



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:21 PM UTC

PDB ID : 7T3A / pdb_00007t3a
EMDB ID : EMD-25652
Title : GATOR1-RAG-RAGULATOR - Inhibitory Complex
Authors : Egri, S.B.; Shen, K.
Deposited on : 2021-12-07
Resolution : 4.00 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:

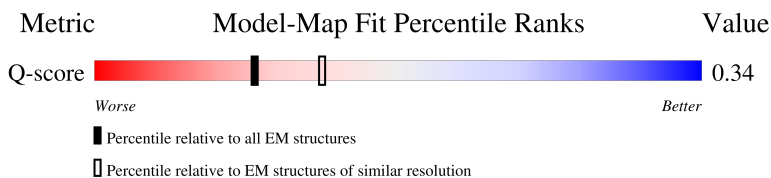
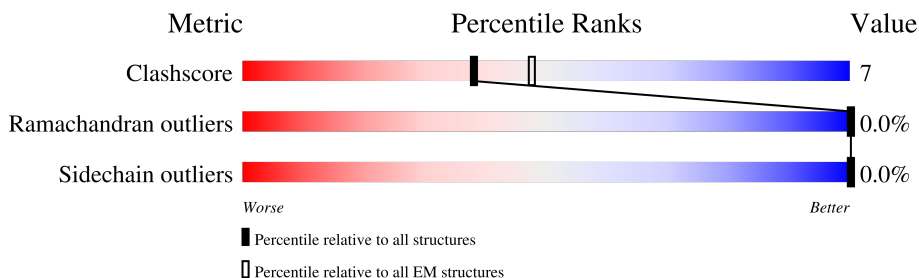
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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.



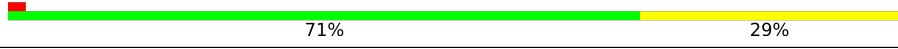
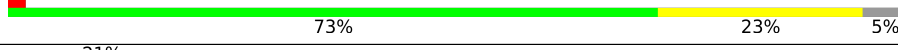
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1603	
2	B	380	
3	C	569	
4	K	313	

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Mol	Chain	Length	Quality of chain
5	L	399	
6	M	161	
7	N	125	
8	O	124	
9	P	99	
10	Q	91	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 23310 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 GATOR complex protein DEPDC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	990	Total	C	N	O	S	0	0
			8120	5243	1347	1485	45		

- Molecule 2 is a protein called GATOR complex protein NPRL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	362	Total	C	N	O	S	0	0
			2926	1873	489	546	18		

- Molecule 3 is a protein called GATOR complex protein NPRL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	406	Total	C	N	O	S	0	0
			3242	2087	568	568	19		

- Molecule 4 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	294	Total	C	N	O	S	0	0
			2416	1535	421	444	16		

- Molecule 5 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	299	Total	C	N	O	S	0	0
			2420	1557	389	460	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	75	ASN	SER	engineered mutation	UNP Q9HB90

- Molecule 6 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	115	Total	C	N	O	S	0	0
			892	560	155	175	2		

- Molecule 7 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	125	Total	C	N	O	S	0	0
			940	590	162	182	6		

- Molecule 8 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	118	Total	C	N	O	S	0	0
			918	591	155	171	1		

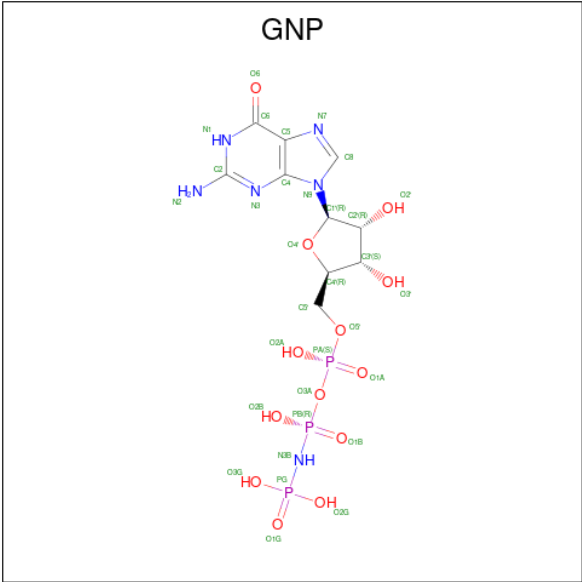
- Molecule 9 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	97	Total	C	N	O	S	0	0
			738	460	135	140	3		

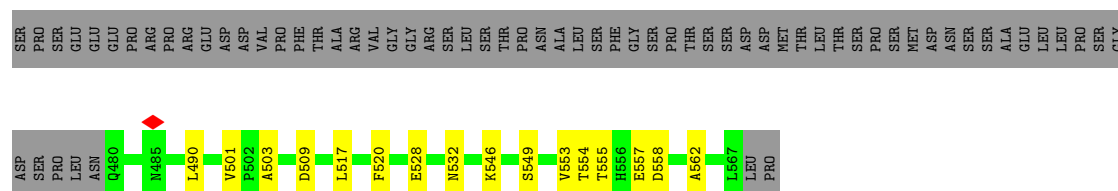
- Molecule 10 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	91	Total	C	N	O	S	0	0
			666	406	115	138	7		

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

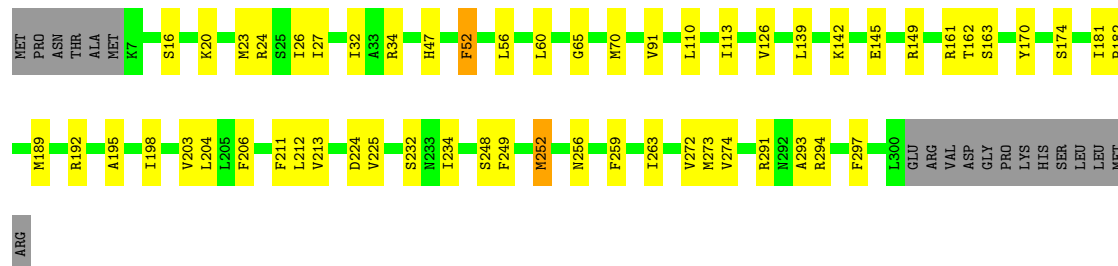


Mol	Chain	Residues	Atoms					AltConf
11	K	1	Total	C	N	O	P	0
			32	10	6	13	3	



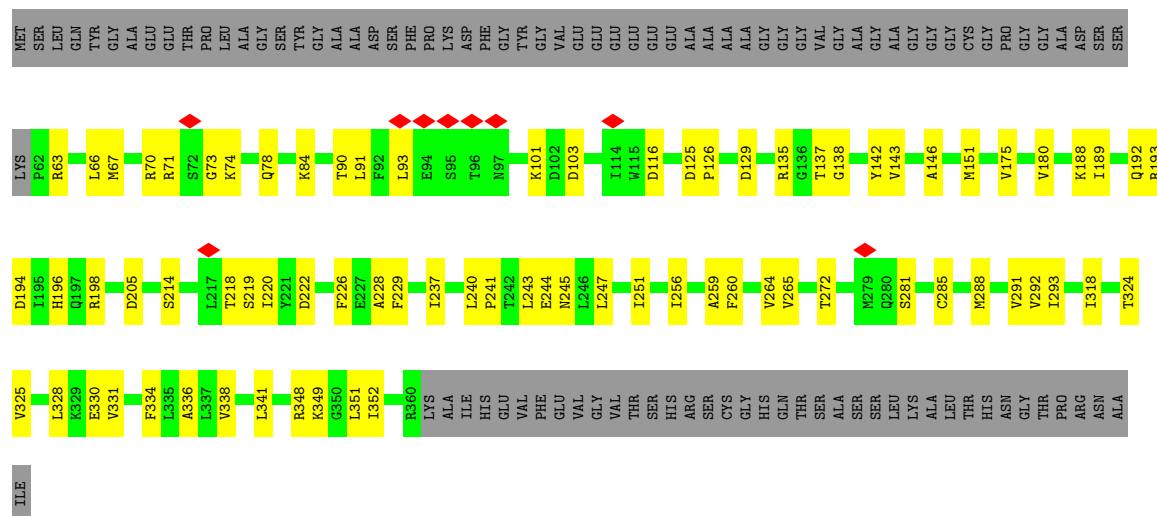
• Molecule 4: Ras-related GTP-binding protein A

Chain K: 76% 17% 6%



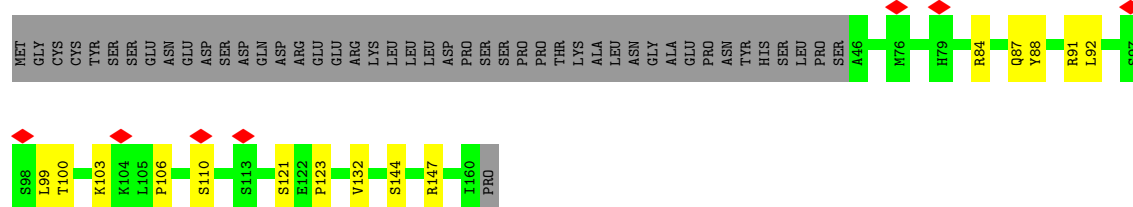
• Molecule 5: Ras-related GTP-binding protein C

Chain L: 56% 19% 25%



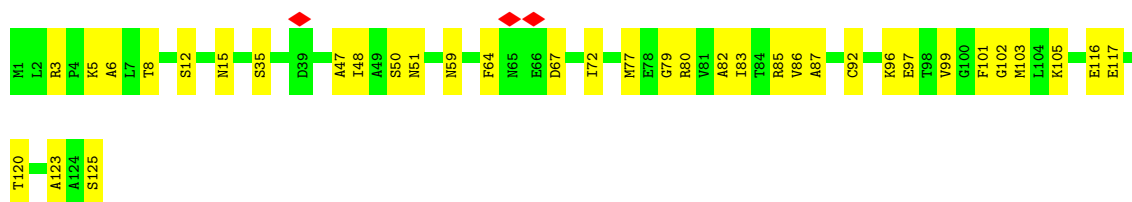
• Molecule 6: Ragulator complex protein LAMTOR1

