



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 07:19 PM UTC

PDB ID : 4V1A / pdb_00004v1a
EMDB ID : EMD-2787
Title : Structure of the large subunit of the mammalian mitoribosome, part 2 of 2
Authors : Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N.
Deposited on : 2014-09-25
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

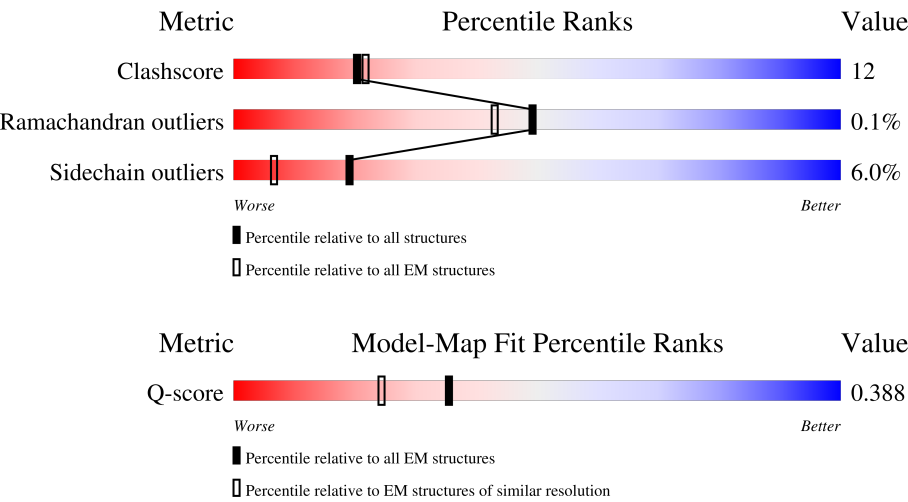
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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 <=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	423	9% 64% 27% 7%
2	b	380	8% 67% 23% 7%
3	c	334	25% 63% 23% 12%
4	d	206	31% 16% 52%

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Mol	Chain	Length	Quality of chain
5	e	135	
6	f	142	
7	g	159	
8	h	332	
9	i	312	
10	j	279	
11	k	212	
12	l	166	
13	m	159	
14	n	128	
15	o	124	
16	p	112	
17	q	138	
18	t	102	
19	u	205	
20	v	222	
21	w	433	
22	x	196	
23	z	47	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 31917 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 MITORIBOSOMAL PROTEIN ML37, MRPL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	121	Total	C	N	O	S	0	0
			968	626	167	172	3		

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	108	Total	C	N	O	S	0	0
			852	544	154	150	4		

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	242	Total	C	N	O	S	0	0
			1979	1266	352	351	10		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	131	Total	C	N	O	S	0	0
			1050	671	178	196	5		

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	94	Total	C	N	O	S	0	0
			747	466	143	136	2		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	q	37	Total	C	N	O	0	0
			336	214	69	53		

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	151	Total	C	N	O	S	0	0
			1208	748	233	222	5		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	131	Total	C	N	O	S	0	0
			1068	662	206	195	5		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	w	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 23 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	z	47	Total	C	N	O	0	0
			282	188	47	47		

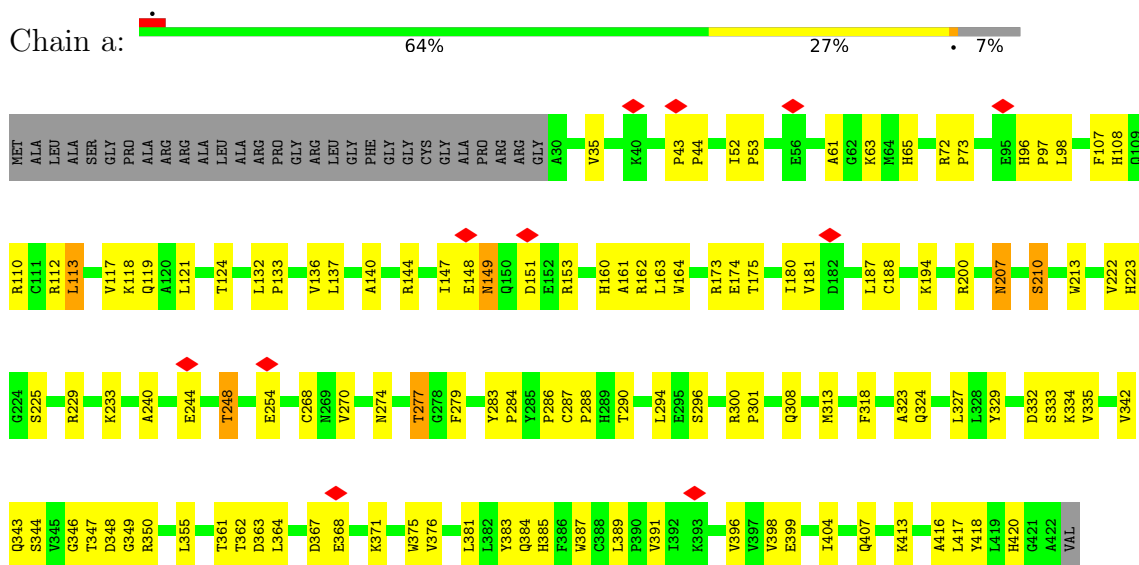
- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	x	1	Total	Zn	0
			1	1	

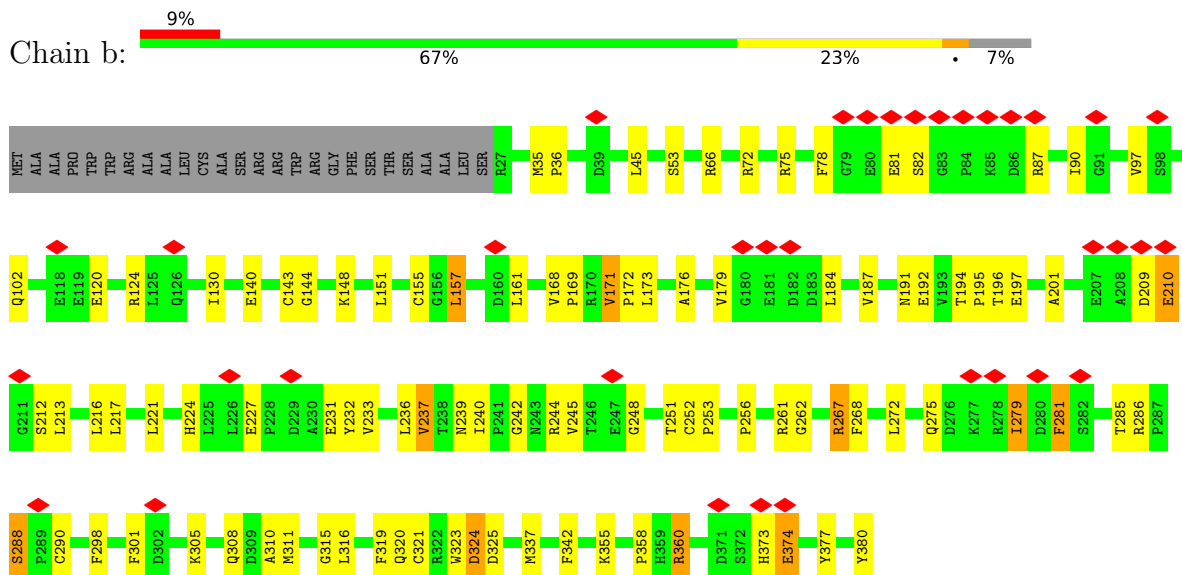
3 Residue-property plots

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.

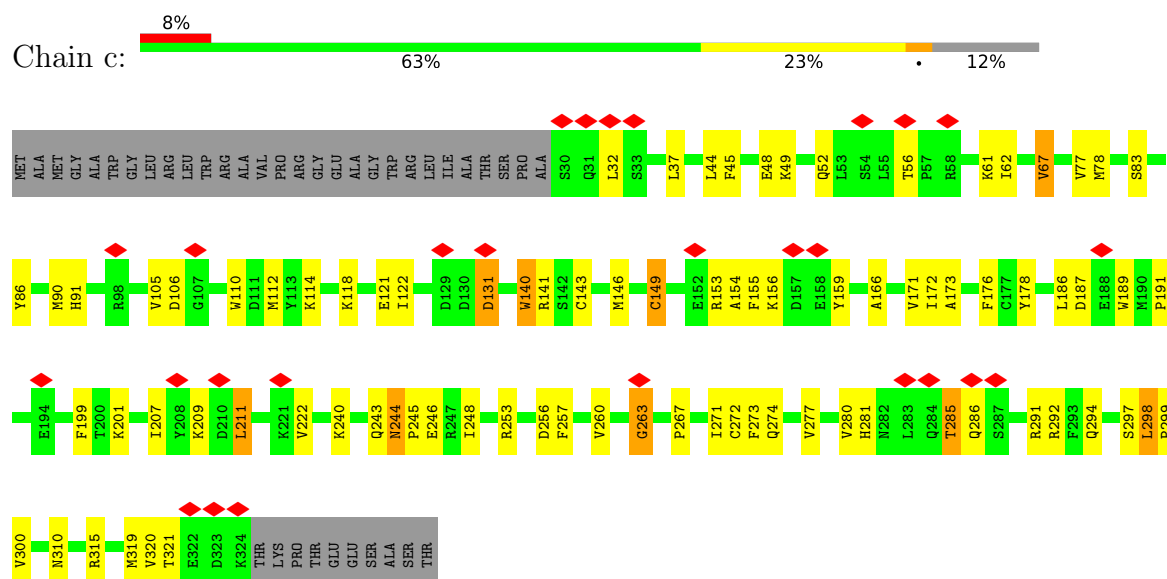
- Molecule 1: MITORIBOSOMAL PROTEIN ML37, MRPL37



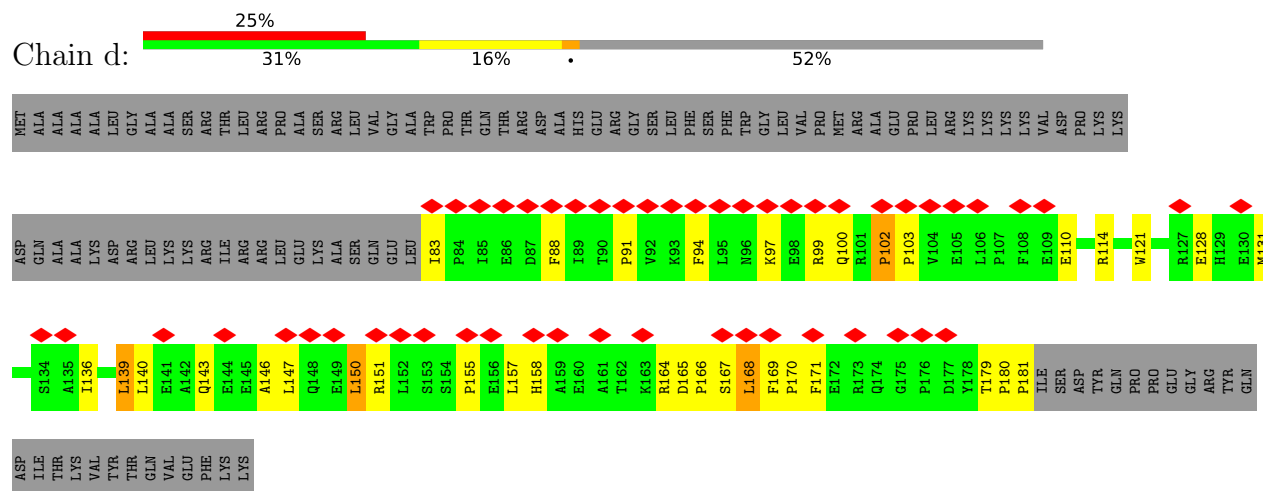
- Molecule 2: MITORIBOSOMAL PROTEIN ML38, MRPL38



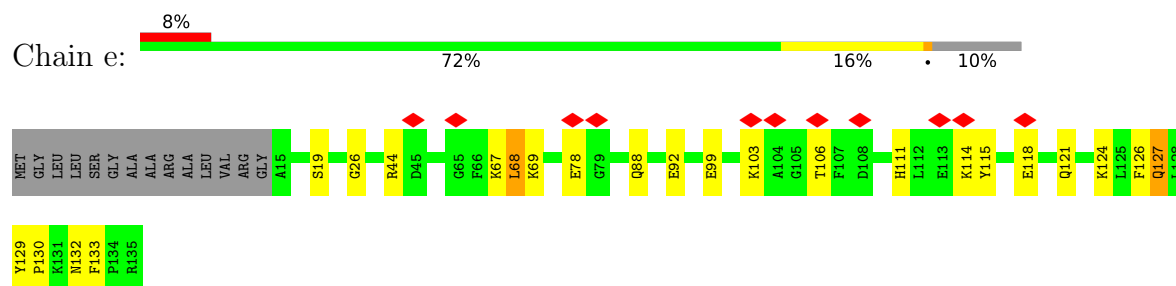
- Molecule 3: MITORIBOSOMAL PROTEIN ML39, MRPL39



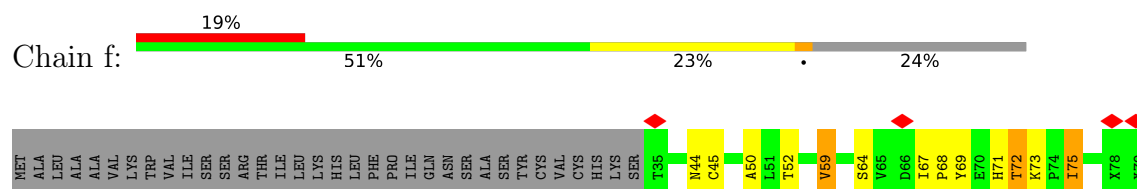
- Molecule 4: MITORIBOSOMAL PROTEIN ML40, MRPL40

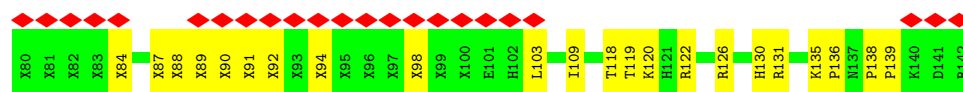


- Molecule 5: MITORIBOSOMAL PROTEIN ML41, MRPL41

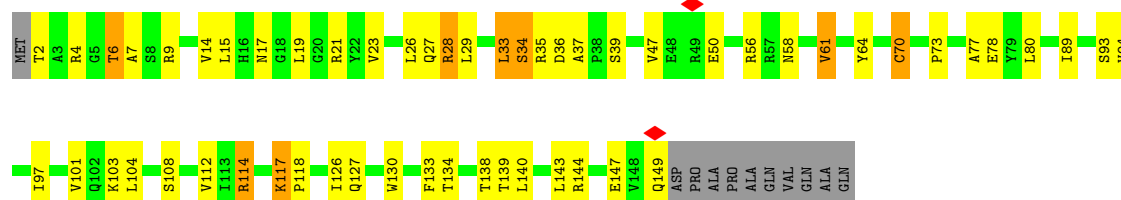


- Molecule 6: MITORIBOSOMAL PROTEIN ML42, MRPL42

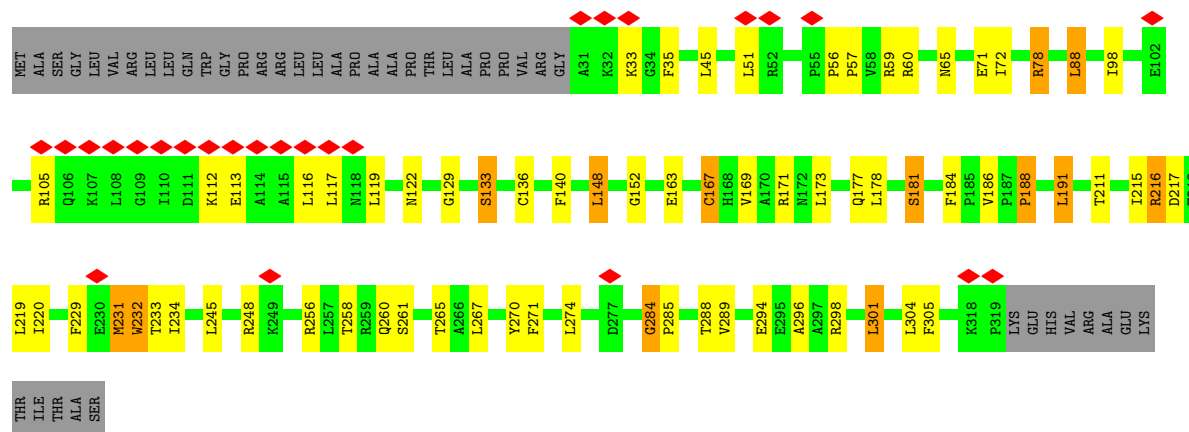




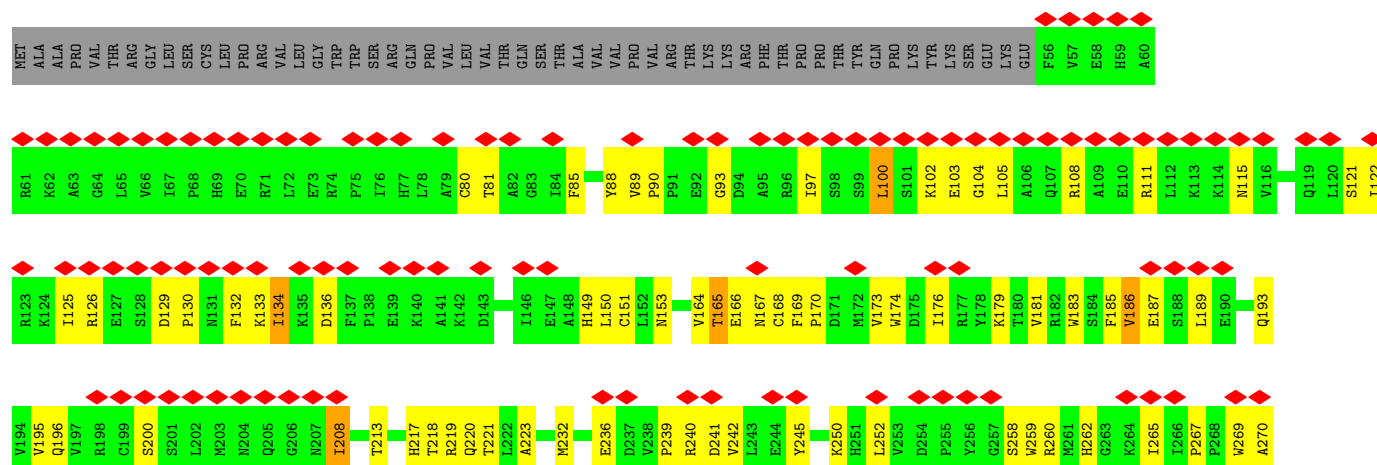
• Molecule 7: MITORIBOSOMAL PROTEIN ML43, MRPL43



