



## Full wwPDB EM Validation Report ⓘ

Apr 14, 2025 – 04:12 PM JST

PDB ID : 9L7M / pdb\_00009l7m  
EMDB ID : EMD-62874  
Title : Nucleotide-free kinesin-1 motor domain bound to the microtubule  
Authors : Makino, T.; Komori, Y.; Yanagisawa, H.; Tomishige, M.; Kikkawa, M.  
Deposited on : 2024-12-26  
Resolution : 3.48 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

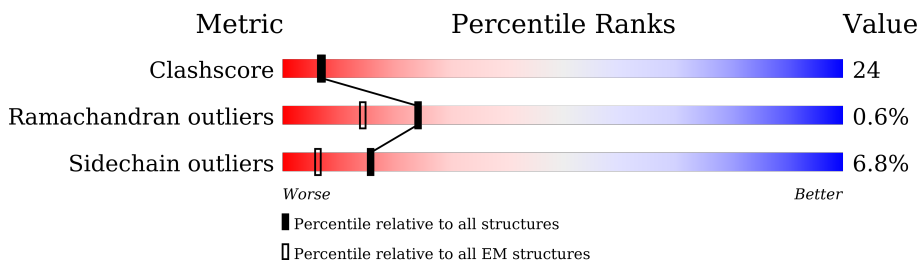
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.48 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>5%</div> <div>50%</div> <div>42%</div> <div>6%</div> <div>.</div> </div>
1	C	451	<div> <div>.</div> <div>49%</div> <div>43%</div> <div>5%</div> <div>.</div> </div>
2	B	445	<div> <div>.</div> <div>51%</div> <div>40%</div> <div>5%</div> <div>.</div> </div>
2	D	445	<div> <div>6%</div> <div>54%</div> <div>37%</div> <div>5%</div> <div>.</div> </div>
3	K	357	<div> <div>9%</div> <div>48%</div> <div>39%</div> <div>.</div> <div>11%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16181 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3430	2170	583	655	22		
1	C	439	Total	C	N	O	S	0	0
			3430	2170	583	655	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3351	2106	575	644	26		
2	D	426	Total	C	N	O	S	0	0
			3351	2106	575	644	26		

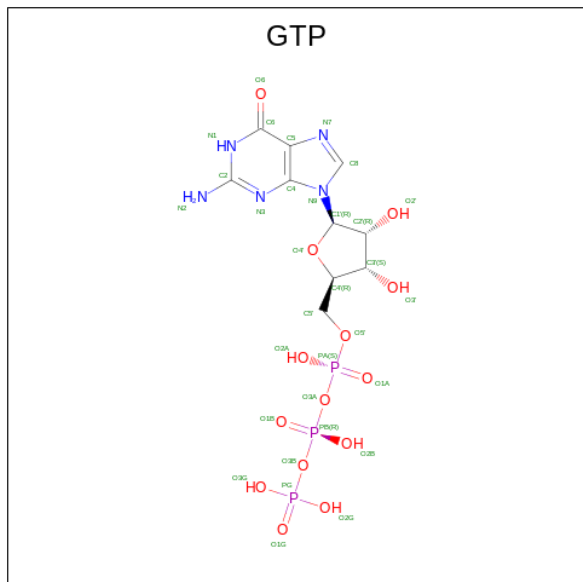
- Molecule 3 is a protein called Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	317	Total	C	N	O	S	0	0
			2487	1548	428	496	15		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	330	SER	CYS	conflict	UNP P33176
K	347	CYS	GLU	conflict	UNP P33176
K	350	GLY	-	expression tag	UNP P33176
K	351	THR	-	expression tag	UNP P33176
K	352	HIS	-	expression tag	UNP P33176
K	353	HIS	-	expression tag	UNP P33176
K	354	HIS	-	expression tag	UNP P33176
K	355	HIS	-	expression tag	UNP P33176
K	356	HIS	-	expression tag	UNP P33176
K	357	HIS	-	expression tag	UNP P33176

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	D	1	Total	C	N	O	P	0
			32	10	5	14	3	

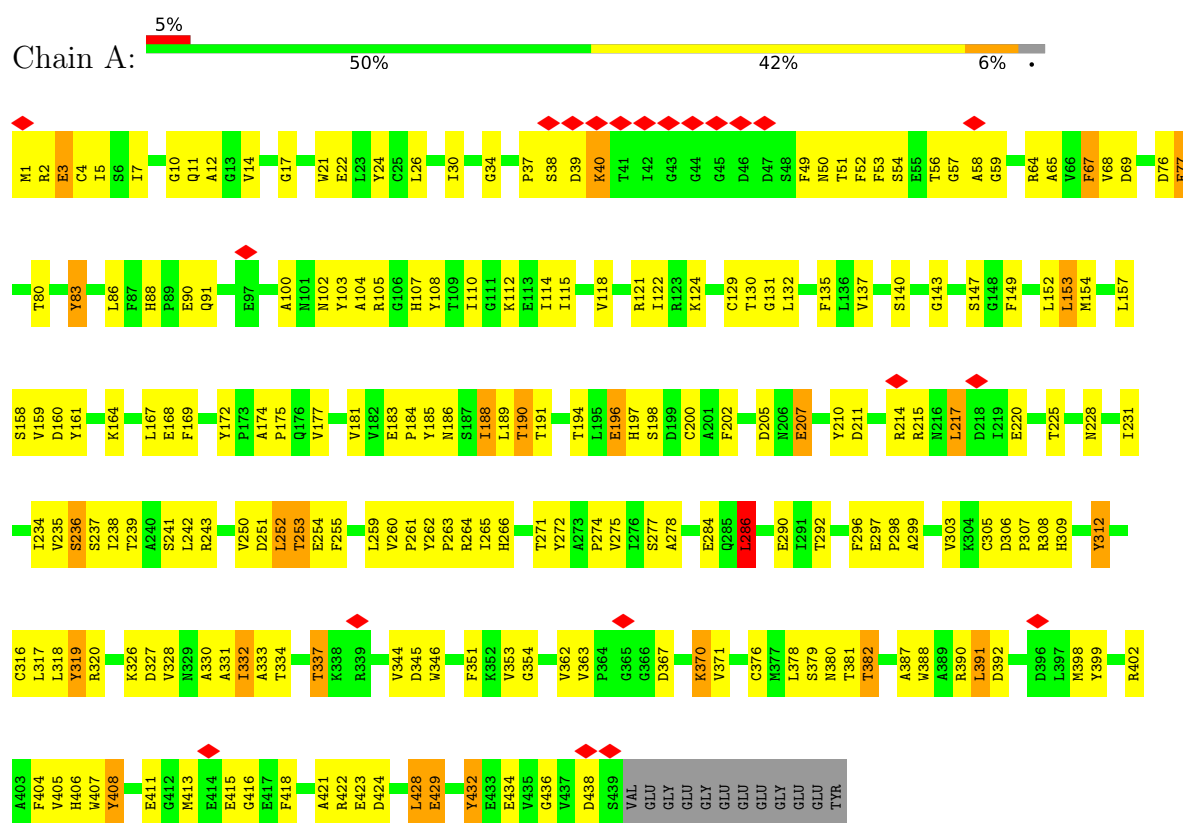
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

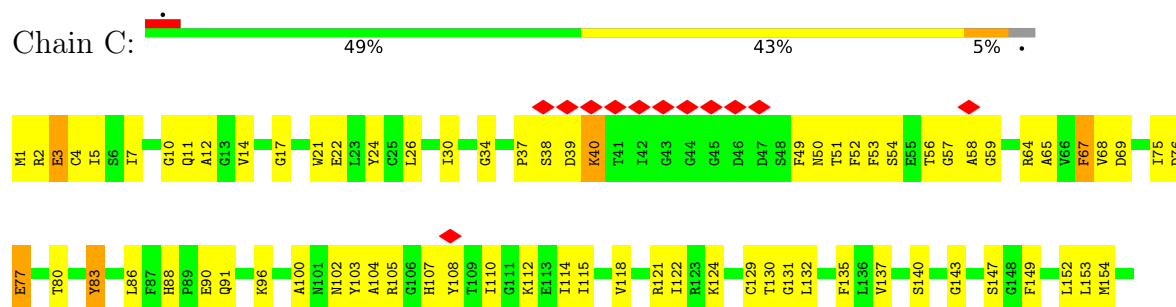
### 3 Residue-property plots

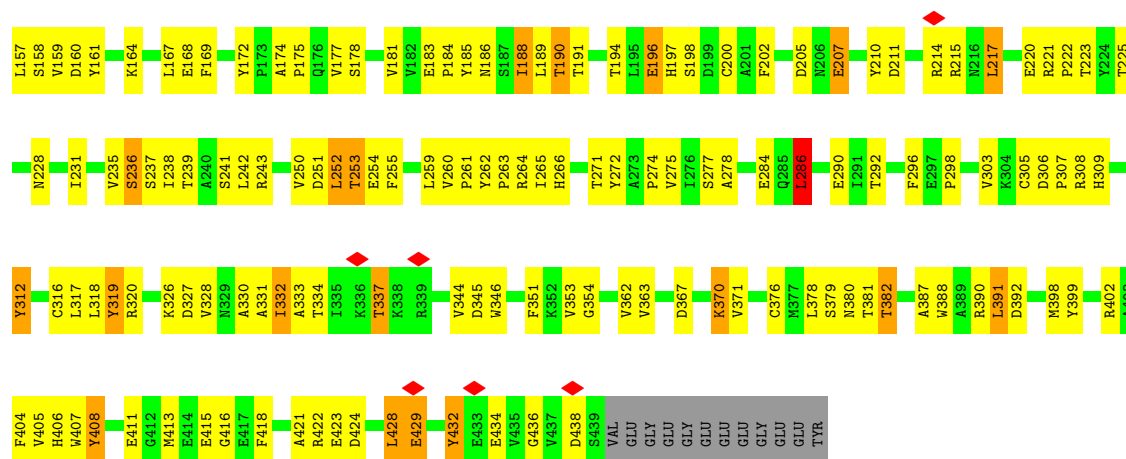
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tubulin alpha-1B chain

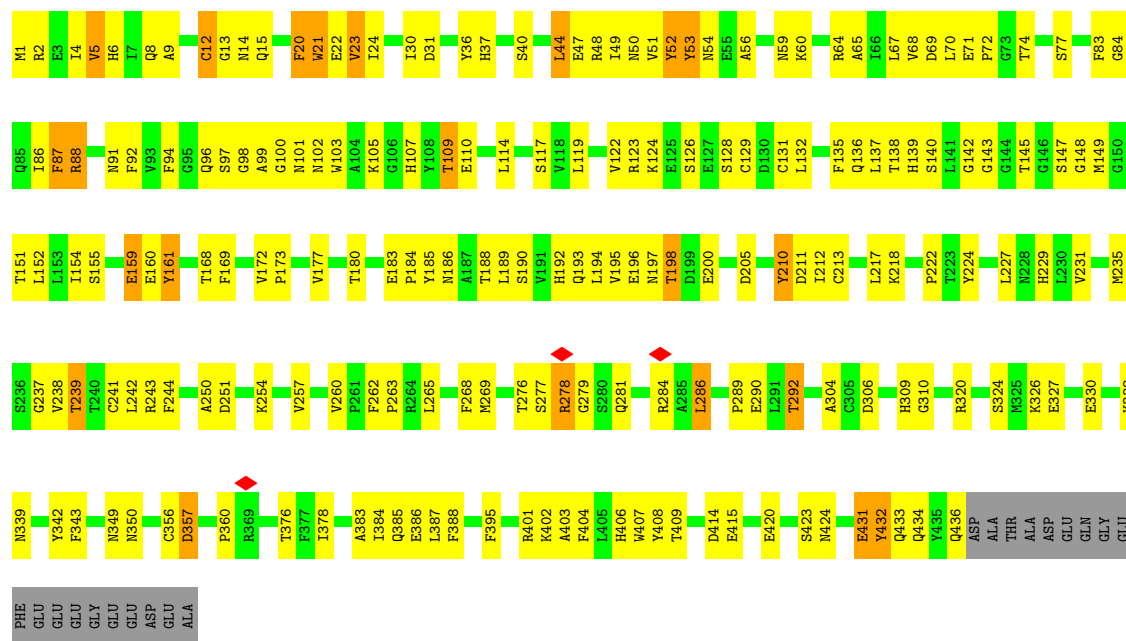


#### • Molecule 1: Tubulin alpha-1B chain

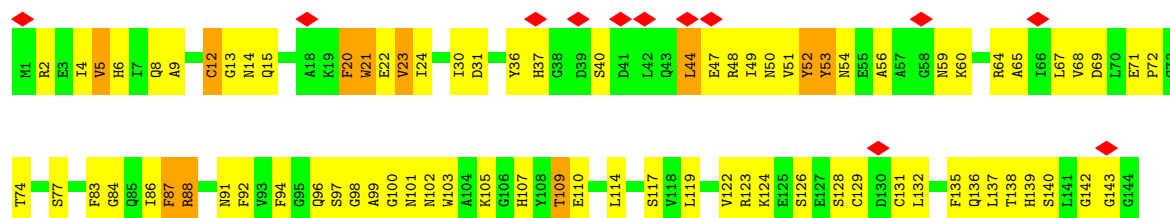


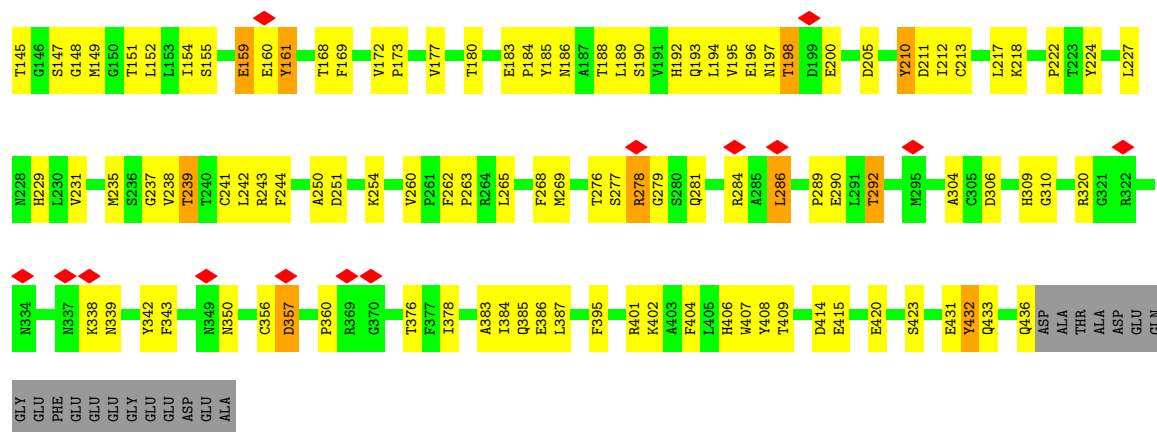


• Molecule 2: Tubulin beta chain

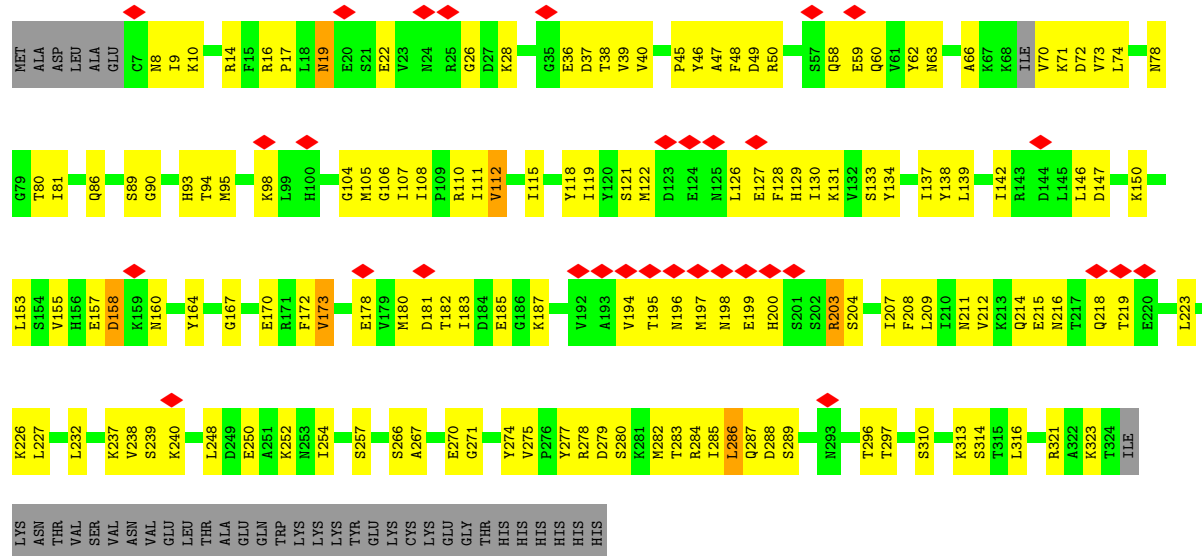


• Molecule 2: Tubulin beta chain





• Molecule 3: Kinesin-1 heavy chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74859	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.601	Depositor
Minimum map value	-3.109	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	1.34	24/3508 (0.7%)	0.84	4/4762 (0.1%)
1	C	1.34	24/3508 (0.7%)	0.84	4/4762 (0.1%)
2	B	1.26	23/3426 (0.7%)	0.78	0/4641
2	D	1.26	23/3426 (0.7%)	0.78	0/4641
3	K	0.92	0/2525	0.75	0/3401
All	All	1.25	94/16393 (0.6%)	0.80	8/22207 (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	C	0	1
2	B	0	3
2	D	0	3
3	K	0	1
All	All	0	9

