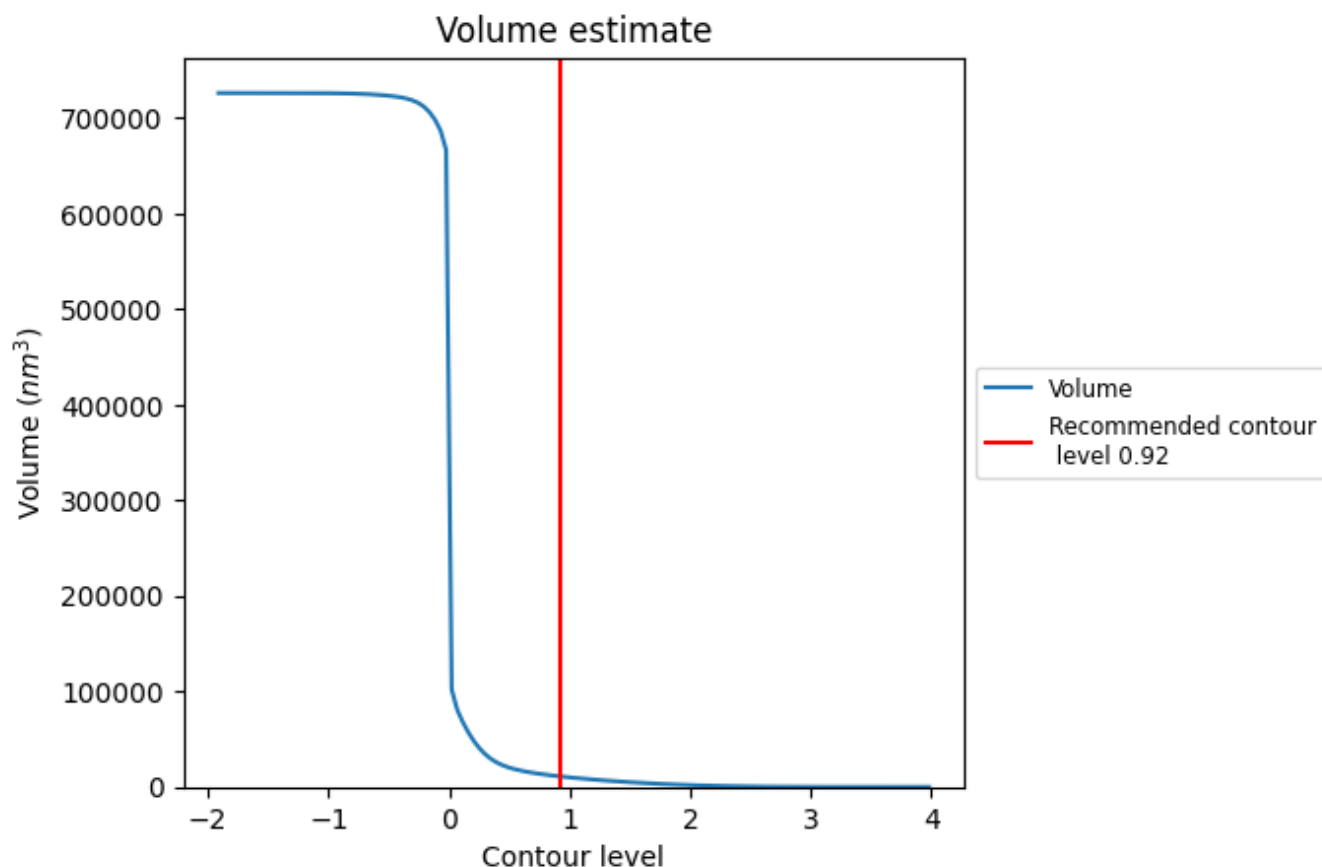
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

