



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:15 AM UTC

PDB ID : 9S0U / pdb_00009s0u
EMDB ID : EMD-54425
Title : State 3 MAP 3 RNA Pol II activated elongation complex with SETD2 bound to distal upstream H3
Authors : Walshe, J.L.; Ochmann, M.; Dienemann, C.; Cramer, P.
Deposited on : 2025-07-17
Resolution : 6.72 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

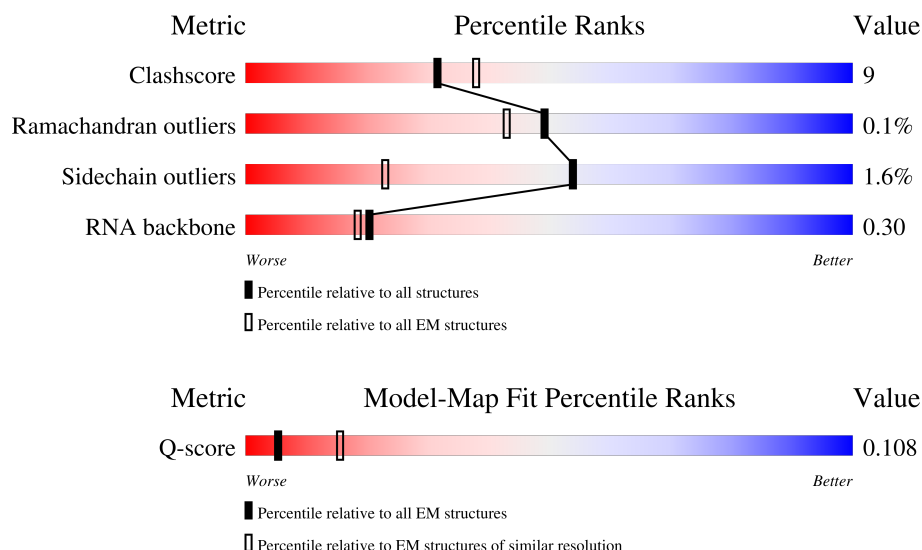
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.72 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.



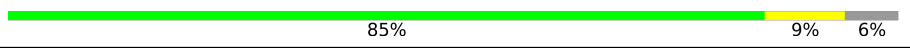
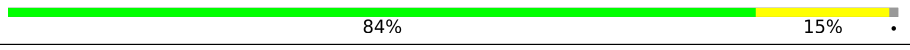
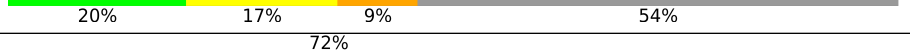
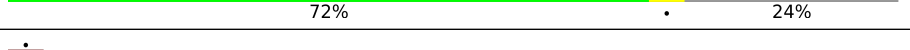
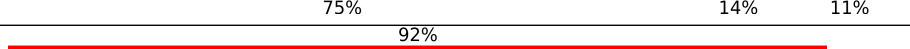
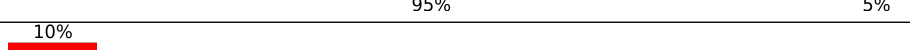
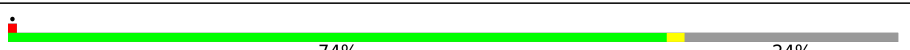
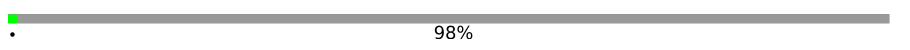
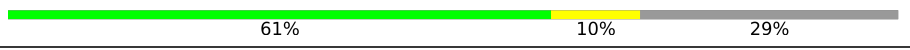
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	481 (6.22 - 7.20)

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	D	142	65% 24% 11%
2	E	210	85% 14%
3	F	127	53% 9% 39%

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Mol	Chain	Length	Quality of chain
4	G	172	
5	H	150	
6	I	125	
7	J	67	
8	K	117	
9	L	58	
10	P	46	
11	Q	1179	
12	T	197	
13	W	305	
14	X	531	
15	Y	121	
16	a	136	
16	e	136	
17	b	103	
17	f	103	
18	c	135	
18	g	135	
19	d	126	
19	h	126	
20	k	1049	
21	A	1970	
22	B	1174	
23	C	275	
24	M	1729	

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Mol	Chain	Length	Quality of chain
25	N	197	5% 71% 13% 17%
26	O	1133	18% 20% 77%
27	R	713	28% 25% 9% 66%
28	S	304	29% 8% 63%
29	U	666	5% 13% 84%
30	V	531	27% 42% 54%
31	Z	1087	16% 37% 9% 53%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 73121 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 RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	149	Total	C	N	O	S	0	0
			1198	759	195	239	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 9 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	47	Total	C	N	O	S	0	0
			398	246	77	69	6		

- Molecule 10 is a RNA chain called RNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 11 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	892	Total	C	N	O	S	0	0
			7240	4587	1266	1355	32		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 12 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	175	Total	C	N	O	P	0	0
			3564	1690	644	1055	175		

- Molecule 13 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	305	Total	C	N	O	S	0	0
			2373	1507	399	462	5		

- Molecule 14 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	53	Total	C	N	O	0	0
			434	268	85	81		

- Molecule 15 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	116	Total	C	N	O	S	0	0
			912	570	159	174	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP Q4R941
Y	-2	PRO	-	expression tag	UNP Q4R941
Y	-1	GLY	-	expression tag	UNP Q4R941
Y	0	SER	-	expression tag	UNP Q4R941

- Molecule 16 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	101	Total	C	N	O	S	0	0
			821	519	157	142	3		
16	e	95	Total	C	N	O	S	0	0
			782	494	150	136	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP Q71DI3
a	110	ALA	CYS	engineered mutation	UNP Q71DI3

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Chain	Residue	Modelled	Actual	Comment	Reference
e	36	MET	LYS	engineered mutation	UNP Q71DI3
e	110	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
17	f	78	Total	C	N	O	S	0	0
			622	393	120	108	1		

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	104	Total	C	N	O		0	0
			801	505	156	140			
18	g	103	Total	C	N	O		0	0
			796	502	155	139			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-5	SER	-	expression tag	UNP P04908
c	-4	ASN	-	expression tag	UNP P04908
c	-3	ALA	-	expression tag	UNP P04908
c	-2	PRO	-	expression tag	UNP P04908
c	-1	TRP	-	expression tag	UNP P04908
g	-5	SER	-	expression tag	UNP P04908
g	-4	ASN	-	expression tag	UNP P04908
g	-3	ALA	-	expression tag	UNP P04908
g	-2	PRO	-	expression tag	UNP P04908
g	-1	TRP	-	expression tag	UNP P04908

- Molecule 19 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	92	Total	C	N	O	S	0	0
			719	452	129	136	2		
19	h	89	Total	C	N	O	S	0	0
			693	437	122	132	2		

- Molecule 20 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	k	18	Total	C	N	O	0	0
			138	80	19	39		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-1	SER	-	expression tag	UNP Q9Y5B9
k	0	ASN	-	expression tag	UNP Q9Y5B9

- Molecule 21 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	1390	Total	C	N	O	S	0	0
			11015	6932	1976	2038	69		

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B	1120	Total	C	N	O	S	0	0
			8964	5675	1574	1651	64		

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 24 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	816	Total	C	N	O	S	0	0
			6687	4245	1153	1258	31		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 25 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	164	Total	C	N	O	P	0	0
			3390	1599	645	982	164		

- Molecule 26 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	261	Total	C	N	O	S	0	0
			2131	1320	389	401	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1569	SER	-	expression tag	UNP Q9BYW2
O	1570	ASN	-	expression tag	UNP Q9BYW2
O	1571	ALA	-	expression tag	UNP Q9BYW2
O	1843F	LEU	PRO	variant	UNP Q9BYW2

- Molecule 27 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	244	Total	C	N	O	S	0	0
			1836	1152	340	337	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 28 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	113	Total	C	N	O	S	0	0
			909	554	169	179	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 29 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	104	Total	C	N	O	S	0	0
			751	475	130	145	1		

- Molecule 30 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	242	Total	C	N	O	S	0	0
			1687	1055	302	326	4		

- Molecule 31 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Z	510	Total	C	N	O	P	S	0	0
			4025	2552	709	745	1	18		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	I	2	Total	Zn	0
			2	2	
32	J	1	Total	Zn	0
			1	1	
32	L	1	Total	Zn	0
			1	1	
32	Y	1	Total	Zn	0
			1	1	
32	A	2	Total	Zn	0
			2	2	
32	B	1	Total	Zn	0
			1	1	
32	C	1	Total	Zn	0
			1	1	

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

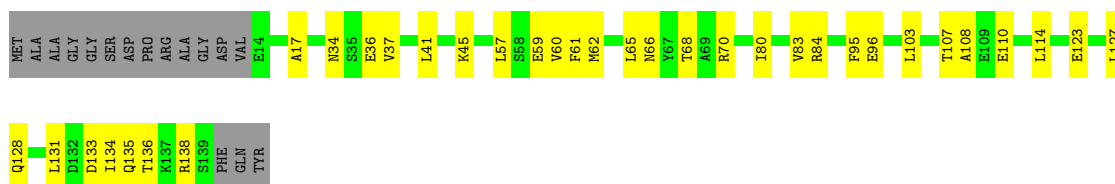
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

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: RNA polymerase II subunit D

Chain D: 



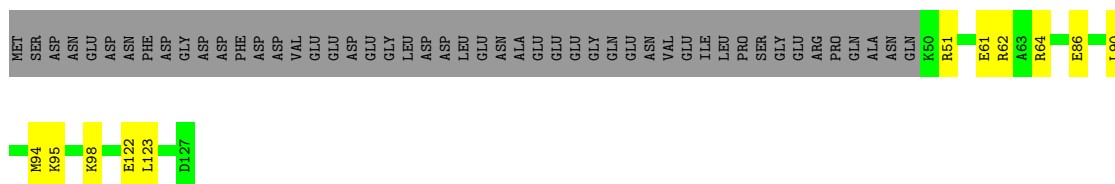
- Molecule 2: DNA-directed RNA polymerase II subunit E

Chain E: 



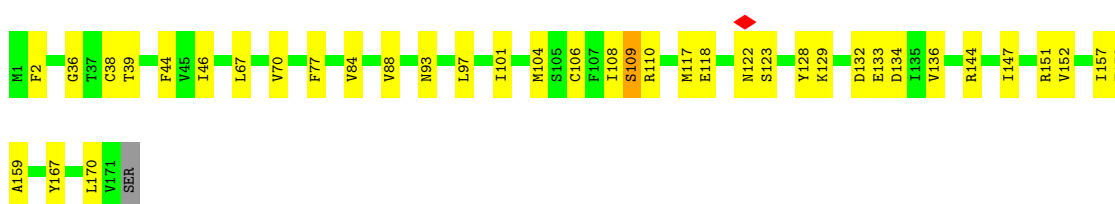
- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 

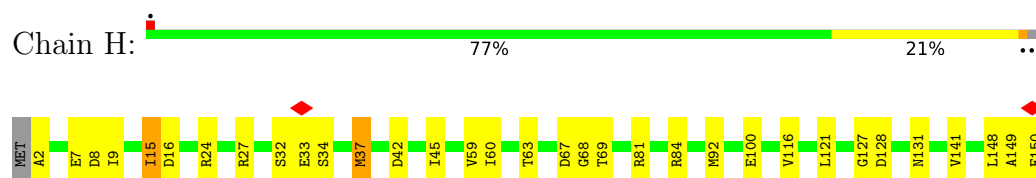


- Molecule 4: DNA-directed RNA polymerase II subunit RPB7

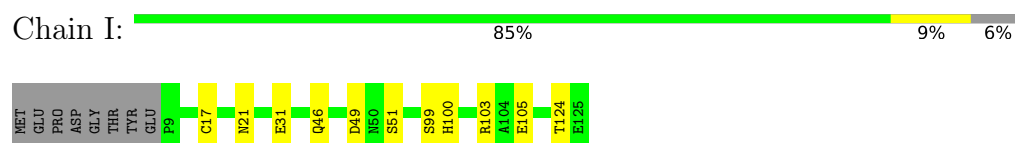
Chain G: 



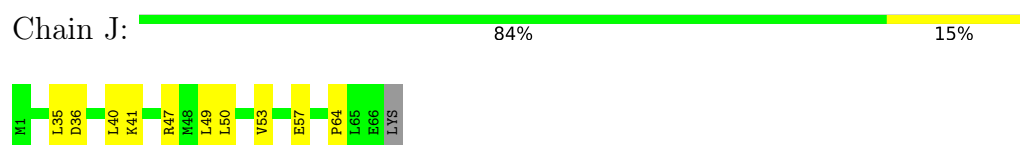
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3



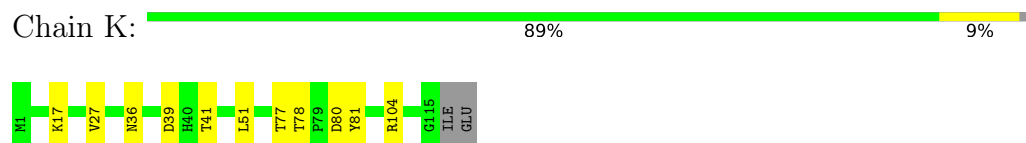
- Molecule 6: DNA-directed RNA polymerase II subunit RPB9



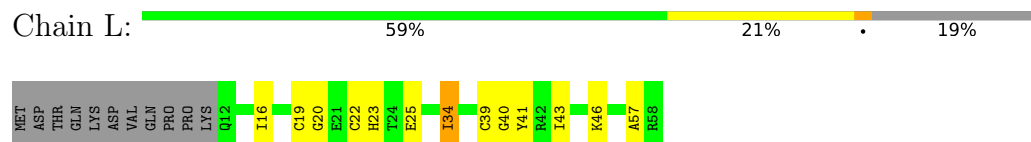
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5



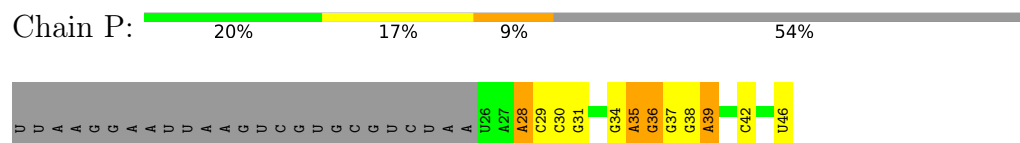
- Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a



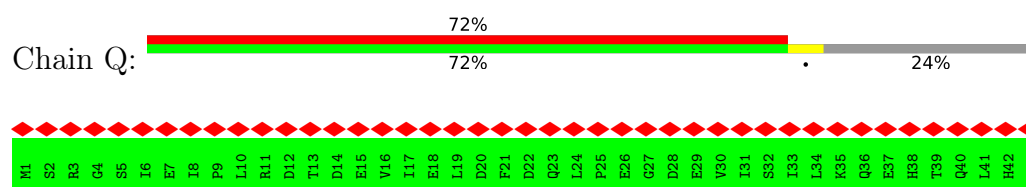
- Molecule 9: RNA polymerase II subunit K



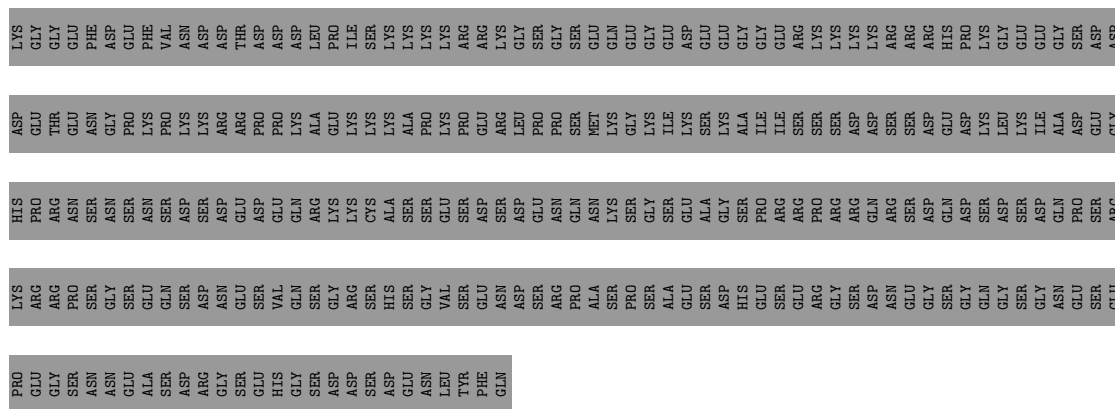
- Molecule 10: RNA (46-MER)



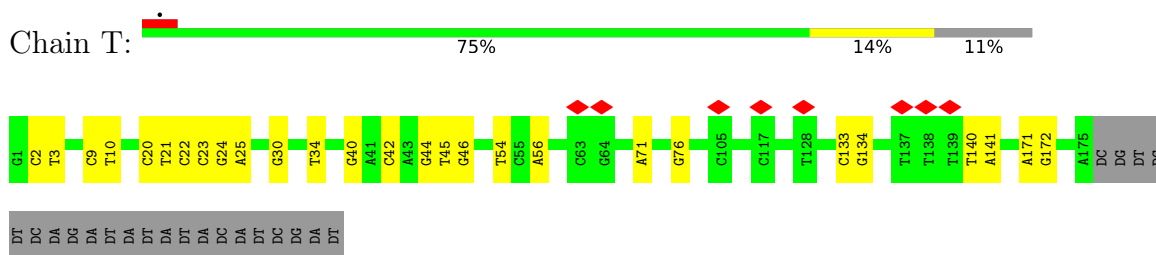
- Molecule 11: RNA polymerase-associated protein CTR9 homolog