• Molecule 8: MITORIBOSOMAL PROTEIN ML44, MRPL44

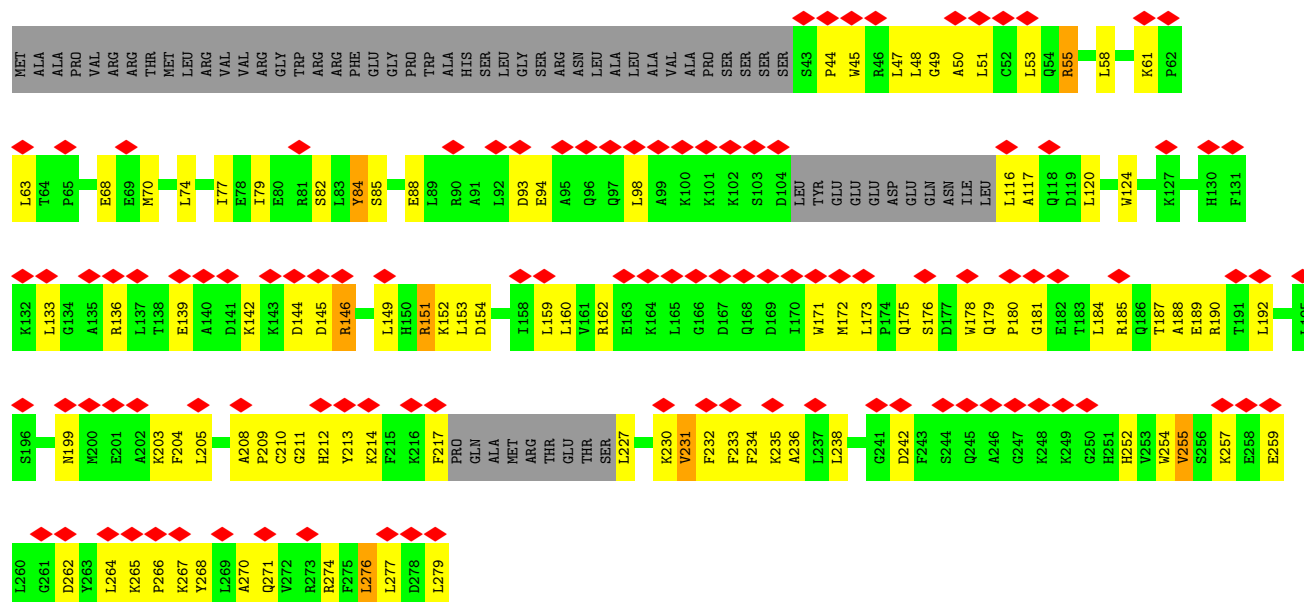
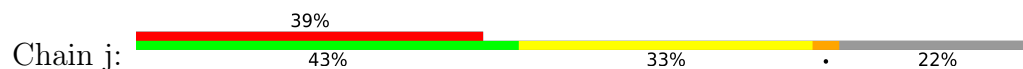


• Molecule 9: MITORIBOSOMAL PROTEIN ML45, MRPL45

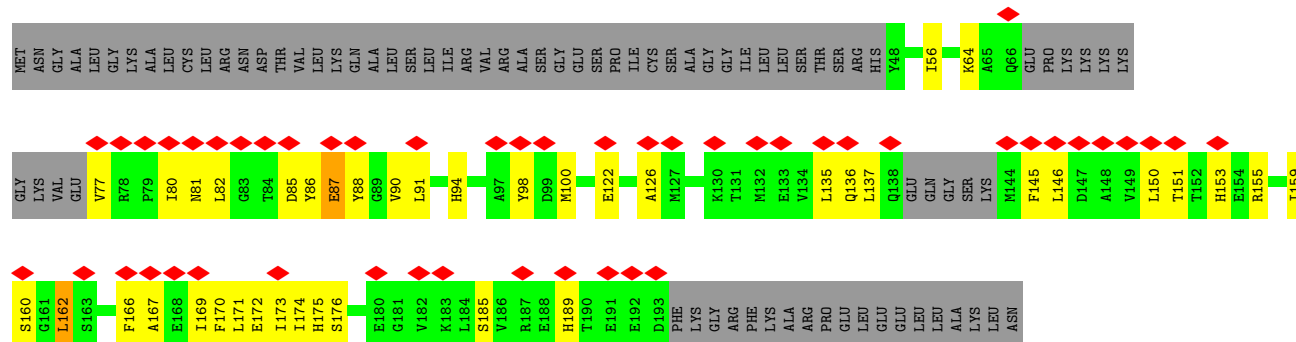
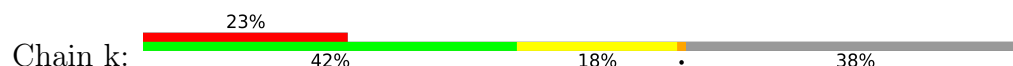




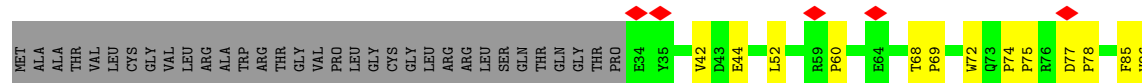
• Molecule 10: MITORIBOSOMAL PROTEIN ML46, MRPL46

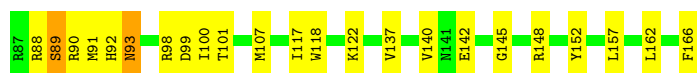


• Molecule 11: MITORIBOSOMAL PROTEIN ML48, MRPL48

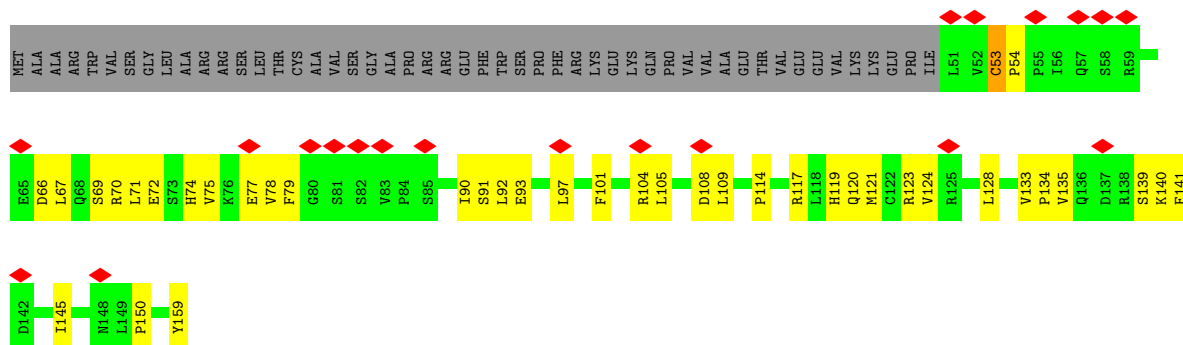
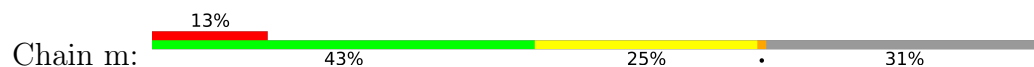


• Molecule 12: MITORIBOSOMAL PROTEIN ML49, MRPL49

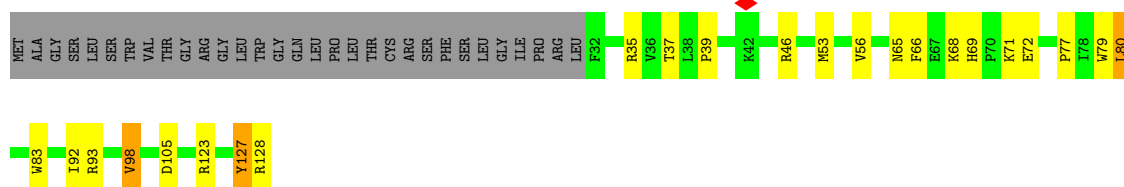




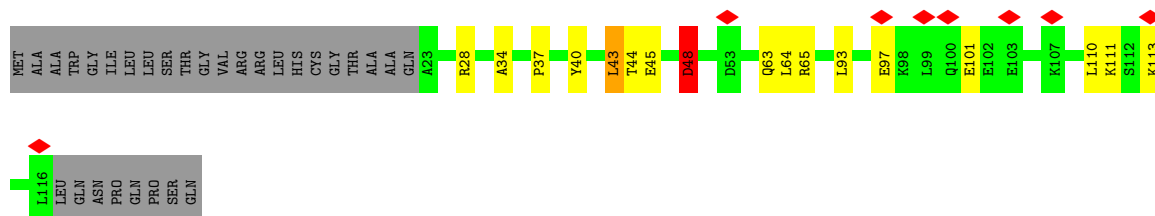
• Molecule 13: MITORIBOSOMAL PROTEIN ML50, MRPL50



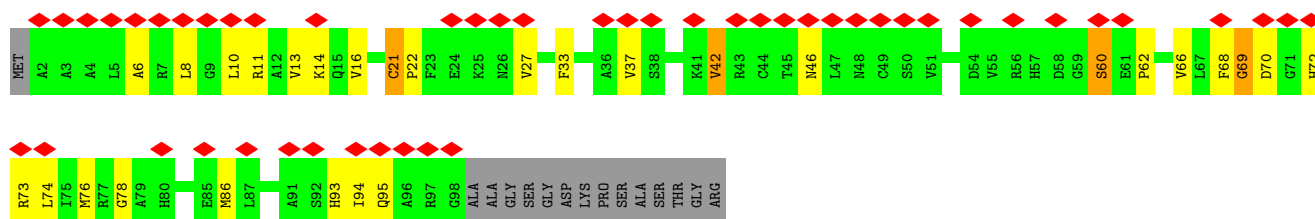
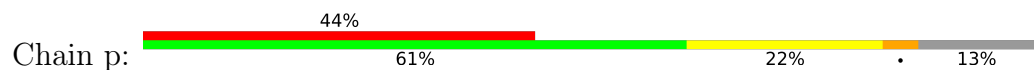
• Molecule 14: MITORIBOSOMAL PROTEIN ML51, MRPL51



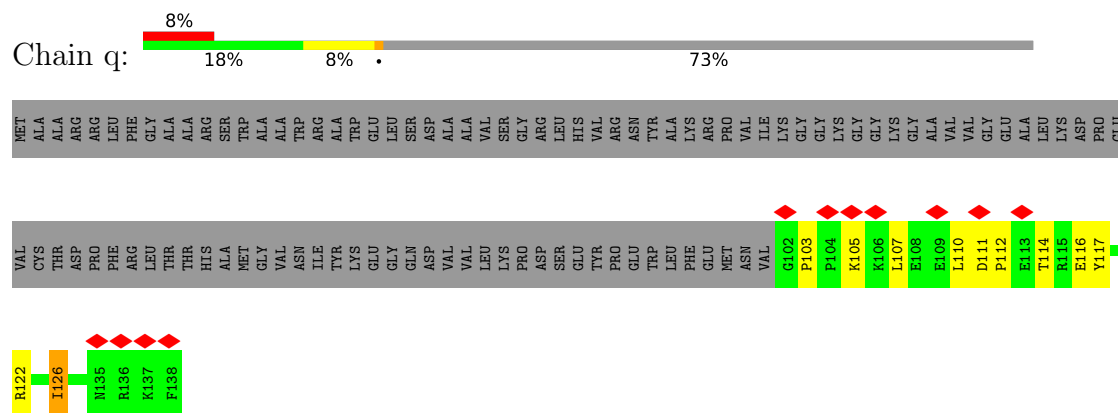
• Molecule 15: MITORIBOSOMAL PROTEIN ML52, MRPL52



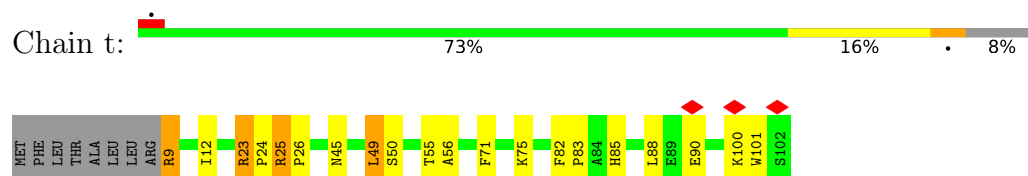
• Molecule 16: MITORIBOSOMAL PROTEIN ML53, MRPL53



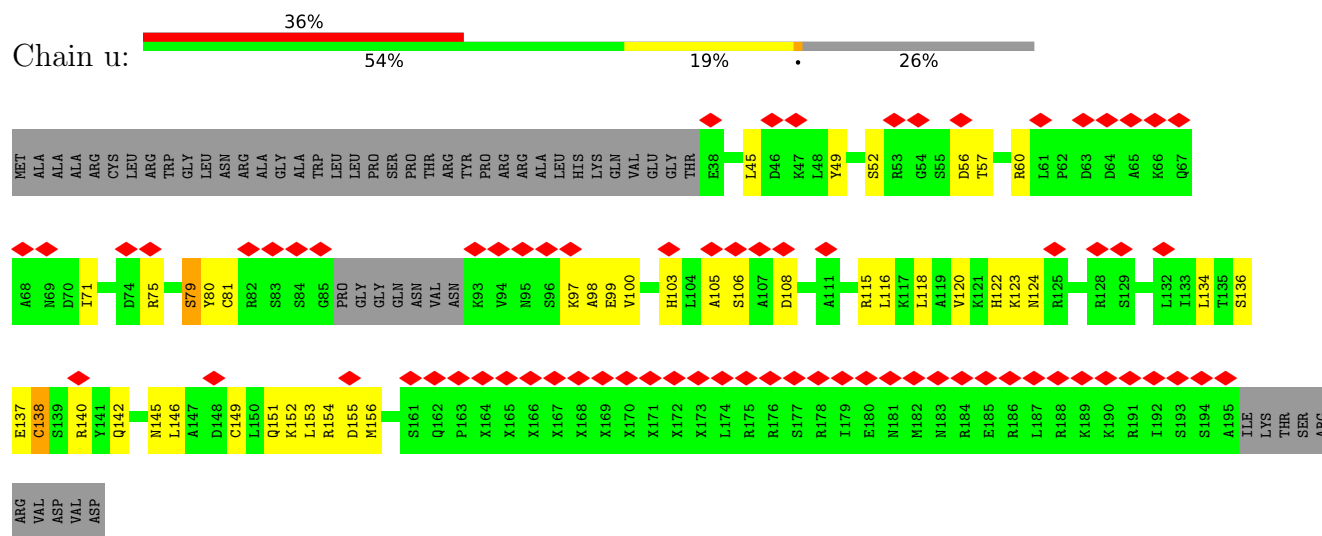
• Molecule 17: MITORIBOSOMAL PROTEIN ML54, MRPL54



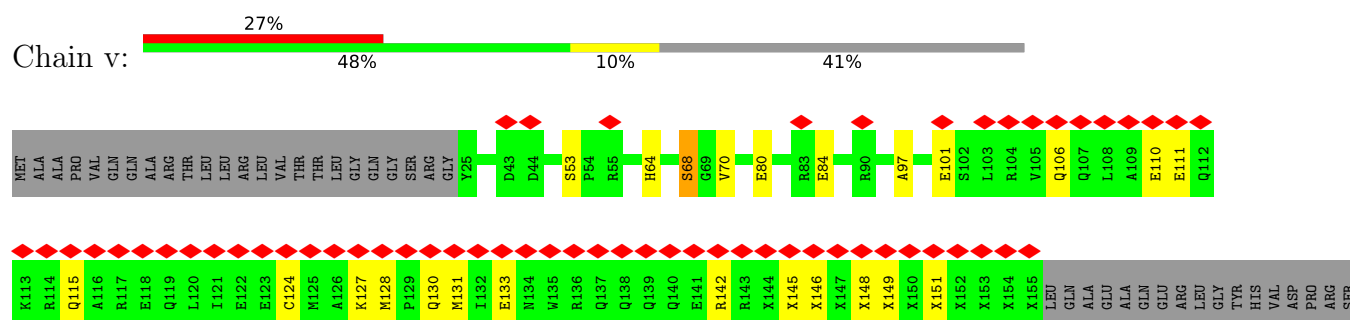
• Molecule 18: MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63