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	TYR	CE1-CZ	-7.47	1.28	1.38
1	C	319	TYR	CE1-CZ	-7.43	1.28	1.38
1	C	24	TYR	CE2-CZ	-7.42	1.28	1.38
1	A	24	TYR	CE2-CZ	-7.36	1.28	1.38
1	A	312	TYR	CE2-CZ	-7.19	1.29	1.38
1	C	312	TYR	CE2-CZ	-7.17	1.29	1.38
1	C	236	SER	CA-C	-6.99	1.34	1.52
1	A	236	SER	CA-C	-6.95	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	269	MET	C-N	-6.84	1.21	1.34
2	B	269	MET	C-N	-6.79	1.21	1.34
2	B	52	TYR	CD2-CE2	-6.47	1.29	1.39
2	D	52	TYR	CD2-CE2	-6.45	1.29	1.39
1	A	24	TYR	CG-CD1	-6.34	1.30	1.39
2	D	53	TYR	CE2-CZ	-6.32	1.30	1.38
2	B	53	TYR	CE2-CZ	-6.29	1.30	1.38
1	C	24	TYR	CG-CD1	-6.25	1.31	1.39
1	C	24	TYR	CD2-CE2	-6.24	1.29	1.39
1	A	24	TYR	CD2-CE2	-6.22	1.30	1.39
1	A	312	TYR	CD2-CE2	-6.21	1.30	1.39
2	D	21	TRP	CA-C	-6.21	1.36	1.52
2	B	21	TRP	CA-C	-6.19	1.36	1.52
1	C	312	TYR	CD2-CE2	-6.19	1.30	1.39
1	C	432	TYR	CE2-CZ	-6.16	1.30	1.38
1	A	432	TYR	CE2-CZ	-6.14	1.30	1.38
1	C	408	TYR	CE1-CZ	-6.12	1.30	1.38
2	B	52	TYR	CD1-CE1	-6.07	1.30	1.39
1	A	319	TYR	CD1-CE1	-6.06	1.30	1.39
2	D	52	TYR	CD1-CE1	-6.05	1.30	1.39
1	C	319	TYR	CD1-CE1	-6.04	1.30	1.39
1	A	408	TYR	CE1-CZ	-6.04	1.30	1.38
1	A	161	TYR	CB-CG	-6.02	1.42	1.51
1	C	161	TYR	CB-CG	-6.01	1.42	1.51
2	D	161	TYR	CD1-CE1	-5.91	1.30	1.39
2	B	161	TYR	CD1-CE1	-5.86	1.30	1.39
2	D	408	TYR	CE2-CZ	-5.83	1.30	1.38
2	B	408	TYR	CE2-CZ	-5.78	1.31	1.38
2	B	408	TYR	CE1-CZ	-5.78	1.31	1.38
2	D	432	TYR	CD2-CE2	-5.75	1.30	1.39
2	B	432	TYR	CD2-CE2	-5.74	1.30	1.39
2	D	408	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	432	TYR	CB-CG	-5.72	1.43	1.51
2	B	185	TYR	CD2-CE2	-5.71	1.30	1.39
1	C	432	TYR	CB-CG	-5.69	1.43	1.51
2	D	5	VAL	CB-CG1	-5.67	1.41	1.52
1	A	161	TYR	CD1-CE1	-5.65	1.30	1.39
1	C	319	TYR	CD2-CE2	-5.65	1.30	1.39
2	D	432	TYR	CB-CG	-5.64	1.43	1.51
2	D	52	TYR	CE1-CZ	-5.64	1.31	1.38
1	C	161	TYR	CD1-CE1	-5.64	1.30	1.39
2	B	52	TYR	CE1-CZ	-5.63	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	432	TYR	CB-CG	-5.63	1.43	1.51
1	A	168	GLU	CB-CG	-5.63	1.41	1.52
1	C	168	GLU	CB-CG	-5.62	1.41	1.52
2	D	161	TYR	CD2-CE2	-5.61	1.30	1.39
2	B	5	VAL	CB-CG1	-5.60	1.41	1.52
2	D	224	TYR	CE2-CZ	-5.57	1.31	1.38
2	D	185	TYR	CD2-CE2	-5.56	1.31	1.39
2	B	161	TYR	CD2-CE2	-5.55	1.31	1.39
1	A	210	TYR	CD1-CE1	-5.54	1.31	1.39
1	A	319	TYR	CD2-CE2	-5.52	1.31	1.39
1	C	210	TYR	CD1-CE1	-5.52	1.31	1.39
2	B	224	TYR	CE2-CZ	-5.50	1.31	1.38
2	D	210	TYR	CD1-CE1	-5.49	1.31	1.39
2	D	432	TYR	CE2-CZ	-5.49	1.31	1.38
2	B	87	PHE	CD1-CE1	-5.48	1.28	1.39
2	D	87	PHE	CD1-CE1	-5.47	1.28	1.39
2	B	210	TYR	CD1-CE1	-5.47	1.31	1.39
1	C	408	TYR	CD1-CE1	-5.45	1.31	1.39
1	A	124	LYS	CA-C	-5.43	1.38	1.52
1	A	83	TYR	CD1-CE1	-5.40	1.31	1.39
1	C	124	LYS	CA-C	-5.40	1.39	1.52
1	A	408	TYR	CD1-CE1	-5.39	1.31	1.39
1	C	83	TYR	CD1-CE1	-5.37	1.31	1.39
2	B	432	TYR	CE2-CZ	-5.35	1.31	1.38
1	A	408	TYR	CE2-CZ	-5.30	1.31	1.38
1	C	399	TYR	CD2-CE2	-5.26	1.31	1.39
1	C	408	TYR	CE2-CZ	-5.26	1.31	1.38
1	C	432	TYR	CD1-CE1	-5.25	1.31	1.39
1	C	432	TYR	CD2-CE2	-5.25	1.31	1.39
1	A	399	TYR	CD2-CE2	-5.21	1.31	1.39
1	A	432	TYR	CD1-CE1	-5.20	1.31	1.39
1	A	432	TYR	CD2-CE2	-5.20	1.31	1.39
2	B	404	PHE	CB-CG	-5.20	1.42	1.51
2	B	210	TYR	CD2-CE2	-5.19	1.31	1.39
2	D	210	TYR	CD2-CE2	-5.17	1.31	1.39
2	D	404	PHE	CB-CG	-5.16	1.42	1.51
1	C	67	PHE	CE2-CZ	-5.16	1.27	1.37
2	B	200	GLU	CB-CG	-5.15	1.42	1.52
2	D	200	GLU	CB-CG	-5.14	1.42	1.52
2	B	224	TYR	CD2-CE2	-5.11	1.31	1.39
2	D	161	TYR	CE2-CZ	-5.09	1.31	1.38
1	A	67	PHE	CE2-CZ	-5.07	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	161	TYR	CE2-CZ	-5.04	1.31	1.38
2	D	224	TYR	CD2-CE2	-5.02	1.31	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	LEU	CA-CB-CG	-6.88	99.48	115.30
1	C	391	LEU	CA-CB-CG	-6.85	99.54	115.30
1	A	286	LEU	CA-CB-CG	6.21	129.59	115.30
1	C	286	LEU	CA-CB-CG	6.20	129.56	115.30
1	C	153	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	153	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	C	428	LEU	CB-CG-CD1	-5.32	101.97	111.00
1	A	428	LEU	CB-CG-CD1	-5.30	101.99	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	PRO	Peptide
2	B	278	ARG	Peptide
2	B	431	GLU	Peptide
2	B	88	ARG	Peptide
1	C	37	PRO	Peptide
2	D	278	ARG	Peptide
2	D	431	GLU	Peptide
2	D	88	ARG	Peptide
3	K	286	LEU	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	3430	0	3340	171	0
1	C	3430	0	3340	184	0
2	B	3351	0	3236	163	0
2	D	3351	0	3236	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2487	0	2455	131	0
4	A	32	0	12	7	0
4	B	32	0	12	1	0
4	C	32	0	12	7	0
4	D	32	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	16181	0	15655	768	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 24.

