



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:38 AM UTC

PDB ID : 7AQO / pdb_00007aqo
EMDB ID : EMD-11871
Title : yeast THO-Sub2 complex dimer
Authors : Schuller, S.K.; Schuller, J.M.; Prabu, R.J.; Baumgartner, M.; Bonneau, F.;
basquin, J.; Conti, E.
Deposited on : 2020-10-22
Resolution : 4.50 Å(reported)
Based on initial model : 7APX

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

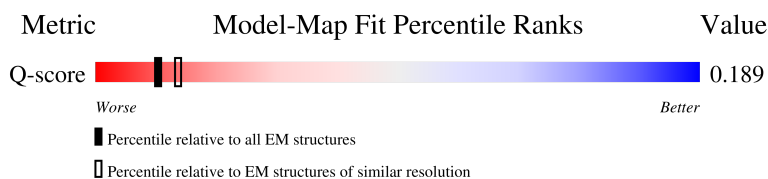
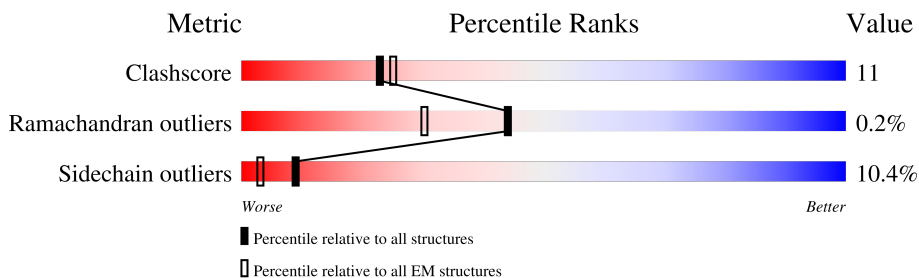
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	1601	
1	G	1601	
2	B	720	
2	H	720	

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Mol	Chain	Length	Quality of chain
3	E	380	76% 14% • 8%
3	K	380	• 75% 15% • 8%
4	F	400	8% 54% 35% • 10%
4	L	400	80% 55% 34% • 10%
5	C	261	60% 19% 7% 13%
5	J	261	20% 61% 20% 7% 12%
6	D	392	45% 10% • 43%
6	I	392	18% 46% 9% • 42%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 40261 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 THO complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	1079	Total	C	N	O	S	0	0
			7785	5074	1304	1379	28		
1	A	1079	Total	C	N	O	S	0	0
			7785	5074	1304	1379	28		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP A0A6A5Q535
G	-2	ALA	-	expression tag	UNP A0A6A5Q535
G	-1	ALA	-	expression tag	UNP A0A6A5Q535
G	0	SER	-	expression tag	UNP A0A6A5Q535
A	-3	GLY	-	expression tag	UNP A0A6A5Q535
A	-2	ALA	-	expression tag	UNP A0A6A5Q535
A	-1	ALA	-	expression tag	UNP A0A6A5Q535
A	0	SER	-	expression tag	UNP A0A6A5Q535

- Molecule 2 is a protein called THO complex subunit HPR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	563	Total	C	N	O	S	0	0
			4143	2713	693	721	16		
2	B	563	Total	C	N	O	S	0	0
			4143	2713	693	721	16		

- Molecule 3 is a protein called TEX1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	348	Total	C	N	O	S	0	0
			2357	1530	402	414	11		
3	E	348	Total	C	N	O	S	0	0
			2357	1530	402	414	11		

- Molecule 4 is a protein called EM14S01-3B_G0007820.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	361	Total	C	N	O	S	0	0
			2818	1783	491	535	9		
4	F	361	Total	C	N	O	S	0	0
			2818	1783	491	535	9		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	GLY	-	expression tag	UNP A0A6A5Q316
L	48	ALA	-	expression tag	UNP A0A6A5Q316
L	49	ALA	-	expression tag	UNP A0A6A5Q316
L	50	SER	-	expression tag	UNP A0A6A5Q316
F	47	GLY	-	expression tag	UNP A0A6A5Q316
F	48	ALA	-	expression tag	UNP A0A6A5Q316
F	49	ALA	-	expression tag	UNP A0A6A5Q316
F	50	SER	-	expression tag	UNP A0A6A5Q316

- Molecule 5 is a protein called BJ4_G0025130.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	230	Total	C	N	O	S	1	0
			1588	997	278	310	3		
5	C	227	Total	C	N	O	S	1	0
			1573	988	275	307	3		

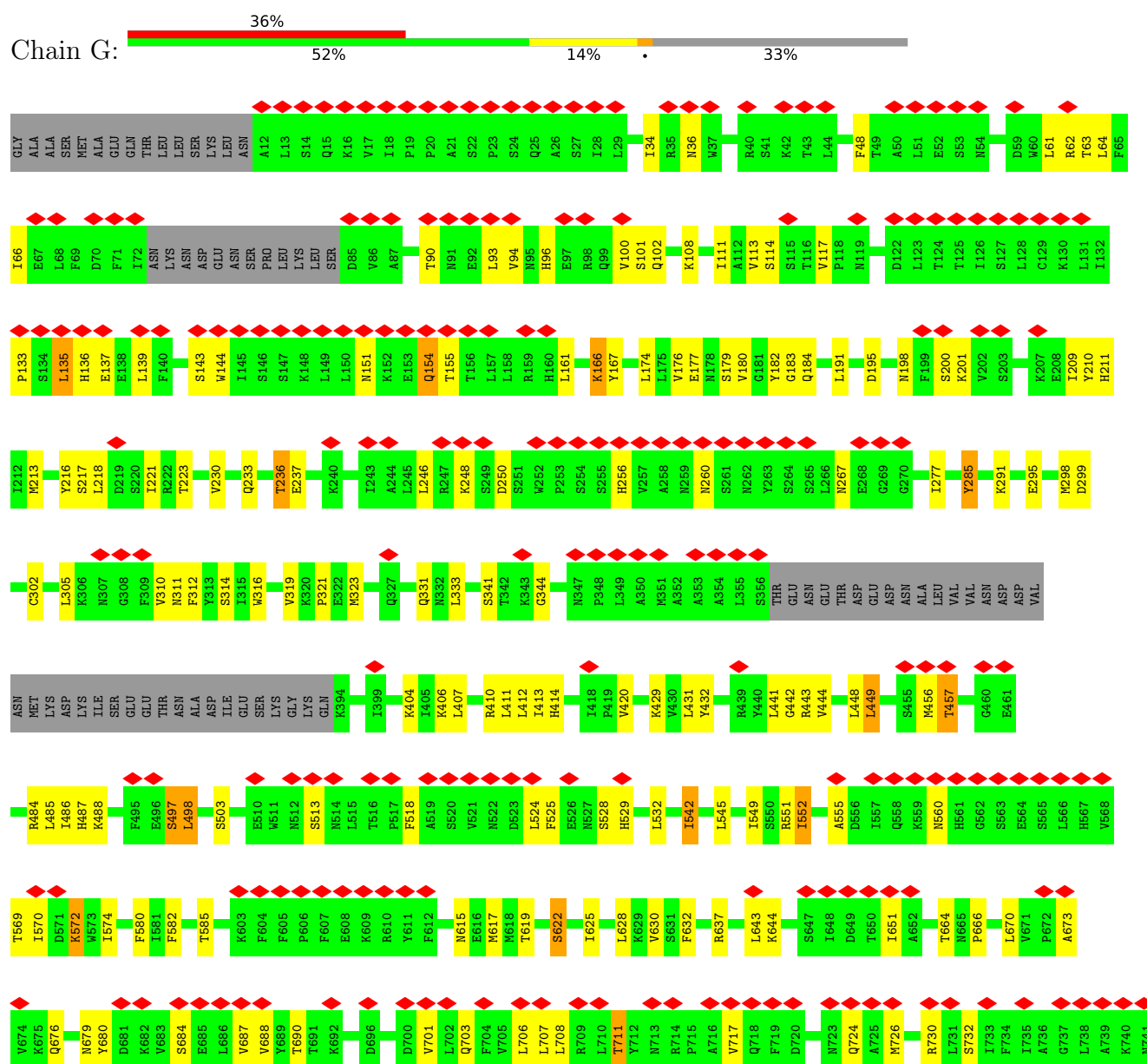
- Molecule 6 is a protein called THO complex subunit MFT1.

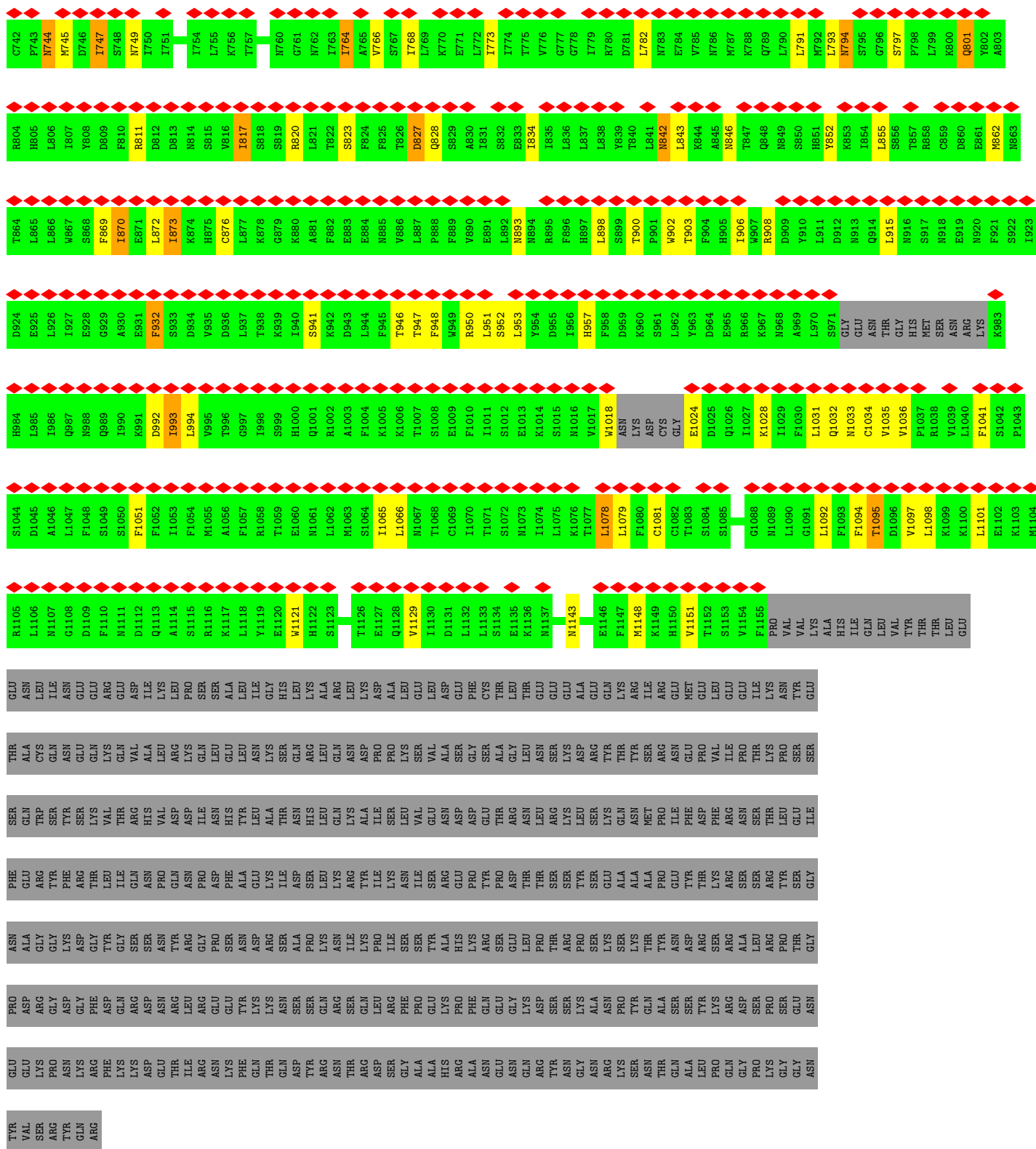
Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	227	Total	C	N	O	S	0	0
			1452	902	267	282	1		
6	D	225	Total	C	N	O	S	0	0
			1442	896	265	280	1		

3 Residue-property plots [i](#)

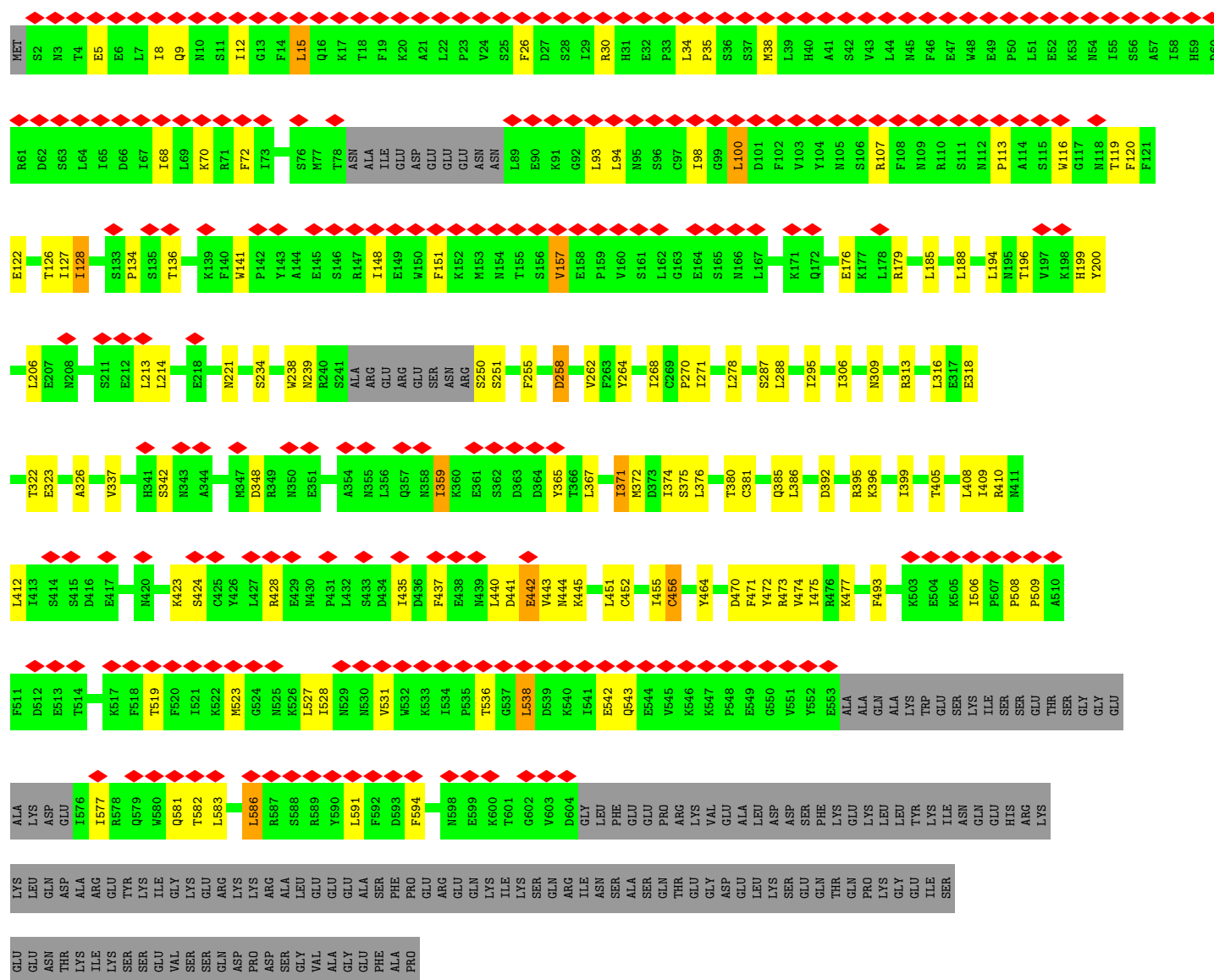
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: THO complex subunit 2