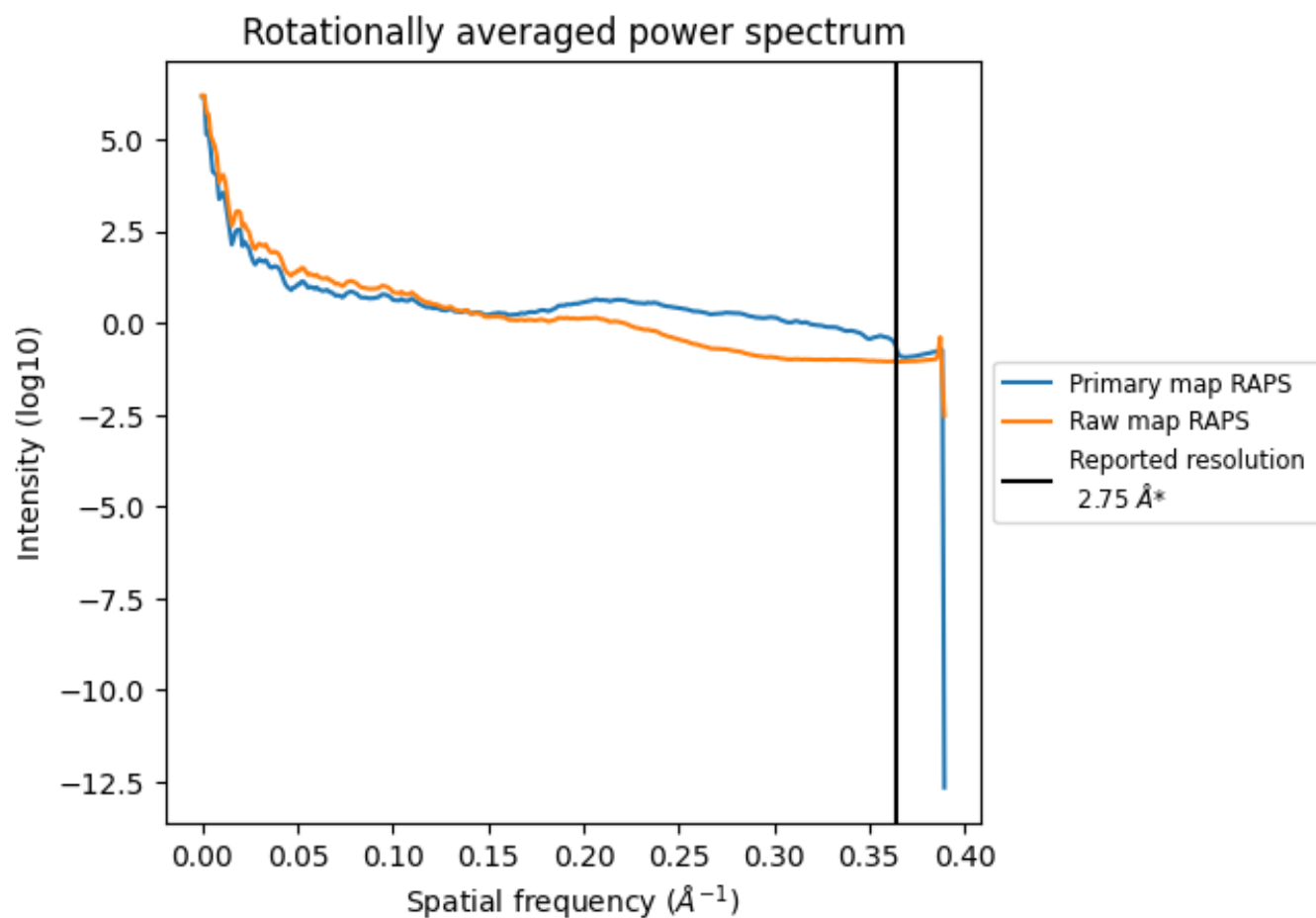
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11060 nm³; this corresponds to an approximate mass of 9991 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 ⓘ