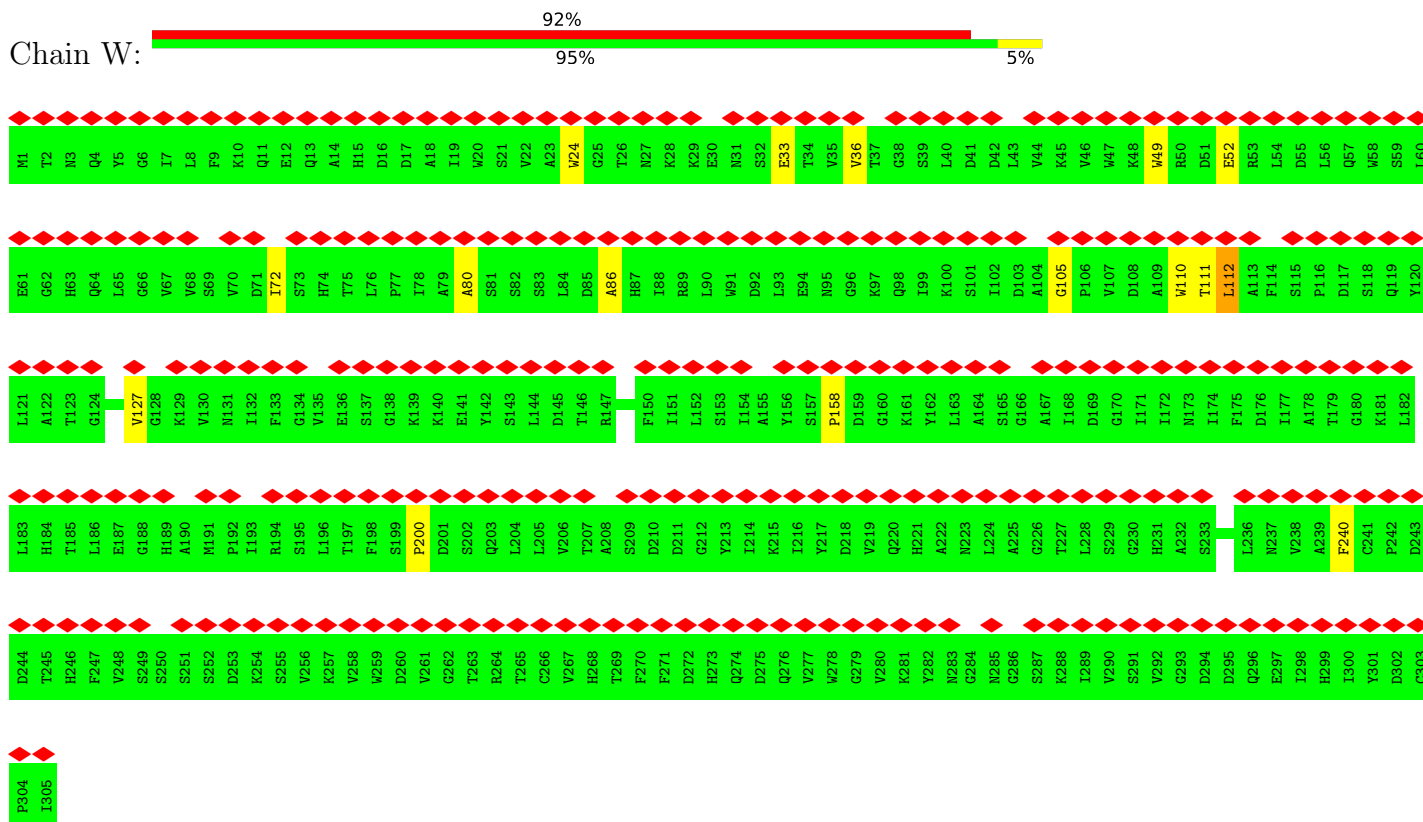




- Molecule 12: Template DNA

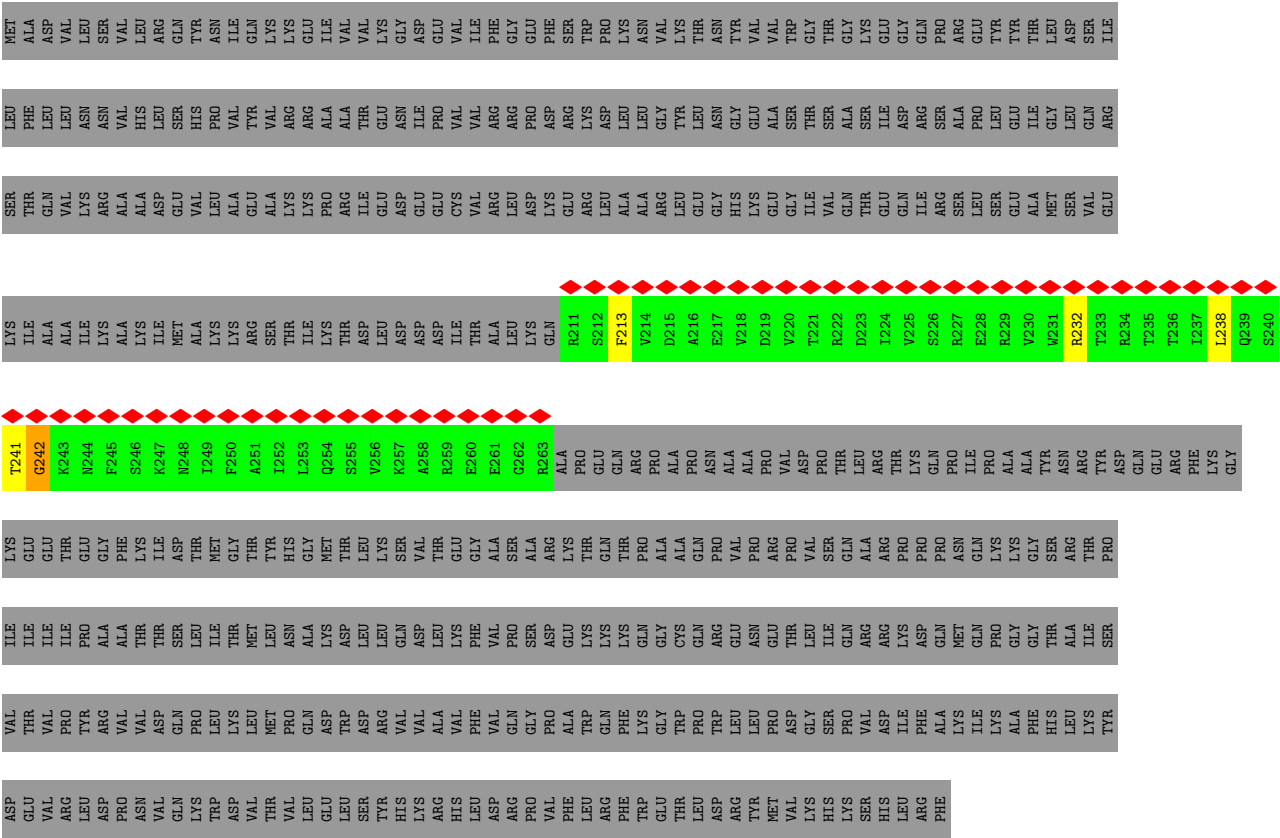


- Molecule 13: WD repeat-containing protein 61

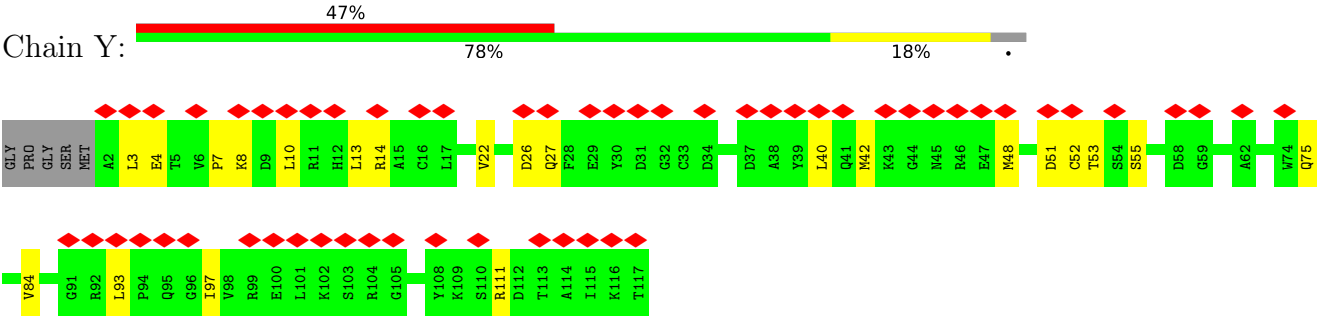


- Molecule 14: Parafibromin

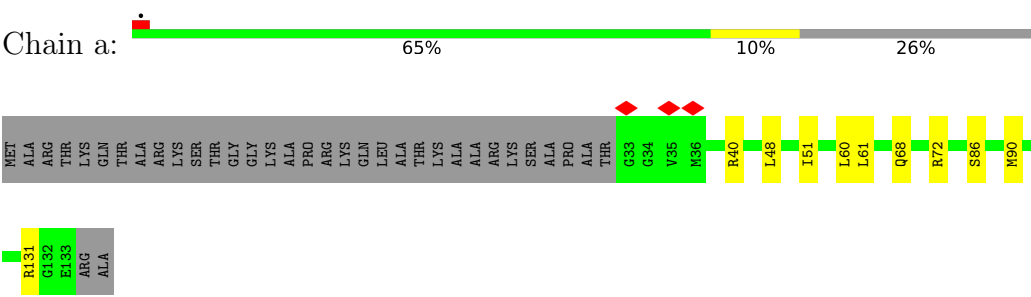




• Molecule 15: Transcription elongation factor SPT4

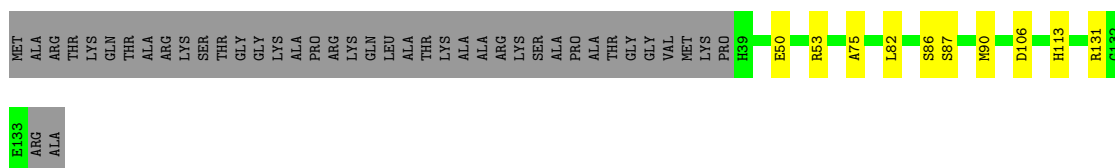


• Molecule 16: Histone H3.2

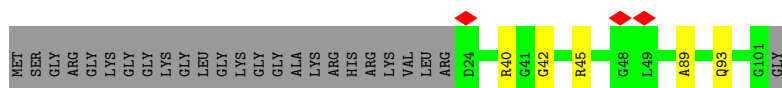


• Molecule 16: Histone H3.2

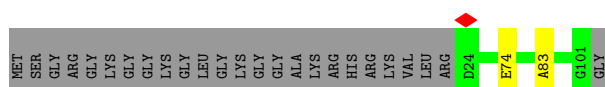




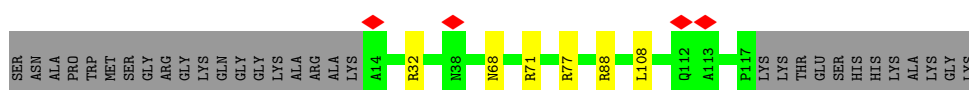
- Molecule 17: Histone H4



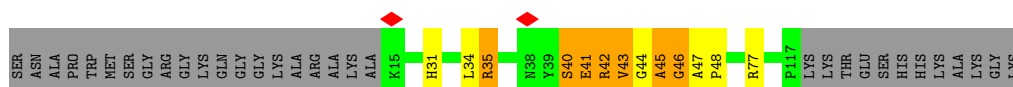
- Molecule 17: Histone H4



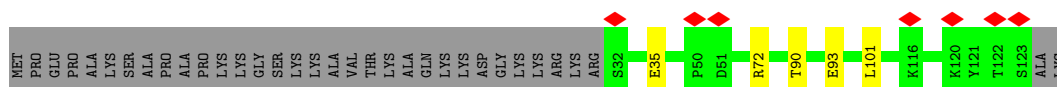
- Molecule 18: Histone H2A type 1-B/E



- Molecule 18: Histone H2A type 1-B/E



- Molecule 19: Histone H2B type 1-K



- Molecule 19: Histone H2B type 1-K





SER
GLY
ARG
GLY
GLY
SER
ASN
ARG
GLY
SER
ARG
HIS
SER
SER
ALA
PRO
PRO
LYS
LYS
LYS
ARG
LYS

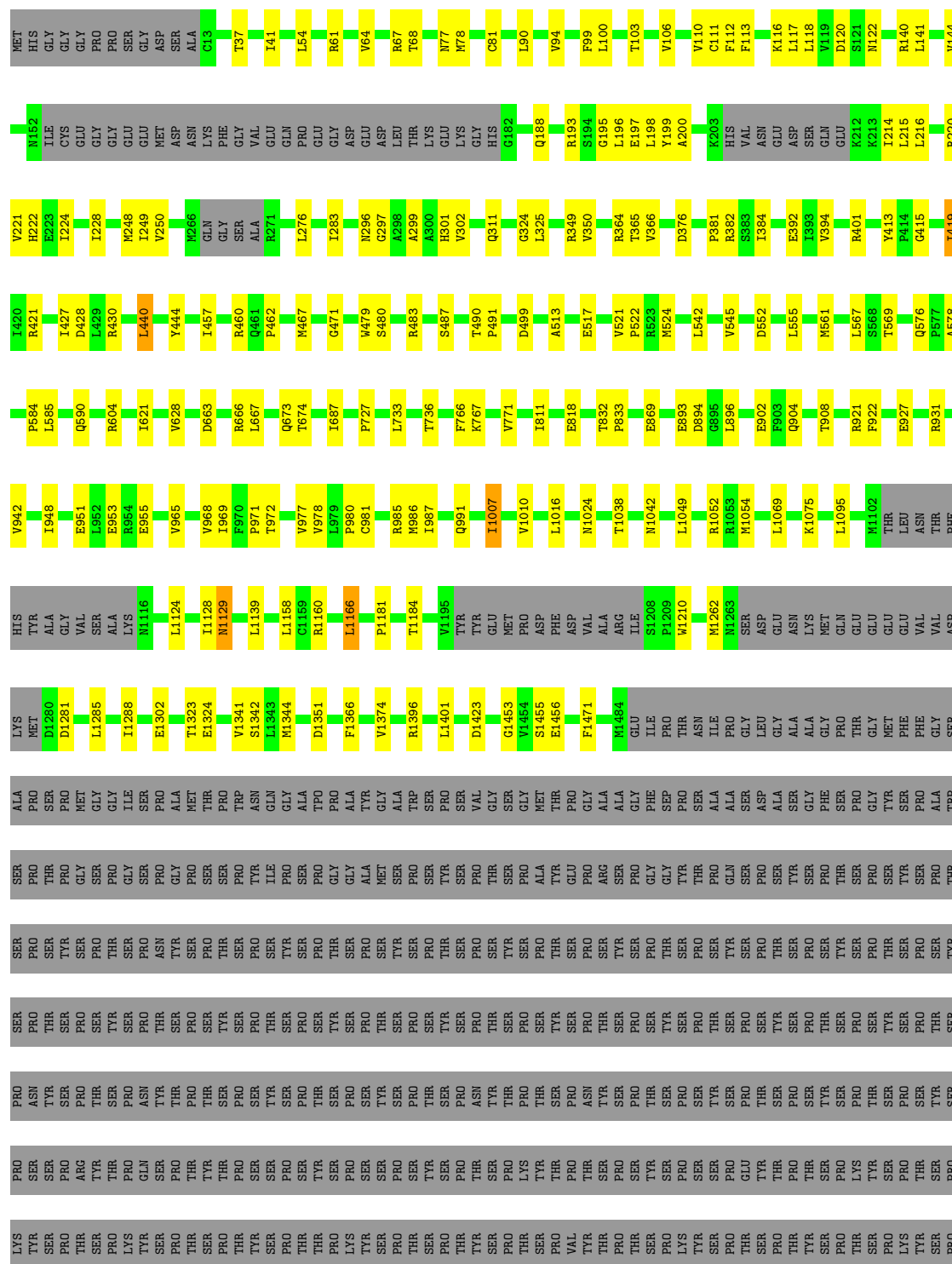
● Molecule 21: DNA-directed RNA polymerase subunit

Chain A:

61%

10%

29%

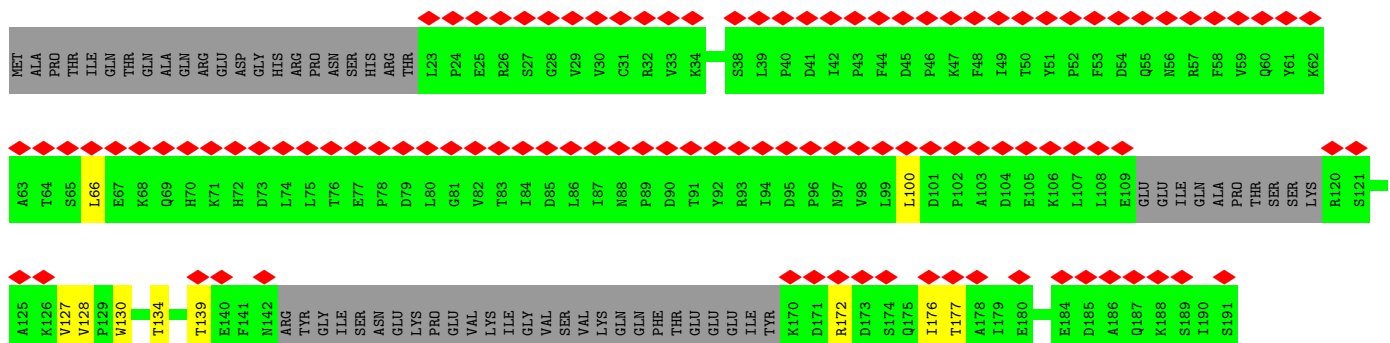
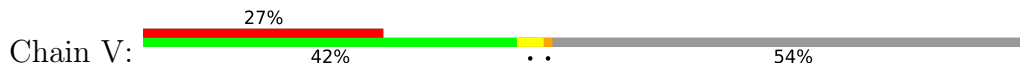


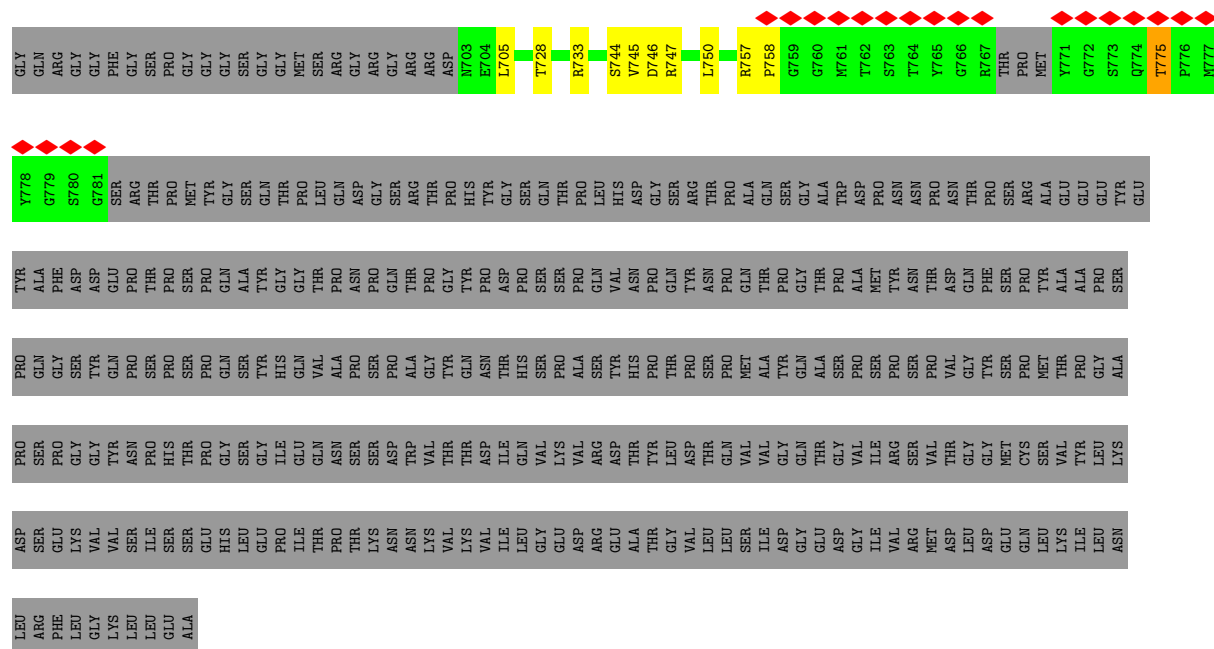






Chain U: 5% 13% 84%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.83	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size ($\text{\AA}$)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.14	0/1017	0.36	0/1368
2	E	0.17	0/1752	0.45	0/2366
3	F	0.18	0/637	0.47	0/859
4	G	0.15	0/1364	0.35	0/1853
5	H	0.17	0/1220	0.44	0/1644
6	I	0.17	0/973	0.46	0/1316
7	J	0.17	0/533	0.43	0/719
8	K	0.17	0/939	0.35	0/1271
9	L	0.20	0/404	0.59	0/536
10	P	0.53	0/506	0.88	1/787 (0.1%)
11	Q	0.42	1/7379 (0.0%)	0.77	13/9945 (0.1%)
12	T	0.33	0/3991	0.65	0/6152
13	W	0.28	0/2432	0.66	0/3311
14	X	0.29	0/438	0.77	0/587
15	Y	0.13	0/928	0.37	0/1250
16	a	0.22	0/833	0.48	0/1117
16	e	0.57	0/793	0.97	3/1064 (0.3%)
17	b	0.23	0/629	0.46	0/843
17	f	0.44	0/629	0.70	0/843
18	c	0.20	0/811	0.42	0/1096
18	g	0.35	0/806	0.74	1/1089 (0.1%)
19	d	0.19	0/730	0.43	0/982
19	h	0.40	0/704	0.76	4/949 (0.4%)
20	k	0.29	0/139	0.79	0/187
21	A	0.19	0/11213	0.47	1/15132 (0.0%)
22	B	0.24	0/9142	0.52	1/12337 (0.0%)
23	C	0.17	0/2115	0.42	0/2873
24	M	0.45	2/6812 (0.0%)	1.08	14/9187 (0.2%)
25	N	0.28	0/3808	0.56	0/5880
26	O	0.27	0/2171	0.56	0/2905
27	R	0.17	0/1866	0.50	3/2519 (0.1%)
28	S	0.19	0/915	0.52	0/1221

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	U	0.19	0/766	0.52	4/1039 (0.4%)
30	V	0.26	0/1715	0.61	3/2343 (0.1%)
31	Z	0.14	0/4084	0.38	2/5498 (0.0%)
All	All	0.29	3/75194 (0.0%)	0.63	50/103068 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	P	0	2
12	T	0	4
14	X	0	1
18	g	0	1
19	h	0	1
24	M	0	4
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	992	LEU	N-CA	9.29	1.57	1.46
24	M	992	LEU	CA-C	9.13	1.66	1.52
11	Q	824	ALA	CA-CB	-6.82	1.42	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	471	TYR	O-C-N	-52.02	50.59	122.37
24	M	572	ASP	O-C-N	-35.24	81.97	122.15
24	M	462	ASP	O-C-N	-35.11	84.91	122.12
24	M	992	LEU	CA-C-N	19.36	152.26	121.87
24	M	992	LEU	C-N-CA	19.36	152.26	121.87
24	M	992	LEU	N-CA-C	13.55	129.78	112.03
19	h	87	SER	CA-C-N	-9.71	105.23	122.32
19	h	87	SER	C-N-CA	-9.71	105.23	122.32
18	g	41	GLU	N-CA-C	-9.23	102.60	113.21
30	V	237	LEU	C-N-CD	-8.42	90.49	125.00
27	R	506	PRO	C-N-CD	-8.03	92.08	125.00
10	P	36	G	P-O3'-C3'	7.75	131.82	120.20
16	e	82	LEU	CA-C-N	7.61	134.36	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	e	82	LEU	C-N-CA	7.61	134.36	122.94
11	Q	816	GLN	CA-C-N	7.50	130.33	120.28
11	Q	816	GLN	C-N-CA	7.50	130.33	120.28
19	h	90	THR	CB-CA-C	-7.20	94.62	110.67
24	M	991	GLY	O-C-N	-6.60	114.38	122.23
24	M	1014	ARG	NE-CZ-NH2	6.44	125.00	119.20
19	h	88	THR	CB-CA-C	-6.15	99.37	112.78
29	U	462	ALA	C-N-CD	-6.00	100.40	125.00
31	Z	757	ARG	C-N-CD	-5.78	101.32	125.00
24	M	1056	SER	N-CA-C	5.77	117.55	108.96
27	R	507	PRO	CA-N-CD	-5.61	104.14	112.00
11	Q	808	ALA	N-CA-C	5.60	118.15	111.71
24	M	1047	ASP	CA-C-N	5.59	128.33	120.28
24	M	1047	ASP	C-N-CA	5.59	128.33	120.28
29	U	493	PRO	CA-N-CD	-5.58	104.19	112.00
27	R	506	PRO	CA-N-CD	-5.57	104.20	112.00
30	V	258	PRO	CA-N-CD	-5.54	104.25	112.00
30	V	238	PRO	CA-N-CD	-5.54	104.25	112.00
31	Z	758	PRO	CA-N-CD	-5.53	104.26	112.00
29	U	463	PRO	CA-N-CD	-5.53	104.26	112.00
11	Q	819	ASP	CA-C-N	5.50	127.58	120.44
11	Q	819	ASP	C-N-CA	5.50	127.58	120.44
22	B	897	ARG	NE-CZ-NH2	5.43	124.08	119.20
21	A	364	ARG	NE-CZ-NH2	5.42	124.08	119.20
29	U	492	ARG	C-N-CD	-5.28	103.37	125.00
24	M	1059	HIS	CA-C-N	5.27	126.43	119.84
24	M	1059	HIS	C-N-CA	5.27	126.43	119.84
16	e	75	ALA	N-CA-C	5.21	116.96	111.28
24	M	1138	ARG	NE-CZ-NH2	5.21	123.89	119.20
11	Q	823	GLN	CA-C-N	5.09	127.06	120.44
11	Q	823	GLN	C-N-CA	5.09	127.06	120.44
11	Q	817	CYS	CA-C-N	5.06	127.33	120.65
11	Q	817	CYS	C-N-CA	5.06	127.33	120.65
11	Q	822	SER	CA-C-N	5.05	127.05	120.28
11	Q	822	SER	C-N-CA	5.05	127.05	120.28
11	Q	820	LEU	CA-C-N	5.04	126.99	120.44
11	Q	820	LEU	C-N-CA	5.04	126.99	120.44

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	M	1098	ARG	Sidechain
24	M	462	ASP	Mainchain
24	M	471	TYR	Mainchain
24	M	572	ASP	Mainchain
10	P	39	A	Sidechain
10	P	42	C	Sidechain
12	T	30	DG	Sidechain
12	T	34	DT	Sidechain
12	T	54	DT	Sidechain
12	T	56	DA	Sidechain
14	X	232	ARG	Sidechain
18	g	40	SER	Mainchain
19	h	87	SER	Mainchain

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	D	1004	0	980	29	0
2	E	1721	0	1737	21	0
3	F	627	0	657	8	0
4	G	1333	0	1321	41	0
5	H	1198	0	1156	32	0
6	I	950	0	880	6	0
7	J	524	0	541	8	0
8	K	920	0	942	7	0
9	L	398	0	404	14	0
10	P	452	0	230	3	0
11	Q	7240	0	7186	37	0
12	T	3564	0	1963	22	0
13	W	2373	0	2290	9	0
14	X	434	0	443	7	0
15	Y	912	0	907	15	0
16	a	821	0	862	9	0
16	e	782	0	818	5	0
17	b	622	0	660	4	0
17	f	622	0	660	1	0
18	c	801	0	853	4	0
18	g	796	0	848	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	d	719	0	738	3	0
19	h	693	0	707	37	0
20	k	138	0	106	33	0
21	A	11015	0	11171	115	0
22	B	8964	0	9013	90	0
23	C	2072	0	2019	20	0
24	M	6687	0	6646	515	0
25	N	3390	0	1837	33	0
26	O	2131	0	2071	93	0
27	R	1836	0	1699	71	0
28	S	909	0	919	14	0
29	U	751	0	633	15	0
30	V	1687	0	1425	20	0
31	Z	4025	0	4041	79	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	Y	1	0	0	0	0
33	A	1	0	0	0	0
All	All	73121	0	69363	1238	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 9.