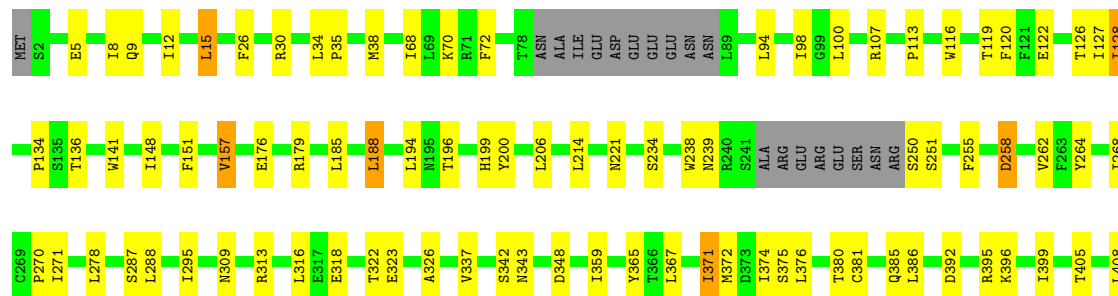


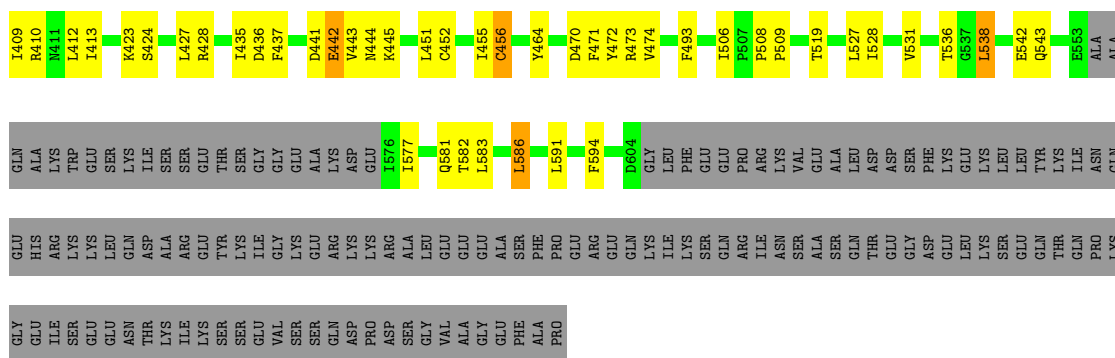


- Molecule 2: THO complex subunit HPR1



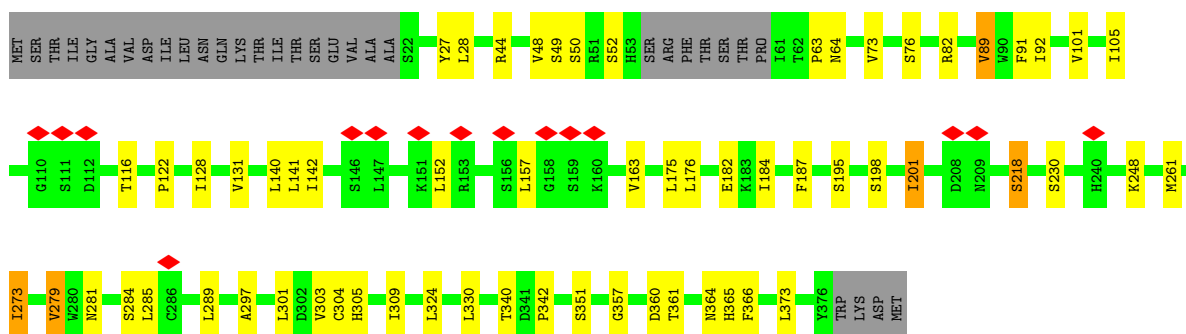
• Molecule 2: THO complex subunit HPR1





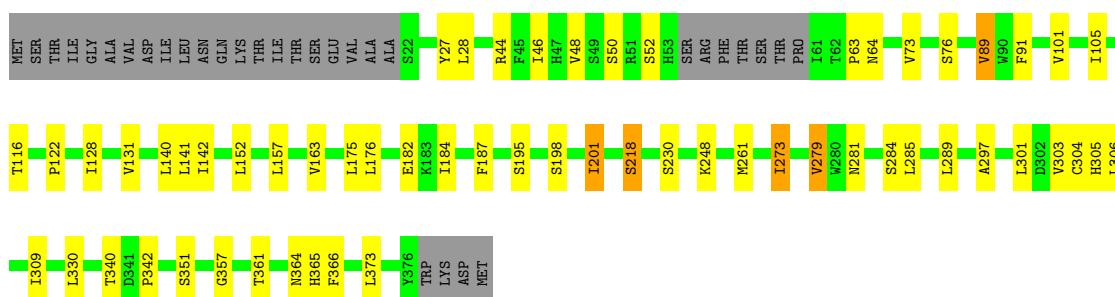
• Molecule 3: TEX1 isoform 1

Chain K: 75% 15% 8%



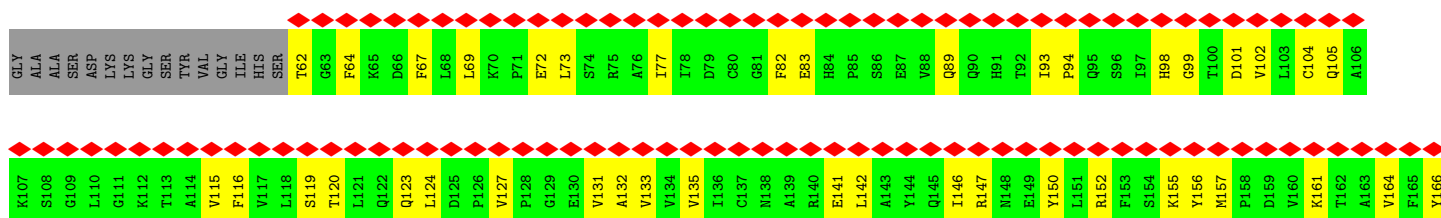
• Molecule 3: TEX1 isoform 1

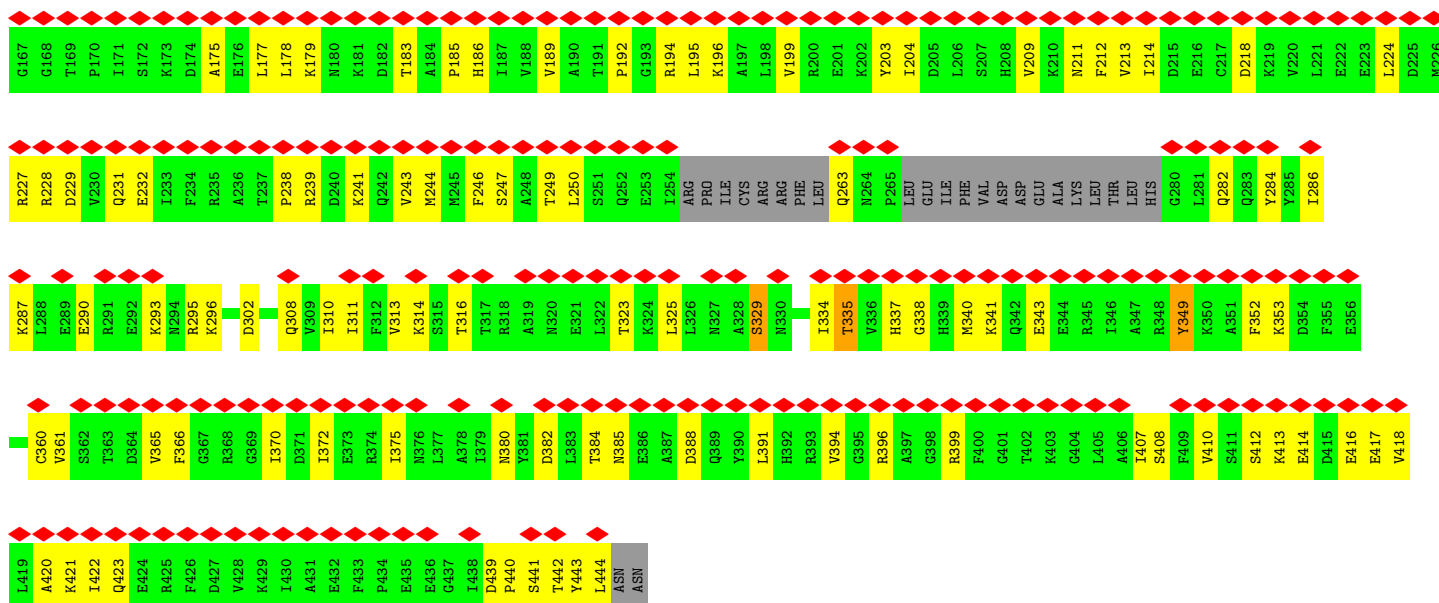
Chain E: 76% 14% 8%



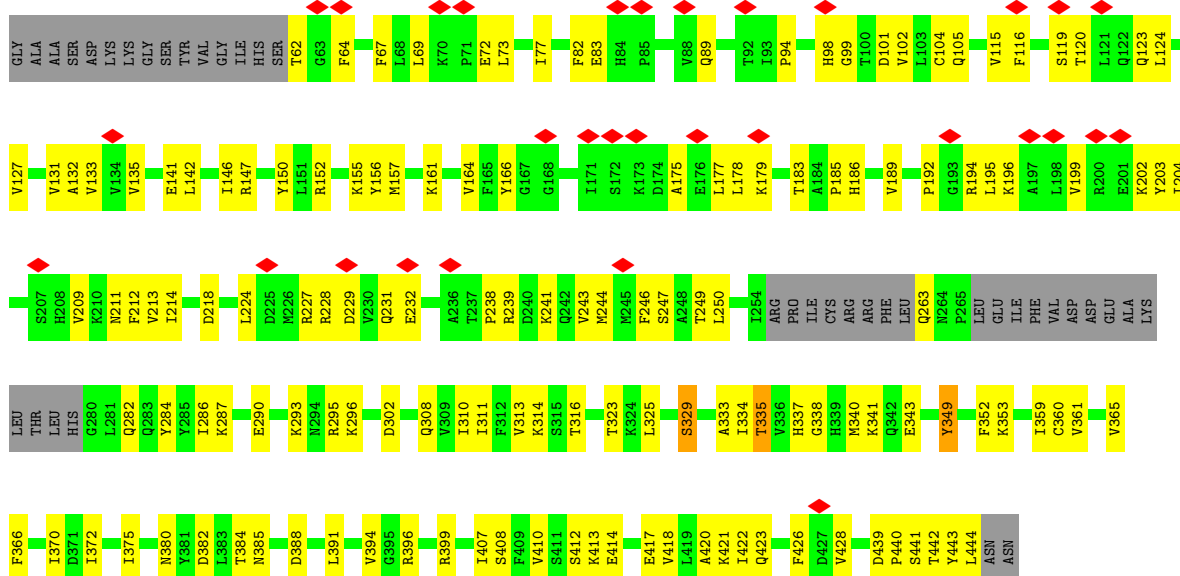
• Molecule 4: EM14S01-3B_G0007820.mRNA.1.CDS.1

Chain L: 55% 34% 10%

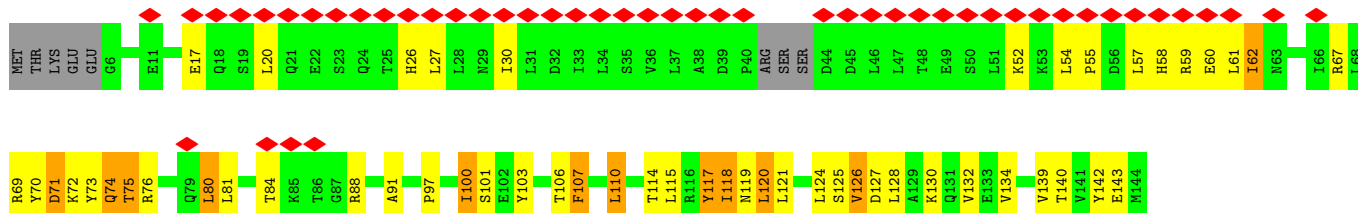




• Molecule 4: EM14S01-3B_G0007820.mRNA.1.CDS.1

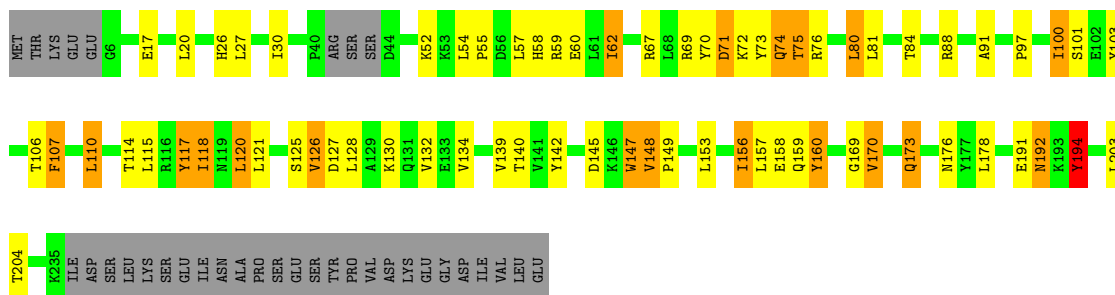


• Molecule 5: BJ4_G0025130.mRNA.1.CDS.1

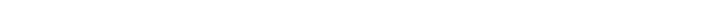


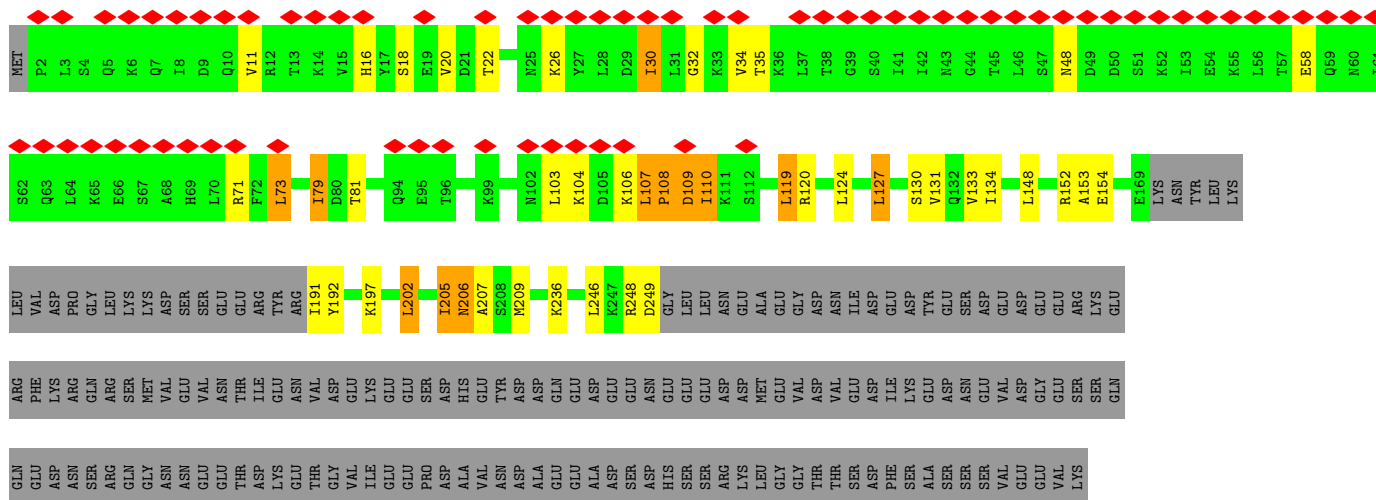
- Molecule 5: BJ4 G0025130.mRNA.1.CDS.1

Chain C: 60% 19% 7% 13%



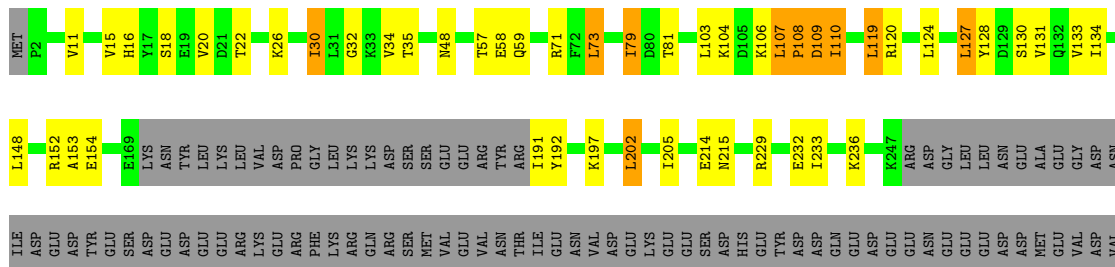
- Molecule 6: THO complex subunit MFT1

Chain I: 



- Molecule 6: THO complex subunit MFT1

Chain D: 45% 10% . 43%



GLU ASP ILE LYS GLU ASP ASN GLU SER SER GLN GLN GLU ASP ASN SER SER ARG GLN GLY ASN ASN GLU GLU THR ASP LYS GLU THR GLY VAL ILE GLU GLU PRO ASP ALA VAL ASN ASP ALA GLU GLU ALA ASP SER ASP HIS SER SER ARG LYS LEU GLY GLY THR THR

SER ASP PHE SER ALA SER SER SER VAL GLU GLU VAL LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113076	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 ($e^-/\text{\AA}^2$)	55.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.789	Depositor
Minimum map value	-0.636	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	414.0, 414.0, 414.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/7953	0.54	3/10871 (0.0%)
1	G	0.34	0/7953	0.54	3/10871 (0.0%)
2	B	0.31	0/4246	0.51	0/5811
2	H	0.31	0/4246	0.51	0/5811
3	E	0.23	0/2411	0.46	0/3318
3	K	0.23	0/2411	0.46	0/3318
4	F	0.15	0/2862	0.39	0/3865
4	L	0.15	0/2862	0.39	0/3865
5	C	1.10	1/1595 (0.1%)	1.47	5/2184 (0.2%)
5	J	1.09	0/1609	1.47	6/2202 (0.3%)
6	D	1.06	3/1454 (0.2%)	1.49	10/1989 (0.5%)
6	I	1.02	1/1464 (0.1%)	1.49	7/2003 (0.3%)
All	All	0.50	5/41066 (0.0%)	0.73	34/56108 (0.1%)

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
6	I	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	236	LYS	C-O	7.42	1.32	1.24
6	D	229	ARG	C-O	7.05	1.32	1.24
6	D	233	ILE	C-O	6.62	1.31	1.24
6	I	236	LYS	C-O	5.66	1.30	1.24
5	C	194	TYR	C-O	5.59	1.31	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	81	THR	CB-CA-C	-9.86	95.40	110.88
6	D	81	THR	CB-CA-C	-9.82	95.47	110.88
1	G	36	ASN	N-CA-C	-7.64	103.26	112.58
1	A	36	ASN	N-CA-C	-7.62	103.28	112.58
5	C	114	THR	CB-CA-C	-6.62	99.80	110.79
5	J	114	THR	CB-CA-C	-6.59	99.85	110.79
1	G	34	ILE	N-CA-C	-6.09	105.09	113.00
1	A	34	ILE	N-CA-C	-6.08	105.10	113.00
6	D	108	PRO	CB-CA-C	-5.95	103.60	113.06
6	I	108	PRO	CB-CA-C	-5.95	103.61	113.06
6	D	16	HIS	CA-C-N	-5.87	112.83	121.99
6	D	16	HIS	C-N-CA	-5.87	112.83	121.99
6	I	16	HIS	CA-C-N	-5.81	112.85	122.08
6	I	16	HIS	C-N-CA	-5.81	112.85	122.08
6	D	236	LYS	CA-C-N	-5.58	112.82	120.46
6	D	236	LYS	C-N-CA	-5.58	112.82	120.46
6	D	232	GLU	CA-C-N	-5.56	112.84	120.46
6	D	232	GLU	C-N-CA	-5.56	112.84	120.46
5	C	160	TYR	CB-CA-C	-5.50	101.65	110.79
5	J	160	TYR	CB-CA-C	-5.49	101.68	110.79
6	D	58	GLU	CA-C-N	-5.37	112.62	121.92
6	D	58	GLU	C-N-CA	-5.37	112.62	121.92
6	I	58	GLU	CA-C-N	-5.35	112.66	121.92
6	I	58	GLU	C-N-CA	-5.35	112.66	121.92
1	G	993	ILE	CA-C-O	-5.32	114.13	120.78
1	A	993	ILE	CA-C-O	-5.31	114.15	120.78
5	C	145	ASP	N-CA-C	-5.28	107.50	114.31
5	J	145	ASP	N-CA-C	-5.27	107.52	114.31
5	C	75	THR	CA-CB-OG1	-5.19	101.81	109.60
5	J	75	THR	CA-CB-OG1	-5.19	101.82	109.60
5	J	119	ASN	O-C-N	5.12	127.55	122.12
6	I	236	LYS	N-CA-C	-5.06	105.85	111.36
5	J	117	TYR	CB-CA-C	-5.02	103.00	110.88
5	C	117	TYR	CB-CA-C	-5.01	103.01	110.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	206	ASN	Mainchain

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	7785	0	7050	144	0
1	G	7785	0	7050	137	0
2	B	4143	0	3661	76	0
2	H	4143	0	3661	78	0
3	E	2357	0	1985	30	0
3	K	2357	0	1985	32	0
4	F	2818	0	2793	104	0
4	L	2818	0	2793	102	0
5	C	1573	0	1319	80	0
5	J	1588	0	1324	79	0
6	D	1442	0	1153	49	0
6	I	1452	0	1157	49	0
All	All	40261	0	35931	852	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 11.