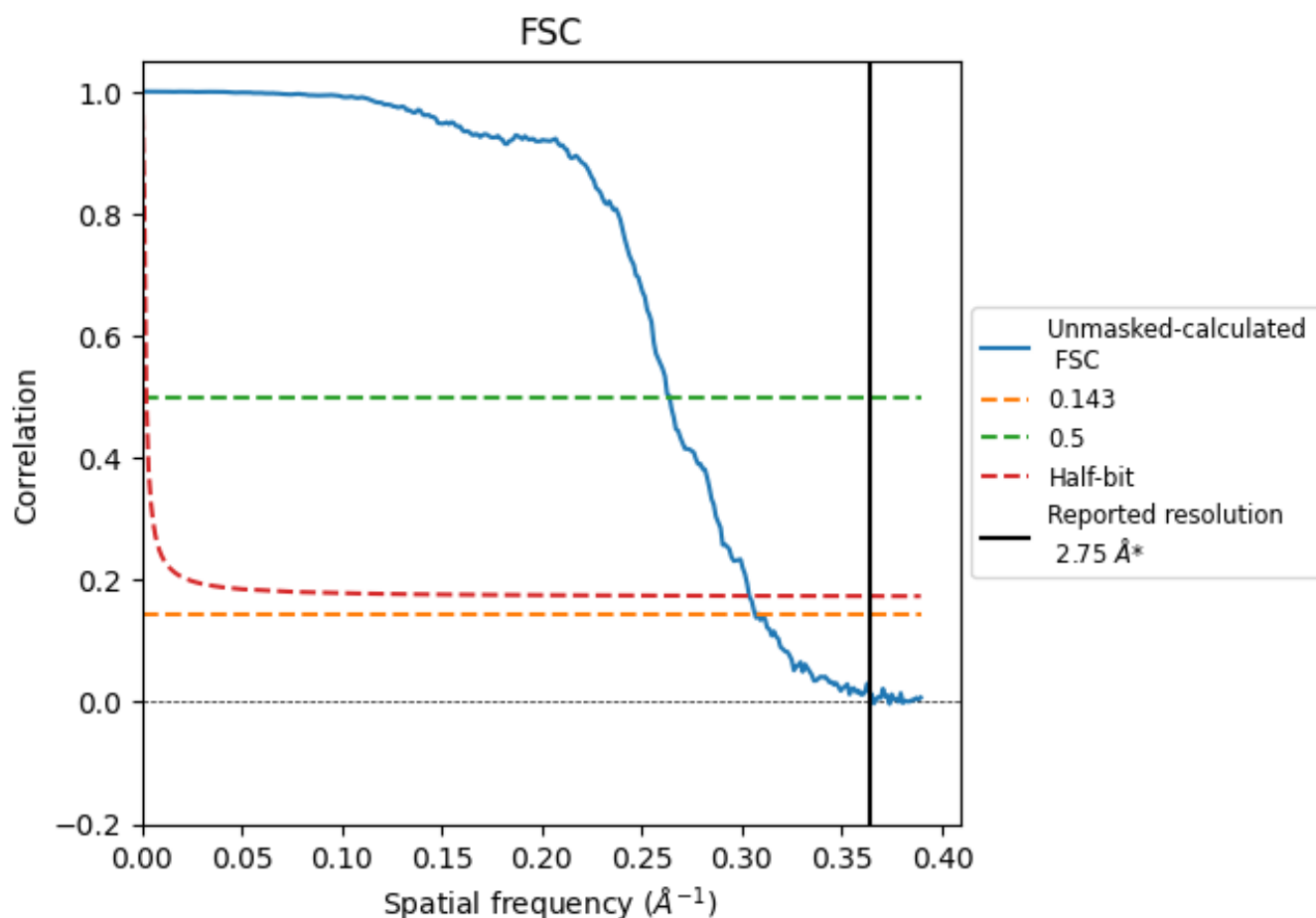


*Reported resolution corresponds to spatial frequency of 0.364 Å⁻¹

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 $0.364 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.79	3.29