All (1238) 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)
24:M:1100:LYS:HB3	26:O:2033:LYS:CA	1.33	1.58
25:N:156:DG:C2'	25:N:157:DT:H71	1.35	1.56
27:R:504:LYS:HG3	27:R:507:PRO:CG	1.36	1.53
24:M:1107:PHE:CE1	26:O:2025:ILE:HG12	1.43	1.52
27:R:504:LYS:HZ3	27:R:507:PRO:CD	1.31	1.41
24:M:1107:PHE:CD1	26:O:2025:ILE:HG12	1.53	1.41
27:R:504:LYS:CG	27:R:507:PRO:HG2	1.53	1.37
27:R:504:LYS:NZ	27:R:507:PRO:HD3	1.39	1.36
30:V:236:PHE:C	30:V:238:PRO:HD2	1.50	1.36
24:M:1100:LYS:HB3	26:O:2033:LYS:C	1.15	1.35
24:M:1107:PHE:CE1	26:O:2025:ILE:CG1	2.10	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:504:LYS:NZ	27:R:507:PRO:CD	1.90	1.31
24:M:1078:GLU:CG	26:O:2024:ARG:HG3	1.60	1.31
24:M:1100:LYS:CB	26:O:2033:LYS:CA	2.07	1.29
24:M:1078:GLU:HG3	26:O:2024:ARG:CG	1.60	1.29
24:M:1100:LYS:CB	26:O:2033:LYS:C	1.95	1.28
24:M:1078:GLU:OE1	26:O:2022:VAL:CG1	1.79	1.28
24:M:1100:LYS:CB	26:O:2033:LYS:HA	1.63	1.28
25:N:156:DG:H2'	25:N:157:DT:C7	1.64	1.26
25:N:156:DG:C2'	25:N:157:DT:C7	2.13	1.26
18:g:45:ALA:O	18:g:48:PRO:HD2	1.45	1.17
19:h:54:ILE:O	20:k:947:THR:CG2	1.94	1.16
24:M:1078:GLU:OE1	26:O:2022:VAL:HG12	0.99	1.14
24:M:1107:PHE:CE1	26:O:2025:ILE:CD1	2.31	1.13
24:M:1078:GLU:CD	26:O:2024:ARG:HG3	1.73	1.12
24:M:1101:ASP:O	26:O:2029:SER:OG	1.66	1.12
19:h:54:ILE:O	20:k:947:THR:HG23	0.97	1.12
24:M:1100:LYS:HB3	26:O:2033:LYS:HA	1.16	1.10
19:h:55:SER:HA	20:k:947:THR:HA	1.09	1.08
24:M:1100:LYS:C	26:O:2033:LYS:HA	1.80	1.07
24:M:1078:GLU:HG3	26:O:2024:ARG:HG3	1.11	1.06
27:R:504:LYS:HZ3	27:R:507:PRO:HD2	1.21	1.06
24:M:1107:PHE:CD1	26:O:2025:ILE:CG1	2.36	1.05
9:L:22:CYS:SG	9:L:41:TYR:CE1	2.50	1.04
19:h:55:SER:CA	20:k:947:THR:HA	1.88	1.04
25:N:156:DG:H2'	25:N:157:DT:C7	1.90	1.01
27:R:504:LYS:CG	27:R:507:PRO:CG	2.21	1.00
24:M:618:ILE:HD12	24:M:640:LEU:HD12	1.45	0.99
25:N:156:DG:H2'	25:N:157:DT:H71	1.42	0.99
24:M:1103:ASP:HB2	26:O:2029:SER:HB3	1.41	0.98
11:Q:772:GLU:O	11:Q:830:ARG:CZ	2.12	0.98
29:U:461:LYS:O	29:U:463:PRO:CD	2.12	0.98
24:M:1078:GLU:HB3	26:O:2022:VAL:HG13	1.47	0.97
27:R:504:LYS:NZ	27:R:507:PRO:CG	2.28	0.97
30:V:236:PHE:C	30:V:238:PRO:CD	2.37	0.96
27:R:504:LYS:HZ2	27:R:507:PRO:HG3	1.30	0.96
24:M:1100:LYS:HB2	26:O:2033:LYS:HB2	1.48	0.96
24:M:1072:ASP:CG	26:O:2025:ILE:H	1.62	0.96
29:U:461:LYS:O	29:U:463:PRO:HD3	1.65	0.96
24:M:1078:GLU:H	26:O:2024:ARG:HE	1.08	0.95
24:M:1102:LEU:HD11	26:O:2025:ILE:CG2	1.96	0.95
24:M:618:ILE:HG12	24:M:667:THR:HG22	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:h:55:SER:HA	20:k:947:THR:CA	1.98	0.93
24:M:469:LEU:HD22	24:M:598:ARG:HG3	1.49	0.93
27:R:387:VAL:HG13	27:R:405:ILE:HD11	1.51	0.93
27:R:504:LYS:HZ2	27:R:507:PRO:CG	1.81	0.92
24:M:1102:LEU:HD11	26:O:2025:ILE:HG21	1.53	0.91
24:M:1107:PHE:CE1	26:O:2025:ILE:HD11	2.03	0.91
18:g:34:LEU:HD13	18:g:43:VAL:HG11	1.54	0.90
30:V:257:ALA:HB3	30:V:258:PRO:HD2	1.52	0.89
24:M:1107:PHE:HE1	26:O:2025:ILE:CG1	1.73	0.89
24:M:1107:PHE:HE1	26:O:2025:ILE:HG12	1.25	0.89
19:h:57:LYS:HB2	20:k:945:ASP:OD2	1.72	0.89
8:K:77:THR:OG1	8:K:81:TYR:O	1.89	0.88
24:M:606:LEU:HD23	24:M:721:LEU:HB3	1.56	0.87
24:M:301:ARG:HD2	24:M:401:GLU:HG2	1.55	0.87
24:M:320:ILE:HD12	24:M:363:LEU:HD11	1.55	0.87
24:M:550:LEU:HD22	24:M:689:ILE:HD12	1.55	0.87
24:M:1072:ASP:CG	26:O:2025:ILE:N	2.22	0.87
18:g:31:HIS:CD2	18:g:35:ARG:HH11	1.94	0.86
27:R:504:LYS:HZ2	27:R:507:PRO:HD3	1.40	0.86
22:B:953:ASP:OD1	23:C:36:ARG:NH1	2.08	0.86
19:h:59:MET:HG2	20:k:948:PHE:CG	2.11	0.85
24:M:1103:ASP:HB2	26:O:2029:SER:CB	2.06	0.85
27:R:504:LYS:CD	27:R:507:PRO:HG3	2.06	0.85
24:M:1100:LYS:CA	26:O:2033:LYS:HA	2.05	0.85
24:M:316:GLU:OE2	24:M:367:ARG:NH2	2.10	0.85
4:G:132:ASP:O	24:M:416:LEU:HB2	1.77	0.84
24:M:1103:ASP:CB	26:O:2029:SER:HB3	2.07	0.84
24:M:851:ALA:HB2	24:M:916:LEU:HD11	1.59	0.84
18:g:77:ARG:NH1	20:k:947:THR:OG1	2.09	0.84
19:h:56:SER:N	20:k:946:GLU:O	2.10	0.84
24:M:850:VAL:HG13	24:M:860:LEU:HD23	1.59	0.84
24:M:1101:ASP:OD1	26:O:2033:LYS:HB3	1.78	0.83
30:V:237:LEU:N	30:V:238:PRO:HD2	1.91	0.83
24:M:1078:GLU:CG	26:O:2024:ARG:CG	2.37	0.83
24:M:561:GLN:NE2	24:M:697:GLU:OE2	2.12	0.83
24:M:1078:GLU:HG3	26:O:2024:ARG:HG2	1.59	0.83
2:E:55:ARG:O	2:E:56:THR:OG1	1.98	0.82
22:B:765:GLU:OE1	22:B:770:ARG:NE	2.13	0.82
24:M:1100:LYS:HB2	26:O:2033:LYS:CB	2.09	0.82
24:M:1107:PHE:HD1	26:O:2025:ILE:HG12	1.43	0.82
15:Y:93:LEU:HD22	15:Y:97:ILE:HD11	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:810:ARG:HG2	24:M:812:PRO:HD3	1.58	0.82
29:U:450:LEU:HD21	29:U:452:LEU:HD23	1.61	0.81
24:M:784:ILE:HG21	24:M:860:LEU:HD21	1.61	0.81
24:M:471:TYR:O	24:M:473:ARG:N	1.99	0.81
18:g:45:ALA:O	18:g:47:ALA:N	2.14	0.81
22:B:387:HIS:NE2	22:B:671:GLU:OE2	2.14	0.81
24:M:1107:PHE:CZ	26:O:2025:ILE:HD11	2.16	0.81
24:M:1100:LYS:HB2	26:O:2033:LYS:CA	2.11	0.80
12:T:40:DG:C2	25:N:159:DG:C2	2.69	0.80
24:M:1150:PHE:O	24:M:1154:THR:OG1	1.99	0.80
22:B:613:ARG:NH2	22:B:615:TYR:OH	2.14	0.80
24:M:1103:ASP:N	26:O:2029:SER:HB3	1.97	0.80
31:Z:554:GLU:OE2	31:Z:559:GLN:NE2	2.14	0.80
29:U:461:LYS:O	29:U:463:PRO:HD2	1.81	0.79
18:g:42:ARG:HH22	25:N:38:DG:H4'	1.46	0.79
25:N:154:DC:H2''	25:N:155:DT:C6	2.18	0.79
27:R:405:ILE:HG23	27:R:426:LEU:HD11	1.63	0.79
5:H:8:ASP:OD2	5:H:32:SER:OG	2.00	0.79
19:h:42:TYR:OH	20:k:948:PHE:O	2.01	0.79
24:M:1258:LYS:HA	24:M:1258:LYS:HE2	1.63	0.79
11:Q:774:SER:O	11:Q:830:ARG:NH1	2.11	0.78
22:B:169:ARG:NH1	30:V:139:THR:O	2.16	0.78
24:M:413:LEU:HD12	24:M:460:LEU:HD11	1.65	0.78
24:M:552:ASP:OD2	24:M:556:ARG:NE	2.17	0.78
30:V:236:PHE:O	30:V:238:PRO:HD2	1.82	0.78
15:Y:75:GLN:O	15:Y:111:ARG:NH2	2.15	0.78
18:g:45:ALA:C	18:g:47:ALA:H	1.92	0.78
24:M:1241:PRO:HG2	24:M:1244:PHE:HD1	1.47	0.77
18:g:42:ARG:HB3	19:h:87:SER:O	1.85	0.77
25:N:156:DG:H2''	25:N:157:DT:H71	0.77	0.76
30:V:236:PHE:O	30:V:238:PRO:CD	2.31	0.76
24:M:475:ILE:HG13	24:M:476:PRO:HD3	1.68	0.76
24:M:859:MET:O	24:M:862:GLU:HG3	1.86	0.76
24:M:1069:MET:HA	26:O:2025:ILE:CD1	2.16	0.76
27:R:504:LYS:NZ	27:R:507:PRO:HG3	1.92	0.76
5:H:37:MET:HE2	5:H:127:GLY:HA3	1.67	0.76
19:h:38:SER:OG	20:k:948:PHE:CD2	2.37	0.76
24:M:1110:GLU:HG2	26:O:2023:TYR:CE1	2.19	0.76
24:M:1100:LYS:HG2	26:O:2034:GLU:HB3	1.65	0.76
24:M:1103:ASP:HB2	26:O:2029:SER:CA	2.16	0.76
31:Z:282:LYS:O	31:Z:287:LYS:NZ	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:462:ASP:O	24:M:463:VAL:C	2.26	0.75
24:M:1078:GLU:H	26:O:2024:ARG:NE	1.84	0.75
24:M:1103:ASP:CA	26:O:2029:SER:HB3	2.17	0.75
29:U:376:VAL:HG13	29:U:493:PRO:HB2	1.69	0.74
8:K:41:THR:OG1	23:C:36:ARG:NH2	2.20	0.74
24:M:792:HIS:HE1	24:M:909:VAL:HG21	1.53	0.74
9:L:22:CYS:SG	9:L:41:TYR:CD1	2.76	0.74
2:E:162:ARG:NH1	21:A:1024:ASN:O	2.21	0.73
24:M:455:GLN:N	24:M:459:GLU:OE2	2.19	0.73
24:M:1102:LEU:HD11	26:O:2025:ILE:HG22	1.70	0.73
5:H:128:ASP:OD1	5:H:131:ASN:ND2	2.20	0.73
22:B:228:SER:O	22:B:405:ARG:NH2	2.20	0.73
24:M:574:VAL:HG23	24:M:578:PHE:O	1.89	0.73
24:M:324:ALA:HB1	24:M:395:ARG:HE	1.52	0.73
24:M:1078:GLU:HB3	26:O:2022:VAL:CG1	2.17	0.73
24:M:1167:ILE:HD12	24:M:1232:LEU:HD11	1.70	0.73
21:A:197:GLU:HB2	21:A:215:LEU:HD11	1.71	0.73
24:M:1103:ASP:HB2	26:O:2029:SER:HA	1.71	0.73
24:M:313:LEU:HG	24:M:360:LYS:HD2	1.69	0.72
21:A:299:ALA:HB3	21:A:302:VAL:HG12	1.71	0.72
18:g:40:SER:C	18:g:42:ARG:H	1.96	0.72
24:M:330:ILE:HG22	24:M:648:LEU:HB2	1.71	0.72
25:N:156:DG:H2'	25:N:157:DT:H73	1.71	0.72
1:D:108:ALA:N	1:D:128:GLN:OE1	2.22	0.72
1:D:123:GLU:N	1:D:123:GLU:OE1	2.22	0.72
27:R:504:LYS:CG	27:R:507:PRO:HG3	2.15	0.71
24:M:693:TYR:HB3	24:M:713:ILE:HD11	1.72	0.71
24:M:551:ARG:HD3	24:M:601:LEU:HD11	1.72	0.71
4:G:93:ASN:O	4:G:128:TYR:OH	2.09	0.71
9:L:57:ALA:O	23:C:175:LYS:NZ	2.18	0.71
10:P:28:A:OP2	24:M:790:ARG:NH2	2.23	0.71
27:R:388:ARG:NH2	27:R:446:GLU:O	2.23	0.70
24:M:693:TYR:CD2	24:M:709:ARG:HB3	2.27	0.70
24:M:1078:GLU:N	26:O:2024:ARG:HE	1.86	0.70
24:M:1100:LYS:CB	26:O:2033:LYS:CB	2.67	0.70
24:M:1110:GLU:HG2	26:O:2023:TYR:CZ	2.26	0.70
24:M:784:ILE:HG13	24:M:796:CYS:HB3	1.72	0.70
24:M:833:ILE:HG23	24:M:867:ILE:HD11	1.74	0.70
26:O:1679:ARG:HH12	26:O:1683:ARG:HH11	1.38	0.70
24:M:1078:GLU:CB	26:O:2022:VAL:CG1	2.70	0.70
24:M:1100:LYS:O	26:O:2033:LYS:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:HG21	4:G:2:PHE:CD2	2.26	0.70
24:M:1165:LYS:HE3	24:M:1167:ILE:CG2	2.22	0.70
24:M:582:GLU:N	24:M:582:GLU:OE1	2.25	0.70
30:V:257:ALA:HB3	30:V:258:PRO:CD	2.20	0.70
31:Z:426:VAL:HG13	31:Z:440:ILE:HD11	1.74	0.70
24:M:1078:GLU:CB	26:O:2022:VAL:HG13	2.22	0.69
24:M:784:ILE:CG2	24:M:860:LEU:HD21	2.22	0.69
19:h:38:SER:OG	20:k:948:PHE:CE2	2.42	0.69
24:M:541:LEU:HB3	24:M:693:TYR:HE1	1.57	0.69
31:Z:478:VAL:HG21	31:Z:502:LEU:HD22	1.74	0.69
21:A:1038:THR:O	21:A:1042:ASN:ND2	2.25	0.69
15:Y:3:LEU:O	15:Y:8:LYS:NZ	2.25	0.69
22:B:783:ALA:O	22:B:789:ASN:ND2	2.26	0.69
24:M:574:VAL:HG23	24:M:579:PRO:HA	1.74	0.69
24:M:448:MET:HA	24:M:452:LYS:HD3	1.73	0.68
24:M:617:ASN:HB2	24:M:668:ASP:OD1	1.93	0.68
24:M:870:GLU:OE1	24:M:870:GLU:N	2.26	0.68
23:C:193:ARG:NH1	23:C:218:ALA:O	2.26	0.68
9:L:16:ILE:HD11	9:L:25:GLU:HB3	1.76	0.68
21:A:54:LEU:O	21:A:61:ARG:NH1	2.26	0.68
24:M:808:PHE:HB2	24:M:910:LEU:HD21	1.75	0.68
31:Z:563:MET:HA	31:Z:637:VAL:HG11	1.76	0.68
22:B:237:VAL:HG11	22:B:369:VAL:HG22	1.76	0.68
24:M:781:VAL:HG11	24:M:920:ILE:CG2	2.24	0.68
11:Q:856:LEU:HD23	11:Q:857:LEU:HD22	1.76	0.68
22:B:59:VAL:HG23	22:B:408:PHE:CZ	2.29	0.68
24:M:330:ILE:HG12	24:M:736:GLU:OE1	1.95	0.67
24:M:570:ALA:O	24:M:574:VAL:HG12	1.93	0.67
21:A:112:PHE:N	21:A:188:GLN:OE1	2.27	0.67
22:B:756:LYS:NZ	30:V:134:THR:OG1	2.27	0.67
19:h:56:SER:HA	20:k:948:PHE:HB2	1.76	0.67
24:M:1072:ASP:HB2	26:O:2025:ILE:HD12	1.75	0.67
31:Z:478:VAL:HB	31:Z:518:LEU:HD11	1.77	0.67
5:H:2:ALA:O	5:H:84:ARG:NH1	2.28	0.67
22:B:565:THR:HG21	22:B:580:PRO:HB3	1.77	0.67
24:M:621:THR:O	24:M:625:ARG:HD3	1.93	0.67
24:M:624:GLY:HA2	24:M:664:LEU:HB2	1.77	0.67
27:R:504:LYS:HG3	27:R:507:PRO:CD	2.19	0.67
22:B:591:ARG:HE	22:B:603:MET:HE1	1.60	0.66
23:C:31:ALA:O	23:C:231:TYR:OH	2.12	0.66
24:M:313:LEU:HD23	24:M:360:LYS:HE2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:608:GLN:HG2	24:M:612:GLU:OE1	1.94	0.66
24:M:693:TYR:CB	24:M:713:ILE:HD11	2.25	0.66
29:U:378:LEU:HD23	29:U:382:LEU:O	1.95	0.66
22:B:854:ILE:HD11	22:B:858:VAL:HG11	1.76	0.66
24:M:581:PRO:O	24:M:584:VAL:HG12	1.95	0.66
24:M:781:VAL:HG11	24:M:920:ILE:HG21	1.77	0.66
18:g:45:ALA:C	18:g:47:ALA:N	2.49	0.66
24:M:541:LEU:HD22	24:M:693:TYR:HD1	1.60	0.66
31:Z:353:ALA:HB3	31:Z:360:ILE:HB	1.77	0.66
24:M:321:TYR:HB2	24:M:359:ILE:HD12	1.77	0.66
24:M:618:ILE:HG23	24:M:665:LEU:HD21	1.77	0.66
25:N:156:DG:H2"	25:N:157:DT:C5	2.29	0.66
27:R:505:ALA:HB3	27:R:506:PRO:CD	2.24	0.66
31:Z:519:GLN:NE2	31:Z:521:CYS:SG	2.68	0.66
18:g:44:GLY:N	19:h:89:ILE:O	2.29	0.66
1:D:135:GLN:OE1	1:D:138:ARG:NH2	2.29	0.66
4:G:152:VAL:HG22	4:G:157:ILE:HG22	1.78	0.66
24:M:301:ARG:NH1	24:M:305:VAL:HG22	2.10	0.66
24:M:330:ILE:HG13	24:M:332:LEU:CD2	2.25	0.66
24:M:565:GLU:N	24:M:565:GLU:OE1	2.29	0.66
24:M:462:ASP:OD2	24:M:607:ARG:NH1	2.27	0.66
12:T:45:DT:H2"	12:T:46:DG:C8	2.31	0.66
27:R:410:GLU:OE2	27:R:423:ASN:ND2	2.29	0.66
5:H:33:GLU:O	11:Q:684:TRP:HH2	1.78	0.65
31:Z:474:MET:HE2	31:Z:494:ARG:HA	1.78	0.65
18:g:34:LEU:HD13	18:g:43:VAL:CG1	2.26	0.65
24:M:301:ARG:HD2	24:M:401:GLU:CG	2.26	0.65
24:M:849:THR:HB	24:M:885:VAL:HG21	1.77	0.65
4:G:132:ASP:OD2	24:M:419:LYS:HE2	1.97	0.65
21:A:349:ARG:HE	22:B:1157:LEU:HD22	1.61	0.65
27:R:406:THR:OG1	27:R:427:GLN:O	2.14	0.65
31:Z:478:VAL:HG22	31:Z:490:GLY:O	1.95	0.65
2:E:2:ASP:OD1	2:E:3:ASP:N	2.30	0.65
24:M:409:ARG:HB3	24:M:460:LEU:HD21	1.79	0.65
24:M:650:ASP:HB2	24:M:740:TYR:CD2	2.31	0.65
24:M:926:GLU:O	24:M:930:VAL:HG12	1.96	0.65
24:M:959:TYR:O	24:M:963:ILE:HG13	1.95	0.65
7:J:64:PRO:O	9:L:23:HIS:NE2	2.30	0.65
31:Z:542:LEU:HD21	31:Z:560:VAL:HG11	1.79	0.65
2:E:96:GLU:OE1	2:E:96:GLU:N	2.30	0.64
24:M:541:LEU:HB3	24:M:693:TYR:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:192:THR:HG23	31:Z:245:LEU:HD21	1.79	0.64
31:Z:525:ALA:HB1	31:Z:552:ARG:HH12	1.63	0.64
12:T:76:DG:H1	25:N:122:DC:H42	1.43	0.64
27:R:366:ARG:NH2	31:Z:775:TPO:OG1	2.30	0.64
18:g:35:ARG:HB2	18:g:35:ARG:CZ	2.27	0.64
9:L:19:CYS:SG	9:L:20:GLY:N	2.71	0.64
11:Q:674:ARG:HG2	11:Q:674:ARG:HH21	1.62	0.64
23:C:131:THR:HG22	23:C:147:ASP:OD1	1.98	0.64
24:M:287:ASN:O	24:M:290:ARG:HG2	1.98	0.64
30:V:236:PHE:O	30:V:238:PRO:HD3	1.98	0.64
31:Z:184:CYS:SG	31:Z:185:LYS:N	2.71	0.64
27:R:485:TYR:OH	27:R:489:ASP:OD2	2.14	0.64
4:G:132:ASP:CG	24:M:416:LEU:HA	2.22	0.64
11:Q:769:LEU:HD22	11:Q:824:ALA:HB2	1.79	0.64
12:T:20:DC:H2"	12:T:21:DT:H71	1.79	0.64
21:A:296:ASN:OD1	21:A:297:GLY:N	2.31	0.63
24:M:851:ALA:HB2	24:M:916:LEU:CD1	2.25	0.63
7:J:57:GLU:OE2	23:C:152:LYS:NZ	2.22	0.63
21:A:767:LYS:O	21:A:771:VAL:HG22	1.98	0.63
24:M:541:LEU:HD22	24:M:693:TYR:CD1	2.33	0.63
11:Q:772:GLU:HG2	11:Q:827:HIS:CE1	2.34	0.63
24:M:392:ASP:O	24:M:396:VAL:HG23	1.99	0.63
24:M:450:ARG:O	24:M:454:VAL:HG23	1.98	0.63
31:Z:728:THR:O	31:Z:747:ARG:NH2	2.32	0.63
16:a:60:LEU:HD11	16:a:90:MET:HE1	1.79	0.63
24:M:899:SER:HB2	24:M:911:ARG:HD3	1.81	0.63
24:M:749:LEU:HD22	24:M:958:LEU:HD22	1.81	0.63
27:R:504:LYS:HG3	27:R:507:PRO:HG2	0.65	0.63
1:D:107:THR:HG23	1:D:110:GLU:H	1.64	0.63
15:Y:4:GLU:O	15:Y:27:GLN:NE2	2.32	0.62
21:A:120:ASP:O	21:A:122:ASN:ND2	2.32	0.62
5:H:9:ILE:HD12	5:H:148:LEU:HD11	1.80	0.62
24:M:714:GLU:O	24:M:718:GLN:HG2	1.98	0.62
27:R:504:LYS:HD3	27:R:507:PRO:HG3	1.79	0.62
31:Z:505:ASP:OD2	31:Z:525:ALA:HB2	1.98	0.62
22:B:817:GLN:N	22:B:817:GLN:OE1	2.32	0.62
24:M:1269:LYS:HB3	24:M:1278:ASP:HB2	1.80	0.62
18:g:34:LEU:CD1	18:g:43:VAL:HG11	2.29	0.62
24:M:469:LEU:HD22	24:M:598:ARG:CG	2.27	0.62
31:Z:279:VAL:HA	31:Z:386:VAL:HG21	1.82	0.62
19:h:59:MET:CB	20:k:948:PHE:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:618:ILE:HG12	24:M:667:THR:CG2	2.26	0.62
24:M:644:PRO:HG2	24:M:647:GLU:HG3	1.82	0.62
24:M:1271:ASP:HB3	24:M:1276:SER:HB2	1.80	0.62
24:M:1162:TYR:HB3	24:M:1165:LYS:HB2	1.82	0.62
24:M:865:LYS:O	24:M:869:HIS:ND1	2.24	0.61
27:R:359:LEU:HD11	27:R:386:PHE:CE2	2.35	0.61
21:A:487:SER:OG	21:A:673:GLN:NE2	2.34	0.61
10:P:46:U:O2'	21:A:499:ASP:OD2	2.18	0.61
4:G:36:GLY:O	31:Z:628:LYS:NZ	2.26	0.61
24:M:416:LEU:HD21	24:M:467:PHE:CE2	2.35	0.61
24:M:1169:CYS:HB3	24:M:1232:LEU:HD13	1.80	0.61
24:M:940:LEU:HD12	24:M:940:LEU:H	1.65	0.61
12:T:44:DG:H2''	12:T:45:DT:H5''	1.82	0.61
24:M:542:THR:OG1	24:M:543:PRO:HD2	2.00	0.61
24:M:610:PHE:O	24:M:614:ALA:HB2	2.01	0.61
24:M:1245:LEU:CD2	24:M:1247:ASP:HB2	2.31	0.61
24:M:373:VAL:HG13	24:M:393:LEU:HB2	1.82	0.61
4:G:132:ASP:CG	24:M:419:LYS:HE2	2.26	0.61
24:M:541:LEU:HD21	24:M:546:PHE:HA	1.83	0.61
6:I:103:ARG:NH1	6:I:105:GLU:OE2	2.34	0.60
24:M:951:LYS:O	24:M:955:LEU:HD23	2.00	0.60
4:G:147:ILE:HG23	4:G:159:ALA:HB1	1.82	0.60
24:M:828:LYS:O	24:M:831:GLN:HG2	2.01	0.60
27:R:455:TRP:CD1	27:R:459:MET:HE3	2.36	0.60
31:Z:192:THR:OG1	31:Z:244:ASN:ND2	2.34	0.60
22:B:179:LEU:HD22	22:B:768:ARG:HD3	1.82	0.60
24:M:1078:GLU:CD	26:O:2024:ARG:CG	2.63	0.60
5:H:150:PHE:HD1	14:X:241:THR:CB	2.14	0.60
21:A:67:ARG:O	21:A:68:THR:OG1	2.16	0.60
31:Z:554:GLU:OE1	31:Z:557:THR:OG1	2.19	0.60
5:H:69:THR:OG1	5:H:81:ARG:NH1	2.32	0.60
24:M:580:THR:O	24:M:582:GLU:N	2.34	0.60
24:M:860:LEU:O	24:M:864:VAL:HG23	2.01	0.60
24:M:1228:VAL:HG23	24:M:1245:LEU:HD12	1.83	0.60
24:M:372:GLU:OE1	24:M:991:GLY:N	2.27	0.60
27:R:504:LYS:CD	27:R:507:PRO:CG	2.69	0.60
24:M:622:LYS:HA	24:M:625:ARG:HE	1.67	0.60
27:R:506:PRO:N	27:R:507:PRO:HD2	2.17	0.60
31:Z:539:LEU:HD22	31:Z:616:HIS:HB3	1.83	0.60
19:h:55:SER:C	20:k:947:THR:HA	2.26	0.60
24:M:734:LEU:HD11	24:M:738:LYS:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:MET:O	1:D:66:ASN:ND2	2.34	0.60
24:M:606:LEU:CD2	24:M:721:LEU:HB3	2.29	0.60
24:M:792:HIS:CE1	24:M:909:VAL:HG21	2.36	0.60
29:U:375:PHE:O	29:U:493:PRO:HG2	2.02	0.60
1:D:59:GLU:OE1	1:D:59:GLU:N	2.34	0.59
18:g:42:ARG:NH2	25:N:38:DG:H4'	2.17	0.59
5:H:33:GLU:HB3	11:Q:674:ARG:HH12	1.66	0.59
24:M:384:VAL:HB	24:M:388:LEU:HB2	1.83	0.59
5:H:7:GLU:HG2	5:H:59:VAL:HG22	1.84	0.59
24:M:413:LEU:HD12	24:M:460:LEU:CD1	2.31	0.59
24:M:824:GLU:HG3	24:M:825:GLU:H	1.67	0.59
24:M:995:ARG:H	24:M:995:ARG:HD2	1.66	0.59
24:M:1240:ILE:HD13	24:M:1281:CYS:SG	2.42	0.59
27:R:569:GLU:O	27:R:573:VAL:HG23	2.01	0.59
24:M:857:ALA:O	24:M:861:ILE:HG23	2.02	0.59
24:M:886:ASP:HA	24:M:1152:MET:SD	2.43	0.59
31:Z:542:LEU:HD22	31:Z:570:VAL:HG11	1.83	0.59
22:B:939:HIS:NE2	22:B:983:GLU:OE1	2.30	0.59
24:M:917:ALA:O	24:M:921:GLN:HG3	2.01	0.59
24:M:589:ARG:HD3	24:M:708:GLN:OE1	2.02	0.59
24:M:1145:ASN:HB3	24:M:1148:GLU:OE1	2.02	0.59
24:M:1278:ASP:OD1	24:M:1279:LEU:N	2.36	0.59
31:Z:745:VAL:HG11	31:Z:750:LEU:HD21	1.83	0.59
24:M:628:VAL:HG13	24:M:632:HIS:HB3	1.83	0.59
24:M:1171:VAL:HG12	24:M:1261:MET:O	2.03	0.59
29:U:450:LEU:CD2	29:U:452:LEU:HD23	2.32	0.59
21:A:955:GLU:OE1	21:A:1010:VAL:HG22	2.03	0.58
4:G:134:ASP:O	24:M:464:TYR:OH	2.20	0.58
6:I:31:GLU:N	6:I:31:GLU:OE1	2.37	0.58
12:T:9:DC:H2'	12:T:10:DT:H71	1.85	0.58
21:A:110:VAL:HG11	21:A:228:ILE:HD11	1.85	0.58
21:A:419:ILE:HG23	21:A:427:ILE:HB	1.84	0.58
24:M:685:TYR:CZ	24:M:689:ILE:HD11	2.38	0.58
22:B:1009:GLN:NE2	22:B:1013:ASN:OD1	2.35	0.58
23:C:56:SER:OG	23:C:158:GLU:N	2.34	0.58
24:M:648:LEU:HD13	24:M:653:PHE:HB2	1.85	0.58
1:D:114:LEU:HD21	4:G:167:TYR:HB2	1.84	0.58
24:M:783:GLY:O	24:M:913:ALA:HB1	2.03	0.58
28:S:194:ARG:NH2	28:S:226:GLU:OE1	2.35	0.58
22:B:411:LEU:HD12	22:B:411:LEU:C	2.27	0.58
24:M:574:VAL:CG2	24:M:579:PRO:HA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:589:ARG:HD2	24:M:711:MET:HG3	1.86	0.58
24:M:1167:ILE:HD12	24:M:1232:LEU:CD1	2.32	0.58
22:B:207:VAL:HG11	22:B:375:ALA:CB	2.33	0.58
24:M:734:LEU:O	24:M:738:LYS:HG2	2.04	0.58
5:H:150:PHE:O	14:X:241:THR:N	2.36	0.58
22:B:177:CYS:SG	22:B:737:ILE:HD11	2.43	0.58
24:M:1100:LYS:HG2	26:O:2034:GLU:CB	2.32	0.58
13:W:80:ALA:HB1	13:W:112:LEU:HD21	1.84	0.58
5:H:150:PHE:HD1	14:X:241:THR:OG1	1.87	0.57
24:M:406:LEU:CA	24:M:457:MET:HE1	2.34	0.57
24:M:570:ALA:HB2	24:M:585:LEU:CD2	2.34	0.57
31:Z:424:ASP:HB2	31:Z:440:ILE:HD12	1.85	0.57
24:M:889:LEU:HG	24:M:930:VAL:HG11	1.87	0.57
24:M:738:LYS:O	24:M:742:ILE:HG13	2.04	0.57
24:M:1230:THR:O	24:M:1238:GLY:N	2.33	0.57
16:e:86:SER:O	16:e:90:MET:HG2	2.04	0.57
24:M:650:ASP:HB2	24:M:740:TYR:CG	2.40	0.57
24:M:850:VAL:CG1	24:M:860:LEU:HD23	2.32	0.57
31:Z:523:GLU:N	31:Z:523:GLU:OE1	2.37	0.57
13:W:36:VAL:HG23	13:W:72:ILE:HD11	1.85	0.57
15:Y:14:ARG:NH2	31:Z:300:GLN:OE1	2.38	0.57
15:Y:48:MET:HE3	15:Y:48:MET:HA	1.86	0.57
30:V:257:ALA:CB	30:V:258:PRO:CD	2.82	0.57
24:M:785:ALA:O	24:M:794:VAL:HG13	2.03	0.57
31:Z:492:ILE:HG22	31:Z:502:LEU:HB3	1.85	0.57
18:g:40:SER:C	18:g:42:ARG:N	2.56	0.57
19:h:88:THR:OG1	19:h:89:ILE:N	2.36	0.57
21:A:120:ASP:O	21:A:122:ASN:N	2.37	0.57
24:M:410:LYS:HE3	24:M:451:LEU:O	2.04	0.57
24:M:450:ARG:NH2	24:M:600:PRO:HG2	2.19	0.57
24:M:687:GLU:OE1	24:M:690:LYS:HD3	2.05	0.57
24:M:1107:PHE:CD1	26:O:2025:ILE:CD1	2.82	0.57
27:R:575:SER:O	27:R:579:LEU:HD13	2.04	0.57
22:B:177:CYS:SG	22:B:180:ASP:N	2.78	0.57
24:M:641:LYS:NZ	24:M:642:ASN:OD1	2.37	0.57
26:O:1602:LYS:HE2	26:O:1699:TRP:HE1	1.69	0.57
24:M:573:TYR:HB2	24:M:584:VAL:HG21	1.87	0.57
24:M:1076:TYR:O	26:O:2024:ARG:NH1	2.30	0.57
24:M:1241:PRO:HD3	24:M:1278:ASP:OD1	2.04	0.57
24:M:717:LEU:HD23	24:M:721:LEU:HD12	1.87	0.56
24:M:1007:ASN:O	24:M:1009:THR:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:404:GLU:OE2	27:R:455:TRP:NE1	2.38	0.56