All (852) 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)
5:C:67:ARG:O	5:C:71:ASP:OD1	1.58	1.21
5:J:67:ARG:O	5:J:71:ASP:OD1	1.58	1.20
3:K:50:SER:CB	3:E:46:ILE:HD12	1.71	1.20
5:C:117:TYR:CZ	6:D:120:ARG:HD3	1.84	1.12
5:J:117:TYR:CZ	6:I:120:ARG:HD3	1.84	1.11
5:J:117:TYR:OH	6:I:120:ARG:HD3	1.50	1.10
5:C:117:TYR:OH	6:D:120:ARG:HD3	1.50	1.08
3:K:50:SER:HB2	3:E:46:ILE:HD12	1.29	1.05
3:K:50:SER:HB2	3:E:46:ILE:CD1	1.96	0.94
5:J:74:GLN:HA	5:J:74:GLN:HE21	1.31	0.93
5:J:62:ILE:HD13	5:J:62:ILE:H	1.33	0.93
5:C:74:GLN:HE21	5:C:74:GLN:HA	1.32	0.92
5:C:62:ILE:HD13	5:C:62:ILE:H	1.33	0.91
2:H:239:ASN:CA	5:J:101:SER:OG	2.21	0.89
2:H:239:ASN:CB	5:J:101:SER:OG	2.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:SER:HB3	3:E:46:ILE:HD12	1.55	0.88
6:D:104:LYS:HA	6:D:107:LEU:HD12	1.56	0.88
5:J:160:TYR:CE2	6:I:127:LEU:HA	2.09	0.87
5:C:160:TYR:CE2	6:D:127:LEU:HA	2.09	0.86
6:I:104:LYS:HA	6:I:107:LEU:HD12	1.56	0.86
6:D:120:ARG:HB2	6:D:120:ARG:NH1	1.90	0.86
6:I:120:ARG:HB2	6:I:120:ARG:NH1	1.90	0.86
5:C:110:LEU:O	5:C:110:LEU:HD12	1.76	0.85
6:I:127:LEU:HD12	6:I:127:LEU:O	1.76	0.85
6:D:120:ARG:HB2	6:D:120:ARG:HH11	1.41	0.85
2:H:313:ARG:NH2	5:J:127:ASP:OD1	2.10	0.85
6:I:120:ARG:HB2	6:I:120:ARG:HH11	1.41	0.85
3:K:49:SER:CB	3:E:50:SER:HB2	2.07	0.85
2:B:239:ASN:CA	5:C:101:SER:OG	2.26	0.84
5:J:110:LEU:O	5:J:110:LEU:HD12	1.76	0.84
1:A:113:VAL:HG13	5:C:69:ARG:HD3	1.59	0.83
6:D:127:LEU:HD12	6:D:127:LEU:O	1.76	0.82
4:L:323:THR:HG21	4:L:335:THR:HB	1.62	0.82
5:C:71:ASP:OD1	5:C:71:ASP:N	2.13	0.81
4:F:323:THR:HG21	4:F:335:THR:HB	1.62	0.80
2:B:239:ASN:CB	5:C:101:SER:OG	2.29	0.80
6:I:248:ARG:O	6:I:249:ASP:C	2.25	0.80
1:G:113:VAL:HG13	5:J:69:ARG:HD3	1.64	0.79
4:L:131:VAL:HG21	4:L:204:ILE:HD11	1.66	0.78
2:H:239:ASN:HA	5:J:101:SER:OG	1.83	0.78
2:B:313:ARG:NH2	5:C:127:ASP:OD1	2.16	0.78
4:F:131:VAL:HG21	4:F:204:ILE:HD11	1.66	0.77
5:C:153:LEU:HD12	5:C:153:LEU:O	1.85	0.77
1:G:744:ASN:N	1:G:744:ASN:OD1	2.18	0.77
5:J:153:LEU:HD12	5:J:153:LEU:O	1.84	0.76
1:A:744:ASN:OD1	1:A:744:ASN:N	2.18	0.75
5:J:71:ASP:OD1	5:J:71:ASP:N	2.13	0.75
5:J:118:ILE:C	5:J:118:ILE:HD13	2.11	0.75
5:C:118:ILE:C	5:C:118:ILE:HD13	2.11	0.75
1:G:166:LYS:NZ	6:I:18:SER:OG	2.20	0.75
4:L:104:CYS:HB3	4:L:246:PHE:HD2	1.51	0.75
2:B:239:ASN:HA	5:C:101:SER:OG	1.86	0.73
4:F:104:CYS:HB3	4:F:246:PHE:HD2	1.51	0.73
1:A:794:ASN:HD21	1:A:953:LEU:HD23	1.54	0.73
6:D:109:ASP:OD1	6:D:109:ASP:N	2.19	0.72
1:A:260:ASN:ND2	1:A:305:LEU:O	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:109:ASP:OD1	6:I:109:ASP:N	2.19	0.72
3:K:44:ARG:HH22	3:K:63:PRO:HA	1.54	0.72
4:L:380:ASN:ND2	4:L:408:SER:OG	2.20	0.72
1:G:260:ASN:ND2	1:G:305:LEU:O	2.20	0.72
3:K:44:ARG:HH12	3:K:64:ASN:H	1.38	0.72
1:G:794:ASN:HD21	1:G:953:LEU:HD23	1.54	0.71
3:E:44:ARG:HH22	3:E:63:PRO:HA	1.54	0.71
3:E:44:ARG:HH12	3:E:64:ASN:H	1.38	0.71
1:A:524:LEU:O	1:A:528:SER:OG	2.09	0.70
2:B:270:PRO:HB3	2:B:405:THR:HG23	1.74	0.70
1:A:108:LYS:O	1:A:111:ILE:HG22	1.91	0.70
4:F:380:ASN:ND2	4:F:408:SER:OG	2.21	0.70
4:L:132:ALA:HA	4:L:209:VAL:HA	1.74	0.70
6:D:127:LEU:HD12	6:D:127:LEU:C	2.16	0.70
6:I:127:LEU:HD12	6:I:127:LEU:C	2.16	0.70
1:G:108:LYS:O	1:G:111:ILE:HG22	1.91	0.69
5:C:62:ILE:HD13	5:C:62:ILE:N	2.04	0.69
1:A:166:LYS:NZ	6:D:18:SER:OG	2.24	0.69
1:G:1032:GLN:HE22	2:H:591:LEU:H	1.39	0.69
1:A:221:ILE:HG23	1:A:277:ILE:HD11	1.75	0.69
4:F:132:ALA:HA	4:F:209:VAL:HA	1.74	0.69
2:H:270:PRO:HB3	2:H:405:THR:HG23	1.74	0.68
1:A:1032:GLN:HE22	2:B:591:LEU:H	1.39	0.68
5:C:107:PHE:CE2	6:D:110:ILE:HD11	2.29	0.68
1:G:221:ILE:HG23	1:G:277:ILE:HD11	1.75	0.68
5:J:62:ILE:HD13	5:J:62:ILE:N	2.04	0.68
1:G:524:LEU:O	1:G:528:SER:OG	2.09	0.68
1:A:93:LEU:HD21	1:A:133:PRO:HD2	1.76	0.68
1:A:551:ARG:NH1	3:E:285:LEU:O	2.21	0.68
5:J:110:LEU:HD12	5:J:110:LEU:C	2.15	0.68
1:G:551:ARG:NH1	3:K:285:LEU:O	2.21	0.68
5:C:110:LEU:HD12	5:C:110:LEU:C	2.15	0.68
3:K:49:SER:CB	3:E:50:SER:CB	2.71	0.68
5:C:74:GLN:HA	5:C:74:GLN:NE2	2.07	0.68
2:H:250:SER:OG	2:H:251:SER:N	2.27	0.68
2:H:392:ASP:OD2	2:H:396:LYS:NZ	2.27	0.68
5:J:107:PHE:CE2	6:I:110:ILE:HD11	2.29	0.68
1:G:93:LEU:HD21	1:G:133:PRO:HD2	1.76	0.68
5:J:76:ARG:HD2	5:J:76:ARG:O	1.94	0.67
5:J:160:TYR:OH	6:I:130:SER:HB2	1.94	0.67
5:C:76:ARG:HD2	5:C:76:ARG:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:102:VAL:HB	4:L:244:MET:HG3	1.77	0.67
1:A:726:MET:O	1:A:730:ARG:NH2	2.28	0.67
1:G:1148:MET:HA	1:G:1151:VAL:HG12	1.76	0.66
1:A:1148:MET:HA	1:A:1151:VAL:HG12	1.76	0.66
2:B:392:ASP:OD2	2:B:396:LYS:NZ	2.27	0.66
4:F:102:VAL:HB	4:F:244:MET:HG3	1.77	0.66
1:G:176:VAL:HG21	2:H:408:LEU:HD22	1.77	0.66
5:C:160:TYR:CE2	6:D:127:LEU:CA	2.79	0.66
2:B:250:SER:OG	2:B:251:SER:N	2.27	0.66
1:G:726:MET:O	1:G:730:ARG:NH2	2.28	0.66
1:A:703:GLN:NE2	1:A:749:ASN:HB2	2.11	0.66
5:C:160:TYR:OH	6:D:130:SER:HB2	1.94	0.66
1:G:797:SER:O	1:G:801:GLN:NE2	2.30	0.65
2:H:35:PRO:HG2	2:H:38:MET:HG3	1.78	0.65
1:G:703:GLN:NE2	1:G:749:ASN:HB2	2.11	0.65
6:I:120:ARG:HH11	6:I:120:ARG:CB	2.10	0.65
4:L:67:PHE:HB3	4:L:69:LEU:HD13	1.79	0.65
1:A:797:SER:O	1:A:801:GLN:NE2	2.30	0.65
1:A:1031:LEU:HA	1:A:1035:VAL:HG12	1.79	0.65
2:B:35:PRO:HG2	2:B:38:MET:HG3	1.78	0.65
5:J:117:TYR:OH	6:I:120:ARG:CD	2.39	0.65
5:J:160:TYR:CE2	6:I:127:LEU:CA	2.79	0.65
1:A:176:VAL:HG21	2:B:408:LEU:HD22	1.77	0.65
1:A:195:ASP:HB3	1:A:198:ASN:HB3	1.79	0.65
1:A:952:SER:OG	1:A:953:LEU:N	2.28	0.65
3:K:218:SER:HA	3:K:261:MET:HE2	1.79	0.65
1:A:114:SER:HA	1:A:117:VAL:HG12	1.79	0.65
5:J:160:TYR:CD2	6:I:127:LEU:CA	2.80	0.65
4:F:101:ASP:HA	4:F:243:VAL:O	1.97	0.64
1:A:195:ASP:OD2	1:A:201:LYS:NZ	2.30	0.64
3:E:273:ILE:HG13	3:E:297:ALA:HB1	1.79	0.64
3:K:364:ASN:OD1	3:K:365:HIS:N	2.30	0.64
4:F:67:PHE:HB3	4:F:69:LEU:HD13	1.79	0.64
5:C:160:TYR:CD2	6:D:127:LEU:CA	2.80	0.64
3:E:218:SER:HA	3:E:261:MET:HE2	1.78	0.64
1:G:1031:LEU:HA	1:G:1035:VAL:HG12	1.79	0.64
3:K:89:VAL:HG11	3:K:142:ILE:HD13	1.80	0.64
3:E:364:ASN:OD1	3:E:365:HIS:N	2.30	0.64
6:D:120:ARG:HH11	6:D:120:ARG:CB	2.10	0.64
1:G:195:ASP:OD2	1:G:201:LYS:NZ	2.31	0.64
4:L:101:ASP:HA	4:L:243:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:58:HIS:O	5:J:62:ILE:HD11	1.98	0.64
5:C:58:HIS:O	5:C:62:ILE:HD11	1.98	0.63
1:G:114:SER:HA	1:G:117:VAL:HG12	1.79	0.63
5:J:74:GLN:HA	5:J:74:GLN:NE2	2.07	0.63
1:G:195:ASP:HB3	1:G:198:ASN:HB3	1.79	0.63
2:H:365:TYR:CE2	6:I:106:LYS:HB3	2.33	0.63
4:L:142:LEU:O	4:L:146:ILE:HG12	1.98	0.63
1:G:1079:LEU:O	1:G:1143:ASN:ND2	2.32	0.63
5:C:117:TYR:OH	6:D:120:ARG:CD	2.39	0.63
3:K:273:ILE:HG13	3:K:297:ALA:HB1	1.79	0.63
3:E:304:CYS:SG	3:E:305:HIS:N	2.72	0.62
2:B:214:LEU:HB2	2:B:221:ASN:HD22	1.64	0.62
4:F:142:LEU:O	4:F:146:ILE:HG12	1.98	0.62
5:J:70:TYR:CZ	5:J:74:GLN:OE1	2.52	0.62
2:H:5:GLU:O	2:H:9:GLN:NE2	2.33	0.62
3:K:304:CYS:SG	3:K:305:HIS:N	2.72	0.62
4:L:135:VAL:HB	4:L:189:VAL:HG12	1.80	0.62
1:A:111:ILE:HG21	1:A:135:LEU:CD1	2.29	0.62
3:E:89:VAL:HG11	3:E:142:ILE:HD13	1.80	0.62
4:F:135:VAL:HB	4:F:189:VAL:HG12	1.80	0.62
1:G:111:ILE:HG21	1:G:135:LEU:CD1	2.29	0.62
2:H:410:ARG:NH1	2:H:456:CYS:SG	2.73	0.62
4:F:439:ASP:O	4:F:442:THR:OG1	2.16	0.62
5:C:70:TYR:CZ	5:C:74:GLN:OE1	2.52	0.62
2:H:313:ARG:NH2	5:J:127:ASP:CG	2.58	0.61
2:B:410:ARG:NH1	2:B:456:CYS:SG	2.73	0.61
5:C:160:TYR:CD2	6:D:127:LEU:HA	2.34	0.61
2:B:5:GLU:O	2:B:9:GLN:NE2	2.33	0.61
1:G:946:THR:O	1:G:950:ARG:HB2	2.01	0.61
2:H:214:LEU:HB2	2:H:221:ASN:HD22	1.65	0.61
1:A:1078:LEU:HD12	2:B:591:LEU:HD11	1.82	0.61
4:L:439:ASP:O	4:L:442:THR:OG1	2.16	0.60
5:J:160:TYR:CD2	6:I:127:LEU:HA	2.34	0.60
6:I:152:ARG:C	6:I:154:GLU:H	2.08	0.60
1:G:1078:LEU:HD12	2:H:591:LEU:HD11	1.82	0.60
1:G:703:GLN:HE21	1:G:749:ASN:HB2	1.66	0.60
5:J:81:LEU:O	5:J:84:THR:HG22	2.02	0.60
1:A:946:THR:O	1:A:950:ARG:HB2	2.01	0.60
5:J:120:LEU:HD23	6:I:124:LEU:HD23	1.83	0.60
6:D:152:ARG:C	6:D:154:GLU:H	2.08	0.60
1:A:1081:CYS:SG	2:B:583:LEU:HB3	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:GLN:HE21	1:A:749:ASN:HB2	1.66	0.59
5:J:117:TYR:CE2	6:I:120:ARG:HD3	2.34	0.59
6:D:32:GLY:HA2	6:D:35:THR:HG22	1.84	0.59
2:H:313:ARG:HH21	2:H:313:ARG:HG3	1.68	0.59
2:H:348:ASP:OD1	6:I:120:ARG:NH2	2.34	0.59
1:G:952:SER:OG	1:G:953:LEU:N	2.28	0.59
2:B:258:ASP:OD1	2:B:287:SER:OG	2.18	0.59
5:C:120:LEU:HD23	6:D:124:LEU:HD23	1.83	0.59
6:I:32:GLY:HA2	6:I:35:THR:HG22	1.84	0.59
1:G:143:SER:OG	1:G:144:TRP:N	2.35	0.59
4:L:175:ALA:O	4:L:179:LYS:HG2	2.03	0.59
1:A:1079:LEU:O	1:A:1143:ASN:ND2	2.32	0.59
2:H:258:ASP:OD1	2:H:287:SER:OG	2.18	0.59
4:L:177:LEU:O	4:L:183:THR:OG1	2.19	0.59
1:G:1081:CYS:SG	2:H:583:LEU:HB3	2.42	0.59
2:H:262:VAL:HG21	2:H:288:LEU:HD12	1.84	0.59
1:A:143:SER:OG	1:A:144:TRP:N	2.35	0.59
4:F:175:ALA:O	4:F:179:LYS:HG2	2.03	0.59
5:J:72:LYS:O	5:J:75:THR:OG1	2.20	0.58
5:C:81:LEU:O	5:C:84:THR:HG22	2.02	0.58
5:C:117:TYR:CE2	6:D:120:ARG:HD3	2.34	0.58
2:B:313:ARG:HH21	2:B:313:ARG:HG3	1.68	0.58
5:J:62:ILE:H	5:J:62:ILE:CD1	2.01	0.58
1:A:820:ARG:O	1:A:823:SER:OG	2.18	0.58
5:C:72:LYS:O	5:C:75:THR:OG1	2.20	0.58
2:B:262:VAL:HG21	2:B:288:LEU:HD12	1.84	0.58
5:J:121:LEU:O	5:J:125:SER:HB3	2.04	0.58
2:B:214:LEU:HB2	2:B:221:ASN:ND2	2.19	0.57
4:F:177:LEU:O	4:F:183:THR:OG1	2.19	0.57
4:F:178:LEU:HD13	4:F:204:ILE:HD13	1.86	0.57
5:J:97:PRO:O	5:J:100:ILE:HB	2.04	0.57
5:C:121:LEU:O	5:C:125:SER:HB3	2.04	0.57
6:D:148:LEU:HA	6:D:191:ILE:N	2.20	0.57
6:I:205:ILE:O	6:I:209:MET:N	2.32	0.57
5:C:73:TYR:N	5:C:73:TYR:CD1	2.73	0.57
1:A:111:ILE:HG21	1:A:135:LEU:HD12	1.87	0.57
5:J:76:ARG:HD2	5:J:76:ARG:C	2.29	0.57
4:L:178:LEU:HD13	4:L:204:ILE:HD13	1.86	0.57
2:B:365:TYR:CE2	6:D:106:LYS:HB3	2.40	0.57
5:C:62:ILE:H	5:C:62:ILE:CD1	2.01	0.57
2:B:313:ARG:NH2	5:C:127:ASP:CG	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:64:PHE:O	4:L:67:PHE:HB2	2.05	0.56
2:B:134:PRO:HG2	2:B:199:HIS:CD2	2.40	0.56
5:J:178:LEU:HD21	6:I:134:ILE:HG13	1.88	0.56
2:H:134:PRO:HG2	2:H:199:HIS:CD2	2.40	0.56
5:J:73:TYR:N	5:J:73:TYR:CD1	2.73	0.56
6:I:148:LEU:HA	6:I:191:ILE:N	2.20	0.56
5:C:97:PRO:O	5:C:100:ILE:HB	2.04	0.56
4:F:195:LEU:O	4:F:199:VAL:HG23	2.05	0.56
1:G:111:ILE:HG21	1:G:135:LEU:HD12	1.87	0.56
2:H:214:LEU:HB2	2:H:221:ASN:ND2	2.19	0.56
5:J:74:GLN:HE21	5:J:74:GLN:CA	2.13	0.56
4:F:64:PHE:O	4:F:67:PHE:HB2	2.05	0.56
4:L:195:LEU:O	4:L:199:VAL:HG23	2.05	0.56
1:G:820:ARG:O	1:G:823:SER:OG	2.18	0.56
1:A:846:ASN:O	2:B:581:GLN:NE2	2.40	0.55
1:A:48:PHE:CE1	1:A:61:LEU:HD21	2.42	0.55
1:G:842:ASN:OD1	1:G:843:LEU:N	2.40	0.55
5:C:178:LEU:HD21	6:D:134:ILE:HG13	1.88	0.55
1:G:846:ASN:O	2:H:581:GLN:NE2	2.40	0.55
1:G:902:TRP:O	1:G:906:ILE:HG13	2.07	0.55
1:G:429:LYS:HD3	1:G:432:TYR:HE2	1.72	0.55
5:C:73:TYR:N	5:C:73:TYR:HD1	2.05	0.55
4:F:127:VAL:H	4:F:186:HIS:CE1	2.25	0.55
4:F:420:ALA:HA	4:F:423:GLN:HE21	1.72	0.55
1:G:794:ASN:OD1	1:G:794:ASN:N	2.40	0.55
4:L:441:SER:HA	4:L:444:LEU:HG	1.88	0.55
1:G:48:PHE:CE1	1:G:61:LEU:HD21	2.42	0.54
1:A:90:THR:O	1:A:94:VAL:HG23	2.07	0.54
1:A:113:VAL:CG1	5:C:69:ARG:HD3	2.32	0.54
1:A:429:LYS:HD3	1:A:432:TYR:HE2	1.72	0.54
1:A:842:ASN:OD1	1:A:843:LEU:N	2.40	0.54
4:L:286:ILE:O	4:L:410:VAL:N	2.37	0.54
1:A:174:LEU:HB3	1:A:177:GLU:HG3	1.89	0.54
1:A:643:LEU:HD11	1:A:673:ALA:HA	1.89	0.54
1:A:666:PRO:HB2	1:A:701:VAL:HG11	1.89	0.54
4:L:418:VAL:O	4:L:422:ILE:HG23	2.08	0.54
3:E:73:VAL:HG21	3:E:122:PRO:HB3	1.88	0.54
4:F:73:LEU:O	4:F:77:ILE:HG12	2.08	0.54
4:F:441:SER:HA	4:F:444:LEU:HG	1.88	0.54
5:J:160:TYR:CD2	6:I:127:LEU:HB2	2.43	0.54
4:L:420:ALA:HA	4:L:423:GLN:HE21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:LEU:O	1:A:711:THR:OG1	2.22	0.54
1:A:902:TRP:O	1:A:906:ILE:HG13	2.07	0.54
2:B:264:TYR:O	2:B:268:ILE:HB	2.07	0.54
1:G:457:THR:O	1:G:457:THR:OG1	2.25	0.54
2:H:264:TYR:O	2:H:268:ILE:HB	2.07	0.54
1:A:617:MET:HE1	1:A:628:LEU:HD13	1.89	0.54
1:A:745:MET:HG3	1:A:747:ILE:HG23	1.90	0.54
5:C:160:TYR:CD2	6:D:127:LEU:HB2	2.42	0.54
1:G:670:LEU:HD12	1:G:701:VAL:HG12	1.89	0.54
2:H:194:LEU:HD21	5:J:91:ALA:HB2	1.90	0.54
1:A:794:ASN:OD1	1:A:794:ASN:N	2.40	0.54
4:F:239:ARG:HA	4:F:239:ARG:NH1	2.23	0.54
5:J:73:TYR:N	5:J:73:TYR:HD1	2.05	0.54
5:C:76:ARG:HD2	5:C:76:ARG:C	2.29	0.54
4:L:310:ILE:HG22	4:L:360:CYS:SG	2.48	0.54
4:F:77:ILE:HG23	4:F:82:PHE:HD2	1.72	0.54
1:G:442:GLY:HA3	1:G:542:ILE:HD13	1.90	0.54
1:G:582:PHE:HA	1:G:585:THR:HG22	1.90	0.54
1:G:745:MET:HG3	1:G:747:ILE:HG23	1.90	0.54
6:D:20:VAL:HG12	6:D:20:VAL:O	2.08	0.54
1:G:174:LEU:HB3	1:G:177:GLU:HG3	1.89	0.53
1:G:666:PRO:HB2	1:G:701:VAL:HG11	1.89	0.53
1:G:707:LEU:O	1:G:711:THR:OG1	2.22	0.53
1:A:442:GLY:HA3	1:A:542:ILE:HD13	1.90	0.53
1:A:670:LEU:HD12	1:A:701:VAL:HG12	1.89	0.53
4:F:418:VAL:O	4:F:422:ILE:HG23	2.08	0.53
4:L:239:ARG:NH1	4:L:239:ARG:HA	2.23	0.53
2:H:464:TYR:O	2:H:472:TYR:HB2	2.08	0.53
3:K:73:VAL:HG21	3:K:122:PRO:HB3	1.88	0.53
4:L:127:VAL:H	4:L:186:HIS:CE1	2.25	0.53
3:E:281:ASN:HD22	3:E:284:SER:H	1.57	0.53
5:J:148:VAL:HB	5:J:149:PRO:HD2	1.91	0.53
4:L:73:LEU:O	4:L:77:ILE:HG12	2.08	0.53
1:G:643:LEU:HD11	1:G:673:ALA:HA	1.89	0.53
4:L:77:ILE:HG23	4:L:82:PHE:HD2	1.72	0.53
2:B:107:ARG:NH1	2:B:157:VAL:O	2.42	0.53
4:F:310:ILE:HG22	4:F:360:CYS:SG	2.48	0.53
2:H:107:ARG:NH1	2:H:157:VAL:O	2.42	0.53
2:H:342:SER:HB2	5:J:158:GLU:OE2	2.09	0.53
1:A:582:PHE:HA	1:A:585:THR:HG22	1.90	0.53
2:B:464:TYR:O	2:B:472:TYR:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:THR:O	1:G:94:VAL:HG23	2.07	0.53
4:L:337:HIS:HA	4:L:365:VAL:HG21	1.91	0.53
4:L:417:GLU:O	4:L:421:LYS:HG2	2.09	0.53
6:I:20:VAL:HG12	6:I:20:VAL:O	2.08	0.53
1:G:617:MET:HE1	1:G:628:LEU:HD13	1.89	0.53
1:G:167:TYR:OH	2:H:179:ARG:NH2	2.27	0.52
4:F:311:ILE:HB	4:F:361:VAL:HG22	1.91	0.52
1:G:113:VAL:CG1	5:J:69:ARG:HD3	2.38	0.52
4:L:101:ASP:OD1	4:L:263:GLN:N	2.42	0.52
4:L:213:VAL:O	4:L:214:ILE:HD13	2.09	0.52
4:F:228:ARG:O	4:F:232:GLU:HG2	2.10	0.52
4:F:101:ASP:OD1	4:F:263:GLN:N	2.42	0.52
5:J:17:GLU:HB2	6:I:79:ILE:HD11	1.92	0.52
1:G:210:TYR:OH	1:G:250:ASP:OD1	2.18	0.52
3:K:281:ASN:HD22	3:K:284:SER:H	1.57	0.52
5:J:54:LEU:HB3	5:J:55:PRO:HD3	1.91	0.52
4:L:334:ILE:HD12	4:L:352:PHE:HB2	1.92	0.52
4:F:334:ILE:HD12	4:F:352:PHE:HB2	1.92	0.52
4:F:286:ILE:N	4:F:408:SER:O	2.40	0.52
4:L:228:ARG:O	4:L:232:GLU:HG2	2.10	0.52
1:A:457:THR:O	1:A:457:THR:OG1	2.25	0.52
5:C:148:VAL:HB	5:C:149:PRO:HD2	1.91	0.52
1:A:96:HIS:O	1:A:100:VAL:HG23	2.09	0.52
4:F:164:VAL:HA	4:F:189:VAL:O	2.10	0.52
5:C:17:GLU:HB2	6:D:79:ILE:HD11	1.92	0.52
1:A:1032:GLN:HG3	1:A:1033:ASN:ND2	2.25	0.52
2:B:410:ARG:HB2	2:B:452:CYS:SG	2.50	0.52
4:F:213:VAL:O	4:F:214:ILE:HD13	2.10	0.51
1:A:167:TYR:OH	2:B:179:ARG:NH2	2.27	0.51
2:B:371:ILE:HG23	2:B:372:MET:HG2	1.93	0.51
4:F:337:HIS:HA	4:F:365:VAL:HG21	1.91	0.51
5:J:153:LEU:HD12	5:J:153:LEU:C	2.33	0.51
1:G:497:SER:OG	1:G:498:LEU:N	2.43	0.51
4:L:286:ILE:N	4:L:408:SER:O	2.40	0.51
1:A:497:SER:OG	1:A:498:LEU:N	2.44	0.51
6:I:197:LYS:CB	6:I:202:LEU:HD11	2.41	0.51
5:C:26:HIS:O	5:C:30:ILE:HG13	2.11	0.51
1:G:992:ASP:O	1:G:994:LEU:N	2.43	0.51
1:G:1032:GLN:HG3	1:G:1033:ASN:ND2	2.25	0.51
4:L:311:ILE:HB	4:L:361:VAL:HG22	1.92	0.51
2:H:119:THR:O	2:H:122:GLU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:410:ARG:HB2	2:H:452:CYS:SG	2.50	0.51
1:A:992:ASP:O	1:A:994:LEU:N	2.43	0.51
4:F:152:ARG:HA	4:F:155:LYS:HE3	1.93	0.51
4:F:417:GLU:O	4:F:421:LYS:HG2	2.09	0.51
5:J:26:HIS:O	5:J:30:ILE:HG13	2.11	0.51
1:G:684:SER:O	1:G:688:VAL:HG23	2.10	0.51
2:B:119:THR:O	2:B:122:GLU:HB3	2.11	0.51
1:G:96:HIS:O	1:G:100:VAL:HG23	2.09	0.51
1:G:528:SER:HB3	1:G:532:LEU:HD12	1.92	0.51
1:G:794:ASN:ND2	1:G:953:LEU:HD23	2.25	0.51
2:H:371:ILE:HG23	2:H:372:MET:HG2	1.93	0.51
4:L:164:VAL:HA	4:L:189:VAL:O	2.10	0.51
5:J:74:GLN:NE2	5:J:74:GLN:CA	2.72	0.51
1:A:684:SER:O	1:A:688:VAL:HG23	2.10	0.51
2:B:26:PHE:HA	2:B:94:LEU:HD23	1.93	0.51
4:F:286:ILE:O	4:F:410:VAL:N	2.37	0.51
4:F:104:CYS:HB3	4:F:246:PHE:CD2	2.40	0.51
6:D:197:LYS:CB	6:D:202:LEU:HD11	2.41	0.51
1:G:295:GLU:OE2	1:G:410:ARG:NH1	2.44	0.51
1:A:321:PRO:O	1:A:404:LYS:NZ	2.35	0.51
2:B:441:ASP:O	2:B:442:GLU:HB2	2.11	0.51
4:F:105:GLN:HG3	4:F:250:LEU:HD13	1.93	0.51
5:J:106:THR:HG21	6:I:110:ILE:HG22	1.93	0.51
4:L:349:TYR:O	4:L:353:LYS:HG2	2.10	0.50
4:F:349:TYR:O	4:F:353:LYS:HG2	2.10	0.50
5:C:106:THR:HG21	6:D:110:ILE:HG22	1.93	0.50
4:L:196:LYS:HD3	4:L:229:ASP:HA	1.94	0.50
4:L:372:ILE:H	4:L:399:ARG:NH2	2.09	0.50
2:H:238:TRP:CD2	5:J:100:ILE:HG21	2.46	0.50
2:H:441:ASP:O	2:H:442:GLU:HB2	2.11	0.50
4:L:133:VAL:HG22	4:L:211:ASN:HB3	1.92	0.50
1:A:210:TYR:OH	1:A:250:ASP:OD1	2.18	0.50
5:C:74:GLN:HE21	5:C:74:GLN:CA	2.13	0.50
4:F:282:GLN:HB3	4:F:284:TYR:HE2	1.77	0.50
1:A:295:GLU:OE2	1:A:410:ARG:NH1	2.44	0.50
5:C:54:LEU:HB3	5:C:55:PRO:HD3	1.92	0.50
1:A:216:TYR:O	1:A:218:LEU:N	2.44	0.50
4:L:282:GLN:HB3	4:L:284:TYR:HE2	1.77	0.50
1:A:794:ASN:ND2	1:A:953:LEU:HD23	2.25	0.50
4:F:133:VAL:HG22	4:F:211:ASN:HB3	1.92	0.50
2:H:26:PHE:HA	2:H:94:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:105:GLN:HG3	4:L:250:LEU:HD13	1.93	0.50
4:L:152:ARG:HA	4:L:155:LYS:HE3	1.93	0.50
4:L:218:ASP:OD1	4:L:218:ASP:N	2.45	0.50
1:A:260:ASN:HD21	1:A:305:LEU:HD12	1.77	0.50
1:A:1031:LEU:HD23	1:A:1035:VAL:HG11	1.94	0.50
2:B:423:LYS:HD2	2:B:437:PHE:HB3	1.94	0.50
6:I:206:ASN:O	6:I:207:ALA:C	2.52	0.50
5:C:74:GLN:NE2	5:C:74:GLN:CA	2.72	0.50
4:F:196:LYS:HD3	4:F:229:ASP:HA	1.94	0.50
1:G:1031:LEU:HD23	1:G:1035:VAL:HG11	1.94	0.49
2:H:128:ILE:HD11	2:H:141:TRP:HZ3	1.76	0.49
1:G:216:TYR:O	1:G:218:LEU:N	2.44	0.49
1:G:260:ASN:HD21	1:G:305:LEU:HD12	1.77	0.49
2:H:271:ILE:HD13	2:H:412:LEU:HD21	1.94	0.49
4:L:414:GLU:O	4:L:418:VAL:HG23	2.12	0.49
1:A:528:SER:HB3	1:A:532:LEU:HD12	1.92	0.49
1:A:948:PHE:CD2	1:A:1034:CYS:HB3	2.47	0.49
4:F:316:THR:HB	4:F:337:HIS:CE1	2.47	0.49
5:C:203:LEU:O	5:C:204:THR:C	2.52	0.49
4:L:157:MET:HE2	4:L:157:MET:HA	1.94	0.49
2:B:271:ILE:HD13	2:B:412:LEU:HD21	1.94	0.49
2:B:342:SER:HB2	5:C:158:GLU:OE2	2.12	0.49
4:F:414:GLU:O	4:F:418:VAL:HG23	2.12	0.49
1:A:766:VAL:HG11	1:A:862:MET:HE1	1.95	0.49
2:B:542:GLU:O	2:B:543:GLN:C	2.56	0.49
4:F:372:ILE:H	4:F:399:ARG:NH2	2.09	0.49
2:H:309:ASN:ND2	5:J:126:VAL:HG23	2.27	0.49
4:F:290:GLU:HA	4:F:293:LYS:HE3	1.94	0.49
1:G:191:LEU:HD11	5:J:115:LEU:HD22	1.94	0.49
1:G:679:ASN:O	1:G:680:TYR:HD1	1.96	0.49
1:G:992:ASP:C	1:G:994:LEU:H	2.21	0.49
1:A:1094:PHE:HA	1:A:1097:VAL:HG12	1.94	0.49
2:B:128:ILE:HD11	2:B:141:TRP:HZ3	1.76	0.49
4:L:316:THR:HB	4:L:337:HIS:CE1	2.47	0.49
2:B:238:TRP:CD2	5:C:100:ILE:HG21	2.47	0.49
4:F:119:SER:O	4:F:123:GLN:HG3	2.13	0.49
2:H:239:ASN:CB	5:J:101:SER:HG	2.24	0.49
2:H:255:PHE:HE1	2:H:386:LEU:HD12	1.79	0.48
2:H:423:LYS:HD2	2:H:437:PHE:HB3	1.94	0.48
1:G:948:PHE:CD2	1:G:1034:CYS:HB3	2.47	0.48
1:G:1094:PHE:HA	1:G:1097:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:104:CYS:HB3	4:L:246:PHE:CD2	2.40	0.48
1:G:545:LEU:O	1:G:549:ILE:HG13	2.14	0.48
4:L:290:GLU:HA	4:L:293:LYS:HE3	1.94	0.48
4:L:325:LEU:O	4:L:329:SER:OG	2.29	0.48
4:F:69:LEU:HD23	4:F:73:LEU:HD23	1.96	0.48
1:G:766:VAL:HG11	1:G:862:MET:HE1	1.95	0.48
4:L:69:LEU:HD23	4:L:73:LEU:HD23	1.96	0.48
1:A:703:GLN:NE2	1:A:749:ASN:HD22	2.12	0.48
4:F:157:MET:HA	4:F:157:MET:HE2	1.94	0.48
2:H:542:GLU:O	2:H:543:GLN:C	2.56	0.48