All (768) 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:K:150:LYS:NZ	3:K:167:GLY:O	2.01	0.94
1:A:292:THR:HG21	1:A:331:ALA:HB1	1.55	0.89
1:C:292:THR:HG21	1:C:331:ALA:HB1	1.54	0.89
3:K:71:LYS:NZ	3:K:72:ASP:OD1	2.04	0.89
1:C:237:SER:OG	1:C:320:ARG:NH2	2.06	0.88
1:A:237:SER:OG	1:A:320:ARG:NH2	2.06	0.88
3:K:105:MET:HB2	3:K:110:ARG:HH12	1.38	0.88
2:B:424:ASN:OD1	3:K:278:ARG:NH1	2.06	0.88
1:C:220:GLU:OE1	1:C:220:GLU:N	2.05	0.88
1:A:220:GLU:OE1	1:A:220:GLU:N	2.05	0.88
1:A:54:SER:OG	1:A:64:ARG:NH1	2.09	0.86
1:C:54:SER:OG	1:C:64:ARG:NH1	2.09	0.86
2:B:327:GLU:OE2	1:C:221:ARG:NH1	2.08	0.85
1:A:345:ASP:OD1	1:A:346:TRP:N	2.11	0.84
1:C:345:ASP:OD1	1:C:346:TRP:N	2.11	0.84
3:K:158:ASP:OD1	3:K:160:ASN:N	2.10	0.84
2:D:6:HIS:HD1	2:D:21:TRP:HZ2	1.25	0.83
2:B:6:HIS:HD1	2:B:21:TRP:HZ2	1.25	0.83
2:B:143:GLY:O	2:B:186:ASN:ND2	2.12	0.83
2:D:143:GLY:O	2:D:186:ASN:ND2	2.12	0.83
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.11	0.82
2:D:54:ASN:OD1	2:D:64:ARG:NH2	2.11	0.82
2:B:310:GLY:HA2	2:B:436:GLN:HE22	1.42	0.81
2:D:310:GLY:HA2	2:D:436:GLN:HE22	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:O	2:B:239:THR:OG1	1.94	0.81
2:D:239:THR:O	2:D:239:THR:OG1	1.94	0.80
2:D:356:CYS:SG	2:D:357:ASP:N	2.47	0.79
2:B:356:CYS:SG	2:B:357:ASP:N	2.47	0.79
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.19	0.78
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.19	0.78
2:B:88:ARG:O	2:B:91:ASN:ND2	2.18	0.77
2:D:88:ARG:O	2:D:91:ASN:ND2	2.18	0.76
2:B:142:GLY:O	2:B:186:ASN:ND2	2.17	0.76
2:D:142:GLY:O	2:D:186:ASN:ND2	2.17	0.76
2:B:414:ASP:OD1	2:B:415:GLU:N	2.19	0.75
3:K:22:GLU:O	3:K:26:GLY:N	2.19	0.75
1:C:429:GLU:OE1	1:C:429:GLU:HA	1.84	0.75
2:D:414:ASP:OD1	2:D:415:GLU:N	2.20	0.75
1:A:429:GLU:OE1	1:A:429:GLU:HA	1.85	0.75
1:A:326:LYS:HD3	2:B:222:PRO:HD2	1.68	0.74
3:K:105:MET:HB2	3:K:110:ARG:NH1	2.02	0.74
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.05	0.74
1:A:57:GLY:O	1:A:59:GLY:N	2.21	0.73
1:C:57:GLY:O	1:C:59:GLY:N	2.21	0.73
1:C:255:PHE:HZ	1:C:378:LEU:HD22	1.53	0.72
1:A:255:PHE:HZ	1:A:378:LEU:HD22	1.53	0.72
3:K:254:ILE:O	3:K:257:SER:OG	2.06	0.72
2:B:69:ASP:OD2	2:B:74:THR:OG1	2.05	0.72
1:C:132:LEU:HB3	1:C:164:LYS:HZ1	1.55	0.71
1:A:132:LEU:HB3	1:A:164:LYS:HZ1	1.55	0.71
1:A:217:LEU:HD21	1:A:367:ASP:HB2	1.72	0.71
1:C:217:LEU:HD21	1:C:367:ASP:HB2	1.72	0.71
1:C:402:ARG:NH1	1:C:415:GLU:OE1	2.23	0.71
3:K:10:LYS:HB2	3:K:297:THR:HG22	1.71	0.71
1:A:402:ARG:NH1	1:A:415:GLU:OE1	2.23	0.71
1:C:190:THR:O	1:C:190:THR:OG1	2.08	0.71
1:A:132:LEU:O	1:A:164:LYS:NZ	2.24	0.71
1:A:190:THR:O	1:A:190:THR:OG1	2.08	0.71
1:C:132:LEU:O	1:C:164:LYS:NZ	2.24	0.70
3:K:197:MET:HG3	3:K:198:ASN:H	1.56	0.70
3:K:62:TYR:HD1	3:K:66:ALA:HB3	1.56	0.70
3:K:78:ASN:ND2	3:K:226:LYS:H	1.88	0.70
2:B:257:VAL:HG23	1:C:407:TRP:CD1	2.27	0.70
1:A:236:SER:O	1:A:236:SER:OG	2.01	0.69
1:A:108:TYR:HB3	1:A:112:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:HB3	1:C:112:LYS:NZ	2.07	0.69
1:A:185:TYR:OH	1:A:398:MET:O	2.11	0.69
2:D:250:ALA:HA	2:D:254:LYS:HG3	1.73	0.69
1:C:185:TYR:OH	1:C:398:MET:O	2.11	0.69
1:A:241:SER:OG	1:A:250:VAL:O	2.04	0.69
2:B:250:ALA:HA	2:B:254:LYS:HG3	1.73	0.69
1:C:241:SER:OG	1:C:250:VAL:O	2.05	0.69
2:D:196:GLU:O	2:D:197:ASN:ND2	2.25	0.69
2:B:196:GLU:O	2:B:197:ASN:ND2	2.25	0.69
1:C:108:TYR:OH	3:K:239:SER:HB3	1.93	0.69
3:K:14:ARG:NH2	3:K:58:GLN:OE1	2.25	0.69
2:B:52:TYR:OH	2:B:136:GLN:NE2	2.27	0.68
2:D:52:TYR:OH	2:D:136:GLN:NE2	2.27	0.68
3:K:131:LYS:HE2	3:K:170:GLU:HB3	1.74	0.68
2:B:137:LEU:HD23	2:B:154:ILE:HD12	1.75	0.68
2:D:137:LEU:HD23	2:D:154:ILE:HD12	1.75	0.68
2:D:262:PHE:HB3	2:D:263:PRO:HD2	1.74	0.68
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.74	0.68
3:K:181:ASP:O	3:K:185:GLU:HG2	1.92	0.68
3:K:214:GLN:HE21	3:K:223:LEU:HB2	1.59	0.68
3:K:279:ASP:OD1	3:K:279:ASP:N	2.27	0.67
3:K:286:LEU:O	3:K:288:ASP:N	2.28	0.67
2:B:5:VAL:HG23	2:B:64:ARG:HG2	1.76	0.67
2:D:5:VAL:HG23	2:D:64:ARG:HG2	1.77	0.66
1:C:143:GLY:O	1:C:186:ASN:ND2	2.29	0.66
1:A:143:GLY:O	1:A:186:ASN:ND2	2.29	0.66
1:A:306:ASP:OD2	1:A:309:HIS:ND1	2.29	0.66
1:C:306:ASP:OD2	1:C:309:HIS:ND1	2.29	0.66
2:D:123:ARG:NH2	2:D:160:GLU:OE2	2.24	0.65
2:B:306:ASP:OD1	2:B:309:HIS:ND1	2.30	0.65
2:D:306:ASP:OD1	2:D:309:HIS:ND1	2.30	0.65
2:B:123:ARG:NH2	2:B:160:GLU:OE2	2.24	0.65
1:A:3:GLU:OE1	1:A:64:ARG:NH2	2.29	0.65
1:C:3:GLU:OE1	1:C:64:ARG:NH2	2.29	0.65
1:A:406:HIS:HE1	1:A:407:TRP:CE2	2.16	0.64
1:A:103:TYR:H	1:A:408:TYR:HE1	1.45	0.64
1:C:406:HIS:HE1	1:C:407:TRP:CE2	2.16	0.64
3:K:194:VAL:HA	3:K:200:HIS:HB3	1.80	0.64
1:A:3:GLU:HA	1:A:51:THR:HG23	1.80	0.64
1:C:103:TYR:H	1:C:408:TYR:HE1	1.45	0.64
1:C:3:GLU:HA	1:C:51:THR:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:266:SER:OG	3:K:267:ALA:N	2.30	0.63
1:A:367:ASP:OD1	1:A:367:ASP:N	2.30	0.63
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.16	0.63
1:A:251:ASP:O	1:A:254:GLU:N	2.30	0.63
1:C:251:ASP:O	1:C:254:GLU:N	2.30	0.63
3:K:239:SER:OG	3:K:240:LYS:N	2.31	0.63
1:C:367:ASP:OD1	1:C:367:ASP:N	2.30	0.63
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.16	0.63
1:A:143:GLY:HA3	4:A:501:GTP:O3A	1.98	0.63
1:C:143:GLY:HA3	4:C:501:GTP:O3A	1.98	0.63
3:K:133:SER:OG	3:K:209:LEU:HB2	1.98	0.63
1:A:132:LEU:HB3	1:A:164:LYS:NZ	2.12	0.63
1:C:132:LEU:HB3	1:C:164:LYS:NZ	2.12	0.63
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.33	0.63
1:C:169:PHE:CE2	1:C:235:VAL:HG22	2.33	0.62
1:C:326:LYS:HD3	2:D:222:PRO:HD2	1.80	0.62
3:K:138:TYR:CE1	3:K:139:LEU:HD13	2.35	0.62
2:B:12:CYS:CB	2:B:140:SER:HB2	2.30	0.62
2:B:434:GLN:HE21	3:K:274:TYR:HB3	1.64	0.62
1:A:69:ASP:N	1:A:69:ASP:OD1	2.29	0.62
2:D:12:CYS:CB	2:D:140:SER:HB2	2.30	0.62
3:K:121:SER:O	3:K:121:SER:OG	2.16	0.62
3:K:119:ILE:HD11	3:K:128:PHE:HB2	1.82	0.62
1:C:69:ASP:OD1	1:C:69:ASP:N	2.29	0.61
2:D:172:VAL:HG11	2:D:387:LEU:HD21	1.81	0.61
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.81	0.61
3:K:280:SER:O	3:K:283:THR:HG22	2.00	0.61
1:A:115:ILE:HG21	1:A:152:LEU:HD23	1.82	0.61
2:B:183:GLU:HB2	2:B:184:PRO:HD3	1.82	0.61
2:D:183:GLU:HB2	2:D:184:PRO:HD3	1.82	0.61
1:C:68:VAL:HG11	1:C:149:PHE:CZ	2.36	0.61
1:C:115:ILE:HG21	1:C:152:LEU:HD23	1.82	0.61
3:K:107:ILE:O	3:K:111:ILE:HG13	2.01	0.61
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.36	0.61
3:K:214:GLN:HE21	3:K:223:LEU:HD23	1.64	0.61
3:K:115:ILE:HD11	3:K:212:VAL:HG11	1.83	0.60
1:A:392:ASP:OD1	1:A:422:ARG:NH1	2.33	0.60
2:B:406:HIS:CE1	2:B:407:TRP:CE2	2.89	0.60
1:C:392:ASP:OD1	1:C:422:ARG:NH1	2.33	0.60
2:D:406:HIS:CE1	2:D:407:TRP:CE2	2.89	0.60
3:K:129:HIS:ND1	3:K:172:PHE:HE2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:THR:O	2:D:149:MET:HB3	2.01	0.59
2:B:145:THR:O	2:B:149:MET:HB3	2.01	0.59
3:K:214:GLN:NE2	3:K:223:LEU:HB2	2.17	0.59
2:D:30:ILE:HG13	2:D:53:TYR:CE2	2.38	0.59
1:A:105:ARG:HG3	1:A:411:GLU:HG3	1.83	0.59
2:B:1:MET:CE	1:C:96:LYS:HD3	2.32	0.59
2:B:30:ILE:HG13	2:B:53:TYR:CE2	2.38	0.59
1:A:12:ALA:HB3	1:A:140:SER:OG	2.03	0.59
1:C:12:ALA:HB3	1:C:140:SER:OG	2.03	0.59
3:K:310:SER:HA	3:K:313:LYS:HD2	1.84	0.59
1:C:105:ARG:HG3	1:C:411:GLU:HG3	1.83	0.59
2:D:5:VAL:HG22	2:D:6:HIS:H	1.67	0.59
3:K:73:VAL:HG21	3:K:227:LEU:HD13	1.84	0.59
3:K:128:PHE:CE2	3:K:214:GLN:HB3	2.38	0.59
2:B:385:GLN:NE2	2:B:433:GLN:OE1	2.36	0.58
2:D:385:GLN:NE2	2:D:433:GLN:OE1	2.36	0.58
3:K:62:TYR:CD1	3:K:66:ALA:HB3	2.36	0.58
2:B:5:VAL:HG22	2:B:6:HIS:H	1.67	0.58
2:D:137:LEU:HG	2:D:139:HIS:HD2	1.68	0.58
2:B:137:LEU:HG	2:B:139:HIS:HD2	1.68	0.58
3:K:207:ILE:HD11	3:K:282:MET:HG2	1.85	0.58
1:C:380:ASN:OD1	1:C:381:THR:N	2.37	0.58
1:A:380:ASN:OD1	1:A:381:THR:N	2.37	0.57
2:D:9:ALA:HA	2:D:68:VAL:O	2.04	0.57
1:A:334:THR:O	1:A:337:THR:HG23	2.05	0.57
2:B:9:ALA:HA	2:B:68:VAL:O	2.05	0.57
1:C:108:TYR:HB3	1:C:112:LYS:CE	2.34	0.57
1:C:334:THR:O	1:C:337:THR:HG23	2.05	0.57
2:D:231:VAL:O	2:D:235:MET:HG3	2.04	0.57
3:K:203:ARG:HB3	3:K:250:GLU:OE1	2.04	0.57
1:A:298:PRO:HG3	1:A:308:ARG:NE	2.19	0.57
2:B:231:VAL:O	2:B:235:MET:HG3	2.04	0.57
1:A:108:TYR:HB3	1:A:112:LYS:CE	2.34	0.57
1:C:298:PRO:HG3	1:C:308:ARG:NE	2.19	0.57
3:K:216:ASN:OD1	3:K:219:THR:HG22	2.04	0.57
1:A:251:ASP:O	1:A:253:THR:N	2.37	0.57
1:C:143:GLY:H	4:C:501:GTP:H5'	1.70	0.57
1:A:143:GLY:H	4:A:501:GTP:H5'	1.70	0.57
1:A:250:VAL:HG11	1:A:318:LEU:HD22	1.87	0.57
1:C:250:VAL:HG11	1:C:318:LEU:HD22	1.87	0.57
1:C:251:ASP:O	1:C:253:THR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASP:OD1	1:C:306:ASP:N	2.27	0.57
2:B:169:PHE:CD2	2:B:235:MET:HG2	2.39	0.57
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.39	0.57
3:K:142:ILE:HD13	3:K:285:ILE:HD11	1.86	0.57
1:C:211:ASP:HA	1:C:214:ARG:HG2	1.86	0.57
1:A:211:ASP:HA	1:A:214:ARG:HG2	1.86	0.56
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.40	0.56
1:A:306:ASP:OD1	1:A:306:ASP:N	2.27	0.56
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.40	0.56
2:D:67:LEU:HD12	2:D:92:PHE:CE1	2.39	0.56
2:B:67:LEU:HD12	2:B:92:PHE:CE1	2.39	0.56
2:B:262:PHE:HB3	2:B:263:PRO:CD	2.35	0.56
2:D:109:THR:OG1	2:D:110:GLU:N	2.36	0.56
2:D:262:PHE:HB3	2:D:263:PRO:CD	2.35	0.56
3:K:106:GLY:O	3:K:110:ARG:HD2	2.05	0.56
3:K:158:ASP:CG	3:K:160:ASN:H	2.05	0.56
3:K:238:VAL:HG12	3:K:238:VAL:O	2.06	0.56
2:B:109:THR:OG1	2:B:110:GLU:N	2.36	0.56
3:K:112:VAL:O	3:K:115:ILE:HG22	2.04	0.56
3:K:9:ILE:HG23	3:K:296:THR:HG23	1.87	0.56
3:K:47:ALA:O	3:K:48:PHE:HD1	1.88	0.56
3:K:155:VAL:HG23	3:K:164:TYR:O	2.05	0.56
1:A:88:HIS:O	1:A:90:GLU:N	2.39	0.56
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.88	0.56
1:C:2:ARG:HA	1:C:2:ARG:NE	2.20	0.56
1:C:88:HIS:O	1:C:90:GLU:N	2.39	0.56
1:C:392:ASP:HB3	1:C:422:ARG:HH22	1.71	0.56
1:A:2:ARG:HA	1:A:2:ARG:NE	2.20	0.56
1:C:381:THR:OG1	1:C:382:THR:N	2.37	0.56
1:A:392:ASP:HB3	1:A:422:ARG:HH22	1.71	0.56
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.88	0.56
1:A:381:THR:OG1	1:A:382:THR:N	2.37	0.55
2:B:97:SER:OG	2:B:97:SER:O	2.22	0.55
2:B:284:ARG:NH2	2:B:286:LEU:HD21	2.21	0.55
2:D:97:SER:O	2:D:97:SER:OG	2.22	0.55
2:B:107:HIS:HD2	2:B:152:LEU:HB2	1.70	0.55
2:D:139:HIS:O	2:D:139:HIS:ND1	2.39	0.55
1:A:103:TYR:HE1	1:A:147:SER:O	1.89	0.55
2:B:139:HIS:O	2:B:139:HIS:ND1	2.39	0.55
2:D:284:ARG:NH2	2:D:286:LEU:HD21	2.21	0.55
2:B:180:THR:OG1	2:B:183:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:TYR:HE1	1:C:147:SER:O	1.88	0.55
2:D:107:HIS:HD2	2:D:152:LEU:HB2	1.70	0.55
2:D:180:THR:OG1	2:D:183:GLU:HG3	2.07	0.55
3:K:197:MET:HB3	3:K:199:GLU:OE2	2.07	0.55
3:K:108:ILE:HA	3:K:111:ILE:HD12	1.89	0.54
1:C:265:ILE:HG23	1:C:432:TYR:CE1	2.42	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.42	0.54
1:C:236:SER:O	1:C:236:SER:OG	2.01	0.54
1:C:132:LEU:HD23	1:C:164:LYS:HE3	1.90	0.53
1:A:132:LEU:HD23	1:A:164:LYS:HE3	1.90	0.53
1:A:197:HIS:O	1:A:198:SER:OG	2.19	0.53
2:D:105:LYS:HA	2:D:109:THR:HG23	1.89	0.53
2:B:105:LYS:HA	2:B:109:THR:HG23	1.89	0.53
1:C:49:PHE:O	1:C:51:THR:N	2.41	0.53
1:A:303:VAL:O	1:A:305:CYS:N	2.41	0.53
1:C:303:VAL:O	1:C:305:CYS:N	2.41	0.53
1:A:49:PHE:O	1:A:51:THR:N	2.41	0.53
1:A:188:ILE:O	1:A:421:ALA:HB1	2.08	0.53
1:A:316:CYS:SG	1:A:318:LEU:HD21	2.49	0.53
2:B:147:SER:OG	2:B:190:SER:HB2	2.08	0.53
1:C:188:ILE:O	1:C:421:ALA:HB1	2.08	0.53
1:C:197:HIS:O	1:C:198:SER:OG	2.19	0.53
1:C:316:CYS:SG	1:C:318:LEU:HD21	2.49	0.53
2:D:147:SER:OG	2:D:190:SER:HB2	2.08	0.53
2:D:277:SER:O	2:D:279:GLY:N	2.42	0.53
2:B:1:MET:HE1	1:C:96:LYS:HD3	1.90	0.53
2:B:277:SER:O	2:B:279:GLY:N	2.42	0.53
1:C:100:ALA:O	1:C:102:ASN:N	2.42	0.53
1:A:100:ALA:O	1:A:102:ASN:N	2.42	0.53
2:B:20:PHE:HE1	2:B:24:ILE:HG13	1.74	0.52
2:D:20:PHE:HE1	2:D:24:ILE:HG13	1.74	0.52
2:B:6:HIS:CE1	2:B:21:TRP:NE1	2.78	0.52
2:D:6:HIS:CE1	2:D:21:TRP:NE1	2.78	0.52
2:D:94:PHE:HD1	2:D:94:PHE:O	1.93	0.52
1:A:40:LYS:HD3	1:A:40:LYS:N	2.24	0.52
1:C:40:LYS:HD3	1:C:40:LYS:N	2.24	0.52
3:K:195:THR:OG1	3:K:196:ASN:N	2.42	0.52
2:B:94:PHE:HD1	2:B:94:PHE:O	1.93	0.52
2:B:151:THR:HG21	2:B:193:GLN:HE21	1.73	0.52
1:C:1:MET:SD	1:C:1:MET:N	2.62	0.52
3:K:138:TYR:CD1	3:K:139:LEU:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:ASN:CG	1:C:178:SER:HB3	2.30	0.52
1:C:112:LYS:HZ1	3:K:238:VAL:HG12	1.75	0.52
2:D:151:THR:HG21	2:D:193:GLN:HE21	1.74	0.52
3:K:40:VAL:HG22	3:K:45:PRO:HA	1.92	0.52
1:A:1:MET:SD	1:A:1:MET:N	2.62	0.52
1:A:172:TYR:HB3	1:A:205:ASP:OD1	2.10	0.52
2:B:159:GLU:OE2	2:B:159:GLU:HA	2.01	0.52
1:C:250:VAL:HA	1:C:254:GLU:OE2	2.10	0.52
1:C:277:SER:OG	1:C:278:ALA:N	2.36	0.52
3:K:178:GLU:O	3:K:182:THR:HG23	2.10	0.52
1:A:22:GLU:HG3	1:A:83:TYR:OH	2.10	0.51
1:A:250:VAL:HA	1:A:254:GLU:OE2	2.10	0.51
1:C:22:GLU:HG3	1:C:83:TYR:OH	2.11	0.51
1:C:172:TYR:HB3	1:C:205:ASP:OD1	2.10	0.51
2:D:159:GLU:OE2	2:D:159:GLU:HA	2.01	0.51
1:A:277:SER:OG	1:A:278:ALA:N	2.36	0.51
2:B:289:PRO:HA	2:B:292:THR:HG23	1.92	0.51
1:A:104:ALA:HB2	1:A:413:MET:SD	2.51	0.51
2:B:431:GLU:OE2	3:K:274:TYR:CD2	2.63	0.51
2:D:289:PRO:HA	2:D:292:THR:HG23	1.92	0.51
1:A:5:ILE:HB	1:A:135:PHE:CE1	2.45	0.51
2:B:434:GLN:NE2	3:K:274:TYR:O	2.35	0.51
1:C:5:ILE:HB	1:C:135:PHE:CE1	2.45	0.51
3:K:37:ASP:OD1	3:K:38:THR:N	2.44	0.51
3:K:130:ILE:HB	3:K:173:VAL:O	2.11	0.51
3:K:215:GLU:OE1	3:K:215:GLU:N	2.42	0.51
1:A:296:PHE:CE2	1:A:312:TYR:HE2	2.28	0.51
2:B:1:MET:HE1	1:C:96:LYS:HA	1.93	0.51
1:C:1:MET:N	1:C:242:LEU:O	2.43	0.51
1:C:104:ALA:HB2	1:C:413:MET:SD	2.51	0.51
2:B:406:HIS:HE1	2:B:407:TRP:CE2	2.28	0.51
1:C:296:PHE:CE2	1:C:312:TYR:HE2	2.28	0.51
2:D:406:HIS:HE1	2:D:407:TRP:CE2	2.28	0.51
1:A:1:MET:N	1:A:242:LEU:O	2.43	0.51
2:B:5:VAL:HG11	2:B:135:PHE:CD1	2.45	0.51
3:K:194:VAL:HG22	3:K:200:HIS:CD2	2.45	0.51
1:A:110:ILE:O	1:A:110:ILE:HG22	2.11	0.51
2:B:238:VAL:HG22	2:B:378:ILE:HD11	1.92	0.51
2:D:5:VAL:HG11	2:D:135:PHE:CD1	2.45	0.51
2:D:238:VAL:HG22	2:D:378:ILE:HD11	1.92	0.51
3:K:134:TYR:CE1	3:K:208:PHE:HD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:THR:O	1:C:239:THR:OG1	2.22	0.50
2:B:138:THR:O	2:B:138:THR:OG1	2.28	0.50
1:A:239:THR:O	1:A:239:THR:OG1	2.22	0.50
1:C:110:ILE:HG22	1:C:110:ILE:O	2.12	0.50
2:D:265:LEU:HD22	2:D:432:TYR:CZ	2.47	0.50
1:A:265:ILE:HD12	1:A:432:TYR:CE1	2.46	0.50
2:D:138:THR:O	2:D:138:THR:OG1	2.28	0.50
2:B:12:CYS:O	2:B:15:GLN:N	2.44	0.50
2:B:184:PRO:O	2:B:395:PHE:HD2	1.94	0.50
2:B:265:LEU:HD22	2:B:432:TYR:CZ	2.47	0.50
1:C:167:LEU:HD22	1:C:200:CYS:HB2	1.93	0.50
1:C:254:GLU:HG2	2:D:100:GLY:HA2	1.92	0.50
1:C:265:ILE:HD12	1:C:432:TYR:CE1	2.46	0.50
2:D:30:ILE:HG13	2:D:53:TYR:HE2	1.77	0.50
2:D:184:PRO:O	2:D:395:PHE:HD2	1.94	0.50
3:K:286:LEU:HB3	3:K:289:SER:OG	2.12	0.50
3:K:314:SER:O	3:K:316:LEU:N	2.45	0.50
1:A:167:LEU:HD22	1:A:200:CYS:HB2	1.93	0.50
2:B:30:ILE:HG13	2:B:53:TYR:HE2	1.77	0.50
2:B:36:TYR:CE2	2:B:44:LEU:HD13	2.47	0.50
2:D:12:CYS:O	2:D:15:GLN:N	2.44	0.50
3:K:78:ASN:HD22	3:K:226:LYS:H	1.55	0.50
1:A:107:HIS:HB3	1:A:108:TYR:CD1	2.47	0.50
1:C:103:TYR:CD2	1:C:189:LEU:HD13	2.47	0.50
1:C:107:HIS:HB3	1:C:108:TYR:CD1	2.47	0.50
1:C:77:GLU:OE2	1:C:77:GLU:HA	2.12	0.50
2:D:36:TYR:CE2	2:D:44:LEU:HD13	2.47	0.50
1:A:77:GLU:OE2	1:A:77:GLU:HA	2.12	0.49
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.47	0.49
1:C:317:LEU:HB3	1:C:319:TYR:CE1	2.47	0.49
1:A:11:GLN:HG2	4:A:501:GTP:O1A	2.12	0.49
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.95	0.49
3:K:280:SER:O	3:K:282:MET:N	2.45	0.49
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.47	0.49
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.95	0.49
1:C:11:GLN:HG2	4:C:501:GTP:O1A	2.12	0.49
1:A:332:ILE:HD13	1:A:351:PHE:CD2	2.48	0.49
1:C:332:ILE:HD13	1:C:351:PHE:CD2	2.48	0.49
3:K:81:ILE:HG22	3:K:297:THR:OG1	2.12	0.49
1:A:388:TRP:CZ3	1:A:428:LEU:HD23	2.47	0.49
3:K:94:THR:HG23	3:K:95:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:HE2	1:A:312:TYR:HE2	1.60	0.49
2:B:192:HIS:CG	2:B:192:HIS:O	2.65	0.49
1:C:296:PHE:HE2	1:C:312:TYR:HE2	1.60	0.49
2:D:192:HIS:CG	2:D:192:HIS:O	2.65	0.49
3:K:321:ARG:O	3:K:323:LYS:N	2.46	0.49
1:A:108:TYR:HB3	1:A:112:LYS:HE3	1.95	0.49
1:A:225:THR:O	1:A:225:THR:OG1	2.18	0.49
1:C:108:TYR:HB3	1:C:112:LYS:HE3	1.95	0.49
1:C:225:THR:O	1:C:225:THR:OG1	2.18	0.49
1:C:388:TRP:CZ3	1:C:428:LEU:HD23	2.47	0.49
3:K:134:TYR:CD1	3:K:208:PHE:HD2	2.31	0.49
2:B:177:VAL:HG12	2:B:177:VAL:O	2.12	0.49
3:K:98:LYS:HB3	3:K:104:GLY:O	2.12	0.49
2:D:177:VAL:HG12	2:D:177:VAL:O	2.12	0.49
3:K:59:GLU:CD	3:K:110:ARG:HH21	2.15	0.49
3:K:72:ASP:OD1	3:K:72:ASP:N	2.44	0.49
3:K:127:GLU:HB3	3:K:215:GLU:OE2	2.13	0.49
3:K:8:ASN:OD1	3:K:9:ILE:N	2.42	0.48
3:K:214:GLN:CG	3:K:223:LEU:HB2	2.43	0.48
1:C:68:VAL:HG11	1:C:149:PHE:CE2	2.48	0.48
3:K:130:ILE:HG22	3:K:173:VAL:HG23	1.95	0.48
2:D:107:HIS:CD2	2:D:152:LEU:HB2	2.48	0.48
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.48	0.48
2:B:107:HIS:CD2	2:B:152:LEU:HB2	2.48	0.48
3:K:28:LYS:H	3:K:28:LYS:HD2	1.77	0.48
3:K:59:GLU:OE2	3:K:110:ARG:NH2	2.45	0.48
3:K:80:THR:O	3:K:296:THR:HA	2.12	0.48
1:C:239:THR:O	1:C:243:ARG:NE	2.44	0.48
3:K:237:LYS:HG2	3:K:238:VAL:H	1.77	0.48
1:A:153:LEU:HA	1:A:153:LEU:HD12	1.55	0.48
1:A:239:THR:O	1:A:243:ARG:NE	2.44	0.48
2:B:36:TYR:O	2:B:37:HIS:ND1	2.47	0.48
2:D:36:TYR:O	2:D:37:HIS:ND1	2.47	0.48
2:B:67:LEU:HD12	2:B:92:PHE:HE1	1.78	0.48