• Molecule 19: MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1

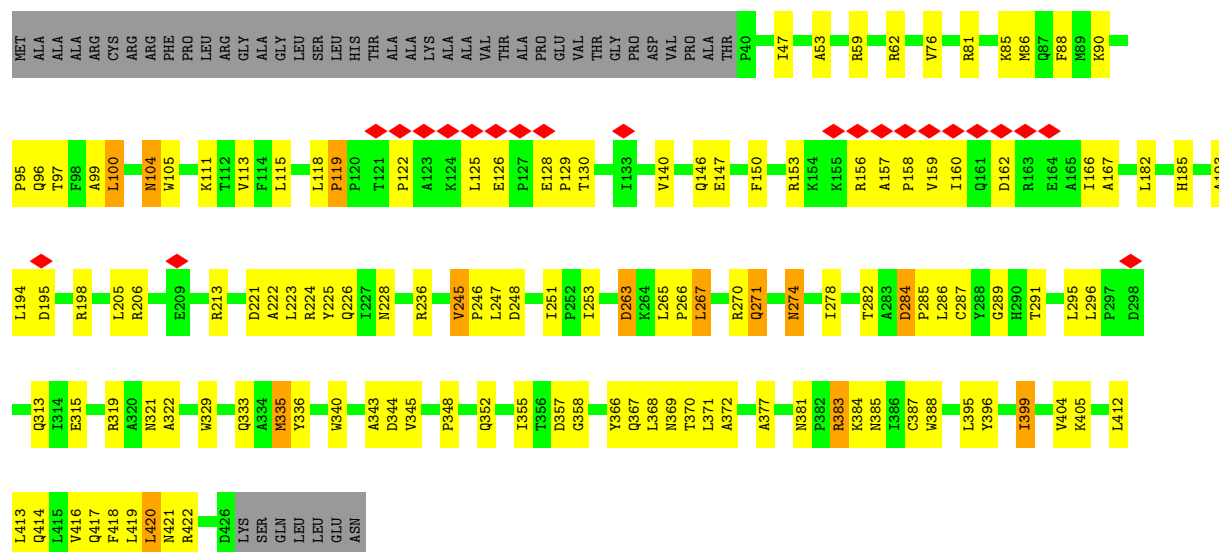


• Molecule 20: MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1

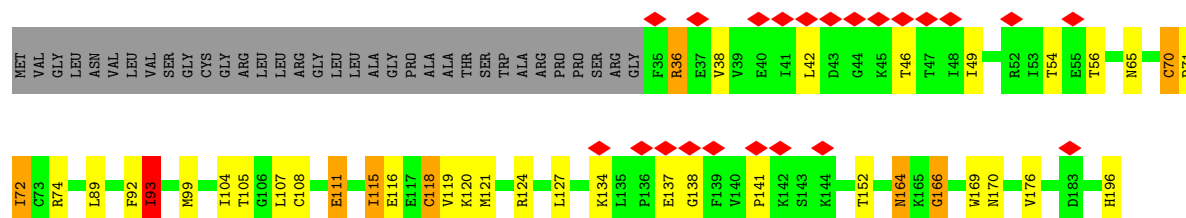




• Molecule 21: MITORIBOSOMAL PROTEIN ML65, MRPS30



• Molecule 22: MITORIBOSOMAL PROTEIN ML66, MRPS18A



• Molecule 23: UNASSIGNED SECONDARY STRUCTURE ELEMENTS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141675	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.560	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	302.4, 302.4, 302.4	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/3267	0.90	3/4455 (0.1%)
2	b	0.45	0/3047	0.93	9/4139 (0.2%)
3	c	0.41	0/2464	0.87	8/3330 (0.2%)
4	d	0.51	0/853	0.94	3/1153 (0.3%)
5	e	0.44	0/996	0.97	4/1340 (0.3%)
6	f	0.44	0/731	0.86	0/990
7	g	0.49	0/1191	0.99	5/1614 (0.3%)
8	h	0.45	0/2372	0.90	4/3211 (0.1%)
9	i	0.44	0/2034	0.89	2/2759 (0.1%)
10	j	0.44	0/1811	0.92	3/2436 (0.1%)
11	k	0.44	0/1070	0.89	2/1448 (0.1%)
12	l	0.49	0/1135	0.87	0/1549
13	m	0.41	0/917	0.87	3/1248 (0.2%)
14	n	0.51	0/860	0.91	1/1150 (0.1%)
15	o	0.48	0/762	0.86	1/1022 (0.1%)
16	p	0.47	0/752	0.98	4/1013 (0.4%)
17	q	0.40	0/346	0.82	0/463
18	t	0.53	0/798	1.09	5/1073 (0.5%)
19	u	0.39	0/1163	0.81	3/1557 (0.2%)
20	v	0.42	0/1022	0.80	0/1382
21	w	0.49	0/3206	0.92	8/4354 (0.2%)
22	x	0.47	0/1364	0.97	3/1849 (0.2%)
All	All	0.45	0/32161	0.91	71/43535 (0.2%)

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
2	b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	1
14	n	0	1
21	w	0	1
All	All	0	4