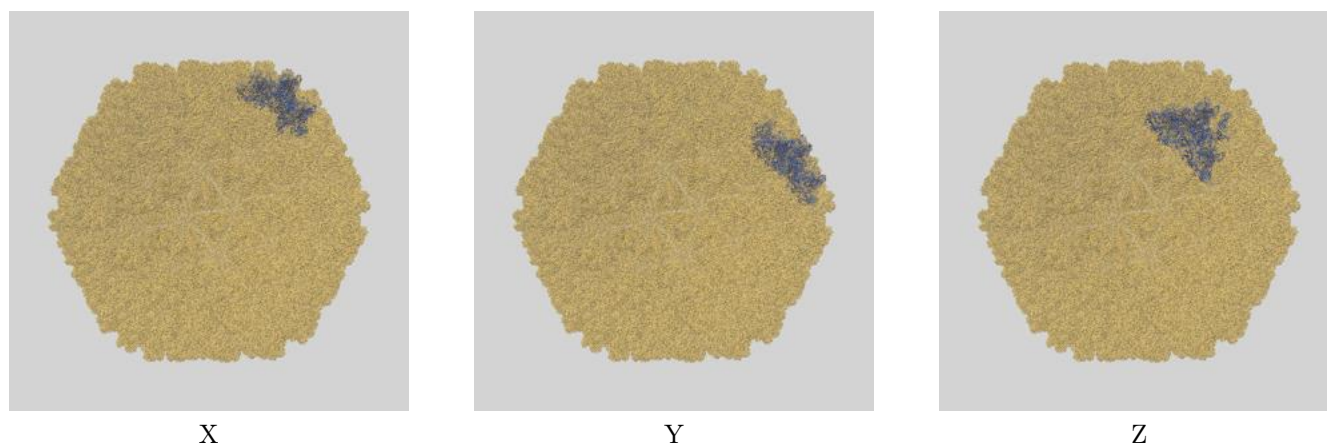
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.75 by more than 10 %

9 Map-model fit [i](#)

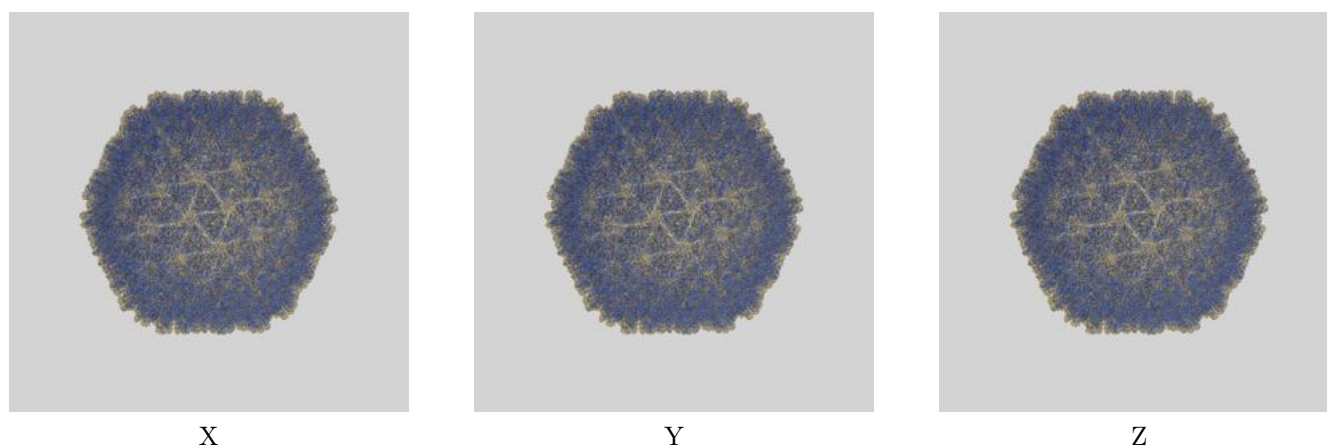
This section contains information regarding the fit between EMDB map EMD-51321 and PDB model 9GG2. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