4:L:119:SER:O	4:L:123:GLN:HG3	2.13	0.48
1:A:679:ASN:O	1:A:680:TYR:HD1	1.96	0.48
2:B:194:LEU:HD21	5:C:91:ALA:HB2	1.95	0.48
3:E:182:GLU:H	3:E:201:ILE:HB	1.77	0.48
1:G:703:GLN:NE2	1:G:749:ASN:HD22	2.12	0.48
3:K:182:GLU:H	3:K:201:ILE:HB	1.78	0.48
1:A:60:TRP:O	1:A:63:THR:OG1	2.28	0.48
1:A:992:ASP:C	1:A:994:LEU:H	2.21	0.48
5:J:191:GLU:O	5:J:192:ASN:C	2.56	0.48
2:H:381:CYS:O	2:H:385:GLN:HG3	2.14	0.48
2:B:381:CYS:O	2:B:385:GLN:HG3	2.14	0.48
1:G:311:ASN:OD1	1:G:311:ASN:N	2.47	0.48
1:A:1031:LEU:HA	1:A:1035:VAL:CG1	2.43	0.48
6:D:148:LEU:HA	6:D:192:TYR:H	1.78	0.48
1:G:992:ASP:C	1:G:994:LEU:N	2.72	0.48
1:G:1031:LEU:HA	1:G:1035:VAL:CG1	2.43	0.48
5:J:160:TYR:CE2	6:I:127:LEU:N	2.82	0.48
5:C:117:TYR:HH	6:D:120:ARG:HD3	1.73	0.48
5:C:191:GLU:O	5:C:192:ASN:C	2.56	0.48
1:A:267:ASN:C	1:A:311:ASN:HD22	2.22	0.47
2:B:309:ASN:ND2	5:C:126:VAL:HG23	2.29	0.47
5:J:58:HIS:O	5:J:60:GLU:N	2.44	0.47
4:F:396:ARG:O	4:F:399:ARG:NH2	2.47	0.47
4:L:396:ARG:O	4:L:399:ARG:NH2	2.47	0.47
4:F:218:ASP:OD2	4:F:249:THR:OG1	2.32	0.47
6:I:119:LEU:HD23	6:I:119:LEU:N	2.29	0.47
4:L:218:ASP:OD2	4:L:249:THR:OG1	2.32	0.47
1:A:545:LEU:O	1:A:549:ILE:HG13	2.14	0.47
1:G:250:ASP:OD1	1:G:250:ASP:N	2.46	0.47
3:K:141:LEU:HD23	3:K:152:LEU:HB2	1.96	0.47
1:A:305:LEU:HD11	1:A:312:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ASP:C	1:A:994:LEU:N	2.72	0.47
5:J:128:LEU:HD23	6:I:131:VAL:HG13	1.97	0.47
5:C:153:LEU:HD12	5:C:153:LEU:C	2.34	0.47
4:F:116:PHE:O	4:F:120:THR:HG22	2.14	0.47
6:D:119:LEU:HD23	6:D:119:LEU:N	2.29	0.47
1:G:305:LEU:HD11	1:G:312:PHE:HA	1.96	0.47
1:G:457:THR:HG22	1:G:555:ALA:HB2	1.96	0.47
4:L:124:LEU:HD21	4:L:133:VAL:HG23	1.96	0.47
4:L:314:LYS:HD2	4:L:382:ASP:HB3	1.95	0.47
2:B:348:ASP:OD1	6:D:120:ARG:NH2	2.40	0.47
3:E:187:PHE:HD1	3:E:195:SER:HA	1.80	0.47
4:F:314:LYS:HD2	4:F:382:ASP:HB3	1.95	0.47
1:G:732:SER:OG	1:G:768:ILE:HA	2.15	0.47
4:L:116:PHE:CD1	4:L:213:VAL:HG11	2.50	0.47
1:A:457:THR:HG22	1:A:555:ALA:HB2	1.96	0.47
2:B:134:PRO:HG2	2:B:199:HIS:HD2	1.80	0.47
5:C:128:LEU:HD23	6:D:131:VAL:HG13	1.97	0.47
4:L:62:THR:N	4:L:83:GLU:OE2	2.48	0.47
2:B:255:PHE:HE1	2:B:386:LEU:HD12	1.79	0.47
2:H:213:LEU:HA	2:H:213:LEU:HD23	1.70	0.47
3:E:27:TYR:OH	3:E:351:SER:O	2.32	0.47
3:E:184:ILE:O	3:E:198:SER:HA	2.15	0.47
5:J:117:TYR:CZ	6:I:120:ARG:CD	2.78	0.47
5:C:58:HIS:O	5:C:60:GLU:N	2.44	0.47
2:H:8:ILE:HG12	2:H:68:ILE:HG22	1.97	0.46
2:H:70:LYS:HB3	2:H:70:LYS:HE2	1.66	0.46
4:F:62:THR:N	4:F:83:GLU:OE2	2.48	0.46
4:F:341:LYS:HG2	4:F:343:GLU:H	1.80	0.46
4:L:341:LYS:HG2	4:L:343:GLU:H	1.80	0.46
3:E:91:PHE:HB2	3:E:101:VAL:HG22	1.97	0.46
4:F:244:MET:HB3	4:F:246:PHE:CZ	2.50	0.46
6:I:148:LEU:HA	6:I:192:TYR:H	1.78	0.46
5:C:160:TYR:CE2	6:D:127:LEU:N	2.82	0.46
1:G:267:ASN:C	1:G:311:ASN:HD22	2.22	0.46
4:L:228:ARG:HH22	4:L:231:GLN:HG3	1.80	0.46
4:L:308:GLN:HB2	4:L:375:ILE:HD13	1.96	0.46
4:F:124:LEU:HD21	4:F:133:VAL:HG23	1.96	0.46
4:L:135:VAL:HG13	4:L:213:VAL:HB	1.98	0.46
1:A:732:SER:OG	1:A:768:ILE:HA	2.15	0.46
2:H:120:PHE:HE2	2:H:151:PHE:CE1	2.33	0.46
3:E:141:LEU:HD23	3:E:152:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:135:VAL:HG13	4:F:213:VAL:HB	1.98	0.46
6:D:214:GLU:O	6:D:215:ASN:C	2.58	0.46
1:A:644:LYS:HE3	4:F:302:ASP:O	2.16	0.46
1:G:179:SER:O	1:G:180:VAL:C	2.59	0.46
2:H:234:SER:HA	2:H:375:SER:HA	1.98	0.46
4:L:116:PHE:O	4:L:120:THR:HG22	2.14	0.46
4:F:228:ARG:HH22	4:F:231:GLN:HG3	1.80	0.46
4:F:308:GLN:HB2	4:F:375:ILE:HD13	1.97	0.46
6:I:107:LEU:N	6:I:108:PRO:CD	2.79	0.46
1:G:644:LYS:HE3	4:L:302:ASP:O	2.16	0.46
4:L:338:GLY:O	4:L:340:MET:HG3	2.16	0.46
4:F:218:ASP:OD1	4:F:218:ASP:N	2.45	0.46
4:F:338:GLY:O	4:F:340:MET:HG3	2.16	0.46
4:F:440:PRO:HA	4:F:443:TYR:CE1	2.51	0.46
6:D:73:LEU:HD23	6:D:73:LEU:O	2.16	0.46
2:B:120:PHE:HE2	2:B:151:PHE:CE1	2.33	0.46
2:B:8:ILE:HG12	2:B:68:ILE:HG22	1.97	0.46
4:F:116:PHE:CD1	4:F:213:VAL:HG11	2.50	0.46
6:I:73:LEU:HD23	6:I:73:LEU:O	2.16	0.46
4:L:244:MET:HB3	4:L:246:PHE:CZ	2.50	0.45
6:D:103:LEU:HD23	6:D:103:LEU:HA	1.86	0.45
3:K:184:ILE:O	3:K:198:SER:HA	2.15	0.45
4:L:440:PRO:HA	4:L:443:TYR:CE1	2.51	0.45
1:A:179:SER:O	1:A:180:VAL:C	2.59	0.45
6:D:107:LEU:N	6:D:108:PRO:CD	2.79	0.45
2:H:134:PRO:HG2	2:H:199:HIS:HD2	1.80	0.45
3:K:187:PHE:HD1	3:K:195:SER:HA	1.80	0.45
1:A:773:ILE:HD11	1:A:869:PHE:HD1	1.81	0.45
1:A:794:ASN:HD22	1:A:953:LEU:HB3	1.81	0.45
2:B:234:SER:HA	2:B:375:SER:HA	1.97	0.45
6:I:30:ILE:HD12	6:I:30:ILE:HA	1.75	0.45
1:G:794:ASN:HD22	1:G:953:LEU:HB3	1.81	0.45
2:H:444:ASN:O	2:H:445:LYS:C	2.59	0.45
4:F:89:GLN:HG3	4:F:115:VAL:HG22	1.99	0.45
4:F:384:THR:OG1	4:F:385:ASN:N	2.50	0.45
1:G:213:MET:SD	1:G:223:THR:HG21	2.57	0.45
1:G:456:MET:HE3	1:G:552:ILE:HG23	1.99	0.45
1:G:687:VAL:HA	1:G:690:THR:HG22	1.99	0.45
4:L:212:PHE:CE2	4:L:214:ILE:HD11	2.52	0.45
1:A:842:ASN:OD1	1:A:842:ASN:C	2.60	0.45
2:B:444:ASN:O	2:B:445:LYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:LEU:HD12	2:B:586:LEU:HA	1.84	0.45
4:F:72:GLU:HB3	4:F:156:TYR:HB3	1.99	0.45
1:G:485:LEU:HD23	5:J:142:TYR:HB3	1.98	0.45
1:G:842:ASN:OD1	1:G:842:ASN:C	2.59	0.45
1:A:101:SER:OG	1:A:102:GLN:NE2	2.50	0.45
4:F:99:GLY:HA2	4:F:123:GLN:HE22	1.82	0.45
5:C:80:LEU:HD12	5:C:80:LEU:HA	1.73	0.45
1:G:773:ILE:HD11	1:G:869:PHE:HD1	1.81	0.45
1:A:687:VAL:HA	1:A:690:THR:HG22	1.99	0.45
4:F:212:PHE:CE2	4:F:214:ILE:HD11	2.52	0.45
1:G:285:TYR:O	1:G:291:LYS:NZ	2.50	0.45
1:G:344:GLY:HA3	1:G:637:ARG:NH1	2.32	0.45
2:B:322:THR:OG1	2:B:323:GLU:N	2.50	0.45
6:D:26:LYS:HB3	6:D:71:ARG:HD3	1.99	0.45
1:G:101:SER:OG	1:G:102:GLN:NE2	2.50	0.44
1:G:855:LEU:HD12	1:G:855:LEU:HA	1.81	0.44
2:H:322:THR:OG1	2:H:323:GLU:N	2.50	0.44
1:A:285:TYR:O	1:A:291:LYS:NZ	2.50	0.44
1:A:773:ILE:HD11	1:A:869:PHE:CD1	2.52	0.44
2:B:451:LEU:O	2:B:455:ILE:HG12	2.17	0.44
4:F:311:ILE:HB	4:F:361:VAL:HG13	1.99	0.44
4:F:325:LEU:O	4:F:329:SER:OG	2.29	0.44
2:H:451:LEU:O	2:H:455:ILE:HG12	2.17	0.44
3:K:91:PHE:HB2	3:K:101:VAL:HG22	1.97	0.44
4:L:384:THR:OG1	4:L:385:ASN:N	2.50	0.44
1:A:151:ASN:O	1:A:154:GLN:N	2.50	0.44
1:A:782:LEU:HD23	1:A:782:LEU:HA	1.84	0.44
3:K:27:TYR:OH	3:K:351:SER:O	2.32	0.44
4:L:72:GLU:HB3	4:L:156:TYR:HB3	1.99	0.44
4:L:99:GLY:HA2	4:L:123:GLN:HE22	1.82	0.44
1:A:191:LEU:HD11	5:C:115:LEU:HD22	2.00	0.44
1:A:529:HIS:HD2	1:A:580:PHE:HZ	1.65	0.44
4:F:420:ALA:HA	4:F:423:GLN:NE2	2.32	0.44
6:I:26:LYS:HB3	6:I:71:ARG:HD3	1.99	0.44
5:C:52:LYS:O	5:C:55:PRO:HD2	2.17	0.44
1:G:299:ASP:OD1	1:G:414:HIS:HE1	2.00	0.44
1:G:321:PRO:O	1:G:404:LYS:NZ	2.35	0.44
1:G:870:ILE:HD13	1:G:906:ILE:HG12	2.00	0.44
2:H:15:LEU:HD13	2:H:15:LEU:HA	1.85	0.44
4:L:311:ILE:HB	4:L:361:VAL:HG13	2.00	0.44
4:F:423:GLN:H	4:F:423:GLN:HG2	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:793:LEU:HD23	1:G:793:LEU:HA	1.75	0.44
2:H:93:LEU:HD23	2:H:93:LEU:HA	1.83	0.44
4:L:440:PRO:HA	4:L:443:TYR:CZ	2.53	0.44
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.86	0.44
1:A:456:MET:HE3	1:A:552:ILE:HG23	1.99	0.44
1:G:764:ILE:O	1:G:768:ILE:HG13	2.18	0.44
1:A:299:ASP:OD1	1:A:414:HIS:HE1	2.00	0.44
4:F:440:PRO:HA	4:F:443:TYR:CZ	2.53	0.44
1:G:333:LEU:HA	1:G:333:LEU:HD23	1.81	0.44
1:G:773:ILE:HD11	1:G:869:PHE:CD1	2.52	0.44
1:A:213:MET:SD	1:A:223:THR:HG21	2.57	0.44
2:B:70:LYS:HB3	2:B:70:LYS:HE2	1.66	0.44
4:F:105:GLN:HA	4:F:247:SER:O	2.18	0.44
2:H:306:ILE:HD11	5:J:124:LEU:HD21	2.00	0.44
4:L:247:SER:HB3	4:L:250:LEU:HD11	2.00	0.44
1:A:449:LEU:HA	1:A:518:PHE:HD2	1.83	0.44
3:E:131:VAL:HG11	3:E:163:VAL:HG23	2.00	0.44
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.71	0.44
1:A:316:TRP:CH2	1:A:404:LYS:HD3	2.53	0.44
4:F:388:ASP:O	4:F:391:LEU:HG	2.18	0.44
5:J:103:TYR:CD1	5:J:103:TYR:C	2.96	0.44
2:H:359:ILE:HD13	2:H:359:ILE:HA	1.92	0.43
4:L:388:ASP:O	4:L:391:LEU:HG	2.18	0.43
1:A:488:LYS:HE2	1:A:488:LYS:HB2	1.86	0.43
3:E:357:GLY:N	3:E:361:THR:O	2.51	0.43
5:J:170:VAL:HA	5:J:173:GLN:NE2	2.33	0.43
1:G:529:HIS:HD2	1:G:580:PHE:HZ	1.65	0.43
1:G:932:PHE:HD1	1:G:932:PHE:HA	1.71	0.43
2:H:523:MET:HE3	2:H:523:MET:HB3	1.90	0.43
4:L:105:GLN:HA	4:L:247:SER:O	2.18	0.43
4:L:175:ALA:HB2	4:L:203:TYR:CD1	2.53	0.43
4:L:224:LEU:O	4:L:228:ARG:HG2	2.18	0.43
1:A:250:ASP:OD1	1:A:250:ASP:N	2.46	0.43
4:F:175:ALA:HB2	4:F:203:TYR:CD1	2.53	0.43
4:F:192:PRO:HB2	4:F:229:ASP:HB2	2.00	0.43
4:F:224:LEU:O	4:F:228:ARG:HG2	2.18	0.43
5:J:52:LYS:O	5:J:55:PRO:HD2	2.18	0.43
6:D:197:LYS:CB	6:D:202:LEU:CD1	2.96	0.43
1:G:873:ILE:HD13	1:G:873:ILE:HA	1.62	0.43
2:H:12:ILE:HD13	2:H:72:PHE:HB2	2.00	0.43
3:K:175:LEU:HD23	3:K:176:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:357:GLY:N	3:K:361:THR:O	2.51	0.43
4:L:238:PRO:O	4:L:241:LYS:HG2	2.18	0.43
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.71	0.43
1:A:412:LEU:HG	1:A:420:VAL:HG21	2.00	0.43
2:B:15:LEU:HD13	2:B:15:LEU:HA	1.85	0.43
5:C:103:TYR:C	5:C:103:TYR:CD1	2.96	0.43
1:G:151:ASN:O	1:G:154:GLN:N	2.50	0.43
3:K:92:ILE:H	3:K:92:ILE:HG12	1.66	0.43
4:F:94:PRO:O	4:F:98:HIS:NE2	2.52	0.43
5:J:67:ARG:HE	5:J:67:ARG:HB2	1.57	0.43
3:K:324:LEU:HD23	3:K:324:LEU:HA	1.80	0.43
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.86	0.43
3:E:175:LEU:HD23	3:E:176:LEU:N	2.33	0.43
5:C:159:GLN:HE21	5:C:159:GLN:HB3	1.56	0.43
5:C:170:VAL:HA	5:C:173:GLN:NE2	2.33	0.43
1:A:211:HIS:CE1	2:B:200:TYR:HD2	2.37	0.43
1:A:344:GLY:HA3	1:A:637:ARG:NH1	2.33	0.43
1:A:731:LEU:HD12	1:A:731:LEU:HA	1.88	0.43
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.75	0.43
2:B:427:LEU:HA	2:B:427:LEU:HD23	1.79	0.43
4:F:161:LYS:HB2	4:F:185:PRO:HA	2.00	0.43
4:F:247:SER:HB3	4:F:250:LEU:HD11	2.00	0.43
5:C:58:HIS:C	5:C:60:GLU:H	2.25	0.43
6:D:30:ILE:HD12	6:D:30:ILE:HA	1.75	0.43
1:G:316:TRP:CH2	1:G:404:LYS:HD3	2.53	0.43
1:G:412:LEU:HG	1:G:420:VAL:HG21	2.01	0.43
1:G:622:SER:HB2	1:G:632:PHE:CD2	2.54	0.43
3:K:131:VAL:HG11	3:K:163:VAL:HG23	2.00	0.43
4:L:89:GLN:HG3	4:L:115:VAL:HG22	1.99	0.43
2:B:577:ILE:O	2:B:581:GLN:HG2	2.18	0.43
1:A:870:ILE:HD13	1:A:906:ILE:HG12	2.00	0.43
3:E:340:THR:O	3:E:342:PRO:HD3	2.19	0.43
4:F:286:ILE:HG13	4:F:407:ILE:HD11	2.01	0.43
1:G:211:HIS:CE1	2:H:200:TYR:HD2	2.37	0.43
2:B:538:LEU:HD13	2:B:538:LEU:HA	1.83	0.43
4:F:238:PRO:O	4:F:241:LYS:HG2	2.18	0.43
5:J:159:GLN:HE21	5:J:159:GLN:HB3	1.57	0.43
6:I:197:LYS:CB	6:I:202:LEU:CD1	2.96	0.43
1:G:246:LEU:HD23	1:G:246:LEU:HA	1.72	0.43
1:G:298:MET:SD	1:G:407:LEU:HD12	2.59	0.43
2:H:440:LEU:HD23	2:H:440:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:538:LEU:HD13	2:H:538:LEU:HA	1.83	0.43
2:H:577:ILE:O	2:H:581:GLN:HG2	2.18	0.43
3:K:340:THR:O	3:K:342:PRO:HD3	2.19	0.43
1:A:622:SER:HB2	1:A:632:PHE:CD2	2.54	0.43
4:F:202:LYS:HD3	4:F:202:LYS:HA	1.85	0.43
5:C:117:TYR:CZ	6:D:120:ARG:CD	2.78	0.43
1:G:817:ILE:H	1:G:817:ILE:HG12	1.70	0.42
2:H:100:LEU:HD23	2:H:100:LEU:HA	1.76	0.42
1:A:764:ILE:O	1:A:768:ILE:HG13	2.18	0.42
2:B:12:ILE:HD13	2:B:72:PHE:HB2	2.00	0.42
5:C:71:ASP:O	5:C:75:THR:HG23	2.19	0.42
2:H:396:LYS:HD2	2:H:471:PHE:CE1	2.55	0.42
4:L:94:PRO:O	4:L:98:HIS:NE2	2.52	0.42
4:L:142:LEU:HD23	4:L:142:LEU:HA	1.89	0.42
1:A:485:LEU:HD23	5:C:142:TYR:HB3	2.01	0.42
2:B:396:LYS:HD2	2:B:471:PHE:CE1	2.54	0.42
2:B:424:SER:OG	2:B:428:ARG:NH2	2.53	0.42
4:F:244:MET:HB3	4:F:246:PHE:CE1	2.54	0.42
5:J:58:HIS:C	5:J:60:GLU:H	2.25	0.42
5:C:156:ILE:CD1	5:C:173:GLN:HB3	2.49	0.42
5:C:157:LEU:HD23	5:C:157:LEU:HA	1.89	0.42
1:G:1098:LEU:HD23	1:G:1098:LEU:HA	1.79	0.42
4:L:141:GLU:HG2	4:L:142:LEU:N	2.35	0.42
4:L:224:LEU:HA	4:L:227:ARG:HG2	2.02	0.42
2:B:413:ILE:HD13	2:B:413:ILE:HA	1.88	0.42
1:A:756:LYS:HE2	1:A:756:LYS:HB2	1.81	0.42
1:A:570:ILE:HD13	1:A:570:ILE:HA	1.86	0.42
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.88	0.42
5:J:156:ILE:CD1	5:J:173:GLN:HB3	2.50	0.42
5:J:160:TYR:HH	6:I:130:SER:HB2	1.85	0.42
1:G:449:LEU:HA	1:G:518:PHE:HD2	1.83	0.42
1:G:525:PHE:CE1	1:G:572:LYS:HE3	2.55	0.42
2:H:176:GLU:N	2:H:176:GLU:OE2	2.52	0.42
2:H:424:SER:OG	2:H:428:ARG:NH2	2.52	0.42
4:L:420:ALA:HA	4:L:423:GLN:NE2	2.32	0.42
1:A:63:THR:O	1:A:64:LEU:C	2.63	0.42
1:A:248:LYS:HB3	1:A:248:LYS:HE3	1.86	0.42
1:A:412:LEU:HA	1:A:412:LEU:HD23	1.64	0.42
1:G:545:LEU:HD23	1:G:545:LEU:HA	1.74	0.42
3:K:48:VAL:O	3:K:52:SER:OG	2.33	0.42
4:L:192:PRO:HB2	4:L:229:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:893:ASN:HD22	1:G:903:THR:HG21	1.84	0.42
4:L:161:LYS:HB2	4:L:185:PRO:HA	2.00	0.42
4:L:287:LYS:HA	4:L:410:VAL:HB	2.02	0.42
1:A:236:THR:O	1:A:237:GLU:HG2	2.20	0.42
2:B:176:GLU:OE2	2:B:176:GLU:N	2.52	0.42
1:G:63:THR:O	1:G:64:LEU:C	2.63	0.42
1:G:248:LYS:HE3	1:G:248:LYS:HB3	1.86	0.42
1:G:486:ILE:O	5:J:143:GLU:O	2.38	0.42
1:G:706:LEU:HD23	1:G:706:LEU:HA	1.82	0.42
1:G:957:HIS:CD2	1:G:1051:PHE:HE2	2.38	0.42
4:L:244:MET:HB3	4:L:246:PHE:CE1	2.54	0.42
1:A:525:PHE:CE1	1:A:572:LYS:HE3	2.55	0.42
2:B:318:GLU:OE1	2:B:326:ALA:N	2.52	0.42
2:B:508:PRO:HA	2:B:509:PRO:HD3	1.91	0.42
4:F:287:LYS:HA	4:F:410:VAL:HB	2.01	0.42
2:H:38:MET:HE2	2:H:38:MET:HB3	1.83	0.42
2:H:508:PRO:HA	2:H:509:PRO:HD3	1.91	0.42
1:A:298:MET:SD	1:A:407:LEU:HD12	2.60	0.42
2:B:395:ARG:O	2:B:399:ILE:HG12	2.20	0.42
4:F:124:LEU:HD11	4:F:133:VAL:HG21	2.02	0.42
1:G:233:GLN:HE22	2:H:473:ARG:HD3	1.85	0.41
1:G:236:THR:O	1:G:237:GLU:HG2	2.20	0.41
4:L:391:LEU:HA	4:L:394:VAL:HG12	2.02	0.41
1:A:62:ARG:O	1:A:66:ILE:HG12	2.20	0.41
1:A:893:ASN:HD22	1:A:903:THR:HG21	1.85	0.41
5:J:169:GLY:O	5:J:173:GLN:NE2	2.52	0.41
5:J:191:GLU:HG3	5:J:192:ASN:H	1.84	0.41
4:L:372:ILE:H	4:L:399:ARG:CZ	2.33	0.41
4:F:341:LYS:HB3	4:F:341:LYS:HE2	1.78	0.41
4:F:353:LYS:HA	4:F:353:LYS:HD3	1.79	0.41
1:G:161:LEU:HD23	1:G:161:LEU:HA	1.72	0.41
1:G:827:ASP:OD1	1:G:827:ASP:N	2.53	0.41
2:H:395:ARG:O	2:H:399:ILE:HG12	2.20	0.41
4:L:286:ILE:HG13	4:L:407:ILE:HD11	2.01	0.41
4:L:412:SER:OG	4:L:413:LYS:N	2.53	0.41
1:A:158:LEU:HD12	6:D:15:VAL:HG22	2.03	0.41
1:A:233:GLN:HE22	2:B:473:ARG:HD3	1.85	0.41
3:E:306:LEU:HD23	3:E:306:LEU:HA	1.87	0.41
4:F:141:GLU:HG2	4:F:142:LEU:N	2.35	0.41
6:D:73:LEU:C	6:D:73:LEU:CD2	2.93	0.41
1:G:1101:LEU:HA	1:G:1101:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:113:PRO:O	2:H:116:TRP:HD1	2.04	0.41
1:A:425:LYS:HE2	1:A:425:LYS:HB2	1.86	0.41
2:B:239:ASN:HA	5:C:101:SER:HG	1.85	0.41
4:F:391:LEU:HA	4:F:394:VAL:HG12	2.02	0.41
5:J:71:ASP:O	5:J:75:THR:HG23	2.19	0.41
5:C:160:TYR:CD2	6:D:127:LEU:N	2.88	0.41
2:H:471:PHE:O	2:H:475:ILE:HG12	2.21	0.41
1:A:108:LYS:O	1:A:111:ILE:CG2	2.64	0.41
1:A:957:HIS:CD2	1:A:1051:PHE:HE2	2.38	0.41
4:F:412:SER:OG	4:F:413:LYS:N	2.53	0.41
6:I:73:LEU:C	6:I:73:LEU:CD2	2.93	0.41
6:I:103:LEU:HA	6:I:103:LEU:HD23	1.86	0.41
6:I:246:LEU:O	6:I:249:ASP:CB	2.68	0.41
1:G:703:GLN:HE22	1:G:749:ASN:HD22	1.69	0.41
1:G:1024:GLU:O	1:G:1028:LYS:N	2.54	0.41
2:H:318:GLU:OE1	2:H:326:ALA:N	2.52	0.41
4:L:147:ARG:HD3	4:L:164:VAL:HB	2.02	0.41
1:A:1024:GLU:O	1:A:1028:LYS:N	2.54	0.41
4:F:142:LEU:HD23	4:F:142:LEU:HA	1.90	0.41
4:F:147:ARG:HD3	4:F:164:VAL:HB	2.02	0.41
5:C:130:LYS:HG2	5:C:147:TRP:CD1	2.56	0.41
5:C:169:GLY:O	5:C:173:GLN:NE2	2.52	0.41
4:L:416:GLU:H	4:L:416:GLU:HG3	1.65	0.41
1:A:183:GLY:O	1:A:184:GLN:C	2.64	0.41
5:J:130:LYS:HG2	5:J:147:TRP:CD1	2.56	0.41
5:C:191:GLU:HG3	5:C:192:ASN:H	1.84	0.41
1:G:801:GLN:HE21	1:G:801:GLN:N	2.19	0.41
4:L:135:VAL:HA	4:L:213:VAL:O	2.21	0.41
4:L:353:LYS:HA	4:L:353:LYS:HD3	1.79	0.41
1:A:1098:LEU:HD23	1:A:1098:LEU:HA	1.79	0.41
2:B:238:TRP:CE3	5:C:100:ILE:HG21	2.55	0.41
5:J:80:LEU:HA	5:J:80:LEU:HD12	1.73	0.41
1:G:62:ARG:O	1:G:66:ILE:HG12	2.20	0.41
1:G:183:GLY:O	1:G:184:GLN:C	2.64	0.41
1:G:628:LEU:HA	1:G:628:LEU:HD23	1.88	0.41
1:G:1101:LEU:HD11	1:G:1121:TRP:HZ3	1.86	0.41
2:H:12:ILE:HD11	2:H:72:PHE:HD1	1.86	0.41
2:H:477:LYS:HA	2:H:477:LYS:HD2	1.80	0.41
4:L:116:PHE:HB3	4:L:246:PHE:CE1	2.56	0.41
4:L:166:TYR:C	4:L:194:ARG:HG3	2.46	0.41
4:L:295:ARG:CZ	4:L:296:LYS:HD3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:366:PHE:HB3	4:L:370:ILE:HD13	2.02	0.41
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.81	0.41
1:A:341:SER:CB	1:A:630:VAL:HG22	2.51	0.41
1:A:534:ILE:HD13	1:A:534:ILE:HA	1.90	0.41
1:A:947:THR:O	1:A:951:LEU:HD12	2.21	0.41
2:B:470:ASP:O	2:B:474:VAL:HG23	2.21	0.41
2:B:582:THR:HG22	2:B:586:LEU:HD22	2.03	0.41
4:F:166:TYR:C	4:F:194:ARG:HG3	2.46	0.41
4:F:224:LEU:HA	4:F:227:ARG:HG2	2.02	0.41
1:G:182:TYR:O	1:G:183:GLY:C	2.64	0.41
1:G:341:SER:CB	1:G:630:VAL:HG22	2.51	0.41
1:G:947:THR:O	1:G:951:LEU:HD12	2.21	0.41
3:K:279:VAL:HG13	3:K:289:LEU:HB3	2.03	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.72	0.41
1:A:851:HIS:O	1:A:854:ILE:HG22	2.21	0.41
2:B:258:ASP:O	2:B:262:VAL:HG12	2.21	0.41
3:E:48:VAL:O	3:E:52:SER:OG	2.33	0.41
4:F:426:PHE:HB3	4:F:428:VAL:HG22	2.03	0.41
1:G:488:LYS:HE2	1:G:488:LYS:HB2	1.86	0.40
1:G:1095:THR:OG1	1:G:1151:VAL:HA	2.21	0.40
2:H:470:ASP:O	2:H:474:VAL:HG23	2.21	0.40
3:K:49:SER:CB	3:E:50:SER:HB3	2.50	0.40
4:L:124:LEU:HD11	4:L:133:VAL:HG21	2.02	0.40
4:F:135:VAL:HA	4:F:213:VAL:O	2.21	0.40
4:F:366:PHE:HB3	4:F:370:ILE:HD13	2.02	0.40
5:J:160:TYR:CD2	6:I:127:LEU:N	2.88	0.40
5:C:194:TYR:N	5:C:194:TYR:CD1	2.89	0.40
1:A:220:SER:O	1:A:223:THR:HG22	2.21	0.40
1:A:831:ILE:HD12	1:A:873:ILE:HD11	2.03	0.40
2:B:12:ILE:HD11	2:B:72:PHE:HD1	1.86	0.40
2:B:342:SER:OG	2:B:343:ASN:N	2.55	0.40
4:F:120:THR:HG21	4:F:150:TYR:OH	2.21	0.40
4:F:372:ILE:H	4:F:399:ARG:CZ	2.33	0.40
5:J:160:TYR:CD2	6:I:127:LEU:CB	3.04	0.40
5:C:160:TYR:CD2	6:D:127:LEU:CB	3.04	0.40
1:G:488:LYS:HD3	1:G:503:SER:OG	2.22	0.40
3:K:82:ARG:NH1	3:K:360:ASP:O	2.55	0.40
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.84	0.40
1:A:855:LEU:HD12	1:A:855:LEU:HA	1.81	0.40
2:B:436:ASP:O	2:B:437:PHE:HB2	2.22	0.40
3:E:279:VAL:HG13	3:E:289:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:295:ARG:CZ	4:F:296:LYS:HD3	2.51	0.40
5:J:30:ILE:HD11	5:J:61:LEU:HB2	2.04	0.40
1:G:200:SER:O	1:G:200:SER:OG	2.38	0.40
2:H:582:THR:HG22	2:H:586:LEU:HD22	2.03	0.40
4:L:93:ILE:HD11	4:L:115:VAL:HA	2.04	0.40
1:A:311:ASN:OD1	1:A:311:ASN:N	2.47	0.40
1:A:1095:THR:OG1	1:A:1151:VAL:HA	2.21	0.40
1:A:1101:LEU:HD11	1:A:1121:TRP:HZ3	1.86	0.40
2:B:113:PRO:O	2:B:116:TRP:HD1	2.04	0.40
4:F:333:ALA:HA	4:F:359:ILE:O	2.22	0.40
6:D:57:THR:C	6:D:59:GLN:H	2.30	0.40
4:L:120:THR:HG21	4:L:150:TYR:OH	2.21	0.40
1:A:545:LEU:HA	1:A:545:LEU:HD23	1.74	0.40
1:A:703:GLN:HE22	1:A:749:ASN:HD22	1.69	0.40
1:A:801:GLN:HE21	1:A:801:GLN:N	2.19	0.40
2:B:188:LEU:HD12	2:B:188:LEU:HA	1.84	0.40
5:C:125:SER:HA	6:D:128:TYR:CZ	2.57	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	1069/1601 (67%)	1002 (94%)	66 (6%)	1 (0%)	48	83
1	G	1069/1601 (67%)	1002 (94%)	66 (6%)	1 (0%)	48	83
2	B	555/720 (77%)	503 (91%)	51 (9%)	1 (0%)	43	77
2	H	555/720 (77%)	503 (91%)	51 (9%)	1 (0%)	43	77
3	E	344/380 (90%)	320 (93%)	24 (7%)	0	100	100
3	K	344/380 (90%)	320 (93%)	24 (7%)	0	100	100
4	F	355/400 (89%)	346 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	355/400 (89%)	346 (98%)	9 (2%)	0	100	100
5	C	224/261 (86%)	211 (94%)	9 (4%)	4 (2%)	6	33
5	J	225/261 (86%)	213 (95%)	9 (4%)	3 (1%)	9	41
6	D	221/392 (56%)	208 (94%)	12 (5%)	1 (0%)	24	63
6	I	223/392 (57%)	210 (94%)	12 (5%)	1 (0%)	30	67
All	All	5539/7508 (74%)	5184 (94%)	342 (6%)	13 (0%)	44	77