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	284	GLY	CA-C-N	10.80	130.89	120.31
8	h	284	GLY	C-N-CA	10.80	130.89	120.31
5	e	26	GLY	CA-C-N	9.87	129.69	120.21
5	e	26	GLY	C-N-CA	9.87	129.69	120.21
10	j	208	ALA	CA-C-N	9.28	130.01	119.99
10	j	208	ALA	C-N-CA	9.28	130.01	119.99
18	t	25	ARG	CA-C-N	9.07	129.76	120.14
18	t	25	ARG	C-N-CA	9.07	129.76	120.14
16	p	21	CYS	CA-C-N	8.63	129.48	119.47
16	p	21	CYS	C-N-CA	8.63	129.48	119.47
7	g	117	LYS	CA-C-N	8.62	128.27	119.82
7	g	117	LYS	C-N-CA	8.62	128.27	119.82
3	c	244	ASN	CA-C-N	7.37	129.06	119.84
3	c	244	ASN	C-N-CA	7.37	129.06	119.84
9	i	89	VAL	CA-C-N	7.28	124.90	119.66
9	i	89	VAL	C-N-CA	7.28	124.90	119.66
3	c	263	GLY	CA-C-N	6.93	126.86	120.21
3	c	263	GLY	C-N-CA	6.93	126.86	120.21
8	h	35	PHE	N-CA-C	-6.87	103.24	111.69
4	d	102	PRO	N-CA-C	6.80	119.00	110.70
21	w	381	ASN	CA-C-N	6.69	126.14	118.85
21	w	381	ASN	C-N-CA	6.69	126.14	118.85
18	t	23	ARG	CA-C-N	6.65	128.15	119.84
18	t	23	ARG	C-N-CA	6.65	128.15	119.84
15	o	48	ASP	N-CA-C	6.65	119.38	111.33
10	j	146	ARG	N-CA-C	-6.46	105.44	113.38
19	u	138	CYS	N-CA-C	6.42	118.81	111.11
4	d	165	ASP	CA-C-N	6.16	125.84	119.56
4	d	165	ASP	C-N-CA	6.16	125.84	119.56
19	u	49	TYR	CA-C-N	6.04	125.59	119.19
19	u	49	TYR	C-N-CA	6.04	125.59	119.19
16	p	69	GLY	N-CA-C	5.92	120.97	114.40
22	x	164	ASN	N-CA-C	5.86	120.59	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	w	88	PHE	N-CA-C	5.77	117.35	110.19
2	b	256	PRO	CA-C-N	5.70	126.03	119.93
2	b	256	PRO	C-N-CA	5.70	126.03	119.93
2	b	171	VAL	CA-C-N	5.68	125.96	119.83
2	b	171	VAL	C-N-CA	5.68	125.96	119.83
2	b	201	ALA	CA-C-N	5.63	125.83	120.31
2	b	201	ALA	C-N-CA	5.63	125.83	120.31
16	p	27	VAL	N-CA-C	5.59	118.89	111.17
7	g	37	ALA	CA-C-N	5.58	124.93	118.85
7	g	37	ALA	C-N-CA	5.58	124.93	118.85
8	h	188	PRO	N-CA-C	5.46	117.37	110.70
13	m	53	CYS	CA-C-N	5.44	123.63	119.66
13	m	53	CYS	C-N-CA	5.44	123.63	119.66
21	w	119	PRO	O-C-N	5.43	123.81	121.31
22	x	166	GLY	N-CA-C	-5.43	106.79	111.95
11	k	87	GLU	CA-C-N	-5.41	115.81	122.84
11	k	87	GLU	C-N-CA	-5.41	115.81	122.84
21	w	381	ASN	N-CA-C	5.39	116.73	109.24
22	x	127	LEU	N-CA-C	-5.27	101.75	109.81
2	b	78	PHE	N-CA-C	5.19	118.64	112.72
5	e	118	GLU	CA-C-N	5.19	124.37	118.97
5	e	118	GLU	C-N-CA	5.19	124.37	118.97
1	a	287	CYS	CA-C-N	5.19	125.44	119.83
1	a	287	CYS	C-N-CA	5.19	125.44	119.83
21	w	284	ASP	CA-C-N	5.19	124.85	119.56
21	w	284	ASP	C-N-CA	5.19	124.85	119.56
21	w	383	ARG	N-CA-C	5.16	117.35	110.53
7	g	50	GLU	N-CA-C	5.14	118.02	111.69
3	c	298	LEU	CA-C-N	5.10	125.00	119.85
3	c	298	LEU	C-N-CA	5.10	125.00	119.85
13	m	93	GLU	N-CA-C	5.07	117.46	111.33
1	a	368	GLU	N-CA-C	5.06	119.44	113.16
14	n	127	TYR	N-CA-C	5.04	119.52	113.17
3	c	131	ASP	CA-C-N	5.03	125.10	119.87
3	c	131	ASP	C-N-CA	5.03	125.10	119.87
2	b	374	GLU	CA-C-N	-5.01	114.79	119.85
2	b	374	GLU	C-N-CA	-5.01	114.79	119.85
18	t	50	SER	N-CA-C	5.00	118.53	112.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	210	GLU	Peptide
10	j	173	LEU	Peptide
14	n	65	ASN	Peptide
21	w	357	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3173	0	3153	82	0
2	b	2952	0	2840	68	0
3	c	2408	0	2415	58	0
4	d	832	0	828	37	0
5	e	968	0	968	13	0
6	f	852	0	834	25	0
7	g	1167	0	1173	42	0
8	h	2319	0	2332	59	0
9	i	1979	0	1974	58	0
10	j	1775	0	1797	83	0
11	k	1050	0	1044	38	0
12	l	1097	0	1080	24	0
13	m	893	0	878	32	0
14	n	837	0	860	13	0
15	o	747	0	748	13	0
16	p	742	0	749	23	0
17	q	336	0	342	6	0
18	t	780	0	792	13	0
19	u	1208	0	1227	26	0
20	v	1068	0	1034	12	0
21	w	3126	0	3153	84	0
22	x	1325	0	1354	25	0
23	z	282	0	294	16	0
24	x	1	0	0	0	0
All	All	31917	0	31869	780	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (780) 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)
14:n:35:ARG:HH12	14:n:39:PRO:HB3	1.20	1.05
4:d:180:PRO:HB2	4:d:181:PRO:HD2	1.36	1.04
5:e:44:ARG:HH12	21:w:157:ALA:HB3	1.23	1.01
11:k:162:LEU:HD21	11:k:167:ALA:HB2	1.46	0.97
11:k:90:VAL:HB	11:k:189:HIS:HB3	1.47	0.96
1:a:347:THR:HG22	1:a:349:GLY:H	1.29	0.96
16:p:11:ARG:HA	16:p:46:ASN:HB3	1.45	0.94
1:a:173:ARG:NH1	1:a:348:ASP:O	2.07	0.88
2:b:161:LEU:HD21	2:b:221:LEU:HD22	1.55	0.86
1:a:387:TRP:HE1	1:a:404:ILE:HD11	1.41	0.85
9:i:80:CYS:HG	9:i:165:THR:HG1	1.05	0.85
15:o:28:ARG:NH1	15:o:37:PRO:HD3	1.92	0.84
21:w:278:ILE:HB	21:w:336:TYR:HE2	1.41	0.84
1:a:248:THR:HG22	1:a:371:LYS:HB2	1.57	0.84
4:d:180:PRO:CB	4:d:181:PRO:HD2	2.07	0.83
1:a:162:ARG:NH1	1:a:383:TYR:OH	2.12	0.82
3:c:294:GLN:HE22	3:c:320:VAL:H	1.28	0.82
1:a:140:ALA:HB2	1:a:416:ALA:HB2	1.60	0.81
2:b:224:HIS:HD2	2:b:227:GLU:H	1.28	0.81
15:o:48:ASP:N	15:o:48:ASP:OD1	2.12	0.80
7:g:28:ARG:HG3	7:g:78:GLU:HB3	1.63	0.80
6:f:69:TYR:OH	8:h:256:ARG:NH1	2.15	0.80
4:d:164:ARG:HH12	11:k:91:LEU:HD21	1.46	0.80
3:c:153:ARG:HH22	3:c:256:ASP:HB2	1.48	0.79
21:w:118:LEU:HG	21:w:119:PRO:HD2	1.63	0.78
2:b:140:GLU:OE2	2:b:172:PRO:HB3	1.82	0.78
4:d:167:SER:O	10:j:203:LYS:NZ	2.14	0.78
19:u:105:ALA:O	19:u:115:ARG:NH1	2.18	0.77
2:b:311:MET:O	15:o:113:LYS:NZ	2.17	0.76
9:i:186:VAL:HG13	9:i:219:ARG:HB3	1.66	0.76
13:m:77:GLU:HG3	13:m:104:ARG:HH11	1.51	0.76
16:p:14:LYS:HE3	16:p:69:GLY:HA2	1.68	0.76
21:w:158:PRO:HB2	21:w:160:ILE:HG22	1.65	0.76
7:g:28:ARG:HB3	7:g:28:ARG:HH11	1.50	0.76
9:i:165:THR:HG23	9:i:167:ASN:H	1.51	0.75
3:c:78:MET:HE3	9:i:279:THR:HG21	1.68	0.75
3:c:155:PHE:HA	6:f:88:UNK:HB1	1.69	0.75
3:c:273:PHE:HD1	3:c:274:GLN:HG3	1.52	0.74
1:a:387:TRP:NE1	1:a:404:ILE:HD11	2.01	0.74
14:n:35:ARG:HH12	14:n:39:PRO:CB	1.98	0.74
1:a:367:ASP:O	1:a:371:LYS:NZ	2.20	0.73
19:u:75:ARG:NH1	19:u:108:ASP:OD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:90:PRO:HB2	9:i:269:TRP:HH2	1.54	0.72
9:i:288:LYS:HB2	9:i:289:PRO:HD2	1.71	0.72
10:j:162:ARG:HD3	10:j:171:TRP:HE3	1.53	0.72
1:a:333:SER:HB3	1:a:363:ASP:HB3	1.70	0.72
9:i:176:ILE:HD11	9:i:181:VAL:HG21	1.72	0.72
7:g:17:ASN:HD21	7:g:23:VAL:H	1.36	0.71
21:w:369:ASN:H	21:w:385:ASN:HD22	1.39	0.71
21:w:213:ARG:HB2	21:w:213:ARG:NH1	2.06	0.71
21:w:53:ALA:O	21:w:62:ARG:NH2	2.23	0.70
18:t:24:PRO:HG2	22:x:169:TRP:HB2	1.71	0.70
21:w:348:PRO:HB3	21:w:367:GLN:HE21	1.55	0.70
16:p:10:LEU:HD22	16:p:42:VAL:HG13	1.73	0.70
2:b:308:GLN:HE22	15:o:111:LYS:H	1.40	0.70
19:u:100:VAL:HB	19:u:134:LEU:HB2	1.72	0.70
22:x:70:CYS:SG	22:x:108:CYS:HB3	2.32	0.70
9:i:150:LEU:HD23	9:i:153:ASN:HD22	1.58	0.69
7:g:2:THR:HG22	7:g:4:ARG:H	1.55	0.69
1:a:288:PRO:HD2	1:a:324:GLN:CD	2.18	0.69
3:c:105:VAL:HG22	3:c:122:ILE:HG12	1.74	0.69
5:e:127:GLN:HG2	5:e:132:ASN:HB2	1.75	0.68
7:g:15:LEU:HD11	8:h:169:VAL:HA	1.76	0.68
8:h:72:ILE:HD13	8:h:178:LEU:HD21	1.75	0.68
8:h:248:ARG:NH1	8:h:304:LEU:HD22	2.09	0.68
1:a:207:ASN:HD22	1:a:229:ARG:HD2	1.59	0.68
7:g:28:ARG:HB3	7:g:28:ARG:NH1	2.08	0.68
3:c:78:MET:HE2	3:c:83:SER:HB3	1.74	0.67
12:l:118:TRP:NE1	12:l:142:GLU:OE2	2.26	0.67
9:i:88:TYR:OH	9:i:108:ARG:NH1	2.28	0.67
10:j:44:PRO:HG2	10:j:227:LEU:HA	1.76	0.67
21:w:97:THR:HG22	21:w:99:ALA:H	1.60	0.67
2:b:355:LYS:HE3	2:b:358:PRO:HA	1.77	0.67
3:c:141:ARG:NH1	3:c:263:GLY:HA3	2.10	0.67
4:d:100:GLN:HG2	10:j:84:TYR:HA	1.75	0.67
4:d:146:ALA:HB2	10:j:211:GLY:HA2	1.77	0.67
1:a:244:GLU:O	1:a:248:THR:OG1	2.13	0.66
2:b:155:CYS:O	2:b:267:ARG:NH1	2.28	0.66
2:b:66:ARG:O	2:b:75:ARG:NH1	2.29	0.65
3:c:267:PRO:HG2	3:c:271:ILE:HD11	1.78	0.65
12:l:107:MET:HE1	12:l:148:ARG:NH1	2.11	0.65
13:m:114:PRO:HG2	13:m:117:ARG:HG3	1.76	0.65
16:p:16:VAL:HG22	16:p:66:VAL:HG13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:76:MET:HE1	16:p:86:MET:HA	1.79	0.65
1:a:347:THR:HG22	1:a:349:GLY:N	2.09	0.65
7:g:89:ILE:HB	7:g:97:ILE:HD12	1.79	0.65
10:j:199:ASN:HB2	10:j:242:ASP:HB2	1.79	0.65
9:i:186:VAL:HG22	9:i:187:GLU:HG3	1.79	0.64
10:j:85:SER:HB3	10:j:88:GLU:HB2	1.79	0.64
16:p:8:LEU:HD13	16:p:95:GLN:HG3	1.78	0.64
21:w:278:ILE:HD11	21:w:333:GLN:HG3	1.79	0.64
12:l:91:MET:HB2	12:l:93:ASN:HD21	1.62	0.64
7:g:34:SER:OG	7:g:70:CYS:O	2.13	0.64
16:p:76:MET:HE3	22:x:49:ILE:HD12	1.80	0.64
21:w:153:ARG:HD2	21:w:156:ARG:HH21	1.63	0.64
6:f:72:THR:HB	8:h:256:ARG:HG3	1.80	0.63
10:j:184:LEU:HB3	10:j:234:PHE:CZ	2.33	0.63
3:c:140:TRP:HE1	3:c:171:VAL:HA	1.62	0.63
21:w:291:THR:HG22	21:w:352:GLN:HB2	1.81	0.63
3:c:48:GLU:O	3:c:52:GLN:HG2	1.99	0.63
14:n:69:HIS:CD2	14:n:71:LYS:H	2.17	0.63
1:a:144:ARG:O	1:a:194:LYS:NZ	2.32	0.62
2:b:212:SER:HB2	2:b:242:GLY:H	1.64	0.62
2:b:224:HIS:CD2	2:b:227:GLU:H	2.12	0.62
7:g:56:ARG:HE	13:m:150:PRO:HG3	1.64	0.62
21:w:185:HIS:O	21:w:422:ARG:NH2	2.32	0.62
3:c:91:HIS:ND1	9:i:281:MET:HB2	2.14	0.62
3:c:172:ILE:O	3:c:315:ARG:NH1	2.23	0.62
14:n:77:PRO:HG2	14:n:80:LEU:HB2	1.81	0.62
21:w:146:GLN:HA	21:w:150:PHE:HB2	1.81	0.62
14:n:69:HIS:HD2	14:n:71:LYS:H	1.45	0.62
4:d:157:LEU:HD21	10:j:178:TRP:CH2	2.35	0.62
8:h:105:ARG:CZ	8:h:113:GLU:HG3	2.29	0.62
12:l:77:ASP:HB2	12:l:78:PRO:HD3	1.81	0.62
2:b:197:GLU:OE1	2:b:197:GLU:N	2.32	0.62
11:k:166:PHE:HA	11:k:169:ILE:HD12	1.82	0.62
6:f:84:UNK:HA	6:f:92:UNK:HB2	1.82	0.61
21:w:366:TYR:HD1	21:w:387:CYS:HB2	1.64	0.61
12:l:140:VAL:H	18:t:85:HIS:HD2	1.47	0.61
2:b:213:LEU:HB3	2:b:275:GLN:HG3	1.80	0.61
4:d:128:GLU:HA	4:d:131:MET:HE3	1.82	0.61
4:d:140:LEU:HD13	11:k:169:ILE:HD11	1.81	0.61
10:j:51:LEU:HD22	10:j:192:LEU:HD21	1.82	0.61
12:l:140:VAL:H	18:t:85:HIS:CD2	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:229:ARG:HH11	1:a:279:PHE:HE2	1.47	0.61
17:q:103:PRO:HG2	17:q:105:LYS:HE3	1.83	0.61
9:i:111:ARG:O	9:i:115:ASN:ND2	2.34	0.61
10:j:265:LYS:HG3	10:j:266:PRO:HD3	1.83	0.61
15:o:97:GLU:O	15:o:101:GLU:HG2	2.01	0.61
13:m:91:SER:HB2	13:m:123:ARG:NH1	2.16	0.61
22:x:99:MET:HE3	22:x:116:GLU:HA	1.82	0.60
19:u:103:HIS:HD2	19:u:106:SER:H	1.50	0.60
4:d:97:LYS:HD3	10:j:84:TYR:CE2	2.37	0.60
20:v:97:ALA:O	20:v:101:GLU:HG2	2.02	0.60
3:c:86:TYR:HB2	3:c:112:MET:HB3	1.84	0.60
18:t:71:PHE:CE2	18:t:75:LYS:HE3	2.36	0.60
12:l:75:PRO:HD3	12:l:88:ARG:NH1	2.17	0.60
14:n:123:ARG:O	14:n:128:ARG:NH2	2.34	0.60
16:p:10:LEU:HD23	16:p:46:ASN:HD21	1.67	0.60
21:w:370:THR:OG1	21:w:383:ARG:HB2	2.01	0.60
4:d:171:PHE:HD1	10:j:203:LYS:HE2	1.67	0.60
7:g:144:ARG:HG2	7:g:147:GLU:CD	2.27	0.60
21:w:111:LYS:HD2	21:w:206:ARG:HH12	1.67	0.60
7:g:36:ASP:O	18:t:100:LYS:NZ	2.29	0.59
9:i:245:TYR:HB3	9:i:265:ILE:O	2.02	0.59
2:b:240:ILE:HG12	2:b:248:GLY:HA3	1.85	0.59
22:x:72:ILE:HD11	22:x:115:ILE:HD11	1.84	0.59
11:k:136:GLN:HB3	11:k:146:LEU:HB2	1.85	0.59
3:c:281:HIS:CG	3:c:319:MET:HG2	2.38	0.59
2:b:120:GLU:HG2	2:b:124:ARG:HE	1.67	0.59
11:k:135:LEU:HD11	11:k:145:PHE:HD1	1.67	0.59
19:u:71:ILE:HD11	19:u:154:ARG:HG3	1.85	0.59
3:c:281:HIS:CD2	3:c:319:MET:HG2	2.38	0.59
9:i:179:LYS:NZ	9:i:232:MET:HE1	2.17	0.58
11:k:98:TYR:OH	11:k:150:LEU:HB3	2.03	0.58
3:c:189:TRP:HZ3	3:c:191:PRO:HA	1.69	0.58
9:i:105:LEU:HD22	9:i:193:GLN:HE21	1.68	0.58
22:x:105:THR:HG22	22:x:107:LEU:HG	1.84	0.58
16:p:21:CYS:SG	16:p:60:SER:N	2.77	0.58
1:a:108:HIS:HD2	1:a:110:ARG:H	1.51	0.58
1:a:210:SER:HB3	1:a:223:HIS:CD2	2.37	0.58
2:b:261:ARG:HA	2:b:323:TRP:CG	2.39	0.58
4:d:169:PHE:HB2	4:d:170:PRO:HD3	1.85	0.58
4:d:180:PRO:CB	4:d:181:PRO:CD	2.80	0.58
1:a:147:ILE:HG22	1:a:148:GLU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:272:LEU:HB2	2:b:315:GLY:H	1.69	0.58
15:o:93:LEU:O	15:o:97:GLU:HG2	2.04	0.58
10:j:160:LEU:HD21	10:j:171:TRP:HE1	1.69	0.58
1:a:213:TRP:HZ3	1:a:222:VAL:HG12	1.69	0.57
8:h:59:ARG:HG2	8:h:184:PHE:CD1	2.39	0.57
11:k:170:PHE:O	11:k:174:ILE:HG13	2.04	0.57
1:a:181:VAL:HG21	1:a:294:LEU:HD21	1.84	0.57
3:c:44:LEU:O	3:c:48:GLU:HG2	2.04	0.57
10:j:49:GLY:N	10:j:176:SER:O	2.37	0.57
21:w:226:GLN:HE21	21:w:228:ASN:HD21	1.51	0.57
10:j:214:LYS:HZ2	10:j:230:LYS:HD3	1.69	0.57
12:l:75:PRO:HD3	12:l:88:ARG:HH12	1.66	0.57
5:e:44:ARG:HH12	21:w:157:ALA:CB	2.09	0.57
9:i:90:PRO:HB2	9:i:269:TRP:CH2	2.38	0.57
12:l:91:MET:HB2	12:l:93:ASN:ND2	2.18	0.57
21:w:85:LYS:HE3	21:w:86:MET:HE3	1.87	0.57
21:w:315:GLU:OE2	21:w:319:ARG:NH2	2.34	0.57
7:g:77:ALA:HB2	7:g:104:LEU:HD13	1.85	0.57
9:i:170:PRO:O	9:i:174:TRP:HB2	2.04	0.57
10:j:63:LEU:HB2	10:j:68:GLU:OE2	2.05	0.57
21:w:167:ALA:HB3	21:w:295:LEU:HD21	1.87	0.57
10:j:235:LYS:HZ2	11:k:172:GLU:HG2	1.70	0.57
1:a:332:ASP:HB3	1:a:334:LYS:HE3	1.85	0.57
8:h:105:ARG:HD2	8:h:112:LYS:HB2	1.87	0.57
13:m:77:GLU:HG3	13:m:104:ARG:NH1	2.20	0.57
10:j:149:LEU:HD13	10:j:254:TRP:CE2	2.41	0.56
1:a:118:LYS:HA	1:a:254:GLU:OE2	2.05	0.56
21:w:247:LEU:HD13	21:w:348:PRO:HG3	1.86	0.56
22:x:89:LEU:HD11	22:x:118:CYS:HB3	1.85	0.56
21:w:369:ASN:H	21:w:385:ASN:ND2	2.03	0.56
1:a:160:HIS:HA	1:a:164:TRP:HB2	1.88	0.56
11:k:94:HIS:HB2	11:k:185:SER:HB3	1.87	0.56
13:m:119:HIS:CE1	13:m:120:GLN:HB2	2.41	0.56
20:v:80:GLU:O	20:v:84:GLU:HG2	2.06	0.56
1:a:112:ARG:HB3	1:a:308:GLN:NE2	2.21	0.56
2:b:217:LEU:HD13	2:b:236:LEU:HD13	1.87	0.56
4:d:168:LEU:HG	10:j:205:LEU:O	2.05	0.56
17:q:122:ARG:O	17:q:126:ILE:HG12	2.06	0.56
10:j:235:LYS:NZ	11:k:172:GLU:HG2	2.19	0.56
21:w:251:ILE:HG22	21:w:253:ILE:H	1.71	0.56
21:w:368:LEU:HD21	21:w:371:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:313:MET:HE1	1:a:346:GLY:HA3	1.88	0.55
5:e:88:GLN:O	5:e:92:GLU:HG2	2.05	0.55
10:j:255:VAL:HG13	10:j:259:GLU:HB2	1.88	0.55
17:q:114:THR:HG22	17:q:116:GLU:H	1.71	0.55
4:d:164:ARG:HB3	11:k:86:TYR:CE1	2.41	0.55
11:k:91:LEU:HD11	11:k:162:LEU:HD22	1.88	0.55
1:a:329:TYR:HB3	1:a:334:LYS:NZ	2.21	0.55
5:e:129:TYR:HB3	5:e:130:PRO:HD3	1.88	0.55
6:f:87:UNK:HG2	6:f:88:UNK:HG2	1.88	0.55
9:i:88:TYR:HD2	9:i:245:TYR:HE2	1.52	0.55
21:w:128:GLU:N	21:w:129:PRO:HD2	2.21	0.55
1:a:355:LEU:HD13	1:a:376:VAL:HG22	1.88	0.55
2:b:157:LEU:HD12	2:b:316:LEU:HD11	1.88	0.55
9:i:183:TRP:CH2	9:i:185:PHE:HB2	2.42	0.55
22:x:108:CYS:SG	22:x:111:GLU:HB2	2.46	0.55
7:g:26:LEU:HD21	7:g:29:LEU:HD13	1.87	0.55
21:w:278:ILE:HB	21:w:336:TYR:CE2	2.31	0.55
19:u:81:CYS:HB2	19:u:97:LYS:HB3	1.88	0.55
8:h:59:ARG:HA	8:h:184:PHE:CE1	2.41	0.55
8:h:136:CYS:HG	8:h:140:PHE:HE2	1.54	0.55
10:j:162:ARG:HD3	10:j:171:TRP:CE3	2.37	0.54
12:l:74:PRO:HA	12:l:88:ARG:HH12	1.71	0.54
21:w:119:PRO:HD3	21:w:388:TRP:HB2	1.88	0.54
10:j:47:LEU:HD12	10:j:180:PRO:HG3	1.89	0.54
8:h:270:TYR:O	8:h:285:PRO:HA	2.07	0.54
13:m:79:PHE:HD1	13:m:97:LEU:HD13	1.70	0.54
7:g:27:GLN:HG3	8:h:78:ARG:HH12	1.72	0.54
2:b:252:CYS:SG	2:b:286:ARG:HG3	2.48	0.54
2:b:191:ASN:OD1	2:b:192:GLU:N	2.40	0.54
7:g:144:ARG:HH12	8:h:260:GLN:HG3	1.73	0.54
10:j:209:PRO:HB2	10:j:212:HIS:NE2	2.23	0.54
13:m:74:HIS:NE2	13:m:108:ASP:OD2	2.33	0.54
21:w:118:LEU:HD22	21:w:414:GLN:HE21	1.72	0.54
10:j:120:LEU:HB3	10:j:124:TRP:CZ2	2.43	0.54
4:d:88:PHE:HE1	11:k:155:ARG:HH12	1.55	0.53
8:h:229:PHE:HZ	8:h:301:LEU:HB3	1.73	0.53
13:m:74:HIS:ND1	13:m:77:GLU:OE2	2.42	0.53
21:w:366:TYR:CD1	21:w:387:CYS:HB2	2.42	0.53
6:f:67:ILE:HD13	8:h:258:THR:HG21	1.90	0.53
9:i:189:LEU:HB2	9:i:217:HIS:CD2	2.43	0.53
20:v:142:ARG:HA	20:v:145:UNK:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:240:ALA:HB2	1:a:375:TRP:HH2	1.73	0.53
2:b:187:VAL:HG13	2:b:319:PHE:HB3	1.89	0.53
7:g:143:LEU:HD21	7:g:149:GLN:HB2	1.90	0.53
11:k:122:GLU:HG2	11:k:160:SER:HB2	1.90	0.53
23:z:17:UNK:HA	23:z:20:UNK:HG3	1.90	0.53
2:b:275:GLN:HA	2:b:310:ALA:O	2.09	0.53
2:b:251:THR:HG23	2:b:285:THR:HA	1.91	0.53
3:c:187:ASP:HA	3:c:291:ARG:NH2	2.24	0.53
9:i:88:TYR:CD2	9:i:195:VAL:HG11	2.44	0.53
1:a:277:THR:HG22	1:a:323:ALA:HB1	1.91	0.53
12:l:98:ARG:HB3	12:l:152:TYR:HE1	1.74	0.53
2:b:267:ARG:HB3	2:b:320:GLN:HE21	1.73	0.53
7:g:56:ARG:NE	13:m:150:PRO:HG3	2.23	0.53
10:j:55:ARG:NH2	10:j:152:LYS:O	2.41	0.53
4:d:99:ARG:NH2	10:j:93:ASP:OD2	2.41	0.53
9:i:219:ARG:NH1	9:i:241:ASP:OD1	2.42	0.53
19:u:134:LEU:HD11	19:u:153:LEU:HD13	1.91	0.53
1:a:63:LYS:HB3	1:a:65:HIS:CE1	2.44	0.52
1:a:188:CYS:HB3	1:a:418:TYR:CD2	2.43	0.52
8:h:105:ARG:HH11	8:h:116:LEU:HD23	1.74	0.52
8:h:265:THR:HG22	8:h:267:LEU:H	1.74	0.52
19:u:98:ALA:HB3	19:u:136:SER:HB3	1.90	0.52
3:c:159:TYR:CE1	3:c:186:LEU:HD13	2.45	0.52
16:p:73:ARG:HB3	22:x:46:THR:HG22	1.90	0.52
10:j:51:LEU:HD13	10:j:192:LEU:HD11	1.90	0.52
21:w:278:ILE:HG12	21:w:329:TRP:CZ3	2.44	0.52
7:g:28:ARG:HH11	7:g:28:ARG:CB	2.20	0.52
8:h:152:GLY:HA2	8:h:232:TRP:NE1	2.24	0.52
9:i:245:TYR:CD1	9:i:265:ILE:HB	2.44	0.52
10:j:47:LEU:HB3	10:j:178:TRP:NE1	2.24	0.52
13:m:78:VAL:HG21	13:m:101:PHE:HA	1.91	0.52
6:f:126:ARG:HE	6:f:130:HIS:CD2	2.27	0.52
9:i:165:THR:HG21	9:i:262:HIS:ND1	2.25	0.52
10:j:53:LEU:HD21	10:j:238:LEU:HD11	1.91	0.52
23:z:206:UNK:HA	23:z:209:UNK:HG3	1.92	0.52
1:a:333:SER:HB3	1:a:363:ASP:CB	2.39	0.52
15:o:45:GLU:HA	15:o:63:GLN:NE2	2.24	0.52
4:d:128:GLU:O	4:d:131:MET:HG2	2.09	0.52
8:h:152:GLY:HA2	8:h:232:TRP:HE1	1.75	0.52
8:h:294:GLU:O	8:h:298:ARG:HG2	2.10	0.52
11:k:166:PHE:O	11:k:170:PHE:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:83:TRP:CD1	14:n:93:ARG:NH1	2.77	0.52
19:u:103:HIS:HB3	19:u:106:SER:HB3	1.91	0.52
11:k:82:LEU:HD12	11:k:85:ASP:OD2	2.10	0.52
2:b:35:MET:SD	2:b:36:PRO:HD2	2.50	0.52
9:i:88:TYR:HB3	9:i:245:TYR:OH	2.09	0.52
9:i:164:VAL:HB	9:i:168:CYS:HB3	1.91	0.52
11:k:126:ALA:HB2	11:k:155:ARG:HH11	1.75	0.52
21:w:221:ASP:OD1	21:w:222:ALA:N	2.43	0.52
3:c:156:LYS:HB2	6:f:89:UNK:N	2.26	0.51
7:g:17:ASN:ND2	7:g:23:VAL:H	2.06	0.51
8:h:184:PHE:O	8:h:186:VAL:HG23	2.10	0.51
9:i:165:THR:HA	9:i:260:ARG:HD3	1.92	0.51
10:j:74:LEU:HA	10:j:77:ILE:HG22	1.92	0.51
18:t:90:GLU:N	18:t:90:GLU:OE1	2.44	0.51
10:j:185:ARG:NH2	10:j:204:PHE:HB2	2.25	0.51
13:m:71:LEU:HD13	13:m:128:LEU:HD23	1.91	0.51
13:m:92:LEU:HD21	13:m:124:VAL:HG22	1.92	0.51
1:a:124:THR:HG23	1:a:318:PHE:CG	2.45	0.51
2:b:97:VAL:HG11	2:b:102:GLN:NE2	2.26	0.51
12:l:89:SER:O	12:l:92:HIS:N	2.39	0.51
19:u:153:LEU:HA	19:u:156:MET:HE2	1.92	0.51
21:w:128:GLU:O	21:w:130:THR:N	2.42	0.51
1:a:210:SER:HB3	1:a:223:HIS:HD2	1.75	0.51
9:i:126:ARG:HG3	9:i:132:PHE:HD2	1.75	0.51
13:m:141:PHE:CE2	13:m:145:ILE:HD11	2.45	0.51
1:a:96:HIS:CG	1:a:97:PRO:HD2	2.46	0.51
10:j:47:LEU:HB3	10:j:178:TRP:CE2	2.45	0.51
3:c:240:LYS:O	3:c:243:GLN:HG2	2.10	0.51
12:l:117:ILE:HD11	12:l:145:GLY:HA2	1.93	0.51
1:a:174:GLU:HA	1:a:296:SER:HB2	1.93	0.51
2:b:144:GLY:O	2:b:148:LYS:HG2	2.11	0.51
9:i:208:ILE:HB	9:i:252:LEU:HD12	1.92	0.51
10:j:139:GLU:HB3	10:j:151:ARG:O	2.11	0.51
9:i:104:GLY:O	9:i:108:ARG:HG2	2.11	0.51
21:w:245:VAL:HG12	21:w:246:PRO:HD2	1.91	0.51
1:a:113:LEU:HG	1:a:119:GLN:OE1	2.11	0.51
8:h:60:ARG:HG2	8:h:177:GLN:NE2	2.26	0.51
21:w:115:LEU:HD11	21:w:251:ILE:HD13	1.93	0.50
21:w:289:GLY:H	21:w:333:GLN:CD	2.16	0.50
1:a:136:VAL:HG22	1:a:420:HIS:HD2	1.76	0.50
13:m:69:SER:O	13:m:72:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:v:148:UNK:HA	20:v:151:UNK:HG3	1.93	0.50
21:w:274:ASN:OD1	21:w:274:ASN:N	2.43	0.50
7:g:144:ARG:HH22	8:h:260:GLN:CD	2.19	0.50
3:c:273:PHE:CD1	3:c:274:GLN:HG3	2.41	0.50
4:d:110:GLU:O	4:d:114:ARG:HG3	2.12	0.50
1:a:361:THR:HG22	1:a:363:ASP:H	1.77	0.50
11:k:80:ILE:HB	11:k:87:GLU:HB2	1.94	0.50
1:a:133:PRO:HG3	1:a:375:TRP:CD2	2.47	0.50
4:d:155:PRO:O	4:d:158:HIS:ND1	2.45	0.50
21:w:96:GLN:HG2	21:w:321:ASN:ND2	2.26	0.50
22:x:138:GLY:C	22:x:141:PRO:HD2	2.37	0.50
2:b:233:VAL:HG23	2:b:298:PHE:CG	2.47	0.50
3:c:153:ARG:NH2	3:c:256:ASP:HB2	2.23	0.50
3:c:187:ASP:HA	3:c:291:ARG:HH22	1.77	0.50
2:b:216:LEU:HD12	2:b:272:LEU:HD21	1.94	0.49
6:f:68:PRO:HG2	6:f:71:HIS:CD2	2.47	0.49
21:w:118:LEU:CG	21:w:119:PRO:HD2	2.39	0.49
1:a:344:SER:HB3	1:a:355:LEU:HD23	1.94	0.49
10:j:217:PHE:HD2	10:j:227:LEU:HD23	1.77	0.49
1:a:96:HIS:CD2	1:a:97:PRO:HD2	2.47	0.49
2:b:194:THR:HG22	2:b:196:THR:H	1.77	0.49
9:i:267:PRO:HG2	9:i:270:ALA:HB2	1.93	0.49
2:b:176:ALA:HB1	2:b:184:LEU:HD11	1.94	0.49
3:c:110:TRP:HE3	3:c:114:LYS:HB3	1.77	0.49
4:d:150:LEU:HD12	10:j:232:PHE:CZ	2.47	0.49
10:j:187:THR:HG23	10:j:190:ARG:HH21	1.76	0.49
20:v:68:SER:OG	20:v:70:VAL:HG23	2.13	0.49
20:v:127:LYS:HG3	20:v:131:MET:HG3	1.94	0.49
23:z:204:UNK:HA	23:z:207:UNK:HG3	1.93	0.49
2:b:324:ASP:OD1	2:b:325:ASP:N	2.44	0.49
3:c:201:LYS:NZ	6:f:98:UNK:HB2	2.28	0.49
4:d:168:LEU:HD11	11:k:171:LEU:HD11	1.95	0.49
10:j:184:LEU:HD21	10:j:232:PHE:HD2	1.77	0.49
10:j:213:TYR:CE2	10:j:271:GLN:HB2	2.48	0.49
3:c:186:LEU:CD1	3:c:189:TRP:HE1	2.26	0.49
6:f:122:ARG:NH1	6:f:122:ARG:HG3	2.28	0.49
7:g:28:ARG:HH22	8:h:71:GLU:CD	2.21	0.49
17:q:107:LEU:HD13	17:q:120:LEU:HB2	1.92	0.49
23:z:22:UNK:HA	23:z:25:UNK:HG3	1.94	0.49
1:a:132:LEU:HB2	1:a:137:LEU:HD13	1.95	0.49
1:a:391:VAL:CG1	1:a:399:GLU:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:159:LEU:HD11	10:j:252:HIS:HB2	1.95	0.49
16:p:74:LEU:HD22	16:p:93:HIS:HD2	1.77	0.49
18:t:9:ARG:NH1	22:x:164:ASN:ND2	2.61	0.49
3:c:105:VAL:HB	3:c:110:TRP:CD1	2.47	0.49