24:M:473:ARG:NE	24:M:473:ARG:HA	2.19	0.56
30:V:127:VAL:HG23	30:V:128:VAL:H	1.69	0.56
31:Z:188:GLU:O	31:Z:192:THR:OG1	2.20	0.56
24:M:650:ASP:HB2	24:M:740:TYR:CE2	2.41	0.56
24:M:687:GLU:O	24:M:690:LYS:HG2	2.05	0.56
27:R:577:LYS:O	27:R:580:VAL:HG22	2.05	0.56
30:V:237:LEU:N	30:V:238:PRO:CD	2.61	0.56
5:H:34:SER:O	11:Q:706:ASN:ND2	2.39	0.56
7:J:36:ASP:OD1	7:J:41:LYS:NZ	2.34	0.56
16:e:87:SER:OG	17:f:83:ALA:HB2	2.05	0.56
24:M:416:LEU:HD12	24:M:416:LEU:O	2.05	0.56
24:M:963:ILE:HA	24:M:988:TYR:HB3	1.88	0.56
26:O:1817:CYS:SG	26:O:1818:GLY:N	2.79	0.56
27:R:505:ALA:HB3	27:R:506:PRO:HD2	1.88	0.56
24:M:285:GLN:HA	24:M:288:GLU:OE2	2.06	0.56
24:M:544:GLU:HG3	24:M:599:GLU:OE2	2.06	0.56
24:M:811:LEU:HD21	24:M:832:ASP:HB3	1.87	0.56
24:M:1171:VAL:HG13	24:M:1260:GLY:H	1.70	0.56
24:M:1242:THR:HA	24:M:1245:LEU:HB3	1.88	0.56
19:h:56:SER:HB3	20:k:948:PHE:HA	1.88	0.56
21:A:110:VAL:HG11	21:A:228:ILE:CD1	2.36	0.56
24:M:1110:GLU:HG2	26:O:2023:TYR:OH	2.04	0.56
3:F:62:ARG:NH2	21:A:517:GLU:OE1	2.39	0.56
22:B:565:THR:HG22	22:B:577:HIS:O	2.06	0.56
24:M:999:HIS:O	24:M:1003:ILE:HG13	2.06	0.56
26:O:1633:ARG:HB2	26:O:1635:GLN:HE21	1.71	0.56
24:M:570:ALA:HB1	24:M:584:VAL:CG1	2.36	0.55
24:M:887:ASN:OD1	24:M:890:ALA:HB3	2.06	0.55
24:M:1245:LEU:HD11	24:M:1253:PRO:HG3	1.89	0.55
9:L:40:GLY:O	9:L:41:TYR:CG	2.59	0.55
31:Z:733:ARG:NH2	31:Z:744:SER:OG	2.38	0.55
5:H:150:PHE:CD1	14:X:241:THR:OG1	2.59	0.55
24:M:294:LEU:HB2	24:M:299:GLN:NE2	2.22	0.55
24:M:417:PHE:O	24:M:421:GLN:HG3	2.06	0.55
9:L:40:GLY:O	9:L:41:TYR:CD1	2.59	0.55
24:M:373:VAL:HG13	24:M:393:LEU:CB	2.37	0.55
24:M:541:LEU:HD11	24:M:549:ASN:ND2	2.21	0.55
24:M:653:PHE:HZ	24:M:730:LYS:HG3	1.71	0.55
24:M:1078:GLU:OE2	26:O:2024:ARG:HG3	2.05	0.55
31:Z:421:GLN:N	31:Z:421:GLN:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:623:LYS:HE2	31:Z:608:SER:CB	2.37	0.55
24:M:1107:PHE:CD1	26:O:2025:ILE:HG23	2.41	0.55
31:Z:478:VAL:HG11	31:Z:492:ILE:HG23	1.89	0.55
18:g:44:GLY:HA3	19:h:89:ILE:O	2.07	0.55
26:O:1653:CYS:SG	26:O:1672:ASN:ND2	2.80	0.55
31:Z:542:LEU:CD2	31:Z:560:VAL:HG11	2.36	0.55
4:G:170:LEU:CD2	24:M:473:ARG:HH12	2.20	0.55
22:B:388:TYR:CE1	22:B:505:LEU:HD21	2.42	0.55
27:R:504:LYS:HZ2	27:R:507:PRO:CD	1.84	0.55
4:G:46:ILE:HD11	4:G:77:PHE:HB2	1.89	0.55
15:Y:14:ARG:NH2	15:Y:55:SER:OG	2.39	0.55
24:M:652:GLN:O	24:M:656:ILE:HG13	2.06	0.55
24:M:783:GLY:O	24:M:796:CYS:HA	2.06	0.55
21:A:687:ILE:HD11	21:A:766:PHE:CZ	2.42	0.55
31:Z:206:THR:HG23	31:Z:208:THR:H	1.71	0.55
9:L:25:GLU:N	9:L:25:GLU:OE1	2.40	0.54
11:Q:772:GLU:HG2	11:Q:827:HIS:ND1	2.22	0.54
24:M:739:GLU:O	24:M:743:LYS:HG3	2.06	0.54
27:R:493:GLU:O	27:R:496:VAL:HG22	2.06	0.54
28:S:203:ASN:ND2	28:S:205:ASN:OD1	2.40	0.54
19:h:38:SER:CB	20:k:948:PHE:CE2	2.90	0.54
24:M:795:PHE:HE1	24:M:810:ARG:HG3	1.72	0.54
24:M:1069:MET:HA	26:O:2025:ILE:HD12	1.87	0.54
24:M:1076:TYR:O	26:O:2024:ARG:CZ	2.56	0.54
18:c:32:ARG:NH1	19:d:35:GLU:OE2	2.41	0.54
16:e:106:ASP:OD2	16:e:131:ARG:NH1	2.40	0.54
19:h:59:MET:HB3	20:k:948:PHE:HB2	1.89	0.54
21:A:869:GLU:OE2	21:A:1455:SER:OG	2.15	0.54
24:M:406:LEU:O	24:M:410:LYS:HG3	2.08	0.54
24:M:475:ILE:HG13	24:M:476:PRO:CD	2.37	0.54
21:A:733:LEU:O	21:A:736:THR:HG22	2.08	0.54
24:M:559:THR:O	24:M:695:ARG:NH1	2.40	0.54
23:C:48:ASP:OD1	23:C:175:LYS:NZ	2.38	0.54
24:M:858:GLN:O	24:M:861:ILE:HG12	2.08	0.54
24:M:1242:THR:O	24:M:1246:SER:N	2.28	0.54
15:Y:10:LEU:O	15:Y:13:LEU:HD22	2.08	0.54
21:A:100:LEU:HD23	21:A:193:ARG:HE	1.72	0.54
22:B:502:HIS:ND1	22:B:504:THR:HG22	2.22	0.54
24:M:917:ALA:O	24:M:920:ILE:HG22	2.07	0.54
24:M:417:PHE:HD2	24:M:443:LEU:HD13	1.72	0.54
31:Z:529:ASP:HB3	31:Z:553:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:133:GLU:O	24:M:416:LEU:HD22	2.08	0.54
17:b:45:ARG:HE	25:N:80:DC:H4'	1.73	0.54
24:M:550:LEU:HD22	24:M:689:ILE:CD1	2.33	0.54
4:G:46:ILE:HD11	4:G:77:PHE:CB	2.38	0.53
21:A:421:ARG:HE	21:A:427:ILE:HD11	1.73	0.53
24:M:285:GLN:HA	24:M:288:GLU:CD	2.33	0.53
24:M:1148:GLU:OE1	24:M:1148:GLU:N	2.40	0.53
27:R:504:LYS:HZ3	27:R:507:PRO:HD3	1.08	0.53
21:A:576:GLN:O	21:A:590:GLN:NE2	2.42	0.53
22:B:785:TYR:O	22:B:786:THR:HG22	2.08	0.53
24:M:303:ILE:HG21	24:M:404:THR:HG21	1.90	0.53
24:M:316:GLU:HB3	24:M:363:LEU:HD13	1.89	0.53
24:M:1107:PHE:CD1	26:O:2025:ILE:CG2	2.91	0.53
24:M:1270:ILE:HG22	24:M:1272:ILE:HG23	1.90	0.53
31:Z:433:LEU:HB3	31:Z:436:LEU:HD12	1.90	0.53
31:Z:470:LYS:NZ	31:Z:518:LEU:O	2.41	0.53
18:g:31:HIS:CG	18:g:35:ARG:HH11	2.26	0.53
18:g:77:ARG:HH11	20:k:947:THR:HG1	1.50	0.53
21:A:896:LEU:HD13	21:A:980:PRO:HG3	1.90	0.53
22:B:854:ILE:HG12	22:B:904:VAL:HG21	1.90	0.53
24:M:615:LYS:HB3	24:M:642:ASN:HA	1.89	0.53
24:M:837:LYS:HD3	24:M:867:ILE:HG23	1.91	0.53
31:Z:492:ILE:HD12	31:Z:495:VAL:CG1	2.37	0.53
5:H:63:THR:HG21	5:H:68:GLY:HA2	1.91	0.53
24:M:799:VAL:HA	24:M:805:VAL:HA	1.90	0.53
24:M:1062:THR:HG22	24:M:1065:TRP:CZ3	2.43	0.53
26:O:2027:LYS:O	26:O:2027:LYS:HG2	2.07	0.53
9:L:40:GLY:C	9:L:41:TYR:CD1	2.86	0.53
16:a:40:ARG:NH1	25:N:82:DT:O2	2.40	0.53
22:B:591:ARG:NE	22:B:603:MET:HE1	2.22	0.53
24:M:759:ARG:HD3	24:M:759:ARG:C	2.33	0.53
31:Z:450:ILE:HG23	31:Z:452:PRO:HD3	1.91	0.53
31:Z:504:SER:OG	31:Z:507:THR:O	2.21	0.53
24:M:406:LEU:HA	24:M:457:MET:HE1	1.91	0.53
26:O:1715:GLU:O	26:O:1759:ASN:ND2	2.39	0.53
26:O:1733:TYR:OH	26:O:1738:ASN:ND2	2.42	0.53
28:S:200:ASP:HB3	28:S:228:MET:HE1	1.90	0.53
1:D:34:ASN:O	1:D:68:THR:OG1	2.27	0.53
1:D:36:GLU:OE1	1:D:84:ARG:NH1	2.42	0.53
12:T:9:DC:C2'	12:T:10:DT:H71	2.39	0.53
12:T:40:DG:N1	25:N:159:DG:C2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:221:VAL:HG23	21:A:249:ILE:HD13	1.91	0.53
24:M:316:GLU:HG2	24:M:403:TRP:CD1	2.44	0.53
24:M:833:ILE:HG23	24:M:867:ILE:CD1	2.38	0.53
24:M:849:THR:HB	24:M:885:VAL:CG2	2.38	0.53
24:M:1240:ILE:HG12	24:M:1279:LEU:HB2	1.91	0.53
31:Z:492:ILE:HD12	31:Z:495:VAL:HG13	1.90	0.53
22:B:789:ASN:OD1	22:B:968:ASN:N	2.42	0.53
24:M:475:ILE:CG1	24:M:476:PRO:HD3	2.37	0.53
24:M:889:LEU:CG	24:M:930:VAL:HG11	2.39	0.53
24:M:1174:ILE:HG13	24:M:1227:GLY:O	2.09	0.53
31:Z:478:VAL:CG1	31:Z:518:LEU:HD21	2.39	0.53
8:K:78:THR:OG1	8:K:80:ASP:OD1	2.27	0.52
24:M:607:ARG:O	24:M:611:GLN:HG2	2.09	0.52
24:M:658:LEU:O	24:M:662:GLU:HG3	2.09	0.52
24:M:807:ASP:OD2	24:M:843:LYS:NZ	2.27	0.52
24:M:1270:ILE:CG2	24:M:1272:ILE:HG23	2.39	0.52
31:Z:440:ILE:HA	31:Z:450:ILE:HD11	1.89	0.52
17:b:89:ALA:O	17:b:93:GLN:NE2	2.42	0.52
21:A:951:GLU:HB3	21:A:1007:ILE:HD11	1.91	0.52
27:R:504:LYS:CE	27:R:507:PRO:HG3	2.39	0.52
30:V:233:VAL:CB	30:V:238:PRO:HB2	2.40	0.52
31:Z:469:ARG:NH1	31:Z:497:GLU:O	2.42	0.52
2:E:153:LYS:O	2:E:157:THR:HG23	2.09	0.52
5:H:33:GLU:CB	11:Q:674:ARG:HH12	2.22	0.52
5:H:34:SER:O	11:Q:706:ASN:CG	2.52	0.52
4:G:129:LYS:HE2	24:M:412:ASN:HD22	1.75	0.52
21:A:199:TYR:CZ	21:A:215:LEU:HD13	2.45	0.52
18:g:44:GLY:CA	19:h:89:ILE:O	2.57	0.52
24:M:303:ILE:CG2	24:M:404:THR:HG21	2.39	0.52
1:D:61:PHE:CE2	1:D:65:LEU:HD21	2.45	0.52
24:M:746:SER:OG	24:M:961:GLU:OE2	2.28	0.52
22:B:108:MET:HE2	22:B:113:ALA:HB2	1.92	0.52
24:M:330:ILE:HG13	24:M:332:LEU:HD23	1.91	0.52
24:M:362:ALA:O	24:M:366:MET:HG3	2.10	0.52
24:M:832:ASP:O	24:M:835:THR:HG22	2.10	0.52
24:M:1265:CYS:SG	24:M:1279:LEU:HD13	2.50	0.52
2:E:185:ILE:HD12	2:E:209:VAL:HG21	1.90	0.52
11:Q:769:LEU:HD22	11:Q:824:ALA:CB	2.40	0.52
24:M:406:LEU:HB2	24:M:457:MET:HE1	1.90	0.52
24:M:1265:CYS:SG	24:M:1279:LEU:HD22	2.50	0.52
24:M:448:MET:SD	24:M:452:LYS:HE2	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:1156:GLU:HB2	24:M:1160:THR:HG21	1.93	0.51
27:R:359:LEU:HD22	27:R:452:PHE:CE1	2.45	0.51
15:Y:26:ASP:OD1	15:Y:27:GLN:N	2.43	0.51
24:M:285:GLN:OE1	24:M:285:GLN:N	2.32	0.51
24:M:475:ILE:N	24:M:476:PRO:HD2	2.25	0.51
24:M:613:ARG:O	24:M:613:ARG:HG3	2.10	0.51
24:M:618:ILE:HG21	24:M:665:LEU:HD11	1.92	0.51
24:M:1271:ASP:CB	24:M:1276:SER:HB2	2.40	0.51
26:O:1613:ILE:HB	26:O:1757:LYS:HB3	1.91	0.51
12:T:20:DC:C2'	12:T:21:DT:H71	2.40	0.51
24:M:285:GLN:O	24:M:289:ILE:HG13	2.10	0.51
24:M:313:LEU:HD11	24:M:363:LEU:CB	2.39	0.51
27:R:431:GLY:N	27:R:459:MET:HE1	2.25	0.51
8:K:51:LEU:HD22	21:A:561:MET:HE1	1.92	0.51
21:A:421:ARG:NE	21:A:427:ILE:HD11	2.25	0.51
22:B:743:ARG:NH2	22:B:745:ASP:OD1	2.44	0.51
30:V:193:HIS:HB2	30:V:199:VAL:HG12	1.92	0.51
31:Z:613:GLU:O	31:Z:625:HIS:N	2.42	0.51
25:N:93:DG:H2'	25:N:94:DG:C8	2.46	0.51
2:E:189:GLN:O	2:E:209:VAL:HG23	2.10	0.51
4:G:132:ASP:OD2	24:M:416:LEU:HA	2.11	0.51
24:M:462:ASP:O	24:M:464:TYR:N	2.44	0.51
24:M:1107:PHE:HD1	26:O:2025:ILE:HG23	1.76	0.51
24:M:1250:VAL:HG12	24:M:1251:LYS:H	1.76	0.51
22:B:191:GLU:OE2	22:B:743:ARG:NH1	2.43	0.51
24:M:373:VAL:HG21	24:M:394:TRP:CE3	2.45	0.51
24:M:795:PHE:HE2	24:M:907:PRO:HB2	1.76	0.51
27:R:505:ALA:HB3	27:R:506:PRO:HD3	1.92	0.51
28:S:242:LYS:HA	28:S:245:ILE:HG22	1.92	0.51
29:U:459:VAL:HG23	29:U:494:HIS:C	2.36	0.51
3:F:64:ARG:NH2	21:A:1471:PHE:O	2.43	0.51
24:M:907:PRO:HD2	24:M:910:LEU:HD12	1.92	0.51
15:Y:40:LEU:HD22	15:Y:42:MET:HB3	1.93	0.51
24:M:330:ILE:HG23	24:M:733:LEU:HD22	1.93	0.51
24:M:799:VAL:HG21	24:M:917:ALA:HB3	1.93	0.51
22:B:313:GLU:OE1	22:B:316:VAL:N	2.43	0.51
11:Q:766:THR:OG1	11:Q:820:LEU:HD21	2.11	0.50
21:A:894:ASP:OD2	21:A:1396:ARG:NH1	2.43	0.50
22:B:351:VAL:HG12	22:B:351:VAL:O	2.11	0.50
24:M:934:ASP:O	24:M:937:ILE:HG22	2.12	0.50
24:M:1250:VAL:HG12	24:M:1251:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:O:1771:ASN:ND2	26:O:1798:GLU:O	2.38	0.50
27:R:405:ILE:HG12	27:R:426:LEU:HD21	1.92	0.50
21:A:381:PRO:HB3	21:A:480:SER:HA	1.93	0.50
24:M:697:GLU:OE1	24:M:697:GLU:N	2.24	0.50
28:S:231:ASP:O	28:S:232:GLU:HG3	2.11	0.50
21:A:77:ASN:OD1	21:A:78:MET:N	2.44	0.50
24:M:330:ILE:O	24:M:332:LEU:HD23	2.10	0.50
24:M:1078:GLU:CD	26:O:2022:VAL:CG1	2.78	0.50
27:R:353:VAL:HG23	27:R:456:LYS:NZ	2.27	0.50
27:R:363:ARG:NH1	27:R:444:ASN:O	2.45	0.50
24:M:417:PHE:CD2	24:M:443:LEU:HD13	2.46	0.50
24:M:802:GLU:N	24:M:802:GLU:OE1	2.44	0.50
24:M:886:ASP:OD1	24:M:887:ASN:N	2.44	0.50
27:R:505:ALA:CB	27:R:506:PRO:CD	2.88	0.50
22:B:414:GLU:HG3	22:B:439:ILE:HD11	1.93	0.50
6:I:17:CYS:O	6:I:21:ASN:N	2.41	0.50
19:h:56:SER:N	20:k:947:THR:HA	2.27	0.50
21:A:199:TYR:CE1	21:A:215:LEU:HD13	2.47	0.50
23:C:183:ALA:HB3	23:C:232:ASN:HB3	1.92	0.50
24:M:995:ARG:HD2	24:M:995:ARG:N	2.26	0.50
24:M:1240:ILE:HG21	24:M:1281:CYS:SG	2.52	0.50
25:N:90:DA:H2"	25:N:91:DG:H5"	1.93	0.50
19:h:56:SER:N	20:k:948:PHE:N	2.60	0.50
23:C:190:ASN:ND2	23:C:195:THR:O	2.34	0.50
24:M:547:GLY:HA2	24:M:602:VAL:HG22	1.94	0.50
24:M:784:ILE:N	24:M:784:ILE:HD12	2.27	0.50
24:M:864:VAL:O	24:M:868:VAL:HG13	2.11	0.50
24:M:1271:ASP:N	24:M:1276:SER:O	2.45	0.50
22:B:218:THR:HG23	22:B:238:SER:HB3	1.94	0.50
24:M:602:VAL:HA	24:M:605:VAL:HG12	1.94	0.50
24:M:618:ILE:HB	24:M:640:LEU:HB2	1.93	0.50
24:M:622:LYS:HA	24:M:625:ARG:NE	2.27	0.50
24:M:865:LYS:HA	24:M:868:VAL:HG22	1.94	0.50
24:M:1251:LYS:HD2	24:M:1251:LYS:C	2.36	0.50
26:O:1776:LYS:HB3	26:O:1783:LEU:HD11	1.92	0.50
21:A:64:VAL:HG11	21:A:78:MET:HA	1.94	0.49
24:M:332:LEU:HD11	24:M:740:TYR:HB2	1.93	0.49
24:M:448:MET:O	24:M:452:LYS:HB2	2.12	0.49
24:M:889:LEU:HD11	24:M:930:VAL:CG1	2.41	0.49
24:M:1144:PRO:HB3	24:M:1148:GLU:HB3	1.93	0.49
1:D:103:LEU:O	4:G:144:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:52:CYS:SG	15:Y:53:THR:N	2.86	0.49
22:B:686:GLU:N	22:B:686:GLU:OE1	2.45	0.49
22:B:854:ILE:O	22:B:907:VAL:HG21	2.12	0.49
24:M:934:ASP:OD1	24:M:935:GLU:N	2.45	0.49
24:M:1258:LYS:HE2	24:M:1258:LYS:CA	2.39	0.49
5:H:15:ILE:O	5:H:16:ASP:C	2.55	0.49
5:H:27:ARG:NH2	5:H:42:ASP:OD2	2.46	0.49
22:B:1028:LEU:HD12	22:B:1041:ILE:HG13	1.94	0.49
24:M:669:ILE:HG21	24:M:729:LEU:HD23	1.95	0.49
24:M:841:LEU:C	24:M:841:LEU:HD23	2.37	0.49
24:M:894:MET:CE	24:M:912:GLN:HE21	2.25	0.49
27:R:363:ARG:NH1	27:R:365:SER:OG	2.45	0.49
31:Z:524:THR:HG22	31:Z:525:ALA:N	2.27	0.49
21:A:948:ILE:HG23	21:A:1007:ILE:HD13	1.94	0.49
22:B:591:ARG:NH1	22:B:663:GLU:OE2	2.45	0.49
24:M:538:LYS:HD3	24:M:569:LEU:CD2	2.43	0.49
27:R:569:GLU:O	27:R:572:ILE:HG22	2.12	0.49
31:Z:364:ASN:O	31:Z:374:LYS:NZ	2.42	0.49
4:G:151:ARG:O	4:G:158:PHE:N	2.43	0.49
21:A:111:CYS:HA	21:A:118:LEU:HD21	1.93	0.49
24:M:331:SER:HB3	24:M:649:ARG:NH1	2.26	0.49
24:M:837:LYS:HD3	24:M:867:ILE:CG2	2.42	0.49
31:Z:419:ASN:OD1	31:Z:516:ARG:NH2	2.45	0.49
31:Z:558:PHE:N	31:Z:570:VAL:O	2.43	0.49
16:a:108:ASN:ND2	17:b:42:GLY:O	2.46	0.49
24:M:444:ASP:OD1	24:M:445:THR:N	2.43	0.49
24:M:911:ARG:O	24:M:914:VAL:HG22	2.12	0.49
2:E:173:ILE:O	2:E:173:ILE:HG23	2.12	0.49
16:a:86:SER:O	16:a:90:MET:HG2	2.12	0.49
24:M:443:LEU:HD22	24:M:446:THR:HG21	1.94	0.49
31:Z:546:THR:HG23	31:Z:563:MET:HE2	1.95	0.49
5:H:150:PHE:O	14:X:242:GLY:N	2.44	0.49
9:L:34:ILE:O	9:L:34:ILE:HG22	2.13	0.49
19:h:56:SER:CB	20:k:948:PHE:HA	2.42	0.49
21:A:200:ALA:HB2	21:A:216:LEU:HD21	1.95	0.49
24:M:1107:PHE:CZ	26:O:2025:ILE:CD1	2.83	0.49
21:A:198:LEU:O	21:A:215:LEU:HD12	2.12	0.49
24:M:728:GLU:O	24:M:732:LYS:HG2	2.13	0.49
24:M:1103:ASP:N	26:O:2029:SER:CB	2.72	0.49
25:N:93:DG:H2'	25:N:94:DG:H8	1.78	0.49
27:R:574:GLU:HA	27:R:577:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:674:ARG:HH21	11:Q:674:ARG:CG	2.26	0.49
19:h:57:LYS:CB	20:k:945:ASP:OD2	2.49	0.49
21:A:987:ILE:O	21:A:991:GLN:HG3	2.13	0.49
24:M:296:GLU:OE2	24:M:300:LEU:HD11	2.13	0.49
24:M:620:PRO:HG2	24:M:625:ARG:HG3	1.93	0.49
24:M:623:LYS:HE2	31:Z:608:SER:HB3	1.94	0.49
24:M:758:TYR:CD1	24:M:847:VAL:HG21	2.48	0.49
11:Q:772:GLU:O	11:Q:830:ARG:NH2	2.46	0.48
21:A:902:GLU:OE1	21:A:985:ARG:NH1	2.46	0.48
24:M:296:GLU:HB2	24:M:996:LYS:HD2	1.95	0.48
24:M:1075:GLU:O	24:M:1075:GLU:HG2	2.13	0.48
27:R:364:LEU:HB2	27:R:387:VAL:HG12	1.94	0.48
12:T:140:DT:H2''	12:T:141:DA:C8	2.48	0.48
21:A:195:GLY:C	21:A:196:LEU:HD12	2.38	0.48
21:A:413:TYR:O	21:A:415:GLY:N	2.42	0.48
22:B:801:VAL:HG13	22:B:929:PRO:HD2	1.94	0.48
24:M:1265:CYS:SG	24:M:1279:LEU:HB3	2.52	0.48
24:M:330:ILE:HG13	24:M:332:LEU:HD21	1.94	0.48
24:M:388:LEU:HD22	24:M:392:ASP:HB3	1.95	0.48
29:U:416:VAL:HG13	29:U:417:GLU:N	2.28	0.48
24:M:546:PHE:CE2	24:M:550:LEU:HD11	2.49	0.48
24:M:1232:LEU:HD23	24:M:1236:VAL:O	2.13	0.48
24:M:690:LYS:HE3	24:M:710:THR:HG23	1.96	0.48
31:Z:524:THR:HG22	31:Z:525:ALA:H	1.79	0.48
21:A:727:PRO:HA	21:A:736:THR:HG21	1.96	0.48
31:Z:450:ILE:HG21	31:Z:468:LEU:HD11	1.95	0.48
21:A:392:GLU:OE2	21:A:401:ARG:NH1	2.47	0.48
21:A:621:ILE:HG23	21:A:621:ILE:O	2.14	0.48
21:A:1016:LEU:HD22	21:A:1069:LEU:HD22	1.96	0.48
22:B:241:ALA:O	22:B:242:ARG:C	2.57	0.48
24:M:541:LEU:HD21	24:M:546:PHE:CA	2.43	0.48
24:M:1174:ILE:N	24:M:1174:ILE:HD12	2.28	0.48
27:R:388:ARG:HH22	27:R:448:THR:HG23	1.79	0.48
2:E:41:LYS:NZ	2:E:46:ASP:OD1	2.41	0.48
18:g:45:ALA:O	18:g:46:GLY:C	2.55	0.48
21:A:965:VAL:O	21:A:968:VAL:HG22	2.14	0.48
24:M:684:THR:OG1	24:M:687:GLU:HG2	2.14	0.48
24:M:856:ASP:HA	24:M:859:MET:HG2	1.95	0.48
24:M:883:GLU:OE1	24:M:883:GLU:N	2.47	0.48
24:M:1227:GLY:HA2	24:M:1245:LEU:HD13	1.95	0.48
24:M:1274:LYS:O	24:M:1274:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:192:THR:CG2	31:Z:245:LEU:HD21	2.43	0.48
31:Z:478:VAL:HG12	31:Z:518:LEU:HD21	1.96	0.48
31:Z:746:ASP:OD1	31:Z:747:ARG:N	2.47	0.48
21:A:1302:GLU:OE1	21:A:1302:GLU:N	2.44	0.48
23:C:19:VAL:HG23	23:C:241:PRO:HB2	1.96	0.48
24:M:926:GLU:OE1	24:M:981:TYR:OH	2.22	0.48
15:Y:7:PRO:HD3	15:Y:84:VAL:HG21	1.96	0.48
24:M:693:TYR:HB3	24:M:713:ILE:CD1	2.42	0.48
5:H:92:MET:HE1	5:H:121:LEU:HD22	1.95	0.47
21:A:200:ALA:HB3	21:A:214:ILE:HG12	1.96	0.47
22:B:412:LEU:HA	22:B:415:VAL:HG22	1.96	0.47
21:A:471:GLY:O	21:A:521:VAL:HG23	2.15	0.47
31:Z:244:ASN:C	31:Z:245:LEU:HD22	2.38	0.47
2:E:185:ILE:HD12	2:E:209:VAL:CG2	2.44	0.47
3:F:51:ARG:NH2	3:F:122:GLU:OE1	2.46	0.47
19:h:56:SER:HB3	20:k:947:THR:C	2.40	0.47
22:B:163:LEU:HD21	22:B:176:GLU:CD	2.39	0.47
24:M:443:LEU:HD22	24:M:446:THR:CG2	2.45	0.47
24:M:571:LYS:HA	24:M:574:VAL:CG1	2.44	0.47
24:M:1241:PRO:HG2	24:M:1244:PHE:CD1	2.37	0.47
27:R:359:LEU:HD11	27:R:386:PHE:CD2	2.49	0.47
30:V:127:VAL:HG23	30:V:128:VAL:N	2.29	0.47
1:D:45:LYS:NZ	1:D:62:MET:HE1	2.29	0.47
21:A:832:THR:HG23	21:A:833:PRO:HD2	1.95	0.47
21:A:971:PRO:O	21:A:972:THR:OG1	2.20	0.47
21:A:1166:LEU:HD13	21:A:1166:LEU:O	2.14	0.47
22:B:127:ASP:OD1	22:B:128:ILE:N	2.47	0.47
29:U:372:ASP:OD1	29:U:373:LEU:N	2.46	0.47
2:E:29:THR:HG23	11:Q:877:GLN:HG2	1.97	0.47
3:F:86:GLU:OE2	3:F:95:LYS:NZ	2.26	0.47
11:Q:835:ASP:OD1	11:Q:839:ARG:NE	2.47	0.47
24:M:545:GLN:HG2	24:M:557:HIS:CD2	2.49	0.47
1:D:131:LEU:HA	1:D:134:ILE:HD12	1.97	0.47
3:F:86:GLU:N	3:F:86:GLU:OE1	2.48	0.47
4:G:109:SER:HB3	31:Z:493:VAL:HG21	1.96	0.47
11:Q:856:LEU:CD2	11:Q:857:LEU:HD22	2.42	0.47
19:d:72:ARG:HB3	19:d:101:LEU:HD11	1.96	0.47
24:M:311:ASP:OD1	24:M:312:GLU:N	2.45	0.47
24:M:316:GLU:O	24:M:320:ILE:HG13	2.15	0.47
24:M:541:LEU:HD11	24:M:549:ASN:HD21	1.78	0.47
24:M:625:ARG:HA	24:M:638:LYS:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:687:GLU:HA	24:M:690:LYS:CD	2.45	0.47
24:M:732:LYS:O	24:M:736:GLU:HG3	2.13	0.47
24:M:809:LEU:HD23	24:M:809:LEU:C	2.40	0.47
24:M:1167:ILE:CD1	24:M:1232:LEU:HD11	2.41	0.47
24:M:1286:LEU:C	24:M:1286:LEU:HD23	2.39	0.47
2:E:55:ARG:C	2:E:56:THR:HG1	2.15	0.47
24:M:421:GLN:HE21	24:M:443:LEU:HB2	1.80	0.47
24:M:940:LEU:HD12	24:M:940:LEU:N	2.28	0.47
24:M:1164:GLY:O	24:M:1266:ARG:HG3	2.14	0.47
4:G:109:SER:OG	4:G:110:ARG:N	2.48	0.47
24:M:309:GLU:HB2	24:M:311:ASP:OD1	2.14	0.47
24:M:592:VAL:O	24:M:596:ILE:HG13	2.15	0.47
24:M:1245:LEU:O	24:M:1246:SER:OG	2.26	0.47
28:S:243:GLU:OE1	28:S:246:ARG:NH2	2.47	0.47
11:Q:849:LYS:O	11:Q:852:LEU:HG	2.15	0.47
21:A:479:TRP:O	21:A:483:ARG:NH1	2.46	0.47
21:A:1342:SER:O	21:A:1344:MET:N	2.45	0.47
22:B:17:ILE:HG23	22:B:19:PRO:HD3	1.96	0.47
24:M:698:PHE:HA	24:M:703:GLN:OE1	2.15	0.47
27:R:359:LEU:HD22	27:R:452:PHE:HE1	1.79	0.47
21:A:140:ARG:O	21:A:144:VAL:HG13	2.15	0.46
21:A:467:MET:SD	21:A:524:MET:HE3	2.55	0.46
21:A:818:GLU:OE2	27:R:599:CYS:N	2.48	0.46
22:B:273:PHE:CD2	22:B:284:ILE:HG23	2.51	0.46
24:M:294:LEU:HB2	24:M:299:GLN:HE21	1.79	0.46
24:M:331:SER:O	24:M:332:LEU:HD22	2.15	0.46
5:H:9:ILE:HG13	11:Q:674:ARG:NH2	2.30	0.46
22:B:388:TYR:H	22:B:504:THR:HG21	1.80	0.46
26:O:1602:LYS:HB3	26:O:1699:TRP:HE1	1.79	0.46
27:R:506:PRO:N	27:R:507:PRO:CD	2.78	0.46
24:M:285:GLN:HA	24:M:288:GLU:OE1	2.15	0.46
24:M:322:ARG:O	24:M:326:ALA:HB2	2.15	0.46
24:M:752:TRP:CZ3	24:M:940:LEU:HD23	2.51	0.46
28:S:219:LEU:HD12	28:S:219:LEU:N	2.30	0.46
21:A:1049:LEU:HG	21:A:1054:MET:HE3	1.96	0.46
24:M:624:GLY:HA3	24:M:664:LEU:O	2.15	0.46
28:S:243:GLU:OE1	28:S:246:ARG:NH1	2.47	0.46
2:E:115:LYS:O	2:E:119:VAL:HG22	2.16	0.46
21:A:951:GLU:HG2	21:A:1007:ILE:HD11	1.97	0.46
24:M:625:ARG:O	24:M:638:LYS:NZ	2.48	0.46
24:M:1269:LYS:N	24:M:1278:ASP:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:145:ARG:HB3	28:S:173:GLU:CB	2.46	0.46
11:Q:163:ILE:HB	11:Q:164:PRO:HD3	1.98	0.46
21:A:106:VAL:O	21:A:110:VAL:HG22	2.16	0.46
22:B:365:LEU:O	22:B:369:VAL:HG23	2.15	0.46
24:M:808:PHE:CD2	24:M:910:LEU:HD11	2.51	0.46
24:M:946:GLN:O	24:M:949:VAL:HG22	2.16	0.46
11:Q:855:LYS:O	11:Q:858:LYS:HG3	2.16	0.46
27:R:492:ILE:O	27:R:496:VAL:HG13	2.16	0.46
31:Z:178:ASN:ND2	31:Z:254:MET:SD	2.83	0.46
31:Z:426:VAL:CG1	31:Z:440:ILE:HD11	2.44	0.46
12:T:71:DA:H4'	18:c:77:ARG:HE	1.81	0.46
22:B:67:LEU:H	22:B:83:ARG:HB2	1.81	0.46
22:B:1006:VAL:HG22	30:V:130:TRP:CB	2.45	0.46
24:M:541:LEU:HA	24:M:545:GLN:OE1	2.16	0.46
24:M:855:ARG:HD3	24:M:1235:GLY:O	2.16	0.46
2:E:126:ILE:HD12	2:E:126:ILE:H	1.81	0.46