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	993	ILE
1	A	993	ILE
5	C	194	TYR
2	H	442	GLU
2	B	442	GLU
5	J	192	ASN
5	C	192	ASN
5	J	59	ARG
6	I	153	ALA
5	C	59	ARG
6	D	153	ALA
5	J	139	VAL
5	C	139	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	702/1468 (48%)	618 (88%)	84 (12%)	5	19
1	G	702/1468 (48%)	617 (88%)	85 (12%)	5	18
2	B	367/670 (55%)	327 (89%)	40 (11%)	6	21
2	H	367/670 (55%)	327 (89%)	40 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	186/344 (54%)	166 (89%)	20 (11%)	6	22
3	K	186/344 (54%)	166 (89%)	20 (11%)	6	22
4	F	299/351 (85%)	295 (99%)	4 (1%)	61	72
4	L	299/351 (85%)	295 (99%)	4 (1%)	61	72
5	C	129/242 (53%)	106 (82%)	23 (18%)	2	10
5	J	129/242 (53%)	106 (82%)	23 (18%)	2	10
6	D	102/363 (28%)	87 (85%)	15 (15%)	3	14
6	I	102/363 (28%)	87 (85%)	15 (15%)	3	14
All	All	3570/6876 (52%)	3197 (90%)	373 (10%)	9	22