2:B:74:THR:O	2:B:77:SER:OG	2.26	0.48
1:C:271:THR:HG22	1:C:272:TYR:N	2.29	0.48
3:K:180:MET:SD	3:K:183:ILE:HD12	2.54	0.48
1:A:271:THR:HG22	1:A:272:TYR:N	2.29	0.48
2:D:67:LEU:HD12	2:D:92:PHE:HE1	1.78	0.48
2:D:74:THR:O	2:D:77:SER:OG	2.26	0.48
3:K:250:GLU:O	3:K:254:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:310:SER:HA	3:K:313:LYS:CD	2.43	0.48
3:K:60:GLN:HA	3:K:63:ASN:HB3	1.95	0.47
3:K:131:LYS:HE2	3:K:170:GLU:CB	2.41	0.47
3:K:275:VAL:HB	3:K:277:TYR:CE2	2.49	0.47
1:A:53:PHE:O	1:A:64:ARG:NE	2.43	0.47
1:A:143:GLY:N	4:A:501:GTP:H5'	2.29	0.47
1:A:316:CYS:C	1:A:317:LEU:HD12	2.35	0.47
2:B:237:GLY:O	2:B:239:THR:N	2.48	0.47
1:C:316:CYS:C	1:C:317:LEU:HD12	2.35	0.47
1:A:183:GLU:CB	1:A:184:PRO:HD3	2.44	0.47
1:C:143:GLY:N	4:C:501:GTP:H5'	2.29	0.47
2:D:52:TYR:O	2:D:53:TYR:HD1	1.97	0.47
2:D:237:GLY:O	2:D:239:THR:N	2.48	0.47
2:B:52:TYR:O	2:B:53:TYR:HD1	1.97	0.47
1:C:38:SER:OG	1:C:39:ASP:N	2.48	0.47
1:C:416:GLY:O	1:C:418:PHE:N	2.47	0.47
3:K:270:GLU:OE1	3:K:271:GLY:N	2.47	0.47
1:A:38:SER:OG	1:A:39:ASP:N	2.48	0.47
1:A:379:SER:O	1:A:379:SER:OG	2.30	0.47
1:C:53:PHE:O	1:C:64:ARG:NE	2.43	0.47
1:C:183:GLU:CB	1:C:184:PRO:HD3	2.45	0.47
1:C:379:SER:O	1:C:379:SER:OG	2.30	0.47
3:K:70:VAL:HG21	3:K:111:ILE:HG23	1.96	0.47
1:A:88:HIS:CE1	1:A:121:ARG:HH22	2.33	0.47
1:A:416:GLY:O	1:A:418:PHE:N	2.47	0.47
2:B:1:MET:HE3	1:C:96:LYS:HD3	1.96	0.47
2:B:326:LYS:HG2	1:C:222:PRO:HD2	1.96	0.47
1:C:88:HIS:CE1	1:C:121:ARG:HH22	2.33	0.47
1:A:80:THR:O	1:A:80:THR:OG1	2.33	0.47
1:A:260:VAL:HG13	1:A:266:HIS:HB3	1.97	0.47
2:B:5:VAL:HG11	2:B:135:PHE:HD1	1.80	0.47
1:A:2:ARG:HA	1:A:2:ARG:HE	1.80	0.47
1:C:2:ARG:HA	1:C:2:ARG:HE	1.80	0.47
1:C:260:VAL:HG13	1:C:266:HIS:HB3	1.97	0.47
2:D:5:VAL:HG11	2:D:135:PHE:HD1	1.80	0.47
3:K:183:ILE:HG12	3:K:208:PHE:CE2	2.50	0.47
2:B:257:VAL:HG23	1:C:407:TRP:CG	2.50	0.47
2:B:260:VAL:HG23	2:B:260:VAL:O	2.15	0.47
1:C:108:TYR:HB3	1:C:112:LYS:HZ1	1.75	0.47
3:K:137:ILE:HD11	3:K:207:ILE:HD11	1.95	0.47
2:B:251:ASP:OD1	2:B:254:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD12	1:C:259:LEU:HA	1.64	0.47
2:D:260:VAL:HG23	2:D:260:VAL:O	2.15	0.47
1:A:68:VAL:HG21	1:A:118:VAL:HG21	1.97	0.46
2:B:100:GLY:O	2:B:102:ASN:N	2.48	0.46
2:B:431:GLU:OE2	3:K:274:TYR:HD2	1.98	0.46
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.97	0.46
1:C:317:LEU:HB3	1:C:319:TYR:HE1	1.80	0.46
1:A:143:GLY:HA3	4:A:501:GTP:PB	2.55	0.46
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.80	0.46
1:C:10:GLY:O	1:C:14:VAL:HG23	2.15	0.46
1:A:10:GLY:O	1:A:14:VAL:HG23	2.15	0.46
2:B:217:LEU:HD12	2:B:277:SER:HA	1.97	0.46
1:C:143:GLY:HA3	4:C:501:GTP:PB	2.55	0.46
1:C:174:ALA:HB1	1:C:207:GLU:OE1	2.16	0.46
1:C:326:LYS:HG3	1:C:327:ASP:N	2.29	0.46
2:D:100:GLY:O	2:D:102:ASN:N	2.48	0.46
2:D:251:ASP:OD1	2:D:254:LYS:N	2.30	0.46
1:A:174:ALA:HB1	1:A:207:GLU:OE1	2.16	0.46
1:A:326:LYS:HG3	1:A:327:ASP:N	2.29	0.46
2:B:49:ILE:O	2:B:53:TYR:HB2	2.15	0.46
2:B:87:PHE:HD1	2:B:87:PHE:H	1.64	0.46
2:B:94:PHE:O	2:B:94:PHE:CD1	2.68	0.46
2:D:49:ILE:O	2:D:53:TYR:HB2	2.15	0.46
2:D:87:PHE:HD1	2:D:87:PHE:H	1.64	0.46
2:D:217:LEU:HD12	2:D:277:SER:HA	1.97	0.46
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.97	0.46
1:C:392:ASP:CB	1:C:422:ARG:HH22	2.28	0.46
2:D:94:PHE:O	2:D:94:PHE:CD1	2.68	0.46
3:K:153:LEU:HA	3:K:153:LEU:HD23	1.64	0.46
1:A:392:ASP:CB	1:A:422:ARG:HH22	2.28	0.46
3:K:10:LYS:HA	3:K:10:LYS:HD3	1.80	0.46
1:A:11:GLN:HG3	1:A:12:ALA:N	2.30	0.46
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.98	0.46
2:D:243:ARG:O	2:D:244:PHE:CG	2.69	0.46
2:B:1:MET:CE	1:C:96:LYS:HA	2.46	0.46
2:B:30:ILE:HG22	2:B:31:ASP:O	2.16	0.46
1:C:11:GLN:HG3	1:C:12:ALA:N	2.30	0.46
3:K:19:ASN:H	3:K:22:GLU:CD	2.17	0.46
3:K:39:VAL:CG1	3:K:46:TYR:HB2	2.46	0.46
1:C:211:ASP:O	1:C:214:ARG:N	2.49	0.46
2:D:30:ILE:HG22	2:D:31:ASP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.31	0.46
1:A:211:ASP:O	1:A:214:ARG:N	2.49	0.46
1:A:228:ASN:HD21	4:A:501:GTP:HN1	1.63	0.46
2:B:12:CYS:O	2:B:13:GLY:C	2.53	0.46
2:B:103:TRP:NE1	2:B:148:GLY:HA2	2.31	0.46
2:B:243:ARG:O	2:B:244:PHE:CG	2.69	0.46
3:K:89:SER:O	3:K:89:SER:OG	2.32	0.46
1:A:121:ARG:HD2	1:A:121:ARG:HA	1.36	0.45
1:A:353:VAL:HG12	1:A:354:GLY:N	2.31	0.45
1:C:353:VAL:HG12	1:C:354:GLY:N	2.31	0.45
3:K:277:TYR:O	3:K:283:THR:HG23	2.16	0.45
1:C:228:ASN:HD21	4:C:501:GTP:HN1	1.63	0.45
1:C:121:ARG:HD2	1:C:121:ARG:HA	1.36	0.45
1:C:255:PHE:CZ	1:C:378:LEU:HD22	2.41	0.45
2:D:12:CYS:O	2:D:13:GLY:C	2.53	0.45
1:A:196:GLU:OE1	1:A:196:GLU:N	2.50	0.45
1:A:255:PHE:CZ	1:A:378:LEU:HD22	2.41	0.45
1:A:362:VAL:HG11	1:A:370:LYS:HG3	1.97	0.45
1:C:196:GLU:OE1	1:C:196:GLU:N	2.50	0.45
1:C:274:PRO:HG2	1:C:371:VAL:HG21	1.99	0.45
2:D:100:GLY:O	2:D:101:ASN:C	2.55	0.45
3:K:214:GLN:HG2	3:K:223:LEU:HB2	1.97	0.45
1:A:137:VAL:HG21	1:A:154:MET:SD	2.57	0.45
1:A:274:PRO:HG2	1:A:371:VAL:HG21	1.99	0.45
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.97	0.45
2:B:100:GLY:O	2:B:101:ASN:C	2.55	0.45
1:C:137:VAL:HG21	1:C:154:MET:SD	2.57	0.45
2:D:84:GLY:C	2:D:86:ILE:H	2.20	0.45
1:A:387:ALA:O	1:A:390:ARG:HB2	2.16	0.45
2:B:84:GLY:C	2:B:86:ILE:H	2.20	0.45
2:B:276:THR:O	2:B:276:THR:OG1	2.32	0.45
1:C:362:VAL:HG11	1:C:370:LYS:HG3	1.97	0.45
1:A:88:HIS:HB3	1:A:91:GLN:CD	2.37	0.45
3:K:216:ASN:OD1	3:K:218:GLN:HB3	2.16	0.45
1:A:214:ARG:HG3	1:A:215:ARG:N	2.31	0.45
2:B:60:LYS:HE3	2:B:88:ARG:HH12	1.81	0.45
1:C:88:HIS:HB3	1:C:91:GLN:CD	2.37	0.45
1:C:214:ARG:HG3	1:C:215:ARG:N	2.32	0.45
1:C:387:ALA:O	1:C:390:ARG:HB2	2.16	0.45
3:K:118:TYR:O	3:K:122:MET:HG2	2.16	0.45
3:K:137:ILE:O	3:K:204:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:GLU:HB3	2:B:98:GLY:HA2	1.98	0.45
1:C:298:PRO:HB3	1:C:307:PRO:HD2	1.98	0.45
1:C:416:GLY:C	1:C:418:PHE:N	2.71	0.45
2:D:60:LYS:HE3	2:D:88:ARG:HH12	1.81	0.45
2:D:71:GLU:HB3	2:D:98:GLY:HA2	1.98	0.45
2:D:276:THR:O	2:D:276:THR:OG1	2.33	0.45
3:K:187:LYS:HE2	3:K:187:LYS:HB3	1.62	0.45
1:A:416:GLY:C	1:A:418:PHE:N	2.71	0.45
2:B:53:TYR:O	2:B:64:ARG:NH2	2.50	0.45
1:C:175:PRO:HB3	1:C:390:ARG:HD3	1.99	0.45
2:D:53:TYR:O	2:D:64:ARG:NH2	2.50	0.44
2:D:123:ARG:NE	2:D:160:GLU:OE1	2.36	0.44
3:K:36:GLU:HG2	3:K:50:ARG:NH1	2.32	0.44
1:A:175:PRO:HB3	1:A:390:ARG:HD3	1.99	0.44
1:A:231:ILE:HD12	1:A:231:ILE:HA	1.76	0.44
1:A:286:LEU:HA	1:A:290:GLU:OE2	2.18	0.44
2:B:5:VAL:CG1	2:B:135:PHE:CD1	3.00	0.44
2:D:5:VAL:CG1	2:D:135:PHE:CD1	3.00	0.44
2:D:48:ARG:HG2	2:D:48:ARG:HH11	1.82	0.44
2:B:189:LEU:HA	2:B:189:LEU:HD23	1.59	0.44
2:B:194:LEU:O	2:B:198:THR:HG23	2.17	0.44
1:C:231:ILE:HD12	1:C:231:ILE:HA	1.76	0.44
1:C:286:LEU:HA	1:C:290:GLU:OE2	2.18	0.44
2:D:194:LEU:O	2:D:198:THR:HG23	2.17	0.44
3:K:90:GLY:O	3:K:94:THR:N	2.49	0.44
3:K:129:HIS:CE1	3:K:172:PHE:HE2	2.35	0.44
3:K:146:LEU:HA	3:K:146:LEU:HD23	1.76	0.44
2:B:123:ARG:NE	2:B:160:GLU:OE1	2.36	0.44
2:B:338:LYS:HD2	2:B:339:ASN:OD1	2.17	0.44
1:C:34:GLY:H	1:C:86:LEU:HD12	1.82	0.44
1:C:65:ALA:HB1	1:C:67:PHE:CE1	2.52	0.44
2:D:338:LYS:HD2	2:D:339:ASN:OD1	2.17	0.44
1:A:34:GLY:H	1:A:86:LEU:HD12	1.82	0.44
1:A:65:ALA:HB1	1:A:67:PHE:CE1	2.52	0.44
2:B:48:ARG:HG2	2:B:48:ARG:HH11	1.83	0.44
1:A:434:GLU:O	1:A:436:GLY:N	2.50	0.44
2:B:124:LYS:HE3	2:B:124:LYS:HB2	1.65	0.44
1:C:217:LEU:HD11	1:C:367:ASP:O	2.18	0.44
1:C:434:GLU:O	1:C:436:GLY:N	2.50	0.44
2:D:189:LEU:HA	2:D:189:LEU:HD23	1.60	0.44
1:A:217:LEU:HD11	1:A:367:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:HIS:CE1	1:A:407:TRP:CE2	3.00	0.44
1:C:406:HIS:CE1	1:C:407:TRP:CE2	3.00	0.44
2:D:119:LEU:HD12	2:D:119:LEU:HA	1.55	0.44
1:A:114:ILE:HD13	1:A:114:ILE:HA	1.84	0.44
2:D:67:LEU:HD11	2:D:87:PHE:CD2	2.53	0.44
2:B:67:LEU:HD11	2:B:87:PHE:CD2	2.53	0.44
2:B:172:VAL:HG12	2:B:173:PRO:HD2	2.00	0.44
2:B:324:SER:HA	1:C:223:THR:HG22	2.00	0.44
1:C:228:ASN:ND2	4:C:501:GTP:HN1	2.14	0.44
2:D:172:VAL:HG12	2:D:173:PRO:HD2	2.00	0.44
2:D:241:CYS:HB2	2:D:250:ALA:O	2.17	0.44
1:A:228:ASN:ND2	4:A:501:GTP:HN1	2.14	0.43
3:K:157:GLU:OE1	3:K:284:ARG:NH2	2.51	0.43
2:B:241:CYS:HB2	2:B:250:ALA:O	2.17	0.43
1:C:284:GLU:HB3	1:C:286:LEU:HG	2.00	0.43
2:D:124:LYS:HB2	2:D:124:LYS:HE3	1.64	0.43
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.53	0.43
1:C:114:ILE:HD13	1:C:114:ILE:HA	1.84	0.43
1:A:284:GLU:HB3	1:A:286:LEU:HG	2.01	0.43
1:C:129:CYS:SG	1:C:132:LEU:HD13	2.58	0.43
2:D:12:CYS:HB2	2:D:140:SER:HB2	1.99	0.43
2:D:22:GLU:HG3	2:D:83:PHE:CD1	2.53	0.43
1:A:129:CYS:SG	1:A:132:LEU:HD13	2.58	0.43
1:A:169:PHE:CZ	1:A:235:VAL:HG22	2.53	0.43
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.64	0.43
2:B:12:CYS:HB2	2:B:140:SER:HB2	1.99	0.43
2:B:349:ASN:ND2	1:C:178:SER:HB3	2.33	0.43
1:C:30:ILE:HD12	1:C:53:PHE:CE2	2.54	0.43
1:C:169:PHE:CZ	1:C:235:VAL:HG22	2.53	0.43
1:A:30:ILE:HD12	1:A:53:PHE:CE2	2.54	0.43
1:A:202:PHE:CE2	1:A:238:ILE:HD13	2.54	0.43
2:B:205:ASP:CG	2:B:304:ALA:H	2.22	0.43
1:C:202:PHE:CE2	1:C:238:ILE:HD13	2.54	0.43
1:C:423:GLU:HG3	1:C:424:ASP:OD1	2.19	0.43
2:D:52:TYR:C	2:D:53:TYR:HD1	2.22	0.43
3:K:95:MET:O	3:K:106:GLY:HA3	2.18	0.43
1:A:423:GLU:HG3	1:A:424:ASP:OD1	2.19	0.43
2:B:52:TYR:C	2:B:53:TYR:HD1	2.22	0.43
2:D:205:ASP:CG	2:D:304:ALA:H	2.22	0.43
2:B:99:ALA:HB3	4:B:501:GTP:O2G	2.19	0.43
2:B:114:LEU:O	2:B:114:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:VAL:HG11	1:C:154:MET:SD	2.59	0.43
2:D:99:ALA:HB3	4:D:501:GTP:O2G	2.19	0.43
2:D:384:ILE:HD12	2:D:384:ILE:HG23	1.81	0.43
1:A:137:VAL:HG11	1:A:154:MET:SD	2.59	0.43
2:B:384:ILE:HD12	2:B:384:ILE:HG23	1.81	0.43
3:K:314:SER:C	3:K:316:LEU:N	2.71	0.43
2:B:20:PHE:CE1	2:B:24:ILE:HG13	2.53	0.42
2:B:151:THR:CG2	2:B:193:GLN:HE21	2.31	0.42
2:D:114:LEU:HG	2:D:114:LEU:O	2.19	0.42
2:D:188:THR:HG22	2:D:188:THR:O	2.19	0.42
3:K:19:ASN:HB2	3:K:22:GLU:OE2	2.19	0.42
2:B:20:PHE:O	2:B:23:VAL:HG13	2.19	0.42
2:D:151:THR:CG2	2:D:193:GLN:HE21	2.31	0.42
2:B:72:PRO:HD3	2:B:96:GLN:HA	2.00	0.42
2:B:188:THR:HG22	2:B:188:THR:O	2.19	0.42
2:D:20:PHE:O	2:D:23:VAL:HG13	2.19	0.42
2:D:20:PHE:CE1	2:D:24:ILE:HG13	2.53	0.42
2:D:384:ILE:HD13	2:D:384:ILE:HA	1.83	0.42
3:K:126:LEU:HD11	3:K:216:ASN:HB2	2.01	0.42
2:B:229:HIS:O	2:B:229:HIS:ND1	2.53	0.42
2:D:44:LEU:O	2:D:44:LEU:HG	2.19	0.42
2:D:72:PRO:HD3	2:D:96:GLN:HA	2.00	0.42
2:D:343:PHE:HB3	2:D:350:ASN:ND2	2.34	0.42
2:B:44:LEU:O	2:B:44:LEU:HG	2.19	0.42
2:B:326:LYS:NZ	2:B:330:GLU:OE1	2.49	0.42
2:B:343:PHE:HB3	2:B:350:ASN:ND2	2.34	0.42
2:B:384:ILE:HD13	2:B:384:ILE:HA	1.83	0.42
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.69	0.42
1:C:402:ARG:HG2	3:K:321:ARG:HH21	1.84	0.42
2:D:229:HIS:O	2:D:229:HIS:ND1	2.53	0.42
3:K:232:LEU:HD23	3:K:232:LEU:HA	1.74	0.42
1:A:114:ILE:HD12	1:A:114:ILE:HG23	1.69	0.42
1:A:234:ILE:HD13	1:A:234:ILE:HG21	1.77	0.42
1:C:174:ALA:HB3	1:C:177:VAL:O	2.20	0.42
3:K:93:HIS:O	3:K:93:HIS:ND1	2.52	0.42
1:A:174:ALA:HB3	1:A:177:VAL:O	2.20	0.42
1:A:428:LEU:HD12	1:A:428:LEU:HA	1.66	0.42
2:B:87:PHE:CD1	2:B:87:PHE:N	2.87	0.42
2:D:251:ASP:H	2:D:254:LYS:HB2	1.84	0.42
3:K:86:GLN:HE21	3:K:86:GLN:HB3	1.56	0.42
3:K:248:LEU:HG	3:K:252:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:O	1:A:80:THR:HG22	2.20	0.42
2:B:251:ASP:H	2:B:254:LYS:HB2	1.84	0.42
1:C:76:ASP:O	1:C:80:THR:HG22	2.20	0.42
1:C:114:ILE:HD12	1:C:114:ILE:HG23	1.69	0.42
1:C:115:ILE:HA	1:C:118:VAL:HG12	2.02	0.42
1:A:115:ILE:HA	1:A:118:VAL:HG12	2.02	0.42
2:B:117:SER:O	2:B:117:SER:OG	2.35	0.42
2:B:119:LEU:HD12	2:B:119:LEU:HA	1.54	0.42
1:C:80:THR:O	1:C:80:THR:OG1	2.33	0.42
2:D:87:PHE:CD1	2:D:87:PHE:N	2.87	0.42
2:D:117:SER:O	2:D:117:SER:OG	2.35	0.42
2:D:401:ARG:HD2	2:D:401:ARG:HA	1.88	0.42
3:K:147:ASP:OD2	3:K:150:LYS:HG3	2.20	0.42
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.69	0.42
2:B:2:ARG:HE	2:B:242:LEU:CD2	2.32	0.42
2:D:2:ARG:HE	2:D:242:LEU:CD2	2.32	0.42
1:A:261:PRO:O	1:A:262:TYR:CG	2.73	0.41
1:A:264:ARG:O	1:A:266:HIS:CD2	2.73	0.41
1:C:7:ILE:HG21	1:C:7:ILE:HD13	1.79	0.41
1:C:200:CYS:HB3	1:C:202:PHE:CE1	2.54	0.41
1:C:428:LEU:HD12	1:C:428:LEU:HA	1.66	0.41
2:D:86:ILE:HG21	2:D:86:ILE:HD13	1.83	0.41
3:K:16:ARG:NH1	3:K:17:PRO:O	2.45	0.41
2:B:65:ALA:HB1	2:B:67:LEU:HD21	2.02	0.41
2:B:86:ILE:HG21	2:B:86:ILE:HD13	1.83	0.41
1:C:261:PRO:O	1:C:262:TYR:CG	2.73	0.41
2:D:12:CYS:O	2:D:14:ASN:N	2.53	0.41
2:D:65:ALA:HB1	2:D:67:LEU:HD21	2.02	0.41
2:D:69:ASP:HA	2:D:145:THR:HG21	2.01	0.41
3:K:46:TYR:HE2	3:K:316:LEU:HD13	1.84	0.41
1:A:7:ILE:HG21	1:A:7:ILE:HD13	1.79	0.41
1:A:200:CYS:HB3	1:A:202:PHE:CE1	2.54	0.41
1:A:330:ALA:O	1:A:333:ALA:HB3	2.19	0.41
1:A:416:GLY:C	1:A:418:PHE:H	2.23	0.41
1:A:422:ARG:HD2	1:A:422:ARG:HA	1.60	0.41
2:B:12:CYS:O	2:B:14:ASN:N	2.53	0.41
2:B:69:ASP:HA	2:B:145:THR:HG21	2.01	0.41
2:B:401:ARG:HD2	2:B:401:ARG:HA	1.88	0.41
1:C:264:ARG:O	1:C:266:HIS:CD2	2.73	0.41
2:D:155:SER:O	2:D:155:SER:OG	2.37	0.41
3:K:134:TYR:CD1	3:K:208:PHE:CD2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.75	0.41
2:B:4:ILE:HB	2:B:52:TYR:CE1	2.55	0.41
2:B:268:PHE:N	2:B:268:PHE:CD1	2.87	0.41
1:C:416:GLY:C	1:C:418:PHE:H	2.23	0.41
2:D:4:ILE:HB	2:D:52:TYR:CE1	2.55	0.41
3:K:74:LEU:HD21	3:K:115:ILE:HG13	2.01	0.41
1:A:122:ILE:HD13	1:A:122:ILE:HG21	1.85	0.41
2:B:155:SER:O	2:B:155:SER:OG	2.37	0.41
2:B:212:ILE:O	2:B:212:ILE:HG22	2.21	0.41
1:C:330:ALA:O	1:C:333:ALA:HB3	2.19	0.41
2:D:2:ARG:HE	2:D:242:LEU:HD22	1.85	0.41
2:D:212:ILE:O	2:D:212:ILE:HG22	2.21	0.41
3:K:131:LYS:HB3	3:K:211:ASN:HB3	2.03	0.41
2:B:129:CYS:SG	2:B:132:LEU:HD23	2.60	0.41
2:D:268:PHE:N	2:D:268:PHE:CD1	2.87	0.41
3:K:73:VAL:HG11	3:K:227:LEU:HB2	2.02	0.41
2:B:24:ILE:HD13	2:B:24:ILE:HA	1.94	0.41
2:B:56:ALA:HB3	2:B:60:LYS:HG3	2.03	0.41
2:B:194:LEU:HD23	2:B:194:LEU:HA	1.90	0.41
2:B:339:ASN:HD22	2:B:342:TYR:HD2	1.68	0.41
1:C:392:ASP:CG	1:C:422:ARG:HH22	2.24	0.41
1:C:404:PHE:CD1	1:C:404:PHE:N	2.88	0.41
1:C:422:ARG:HD2	1:C:422:ARG:HA	1.60	0.41
2:D:129:CYS:SG	2:D:132:LEU:HD23	2.60	0.41
2:D:383:ALA:C	2:D:385:GLN:N	2.73	0.41
1:A:404:PHE:CD1	1:A:404:PHE:N	2.88	0.41
1:C:5:ILE:HB	1:C:135:PHE:CD1	2.55	0.41
2:D:56:ALA:HB3	2:D:60:LYS:HG3	2.03	0.41
2:D:183:GLU:CB	2:D:184:PRO:HD3	2.48	0.41
2:D:339:ASN:HD22	2:D:342:TYR:HD2	1.68	0.41
3:K:214:GLN:HE21	3:K:223:LEU:CD2	2.33	0.41
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.55	0.41
1:A:122:ILE:HD13	1:A:157:LEU:HD21	2.03	0.41
1:A:130:THR:OG1	1:A:131:GLY:N	2.54	0.41
1:A:392:ASP:CG	1:A:422:ARG:HH22	2.25	0.41
2:B:2:ARG:HE	2:B:242:LEU:HD22	1.85	0.41
2:B:160:GLU:C	2:B:161:TYR:CD1	2.94	0.41
2:B:183:GLU:CB	2:B:184:PRO:HD3	2.48	0.41
2:B:383:ALA:C	2:B:385:GLN:N	2.73	0.41
2:B:420:GLU:OE2	2:B:420:GLU:HA	2.20	0.41
1:C:26:LEU:HD23	1:C:26:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HD12	1:C:75:ILE:HG23	1.80	0.41
1:C:122:ILE:HD13	1:C:157:LEU:HD21	2.03	0.41
1:C:130:THR:OG1	1:C:131:GLY:N	2.54	0.41
1:C:306:ASP:OD2	1:C:309:HIS:CE1	2.72	0.41
2:D:24:ILE:HD13	2:D:24:ILE:HA	1.94	0.41
3:K:46:TYR:CE2	3:K:316:LEU:HD13	2.55	0.41
3:K:94:THR:O	3:K:107:ILE:HG13	2.21	0.41
3:K:126:LEU:HD13	3:K:216:ASN:HA	2.03	0.41
3:K:321:ARG:C	3:K:323:LYS:H	2.24	0.41
1:A:306:ASP:OD2	1:A:309:HIS:CE1	2.72	0.41
2:B:48:ARG:C	2:B:50:ASN:N	2.74	0.41
1:C:252:LEU:HD12	1:C:252:LEU:HA	1.82	0.41
1:C:271:THR:HG22	1:C:272:TYR:H	1.85	0.41
2:D:48:ARG:C	2:D:50:ASN:N	2.74	0.41
2:D:420:GLU:OE2	2:D:420:GLU:HA	2.20	0.41
3:K:14:ARG:HH11	3:K:94:THR:HB	1.86	0.41
1:A:4:CYS:HG	1:A:52:PHE:HE1	1.69	0.40
1:A:228:ASN:O	1:A:231:ILE:HG22	2.21	0.40
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.82	0.40
1:A:271:THR:HG22	1:A:272:TYR:H	1.85	0.40
1:A:328:VAL:O	1:A:332:ILE:HG13	2.21	0.40
1:C:328:VAL:O	1:C:332:ILE:HG13	2.21	0.40
2:D:160:GLU:C	2:D:161:TYR:CD1	2.94	0.40
2:D:194:LEU:HD23	2:D:194:LEU:HA	1.90	0.40
3:K:48:PHE:HB3	3:K:49:ASP:H	1.71	0.40
1:A:17:GLY:O	1:A:21:TRP:HD1	2.05	0.40
1:A:326:LYS:CD	2:B:222:PRO:HD2	2.46	0.40
2:B:122:VAL:O	2:B:126:SER:N	2.54	0.40
2:B:227:LEU:N	2:B:227:LEU:HD12	2.37	0.40
1:C:17:GLY:O	1:C:21:TRP:HD1	2.05	0.40
1:C:188:ILE:HD12	1:C:188:ILE:HA	1.71	0.40
2:D:8:GLN:NE2	2:D:67:LEU:HD22	2.35	0.40
2:B:67:LEU:HD11	2:B:87:PHE:CE2	2.57	0.40
2:B:70:LEU:HA	2:B:70:LEU:HD12	1.87	0.40
1:C:4:CYS:HG	1:C:52:PHE:HE1	1.69	0.40
1:C:228:ASN:O	1:C:231:ILE:HG22	2.22	0.40
2:D:67:LEU:HD11	2:D:87:PHE:CE2	2.57	0.40
2:D:122:VAL:O	2:D:126:SER:N	2.54	0.40
2:D:227:LEU:N	2:D:227:LEU:HD12	2.36	0.40
2:D:320:ARG:CZ	2:D:360:PRO:HD3	2.52	0.40
1:A:188:ILE:HD12	1:A:188:ILE:HA	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:NE2	2:B:67:LEU:HD22	2.35	0.40
2:B:320:ARG:CZ	2:B:360:PRO:HD3	2.52	0.40
2:B:401:ARG:O	2:B:403:ALA:N	2.55	0.40
2:D:238:VAL:O	2:D:238:VAL:HG12	2.21	0.40
1:A:297:GLU:C	1:A:299:ALA:H	2.23	0.40
2:B:388:PHE:N	2:B:388:PHE:CD1	2.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/451 (97%)	346 (79%)	88 (20%)	3 (1%)	19	53
1	C	437/451 (97%)	347 (79%)	87 (20%)	3 (1%)	19	53
2	B	424/445 (95%)	351 (83%)	71 (17%)	2 (0%)	25	59
2	D	424/445 (95%)	351 (83%)	71 (17%)	2 (0%)	25	59
3	K	313/357 (88%)	264 (84%)	47 (15%)	2 (1%)	22	55
All	All	2035/2149 (95%)	1659 (82%)	364 (18%)	12 (1%)	24	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
1	C	252	LEU
3	K	287	GLN
3	K	203	ARG
2	B	12	CYS
2	B	402	LYS
2	D	12	CYS
2	D	402	LYS