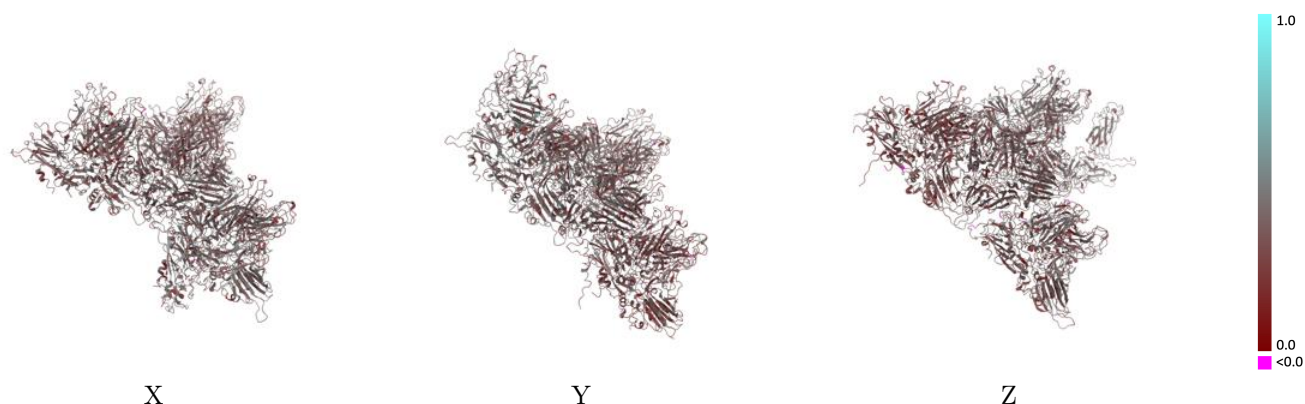


9.1.2 Map-model assembly overlay [i](#)



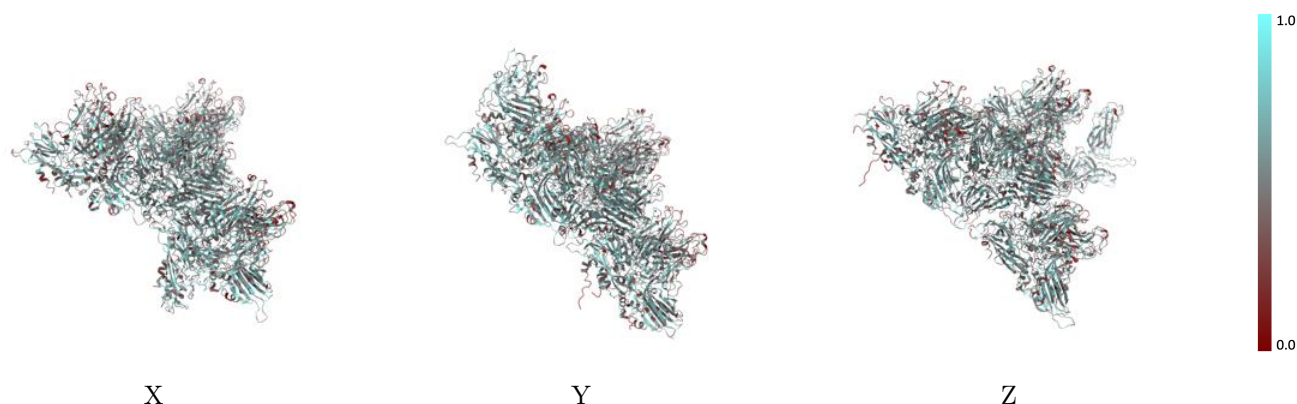
The images above show the 3D surface view of the map at the recommended contour level 0.92 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