Chain M: 62% 9% 29%



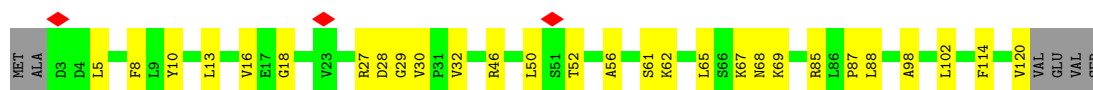
• Molecule 7: Ragulator complex protein LAMTOR2

Chain N:  71% 29%



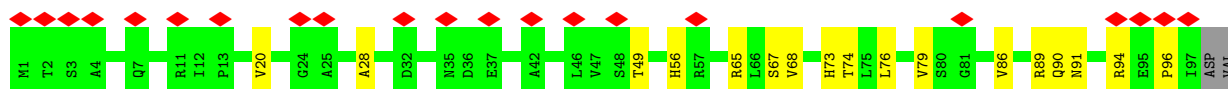
- Molecule 8: Regulator complex protein LAMTOR3

Chain O:  73% 23% 5%



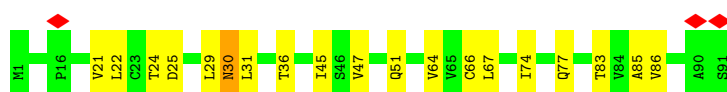
- Molecule 9: Regulator complex protein LAMTOR4

Chain P:  21% 81% 17%



- Molecule 10: Regulator complex protein LAMTOR5

Chain Q:  79% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251583	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 ($e^-/\text{\AA}^2$)	58.3	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.426	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	288.19998, 288.19998, 288.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.655, 0.655, 0.655	Depositor

5 Model quality

5.1 Standard geometry

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

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	1/8337 (0.0%)	0.61	7/11305 (0.1%)
2	B	0.29	0/2985	0.72	2/4044 (0.0%)
3	C	0.23	0/3306	0.63	2/4483 (0.0%)
4	K	0.31	0/2461	0.75	3/3314 (0.1%)
5	L	0.30	1/2471 (0.0%)	0.76	0/3337
6	M	0.21	0/908	0.55	0/1234
7	N	0.31	1/951 (0.1%)	0.66	0/1288
8	O	0.23	0/935	0.58	0/1268
9	P	0.21	0/747	0.54	0/1008
10	Q	0.25	0/672	0.61	0/911
All	All	0.28	3/23773 (0.0%)	0.66	14/32192 (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
2	B	0	1
5	L	0	2
7	N	0	1
8	O	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	733	VAL	C-N	7.89	1.41	1.34
7	N	117	GLU	C-N	5.17	1.40	1.34
5	L	125	ASP	C-N	5.04	1.40	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	52	PHE	CA-C-N	5.67	130.46	122.46
4	K	52	PHE	C-N-CA	5.67	130.46	122.46
1	A	733	VAL	N-CA-C	5.57	120.92	108.88
3	C	226	GLU	CA-C-N	5.55	129.73	120.62
3	C	226	GLU	C-N-CA	5.55	129.73	120.62
1	A	288	GLU	CA-C-N	5.40	131.03	122.61
1	A	288	GLU	C-N-CA	5.40	131.03	122.61
4	K	252	MET	CB-CG-SD	5.30	128.59	112.70
1	A	343	PHE	N-CA-C	5.29	117.10	110.91
1	A	866	LYS	CA-C-N	5.17	130.16	122.82
1	A	866	LYS	C-N-CA	5.17	130.16	122.82
1	A	266	GLU	CA-CB-CG	5.14	124.39	114.10
2	B	59	ALA	CA-C-N	5.09	131.26	121.54
2	B	59	ALA	C-N-CA	5.09	131.26	121.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	VAL	Peptide
2	B	318	LEU	Peptide
5	L	264	VAL	Peptide
5	L	331	VAL	Peptide
7	N	86	VAL	Peptide
8	O	65	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8120	0	7898	98	0
2	B	2926	0	2964	55	0
3	C	3242	0	3342	48	0
4	K	2416	0	2407	37	0
5	L	2420	0	2389	51	0
6	M	892	0	894	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	940	0	947	28	0
8	O	918	0	943	21	0
9	P	738	0	753	12	0
10	Q	666	0	666	18	0
11	K	32	0	13	2	0
All	All	23310	0	23216	346	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 7.