3:F:94:MET:HE3	3:F:98:LYS:HE3	1.98	0.46
4:G:101:ILE:N	4:G:104:MET:O	2.49	0.46
5:H:149:ALA:O	5:H:150:PHE:OXT	2.34	0.46
8:K:39:ASP:OD1	8:K:39:ASP:N	2.47	0.46
11:Q:523:ILE:HG21	11:Q:533:CYS:SG	2.56	0.46
22:B:721:ARG:NH2	22:B:940:GLY:O	2.48	0.46
24:M:466:HIS:HB2	24:M:598:ARG:O	2.15	0.46
24:M:1168:ILE:HG12	24:M:1264:HIS:HB3	1.98	0.46
31:Z:602:VAL:HG21	31:Z:636:PHE:HE2	1.81	0.46
2:E:58:LEU:HD23	2:E:58:LEU:H	1.81	0.46
8:K:104:ARG:NH2	23:C:7:PRO:O	2.48	0.46
22:B:1090:GLU:OE1	22:B:1090:GLU:N	2.44	0.46
24:M:404:THR:O	24:M:408:ILE:HG13	2.16	0.46
24:M:1154:THR:O	24:M:1155:LYS:HB2	2.16	0.46
21:A:1281:ASP:OD1	21:A:1281:ASP:N	2.49	0.45
22:B:166:LEU:HG	22:B:170:ASP:HB2	1.98	0.45
23:C:103:LEU:HD23	23:C:103:LEU:C	2.41	0.45
24:M:355:THR:HA	24:M:387:GLU:OE1	2.17	0.45
24:M:464:TYR:CE2	24:M:468:LEU:HD12	2.51	0.45
24:M:542:THR:HG22	24:M:545:GLN:CD	2.41	0.45
4:G:106:CYS:SG	4:G:159:ALA:HB3	2.56	0.45
19:d:90:THR:OG1	19:d:93:GLU:OE1	2.31	0.45
16:e:50:GLU:HA	16:e:53:ARG:HG2	1.96	0.45
21:A:986:MET:HE2	21:A:1075:LYS:HG3	1.98	0.45
31:Z:199:LYS:HG2	31:Z:210:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASP:O	1:D:136:THR:OG1	2.28	0.45
4:G:122:ASN:HB2	24:M:303:ILE:HD11	1.98	0.45
12:T:40:DG:C6	25:N:159:DG:N1	2.84	0.45
13:W:24:TRP:HE1	13:W:33:GLU:HB3	1.82	0.45
21:A:111:CYS:N	21:A:116:LYS:O	2.44	0.45
21:A:480:SER:O	22:B:1055:VAL:HG21	2.16	0.45
21:A:1095:LEU:HD23	21:A:1401:LEU:HD22	1.97	0.45
24:M:784:ILE:HG13	24:M:796:CYS:CB	2.44	0.45
1:D:135:GLN:HB3	24:M:577:GLN:HE22	1.80	0.45
4:G:134:ASP:HB2	24:M:416:LEU:HD13	1.97	0.45
11:Q:887:ASN:HA	11:Q:890:MET:HG2	1.99	0.45
24:M:715:ARG:O	24:M:719:GLN:HG2	2.16	0.45
21:A:94:VAL:HG21	21:A:311:GLN:HA	1.99	0.45
21:A:1129:ASN:O	21:A:1129:ASN:ND2	2.48	0.45
24:M:758:TYR:OH	24:M:883:GLU:OE2	2.22	0.45
27:R:403:ALA:HB1	27:R:428:LEU:HB3	1.98	0.45
21:A:1262:MET:HE2	21:A:1262:MET:HA	1.97	0.45
22:B:268:PRO:HG2	22:B:271:ILE:HD12	1.98	0.45
21:A:569:THR:CG2	21:A:667:LEU:HD13	2.47	0.45
24:M:329:THR:HG22	24:M:329:THR:O	2.17	0.45
24:M:665:LEU:HD23	24:M:666:THR:N	2.32	0.45
4:G:147:ILE:HD12	4:G:147:ILE:H	1.81	0.45
22:B:407:MET:SD	22:B:444:LEU:HD22	2.57	0.45
24:M:824:GLU:HA	24:M:827:GLU:OE2	2.17	0.45
24:M:1170:ASN:CB	24:M:1262:THR:HG22	2.46	0.45
5:H:150:PHE:O	14:X:241:THR:CA	2.62	0.45
21:A:921:ARG:NH1	21:A:953:GLU:OE2	2.43	0.45
23:C:44:ILE:HG23	23:C:176:TRP:HD1	1.82	0.45
24:M:443:LEU:HD21	24:M:471:TYR:CE2	2.52	0.45
24:M:550:LEU:CD2	24:M:689:ILE:HD12	2.37	0.45
24:M:602:VAL:O	24:M:605:VAL:HG12	2.17	0.45
24:M:938:LEU:O	24:M:946:GLN:NE2	2.50	0.45
24:M:1245:LEU:HG	24:M:1253:PRO:HB3	1.99	0.45
21:A:578:ALA:N	21:A:590:GLN:OE1	2.50	0.44
21:A:604:ARG:O	21:A:628:VAL:N	2.50	0.44
21:A:1181:PRO:O	21:A:1184:THR:HG23	2.16	0.44
24:M:570:ALA:HB2	24:M:585:LEU:HD21	1.98	0.44
24:M:745:CYS:HA	24:M:942:PHE:HB3	1.98	0.44
4:G:38:CYS:SG	4:G:39:THR:N	2.90	0.44
5:H:24:ARG:NH2	21:A:552:ASP:O	2.51	0.44
11:Q:524:LEU:HD21	11:Q:533:CYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:68:GLN:HE21	16:a:72:ARG:HH11	1.64	0.44
21:A:428:ASP:OD1	21:A:430:ARG:NH2	2.50	0.44
21:A:663:ASP:OD1	21:A:666:ARG:NH1	2.50	0.44
24:M:574:VAL:HG22	24:M:574:VAL:O	2.16	0.44
28:S:144:CYS:HB2	28:S:191:VAL:HG11	1.99	0.44
5:H:67:ASP:N	5:H:67:ASP:OD1	2.50	0.44
24:M:1078:GLU:OE2	26:O:2024:ARG:CG	2.64	0.44
24:M:1167:ILE:HD13	24:M:1267:ILE:HD11	1.98	0.44
24:M:1269:LYS:O	24:M:1270:ILE:HD13	2.17	0.44
26:O:1807:ARG:HH11	26:O:1826:LEU:HB2	1.82	0.44
27:R:587:LYS:O	27:R:588:ASN:ND2	2.50	0.44
31:Z:472:PHE:CD2	31:Z:518:LEU:HD23	2.53	0.44
21:A:584:PRO:O	21:A:585:LEU:HD12	2.18	0.44
24:M:779:ILE:HG13	24:M:781:VAL:HG23	1.99	0.44
24:M:887:ASN:ND2	24:M:891:ILE:HD11	2.31	0.44
31:Z:307:MET:O	31:Z:372:LEU:N	2.50	0.44
12:T:24:DG:H2'	12:T:25:DA:H8	1.81	0.44
13:W:86:ALA:HB1	13:W:105:GLY:O	2.17	0.44
21:A:1423:ASP:OD1	21:A:1423:ASP:N	2.50	0.44
22:B:854:ILE:CG1	22:B:904:VAL:HG21	2.47	0.44
31:Z:307:MET:HE3	31:Z:308:ILE:H	1.82	0.44
3:F:61:GLU:HA	21:A:1471:PHE:CZ	2.53	0.44
4:G:101:ILE:HD13	4:G:106:CYS:SG	2.58	0.44
24:M:296:GLU:HA	24:M:299:GLN:OE1	2.17	0.44
24:M:665:LEU:HD23	24:M:665:LEU:C	2.43	0.44
24:M:738:LYS:HD2	24:M:949:VAL:HA	1.99	0.44
4:G:136:VAL:HG23	24:M:464:TYR:OH	2.17	0.44
6:I:49:ASP:OD1	6:I:49:ASP:N	2.49	0.44
12:T:40:DG:C2	25:N:159:DG:N2	2.85	0.44
22:B:1035:ARG:NH2	22:B:1036:LYS:O	2.51	0.44
24:M:1170:ASN:CG	24:M:1262:THR:HG22	2.43	0.44
24:M:1267:ILE:HG21	24:M:1270:ILE:HD11	1.99	0.44
31:Z:470:LYS:HB2	31:Z:516:ARG:HA	1.98	0.44
5:H:24:ARG:O	5:H:45:ILE:N	2.48	0.44
5:H:60:ILE:HG23	5:H:141:VAL:CG2	2.47	0.44
13:W:49:TRP:CZ2	13:W:52:GLU:HA	2.52	0.44
18:c:68:ASN:OD1	18:c:71:ARG:NH1	2.41	0.44
19:h:56:SER:CA	20:k:948:PHE:N	2.80	0.44
22:B:541:ILE:HD12	22:B:616:THR:CG2	2.48	0.44
24:M:588:ALA:O	24:M:592:VAL:HG23	2.18	0.44
24:M:880:ILE:N	24:M:880:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:470:ASP:OD1	27:R:471:GLU:N	2.50	0.44
2:E:197:SER:OG	21:A:893:GLU:OE1	2.32	0.44
21:A:37:THR:HG21	21:A:41:ILE:HD11	2.00	0.44
23:C:151:VAL:HG21	23:C:159:LEU:HD22	1.98	0.44
24:M:303:ILE:HG21	24:M:404:THR:CG2	2.47	0.44
24:M:406:LEU:CB	24:M:457:MET:HE1	2.48	0.44
24:M:850:VAL:O	24:M:884:LEU:HD12	2.18	0.44
27:R:385:CYS:O	27:R:405:ILE:HD12	2.17	0.44
21:A:490:THR:HB	21:A:491:PRO:HD3	2.00	0.43
22:B:907:VAL:HG13	22:B:921:ILE:HG12	2.00	0.43
24:M:394:TRP:O	24:M:398:GLN:HG3	2.18	0.43
24:M:589:ARG:NH2	24:M:708:GLN:OE1	2.40	0.43
24:M:737:ALA:O	24:M:741:VAL:HG23	2.18	0.43
24:M:1078:GLU:HB2	26:O:2022:VAL:CG1	2.46	0.43
24:M:1271:ASP:CG	24:M:1274:LYS:HB3	2.43	0.43
1:D:37:VAL:HG21	4:G:2:PHE:HD2	1.79	0.43
7:J:35:LEU:HD11	7:J:50:LEU:HG	2.00	0.43
22:B:550:MET:CE	22:B:567:ILE:HG21	2.48	0.43
24:M:550:LEU:HD12	24:M:602:VAL:HG13	2.00	0.43
24:M:591:MET:O	24:M:595:GLN:HG3	2.18	0.43
24:M:848:VAL:HG11	24:M:864:VAL:HG11	2.01	0.43
24:M:1078:GLU:HB2	26:O:2022:VAL:HG11	1.98	0.43
24:M:1156:GLU:HG2	24:M:1161:PHE:CE2	2.53	0.43
31:Z:473:LYS:O	31:Z:492:ILE:HD11	2.17	0.43
15:Y:22:VAL:HB	15:Y:84:VAL:HG12	2.01	0.43
16:a:48:LEU:HD23	16:a:51:ILE:HD12	2.00	0.43
20:k:938:ASP:H	26:O:1632:LYS:HD3	1.82	0.43
24:M:413:LEU:O	24:M:417:PHE:HD1	2.00	0.43
25:N:81:DG:H2'	25:N:82:DT:C6	2.54	0.43
1:D:45:LYS:HZ2	1:D:62:MET:HE1	1.83	0.43
1:D:60:VAL:HG11	4:G:44:PHE:CZ	2.53	0.43
18:g:34:LEU:HB3	18:g:43:VAL:HG11	1.99	0.43
21:A:1366:PHE:HB2	21:A:1374:VAL:HG21	2.00	0.43
24:M:541:LEU:HD23	24:M:546:PHE:HB2	2.00	0.43
3:F:90:LEU:HD21	21:A:513:ALA:HB2	1.99	0.43
15:Y:10:LEU:H	15:Y:10:LEU:HD23	1.84	0.43
21:A:457:ILE:HG21	22:B:1102:PHE:CZ	2.54	0.43
21:A:1285:LEU:HA	21:A:1288:ILE:HG12	2.01	0.43
22:B:552:ASN:OD1	22:B:553:LEU:N	2.52	0.43
24:M:427:GLN:OE1	24:M:427:GLN:HA	2.19	0.43
24:M:464:TYR:OH	24:M:468:LEU:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:786:PHE:HB3	24:M:794:VAL:HG22	1.99	0.43
24:M:855:ARG:NE	24:M:1275:PHE:HD2	2.17	0.43
24:M:1245:LEU:HD23	24:M:1245:LEU:C	2.44	0.43
11:Q:858:LYS:HA	11:Q:861:GLU:HG3	2.00	0.43
19:h:56:SER:N	20:k:947:THR:C	2.77	0.43
21:A:103:THR:HG22	21:A:248:MET:HE3	2.01	0.43
21:A:1323:THR:HG22	21:A:1324:GLU:N	2.34	0.43
24:M:321:TYR:HA	24:M:325:PHE:HD2	1.83	0.43
24:M:567:LEU:O	24:M:570:ALA:HB3	2.17	0.43
24:M:654:LEU:CD2	24:M:741:VAL:HG21	2.48	0.43
24:M:1268:MET:O	24:M:1268:MET:HG3	2.17	0.43
31:Z:705:LEU:HD21	31:Z:747:ARG:HD2	2.01	0.43
22:B:1040:GLN:NE2	23:C:195:THR:OG1	2.49	0.43
24:M:331:SER:C	24:M:332:LEU:HD22	2.43	0.43
24:M:401:GLU:O	24:M:405:GLN:HG3	2.19	0.43
24:M:570:ALA:HB2	24:M:585:LEU:HD22	1.99	0.43
28:S:165:GLU:OE1	28:S:165:GLU:N	2.40	0.43
18:c:88:ARG:HB3	18:c:108:LEU:HD11	2.01	0.43
21:A:64:VAL:HG12	21:A:81:CYS:SG	2.59	0.43
21:A:394:VAL:HG23	21:A:444:TYR:O	2.19	0.43
22:B:785:TYR:C	22:B:786:THR:HG22	2.43	0.43
23:C:201:GLU:OE1	23:C:201:GLU:N	2.44	0.43
24:M:465:ASN:HB3	24:M:598:ARG:NH2	2.33	0.43
25:N:34:DT:H2"	25:N:35:DA:C8	2.53	0.43
28:S:239:ASN:O	28:S:243:GLU:HG2	2.19	0.43
5:H:33:GLU:O	11:Q:684:TRP:CH2	2.67	0.43
21:A:324:GLY:O	21:A:325:LEU:HD22	2.19	0.43
22:B:596:ILE:N	22:B:596:ILE:HD12	2.34	0.43
24:M:550:LEU:HD21	24:M:689:ILE:HG23	2.00	0.43
24:M:650:ASP:HB2	24:M:740:TYR:CD1	2.54	0.43
24:M:1169:CYS:HB3	24:M:1232:LEU:CD1	2.48	0.43
25:N:156:DG:H2"	25:N:157:DT:C6	2.54	0.43
29:U:394:TYR:O	30:V:172:ARG:NH1	2.50	0.43
11:Q:833:LYS:O	11:Q:836:GLU:HG3	2.18	0.43
24:M:316:GLU:HG2	24:M:403:TRP:CE2	2.54	0.43
24:M:357:GLN:O	24:M:361:GLU:HG2	2.19	0.43
24:M:748:LYS:HD3	24:M:942:PHE:HA	2.01	0.43
24:M:853:GLU:OE1	24:M:854:ASN:ND2	2.52	0.43
24:M:940:LEU:H	24:M:940:LEU:CD1	2.30	0.43
24:M:994:PRO:O	24:M:998:THR:HG23	2.19	0.43
24:M:1147:GLU:OE2	24:M:1158:PRO:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:1245:LEU:O	24:M:1245:LEU:HD23	2.19	0.43
27:R:576:GLU:O	27:R:580:VAL:HG13	2.19	0.43
22:B:226:GLU:O	22:B:227:ASN:C	2.62	0.42
22:B:265:GLN:N	22:B:265:GLN:OE1	2.51	0.42
22:B:1142:ASN:O	22:B:1144:THR:HG22	2.19	0.42
24:M:313:LEU:HD11	24:M:363:LEU:HB2	2.00	0.42
25:N:68:DG:H2''	25:N:69:DG:C8	2.54	0.42
25:N:180:DC:H2''	25:N:181:DA:C8	2.53	0.42
18:g:41:GLU:O	18:g:42:ARG:HB2	2.19	0.42
19:h:98:VAL:HG13	19:h:102:LEU:HD12	2.02	0.42
21:A:1158:LEU:C	21:A:1158:LEU:HD23	2.44	0.42
24:M:938:LEU:HD11	24:M:955:LEU:HD21	2.00	0.42
25:N:158:DC:H5'	25:N:158:DC:C6	2.55	0.42
4:G:97:LEU:N	4:G:108:ILE:O	2.40	0.42
21:A:141:LEU:HA	21:A:144:VAL:HG22	2.01	0.42
22:B:1022:LEU:HD23	22:B:1022:LEU:H	1.84	0.42
24:M:313:LEU:HD11	24:M:363:LEU:HB3	2.00	0.42
25:N:128:DC:H2''	25:N:129:DG:C8	2.54	0.42
2:E:73:PHE:CD2	2:E:99:ILE:HD12	2.54	0.42
4:G:84:VAL:HG23	4:G:84:VAL:O	2.19	0.42
18:g:44:GLY:O	18:g:45:ALA:HB2	2.20	0.42
24:M:541:LEU:HD23	24:M:541:LEU:O	2.20	0.42
24:M:1164:GLY:HA2	24:M:1266:ARG:HG2	2.01	0.42
27:R:378:PHE:O	27:R:382:VAL:HG22	2.19	0.42
27:R:428:LEU:HB2	27:R:437:PHE:CD1	2.54	0.42
29:U:373:LEU:HD23	29:U:375:PHE:H	1.84	0.42
30:V:236:PHE:CA	30:V:238:PRO:HD2	2.40	0.42
31:Z:176:ASP:OD1	31:Z:176:ASP:N	2.51	0.42
21:A:220:ARG:O	21:A:224:ILE:HG13	2.20	0.42
24:M:406:LEU:HB2	24:M:457:MET:CE	2.49	0.42
24:M:649:ARG:NE	24:M:649:ARG:HA	2.34	0.42
1:D:103:LEU:HD11	4:G:84:VAL:HG23	2.01	0.42
7:J:64:PRO:O	9:L:23:HIS:CE1	2.72	0.42
12:T:42:DC:H6	12:T:42:DC:H2'	1.75	0.42
22:B:407:MET:HE1	22:B:443:GLY:C	2.45	0.42
22:B:587:LEU:HB3	22:B:603:MET:HE3	2.01	0.42
24:M:787:SER:OG	24:M:792:HIS:ND1	2.51	0.42
24:M:983:GLN:OE1	24:M:1001:LEU:HD13	2.20	0.42
31:Z:592:ASN:OD1	31:Z:593:ASN:N	2.51	0.42
2:E:20:LEU:C	2:E:20:LEU:HD23	2.44	0.42
4:G:109:SER:HB3	31:Z:493:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:922:PHE:H	21:A:1052:ARG:HD2	1.85	0.42
21:A:1453:GLY:N	21:A:1456:GLU:OE1	2.44	0.42
22:B:541:ILE:HD12	22:B:616:THR:HG21	2.01	0.42
24:M:390:ILE:HG23	24:M:391:ASN:N	2.35	0.42
24:M:606:LEU:CD2	24:M:721:LEU:HD13	2.50	0.42
24:M:782:LEU:HD11	24:M:796:CYS:HB2	2.01	0.42
9:L:46:LYS:NZ	22:B:849:ASP:OD2	2.49	0.42
15:Y:48:MET:HE3	15:Y:51:ASP:HB2	2.01	0.42
21:A:965:VAL:O	21:A:969:ILE:HG12	2.20	0.42
24:M:316:GLU:HG2	24:M:403:TRP:NE1	2.34	0.42
24:M:382:GLU:OE1	24:M:382:GLU:N	2.35	0.42
24:M:629:ASP:C	24:M:631:ALA:H	2.28	0.42
24:M:827:GLU:OE1	24:M:827:GLU:N	2.41	0.42
24:M:1145:ASN:OD1	24:M:1146:THR:N	2.52	0.42
21:A:99:PHE:O	21:A:103:THR:HG23	2.19	0.42
21:A:904:GLN:NE2	21:A:981:CYS:O	2.48	0.42
22:B:497:LYS:CG	22:B:498:PRO:HD3	2.50	0.42
24:M:749:LEU:HD13	24:M:942:PHE:HE2	1.85	0.42
27:R:559:ALA:O	27:R:563:ILE:HG23	2.20	0.42
30:V:176:ILE:HG23	30:V:177:THR:N	2.35	0.42
10:P:35:A:N3	22:B:841:ARG:NH2	2.68	0.42
11:Q:748:PRO:HB3	13:W:110:TRP:CH2	2.55	0.42
12:T:2:DC:H2'	12:T:3:DT:H72	2.02	0.42
24:M:298:PHE:HE2	24:M:370:HIS:HA	1.84	0.42
24:M:614:ALA:HB3	24:M:645:VAL:CG2	2.49	0.42
31:Z:257:ILE:HA	31:Z:260:MET:HE2	2.02	0.42
1:D:61:PHE:O	1:D:65:LEU:HG	2.20	0.41
1:D:70:ARG:NH2	4:G:88:VAL:HG21	2.35	0.41
11:Q:837:GLU:O	11:Q:840:GLU:HG3	2.20	0.41
13:W:36:VAL:CG2	13:W:72:ILE:HD11	2.49	0.41
24:M:449:GLU:O	24:M:453:ASP:HB3	2.20	0.41
24:M:475:ILE:N	24:M:476:PRO:CD	2.82	0.41
24:M:622:LYS:HD3	24:M:622:LYS:C	2.45	0.41
24:M:824:GLU:HG3	24:M:825:GLU:N	2.35	0.41
2:E:2:ASP:OD1	2:E:4:GLU:N	2.52	0.41
5:H:33:GLU:HB3	11:Q:674:ARG:NH1	2.34	0.41
5:H:121:LEU:HD12	5:H:121:LEU:N	2.36	0.41
12:T:21:DT:H2''	12:T:22:DC:C6	2.55	0.41
16:a:61:LEU:HD11	17:b:40:ARG:HH11	1.85	0.41
16:a:106:ASP:OD2	16:a:131:ARG:NH1	2.38	0.41
21:A:117:LEU:O	21:A:118:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:440:LEU:HD12	21:A:440:LEU:O	2.21	0.41
12:T:171:DA:H2''	12:T:172:DG:N7	2.35	0.41
22:B:207:VAL:HG11	22:B:375:ALA:HB3	2.01	0.41
22:B:550:MET:HE1	22:B:567:ILE:HG21	2.02	0.41
24:M:296:GLU:OE1	24:M:993:GLY:HA3	2.20	0.41
24:M:473:ARG:NE	24:M:473:ARG:CA	2.82	0.41
24:M:559:THR:HG22	24:M:560:GLU:N	2.35	0.41
26:O:1660:ARG:HB2	26:O:1678:ASN:HD21	1.84	0.41
28:S:224:THR:HG22	28:S:225:ALA:N	2.36	0.41
4:G:117:MET:HB3	4:G:128:TYR:HB3	2.02	0.41
4:G:122:ASN:OD1	4:G:123:SER:N	2.54	0.41
11:Q:605:LEU:HD12	14:X:238:LEU:HD13	2.03	0.41
11:Q:829:ALA:O	11:Q:833:LYS:HG3	2.21	0.41
12:T:40:DG:N1	25:N:159:DG:N1	2.68	0.41
27:R:492:ILE:H	27:R:492:ILE:HD12	1.85	0.41
28:S:197:ASN:CB	28:S:228:MET:HE3	2.50	0.41
2:E:84:ILE:O	2:E:85:LYS:C	2.63	0.41
12:T:40:DG:N2	25:N:159:DG:N3	2.68	0.41
13:W:110:TRP:CD1	13:W:111:THR:H	2.38	0.41
19:h:56:SER:HA	20:k:948:PHE:CA	2.51	0.41
21:A:222:HIS:HB2	21:A:249:ILE:HD11	2.03	0.41
22:B:588:ARG:O	22:B:592:ARG:HD3	2.20	0.41
22:B:680:ASP:OD1	22:B:681:ASP:N	2.54	0.41
24:M:413:LEU:HB3	24:M:451:LEU:HD11	2.02	0.41
24:M:650:ASP:HB2	24:M:740:TYR:CZ	2.56	0.41
25:N:36:DG:H2''	25:N:37:DG:C8	2.56	0.41
25:N:156:DG:C2'	25:N:157:DT:H73	2.25	0.41
27:R:355:LEU:HD12	27:R:356:PRO:HD2	2.02	0.41
5:H:37:MET:HE1	5:H:131:ASN:HB2	2.02	0.41
11:Q:772:GLU:CG	11:Q:827:HIS:CE1	3.01	0.41
19:h:56:SER:N	20:k:947:THR:CA	2.82	0.41
21:A:381:PRO:CG	21:A:384:ILE:HD12	2.50	0.41
21:A:1139:LEU:HD21	21:A:1341:VAL:HG13	2.01	0.41
22:B:56:GLN:HG2	22:B:91:ILE:HG22	2.02	0.41
23:C:74:THR:O	23:C:74:THR:OG1	2.35	0.41
27:R:504:LYS:CE	27:R:507:PRO:CG	2.96	0.41
1:D:41:LEU:HB3	1:D:65:LEU:CD2	2.50	0.41
4:G:170:LEU:HD22	24:M:473:ARG:HH12	1.85	0.41
19:h:59:MET:HG2	20:k:948:PHE:CD2	2.52	0.41
22:B:22:TRP:O	22:B:26:CYS:N	2.51	0.41
22:B:395:LEU:HD11	22:B:532:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:534:GLY:O	24:M:538:LYS:HG3	2.20	0.41
24:M:624:GLY:CA	24:M:664:LEU:HB2	2.48	0.41
24:M:864:VAL:HG12	24:M:882:VAL:HG21	2.02	0.41
27:R:360:ASN:OD1	27:R:447:PHE:N	2.42	0.41
27:R:458:ALA:HB3	27:R:459:MET:HE2	2.02	0.41
1:D:17:ALA:HB1	1:D:95:PHE:CZ	2.56	0.41
12:T:22:DC:H2'	12:T:23:DC:C6	2.56	0.41
21:A:365:THR:HG22	21:A:366:VAL:N	2.35	0.41
24:M:293:ASP:OD1	24:M:1024:GLY:HA3	2.21	0.41
24:M:594:LEU:HD13	24:M:594:LEU:HA	1.93	0.41
24:M:621:THR:OG1	24:M:664:LEU:HA	2.21	0.41
24:M:889:LEU:HD11	24:M:930:VAL:HG13	2.03	0.41
24:M:1072:ASP:OD1	26:O:2025:ILE:N	2.38	0.41
24:M:1232:LEU:HB2	24:M:1236:VAL:O	2.21	0.41
1:D:96:GLU:N	1:D:96:GLU:OE1	2.54	0.41
2:E:55:ARG:NH1	2:E:132:GLN:OE1	2.50	0.41
4:G:132:ASP:OD1	24:M:416:LEU:HA	2.21	0.41
6:I:99:SER:O	6:I:100:HIS:HB2	2.21	0.41
8:K:17:LYS:O	8:K:36:ASN:ND2	2.42	0.41
11:Q:861:GLU:O	11:Q:865:LEU:HG	2.21	0.41
18:g:41:GLU:O	18:g:42:ARG:CB	2.67	0.41
21:A:376:ASP:HB3	21:A:522:PRO:HD3	2.03	0.41
22:B:285:LEU:HD13	22:B:305:LEU:HD21	2.03	0.41
22:B:651:TYR:HB2	29:U:460:TYR:CZ	2.56	0.41
24:M:606:LEU:HD23	24:M:721:LEU:HD13	2.03	0.41
24:M:618:ILE:CD1	24:M:640:LEU:HD12	2.33	0.41
24:M:1072:ASP:HB2	26:O:2025:ILE:CD1	2.48	0.41
31:Z:475:GLY:HA2	31:Z:491:LEU:HD22	2.03	0.41
1:D:57:LEU:N	1:D:57:LEU:HD12	2.36	0.41
6:I:103:ARG:O	6:I:103:ARG:HG2	2.21	0.41
12:T:133:DC:H2''	12:T:134:DG:C8	2.56	0.41
19:h:56:SER:HA	20:k:948:PHE:CB	2.45	0.41
21:A:542:LEU:O	21:A:545:VAL:HG12	2.21	0.41
24:M:1171:VAL:HA	24:M:1230:THR:HA	2.02	0.41
24:M:1245:LEU:HD21	24:M:1247:ASP:HB2	2.01	0.41
27:R:507:PRO:HA	27:R:508:ASN:HA	1.77	0.41
31:Z:358:PHE:CE2	31:Z:360:ILE:HD11	2.56	0.41
9:L:22:CYS:SG	9:L:41:TYR:HE1	2.30	0.40
24:M:357:GLN:OE1	24:M:357:GLN:HA	2.21	0.40
24:M:1078:GLU:HG3	26:O:2024:ARG:CD	2.41	0.40
27:R:592:ASP:O	27:R:594:PHE:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:239:ILE:O	31:Z:242:VAL:HG22	2.21	0.40
1:D:57:LEU:HD12	1:D:57:LEU:H	1.86	0.40
11:Q:879:ALA:O	11:Q:882:VAL:HG12	2.21	0.40
19:h:59:MET:HB2	20:k:948:PHE:HB2	2.03	0.40
21:A:460:ARG:HG2	21:A:462:PRO:HD2	2.02	0.40
22:B:237:VAL:O	22:B:372:LEU:HD22	2.21	0.40
22:B:567:ILE:N	22:B:567:ILE:HD12	2.36	0.40
24:M:450:ARG:HH21	24:M:600:PRO:HG2	1.85	0.40
24:M:729:LEU:O	24:M:733:LEU:HG	2.21	0.40
25:N:156:DG:C4	25:N:157:DT:C4	3.09	0.40
27:R:402:VAL:HG23	27:R:451:GLU:HG2	2.02	0.40
4:G:110:ARG:HH11	4:G:118:GLU:HA	1.87	0.40
7:J:53:VAL:O	7:J:53:VAL:HG13	2.21	0.40
13:W:158:PRO:HG2	13:W:200:PRO:HA	2.03	0.40
21:A:951:GLU:CB	21:A:1007:ILE:HD11	2.51	0.40
21:A:977:VAL:HG22	21:A:978:VAL:N	2.36	0.40
23:C:205:LYS:NZ	23:C:212:ASP:O	2.54	0.40
24:M:809:LEU:HD23	24:M:810:ARG:O	2.21	0.40
31:Z:188:GLU:N	31:Z:188:GLU:OE1	2.55	0.40
1:D:80:ILE:O	1:D:83:VAL:HG22	2.20	0.40
7:J:47:ARG:NE	22:B:777:ASN:O	2.46	0.40
16:a:126:LEU:HD22	16:e:113:HIS:CG	2.57	0.40
18:g:31:HIS:CD2	18:g:35:ARG:NH1	2.77	0.40
19:h:88:THR:HG23	19:h:89:ILE:N	2.36	0.40
24:M:312:GLU:OE2	24:M:316:GLU:HG3	2.21	0.40
24:M:535:LEU:O	24:M:539:PHE:HD1	2.04	0.40
26:O:1665:GLU:HB2	26:O:1779:VAL:HG22	2.03	0.40
31:Z:506:LEU:HD11	31:Z:552:ARG:HH11	1.86	0.40
1:D:127:LEU:O	1:D:131:LEU:HD13	2.21	0.40
7:J:40:LEU:HD11	7:J:49:LEU:HD12	2.03	0.40
19:h:59:MET:HG2	20:k:948:PHE:CB	2.50	0.40
21:A:927:GLU:O	21:A:931:ARG:NE	2.55	0.40
22:B:649:ASN:HB2	29:U:460:TYR:OH	2.21	0.40
24:M:454:VAL:HG11	24:M:460:LEU:HD13	2.02	0.40
24:M:536:ALA:O	24:M:539:PHE:HB2	2.22	0.40
24:M:538:LYS:HD3	24:M:569:LEU:HD23	2.02	0.40
24:M:996:LYS:HE3	24:M:1027:VAL:HG11	2.03	0.40
31:Z:541:GLN:NE2	31:Z:543:ASP:O	2.49	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	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
2	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	24	63
3	F	76/127 (60%)	72 (95%)	4 (5%)	0	100	100
4	G	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
5	H	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
6	I	115/125 (92%)	106 (92%)	9 (8%)	0	100	100
7	J	64/67 (96%)	60 (94%)	4 (6%)	0	100	100
8	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
9	L	45/58 (78%)	38 (84%)	7 (16%)	0	100	100
11	Q	890/1179 (76%)	880 (99%)	10 (1%)	0	100	100
13	W	303/305 (99%)	296 (98%)	6 (2%)	1 (0%)	36	72
14	X	51/531 (10%)	50 (98%)	0	1 (2%)	6	31
15	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100	100
16	a	99/136 (73%)	97 (98%)	2 (2%)	0	100	100
16	e	93/136 (68%)	93 (100%)	0	0	100	100
17	b	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
17	f	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
18	c	102/135 (76%)	100 (98%)	2 (2%)	0	100	100
18	g	101/135 (75%)	95 (94%)	3 (3%)	3 (3%)	3	22
19	d	90/126 (71%)	90 (100%)	0	0	100	100
19	h	87/126 (69%)	84 (97%)	3 (3%)	0	100	100
20	k	16/1049 (2%)	15 (94%)	1 (6%)	0	100	100
21	A	1376/1970 (70%)	1323 (96%)	53 (4%)	0	100	100
22	B	1110/1174 (94%)	1045 (94%)	65 (6%)	0	100	100
23	C	254/275 (92%)	246 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	M	798/1729 (46%)	749 (94%)	45 (6%)	4 (0%)	24	63
26	O	257/1133 (23%)	231 (90%)	26 (10%)	0	100	100
27	R	240/713 (34%)	235 (98%)	4 (2%)	1 (0%)	30	67
28	S	109/304 (36%)	103 (94%)	6 (6%)	0	100	100
29	U	98/666 (15%)	88 (90%)	10 (10%)	0	100	100
30	V	232/531 (44%)	213 (92%)	19 (8%)	0	100	100
31	Z	497/1087 (46%)	476 (96%)	21 (4%)	0	100	100
All	All	8129/14935 (54%)	7766 (96%)	352 (4%)	11 (0%)	49	83