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Mol	Chain	Res	Type
1	A	58	ALA
1	A	286	LEU
1	C	58	ALA
1	C	286	LEU

### 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	370/379 (98%)	341 (92%)	29 (8%)	10	34
1	C	370/379 (98%)	341 (92%)	29 (8%)	10	34
2	B	367/381 (96%)	338 (92%)	29 (8%)	10	34
2	D	367/381 (96%)	338 (92%)	29 (8%)	10	34
3	K	283/319 (89%)	279 (99%)	4 (1%)	62	79
All	All	1757/1839 (96%)	1637 (93%)	120 (7%)	16	40

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	40	LYS
1	A	50	ASN
1	A	56	THR
1	A	77	GLU
1	A	158	SER
1	A	159	VAL
1	A	160	ASP
1	A	181	VAL
1	A	188	ILE
1	A	190	THR
1	A	191	THR
1	A	194	THR
1	A	196	GLU
1	A	207	GLU

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Mol	Chain	Res	Type
1	A	217	LEU
1	A	253	THR
1	A	275	VAL
1	A	332	ILE
1	A	337	THR
1	A	344	VAL
1	A	363	VAL
1	A	370	LYS
1	A	376	CYS
1	A	382	THR
1	A	391	LEU
1	A	405	VAL
1	A	429	GLU
1	A	438	ASP
2	B	20	PHE
2	B	23	VAL
2	B	40	SER
2	B	44	LEU
2	B	47	GLU
2	B	51	VAL
2	B	59	ASN
2	B	109	THR
2	B	128	SER
2	B	131	CYS
2	B	159	GLU
2	B	168	THR
2	B	195	VAL
2	B	198	THR
2	B	210	TYR
2	B	211	ASP
2	B	213	CYS
2	B	218	LYS
2	B	239	THR
2	B	278	ARG
2	B	281	GLN
2	B	286	LEU
2	B	290	GLU
2	B	292	THR
2	B	357	ASP
2	B	376	THR
2	B	386	GLU
2	B	409	THR

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Mol	Chain	Res	Type
2	B	423	SER
1	C	3	GLU
1	C	40	LYS
1	C	50	ASN
1	C	56	THR
1	C	77	GLU
1	C	158	SER
1	C	159	VAL
1	C	160	ASP
1	C	181	VAL
1	C	188	ILE
1	C	190	THR
1	C	191	THR
1	C	194	THR
1	C	196	GLU
1	C	207	GLU
1	C	217	LEU
1	C	253	THR
1	C	275	VAL
1	C	332	ILE
1	C	337	THR
1	C	344	VAL
1	C	363	VAL
1	C	370	LYS
1	C	376	CYS
1	C	382	THR
1	C	391	LEU
1	C	405	VAL
1	C	429	GLU
1	C	438	ASP
2	D	20	PHE
2	D	23	VAL
2	D	40	SER
2	D	44	LEU
2	D	47	GLU
2	D	51	VAL
2	D	59	ASN
2	D	109	THR
2	D	128	SER
2	D	131	CYS
2	D	159	GLU
2	D	168	THR

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Mol	Chain	Res	Type
2	D	195	VAL
2	D	198	THR
2	D	210	TYR
2	D	211	ASP
2	D	213	CYS
2	D	218	LYS
2	D	239	THR
2	D	278	ARG
2	D	281	GLN
2	D	286	LEU
2	D	290	GLU
2	D	292	THR
2	D	357	ASP
2	D	376	THR
2	D	386	GLU
2	D	409	THR
2	D	423	SER
3	K	19	ASN
3	K	112	VAL
3	K	158	ASP
3	K	173	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	107	HIS
1	A	192	HIS
1	A	197	HIS
1	A	226	ASN
1	A	228	ASN
1	A	249	ASN
1	A	406	HIS
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
2	B	59	ASN
2	B	91	ASN
2	B	101	ASN
2	B	107	HIS
2	B	136	GLN
2	B	192	HIS

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Mol	Chain	Res	Type
2	B	193	GLN
2	B	197	ASN
2	B	247	GLN
2	B	249	ASN
2	B	258	ASN
2	B	266	HIS
2	B	293	GLN
2	B	394	GLN
2	B	406	HIS
1	C	107	HIS
1	C	192	HIS
1	C	197	HIS
1	C	226	ASN
1	C	228	ASN
1	C	249	ASN
1	C	406	HIS
2	D	8	GLN
2	D	11	GLN
2	D	14	ASN
2	D	59	ASN
2	D	91	ASN
2	D	101	ASN
2	D	107	HIS
2	D	136	GLN
2	D	192	HIS
2	D	193	GLN
2	D	197	ASN
2	D	247	GLN
2	D	249	ASN
2	D	266	HIS
2	D	293	GLN
2	D	394	GLN
2	D	406	HIS
3	K	78	ASN
3	K	86	GLN
3	K	198	ASN
3	K	214	GLN
3	K	218	GLN
3	K	287	GLN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GTP	A	501	5	26,34,34	2.02	7 (26%)	32,54,54	2.34	8 (25%)
4	GTP	C	501	5	26,34,34	2.02	7 (26%)	32,54,54	2.35	8 (25%)
4	GTP	D	501	5	26,34,34	2.06	5 (19%)	32,54,54	2.25	10 (31%)
4	GTP	B	501	5	26,34,34	2.05	5 (19%)	32,54,54	2.25	10 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	501	5	-	2/18/38/38	0/3/3/3
4	GTP	C	501	5	-	2/18/38/38	0/3/3/3
4	GTP	D	501	5	-	5/18/38/38	0/3/3/3
4	GTP	B	501	5	-	5/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	GTP	C5-C6	-5.71	1.35	1.47
4	B	501	GTP	C5-C6	-5.65	1.35	1.47
4	C	501	GTP	C5-C6	-5.52	1.36	1.47
4	A	501	GTP	C5-C6	-5.45	1.36	1.47
4	A	501	GTP	C2'-C1'	-4.35	1.47	1.53
4	C	501	GTP	C2'-C1'	-4.33	1.47	1.53
4	D	501	GTP	C2'-C1'	-3.94	1.47	1.53
4	B	501	GTP	C2'-C1'	-3.92	1.47	1.53
4	B	501	GTP	C5-C4	-3.60	1.33	1.43
4	D	501	GTP	C5-C4	-3.56	1.34	1.43
4	A	501	GTP	C5-C4	-3.35	1.34	1.43
4	C	501	GTP	C5-C4	-3.34	1.34	1.43
4	B	501	GTP	C6-N1	-2.59	1.34	1.37
4	D	501	GTP	C6-N1	-2.55	1.34	1.37
4	D	501	GTP	O4'-C4'	-2.51	1.39	1.45
4	A	501	GTP	C6-N1	-2.50	1.34	1.37
4	C	501	GTP	C6-N1	-2.48	1.34	1.37
4	B	501	GTP	O4'-C4'	-2.47	1.39	1.45
4	A	501	GTP	O4'-C4'	-2.29	1.39	1.45
4	C	501	GTP	O4'-C4'	-2.25	1.40	1.45
4	A	501	GTP	O4'-C1'	-2.07	1.38	1.41
4	C	501	GTP	O4'-C1'	-2.03	1.38	1.41
4	A	501	GTP	O2'-C2'	-2.03	1.38	1.43
4	C	501	GTP	O2'-C2'	-2.01	1.38	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GTP	PB-O3B-PG	-6.74	109.70	132.83
4	A	501	GTP	PB-O3B-PG	-6.73	109.74	132.83
4	A	501	GTP	PA-O3A-PB	-5.73	113.15	132.83
4	C	501	GTP	PA-O3A-PB	-5.72	113.18	132.83
4	B	501	GTP	PA-O3A-PB	-5.67	113.36	132.83
4	D	501	GTP	PA-O3A-PB	-5.65	113.44	132.83
4	D	501	GTP	PB-O3B-PG	-4.81	116.34	132.83
4	B	501	GTP	PB-O3B-PG	-4.80	116.37	132.83
4	D	501	GTP	C2-N1-C6	-4.73	116.39	125.10
4	B	501	GTP	C2-N1-C6	-4.67	116.50	125.10
4	D	501	GTP	C5-C6-N1	4.62	122.11	113.95
4	B	501	GTP	C5-C6-N1	4.56	122.01	113.95
4	C	501	GTP	C5-C6-N1	3.96	120.94	113.95
4	C	501	GTP	O4'-C1'-C2'	-3.95	101.16	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	O4'-C1'-C2'	-3.94	101.16	106.93
4	A	501	GTP	C5-C6-N1	3.92	120.87	113.95
4	B	501	GTP	C8-N7-C5	3.67	109.98	102.99
4	D	501	GTP	C8-N7-C5	3.66	109.96	102.99
4	C	501	GTP	C2-N1-C6	-3.55	118.57	125.10
4	A	501	GTP	C2-N1-C6	-3.54	118.58	125.10
4	C	501	GTP	C8-N7-C5	3.50	109.66	102.99
4	A	501	GTP	C8-N7-C5	3.48	109.61	102.99
4	C	501	GTP	O6-C6-N1	-3.09	117.00	120.65
4	A	501	GTP	O6-C6-N1	-3.01	117.10	120.65
4	B	501	GTP	O2'-C2'-C3'	-2.88	102.52	111.82
4	D	501	GTP	O2'-C2'-C3'	-2.86	102.56	111.82
4	D	501	GTP	O6-C6-N1	-2.67	117.50	120.65
4	D	501	GTP	O4'-C1'-C2'	-2.60	103.12	106.93
4	B	501	GTP	O4'-C1'-C2'	-2.60	103.13	106.93
4	B	501	GTP	O6-C6-N1	-2.57	117.61	120.65
4	C	501	GTP	O2'-C2'-C3'	-2.34	104.26	111.82
4	A	501	GTP	O2'-C2'-C3'	-2.31	104.36	111.82
4	B	501	GTP	O3'-C3'-C2'	-2.15	104.87	111.82
4	D	501	GTP	O3'-C3'-C2'	-2.15	104.87	111.82
4	B	501	GTP	O6-C6-C5	-2.04	120.38	124.37
4	D	501	GTP	O6-C6-C5	-2.04	120.39	124.37