10:j:79:ILE:O	10:j:82:SER:OG	2.30	0.49
16:p:70:ASP:HB3	16:p:72:HIS:CD2	2.48	0.49
23:z:24:UNK:HA	23:z:27:UNK:HG3	1.94	0.49
9:i:218:THR:HG22	9:i:220:GLN:HG3	1.95	0.49
21:w:100:LEU:O	21:w:313:GLN:NE2	2.43	0.49
1:a:385:HIS:HB3	1:a:404:ILE:HD12	1.95	0.49
21:w:213:ARG:HB2	21:w:213:ARG:HH11	1.74	0.49
21:w:263:ASP:O	21:w:266:PRO:HA	2.13	0.48
6:f:73:LYS:NZ	8:h:260:GLN:HE21	2.11	0.48
21:w:396:TYR:HE2	21:w:399:ILE:HD11	1.78	0.48
6:f:75:ILE:HG23	8:h:289:VAL:HG11	1.95	0.48
9:i:287:LEU:HD11	9:i:293:PHE:HB2	1.95	0.48
12:l:98:ARG:HB3	12:l:152:TYR:CE1	2.48	0.48
19:u:75:ARG:HH12	19:u:108:ASP:CG	2.22	0.48
5:e:99:GLU:O	5:e:103:LYS:HB2	2.13	0.48
15:o:28:ARG:HH11	15:o:37:PRO:HD3	1.72	0.48
2:b:195:PRO:HG2	2:b:324:ASP:HB3	1.95	0.48
7:g:21:ARG:HD3	8:h:217:ASP:OD2	2.14	0.48
9:i:133:LYS:HD2	9:i:136:ASP:OD2	2.13	0.48
22:x:108:CYS:O	22:x:111:GLU:N	2.43	0.48
23:z:28:UNK:HA	23:z:31:UNK:HG3	1.94	0.48
1:a:229:ARG:NH1	1:a:279:PHE:HE2	2.11	0.48
8:h:248:ARG:HH12	8:h:304:LEU:HD22	1.76	0.48
10:j:146:ARG:O	10:j:254:TRP:N	2.44	0.48
15:o:34:ALA:HB2	15:o:40:TYR:CE2	2.49	0.48
1:a:329:TYR:HB3	1:a:334:LYS:HZ2	1.77	0.48
9:i:176:ILE:CD1	9:i:181:VAL:HG21	2.43	0.48
16:p:10:LEU:O	16:p:13:VAL:HG23	2.13	0.48
16:p:62:PRO:HG2	16:p:78:GLY:O	2.13	0.48
6:f:122:ARG:HG3	6:f:122:ARG:HH11	1.79	0.48
18:t:55:THR:HG22	18:t:56:ALA:H	1.79	0.48
2:b:267:ARG:HB3	2:b:320:GLN:NE2	2.28	0.47
3:c:154:ALA:O	6:f:91:UNK:HB1	2.14	0.47
21:w:157:ALA:N	21:w:158:PRO:HD2	2.29	0.47
21:w:195:ASP:HA	21:w:198:ARG:NH2	2.29	0.47
23:z:29:UNK:HA	23:z:32:UNK:HG3	1.96	0.47
1:a:381:LEU:O	1:a:407:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:308:GLN:NE2	15:o:111:LYS:H	2.07	0.47
11:k:122:GLU:CG	11:k:160:SER:HB2	2.44	0.47
21:w:158:PRO:C	21:w:160:ILE:H	2.23	0.47
23:z:21:UNK:HA	23:z:24:UNK:HG3	1.96	0.47
3:c:173:ALA:HB1	3:c:320:VAL:HG11	1.96	0.47
7:g:144:ARG:HG2	7:g:147:GLU:OE2	2.13	0.47
10:j:51:LEU:HD21	10:j:236:ALA:HB3	1.95	0.47
19:u:151:GLN:NE2	19:u:155:ASP:OD2	2.46	0.47
21:w:226:GLN:HE21	21:w:228:ASN:ND2	2.12	0.47
22:x:92:PHE:O	22:x:93:ILE:HG23	2.15	0.47
1:a:117:VAL:O	1:a:121:LEU:HG	2.15	0.47
1:a:162:ARG:NH1	1:a:383:TYR:CE2	2.83	0.47
3:c:273:PHE:HB2	3:c:300:VAL:HG12	1.96	0.47
9:i:80:CYS:HB2	9:i:166:GLU:HB2	1.97	0.47
10:j:45:TRP:HB3	10:j:230:LYS:HE3	1.96	0.47
10:j:209:PRO:HB3	10:j:234:PHE:CE2	2.49	0.47
21:w:371:LEU:HD12	21:w:371:LEU:HA	1.68	0.47
22:x:65:ASN:HB2	22:x:74:ARG:HA	1.96	0.47
7:g:28:ARG:HH21	8:h:177:GLN:NE2	2.12	0.47
7:g:144:ARG:HB2	7:g:147:GLU:HB2	1.96	0.47
8:h:105:ARG:HB2	8:h:112:LYS:HG3	1.96	0.47
9:i:223:ALA:HB2	9:i:236:GLU:HB2	1.95	0.47
20:v:106:GLN:O	20:v:110:GLU:HG2	2.15	0.47
2:b:240:ILE:HG23	2:b:244:ARG:O	2.14	0.47
3:c:146:MET:HE1	3:c:207:ILE:HG12	1.97	0.47
3:c:149:CYS:SG	3:c:257:PHE:HB2	2.54	0.47
4:d:121:TRP:CG	10:j:70:MET:HE3	2.50	0.47
4:d:166:PRO:HA	4:d:169:PHE:CE1	2.50	0.47
7:g:133:PHE:HZ	8:h:261:SER:HB2	1.78	0.47
8:h:229:PHE:CZ	8:h:301:LEU:HB3	2.48	0.47
11:k:91:LEU:HB2	11:k:159:ILE:HG13	1.96	0.47
13:m:79:PHE:HA	13:m:97:LEU:HD22	1.97	0.47
17:q:110:LEU:HD12	17:q:111:ASP:H	1.79	0.47
20:v:130:GLN:O	20:v:133:GLU:HG2	2.14	0.47
21:w:416:VAL:O	21:w:420:LEU:HB2	2.15	0.47
1:a:283:TYR:CD1	1:a:284:PRO:HD2	2.50	0.47
3:c:244:ASN:HA	3:c:245:PRO:HD3	1.69	0.47
2:b:231:GLU:HG2	2:b:298:PHE:O	2.16	0.47
2:b:373:HIS:O	2:b:374:GLU:HG2	2.14	0.47
4:d:179:THR:HG21	10:j:133:LEU:HD22	1.97	0.47
10:j:149:LEU:HD13	10:j:254:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:u:79:SER:HB2	19:u:99:GLU:HB3	1.97	0.47
21:w:90:LYS:HD2	21:w:226:GLN:HB2	1.97	0.47
7:g:58:ASN:HB3	7:g:61:VAL:HG12	1.98	0.46
7:g:93:SER:O	7:g:97:ILE:HG12	2.14	0.46
9:i:80:CYS:SG	9:i:166:GLU:HG2	2.56	0.46
10:j:53:LEU:HD11	10:j:238:LEU:HD21	1.97	0.46
19:u:56:ASP:OD2	19:u:60:ARG:NH2	2.47	0.46
21:w:322:ALA:HB2	21:w:355:ILE:HD11	1.96	0.46
13:m:78:VAL:HG11	13:m:101:PHE:HB2	1.97	0.46
14:n:68:LYS:HE2	14:n:72:GLU:HB3	1.97	0.46
19:u:108:ASP:HA	19:u:115:ARG:HH21	1.79	0.46
21:w:140:VAL:HG21	21:w:412:LEU:HD21	1.96	0.46
21:w:340:TRP:H	21:w:343:ALA:HB3	1.80	0.46
12:l:85:PHE:HA	12:l:166:PHE:CE1	2.51	0.46
13:m:139:SER:OG	13:m:140:LYS:N	2.49	0.46
16:p:6:ALA:HB2	16:p:42:VAL:HG23	1.97	0.46
21:w:122:PRO:O	21:w:125:LEU:HG	2.14	0.46
9:i:88:TYR:O	9:i:90:PRO:HD3	2.15	0.46
15:o:43:LEU:HD23	15:o:43:LEU:HA	1.76	0.46
4:d:143:GLN:O	4:d:147:LEU:HG	2.16	0.46
9:i:149:HIS:HB3	9:i:183:TRP:CD2	2.51	0.46
9:i:165:THR:HG23	9:i:167:ASN:N	2.25	0.46
10:j:50:ALA:O	10:j:233:PHE:HA	2.15	0.46
14:n:69:HIS:CD2	14:n:71:LYS:HG3	2.51	0.46
18:t:82:PHE:CG	18:t:83:PRO:HD2	2.50	0.46
1:a:161:ALA:CB	1:a:180:ILE:HG13	2.45	0.46
5:e:114:LYS:HE3	5:e:115:TYR:CE2	2.51	0.46
23:z:16:UNK:HA	23:z:19:UNK:HG3	1.98	0.46
3:c:156:LYS:HB3	3:c:159:TYR:CD2	2.51	0.46
21:w:206:ARG:HB3	21:w:225:TYR:HE1	1.80	0.46
10:j:188:ALA:O	10:j:192:LEU:HG	2.16	0.46
12:l:162:LEU:HD23	12:l:162:LEU:HA	1.74	0.46
21:w:270:ARG:HG2	21:w:271:GLN:H	1.81	0.46
22:x:170:ASN:O	22:x:170:ASN:CG	2.59	0.46
1:a:290:THR:HA	1:a:343:GLN:O	2.16	0.46
2:b:179:VAL:HG13	2:b:197:GLU:HG3	1.97	0.46
7:g:6:THR:HG22	7:g:7:ALA:H	1.81	0.46
1:a:161:ALA:HB1	1:a:180:ILE:HG13	1.97	0.46
10:j:162:ARG:HB2	10:j:171:TRP:CZ3	2.51	0.46
11:k:86:TYR:CE1	11:k:88:TYR:HD1	2.34	0.46
13:m:141:PHE:O	13:m:145:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:301:LEU:HD12	8:h:301:LEU:HA	1.76	0.45
4:d:102:PRO:HG2	4:d:103:PRO:HD3	1.97	0.45
1:a:207:ASN:ND2	1:a:229:ARG:HD2	2.29	0.45
1:a:300:ARG:N	1:a:301:PRO:HD2	2.32	0.45
10:j:116:LEU:HG	10:j:117:ALA:H	1.80	0.45
18:t:25:ARG:HA	18:t:26:PRO:HD3	1.76	0.45
11:k:173:ILE:H	11:k:173:ILE:HG13	1.64	0.45
2:b:337:MET:HE2	2:b:337:MET:HB3	1.81	0.45
8:h:163:GLU:O	8:h:167:CYS:HB2	2.15	0.45
10:j:179:GLN:HG2	10:j:181:GLY:H	1.81	0.45
3:c:62:ILE:HD11	3:c:118:LYS:O	2.16	0.45
9:i:221:THR:HG22	9:i:239:PRO:HA	1.98	0.45
21:w:193:ALA:HB3	21:w:236:ARG:HB2	1.99	0.45
3:c:67:VAL:CG2	3:c:121:GLU:HB3	2.47	0.45
6:f:88:UNK:HB2	6:f:91:UNK:HG3	1.97	0.45
9:i:85:PHE:CZ	9:i:200:SER:HB2	2.51	0.45
9:i:271:PRO:HA	9:i:272:PRO:HD3	1.87	0.45
11:k:126:ALA:HB2	11:k:155:ARG:NH1	2.30	0.45
1:a:96:HIS:HE1	1:a:98:LEU:HD12	1.81	0.45
4:d:180:PRO:HG3	10:j:153:LEU:HD13	1.97	0.45
7:g:104:LEU:HD23	7:g:104:LEU:HA	1.80	0.45
10:j:257:LYS:HD3	10:j:276:LEU:HD21	1.99	0.45
16:p:46:ASN:OD1	16:p:46:ASN:N	2.49	0.45
23:z:12:UNK:HA	23:z:15:UNK:HG3	1.98	0.45
2:b:301:PHE:O	2:b:305:LYS:HG2	2.17	0.45
11:k:170:PHE:CD2	11:k:174:ILE:HD11	2.51	0.45
12:l:44:GLU:OE1	12:l:44:GLU:N	2.50	0.45
13:m:74:HIS:HA	13:m:77:GLU:CD	2.42	0.45
10:j:162:ARG:HB2	10:j:171:TRP:HZ3	1.82	0.44
10:j:172:MET:HG3	10:j:175:GLN:CD	2.42	0.44
13:m:133:VAL:HA	13:m:134:PRO:HD3	1.86	0.44
14:n:127:TYR:O	14:n:128:ARG:C	2.60	0.44
9:i:100:LEU:HD13	9:i:103:GLU:HG3	1.99	0.44
12:l:107:MET:HE3	12:l:148:ARG:HD3	2.00	0.44
21:w:95:PRO:O	21:w:321:ASN:HA	2.17	0.44
22:x:71:PRO:HD2	22:x:107:LEU:HD23	1.99	0.44
9:i:250:LYS:HB2	9:i:259:TRP:CD2	2.51	0.44
11:k:170:PHE:CE2	11:k:174:ILE:HD11	2.53	0.44
16:p:68:PHE:CG	16:p:94:ILE:HG13	2.52	0.44
21:w:90:LYS:HB3	21:w:224:ARG:HB2	2.00	0.44
1:a:72:ARG:HA	1:a:73:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:118:LYS:HG2	1:a:254:GLU:CD	2.43	0.44
7:g:33:LEU:HD11	7:g:47:VAL:HG21	1.97	0.44
9:i:165:THR:CG2	9:i:262:HIS:HA	2.47	0.44
14:n:68:LYS:HG2	14:n:72:GLU:HG3	1.98	0.44
16:p:10:LEU:O	16:p:46:ASN:ND2	2.50	0.44
16:p:68:PHE:CD1	16:p:94:ILE:HG13	2.52	0.44
1:a:149:ASN:OD1	1:a:149:ASN:N	2.50	0.44
21:w:335:MET:HE2	21:w:335:MET:HB3	1.82	0.44
22:x:104:ILE:HD13	22:x:104:ILE:HA	1.83	0.44
4:d:150:LEU:HD12	10:j:232:PHE:CE2	2.52	0.44
6:f:89:UNK:HA	6:f:92:UNK:HB1	1.99	0.44
7:g:64:TYR:CD2	8:h:65:ASN:HB3	2.53	0.44
8:h:59:ARG:HG2	8:h:184:PHE:CG	2.53	0.44
9:i:179:LYS:HD3	9:i:232:MET:HE1	2.00	0.44
12:l:60:PRO:HD3	12:l:92:HIS:CE1	2.53	0.44
20:v:124:CYS:O	20:v:128:MET:HG3	2.17	0.44
1:a:61:ALA:HB2	1:a:73:PRO:HB3	2.00	0.44
1:a:391:VAL:HG12	1:a:399:GLU:HB2	1.98	0.44
10:j:213:TYR:HE2	10:j:271:GLN:HB2	1.82	0.44
21:w:344:ASP:HB3	21:w:345:VAL:H	1.62	0.44
2:b:253:PRO:HG2	2:b:288:SER:O	2.18	0.44
18:t:49:LEU:HA	18:t:49:LEU:HD12	1.61	0.44
19:u:52:SER:HB2	19:u:57:THR:HG21	2.00	0.44
19:u:103:HIS:HD2	19:u:106:SER:N	2.15	0.44
22:x:137:GLU:O	22:x:141:PRO:HD3	2.18	0.44
8:h:59:ARG:NH1	8:h:181:SER:O	2.50	0.44
10:j:58:LEU:N	10:j:153:LEU:O	2.47	0.44
1:a:162:ARG:NH1	1:a:383:TYR:CZ	2.85	0.43
10:j:213:TYR:HB3	10:j:268:TYR:HD1	1.83	0.43
14:n:80:LEU:HD23	14:n:80:LEU:HA	1.81	0.43
21:w:113:VAL:HG21	21:w:384:LYS:HD3	1.99	0.43
1:a:277:THR:CG2	1:a:323:ALA:HB1	2.47	0.43
3:c:49:LYS:NZ	3:c:253:ARG:NH1	2.66	0.43
8:h:88:LEU:HD23	8:h:88:LEU:HA	1.80	0.43
8:h:191:LEU:HD23	8:h:191:LEU:HA	1.83	0.43
10:j:61:LYS:HG2	10:j:154:ASP:HB2	1.99	0.43
10:j:94:GLU:O	10:j:98:LEU:HG	2.18	0.43
10:j:189:GLU:HG2	10:j:204:PHE:CZ	2.53	0.43
21:w:368:LEU:HD12	21:w:385:ASN:ND2	2.33	0.43
2:b:237:VAL:HG11	2:b:240:ILE:HD11	2.00	0.43
2:b:239:ASN:HA	2:b:275:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:240:ILE:HD13	2:b:245:VAL:HA	2.00	0.43
2:b:81:GLU:O	2:b:82:SER:HB3	2.18	0.43
5:e:68:LEU:HD12	5:e:68:LEU:HA	1.89	0.43
8:h:173:LEU:HD23	8:h:173:LEU:HA	1.82	0.43
8:h:45:LEU:HD12	8:h:45:LEU:HA	1.79	0.43
10:j:160:LEU:O	10:j:252:HIS:HA	2.18	0.43
13:m:67:LEU:O	13:m:71:LEU:HD12	2.17	0.43
2:b:224:HIS:HA	2:b:232:TYR:CE2	2.53	0.43
12:l:86:VAL:HB	12:l:166:PHE:HB3	2.01	0.43
12:l:157:LEU:HA	12:l:157:LEU:HD23	1.87	0.43
13:m:71:LEU:HD13	13:m:128:LEU:CD2	2.48	0.43
20:v:146:UNK:HA	20:v:149:UNK:HG3	2.00	0.43
3:c:246:GLU:HB2	3:c:248:ILE:HG13	2.00	0.43
3:c:298:LEU:HA	3:c:299:PRO:HD3	1.82	0.43
4:d:100:GLN:CG	10:j:84:TYR:HA	2.48	0.43
7:g:35:ARG:HG2	13:m:159:TYR:CE2	2.54	0.43
19:u:45:LEU:HD12	19:u:45:LEU:HA	1.77	0.43
22:x:138:GLY:O	22:x:141:PRO:HD2	2.18	0.43
22:x:164:ASN:O	22:x:166:GLY:N	2.51	0.43
1:a:162:ARG:HA	1:a:162:ARG:HD2	1.80	0.43
2:b:151:LEU:HD23	2:b:151:LEU:HA	1.65	0.43
3:c:45:PHE:CD2	3:c:253:ARG:HD2	2.53	0.43
3:c:143:CYS:SG	3:c:297:SER:OG	2.62	0.43
7:g:114:ARG:O	7:g:114:ARG:HG3	2.16	0.43
10:j:267:LYS:HA	10:j:270:ALA:HB3	2.00	0.43
1:a:207:ASN:OD1	1:a:207:ASN:N	2.52	0.43
1:a:350:ARG:NH1	1:a:384:GLN:O	2.52	0.43
2:b:261:ARG:HA	2:b:323:TRP:CD1	2.53	0.43
3:c:140:TRP:CE3	3:c:176:PHE:HB3	2.54	0.43
8:h:129:GLY:O	8:h:133:SER:HB2	2.19	0.43
9:i:93:GLY:O	9:i:97:ILE:HG13	2.18	0.43
11:k:100:MET:HG2	11:k:153:HIS:NE2	2.33	0.43
2:b:45:LEU:HD12	11:k:64:LYS:HG3	2.01	0.43
7:g:29:LEU:HD21	7:g:101:VAL:HG13	2.01	0.43
7:g:117:LYS:HA	7:g:118:PRO:HD3	1.78	0.43
8:h:122:ASN:OD1	8:h:122:ASN:N	2.52	0.43
8:h:148:LEU:CD2	8:h:305:PHE:HB3	2.48	0.43
10:j:210:CYS:SG	10:j:235:LYS:HB2	2.59	0.43
14:n:79:TRP:CE3	14:n:98:VAL:HG21	2.54	0.43
16:p:74:LEU:HD22	16:p:93:HIS:CD2	2.53	0.43
19:u:80:TYR:CE1	19:u:146:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:u:116:LEU:O	19:u:120:VAL:HG23	2.19	0.43
21:w:194:LEU:HD12	21:w:194:LEU:HA	1.87	0.43
6:f:73:LYS:C	8:h:256:ARG:HE	2.26	0.42
6:f:118:THR:HG22	6:f:119:THR:N	2.34	0.42
13:m:70:ARG:HH11	13:m:109:LEU:HD23	1.84	0.42
13:m:71:LEU:O	13:m:75:VAL:HG23	2.19	0.42
19:u:134:LEU:HD21	19:u:156:MET:HE1	2.01	0.42
21:w:206:ARG:HB3	21:w:225:TYR:CE1	2.54	0.42
4:d:139:LEU:O	4:d:143:GLN:HG2	2.18	0.42
8:h:271:PHE:HA	8:h:284:GLY:O	2.18	0.42
10:j:209:PRO:HB3	10:j:234:PHE:CZ	2.55	0.42
22:x:120:LYS:O	22:x:124:ARG:HG3	2.19	0.42
1:a:413:LYS:O	1:a:417:LEU:HG	2.19	0.42
3:c:61:LYS:HD2	3:c:77:VAL:HG12	2.00	0.42
8:h:256:ARG:HD2	8:h:256:ARG:HA	1.83	0.42
12:l:72:TRP:CH2	12:l:74:PRO:HB3	2.54	0.42
1:a:318:PHE:HZ	1:a:364:LEU:HD11	1.83	0.42
3:c:156:LYS:HB3	3:c:159:TYR:HD2	1.83	0.42
5:e:121:GLN:OE1	5:e:124:LYS:HE3	2.19	0.42
11:k:172:GLU:HA	11:k:175:HIS:CE1	2.54	0.42
23:z:20:UNK:HA	23:z:23:UNK:HG3	2.01	0.42
21:w:372:ALA:HB1	21:w:377:ALA:CB	2.49	0.42
3:c:45:PHE:O	3:c:48:GLU:HB2	2.18	0.42
4:d:151:ARG:HG2	4:d:158:HIS:HB2	2.01	0.42
4:d:157:LEU:HD21	10:j:178:TRP:HH2	1.81	0.42
8:h:215:ILE:HG23	8:h:219:LEU:HD12	2.01	0.42
9:i:166:GLU:O	9:i:170:PRO:HD3	2.19	0.42
11:k:137:LEU:O	23:z:106:UNK:HG3	2.19	0.42
21:w:193:ALA:HB2	21:w:286:LEU:HD12	2.02	0.42
3:c:209:LYS:HE3	3:c:211:LEU:HD21	2.02	0.42
5:e:126:PHE:HD2	5:e:133:PHE:HB3	1.84	0.42
6:f:138:PRO:HA	6:f:139:PRO:HD3	1.94	0.42
7:g:103:LYS:HA	7:g:103:LYS:HD3	1.73	0.42
10:j:48:LEU:O	10:j:231:VAL:HA	2.20	0.42
21:w:396:TYR:CE2	21:w:399:ILE:HD11	2.55	0.42
2:b:36:PRO:HG3	11:k:56:ILE:HG23	2.01	0.42
2:b:192:GLU:HA	2:b:320:GLN:O	2.19	0.42
2:b:195:PRO:HD2	2:b:324:ASP:HB3	2.01	0.42
2:b:377:TYR:HB3	2:b:380:TYR:HB2	2.00	0.42
6:f:50:ALA:HB3	6:f:59:VAL:HG22	2.00	0.42
12:l:68:THR:HB	12:l:69:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:53:CYS:HA	13:m:54:PRO:HD2	1.91	0.42
18:t:23:ARG:HA	18:t:24:PRO:HD2	1.73	0.42
21:w:413:LEU:O	21:w:417:GLN:HG2	2.20	0.42
2:b:72:ARG:HA	2:b:72:ARG:HD3	1.79	0.42
2:b:87:ARG:HA	2:b:87:ARG:HD3	1.90	0.42
3:c:285:THR:HG22	3:c:286:GLN:H	1.83	0.42
6:f:44:ASN:HB3	6:f:45:CYS:H	1.62	0.42
8:h:56:PRO:HA	8:h:57:PRO:HD3	1.86	0.42
20:v:111:GLU:O	20:v:115:GLN:HG2	2.20	0.42
22:x:36:ARG:HE	22:x:36:ARG:HB3	1.50	0.42
22:x:134:LYS:O	22:x:134:LYS:HG2	2.19	0.42
3:c:62:ILE:HD11	3:c:118:LYS:C	2.44	0.42
19:u:118:LEU:HD22	19:u:122:HIS:CD2	2.55	0.42
20:v:145:UNK:HA	20:v:148:UNK:HG3	2.02	0.42
21:w:182:LEU:HD12	21:w:419:LEU:HD23	2.01	0.42
21:w:352:GLN:HB3	21:w:418:PHE:CD2	2.55	0.42
4:d:146:ALA:C	10:j:212:HIS:HD1	2.25	0.41
5:e:69:LYS:HD3	5:e:69:LYS:HA	1.90	0.41
8:h:119:LEU:HD23	8:h:119:LEU:HA	1.83	0.41
13:m:114:PRO:HG2	13:m:117:ARG:CG	2.49	0.41
19:u:152:LYS:O	19:u:156:MET:HG3	2.19	0.41
21:w:76:VAL:HB	21:w:282:THR:HG21	2.01	0.41
1:a:52:ILE:HA	1:a:53:PRO:HD3	1.85	0.41
2:b:171:VAL:HA	2:b:172:PRO:HD2	1.75	0.41
2:b:213:LEU:HB3	2:b:275:GLN:CG	2.47	0.41
3:c:77:VAL:O	9:i:279:THR:HG23	2.20	0.41
3:c:153:ARG:HH22	3:c:256:ASP:CB	2.24	0.41
16:p:21:CYS:HA	16:p:22:PRO:HD3	1.83	0.41
2:b:279:ILE:HB	2:b:281:PHE:HE1	1.86	0.41
2:b:360:ARG:NH1	2:b:360:ARG:HG2	2.34	0.41
5:e:103:LYS:HD2	5:e:103:LYS:HA	1.92	0.41
8:h:231:MET:HE2	8:h:231:MET:HB3	1.86	0.41
21:w:267:LEU:HD23	21:w:267:LEU:HA	1.55	0.41
1:a:110:ARG:HA	1:a:110:ARG:HD3	1.71	0.41
1:a:153:ARG:HD3	1:a:187:LEU:HD22	2.02	0.41
2:b:239:ASN:HA	2:b:275:GLN:NE2	2.35	0.41
11:k:100:MET:HG2	11:k:153:HIS:CE1	2.55	0.41
17:q:112:PRO:HA	17:q:117:TYR:CD2	2.56	0.41
23:z:25:UNK:HA	23:z:28:UNK:HG3	2.01	0.41
9:i:240:ARG:HD3	9:i:274:GLN:HE21	1.86	0.41
21:w:278:ILE:O	21:w:329:TRP:HZ3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:w:348:PRO:CB	21:w:367:GLN:HE21	2.28	0.41
1:a:286:PRO:O	1:a:288:PRO:HD3	2.20	0.41
2:b:253:PRO:HD2	2:b:290:CYS:SG	2.60	0.41
2:b:261:ARG:NH2	19:u:124:ASN:HB3	2.36	0.41
7:g:139:THR:OG1	7:g:140:LEU:N	2.54	0.41
21:w:419:LEU:HA	21:w:419:LEU:HD12	1.82	0.41
2:b:268:PHE:HB2	2:b:319:PHE:CE1	2.55	0.41
3:c:292:ARG:HH12	3:c:321:THR:HG22	1.86	0.41
9:i:169:PHE:CZ	9:i:173:VAL:HG21	2.56	0.41
10:j:184:LEU:HB3	10:j:234:PHE:HZ	1.84	0.41
10:j:255:VAL:HG22	10:j:259:GLU:HB3	2.03	0.41
11:k:135:LEU:HD11	11:k:145:PHE:CD1	2.53	0.41
13:m:79:PHE:CD1	13:m:97:LEU:HD13	2.53	0.41
1:a:136:VAL:HG13	1:a:416:ALA:HB1	2.02	0.41
1:a:381:LEU:HD12	1:a:381:LEU:HA	1.93	0.41
5:e:44:ARG:HH22	21:w:157:ALA:HB1	1.85	0.41
22:x:70:CYS:HA	22:x:71:PRO:HD3	1.96	0.41
1:a:327:LEU:HA	1:a:327:LEU:HD23	1.80	0.41
2:b:360:ARG:CG	2:b:360:ARG:HH11	2.34	0.41
4:d:91:PRO:HB2	4:d:94:PHE:CD1	2.56	0.41
4:d:100:GLN:HB3	10:j:84:TYR:HA	2.03	0.41
8:h:113:GLU:O	8:h:117:LEU:HG	2.21	0.41
8:h:245:LEU:HD23	8:h:245:LEU:HA	1.83	0.41
9:i:102:LYS:HD2	9:i:102:LYS:HA	1.78	0.41
9:i:121:SER:O	9:i:125:ILE:HG13	2.20	0.41
10:j:279:LEU:HD22	11:k:176:SER:HB3	2.03	0.41
12:l:142:GLU:OE1	18:t:88:LEU:HB2	2.21	0.41
13:m:66:ASP:OD2	13:m:70:ARG:HG3	2.21	0.41
16:p:8:LEU:HB3	16:p:95:GLN:HG3	2.03	0.41
19:u:142:GLN:HA	19:u:145:ASN:HD22	1.84	0.41
21:w:284:ASP:HA	21:w:285:PRO:HD2	1.82	0.41
1:a:283:TYR:HA	1:a:284:PRO:HD2	1.89	0.41
2:b:168:VAL:HA	2:b:169:PRO:HD3	1.81	0.41
4:d:164:ARG:NH1	11:k:88:TYR:HB3	2.35	0.41
10:j:142:LYS:C	10:j:144:ASP:H	2.29	0.41
13:m:105:LEU:HD23	13:m:105:LEU:HA	1.87	0.41
15:o:64:LEU:HD12	15:o:64:LEU:HA	1.77	0.41
21:w:206:ARG:O	21:w:223:LEU:HB2	2.21	0.41
1:a:200:ARG:HD3	1:a:233:LYS:HD3	2.03	0.40
2:b:90:ILE:HD11	15:o:110:LEU:HD23	2.04	0.40
6:f:89:UNK:O	6:f:92:UNK:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:130:TRP:CD1	7:g:134:THR:HG21	2.56	0.40
8:h:274:LEU:HG	8:h:296:ALA:HB1	2.02	0.40
9:i:129:ASP:HA	9:i:130:PRO:HD2	1.95	0.40
10:j:133:LEU:HD23	10:j:133:LEU:HA	1.91	0.40
10:j:136:ARG:O	10:j:153:LEU:HD12	2.21	0.40
10:j:146:ARG:NH1	10:j:259:GLU:OE2	2.54	0.40
11:k:81:ASN:HB3	11:k:86:TYR:CE2	2.56	0.40
21:w:105:TRP:CG	21:w:265:LEU:HD13	2.56	0.40
21:w:372:ALA:HB1	21:w:377:ALA:HB1	2.02	0.40
22:x:176:VAL:HG21	22:x:196:HIS:NE2	2.36	0.40
23:z:205:UNK:HA	23:z:208:UNK:HG3	2.02	0.40
2:b:262:GLY:HA3	2:b:342:PHE:O	2.22	0.40
3:c:166:ALA:HB2	3:c:178:TYR:CE1	2.57	0.40
3:c:199:PHE:HB3	3:c:277:VAL:HG21	2.02	0.40
7:g:19:LEU:HD12	7:g:19:LEU:HA	1.92	0.40
7:g:73:PRO:HB2	7:g:89:ILE:HG13	2.04	0.40
16:p:33:PHE:O	16:p:37:VAL:HG23	2.22	0.40
1:a:389:LEU:HD23	1:a:389:LEU:HA	1.88	0.40
3:c:32:LEU:HD13	3:c:37:LEU:HD21	2.04	0.40
8:h:105:ARG:NH1	8:h:113:GLU:HA	2.37	0.40
8:h:163:GLU:OE2	8:h:188:PRO:HB2	2.21	0.40
8:h:231:MET:H	8:h:231:MET:HG2	1.63	0.40
9:i:122:ILE:HG23	9:i:134:ILE:HD11	2.03	0.40
9:i:213:THR:HG21	9:i:245:TYR:CZ	2.57	0.40
21:w:104:ASN:HD22	21:w:104:ASN:HA	1.53	0.40
21:w:296:LEU:HD23	21:w:296:LEU:HA	1.82	0.40
1:a:43:PRO:HA	1:a:44:PRO:HD3	1.91	0.40
1:a:107:PHE:HE1	1:a:113:LEU:HD13	1.87	0.40
1:a:163:LEU:HA	1:a:163:LEU:HD23	1.88	0.40
3:c:146:MET:HE2	3:c:146:MET:HB3	1.91	0.40
6:f:90:UNK:O	6:f:94:UNK:HB1	2.21	0.40
7:g:80:LEU:HD12	7:g:80:LEU:HA	1.88	0.40
19:u:136:SER:HB2	19:u:149:CYS:SG	2.60	0.40
23:z:18:UNK:HA	23:z:21:UNK:HG3	2.03	0.40
23:z:23:UNK:HA	23:z:26:UNK:HG3	2.04	0.40
3:c:273:PHE:HD2	3:c:300:VAL:HG12	1.87	0.40
6:f:135:LYS:HA	6:f:136:PRO:HD3	1.87	0.40
8:h:59:ARG:HE	8:h:184:PHE:HB2	1.85	0.40
8:h:216:ARG:HB2	8:h:220:ILE:HD12	2.02	0.40
10:j:47:LEU:O	10:j:48:LEU:HD23	2.22	0.40
13:m:145:ILE:HG13	13:m:145:ILE:H	1.72	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	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
2	b	352/380 (93%)	329 (94%)	23 (6%)	0	100	100
3	c	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
4	d	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
5	e	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
6	f	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
7	g	146/159 (92%)	141 (97%)	5 (3%)	0	100	100
8	h	287/332 (86%)	270 (94%)	17 (6%)	0	100	100
9	i	240/312 (77%)	230 (96%)	10 (4%)	0	100	100
10	j	211/279 (76%)	200 (95%)	9 (4%)	2 (1%)	14	42
11	k	125/212 (59%)	119 (95%)	6 (5%)	0	100	100
12	l	131/166 (79%)	127 (97%)	4 (3%)	0	100	100
13	m	107/159 (67%)	101 (94%)	6 (6%)	0	100	100
14	n	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
15	o	92/124 (74%)	87 (95%)	5 (5%)	0	100	100
16	p	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
17	q	35/138 (25%)	33 (94%)	2 (6%)	0	100	100
18	t	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
19	u	137/205 (67%)	130 (95%)	7 (5%)	0	100	100
20	v	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
21	w	385/433 (89%)	363 (94%)	20 (5%)	2 (0%)	24	54
22	x	160/196 (82%)	155 (97%)	4 (2%)	1 (1%)	21	50
All	All	3790/4899 (77%)	3612 (95%)	173 (5%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	w	159	VAL
22	x	93	ILE
10	j	84	TYR
10	j	151	ARG
21	w	358	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	348/365 (95%)	330 (95%)	18 (5%)	21	48
2	b	310/328 (94%)	295 (95%)	15 (5%)	23	50
3	c	271/299 (91%)	257 (95%)	14 (5%)	21	48
4	d	92/181 (51%)	87 (95%)	5 (5%)	20	47
5	e	100/108 (93%)	93 (93%)	7 (7%)	14	40
6	f	80/110 (73%)	71 (89%)	9 (11%)	5	21
7	g	128/136 (94%)	112 (88%)	16 (12%)	4	18
8	h	251/284 (88%)	232 (92%)	19 (8%)	12	38
9	i	218/281 (78%)	208 (95%)	10 (5%)	24	50
10	j	190/242 (78%)	181 (95%)	9 (5%)	23	50
11	k	115/181 (64%)	112 (97%)	3 (3%)	40	61
12	l	122/147 (83%)	112 (92%)	10 (8%)	10	35
13	m	103/145 (71%)	100 (97%)	3 (3%)	37	60
14	n	88/113 (78%)	79 (90%)	9 (10%)	7	25
15	o	74/97 (76%)	70 (95%)	4 (5%)	20	47
16	p	79/88 (90%)	77 (98%)	2 (2%)	42	62
17	q	36/114 (32%)	35 (97%)	1 (3%)	38	60
18	t	75/82 (92%)	70 (93%)	5 (7%)	15	41
19	u	126/169 (75%)	121 (96%)	5 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	v	102/173 (59%)	99 (97%)	3 (3%)	37 60
21	w	340/373 (91%)	316 (93%)	24 (7%)	13 39
22	x	149/173 (86%)	135 (91%)	14 (9%)	8 29
All	All	3397/4189 (81%)	3192 (94%)	205 (6%)	19 43