All (346) 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)
3:C:9:SER:O	3:C:129:ALA:HB3	1.97	0.64
7:N:8:THR:O	7:N:12:SER:HB3	1.97	0.64
1:A:307:LEU:HD23	1:A:345:VAL:HG11	1.81	0.62
6:M:132:VAL:HG13	10:Q:77:GLN:HE22	1.64	0.62
5:L:70:ARG:HG2	5:L:73:GLY:H	1.65	0.62
5:L:240:LEU:O	5:L:244:GLU:HB2	2.00	0.62
9:P:20:VAL:HB	9:P:28:ALA:HB3	1.82	0.61
1:A:1422:GLY:HA3	1:A:1431:TYR:HB3	1.82	0.61
3:C:224:TRP:HB2	3:C:227:VAL:HG12	1.83	0.60
5:L:214:SER:HB3	5:L:228:ALA:HB1	1.82	0.60
7:N:77:MET:HE1	8:O:67:LYS:HB3	1.84	0.60
2:B:89:CYS:SG	2:B:90:ASP:N	2.75	0.59
5:L:348:ARG:NH1	5:L:349:LYS:O	2.35	0.59
4:K:204:LEU:HB2	4:K:273:MET:HB3	1.84	0.59
3:C:15:SER:HA	3:C:20:ASN:HA	1.84	0.59
5:L:70:ARG:HB3	5:L:74:LYS:H	1.66	0.59
1:A:1512:GLN:HB3	1:A:1547:ASN:HB2	1.84	0.58
2:B:351:TYR:O	2:B:355:CYS:HB3	2.04	0.58
5:L:151:MET:SD	5:L:198:ARG:NE	2.76	0.57
4:K:203:VAL:HG22	4:K:274:VAL:HG12	1.85	0.57
3:C:348:LEU:HD12	3:C:351:GLN:HE22	1.68	0.57
1:A:764:GLN:O	1:A:768:ASN:ND2	2.38	0.57
7:N:3:ARG:HG3	7:N:6:ALA:H	1.70	0.56
4:K:291:ARG:NH1	7:N:125:SER:OG	2.39	0.56
5:L:180:VAL:H	5:L:218:THR:HB	1.70	0.56
2:B:94:LYS:HD2	2:B:96:CYS:H	1.69	0.56
5:L:260:PHE:HB2	5:L:338:VAL:HB	1.87	0.56
3:C:309:VAL:HA	3:C:312:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:67:LEU:HD23	10:Q:74:ILE:HD12	1.87	0.56
6:M:144:SER:O	6:M:147:ARG:NH2	2.39	0.56
3:C:401:ARG:HH12	3:C:562:ALA:HA	1.71	0.55
8:O:85:ARG:O	8:O:88:LEU:HB2	2.06	0.55
10:Q:30:ASN:ND2	10:Q:30:ASN:H	2.04	0.55
4:K:20:LYS:HB3	4:K:91:VAL:HG21	1.88	0.55
1:A:221:PHE:HA	1:A:254:PHE:O	2.06	0.55
1:A:733:VAL:HG11	2:B:215:VAL:HG12	1.89	0.55
7:N:64:PHE:HD2	7:N:67:ASP:H	1.53	0.55
5:L:71:ARG:HD2	5:L:116:ASP:HA	1.88	0.54
5:L:241:PRO:O	5:L:245:ASN:ND2	2.40	0.54
4:K:263:ILE:HA	4:K:272:VAL:O	2.06	0.54
5:L:349:LYS:NZ	7:N:50:SER:OG	2.41	0.54
1:A:24:VAL:HG12	1:A:62:LEU:HD11	1.90	0.54
1:A:219:VAL:HG11	1:A:1435:LEU:HD21	1.89	0.54
5:L:219:SER:HB3	5:L:222:ASP:HB2	1.89	0.54
8:O:27:ARG:HB2	8:O:87:PRO:HB2	1.90	0.54
1:A:256:LYS:HE2	1:A:277:LEU:HD11	1.90	0.54
1:A:814:ILE:HD11	1:A:855:SER:HB3	1.89	0.54
2:B:316:PHE:HA	2:B:319:MET:HG2	1.90	0.54
4:K:34:ARG:HH12	5:L:220:ILE:HG23	1.73	0.54
2:B:6:ARG:N	2:B:140:ASN:OD1	2.41	0.54
4:K:139:LEU:HA	4:K:142:LYS:HE2	1.90	0.54
10:Q:22:LEU:HB2	10:Q:85:ALA:HB3	1.89	0.54
10:Q:24:THR:HG23	10:Q:83:THR:HB	1.89	0.54
1:A:215:GLU:OE2	1:A:263:ARG:NE	2.39	0.53
1:A:262:GLU:OE1	1:A:264:ARG:NH1	2.40	0.53
5:L:188:LYS:NZ	5:L:218:THR:OG1	2.41	0.53
1:A:239:ARG:NH1	1:A:251:TYR:OH	2.40	0.53
2:B:187:SER:OG	2:B:188:GLN:OE1	2.26	0.53
2:B:279:ARG:HA	3:C:413:MET:HE2	1.90	0.53
4:K:162:THR:OG1	4:K:163:SER:N	2.41	0.53
3:C:84:PHE:HB3	3:C:95:GLY:O	2.09	0.53
3:C:160:CYS:SG	3:C:165:ARG:NH2	2.81	0.53
6:M:121:SER:OG	9:P:65:ARG:NH1	2.42	0.53
1:A:801:GLU:OE1	1:A:1366:ARG:NH1	2.42	0.53
2:B:128:LEU:HA	2:B:131:ILE:HD12	1.89	0.53
4:K:291:ARG:HA	4:K:294:ARG:HE	1.74	0.53
5:L:126:PRO:HA	5:L:129:ASP:HB2	1.91	0.53
2:B:63:LYS:HG3	2:B:91:ALA:HA	1.90	0.53
3:C:406:LEU:HD12	3:C:555:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:224:ASP:OD2	4:K:225:VAL:N	2.41	0.53
1:A:223:ARG:HD3	1:A:303:GLN:HB3	1.89	0.53
1:A:243:ARG:HH21	1:A:384:ASN:H	1.57	0.53
2:B:175:PRO:HB3	2:B:224:ILE:HD11	1.91	0.53
4:K:145:GLU:OE2	4:K:149:ARG:NH2	2.42	0.53
1:A:107:GLN:HE22	1:A:138:ARG:H	1.58	0.52
3:C:155:HIS:HA	3:C:158:ARG:HD2	1.91	0.52
7:N:59:ASN:OD1	8:O:46:ARG:NH2	2.41	0.52
1:A:1375:HIS:CE1	1:A:1385:GLU:HG3	2.44	0.52
2:B:12:PHE:HB3	2:B:25:TYR:HB2	1.90	0.52
3:C:255:ILE:O	3:C:256:ARG:NH1	2.43	0.52
1:A:1560:SER:OG	1:A:1561:SER:N	2.41	0.52
6:M:91:ARG:HG2	8:O:120:VAL:HG13	1.90	0.52
7:N:72:ILE:HB	7:N:83:ILE:HB	1.91	0.52
2:B:265:LEU:HG	2:B:275:ARG:HH11	1.75	0.52
3:C:282:LEU:HD13	3:C:312:LEU:HD12	1.92	0.52
4:K:24:ARG:HG3	4:K:60:LEU:HD21	1.92	0.52
4:K:248:SER:OG	4:K:249:PHE:N	2.42	0.52
1:A:1448:LEU:HD11	1:A:1588:VAL:HA	1.92	0.51
6:M:123:PRO:HB3	9:P:89:ARG:HH22	1.74	0.51
1:A:298:ASN:ND2	1:A:299:SER:O	2.43	0.51
1:A:334:VAL:HA	1:A:364:VAL:O	2.11	0.51
1:A:27:PRO:HD3	1:A:58:LEU:HB2	1.93	0.51
7:N:102:GLY:HA3	10:Q:31:LEU:HA	1.92	0.51
1:A:207:TRP:HE1	1:A:748:THR:HA	1.75	0.51
5:L:226:PHE:HA	5:L:229:PHE:HB2	1.92	0.51
7:N:59:ASN:ND2	8:O:52:THR:OG1	2.43	0.51
4:K:65:GLY:HA2	4:K:70:MET:HE3	1.93	0.50
5:L:251:ILE:HG23	5:L:256:ILE:HB	1.93	0.50
4:K:181:ILE:HD12	4:K:182:PRO:HD2	1.93	0.50
1:A:1193:LEU:HD13	1:A:1205:PHE:HB3	1.92	0.50
1:A:406:SER:HB2	1:A:742:VAL:HA	1.94	0.50
2:B:119:VAL:O	2:B:125:LYS:NZ	2.38	0.50
1:A:38:ILE:HA	1:A:53:LEU:O	2.12	0.50
4:K:293:ALA:O	4:K:297:PHE:HB2	2.12	0.50
2:B:71:ILE:H	2:B:80:ALA:HB1	1.75	0.50
2:B:77:SER:OG	2:B:78:ARG:N	2.45	0.50
4:K:234:ILE:HG22	5:L:291:VAL:HG23	1.94	0.50
1:A:217:THR:O	1:A:217:THR:OG1	2.25	0.50
1:A:1420:LEU:HD22	1:A:1553:MET:HG2	1.92	0.50
1:A:1427:PRO:HB3	1:A:1434:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:MET:HE3	1:A:797:GLN:HG3	1.94	0.49
4:K:32:ILE:HG23	4:K:34:ARG:H	1.76	0.49
1:A:213:SER:OG	1:A:328:ARG:NH1	2.42	0.49
1:A:242:ILE:HG13	1:A:247:LYS:HB3	1.92	0.49
1:A:260:GLN:NE2	1:A:1435:LEU:O	2.45	0.49
1:A:1556:LYS:HA	1:A:1559:ARG:HG3	1.94	0.49
2:B:166:PRO:HG2	2:B:225:GLN:HE21	1.78	0.49
2:B:279:ARG:NH2	3:C:549:SER:O	2.37	0.49
1:A:762:ASP:OD1	1:A:762:ASP:N	2.44	0.49
1:A:772:GLU:HA	1:A:874:ARG:O	2.11	0.49
3:C:148:ARG:NH1	3:C:318:TYR:OH	2.45	0.49
8:O:61:SER:HA	8:O:67:LYS:H	1.77	0.49
8:O:85:ARG:NH1	8:O:114:PHE:O	2.46	0.49
10:Q:21:VAL:HG23	10:Q:86:VAL:HG22	1.94	0.49
2:B:32:ILE:HG23	2:B:36:LEU:HD12	1.94	0.49
7:N:47:ALA:O	7:N:50:SER:OG	2.29	0.49
1:A:410:SER:OG	1:A:411:LYS:N	2.44	0.49
1:A:1213:TRP:O	1:A:1217:HIS:HB3	2.13	0.49
2:B:63:LYS:NZ	2:B:93:ALA:O	2.42	0.49
1:A:109:ILE:H	1:A:329:THR:HG22	1.77	0.49
1:A:347:ARG:HD3	1:A:382:LEU:HD21	1.93	0.49
1:A:780:GLU:HA	1:A:783:ILE:HD12	1.94	0.49
2:B:351:TYR:O	2:B:355:CYS:CB	2.61	0.49
5:L:240:LEU:HA	5:L:243:LEU:HG	1.94	0.49
1:A:189:ASP:OD1	1:A:189:ASP:N	2.43	0.49
4:K:110:LEU:HA	4:K:113:ILE:HG22	1.95	0.49
10:Q:30:ASN:ND2	10:Q:30:ASN:N	2.58	0.49
2:B:257:ASP:O	2:B:261:GLN:NE2	2.46	0.49
4:K:256:ASN:HB3	4:K:259:PHE:HB3	1.95	0.49
10:Q:64:VAL:HG13	10:Q:77:GLN:HB3	1.94	0.49
1:A:127:TYR:HB2	1:A:130:GLN:HB2	1.93	0.48
2:B:46:THR:OG1	2:B:47:LYS:N	2.46	0.48
3:C:92:ARG:O	3:C:129:ALA:HA	2.12	0.48
1:A:98:ASP:OD1	1:A:98:ASP:N	2.44	0.48
1:A:1194:LEU:HD23	1:A:1205:PHE:HA	1.95	0.48
5:L:351:LEU:HD21	8:O:62:LYS:HB3	1.95	0.48
6:M:99:LEU:HD23	6:M:100:THR:H	1.78	0.48
3:C:91:VAL:HG22	3:C:131:ARG:HH22	1.76	0.48
4:K:198:ILE:O	7:N:3:ARG:NH1	2.45	0.48
5:L:194:ASP:O	5:L:198:ARG:HB2	2.13	0.48
9:P:74:THR:OG1	9:P:91:ASN:OD1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:76:LEU:O	9:P:86:VAL:HA	2.14	0.48
1:A:814:ILE:HD13	1:A:853:TRP:HB3	1.96	0.48
6:M:99:LEU:HD22	6:M:103:LYS:HG3	1.96	0.48
8:O:56:ALA:O	8:O:68:ASN:ND2	2.43	0.48
3:C:257:PRO:HA	3:C:295:LEU:HD12	1.95	0.48
5:L:90:THR:HA	5:L:93:LEU:HD23	1.96	0.48
7:N:85:ARG:NE	7:N:87:ALA:O	2.42	0.48
5:L:74:LYS:HE3	5:L:143:VAL:HG11	1.96	0.48
4:K:206:PHE:HB3	4:K:213:VAL:HA	1.96	0.47
2:B:285:TYR:OH	2:B:313:LEU:O	2.31	0.47
7:N:116:GLU:O	7:N:120:THR:OG1	2.29	0.47
2:B:286:CYS:HB2	3:C:554:THR:HB	1.96	0.47
3:C:404:ILE:HD12	3:C:557:GLU:HB3	1.96	0.47
4:K:252:MET:HE3	4:K:263:ILE:HD13	1.96	0.47
5:L:66:LEU:HG	5:L:78:GLN:HE21	1.79	0.47
1:A:1433:ASP:N	1:A:1433:ASP:OD1	2.48	0.47
2:B:253:ASP:OD1	2:B:253:ASP:N	2.46	0.47
3:C:410:VAL:HG22	3:C:553:VAL:HG12	1.95	0.47
5:L:288:MET:HA	5:L:291:VAL:HG12	1.95	0.47
1:A:179:CYS:N	1:A:298:ASN:O	2.44	0.47
10:Q:67:LEU:HB3	10:Q:74:ILE:HB	1.97	0.47
1:A:1357:ASP:OD1	1:A:1357:ASP:N	2.47	0.47
3:C:144:ASN:OD1	3:C:147:ARG:NH2	2.46	0.47
5:L:84:LYS:HZ1	5:L:220:ILE:HD12	1.79	0.47
7:N:80:ARG:HH12	7:N:101:PHE:HB2	1.80	0.47
8:O:102:LEU:HD22	10:Q:47:VAL:HG21	1.95	0.47
2:B:15:PHE:HZ	2:B:78:ARG:HH22	1.62	0.47
2:B:85:LEU:HD23	2:B:105:LEU:HD21	1.97	0.47
3:C:528:GLU:OE2	3:C:532:ASN:ND2	2.47	0.47
7:N:82:ALA:O	7:N:92:CYS:HA	2.15	0.47
4:K:27:ILE:HD11	4:K:212:LEU:HD11	1.98	0.46
5:L:324:THR:HA	5:L:341:LEU:O	2.15	0.46
10:Q:30:ASN:N	10:Q:30:ASN:HD22	2.12	0.46
1:A:175:ILE:HG12	1:A:336:ILE:HD12	1.98	0.46
1:A:775:TYR:HB2	1:A:872:VAL:HB	1.97	0.46
1:A:923:GLN:OE1	4:K:47:HIS:NE2	2.44	0.46
2:B:30:ASP:OD1	2:B:30:ASP:N	2.48	0.46
1:A:1420:LEU:HD21	1:A:1552:THR:HB	1.98	0.46
2:B:104:LYS:O	2:B:108:TYR:HB2	2.16	0.46
3:C:412:LEU:HD22	3:C:520:PHE:HB2	1.98	0.46