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	O4'-C4'-C5'-O5'
4	B	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	O4'-C4'-C5'-O5'
4	D	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C3'-C4'-C5'-O5'
4	C	501	GTP	C3'-C4'-C5'-O5'
4	B	501	GTP	PA-O3A-PB-O2B
4	D	501	GTP	PA-O3A-PB-O2B
4	B	501	GTP	C4'-C5'-O5'-PA
4	D	501	GTP	C4'-C5'-O5'-PA
4	B	501	GTP	PA-O3A-PB-O1B
4	D	501	GTP	PA-O3A-PB-O1B
4	B	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O2G

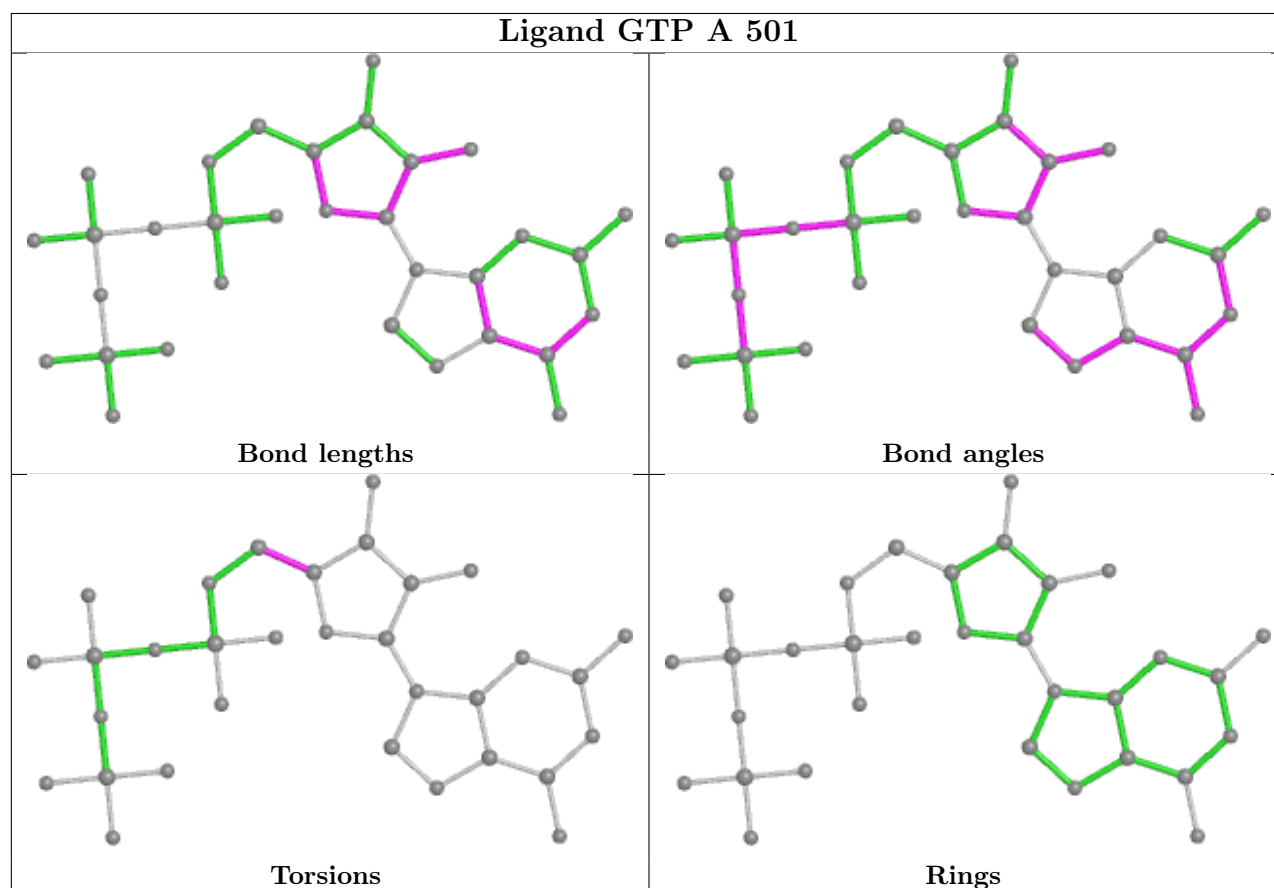


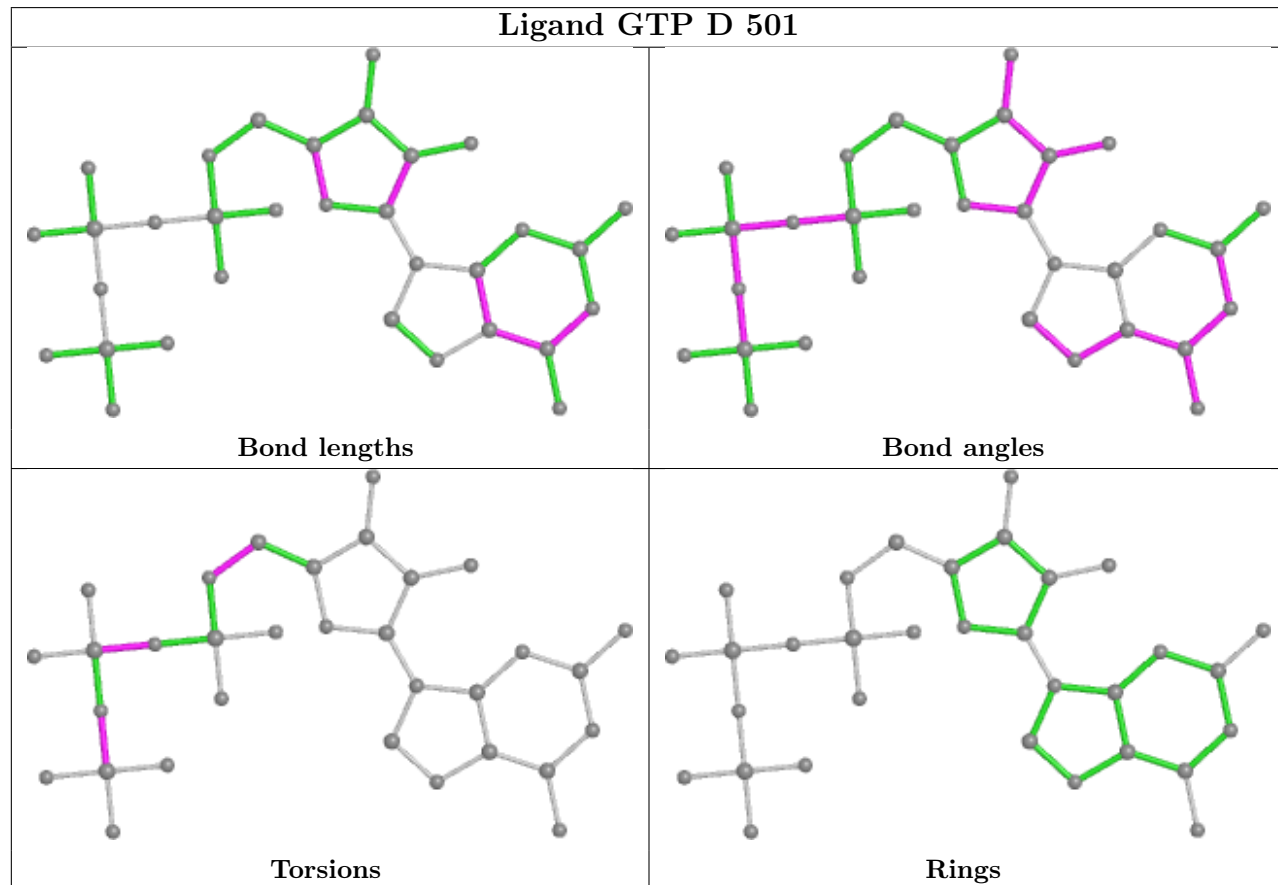
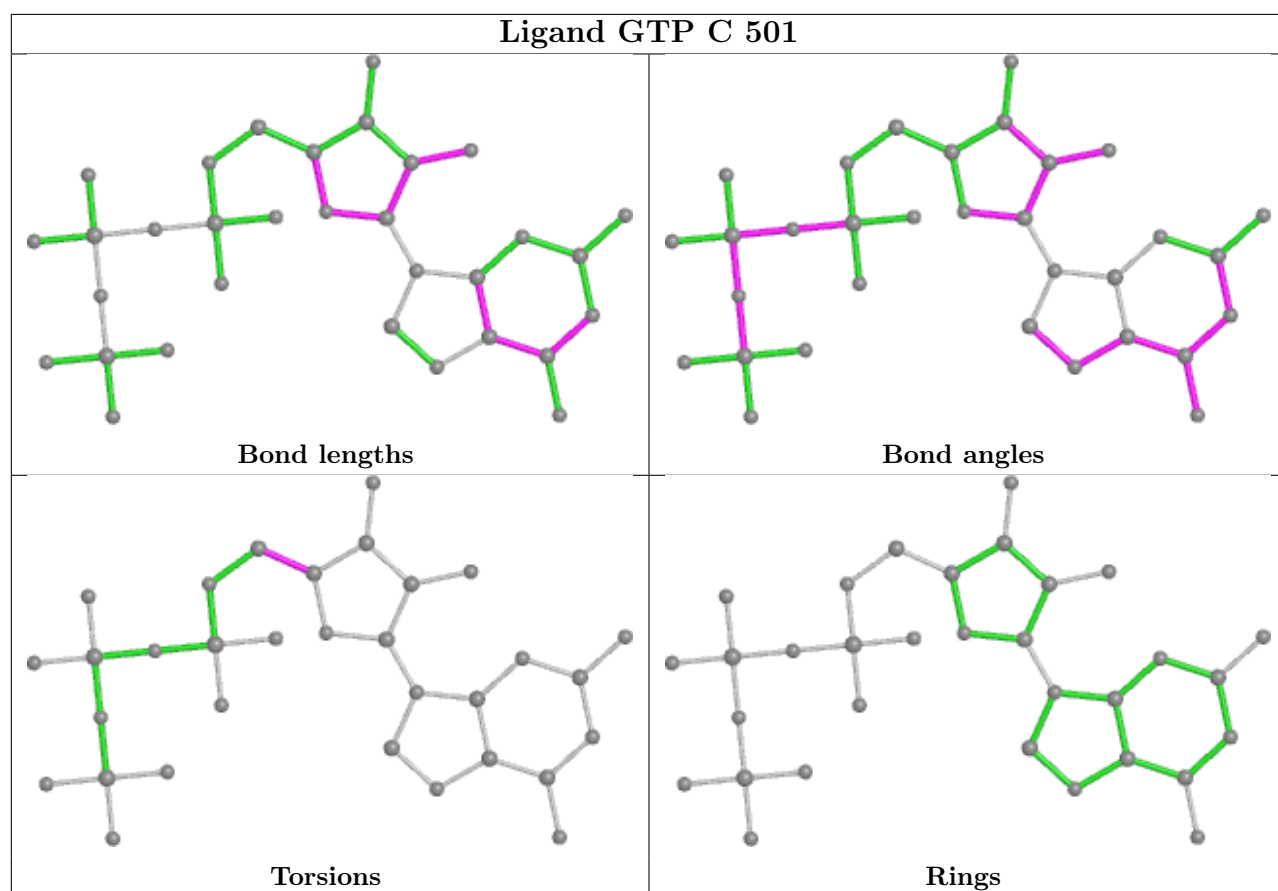
There are no ring outliers.

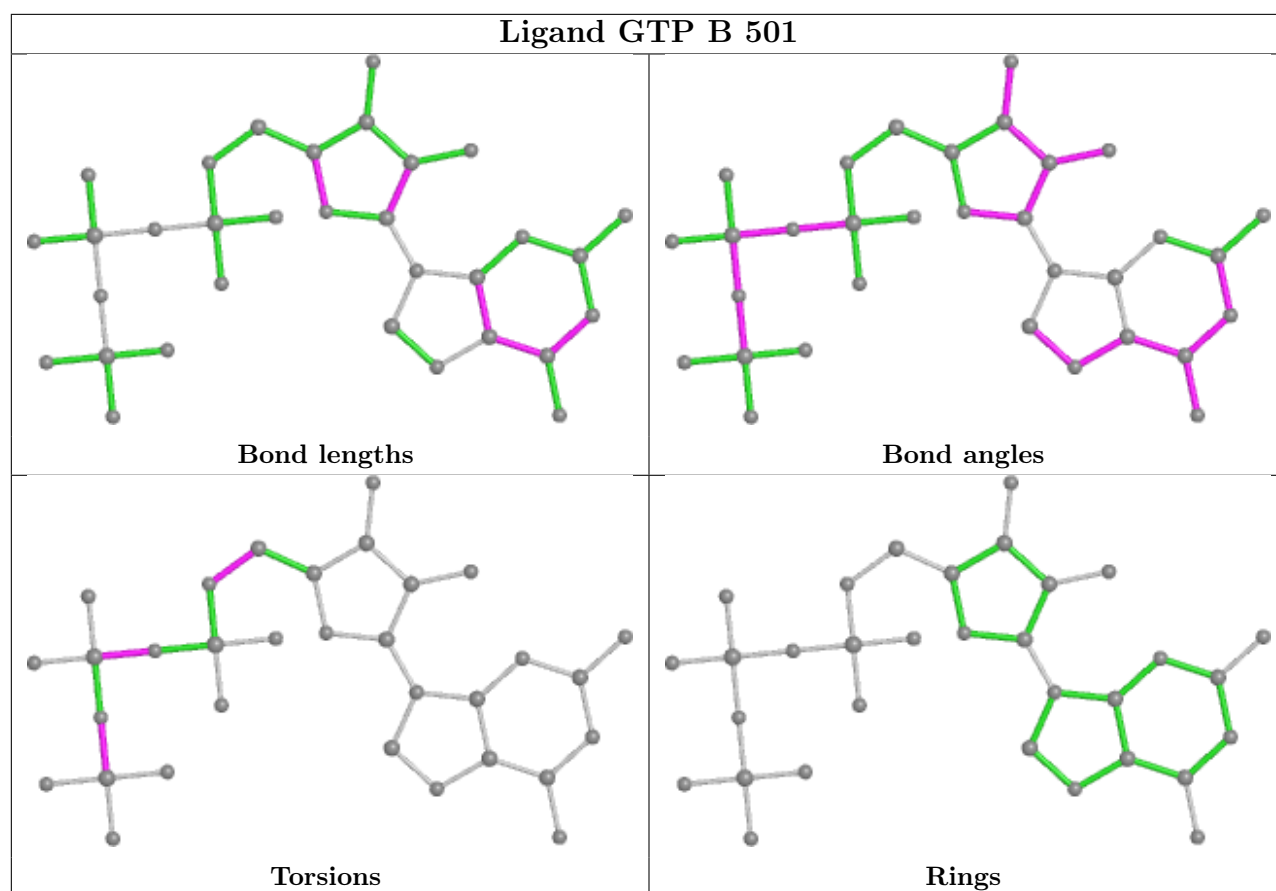
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GTP	7	0
4	C	501	GTP	7	0
4	D	501	GTP	1	0
4	B	501	GTP	1	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.

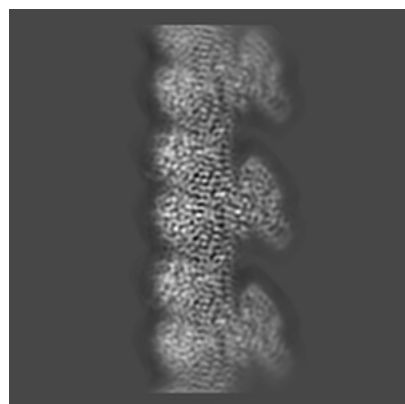
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62874. These allow visual inspection of the internal detail of the map and identification of artifacts.

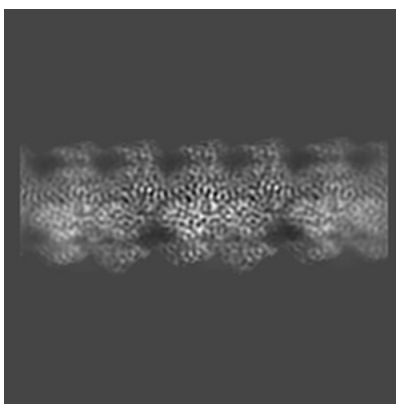
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

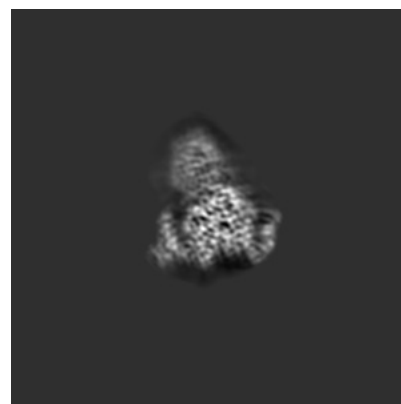
#### 6.1.1 Primary map



X

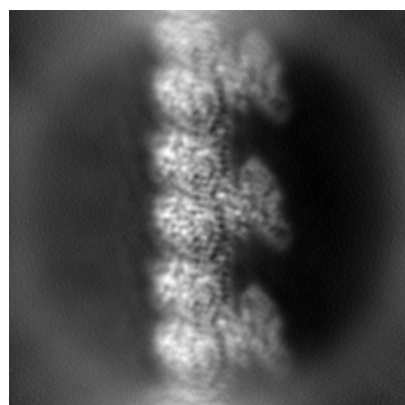


Y

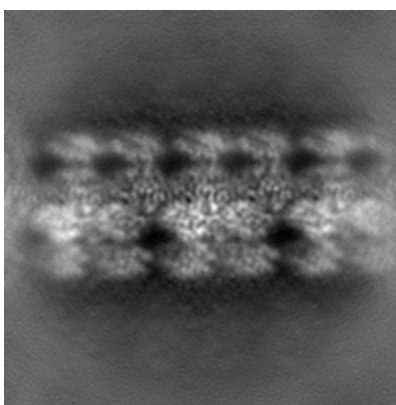


Z

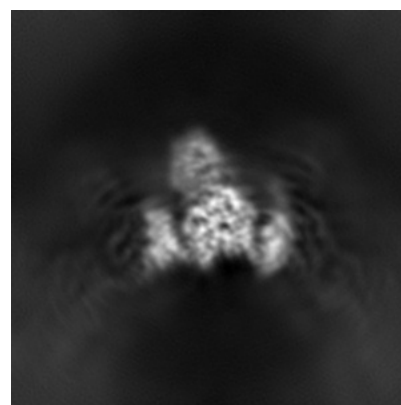
#### 6.1.2 Raw map



X



Y



Z

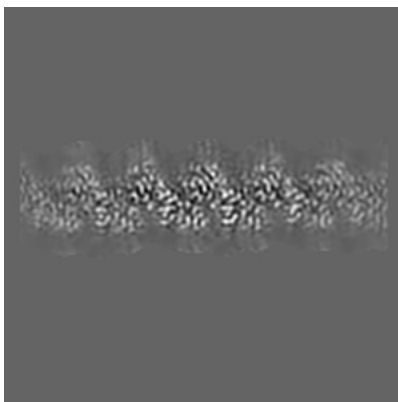
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