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	135	LEU
1	G	136	HIS
1	G	137	GLU
1	G	139	LEU
1	G	154	GLN
1	G	155	THR
1	G	166	LYS
1	G	209	ILE
1	G	217	SER
1	G	230	VAL
1	G	236	THR
1	G	256	HIS
1	G	285	TYR
1	G	302	CYS
1	G	310	VAL
1	G	314	SER
1	G	319	VAL
1	G	323	MET
1	G	331	GLN
1	G	406	LYS
1	G	411	LEU
1	G	413	ILE
1	G	431	LEU
1	G	441	LEU
1	G	443	ARG
1	G	444	VAL

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Mol	Chain	Res	Type
1	G	448	LEU
1	G	449	LEU
1	G	457	THR
1	G	484	ARG
1	G	487	HIS
1	G	497	SER
1	G	498	LEU
1	G	513	SER
1	G	542	ILE
1	G	552	ILE
1	G	560	ASN
1	G	569	THR
1	G	570	ILE
1	G	572	LYS
1	G	574	ILE
1	G	615	ASN
1	G	619	THR
1	G	622	SER
1	G	625	ILE
1	G	651	ILE
1	G	664	THR
1	G	676	GLN
1	G	708	LEU
1	G	711	THR
1	G	717	VAL
1	G	724	GLN
1	G	744	ASN
1	G	747	ILE
1	G	764	ILE
1	G	782	LEU
1	G	791	LEU
1	G	794	ASN
1	G	801	GLN
1	G	811	ARG
1	G	817	ILE
1	G	827	ASP
1	G	828	GLN
1	G	834	ILE
1	G	842	ASN
1	G	852	TYR
1	G	870	ILE
1	G	872	LEU