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	g	45	ALA
18	g	46	GLY
24	M	993	GLY
24	M	757	PRO
24	M	1060	PRO
18	g	42	ARG
14	X	242	GLY
13	W	127	VAL
2	E	45	GLY
27	R	507	PRO
24	M	581	PRO

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	D	109/126 (86%)	109 (100%)	0	100	100
2	E	191/192 (100%)	188 (98%)	3 (2%)	55	70
3	F	68/111 (61%)	67 (98%)	1 (2%)	57	72
4	G	146/153 (95%)	143 (98%)	3 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	130/131 (99%)	126 (97%)	4 (3%)	35	56
6	I	105/112 (94%)	102 (97%)	3 (3%)	37	58
7	J	55/56 (98%)	55 (100%)	0	100	100
8	K	104/106 (98%)	103 (99%)	1 (1%)	68	78
9	L	44/55 (80%)	41 (93%)	3 (7%)	14	36
11	Q	763/1011 (76%)	754 (99%)	9 (1%)	63	75
13	W	260/260 (100%)	258 (99%)	2 (1%)	73	80
14	X	48/467 (10%)	47 (98%)	1 (2%)	47	65
15	Y	102/105 (97%)	102 (100%)	0	100	100
16	a	86/110 (78%)	86 (100%)	0	100	100
16	e	82/110 (74%)	82 (100%)	0	100	100
17	b	64/79 (81%)	64 (100%)	0	100	100
17	f	64/79 (81%)	63 (98%)	1 (2%)	55	70
18	c	82/104 (79%)	82 (100%)	0	100	100
18	g	82/104 (79%)	80 (98%)	2 (2%)	43	64
19	d	79/105 (75%)	79 (100%)	0	100	100
19	h	76/105 (72%)	76 (100%)	0	100	100
20	k	16/929 (2%)	16 (100%)	0	100	100
21	A	1225/1747 (70%)	1201 (98%)	24 (2%)	48	66
22	B	984/1027 (96%)	944 (96%)	40 (4%)	27	49
23	C	235/252 (93%)	232 (99%)	3 (1%)	61	74
24	M	726/1524 (48%)	720 (99%)	6 (1%)	73	80
26	O	233/1017 (23%)	232 (100%)	1 (0%)	84	84
27	R	170/625 (27%)	169 (99%)	1 (1%)	78	83
28	S	98/268 (37%)	96 (98%)	2 (2%)	48	66
29	U	65/590 (11%)	65 (100%)	0	100	100
30	V	144/462 (31%)	142 (99%)	2 (1%)	59	72
31	Z	435/939 (46%)	433 (100%)	2 (0%)	81	83
All	All	7071/13061 (54%)	6957 (98%)	114 (2%)	54	70