7:N:80:ARG:HH22	7:N:101:PHE:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:ASP:OD1	1:A:1233:LYS:NZ	2.49	0.46
2:B:331:VAL:HG22	2:B:347:GLY:HA2	1.98	0.46
5:L:247:LEU:HD13	5:L:272:THR:HG21	1.97	0.46
1:A:1358:VAL:HB	1:A:1368:GLU:HB2	1.98	0.46
1:A:14:LYS:HA	1:A:14:LYS:HD3	1.78	0.46
5:L:192:GLN:O	5:L:196:HIS:ND1	2.48	0.46
5:L:349:LYS:HD2	7:N:51:ASN:HB2	1.97	0.46
7:N:103:MET:SD	7:N:103:MET:N	2.89	0.46
2:B:193:THR:HA	2:B:196:ILE:HG22	1.99	0.46
3:C:257:PRO:HG3	3:C:310:PHE:HZ	1.81	0.46
1:A:1375:HIS:HE2	1:A:1486:LYS:HB2	1.81	0.45
4:K:291:ARG:HH22	7:N:123:ALA:HA	1.81	0.45
4:K:23:MET:HA	4:K:26:ILE:HG22	1.98	0.45
1:A:775:TYR:O	1:A:871:THR:HA	2.17	0.45
1:A:1181:LEU:HD13	1:A:1260:ILE:HD11	1.97	0.45
1:A:1365:ASP:OD1	1:A:1365:ASP:N	2.47	0.45
4:K:16:SER:OG	11:K:500:GNP:O2B	2.33	0.45
4:K:52:PHE:HB3	4:K:56:LEU:HB3	1.97	0.45
10:Q:45:ILE:HG21	10:Q:85:ALA:HB2	1.97	0.45
1:A:858:ARG:NE	1:A:881:TYR:OH	2.45	0.45
1:A:353:THR:O	1:A:357:MET:HB2	2.16	0.45
4:K:211:PHE:O	4:K:232:SER:OG	2.35	0.45
9:P:49:THR:HB	10:Q:51:GLN:HE22	1.81	0.45
10:Q:25:ASP:OD1	10:Q:25:ASP:N	2.48	0.45
1:A:319:LYS:NZ	1:A:1430:LEU:O	2.44	0.45
1:A:342:VAL:HG12	1:A:379:LEU:HD21	1.99	0.45
3:C:126:VAL:HG11	3:C:149:ILE:HD11	1.99	0.45
5:L:142:TYR:HB3	5:L:175:VAL:HG12	1.99	0.45
6:M:110:SER:HA	9:P:79:VAL:HG12	1.99	0.45
2:B:23:ILE:HG21	2:B:32:ILE:HG21	1.99	0.45
2:B:269:THR:HG21	2:B:275:ARG:HD3	1.98	0.45
3:C:293:LYS:HE2	3:C:297:GLN:HB3	1.99	0.45
9:P:68:VAL:O	9:P:74:THR:HA	2.17	0.45
4:K:195:ALA:HA	4:K:198:ILE:HG22	1.99	0.45
1:A:44:PRO:HD3	1:A:85:VAL:HA	1.99	0.44
1:A:1439:LEU:HB3	1:A:1548:TRP:HB3	1.99	0.44
4:K:170:TYR:O	4:K:174:SER:HB3	2.16	0.44
6:M:84:ARG:HH21	8:O:30:VAL:HG21	1.82	0.44
2:B:332:ARG:HG2	2:B:346:THR:HA	1.99	0.44
3:C:84:PHE:CB	3:C:95:GLY:O	2.65	0.44
3:C:173:LEU:HD13	3:C:194:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LYS:HA	2:B:261:GLN:HB2	1.98	0.44
3:C:7:PRO:HA	3:C:130:LEU:HG	1.99	0.44
8:O:18:GLY:HA3	8:O:98:ALA:HB2	1.99	0.44
9:P:73:HIS:HA	9:P:90:GLN:HA	1.98	0.44
1:A:235:PRO:HB2	1:A:237:ILE:HG12	1.98	0.44
5:L:103:ASP:N	5:L:103:ASP:OD1	2.49	0.44
5:L:281:SER:O	5:L:285:CYS:HB2	2.17	0.44
9:P:67:SER:HB2	10:Q:66:CYS:HB2	1.98	0.44
1:A:921:LEU:HD11	1:A:1391:MET:HG2	1.99	0.44
3:C:265:SER:OG	3:C:266:ASP:N	2.49	0.44
1:A:171:VAL:HG12	1:A:332:MET:HG2	2.00	0.44
3:C:501:VAL:HG12	3:C:503:ALA:H	1.83	0.44
1:A:803:ILE:HG13	1:A:852:TYR:HD2	1.81	0.44
3:C:348:LEU:HD21	3:C:402:LEU:HD11	1.99	0.44
4:K:47:HIS:HA	4:K:60:LEU:O	2.17	0.44
1:A:337:THR:HG21	1:A:343:PHE:HZ	1.83	0.43
3:C:379:ASN:HB3	3:C:382:ALA:HB3	2.00	0.43
4:K:189:MET:HA	4:K:192:ARG:HB3	2.00	0.43
5:L:259:ALA:HA	5:L:338:VAL:O	2.18	0.43
6:M:106:PRO:HD3	8:O:8:PHE:HE1	1.83	0.43
7:N:15:ASN:OD1	7:N:35:SER:OG	2.33	0.43
2:B:210:SER:HB2	2:B:220:VAL:HG11	2.00	0.43
3:C:128:PHE:HE2	3:C:146:SER:HB3	1.83	0.43
5:L:63:ARG:NH1	5:L:135:ARG:O	2.48	0.43
7:N:3:ARG:HE	7:N:5:LYS:H	1.66	0.43
2:B:173:ASP:OD1	2:B:173:ASP:N	2.49	0.43
3:C:386:GLN:HA	3:C:389:GLN:HB2	2.01	0.43
3:C:407:HIS:O	3:C:555:THR:HA	2.19	0.43
6:M:92:LEU:HD13	8:O:5:LEU:HD21	2.00	0.43
3:C:80:CYS:SG	3:C:99:LEU:N	2.92	0.43
3:C:409:TYR:OH	3:C:558:ASP:OD1	2.37	0.43
1:A:35:LEU:HD21	1:A:58:LEU:HD22	2.01	0.43
1:A:133:GLU:HG2	1:A:138:ARG:HA	2.00	0.43
1:A:807:LEU:HD23	1:A:807:LEU:HA	1.88	0.43
2:B:145:CYS:HB2	2:B:157:LEU:HB2	2.00	0.43
3:C:76:LYS:HA	3:C:76:LYS:HD3	1.72	0.43
1:A:181:MET:HE3	1:A:192:PHE:HA	2.01	0.43
1:A:733:VAL:HG21	2:B:215:VAL:HA	2.01	0.43
2:B:27:VAL:HG13	2:B:28:PRO:HD3	2.01	0.43
5:L:63:ARG:HB2	5:L:138:GLY:H	1.83	0.43
5:L:91:LEU:HD13	5:L:334:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:88:TYR:HB3	8:O:32:VAL:HG23	1.99	0.43
2:B:284:LEU:O	2:B:287:SER:OG	2.36	0.43
3:C:509:ASP:OD2	3:C:546:LYS:NZ	2.44	0.43
5:L:292:VAL:HG11	5:L:328:LEU:HD13	2.01	0.42
5:L:352:ILE:H	5:L:352:ILE:HG13	1.63	0.42
1:A:916:TYR:HE1	1:A:939:LEU:HA	1.84	0.42
8:O:29:GLY:HA2	8:O:50:LEU:HB2	2.01	0.42
3:C:136:PRO:HA	3:C:139:ILE:HG12	2.02	0.42
5:L:330:GLU:HA	5:L:336:ALA:HA	2.01	0.42
9:P:56:HIS:NE2	10:Q:36:THR:O	2.46	0.42
7:N:96:LYS:HB2	7:N:99:VAL:HG23	1.99	0.42
8:O:69:LYS:HB3	8:O:69:LYS:HE2	1.87	0.42
1:A:329:THR:OG1	1:A:330:GLY:N	2.52	0.42
1:A:1232:GLN:HE22	1:A:1235:LEU:HD23	1.83	0.42
5:L:205:ASP:OD1	5:L:205:ASP:N	2.51	0.42
1:A:185:ASP:OD1	1:A:185:ASP:N	2.52	0.42
3:C:148:ARG:HH12	3:C:319:TRP:HZ3	1.68	0.42
5:L:67:MET:SD	5:L:67:MET:N	2.92	0.42
6:M:84:ARG:HA	6:M:87:GLN:HG2	2.01	0.42
9:P:94:ARG:HG2	9:P:96:PRO:HD3	2.01	0.42
1:A:229:LYS:HE2	1:A:229:LYS:HB2	1.90	0.42
5:L:137:THR:OG1	5:L:138:GLY:N	2.52	0.42
8:O:10:TYR:HA	8:O:13:LEU:HD12	2.02	0.42
1:A:1408:LYS:HD2	1:A:1408:LYS:HA	1.82	0.42
2:B:71:ILE:HD11	2:B:114:LEU:HD21	2.02	0.42
5:L:192:GLN:HE22	5:L:193:ARG:NH1	2.17	0.42
2:B:205:HIS:HE1	2:B:238:ILE:HG22	1.85	0.42
7:N:48:ILE:O	7:N:51:ASN:HB3	2.19	0.42
8:O:16:VAL:HG13	8:O:102:LEU:HD23	2.02	0.42
1:A:894:PRO:HD2	1:A:897:SER:HB2	2.01	0.41
1:A:1313:LEU:O	1:A:1468:ARG:NH2	2.53	0.41
1:A:1507:GLY:O	1:A:1551:ASN:ND2	2.40	0.41
3:C:12:LEU:HG	3:C:200:LEU:HD21	2.02	0.41
5:L:318:ILE:O	5:L:325:VAL:HA	2.20	0.41
2:B:7:ILE:HD11	2:B:98:LEU:HD11	2.01	0.41
2:B:279:ARG:NH1	3:C:413:MET:O	2.54	0.41
2:B:49:GLU:HG2	2:B:50:LEU:HD12	2.01	0.41
2:B:380:LYS:HA	3:C:336:LEU:HD11	2.02	0.41
4:K:52:PHE:O	4:K:56:LEU:HB3	2.20	0.41
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.97	0.41
1:A:782:ASP:HA	1:A:785:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:GLN:HG2	2:B:278:LEU:HD22	2.02	0.41
5:L:146:ALA:HB2	5:L:180:VAL:HA	2.02	0.41
7:N:79:GLY:N	7:N:97:GLU:OE2	2.54	0.41
1:A:374:LEU:O	2:B:192:THR:OG1	2.37	0.41
5:L:101:LYS:NZ	5:L:237:ILE:O	2.53	0.41
1:A:298:ASN:HD22	1:A:303:GLN:HB2	1.86	0.41
2:B:329:TYR:HB2	2:B:380:LYS:HE3	2.02	0.41
5:L:240:LEU:O	5:L:244:GLU:CB	2.67	0.41
7:N:77:MET:SD	7:N:77:MET:N	2.90	0.41
8:O:28:ASP:OD1	8:O:28:ASP:N	2.54	0.41
1:A:170:MET:HE3	1:A:170:MET:HB2	1.84	0.41
2:B:27:VAL:HB	2:B:132:MET:HE3	2.02	0.41
4:K:16:SER:OG	11:K:500:GNP:O1G	2.38	0.41
5:L:293:ILE:HD12	5:L:293:ILE:HA	1.90	0.41
7:N:105:LYS:HA	7:N:105:LYS:HD2	1.95	0.41
1:A:319:LYS:NZ	1:A:1432:GLY:O	2.42	0.40
3:C:490:LEU:HD21	3:C:517:LEU:HD21	2.03	0.40
5:L:247:LEU:HD11	5:L:259:ALA:HB3	2.02	0.40
7:N:101:PHE:HD2	10:Q:29:LEU:HD11	1.86	0.40
2:B:205:HIS:CE1	2:B:238:ILE:HG22	2.56	0.40
1:A:93:LYS:O	1:A:93:LYS:NZ	2.40	0.40
1:A:337:THR:HA	1:A:338:PRO:HD3	1.80	0.40
1:A:811:TYR:HA	1:A:856:MET:HB2	2.03	0.40
3:C:89:ASP:OD2	3:C:90:ASN:N	2.49	0.40
4:K:126:VAL:O	4:K:161:ARG:HA	2.21	0.40
1:A:947:LEU:HD22	1:A:1383:ALA:HB1	2.03	0.40
2:B:360:MET:HE3	2:B:364:GLU:HG3	2.03	0.40
2:B:369:LEU:HD12	2:B:369:LEU:HA	1.98	0.40
5:L:189:ILE:HD13	5:L:189:ILE:HA	1.97	0.40
1:A:165:ARG:HA	1:A:751:ALA:HA	2.04	0.40
1:A:1185:LYS:HA	1:A:1185:LYS:HD2	1.91	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	974/1603 (61%)	885 (91%)	89 (9%)	0	100	100
2	B	358/380 (94%)	312 (87%)	46 (13%)	0	100	100
3	C	394/569 (69%)	367 (93%)	27 (7%)	0	100	100
4	K	292/313 (93%)	266 (91%)	26 (9%)	0	100	100
5	L	297/399 (74%)	260 (88%)	36 (12%)	1 (0%)	36	70
6	M	113/161 (70%)	104 (92%)	9 (8%)	0	100	100
7	N	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
8	O	116/124 (94%)	108 (93%)	8 (7%)	0	100	100
9	P	95/99 (96%)	87 (92%)	8 (8%)	0	100	100
10	Q	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
All	All	2851/3864 (74%)	2586 (91%)	264 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	265	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	891/1412 (63%)	891 (100%)	0	100	100
2	B	336/351 (96%)	336 (100%)	0	100	100
3	C	363/504 (72%)	363 (100%)	0	100	100
4	K	270/287 (94%)	270 (100%)	0	100	100
5	L	274/340 (81%)	274 (100%)	0	100	100
6	M	99/141 (70%)	99 (100%)	0	100	100
7	N	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	O	103/108 (95%)	103 (100%)	0	100	100
9	P	81/83 (98%)	81 (100%)	0	100	100
10	Q	77/77 (100%)	76 (99%)	1 (1%)	61	72
All	All	2591/3401 (76%)	2590 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	Q	30	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	298	ASN
1	A	311	ASN
1	A	315	ASN
1	A	764	GLN
1	A	768	ASN
1	A	797	GLN
1	A	965	HIS
1	A	1444	ASN
2	B	52	ASN
2	B	140	ASN
2	B	261	GLN
2	B	271	GLN
2	B	327	GLN
3	C	161	GLN
3	C	220	HIS
3	C	222	ASN
3	C	331	ASN
3	C	389	GLN
3	C	485	ASN
3	C	532	ASN
4	K	30	ASN
5	L	83	HIS
5	L	245	ASN
7	N	15	ASN
7	N	51	ASN
9	P	90	GLN