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Mol	Chain	Res	Type
1	G	873	ILE
1	G	876	CYS
1	G	898	LEU
1	G	900	THR
1	G	908	ARG
1	G	915	LEU
1	G	932	PHE
1	G	941	SER
1	G	1018	TRP
1	G	1036	VAL
1	G	1041	PHE
1	G	1065	ILE
1	G	1066	LEU
1	G	1078	LEU
1	G	1092	LEU
1	G	1095	THR
1	G	1129	VAL
2	H	15	LEU
2	H	30	ARG
2	H	34	LEU
2	H	98	ILE
2	H	100	LEU
2	H	126	THR
2	H	127	ILE
2	H	128	ILE
2	H	136	THR
2	H	148	ILE
2	H	157	VAL
2	H	185	LEU
2	H	188	LEU
2	H	196	THR
2	H	206	LEU
2	H	258	ASP
2	H	278	LEU
2	H	295	ILE
2	H	316	LEU
2	H	337	VAL
2	H	359	ILE
2	H	367	LEU
2	H	371	ILE
2	H	374	ILE
2	H	376	LEU

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Mol	Chain	Res	Type
2	H	380	THR
2	H	409	ILE
2	H	435	ILE
2	H	443	VAL
2	H	456	CYS
2	H	493	PHE
2	H	506	ILE
2	H	519	THR
2	H	527	LEU
2	H	528	ILE
2	H	531	VAL
2	H	536	THR
2	H	538	LEU
2	H	586	LEU
2	H	594	PHE
3	K	28	LEU
3	K	76	SER
3	K	89	VAL
3	K	105	ILE
3	K	116	THR
3	K	128	ILE
3	K	140	LEU
3	K	157	LEU
3	K	201	ILE
3	K	218	SER
3	K	230	SER
3	K	248	LYS
3	K	273	ILE
3	K	279	VAL
3	K	301	LEU
3	K	303	VAL
3	K	309	ILE
3	K	330	LEU
3	K	366	PHE
3	K	373	LEU
4	L	313	VAL
4	L	329	SER
4	L	335	THR
4	L	349	TYR
1	A	135	LEU
1	A	136	HIS
1	A	137	GLU

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	154	GLN
1	A	155	THR
1	A	166	LYS
1	A	209	ILE
1	A	217	SER
1	A	230	VAL
1	A	236	THR
1	A	256	HIS
1	A	285	TYR
1	A	302	CYS
1	A	310	VAL
1	A	314	SER
1	A	319	VAL
1	A	323	MET
1	A	331	GLN
1	A	406	LYS
1	A	411	LEU
1	A	413	ILE
1	A	431	LEU
1	A	441	LEU
1	A	443	ARG
1	A	444	VAL
1	A	448	LEU
1	A	449	LEU
1	A	457	THR
1	A	484	ARG
1	A	487	HIS
1	A	497	SER
1	A	498	LEU
1	A	513	SER
1	A	542	ILE
1	A	552	ILE
1	A	560	ASN
1	A	569	THR
1	A	572	LYS
1	A	574	ILE
1	A	615	ASN
1	A	619	THR
1	A	622	SER
1	A	625	ILE
1	A	651	ILE

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Mol	Chain	Res	Type
1	A	664	THR
1	A	676	GLN
1	A	708	LEU
1	A	711	THR
1	A	717	VAL
1	A	724	GLN
1	A	744	ASN
1	A	747	ILE
1	A	764	ILE
1	A	782	LEU
1	A	791	LEU
1	A	794	ASN
1	A	801	GLN
1	A	811	ARG
1	A	817	ILE
1	A	827	ASP
1	A	828	GLN
1	A	834	ILE
1	A	842	ASN
1	A	852	TYR
1	A	870	ILE
1	A	872	LEU
1	A	873	ILE
1	A	876	CYS
1	A	898	LEU
1	A	900	THR
1	A	908	ARG
1	A	915	LEU
1	A	932	PHE
1	A	941	SER
1	A	1018	TRP
1	A	1036	VAL
1	A	1041	PHE
1	A	1065	ILE
1	A	1066	LEU
1	A	1078	LEU
1	A	1092	LEU
1	A	1095	THR
1	A	1129	VAL
2	B	15	LEU
2	B	30	ARG
2	B	34	LEU

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Mol	Chain	Res	Type
2	B	98	ILE
2	B	100	LEU
2	B	126	THR
2	B	127	ILE
2	B	128	ILE
2	B	136	THR
2	B	148	ILE
2	B	157	VAL
2	B	185	LEU
2	B	188	LEU
2	B	196	THR
2	B	206	LEU
2	B	258	ASP
2	B	278	LEU
2	B	295	ILE
2	B	316	LEU
2	B	337	VAL
2	B	359	ILE
2	B	367	LEU
2	B	371	ILE
2	B	374	ILE
2	B	376	LEU
2	B	380	THR
2	B	409	ILE
2	B	435	ILE
2	B	443	VAL
2	B	456	CYS
2	B	493	PHE
2	B	506	ILE
2	B	519	THR
2	B	527	LEU
2	B	528	ILE
2	B	531	VAL
2	B	536	THR
2	B	538	LEU
2	B	586	LEU
2	B	594	PHE
3	E	28	LEU
3	E	76	SER
3	E	89	VAL
3	E	105	ILE
3	E	116	THR

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Mol	Chain	Res	Type
3	E	128	ILE
3	E	140	LEU
3	E	157	LEU
3	E	201	ILE
3	E	218	SER
3	E	230	SER
3	E	248	LYS
3	E	273	ILE
3	E	279	VAL
3	E	301	LEU
3	E	303	VAL
3	E	309	ILE
3	E	330	LEU
3	E	366	PHE
3	E	373	LEU
4	F	313	VAL
4	F	329	SER
4	F	335	THR
4	F	349	TYR
5	J	20	LEU
5	J	27	LEU
5	J	57	LEU
5	J	62	ILE
5	J	71	ASP
5	J	74	GLN
5	J	80	LEU
5	J	88	ARG
5	J	100	ILE
5	J	107	PHE
5	J	110	LEU
5	J	118	ILE
5	J	120	LEU
5	J	126	VAL
5	J	132	VAL
5	J	134	VAL
5	J	140	THR
5	J	147	TRP
5	J	148	VAL
5	J	156	ILE
5	J	170	VAL
5	J	173	GLN
5	J	176	ASN

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Mol	Chain	Res	Type
6	I	11	VAL
6	I	22	THR
6	I	30	ILE
6	I	34	VAL
6	I	48	ASN
6	I	73	LEU
6	I	79	ILE
6	I	107	LEU
6	I	109	ASP
6	I	110	ILE
6	I	119	LEU
6	I	127	LEU
6	I	133	VAL
6	I	202	LEU
6	I	205	ILE
5	C	20	LEU
5	C	27	LEU
5	C	57	LEU
5	C	62	ILE
5	C	71	ASP
5	C	74	GLN
5	C	80	LEU
5	C	88	ARG
5	C	100	ILE
5	C	107	PHE
5	C	110	LEU
5	C	118	ILE
5	C	120	LEU
5	C	126	VAL
5	C	132	VAL
5	C	134	VAL
5	C	140	THR
5	C	147	TRP
5	C	148	VAL
5	C	156	ILE
5	C	170	VAL
5	C	173	GLN
5	C	176	ASN
6	D	11	VAL
6	D	22	THR
6	D	30	ILE
6	D	34	VAL

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Mol	Chain	Res	Type
6	D	48	ASN
6	D	73	LEU
6	D	79	ILE
6	D	107	LEU
6	D	109	ASP
6	D	110	ILE
6	D	119	LEU
6	D	127	LEU
6	D	133	VAL
6	D	202	LEU
6	D	205	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	102	GLN
1	G	211	HIS
1	G	256	HIS
1	G	262	ASN
1	G	318	ASN
1	G	414	HIS
1	G	422	HIS
1	G	529	HIS
1	G	724	GLN
1	G	749	ASN
1	G	759	HIS
1	G	794	ASN
1	G	801	GLN
1	G	893	ASN
1	G	1032	GLN
1	G	1033	ASN
2	H	9	GLN
2	H	208	ASN
2	H	221	ASN
2	H	282	ASN
2	H	350	ASN
2	H	388	GLN
3	K	72	HIS
3	K	223	HIS
3	K	252	HIS
3	K	281	ASN
3	K	305	HIS

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Mol	Chain	Res	Type
4	L	90	GLN
4	L	122	GLN
4	L	123	GLN
4	L	186	HIS
4	L	330	ASN
4	L	380	ASN
4	L	385	ASN
4	L	423	GLN
1	A	102	GLN
1	A	211	HIS
1	A	256	HIS
1	A	262	ASN
1	A	318	ASN
1	A	414	HIS
1	A	422	HIS
1	A	529	HIS
1	A	724	GLN
1	A	749	ASN
1	A	759	HIS
1	A	794	ASN
1	A	801	GLN
1	A	893	ASN
1	A	1032	GLN
1	A	1033	ASN
2	B	9	GLN
2	B	208	ASN
2	B	221	ASN
2	B	282	ASN
2	B	350	ASN
2	B	358	ASN
3	E	72	HIS
3	E	223	HIS
3	E	281	ASN
3	E	305	HIS
4	F	90	GLN
4	F	122	GLN
4	F	123	GLN
4	F	186	HIS
4	F	380	ASN
4	F	385	ASN
4	F	423	GLN
5	J	79	GLN

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Mol	Chain	Res	Type
5	J	109	HIS
5	J	131	GLN
5	J	159	GLN
5	J	173	GLN
5	J	180	GLN
6	I	25	ASN
6	I	48	ASN
6	I	94	GLN
5	C	79	GLN
5	C	109	HIS
5	C	131	GLN
5	C	159	GLN
5	C	173	GLN
5	C	180	GLN
6	D	25	ASN
6	D	48	ASN
6	D	94	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	235:LYS	C	236:ILE	N	3.04

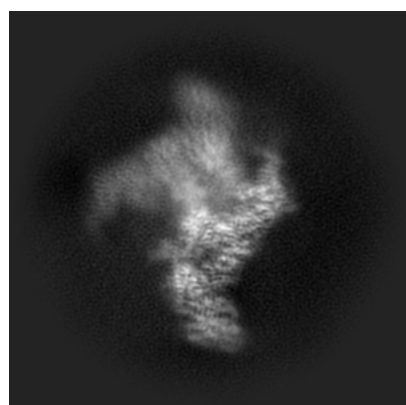
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11871. These allow visual inspection of the internal detail of the map and identification of artifacts.

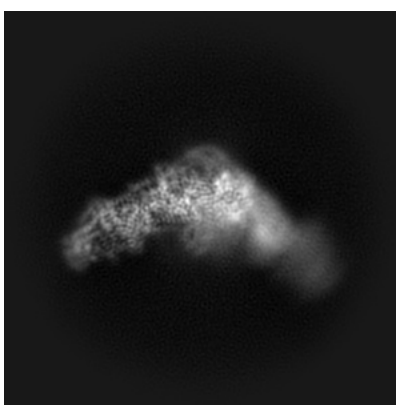
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

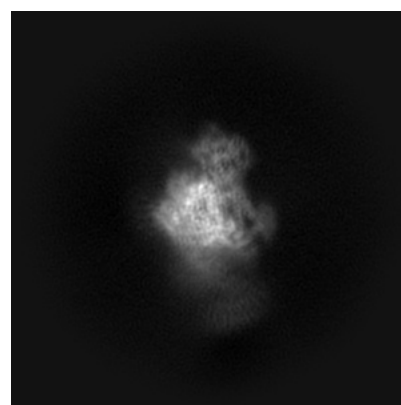
6.1.1 Primary map



X



Y

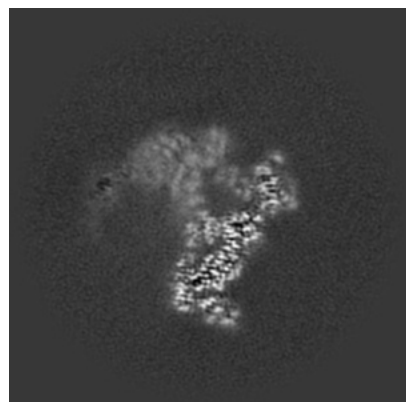


Z

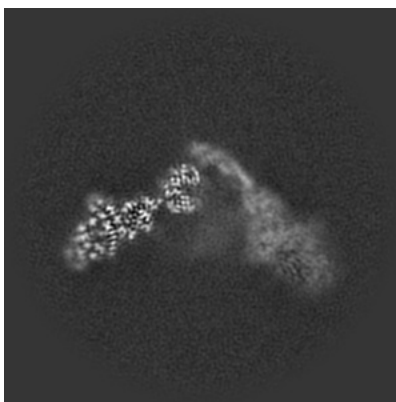
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

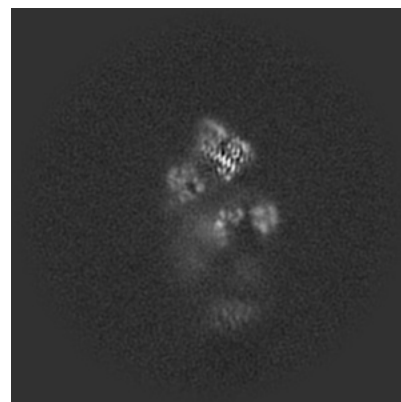
6.2.1 Primary map



X Index: 150



Y Index: 150

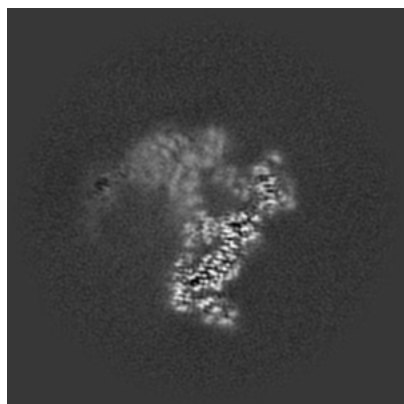


Z Index: 150

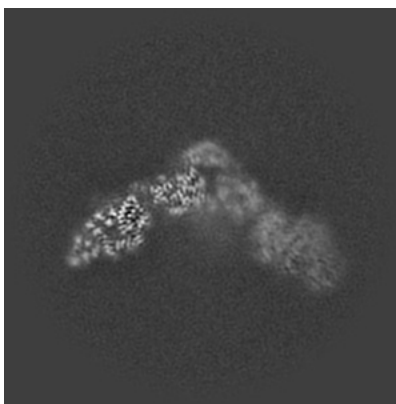
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 150



Y Index: 141



Z Index: 144

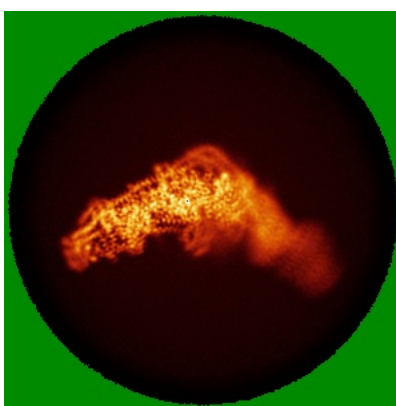
The images above show the largest variance slices of the map in three orthogonal directions.

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

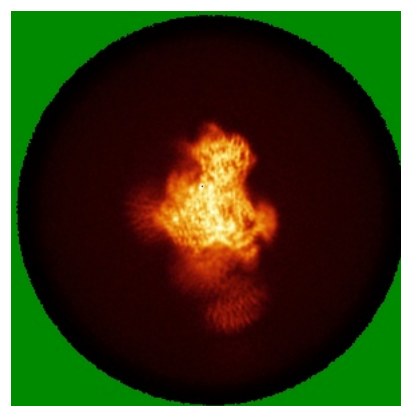
6.4.1 Primary map



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

This section was not generated.