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	35	VAL
1	a	113	LEU
1	a	149	ASN
1	a	151	ASP
1	a	175	THR
1	a	207	ASN
1	a	210	SER
1	a	225	SER
1	a	248	THR
1	a	268	CYS
1	a	270	VAL
1	a	274	ASN
1	a	277	THR
1	a	335	VAL
1	a	342	VAL
1	a	362	THR
1	a	396	VAL
1	a	398	VAL
2	b	53	SER
2	b	130	ILE
2	b	143	CYS
2	b	157	LEU
2	b	173	LEU
2	b	209	ASP
2	b	210	GLU
2	b	237	VAL
2	b	267	ARG
2	b	279	ILE
2	b	281	PHE
2	b	288	SER
2	b	321	CYS
2	b	324	ASP
2	b	360	ARG

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Mol	Chain	Res	Type
3	c	56	THR
3	c	67	VAL
3	c	90	MET
3	c	106	ASP
3	c	131	ASP
3	c	140	TRP
3	c	149	CYS
3	c	211	LEU
3	c	222	VAL
3	c	260	VAL
3	c	272	CYS
3	c	280	VAL
3	c	285	THR
3	c	310	ASN
4	d	83	ILE
4	d	136	ILE
4	d	139	LEU
4	d	150	LEU
4	d	168	LEU
5	e	19	SER
5	e	67	LYS
5	e	68	LEU
5	e	78	GLU
5	e	106	THR
5	e	111	HIS
5	e	127	GLN
6	f	52	THR
6	f	59	VAL
6	f	64	SER
6	f	72	THR
6	f	75	ILE
6	f	103	LEU
6	f	109	ILE
6	f	120	LYS
6	f	131	ARG
7	g	6	THR
7	g	9	ARG
7	g	14	VAL
7	g	28	ARG
7	g	33	LEU
7	g	34	SER
7	g	39	SER