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Mol	Chain	Res	Type
10	Q	30	ASN
10	Q	51	GLN
10	Q	71	ASN
10	Q	77	GLN

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](#)

1 ligand is 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	$\# Z > 2$
11	GNP	K	500	-	34,34,34	1.25	5 (14%)	47,54,54	0.81	2 (4%)

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
11	GNP	K	500	-	-	8/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	500	GNP	PB-O3A	3.97	1.64	1.59
11	K	500	GNP	PG-O1G	2.83	1.50	1.46
11	K	500	GNP	PB-O1B	2.83	1.50	1.46
11	K	500	GNP	PG-N3B	2.81	1.70	1.63
11	K	500	GNP	PB-O2B	-2.36	1.50	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	500	GNP	O1G-PG-N3B	-3.10	107.20	111.77
11	K	500	GNP	O2B-PB-O3A	2.15	111.83	104.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	500	GNP	PB-N3B-PG-O1G
11	K	500	GNP	C5'-O5'-PA-O3A
11	K	500	GNP	C5'-O5'-PA-O2A
11	K	500	GNP	O4'-C4'-C5'-O5'
11	K	500	GNP	C3'-C4'-C5'-O5'
11	K	500	GNP	C5'-O5'-PA-O1A
11	K	500	GNP	PA-O3A-PB-O2B
11	K	500	GNP	PA-O3A-PB-O1B

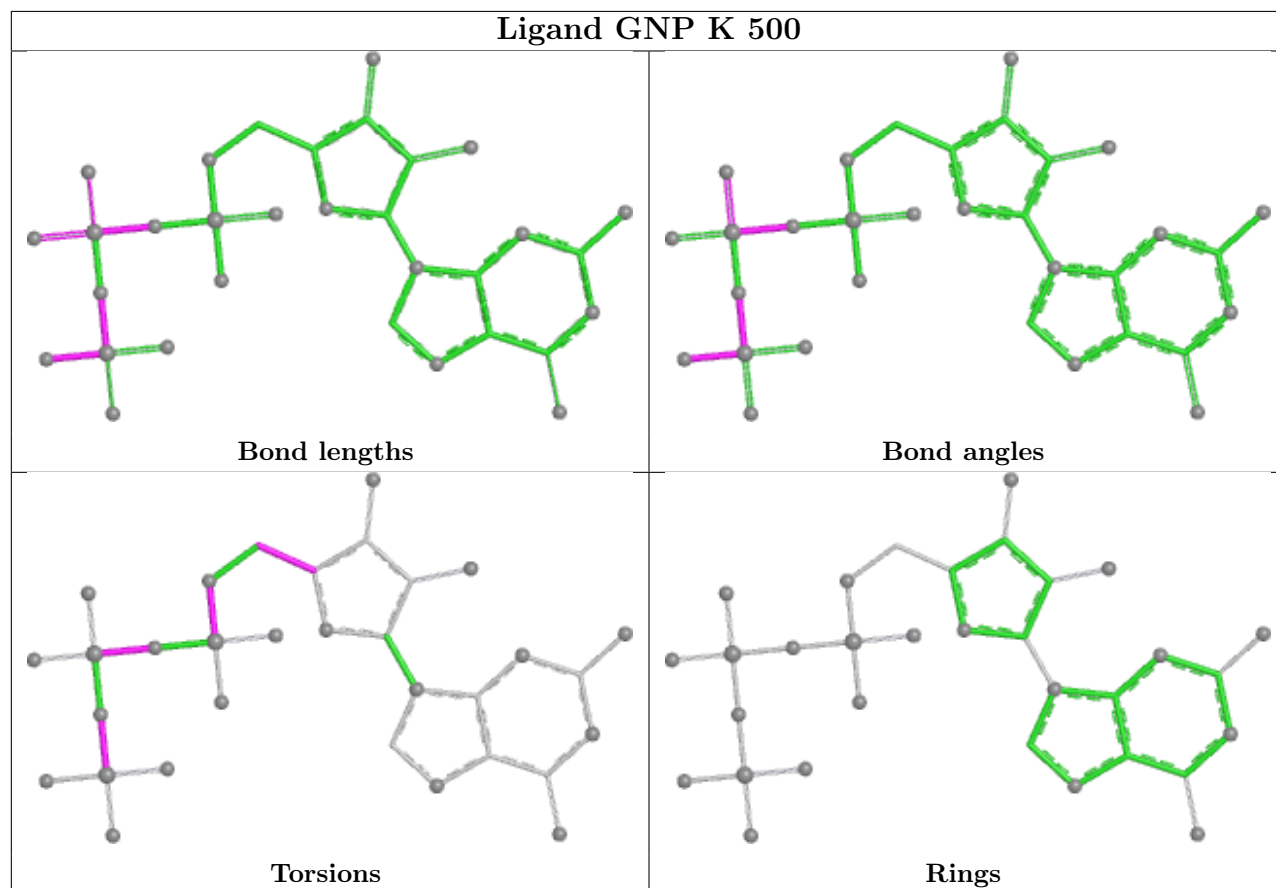
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	500	GNP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