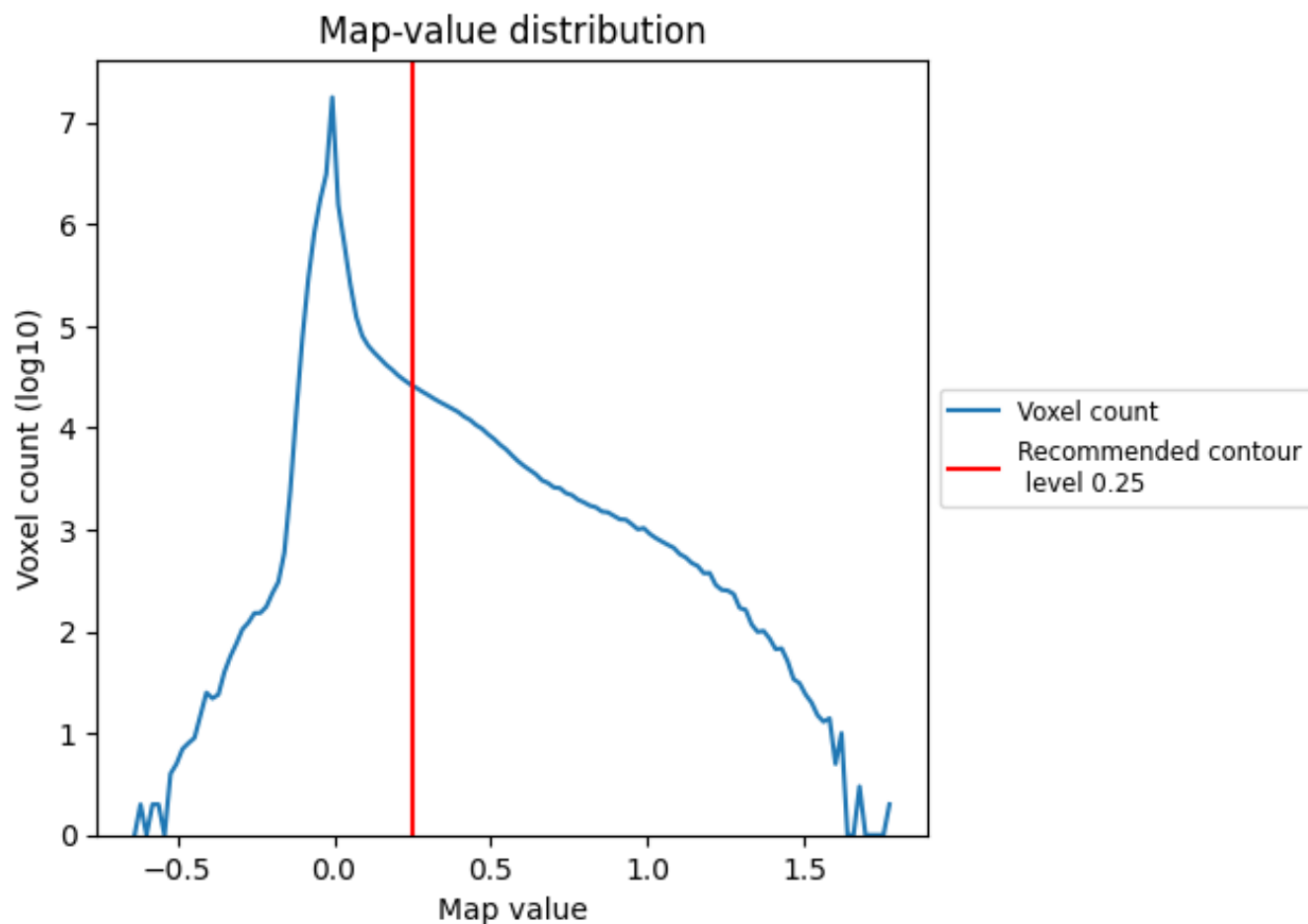
6.6 Mask visualisation

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

7 Map analysis [i](#)

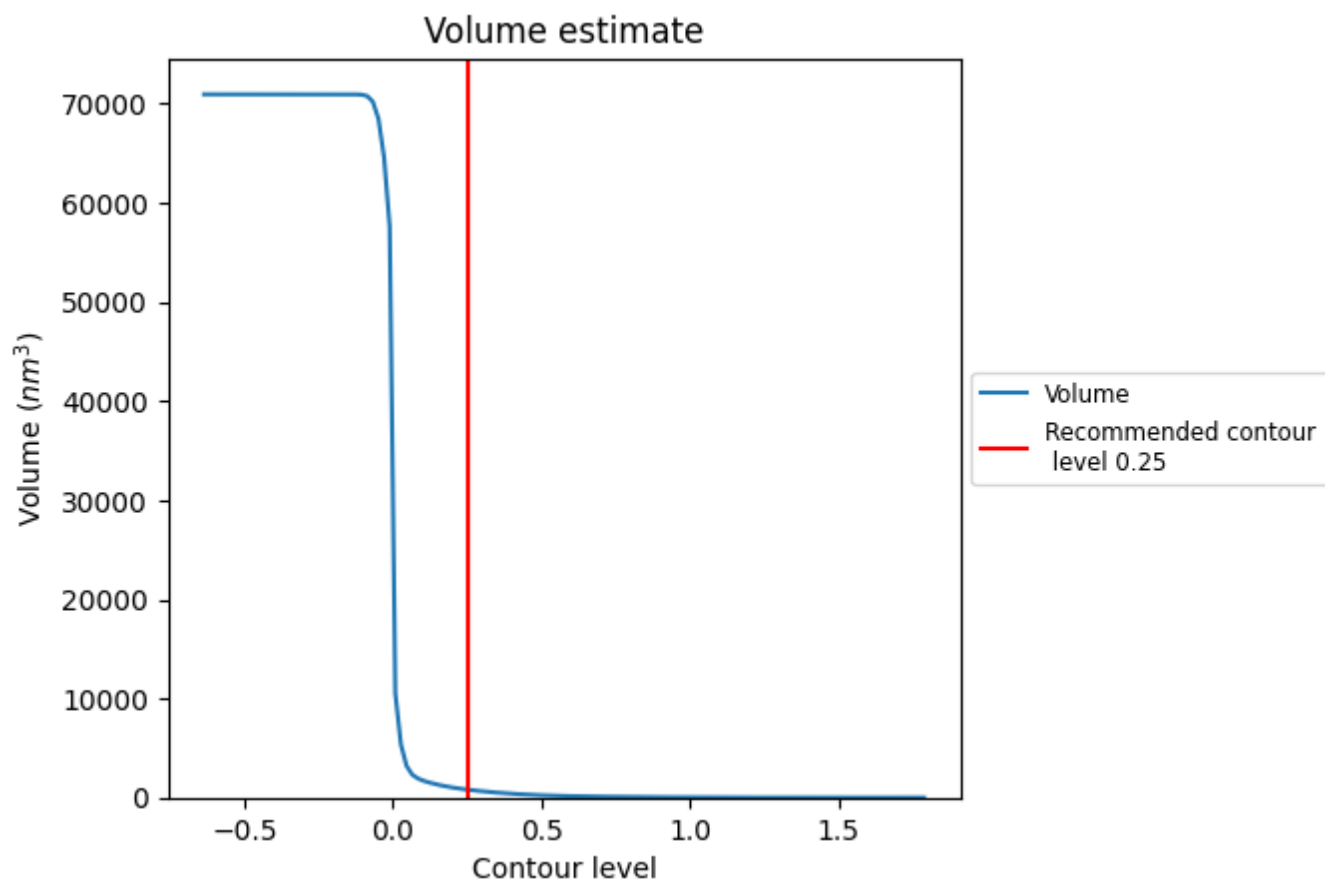
This section contains the results of statistical analysis of the map.

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.

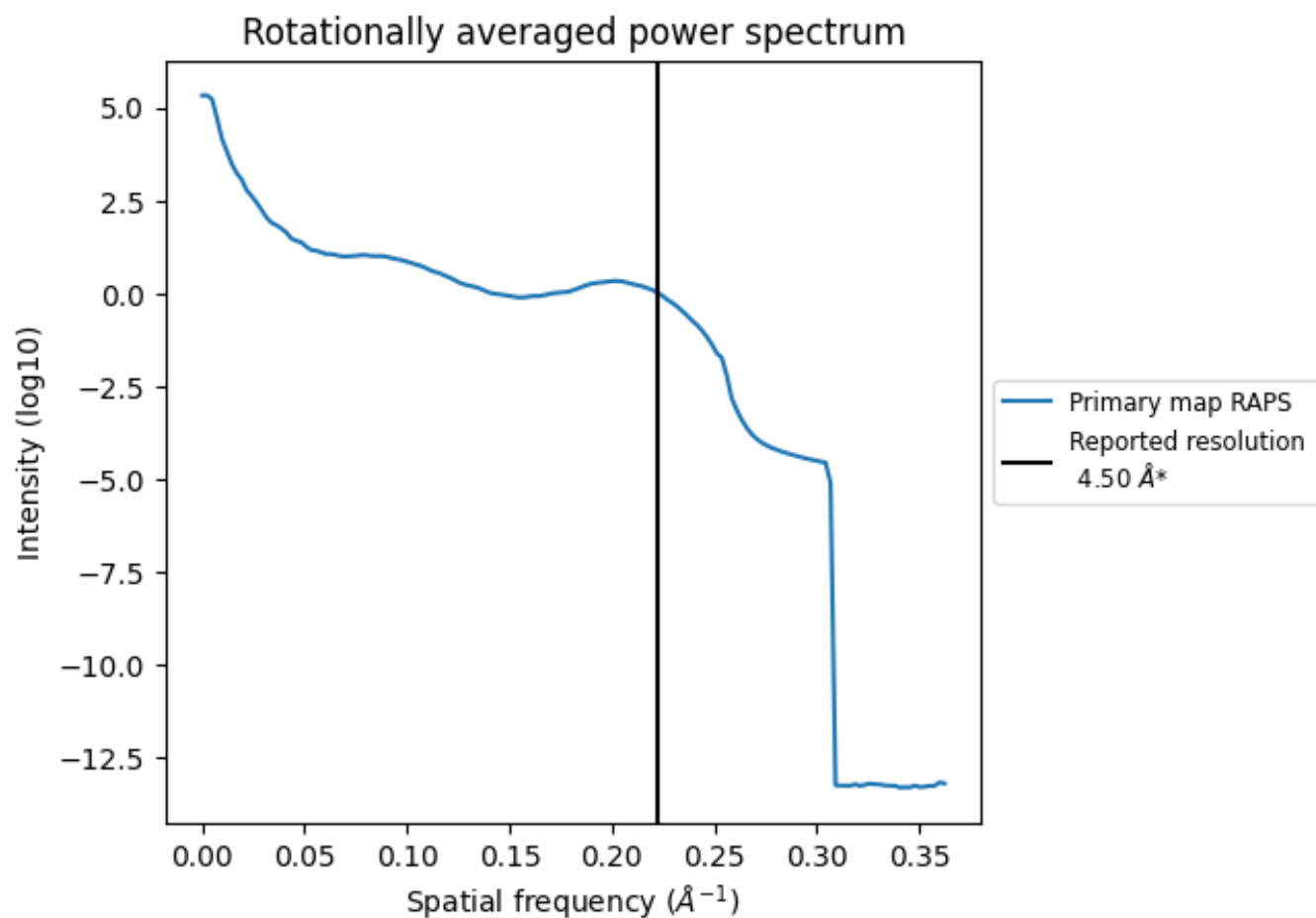
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 804 nm^3 ; this corresponds to an approximate mass of 726 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 0.222 Å⁻¹

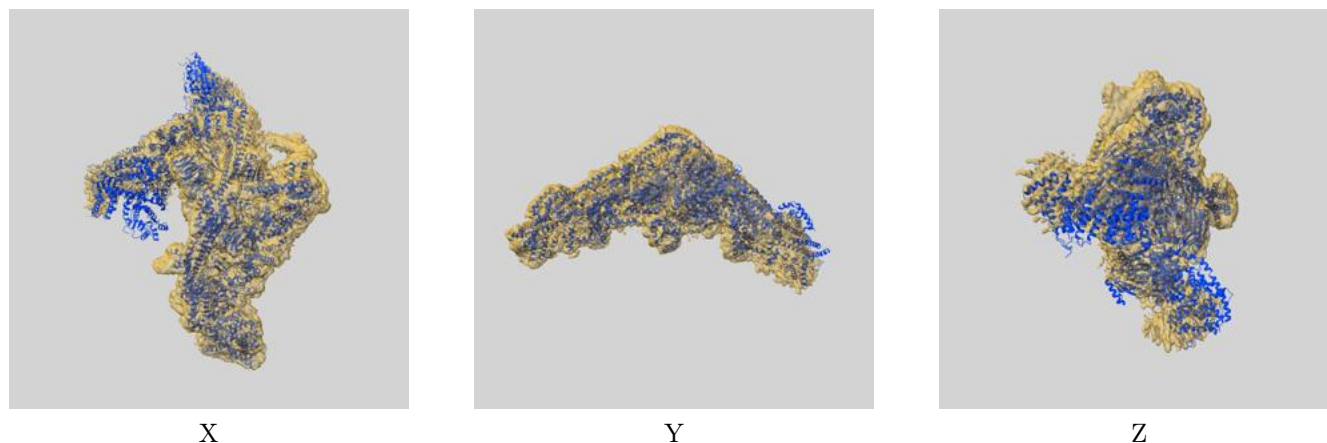
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

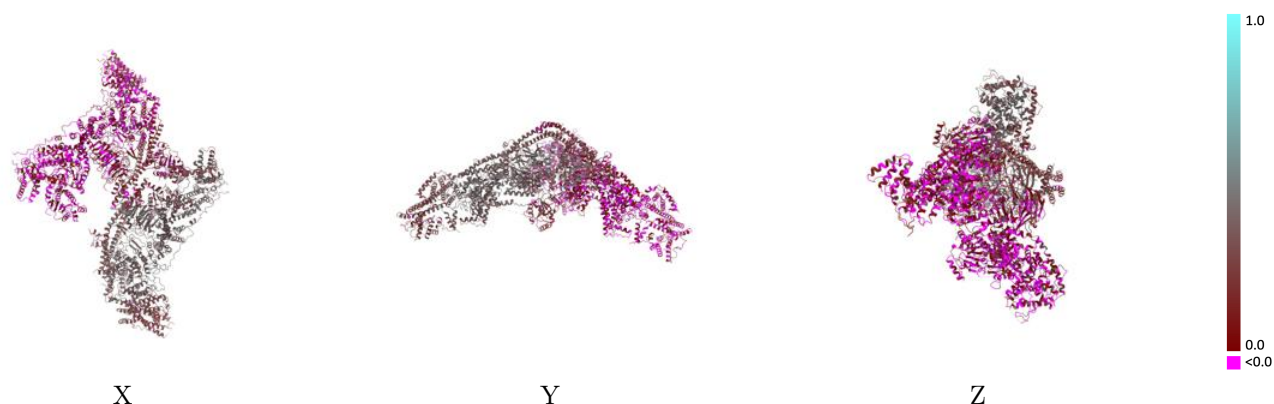
This section contains information regarding the fit between EMDB map EMD-11871 and PDB model 7AQO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



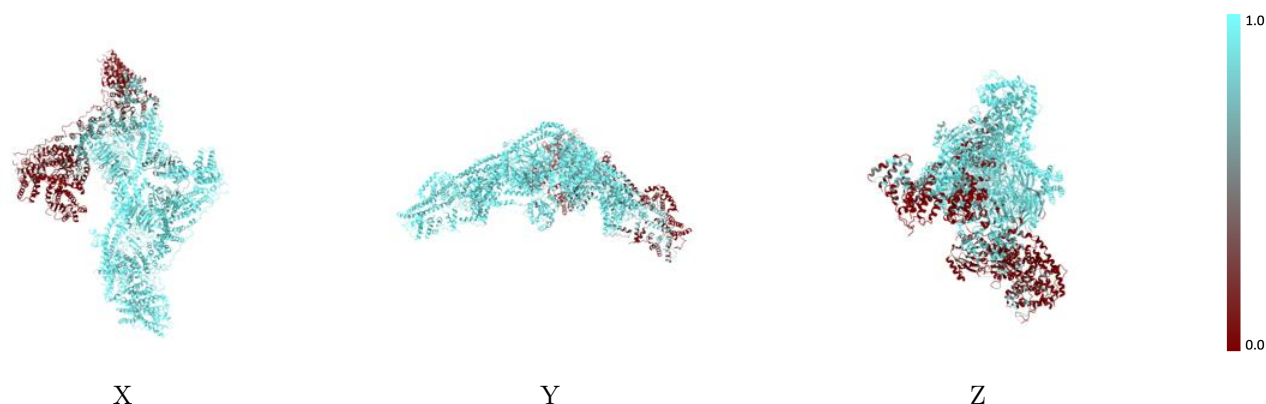
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



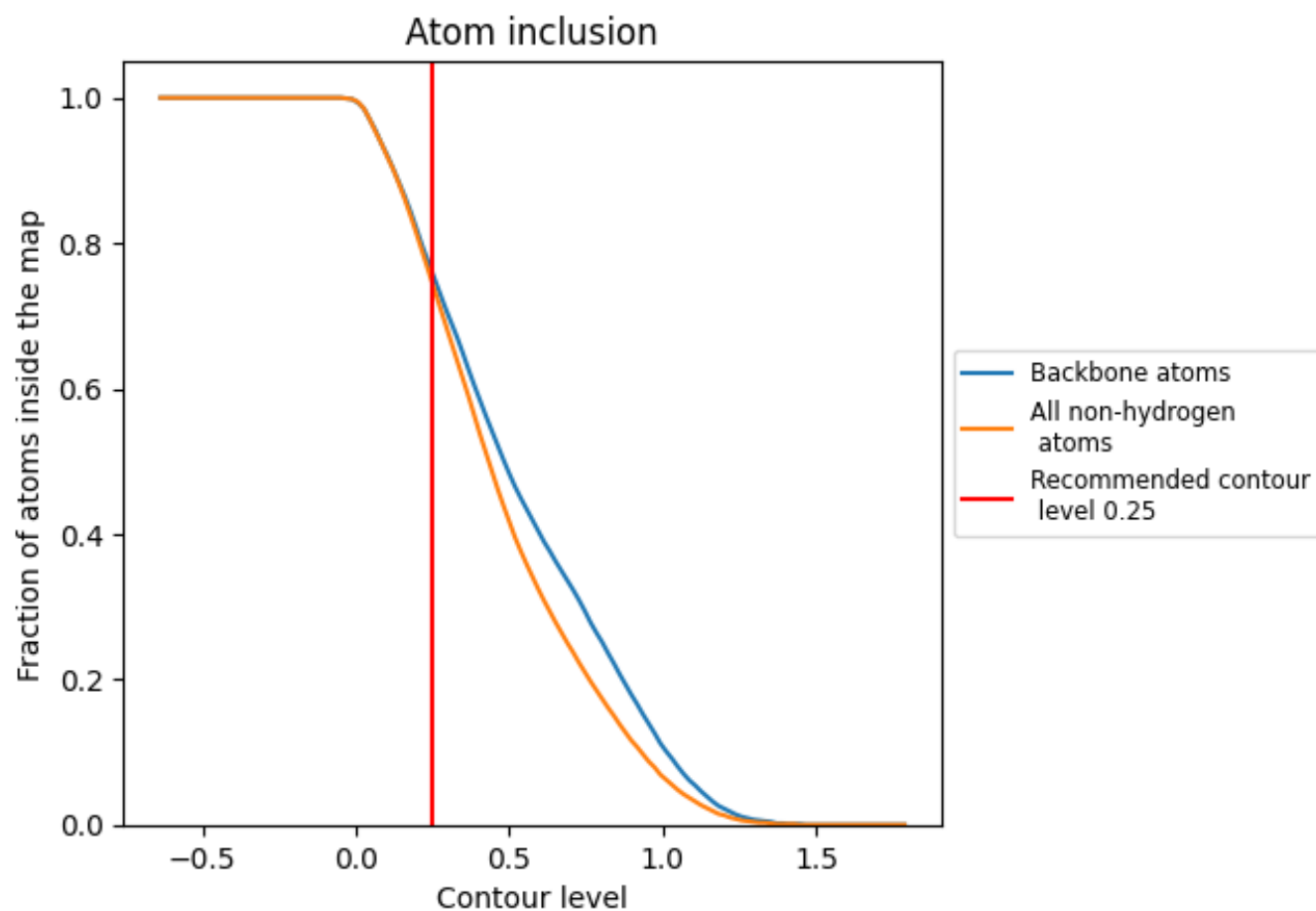
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.1890
A	0.9870	0.3920
B	0.9820	0.3790
C	0.9700	0.3400
D	0.9740	0.3130
E	0.9930	0.4000
F	0.8170	0.1320
G	0.4690	0.0170
H	0.5790	0.0200
I	0.6440	0.0790
J	0.7470	0.0910
K	0.9340	0.0960
L	0.1040	0.0020

1.0

0.0

<0.0