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	36	THR
2	E	73	PHE
2	E	129	GLN
3	F	123	LEU
4	G	67	LEU
4	G	70	VAL
4	G	109	SER
5	H	15	ILE
5	H	37	MET
5	H	100	GLU
5	H	116	VAL
6	I	46	GLN
6	I	51	SER
6	I	124	THR
8	K	27	VAL
9	L	34	ILE
9	L	39	CYS
9	L	43	ILE
11	Q	263	THR
11	Q	293	LEU
11	Q	531	VAL
11	Q	674	ARG
11	Q	698	ILE
11	Q	752	VAL
11	Q	816	GLN
11	Q	817	CYS
11	Q	820	LEU
13	W	112	LEU
13	W	240	PHE
14	X	213	PHE
17	f	74	GLU
18	g	35	ARG
18	g	43	VAL
21	A	90	LEU
21	A	113	PHE
21	A	250	VAL
21	A	276	LEU
21	A	283	ILE
21	A	301	HIS
21	A	350	VAL
21	A	382	ARG
21	A	419	ILE
21	A	440	LEU

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Mol	Chain	Res	Type
21	A	555	LEU
21	A	567	LEU
21	A	674	THR
21	A	811	ILE
21	A	908	THR
21	A	942	VAL
21	A	1007	ILE
21	A	1124	LEU
21	A	1128	ILE
21	A	1129	ASN
21	A	1160	ARG
21	A	1166	LEU
21	A	1210	TRP
21	A	1351	ASP
22	B	21	LEU
22	B	23	GLN
22	B	56	GLN
22	B	90	GLN
22	B	115	LEU
22	B	152	ILE
22	B	176	GLU
22	B	180	ASP
22	B	218	THR
22	B	276	LEU
22	B	285	LEU
22	B	307	GLU
22	B	332	LYS
22	B	371	ARG
22	B	386	ASP
22	B	388	TYR
22	B	411	LEU
22	B	440	ILE
22	B	547	GLU
22	B	576	ILE
22	B	607	ILE
22	B	626	LEU
22	B	647	GLU
22	B	649	ASN
22	B	665	ILE
22	B	685	LYS
22	B	687	VAL
22	B	690	CYS

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Mol	Chain	Res	Type
22	B	731	GLN
22	B	738	THR
22	B	743	ARG
22	B	759	VAL
22	B	838	GLN
22	B	848	LEU
22	B	909	VAL
22	B	931	ILE
22	B	995	GLU
22	B	1006	VAL
22	B	1048	TYR
22	B	1067	ILE
23	C	5	ASN
23	C	75	SER
23	C	169	PHE
24	M	574	VAL
24	M	594	LEU
24	M	672	ASP
24	M	946	GLN
24	M	1012	GLU
24	M	1122	THR
26	O	2029	SER
27	R	570	TRP
28	S	158	TYR
28	S	182	ASN
30	V	66	LEU
30	V	100	LEU
31	Z	216	VAL
31	Z	567	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	30	GLN
2	E	133	GLN
5	H	46	GLN
5	H	133	HIS
6	I	84	HIS
8	K	29	ASN
8	K	69	HIS
11	Q	151	GLN
11	Q	278	HIS

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Mol	Chain	Res	Type
11	Q	373	ASN
11	Q	564	HIS
11	Q	860	GLN
13	W	173	ASN
13	W	184	HIS
16	a	68	GLN
16	a	85	GLN
17	b	93	GLN
19	d	49	HIS
19	d	109	HIS
16	e	39	HIS
18	g	31	HIS
19	h	49	HIS
21	A	96	HIS
21	A	122	ASN
21	A	143	HIS
21	A	152	ASN
21	A	742	ASN
21	A	791	GLN
21	A	804	HIS
21	A	1005	HIS
21	A	1032	GLN
21	A	1044	HIS
21	A	1101	GLN
21	A	1422	GLN
22	B	52	GLN
22	B	175	ASN
22	B	197	GLN
22	B	254	GLN
22	B	486	ASN
22	B	525	ASN
22	B	642	GLN
22	B	649	ASN
22	B	654	GLN
22	B	725	GLN
22	B	749	HIS
22	B	1021	HIS
22	B	1030	ASN
22	B	1040	GLN
22	B	1060	HIS
23	C	6	GLN
23	C	111	GLN

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Mol	Chain	Res	Type
23	C	260	GLN
24	M	287	ASN
24	M	412	ASN
24	M	421	GLN
24	M	561	GLN
24	M	577	GLN
24	M	652	GLN
24	M	921	GLN
24	M	956	ASN
24	M	1007	ASN
24	M	1059	HIS
24	M	1084	ASN
24	M	1151	ASN
26	O	1603	GLN
26	O	1635	GLN
26	O	1672	ASN
26	O	1678	ASN
26	O	1804	GLN
27	R	427	GLN
27	R	432	ASN
27	R	490	GLN
27	R	588	ASN
28	S	239	ASN
30	V	122	GLN
31	Z	234	HIS
31	Z	237	GLN
31	Z	519	GLN
31	Z	572	HIS
31	Z	714	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	P	20/46 (43%)	9 (45%)	3 (15%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	P	28	A
10	P	29	C
10	P	30	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	P	31	G
10	P	34	G
10	P	35	A
10	P	36	G
10	P	37	G
10	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	P	28	A
10	P	36	G
10	P	38	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	TPO	Z	775	31	8,10,11	1.10	0	10,14,16	2.06	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	TPO	Z	775	31	-	2/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
31	Z	775	TPO	P-OG1-CB	-5.94	107.18	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	Z	775	TPO	C-CA-CB-CG2
31	Z	775	TPO	N-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Z	775	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are 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
30	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	299:GLU	C	310:ASN	N	12.62

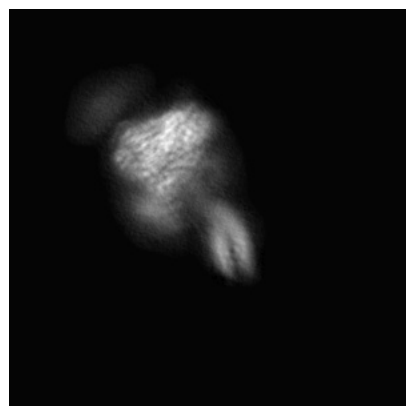
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54425. These allow visual inspection of the internal detail of the map and identification of artifacts.

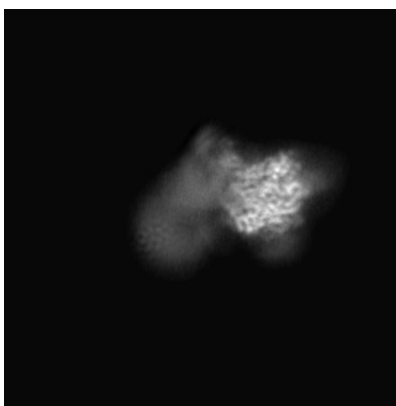
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

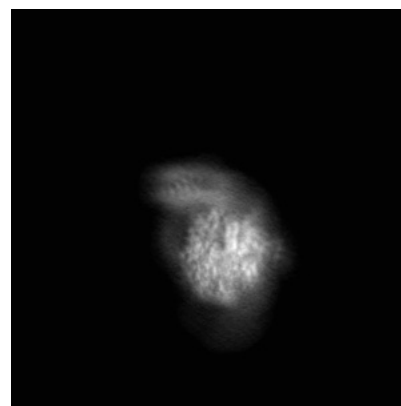
6.1.1 Primary map



X

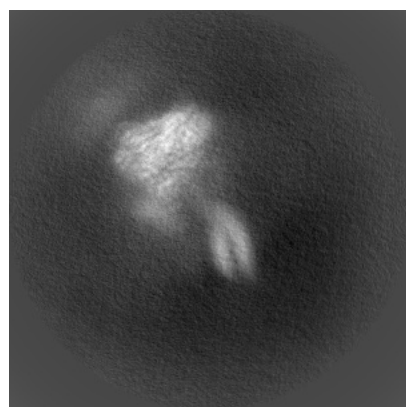


Y

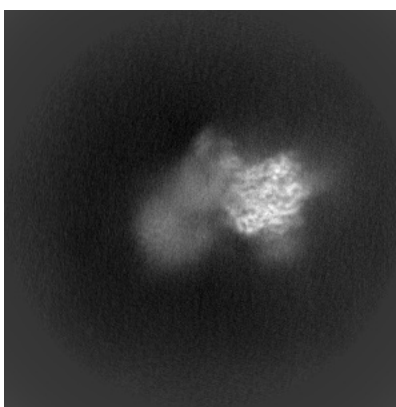


Z

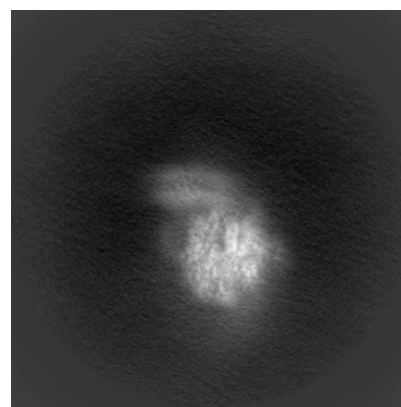
6.1.2 Raw map



X



Y

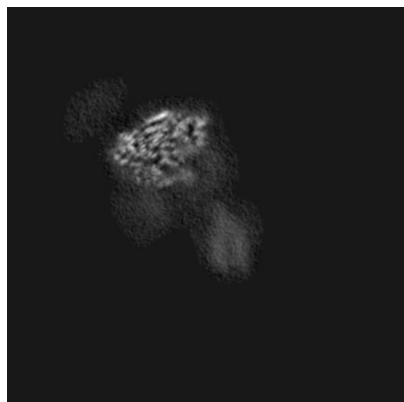


Z

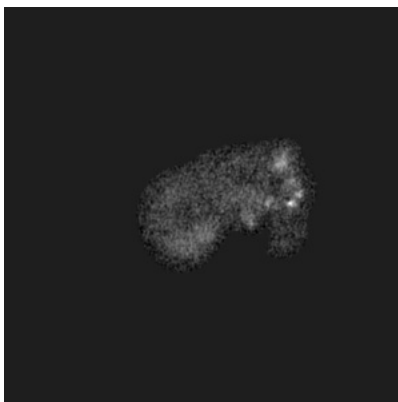
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

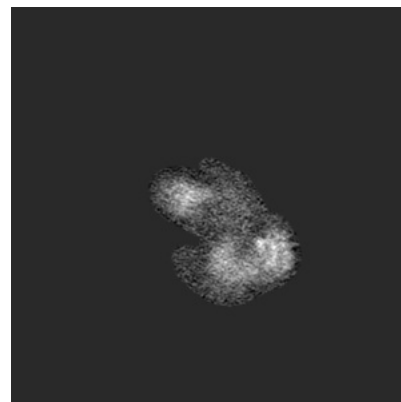
6.2.1 Primary map



X Index: 256

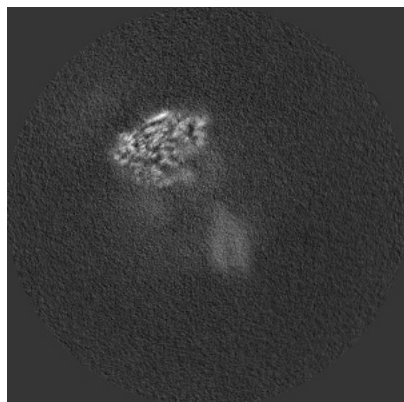


Y Index: 256

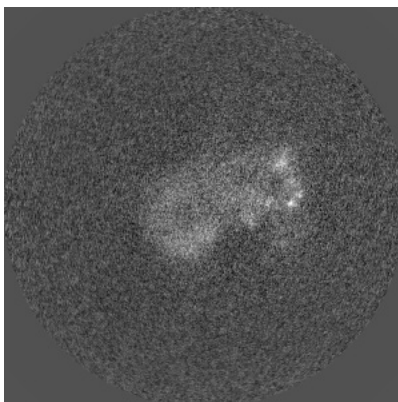


Z Index: 256

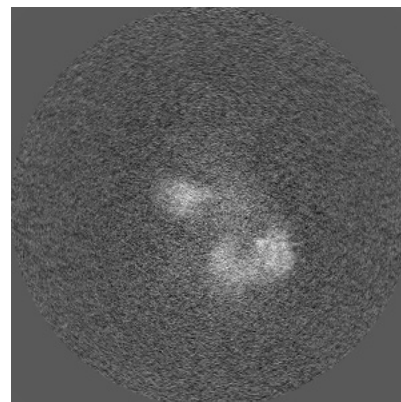
6.2.2 Raw map



X Index: 256



Y Index: 256

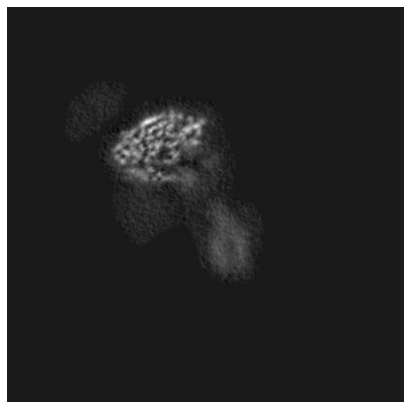


Z Index: 256

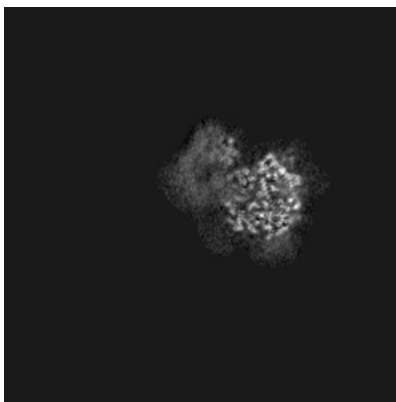
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 252

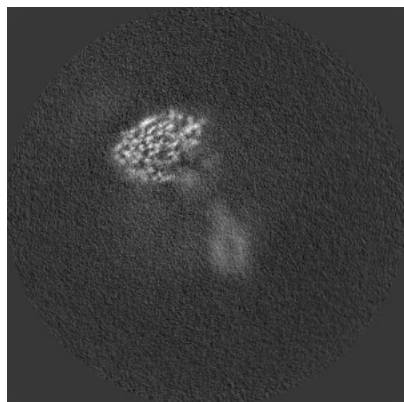


Y Index: 201

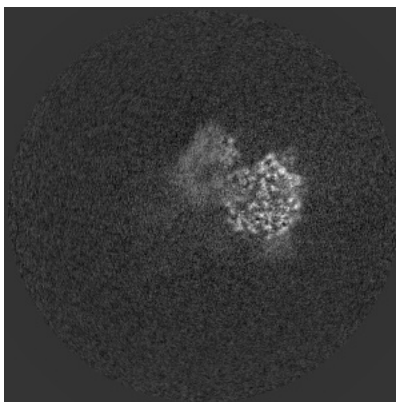


Z Index: 348

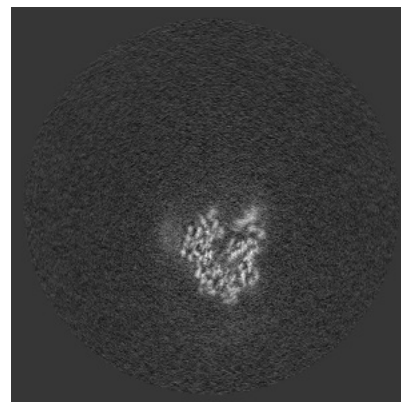
6.3.2 Raw map



X Index: 251



Y Index: 201

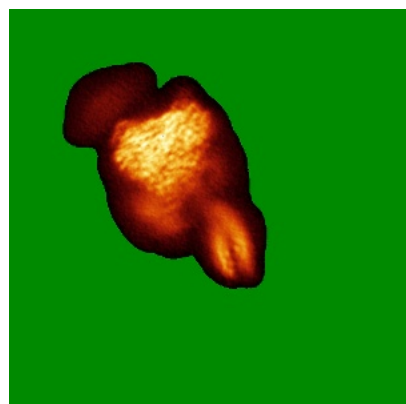


Z Index: 348

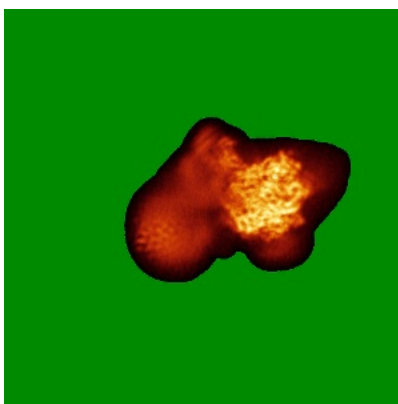
The images above show the largest variance slices of the map in three orthogonal directions.