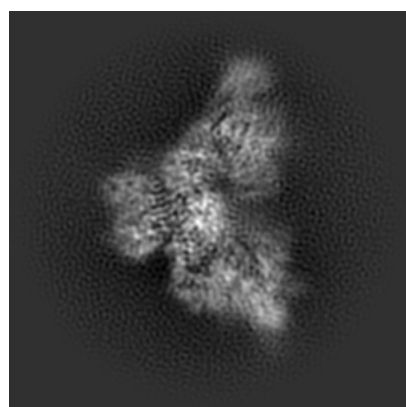
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25652. These allow visual inspection of the internal detail of the map and identification of artifacts.

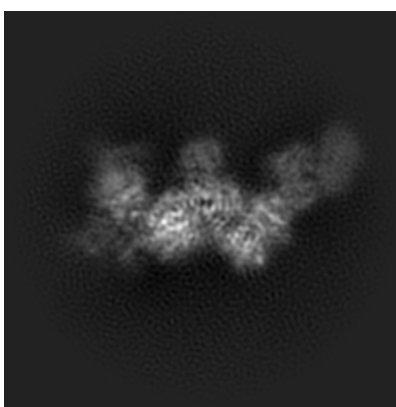
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

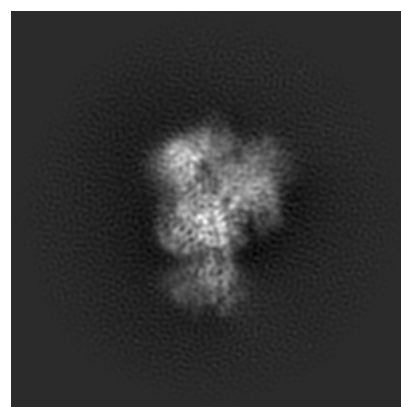
6.1.1 Primary map



X



Y

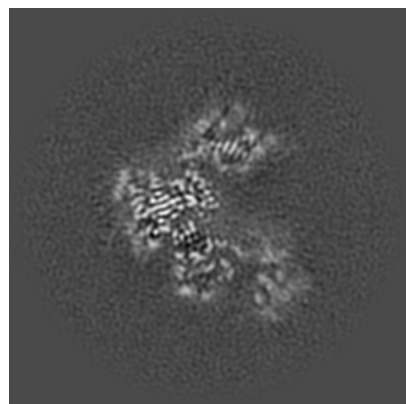


Z

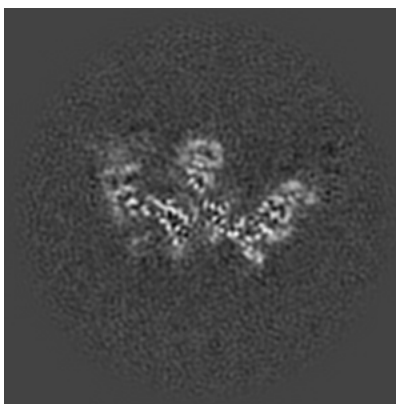
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

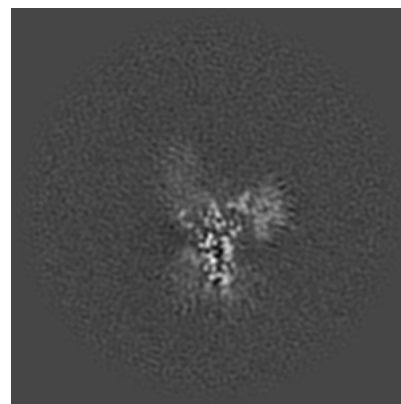
6.2.1 Primary map



X Index: 220



Y Index: 220

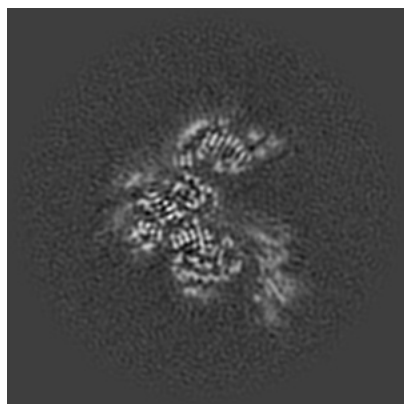


Z Index: 220

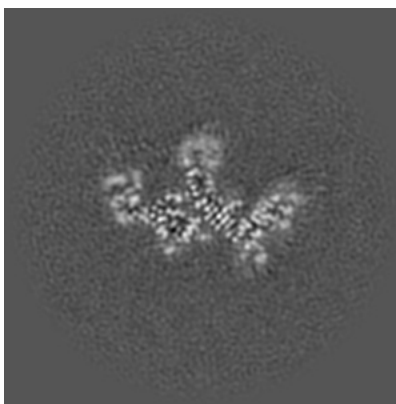
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

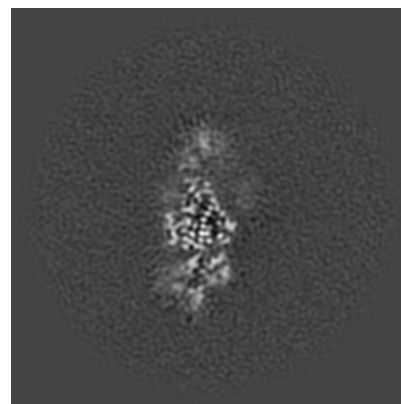
6.3.1 Primary map



X Index: 215



Y Index: 212

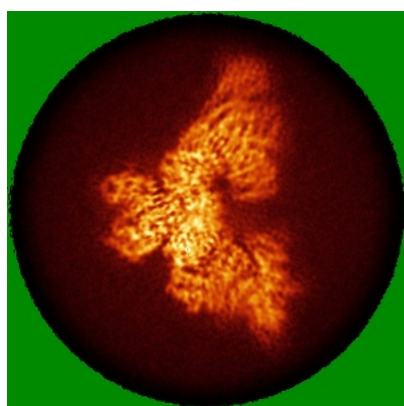


Z Index: 182

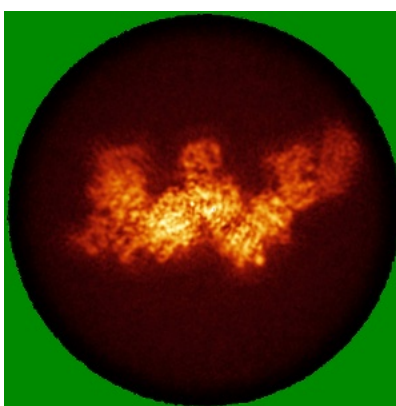
The images above show the largest variance slices of the map in three orthogonal directions.

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

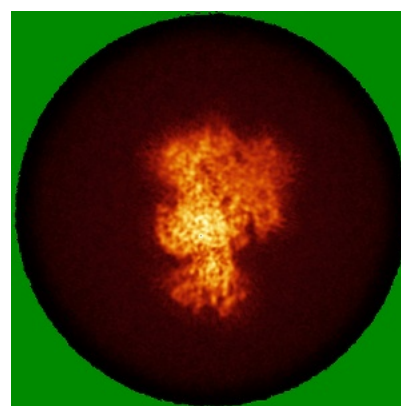
6.4.1 Primary map



X



Y



Z

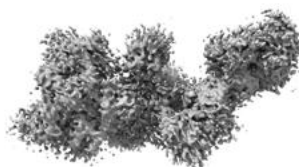
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