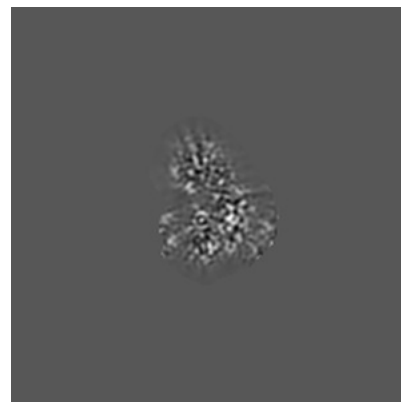
### 6.2.1 Primary map



X Index: 100

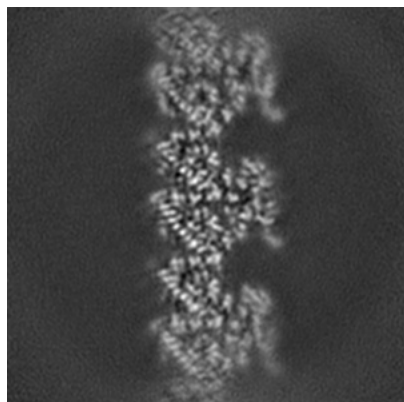


Y Index: 100

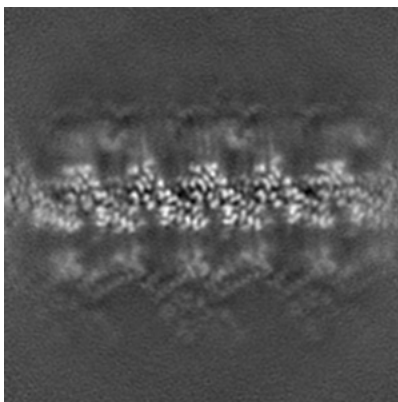


Z Index: 100

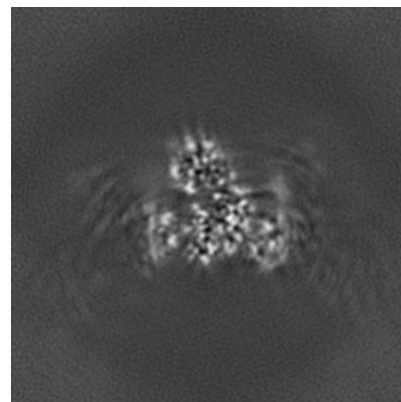
### 6.2.2 Raw map



X Index: 100



Y Index: 100

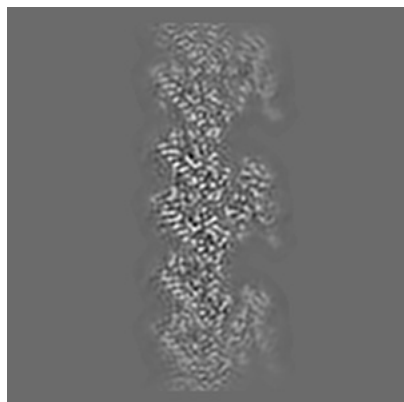


Z Index: 100

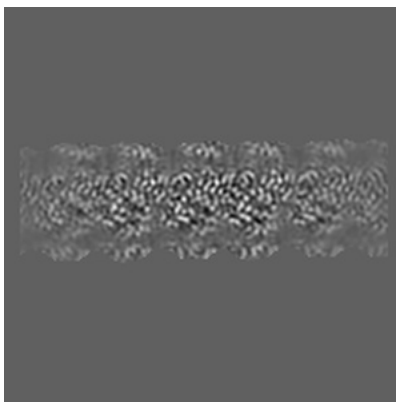
The images above show central slices of the map in three orthogonal directions.

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

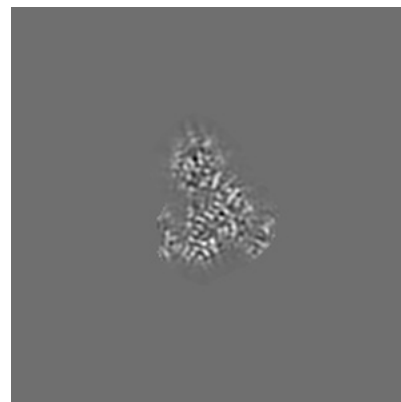
### 6.3.1 Primary map



X Index: 101

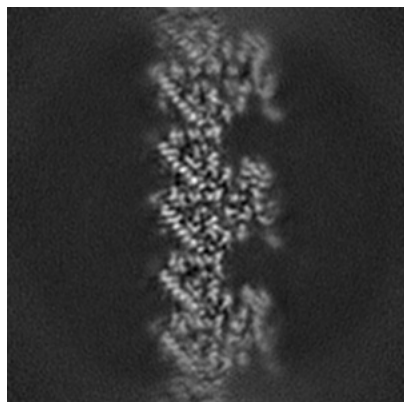


Y Index: 88

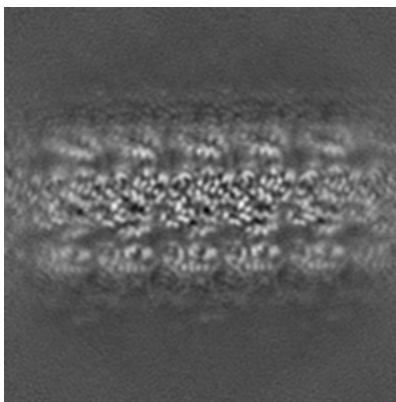


Z Index: 97

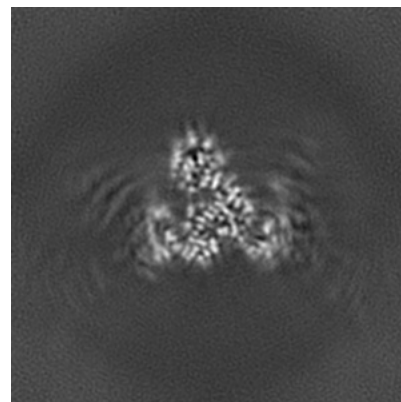
### 6.3.2 Raw map



X Index: 101



Y Index: 88

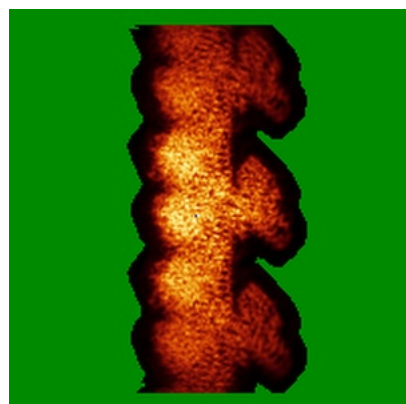


Z Index: 97

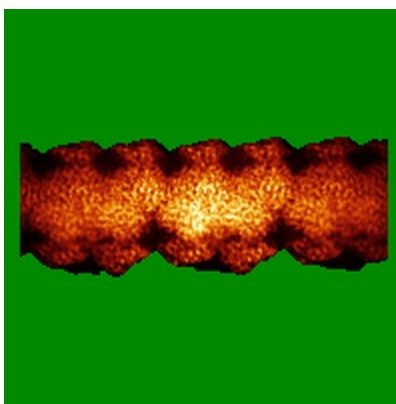
The images above show the largest variance slices of the map in three orthogonal directions.

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

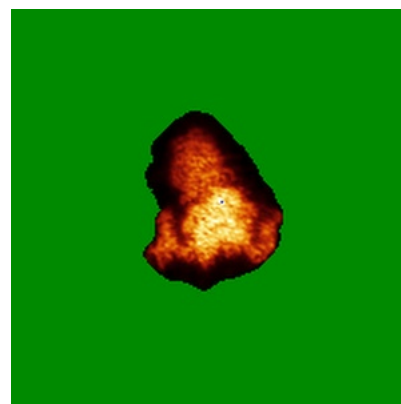
### 6.4.1 Primary map



X

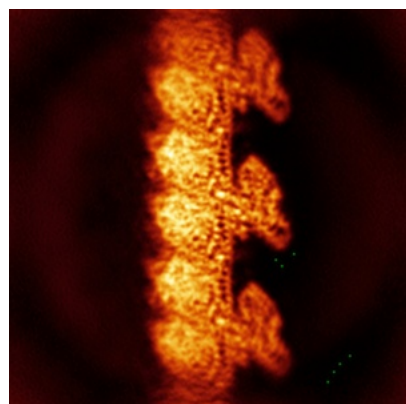


Y

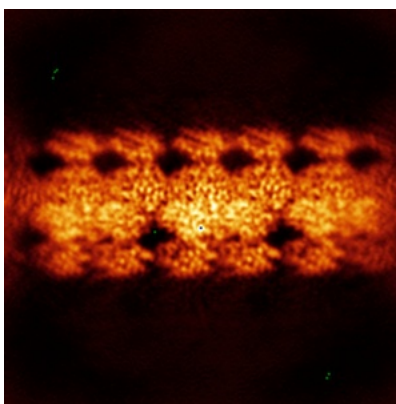


Z

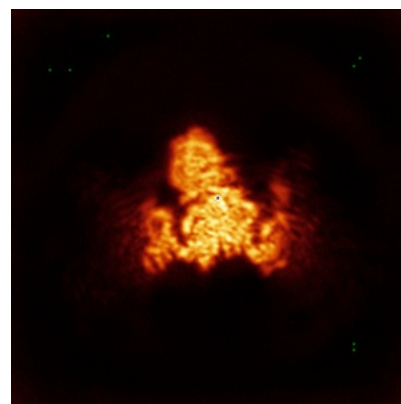
### 6.4.2 Raw map



X



Y



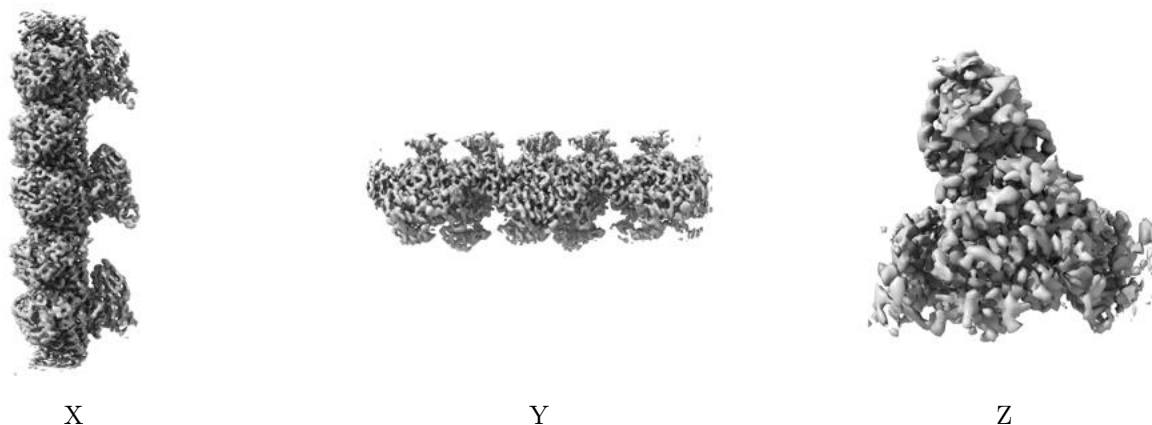
Z

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



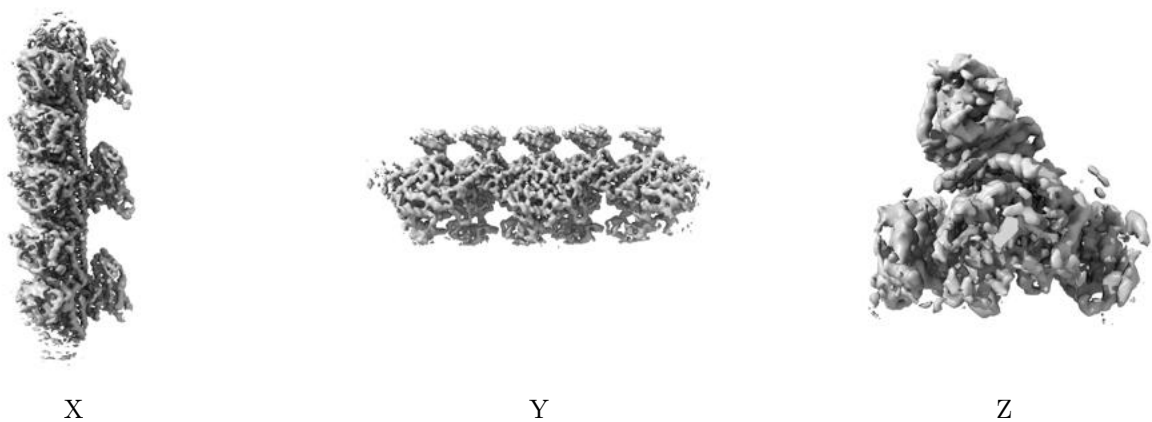
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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



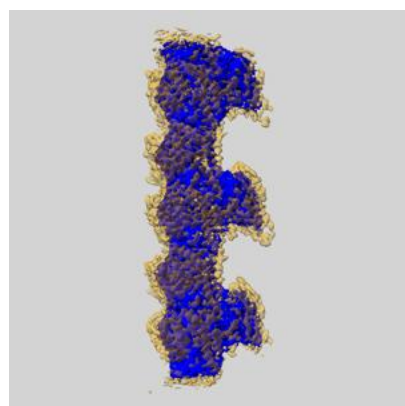
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

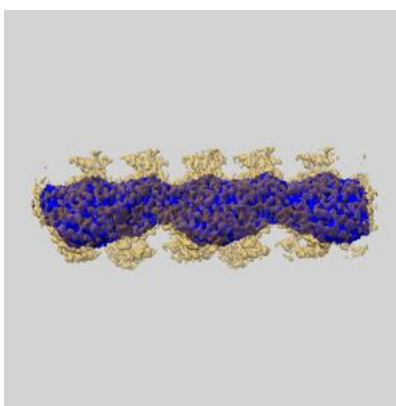
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

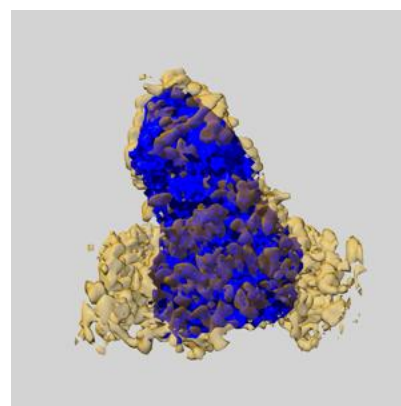
### 6.6.1 emd\_62874\_msk\_1.map [i](#)



X



Y

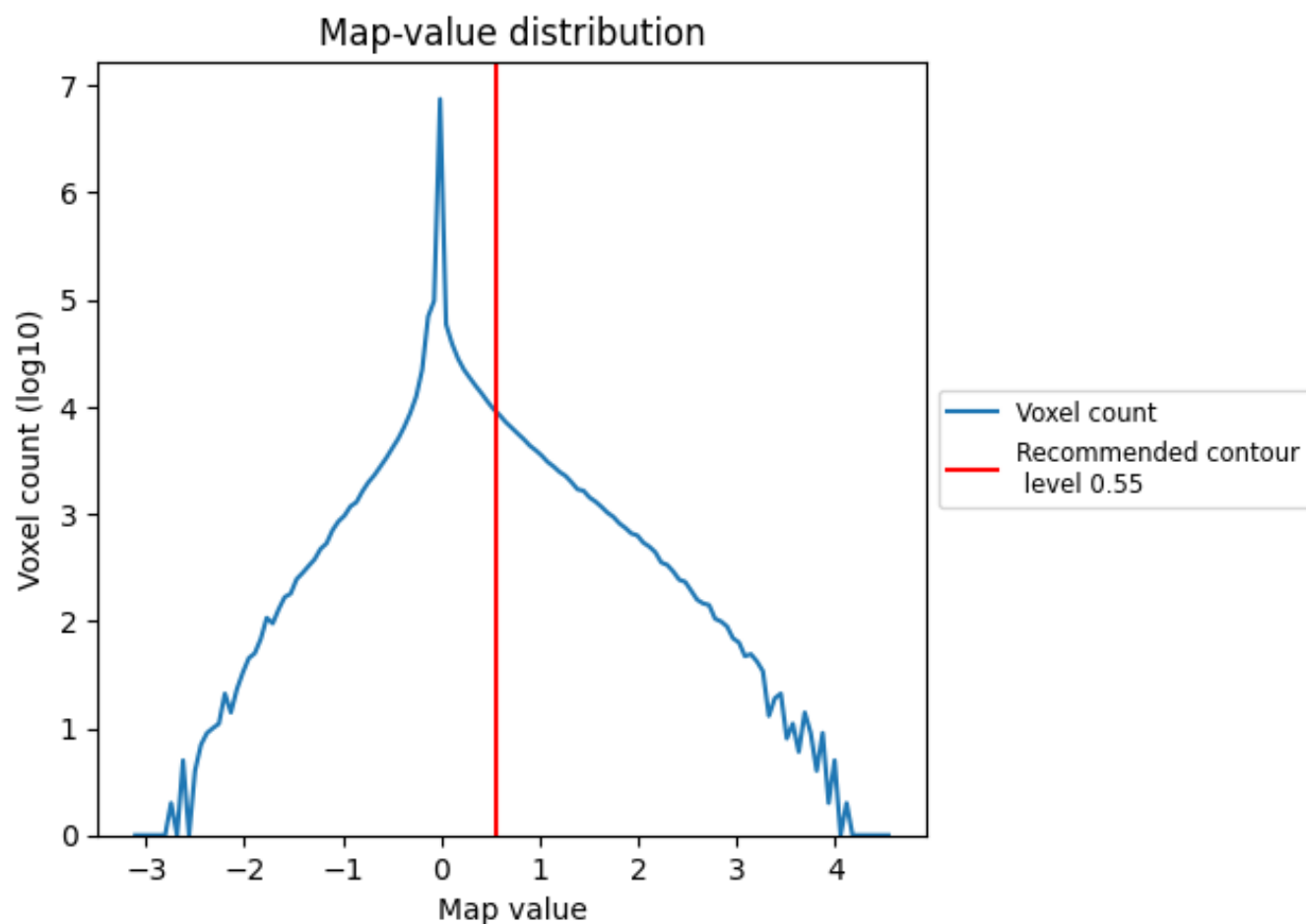


Z

## 7 Map analysis [i](#)

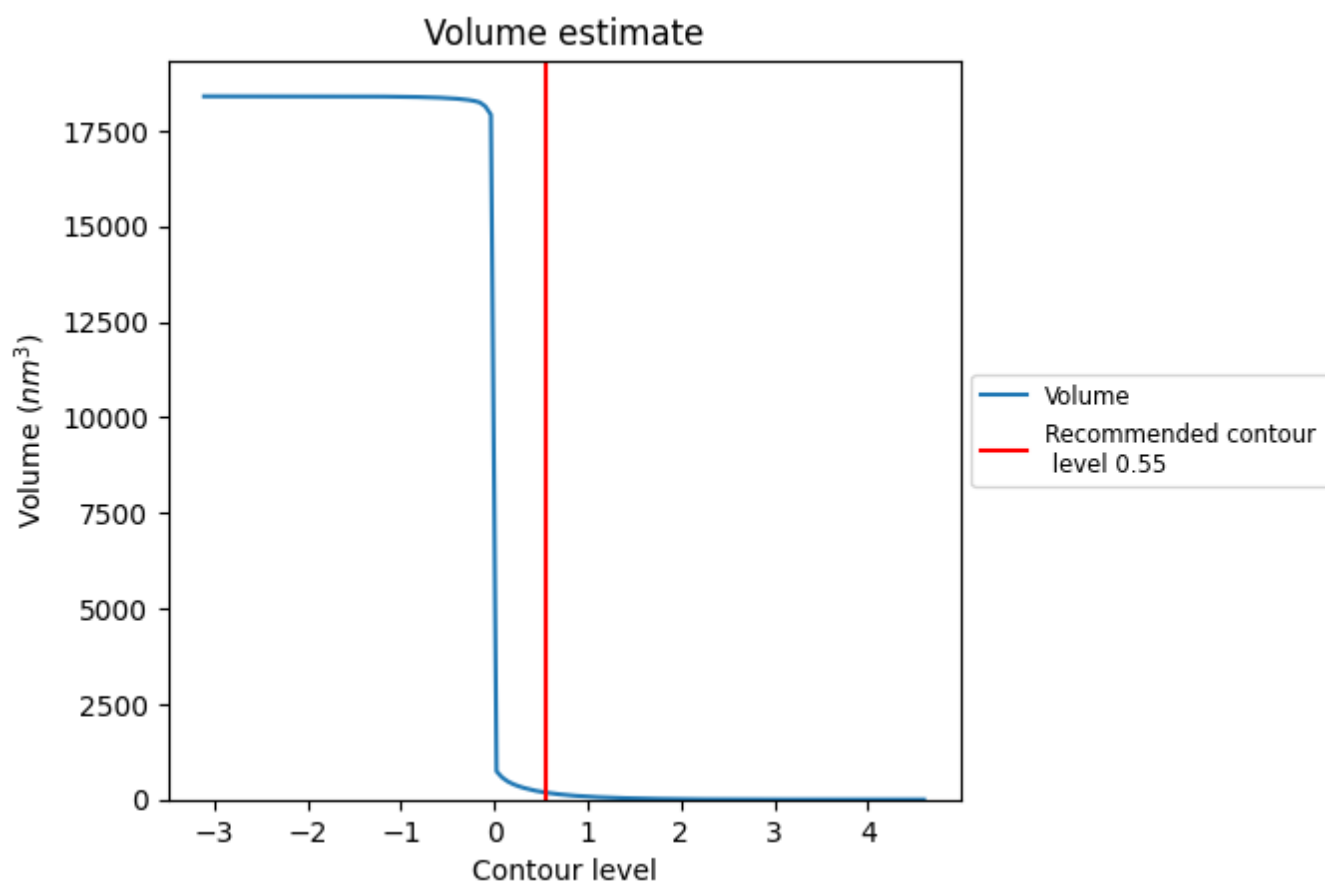
This section contains the results of statistical analysis of the map.