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Mol	Chain	Res	Type
7	g	61	VAL
7	g	70	CYS
7	g	94	VAL
7	g	108	SER
7	g	112	VAL
7	g	114	ARG
7	g	126	ILE
7	g	127	GLN
7	g	138	THR
8	h	33	LYS
8	h	51	LEU
8	h	78	ARG
8	h	88	LEU
8	h	98	ILE
8	h	133	SER
8	h	148	LEU
8	h	167	CYS
8	h	171	ARG
8	h	181	SER
8	h	191	LEU
8	h	211	THR
8	h	216	ARG
8	h	231	MET
8	h	232	TRP
8	h	233	THR
8	h	234	ILE
8	h	288	THR
8	h	301	LEU
9	i	81	THR
9	i	100	LEU
9	i	134	ILE
9	i	151	CYS
9	i	165	THR
9	i	186	VAL
9	i	196	GLN
9	i	208	ILE
9	i	242	VAL
9	i	258	SER
10	j	55	ARG
10	j	145	ASP
10	j	231	VAL
10	j	255	VAL

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Mol	Chain	Res	Type
10	j	262	ASP
10	j	264	LEU
10	j	274	ARG
10	j	276	LEU
10	j	277	LEU
11	k	77	VAL
11	k	151	THR
11	k	162	LEU
12	l	42	VAL
12	l	52	LEU
12	l	89	SER
12	l	90	ARG
12	l	93	ASN
12	l	99	ASP
12	l	100	ILE
12	l	101	THR
12	l	122	LYS
12	l	137	VAL
13	m	90	ILE
13	m	121	MET
13	m	135	VAL
14	n	37	THR
14	n	46	ARG
14	n	53	MET
14	n	56	VAL
14	n	66	PHE
14	n	80	LEU
14	n	92	ILE
14	n	98	VAL
14	n	105	ASP
15	o	43	LEU
15	o	44	THR
15	o	48	ASP
15	o	65	ARG
16	p	42	VAL
16	p	60	SER
17	q	126	ILE
18	t	9	ARG
18	t	12	ILE
18	t	45	ASN
18	t	49	LEU
18	t	101	TRP

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Mol	Chain	Res	Type
19	u	79	SER
19	u	123	LYS
19	u	137	GLU
19	u	138	CYS
19	u	140	ARG
20	v	53	SER
20	v	64	HIS
20	v	68	SER
21	w	47	ILE
21	w	59	ARG
21	w	81	ARG
21	w	100	LEU
21	w	104	ASN
21	w	126	GLU
21	w	147	GLU
21	w	162	ASP
21	w	166	ILE
21	w	205	LEU
21	w	245	VAL
21	w	248	ASP
21	w	263	ASP
21	w	267	LEU
21	w	271	GLN
21	w	274	ASN
21	w	287	CYS
21	w	335	MET
21	w	395	LEU
21	w	399	ILE
21	w	404	VAL
21	w	405	LYS
21	w	420	LEU
21	w	421	ASN
22	x	36	ARG
22	x	38	VAL
22	x	42	LEU
22	x	54	THR
22	x	56	THR
22	x	70	CYS
22	x	72	ILE
22	x	93	ILE
22	x	111	GLU
22	x	115	ILE

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Mol	Chain	Res	Type
22	x	118	CYS
22	x	119	VAL
22	x	121	MET
22	x	152	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	65	HIS
1	a	96	HIS
1	a	108	HIS
1	a	156	ASN
1	a	160	HIS
1	a	207	ASN
1	a	223	HIS
1	a	274	ASN
1	a	289	HIS
1	a	343	GLN
1	a	380	GLN
1	a	385	HIS
1	a	420	HIS
2	b	102	GLN
2	b	116	ASN
2	b	224	HIS
2	b	266	HIS
2	b	275	GLN
2	b	308	GLN
2	b	320	GLN
2	b	373	HIS
3	c	252	HIS
3	c	294	GLN
3	c	305	HIS
3	c	310	ASN
5	e	127	GLN
6	f	44	ASN
6	f	121	HIS
6	f	130	HIS
6	f	137	ASN
7	g	17	ASN
7	g	90	HIS
7	g	131	HIS
8	h	94	ASN

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Mol	Chain	Res	Type
8	h	177	GLN
8	h	260	GLN
8	h	310	ASN
9	i	115	ASN
9	i	193	GLN
9	i	196	GLN
9	i	207	ASN
9	i	217	HIS
11	k	54	HIS
11	k	61	HIS
11	k	177	ASN
12	l	63	HIS
12	l	93	ASN
12	l	141	ASN
13	m	107	ASN
14	n	69	HIS
14	n	122	ASN
14	n	124	HIS
16	p	72	HIS
16	p	80	HIS
16	p	93	HIS
17	q	124	HIS
18	t	34	ASN
18	t	45	ASN
18	t	85	HIS
18	t	91	GLN
19	u	103	HIS
19	u	145	ASN
20	v	130	GLN
21	w	96	GLN
21	w	101	ASN
21	w	104	ASN
21	w	173	GLN
21	w	228	ASN
21	w	233	ASN
21	w	234	GLN
21	w	367	GLN
21	w	385	ASN
21	w	414	GLN
21	w	421	ASN
22	x	131	HIS
22	x	164	ASN

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Mol	Chain	Res	Type
22	x	170	ASN
22	x	184	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	z	5
20	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	36:UNK	C	99:UNK	N	57.05
1	z	106:UNK	C	201:UNK	N	13.00
1	z	105:UNK	C	106:UNK	N	3.37
1	v	154:UNK	C	155:UNK	N	3.12
1	z	35:UNK	C	36:UNK	N	3.12
1	z	210:UNK	C	211:UNK	N	3.12

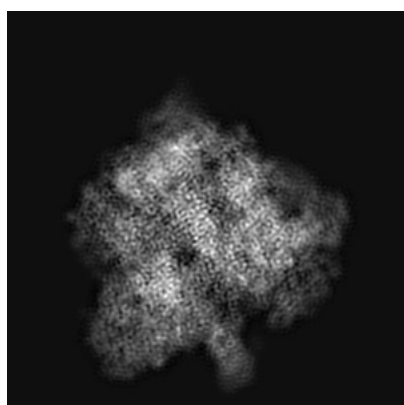
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2787. These allow visual inspection of the internal detail of the map and identification of artifacts.

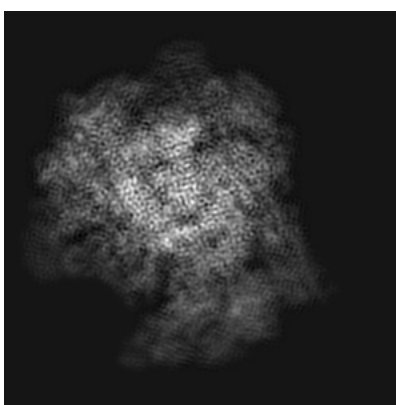
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

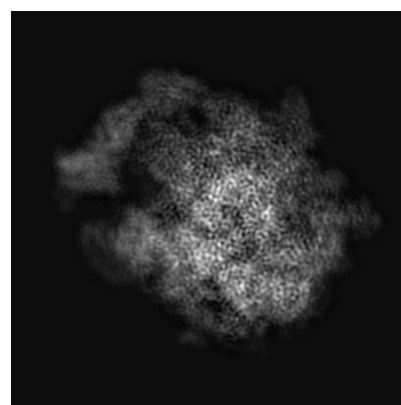
6.1.1 Primary map



X



Y

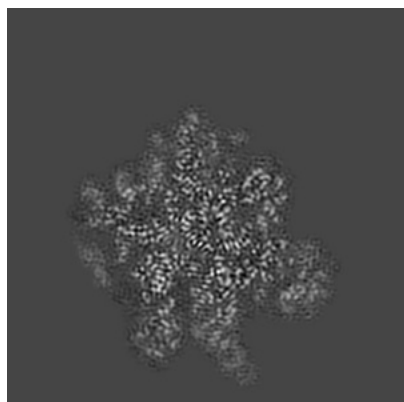


Z

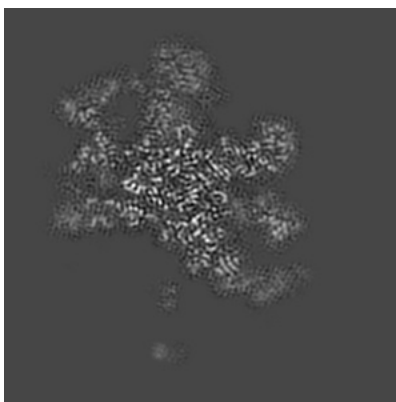
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

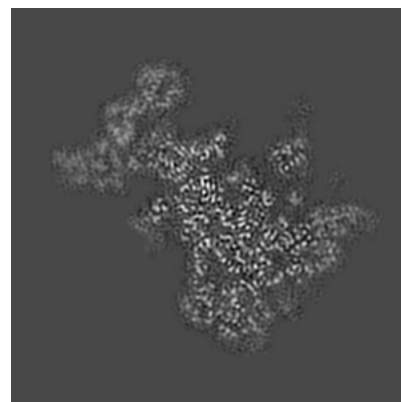
6.2.1 Primary map



X Index: 108



Y Index: 108

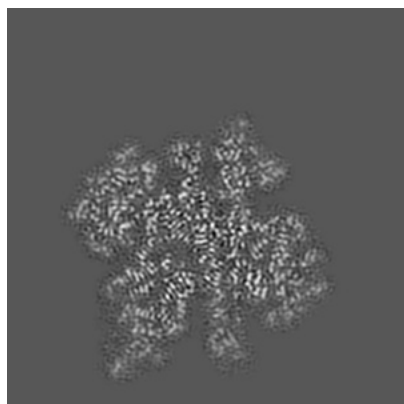


Z Index: 108

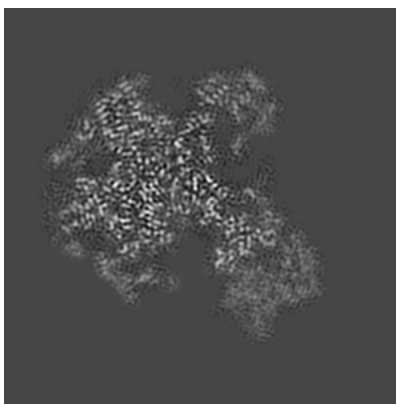
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

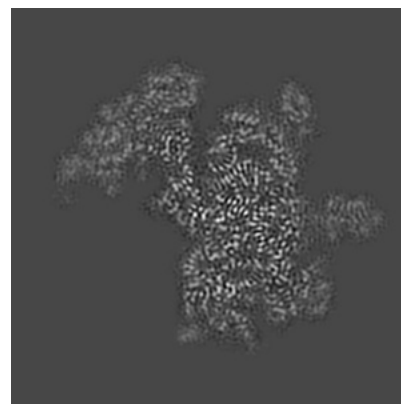
6.3.1 Primary map



X Index: 120



Y Index: 86

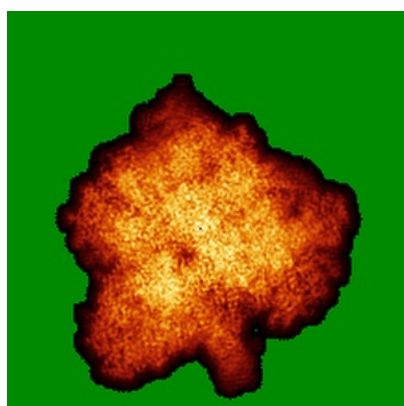


Z Index: 98

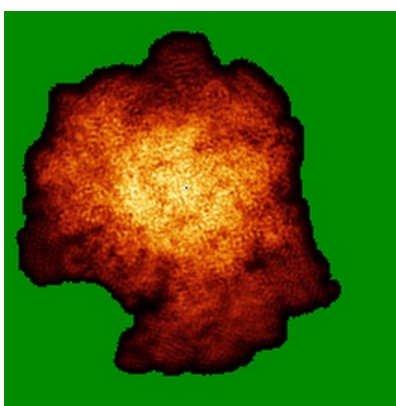
The images above show the largest variance slices of the map in three orthogonal directions.