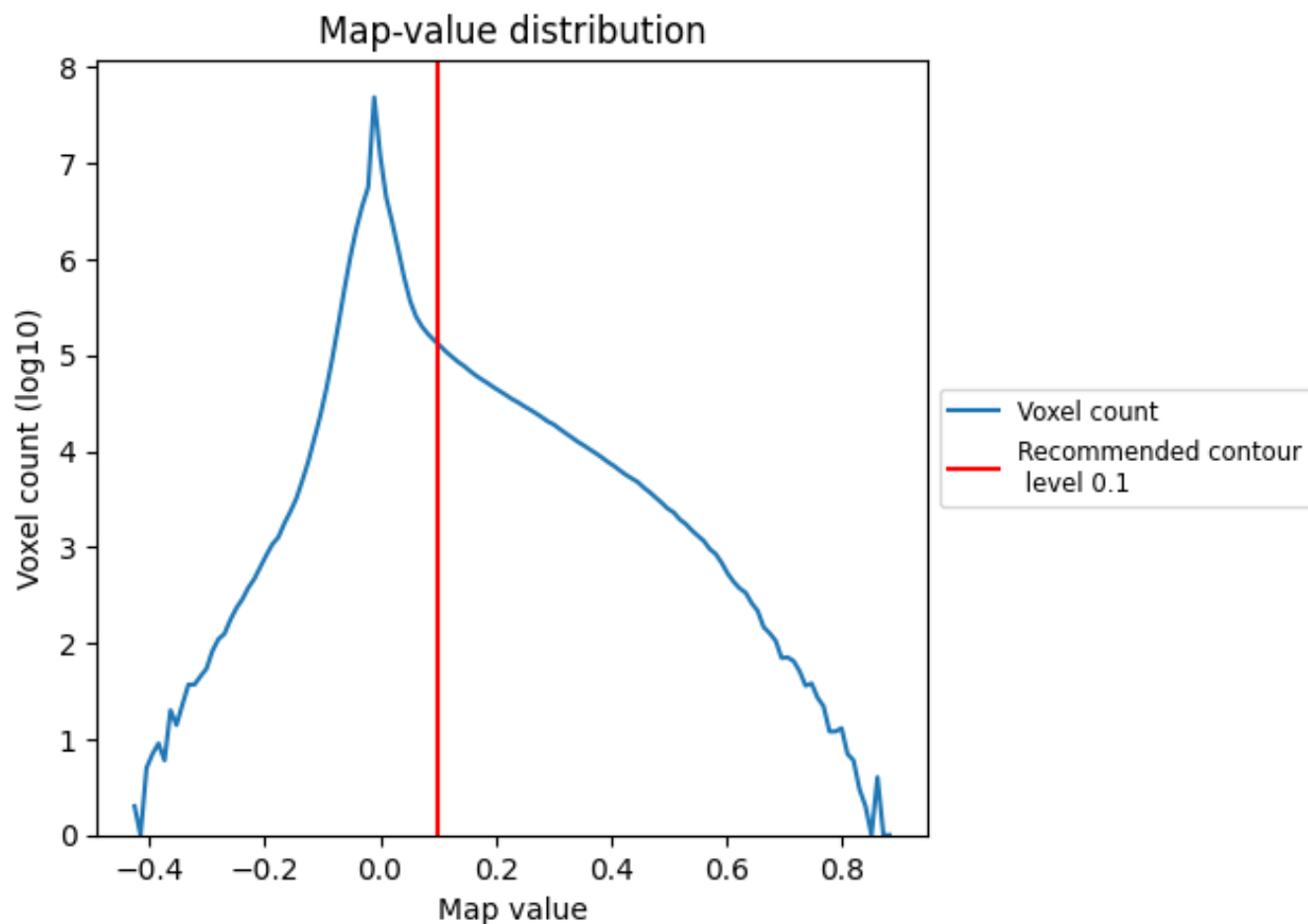
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

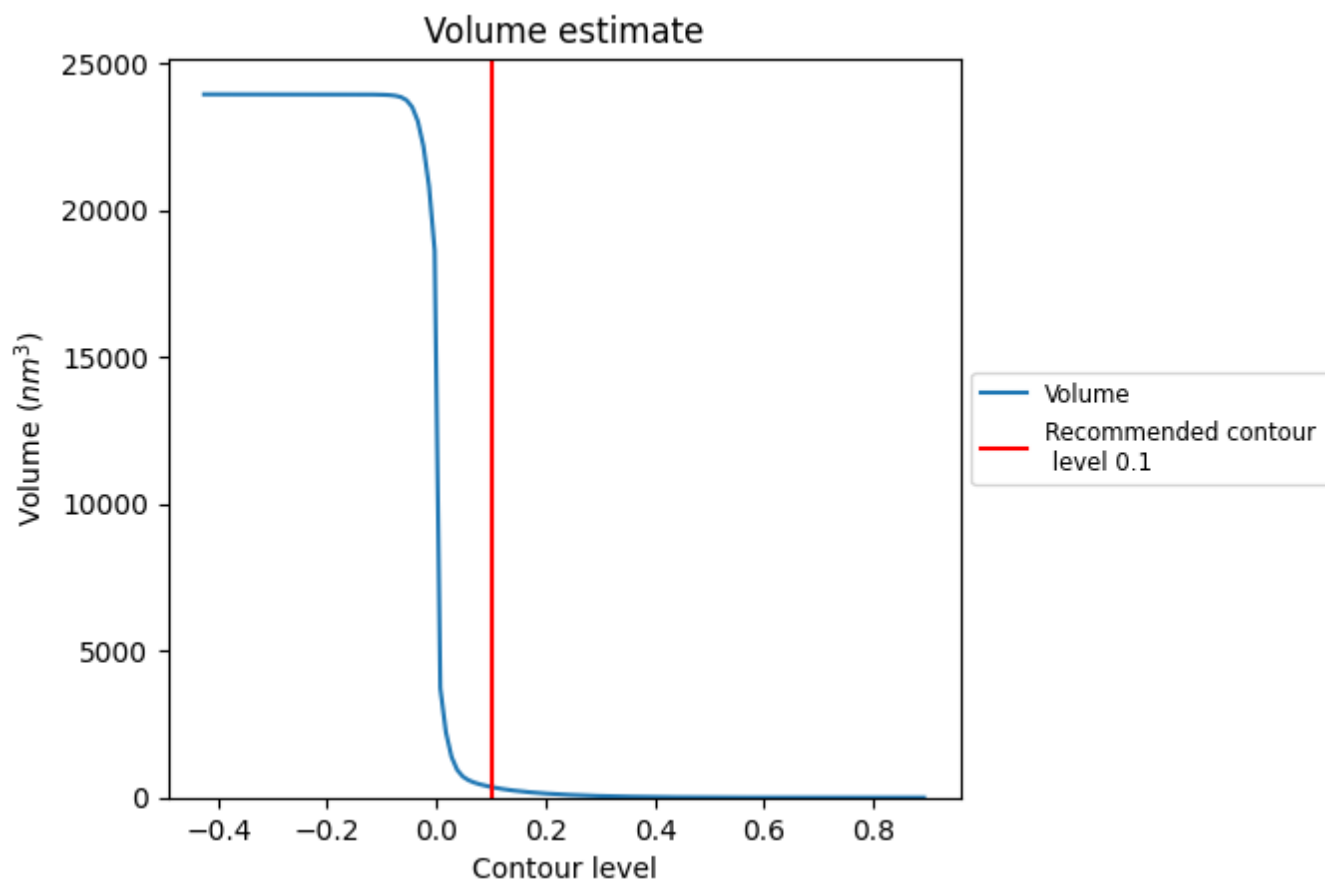
This section contains the results of statistical analysis of the map.

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.

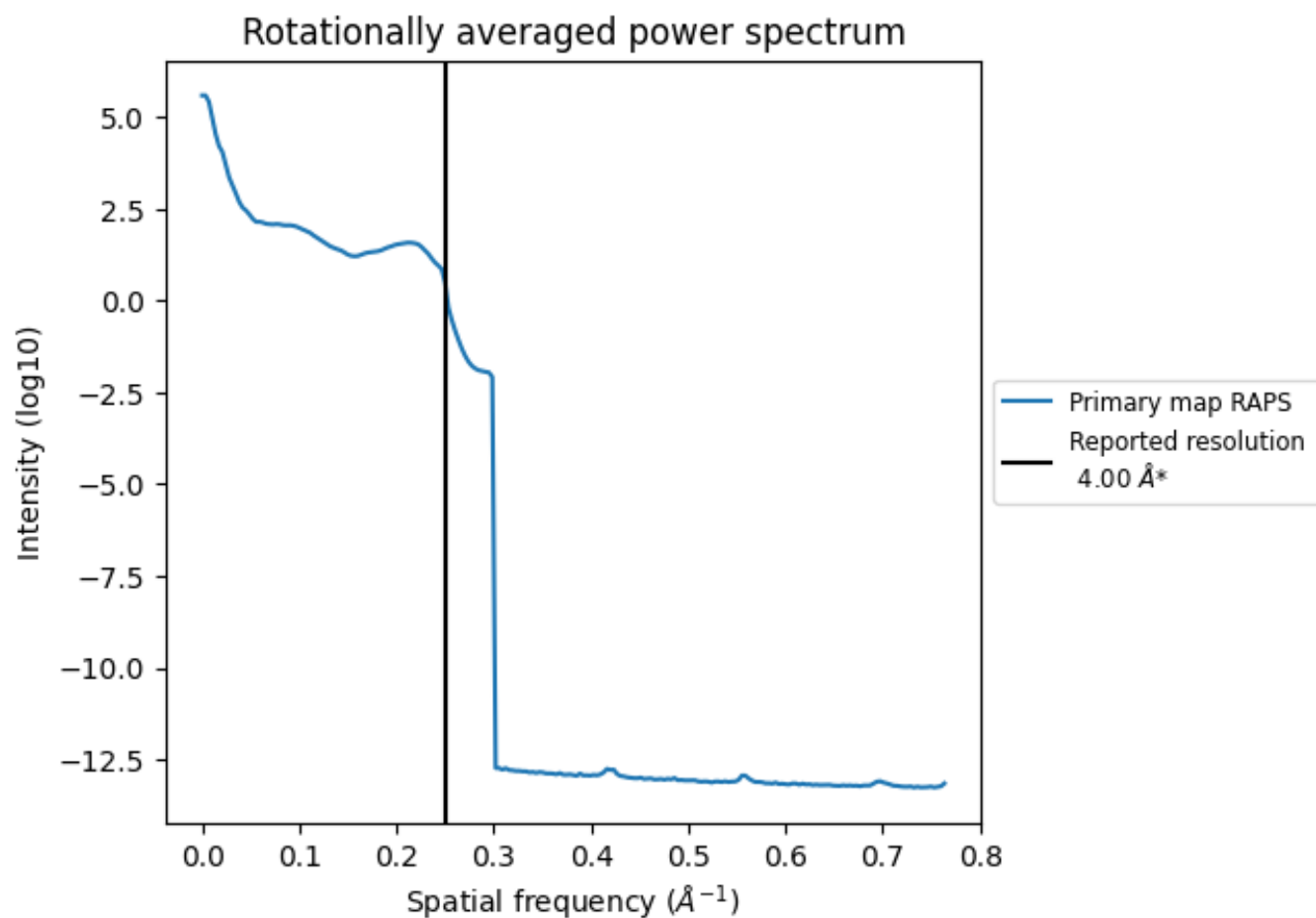
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm³; this corresponds to an approximate mass of 327 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 0.250 Å⁻¹