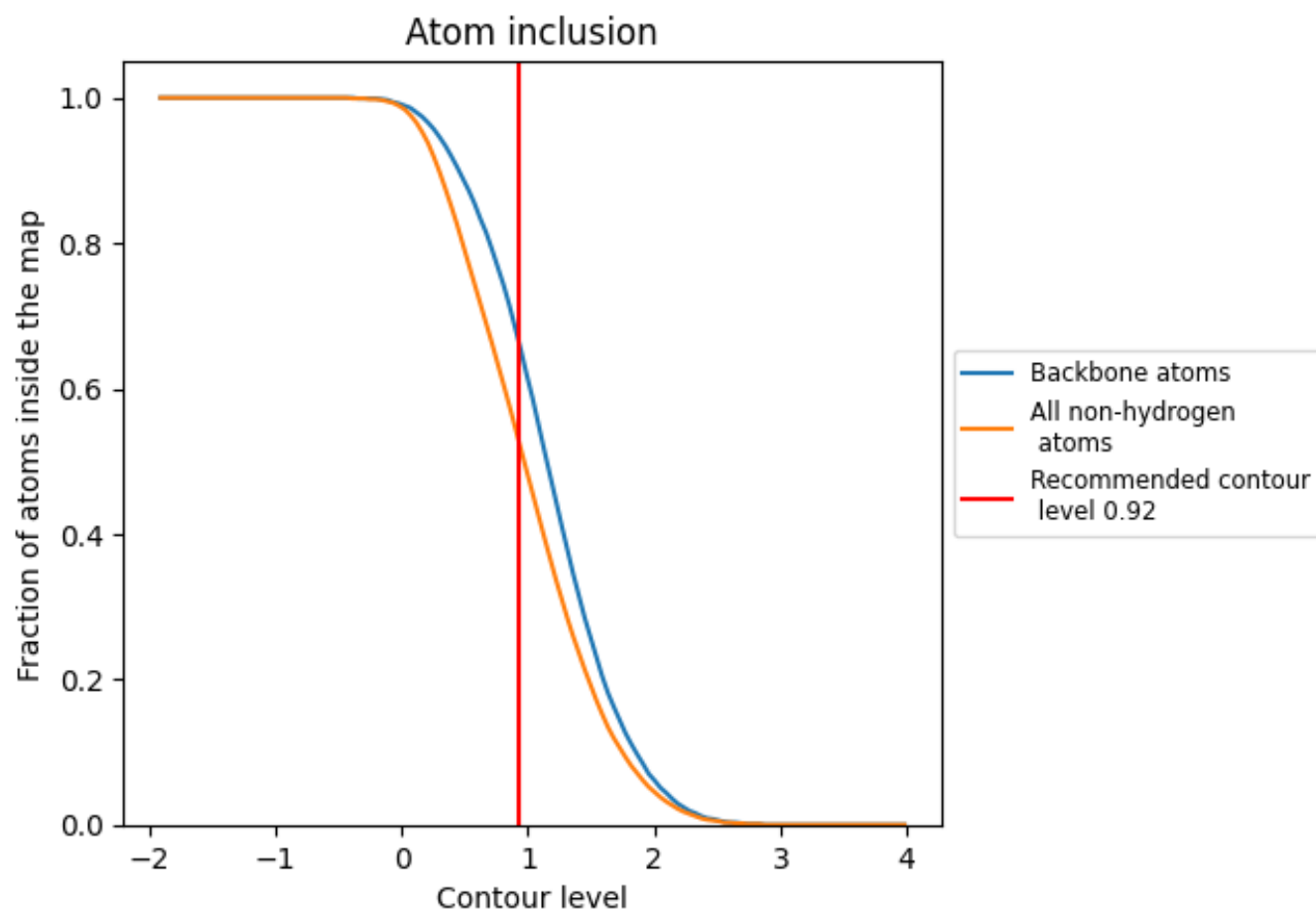
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.92).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 53% 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 (0.92) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5320	0.3630
A	0.5040	0.3210
B	0.5240	0.3330
C	0.5210	0.3390
D	0.5370	0.3610
E	0.5430	0.3570
F	0.5370	0.3710
G	0.5260	0.3690
H	0.5190	0.3560
I	0.5230	0.3650
J	0.5390	0.3890
K	0.5360	0.3840
L	0.5480	0.3860
M	0.5520	0.3900

1.0

0.0

<0.0