### 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.

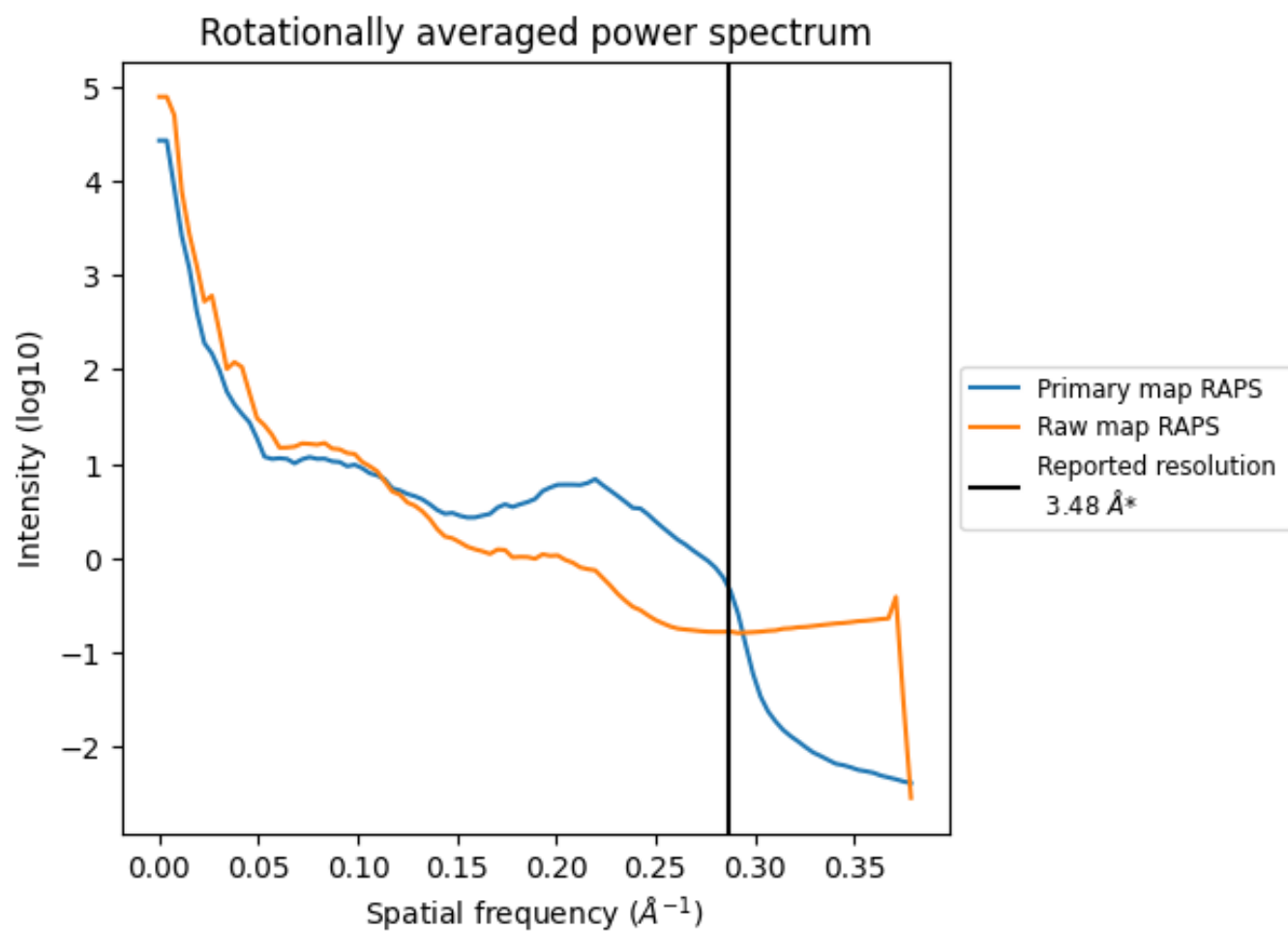
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm<sup>3</sup>; this corresponds to an approximate mass of 166 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 ⓘ

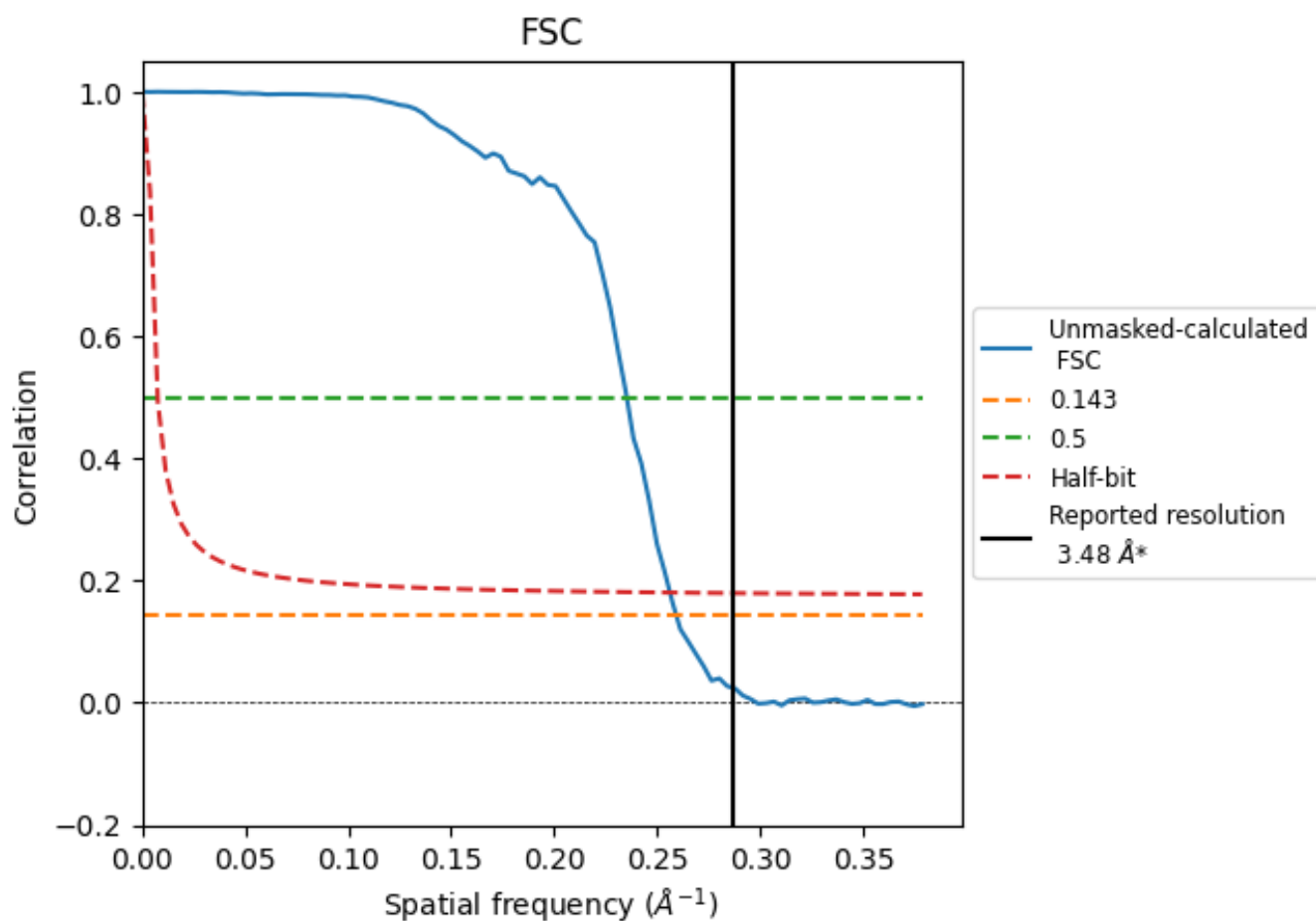


\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.287  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

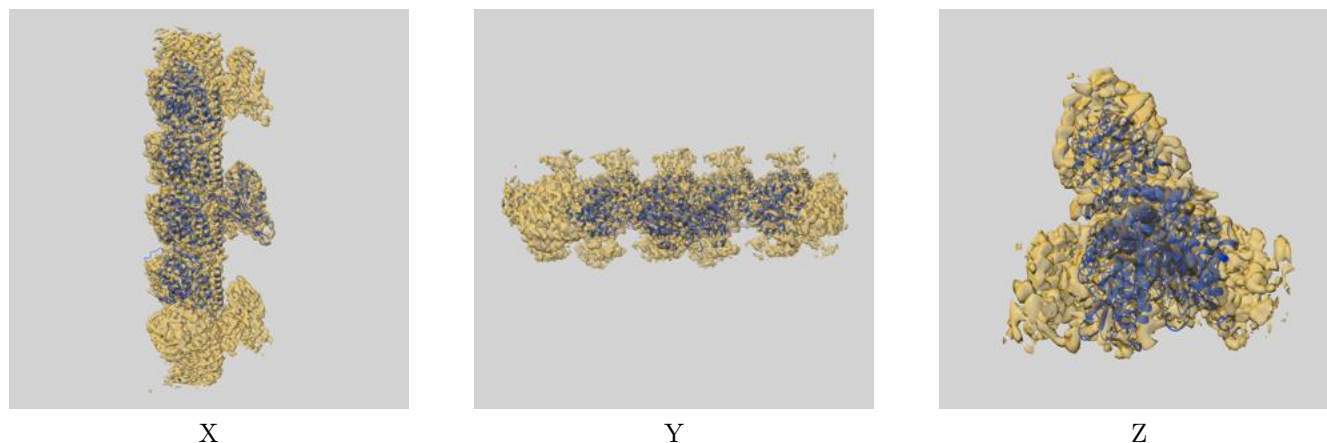
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	4.25	3.90

\*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 3.86 differs from the reported value 3.48 by more than 10 %

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

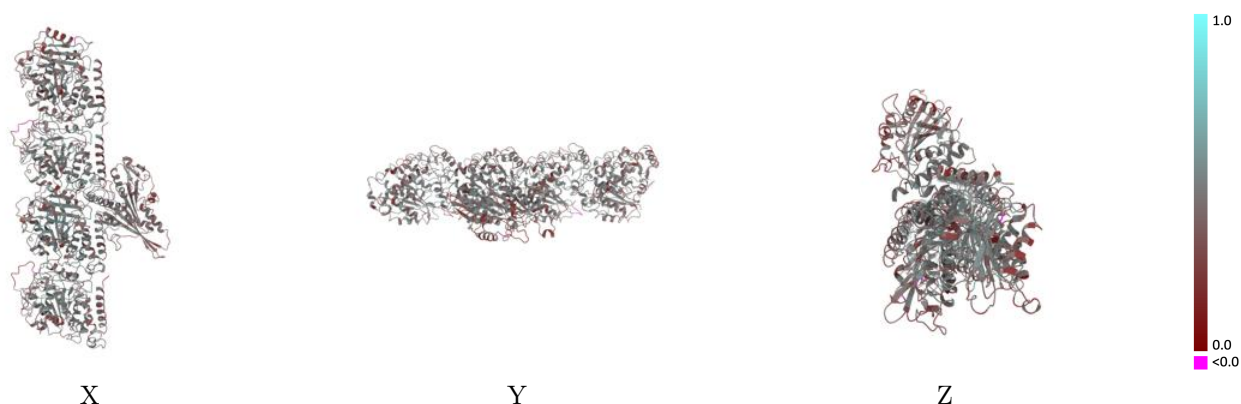
This section contains information regarding the fit between EMDB map EMD-62874 and PDB model 9L7M. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



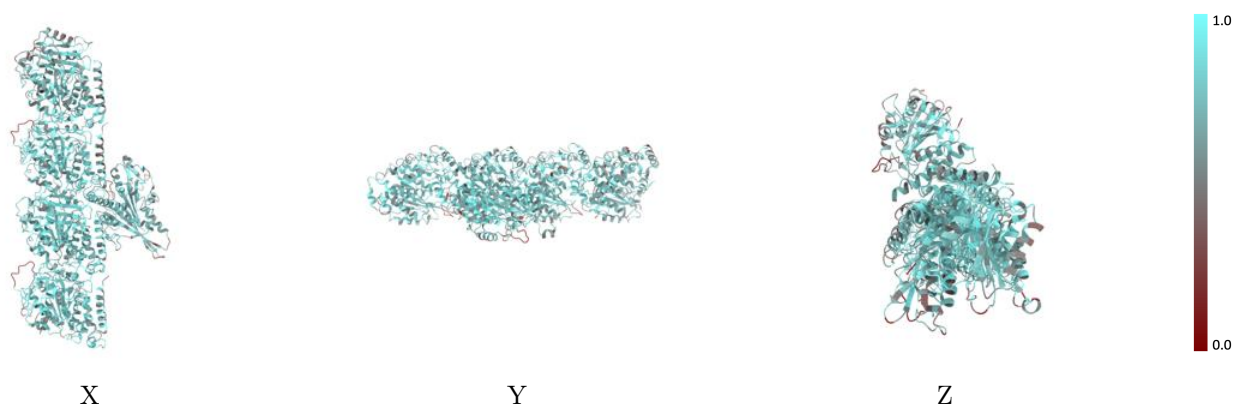
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

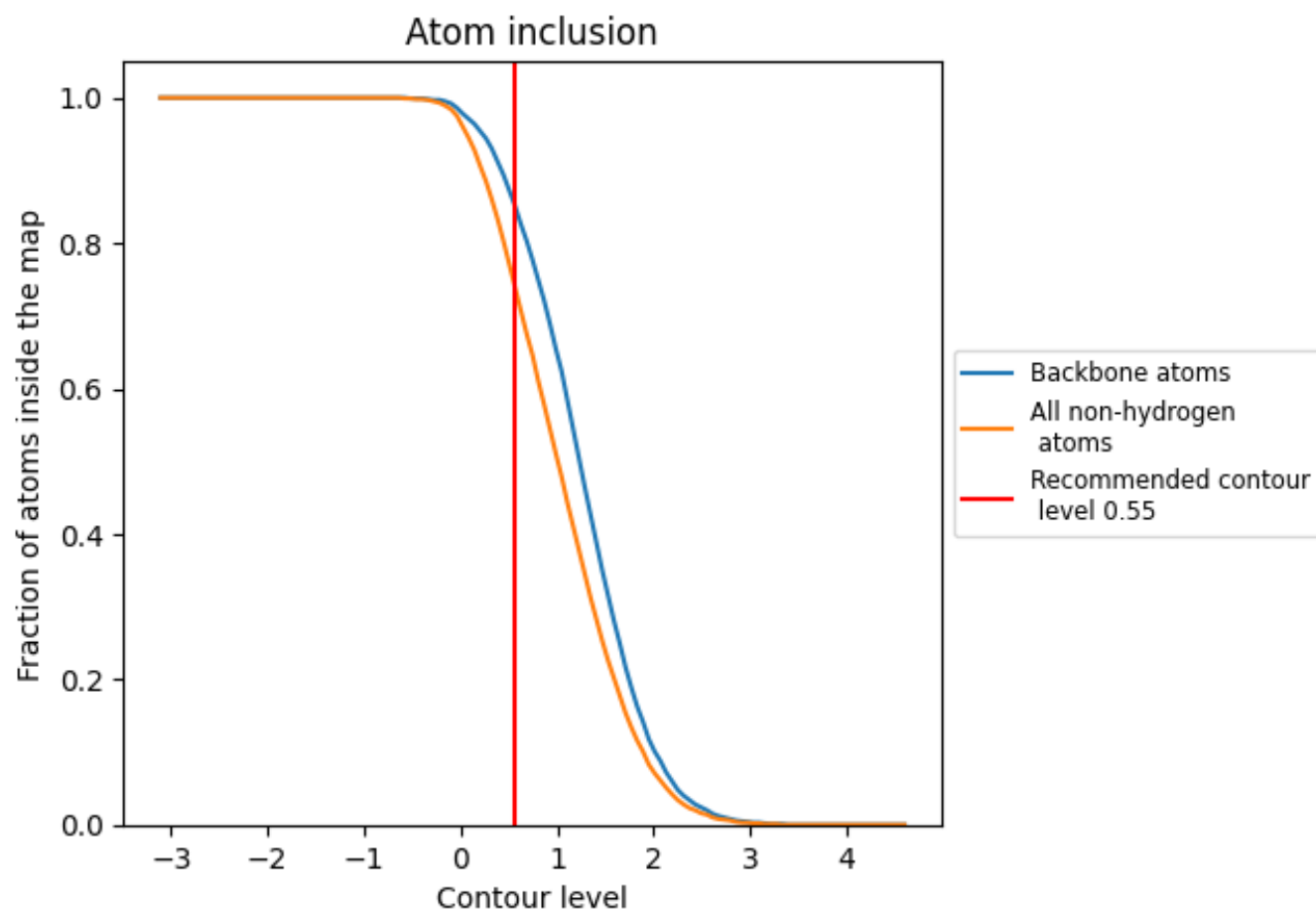
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.55).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7470	<div></div> 0.4340
A	<div></div> 0.7500	<div></div> 0.4360
B	<div></div> 0.8020	<div></div> 0.4630
C	<div></div> 0.7800	<div></div> 0.4500
D	<div></div> 0.7020	<div></div> 0.4240
K	<div></div> 0.6850	<div></div> 0.3860