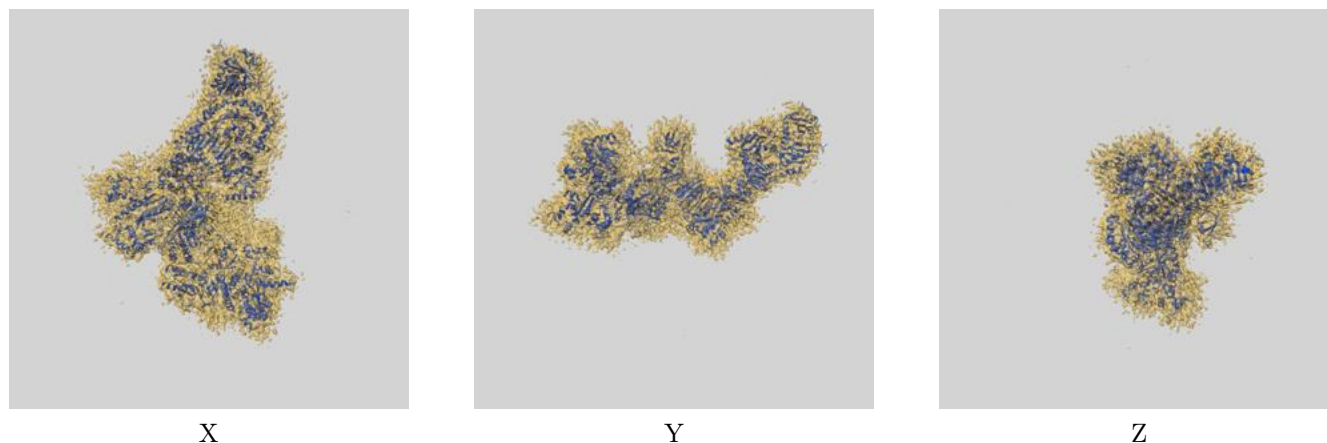
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

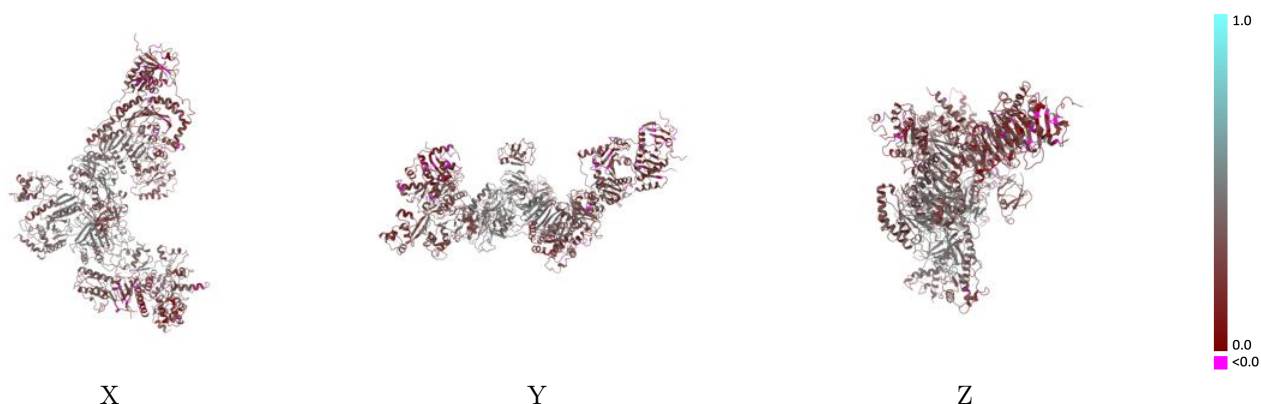
This section contains information regarding the fit between EMDB map EMD-25652 and PDB model 7T3A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



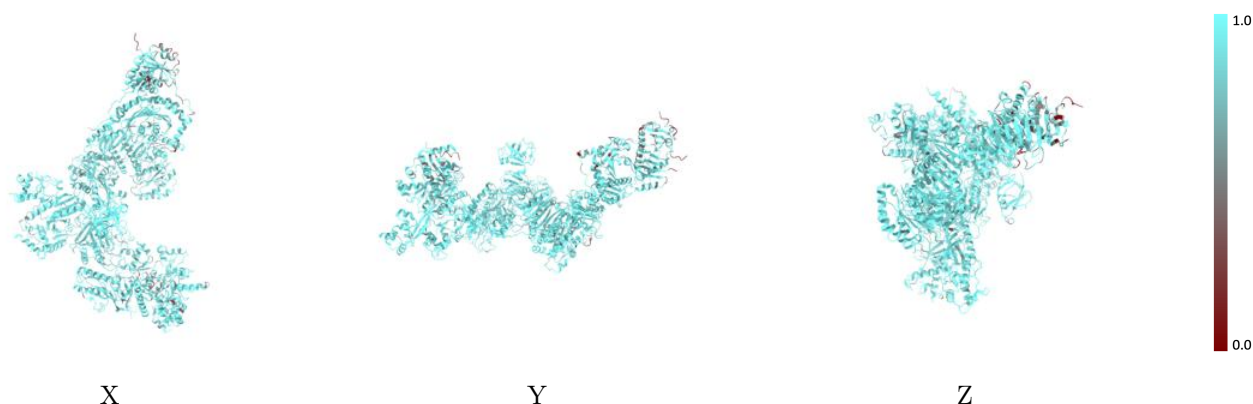
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



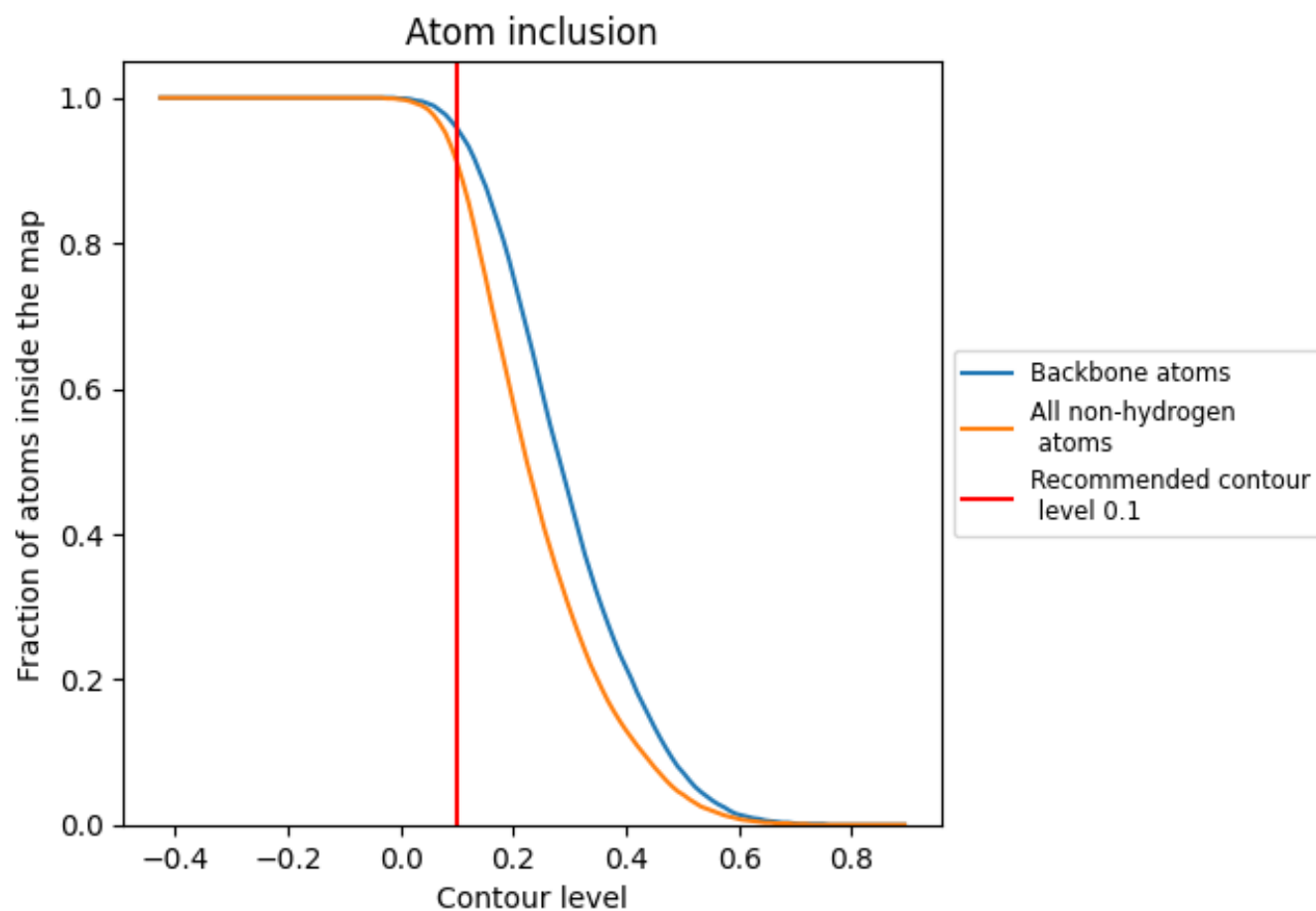
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.3400
A	0.9500	0.4070
B	0.9190	0.3500
C	0.8750	0.2630
K	0.9590	0.3830
L	0.8890	0.2840
M	0.8430	0.2850
N	0.9200	0.2980
O	0.8880	0.2610
P	0.6920	0.2380
Q	0.8430	0.2600

1.0

0.0

<0.0