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

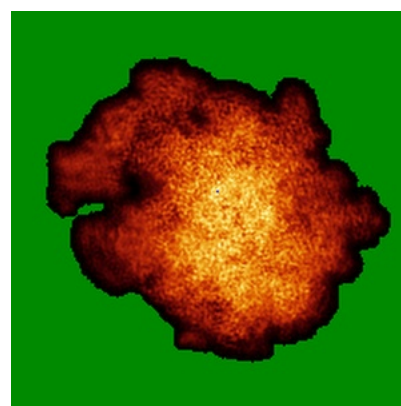
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

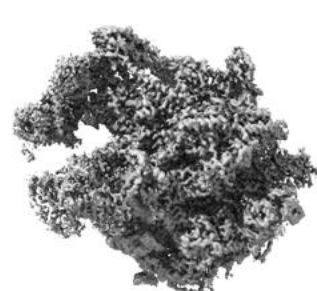
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

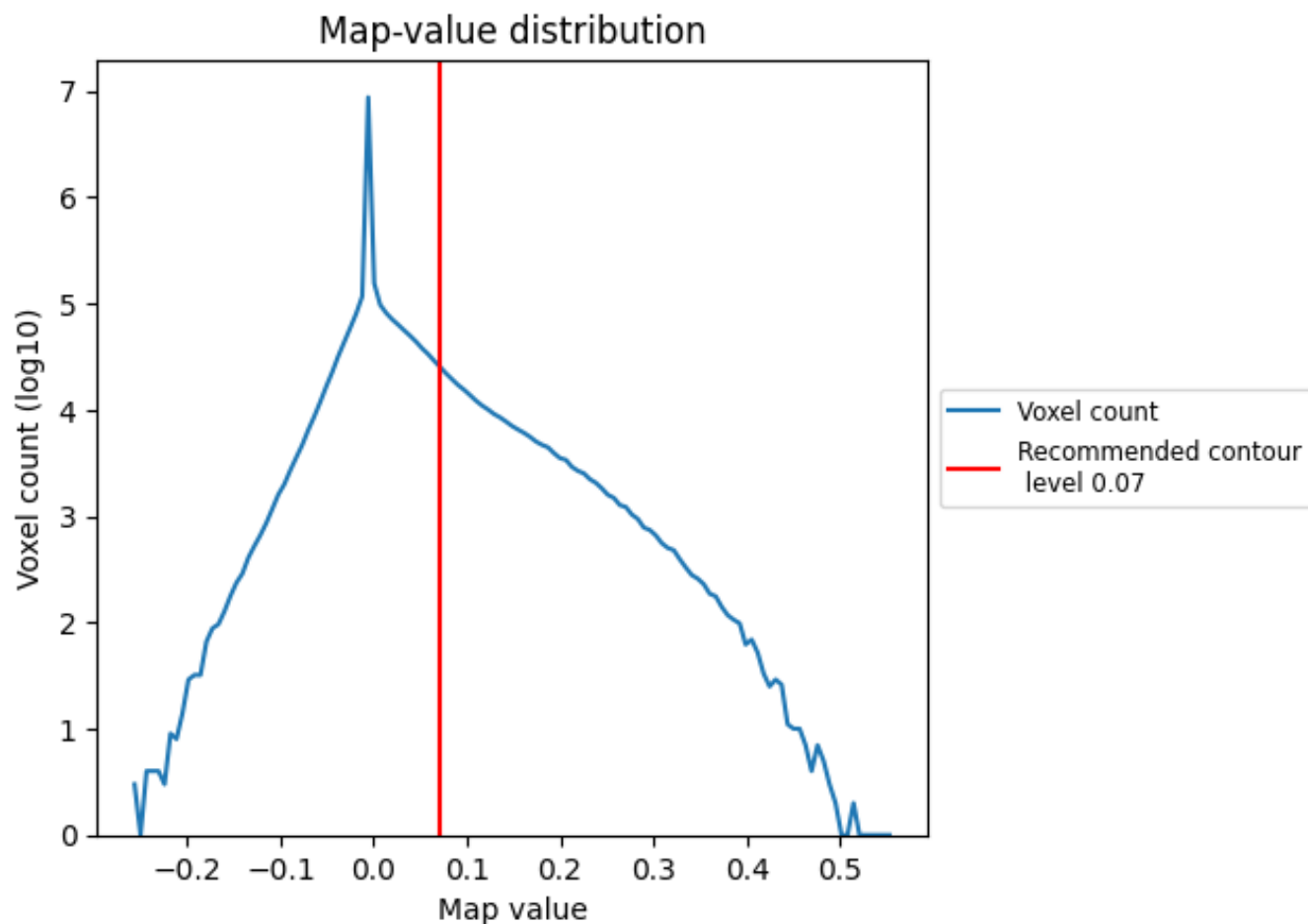
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

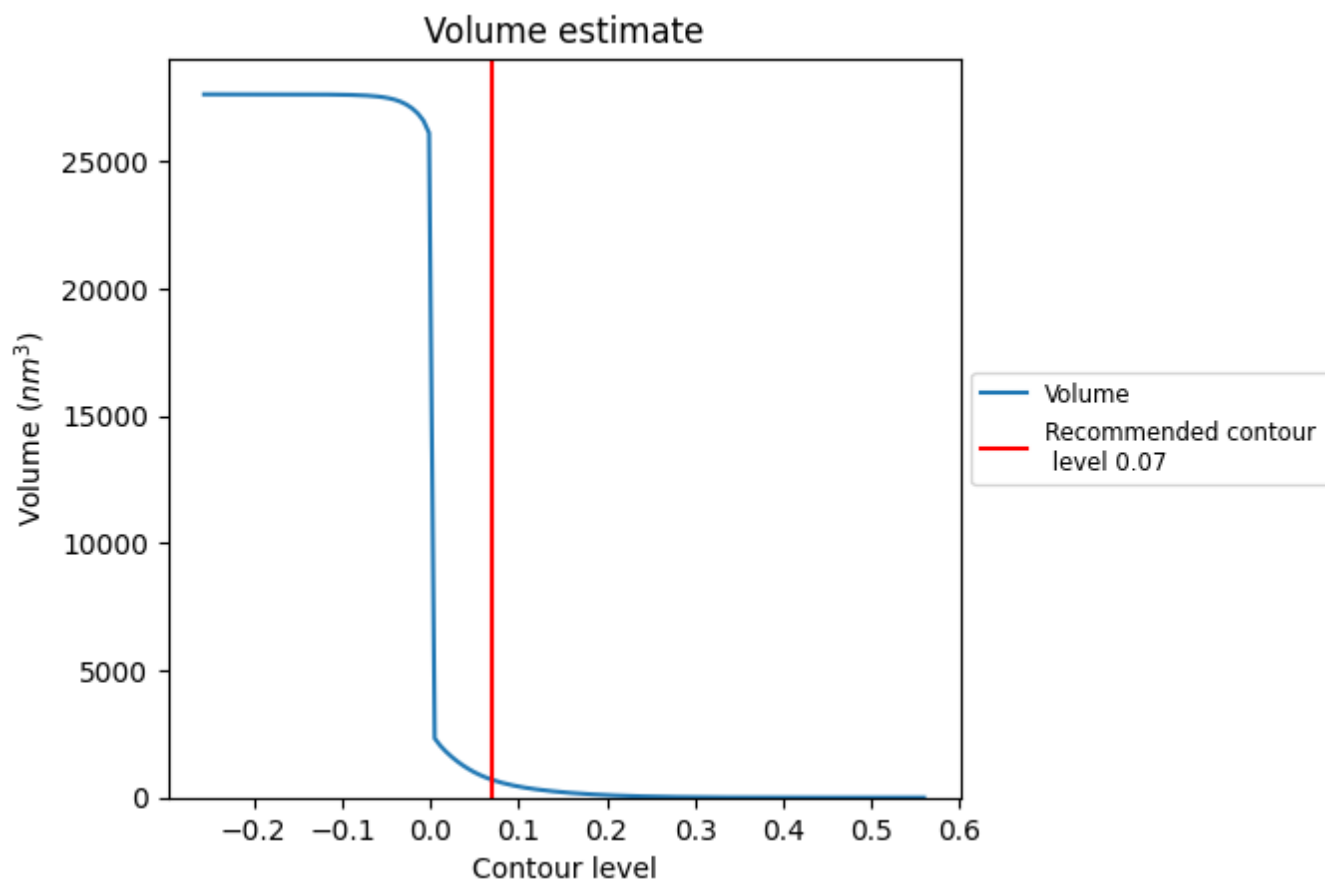
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

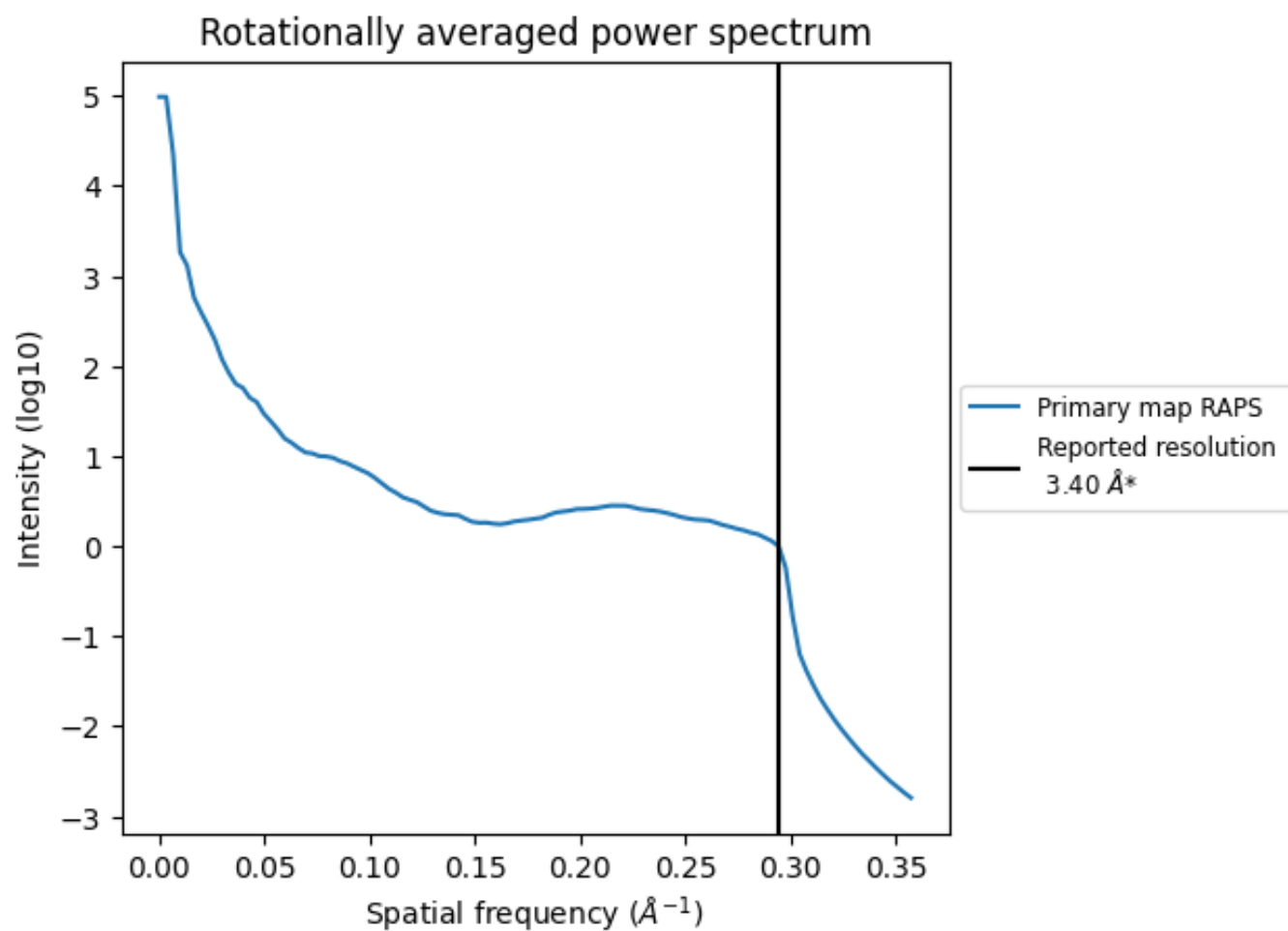
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 700 nm^3 ; this corresponds to an approximate mass of 632 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 0.294 Å⁻¹

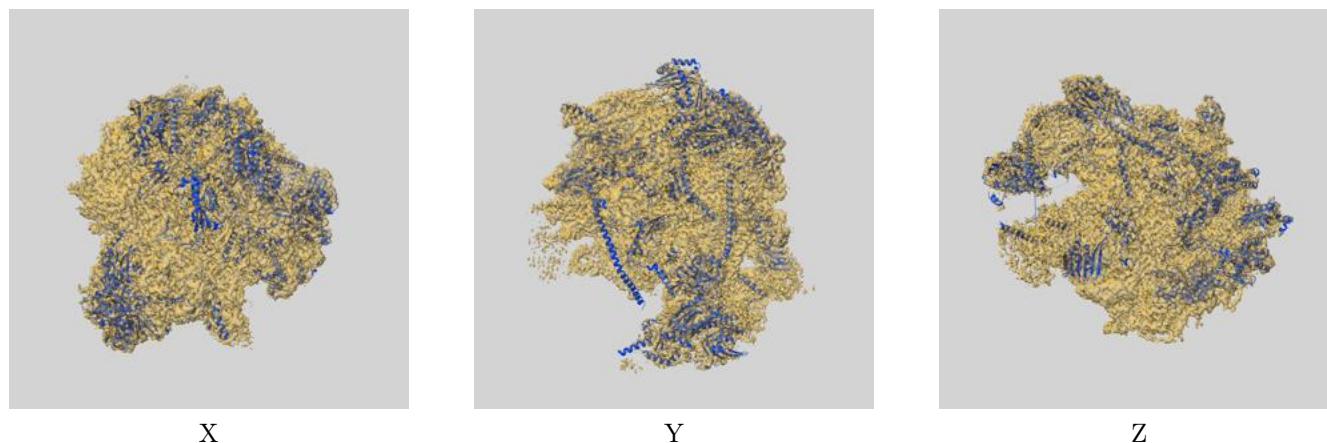
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

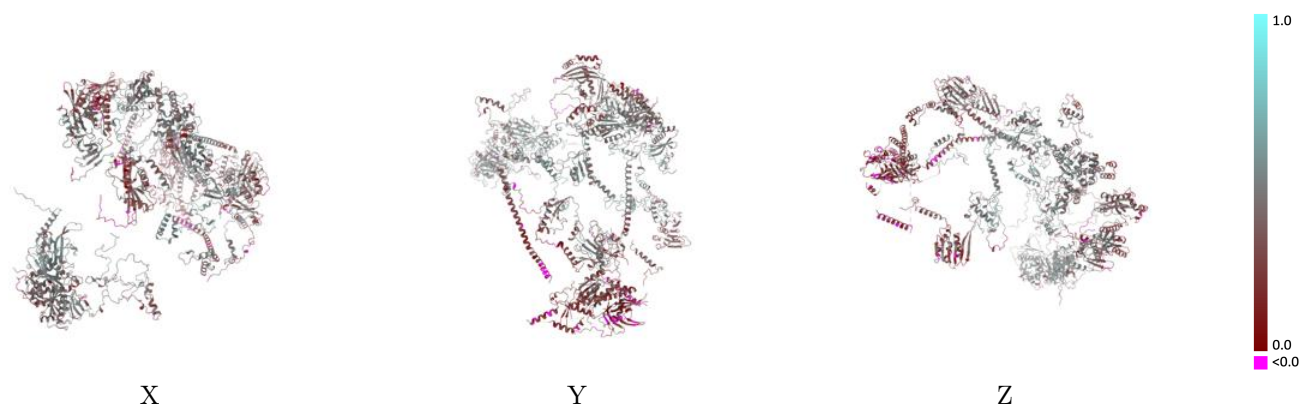
This section contains information regarding the fit between EMDB map EMD-2787 and PDB model 4V1A. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.07 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](#)

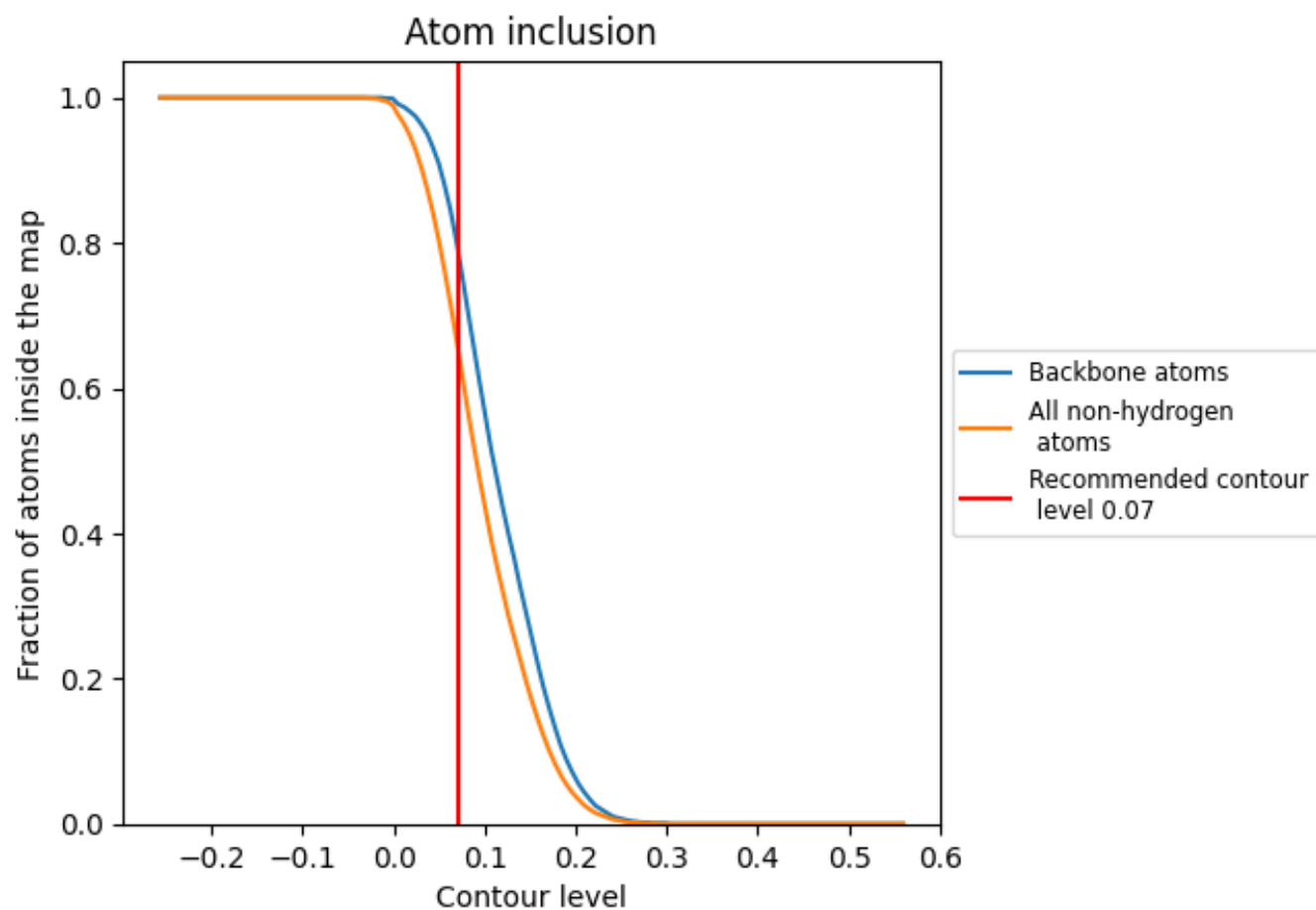


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.3880
a	 0.7830	 0.4530
b	 0.7240	 0.3930
c	 0.6960	 0.3920
d	 0.4400	 0.2390
e	 0.7290	 0.4160
f	 0.6830	 0.4250
g	 0.8320	 0.5020
h	 0.7240	 0.4250
i	 0.4170	 0.3120
j	 0.4130	 0.1810
k	 0.4980	 0.2970
l	 0.8170	 0.4700
m	 0.6160	 0.3680
n	 0.8570	 0.5090
o	 0.7600	 0.4480
p	 0.4210	 0.2680
q	 0.5110	 0.2740
t	 0.8510	 0.5140
u	 0.4020	 0.2990
v	 0.4530	 0.3110
w	 0.7940	 0.4580
x	 0.7540	 0.4420
z	 0.1210	 0.1570