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

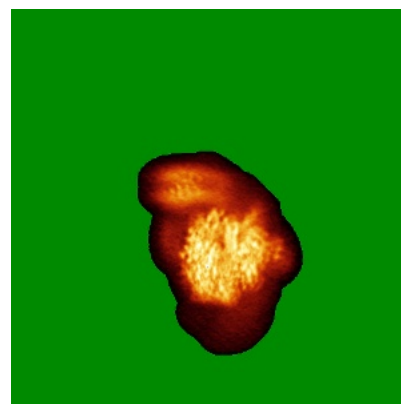
6.4.1 Primary map



X

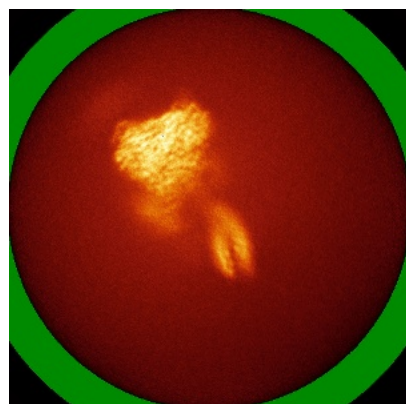


Y

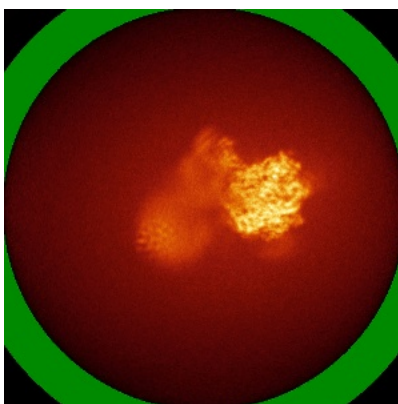


Z

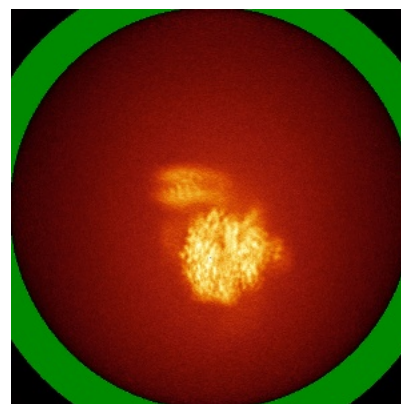
6.4.2 Raw map



X



Y

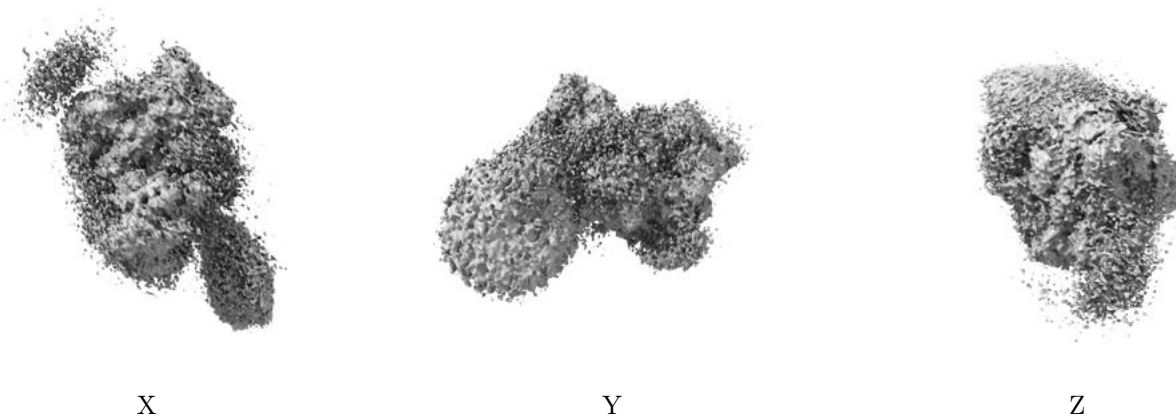


Z

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

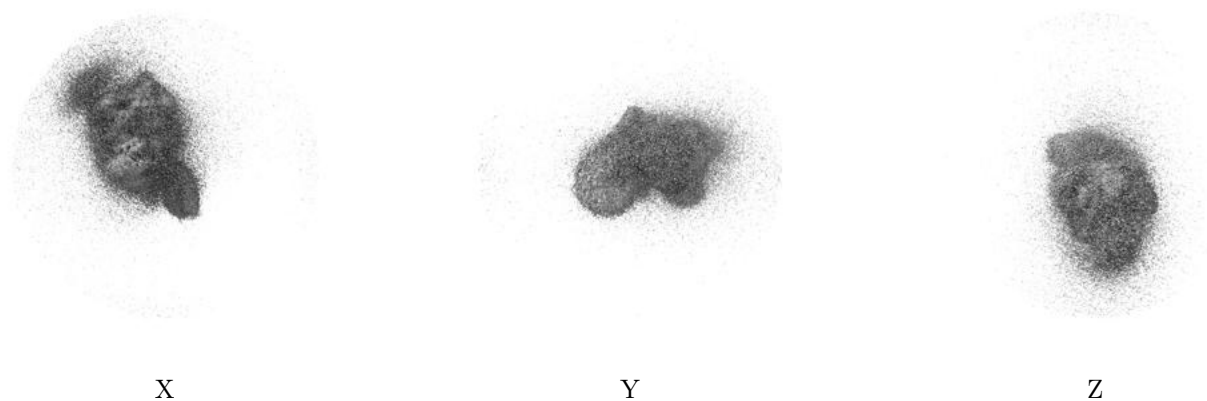
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

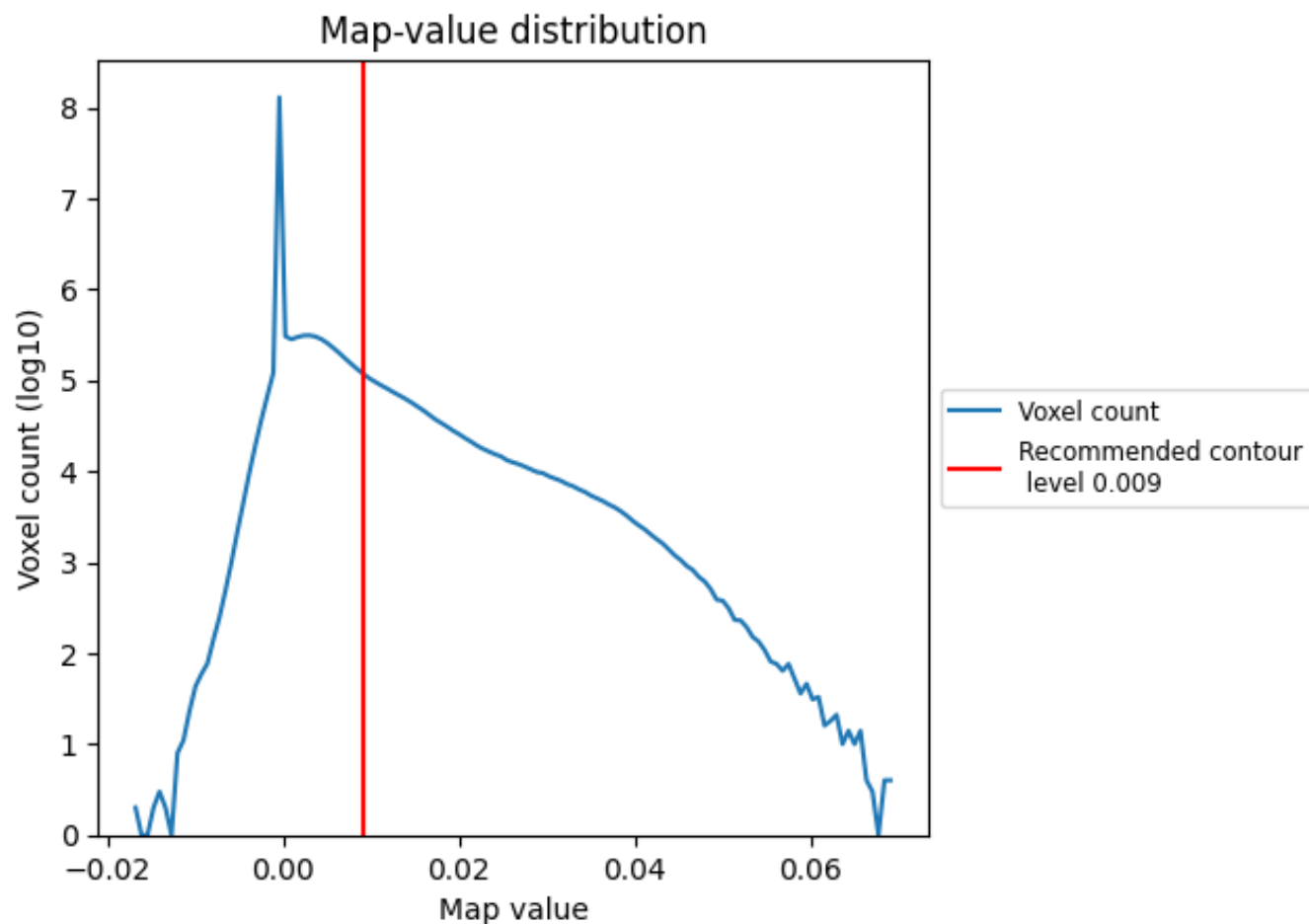
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

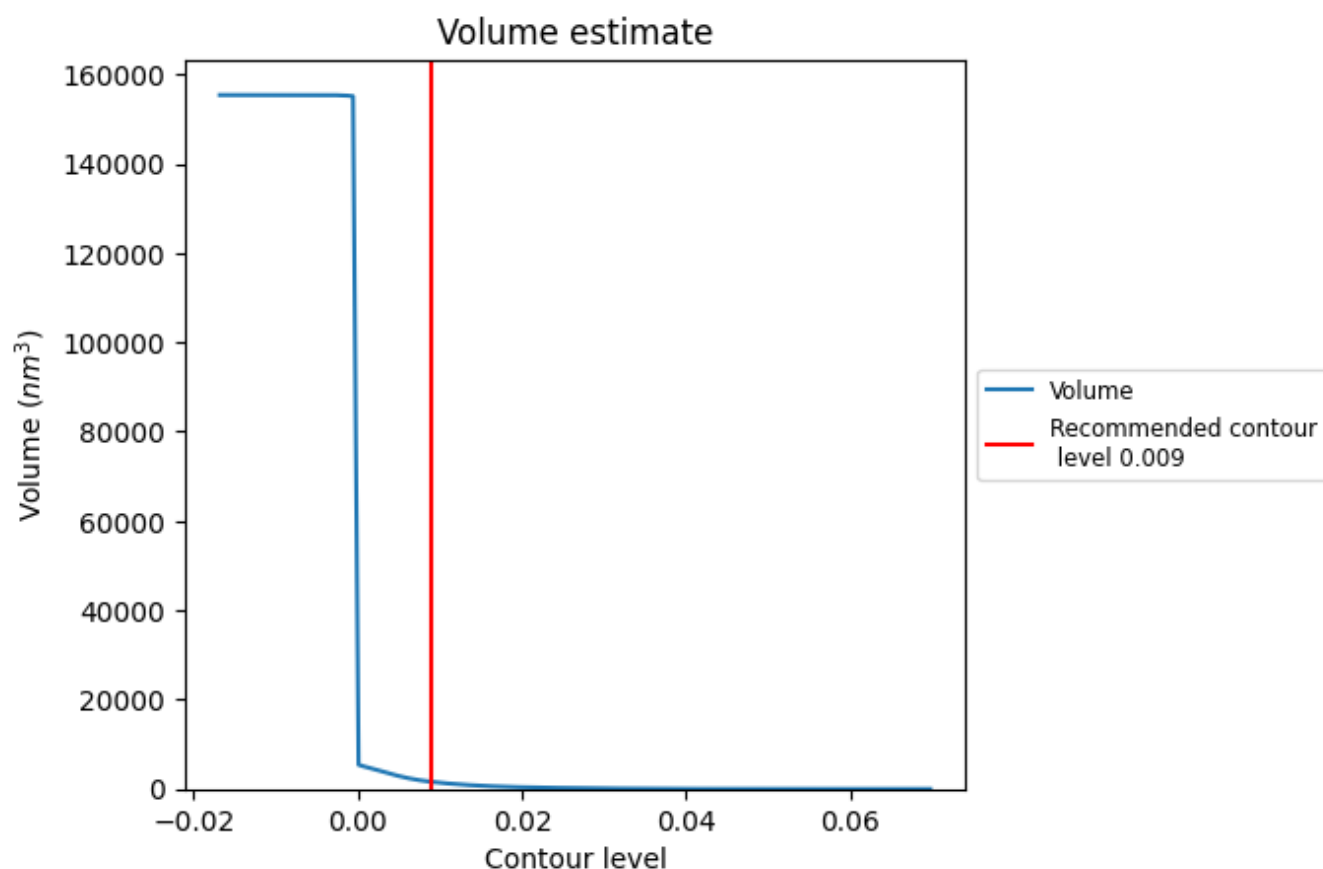
This section contains the results of statistical analysis of the map.

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.

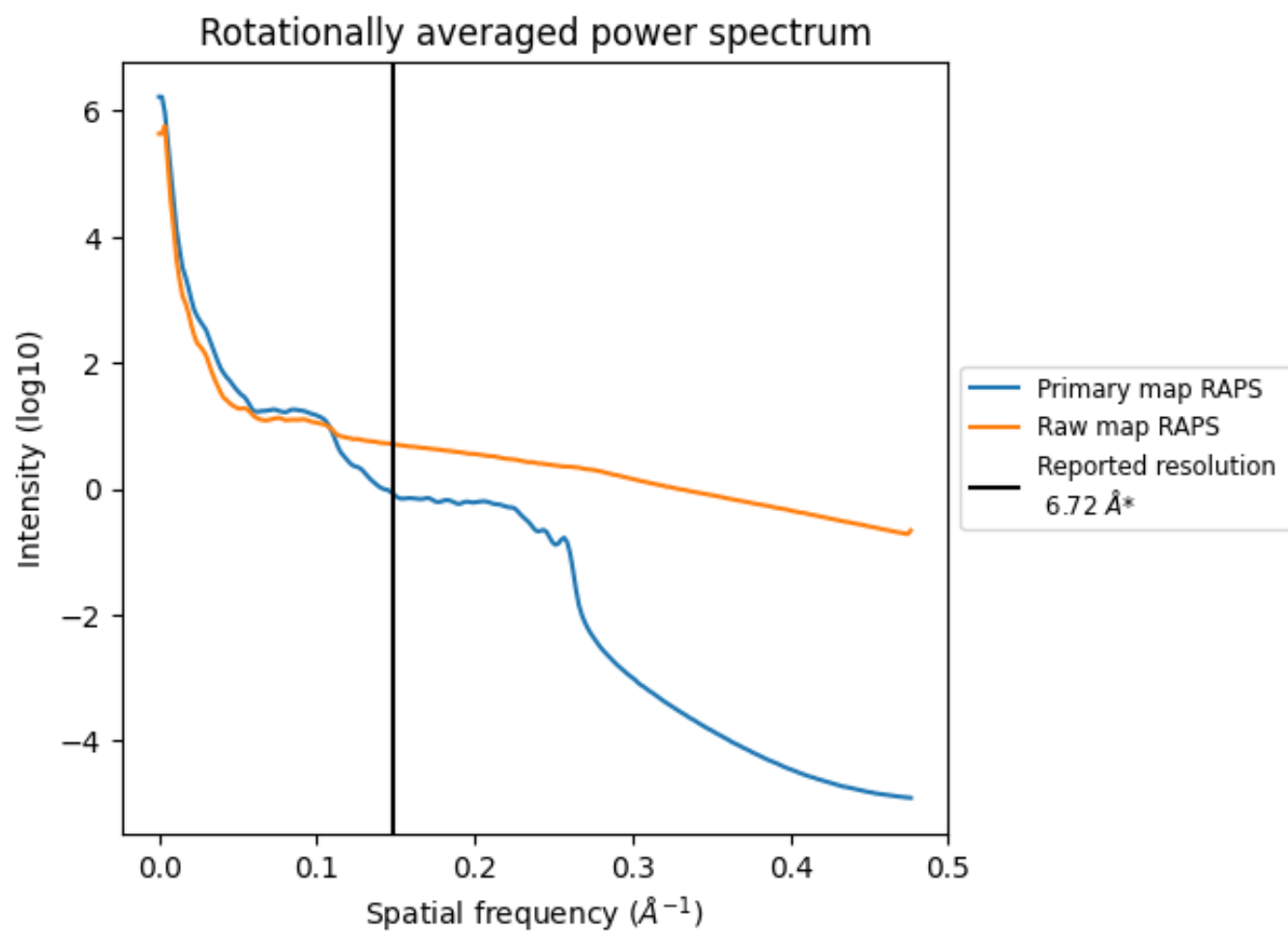
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1588 nm^3 ; this corresponds to an approximate mass of 1435 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 ⓘ

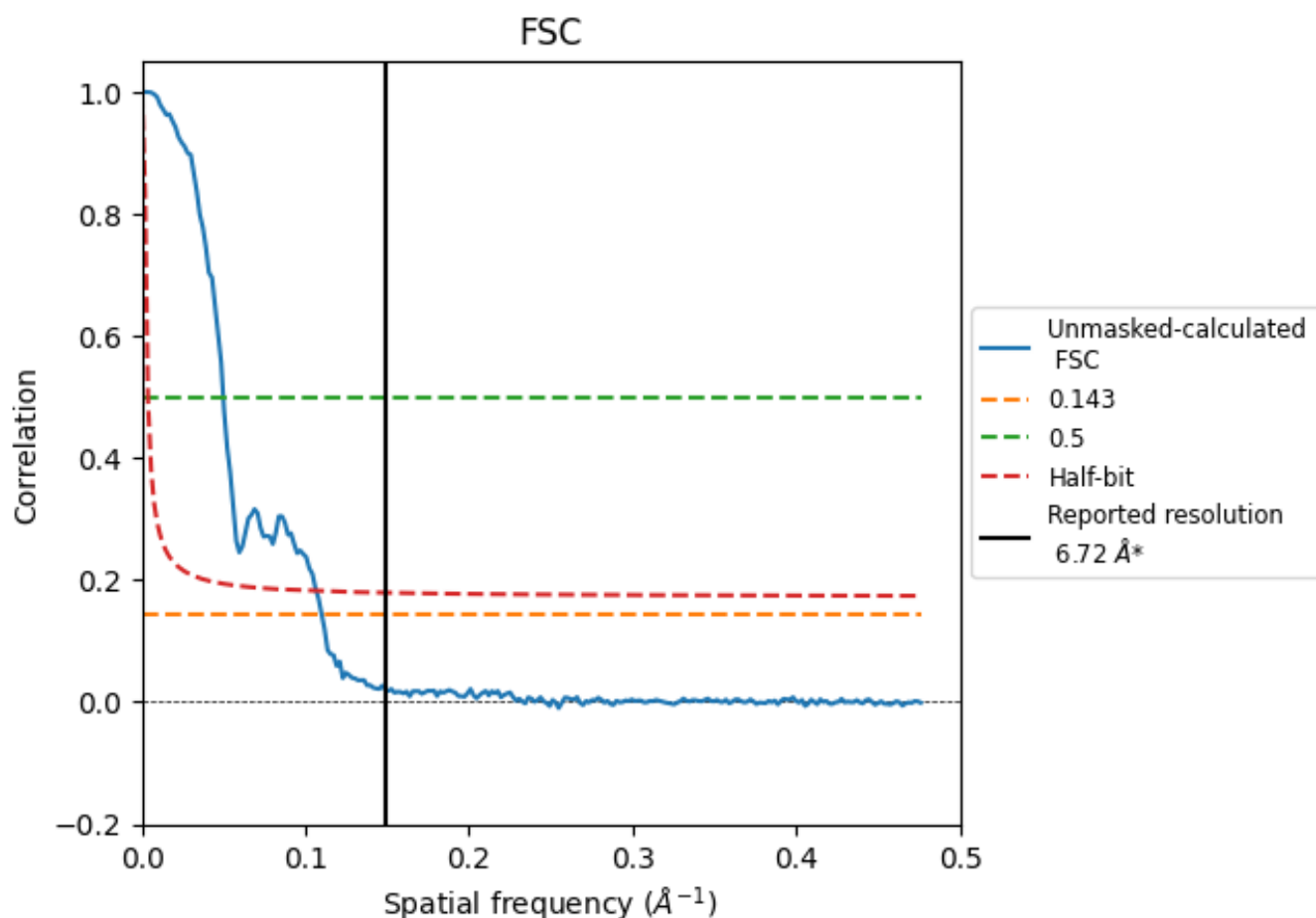


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.149 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

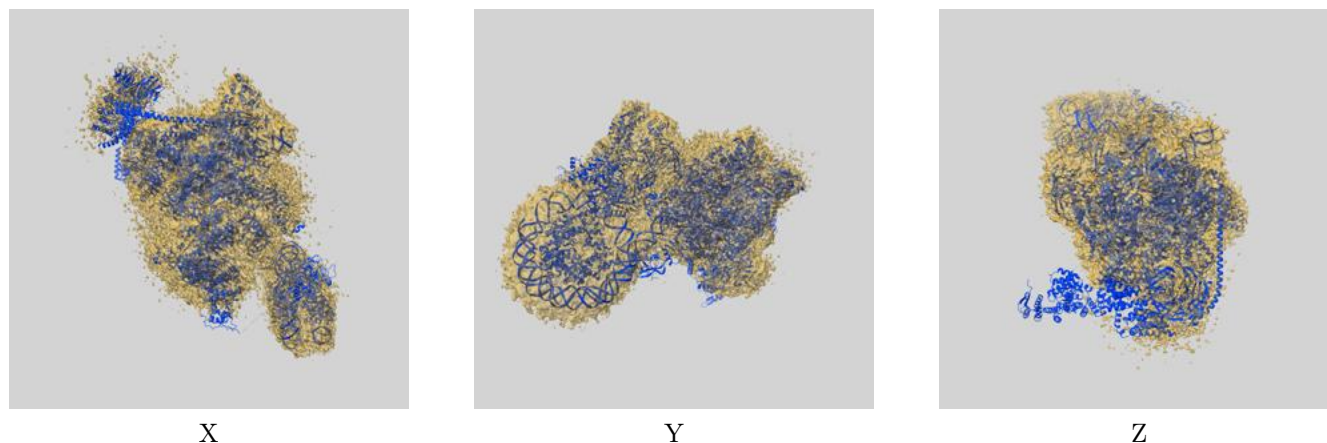
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.10	20.12	9.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.10 differs from the reported value 6.72 by more than 10 %

9 Map-model fit [i](#)

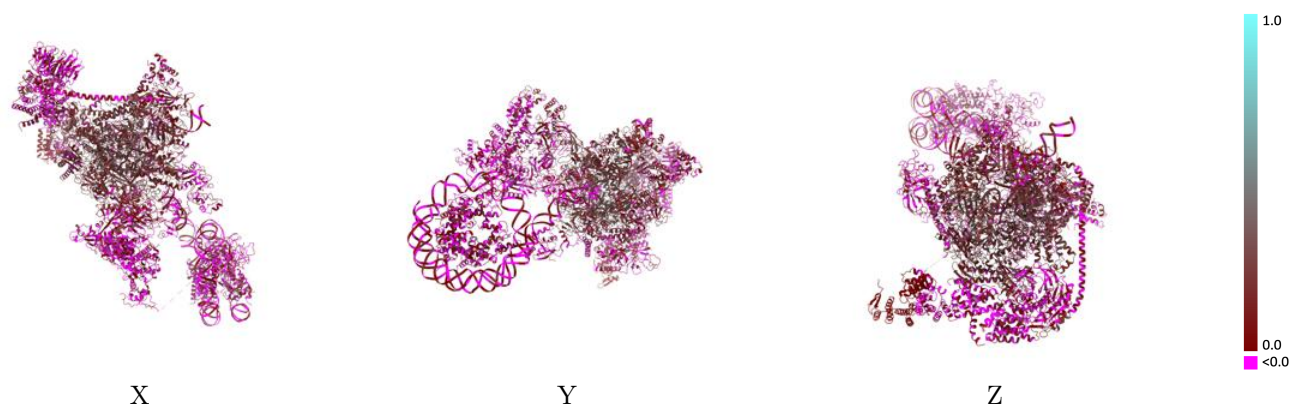
This section contains information regarding the fit between EMDB map EMD-54425 and PDB model 9S0U. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



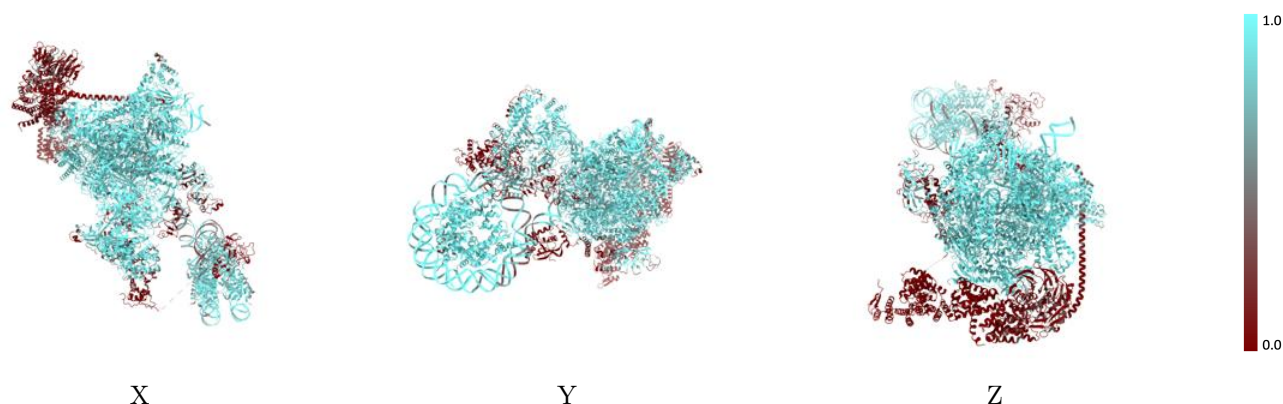
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



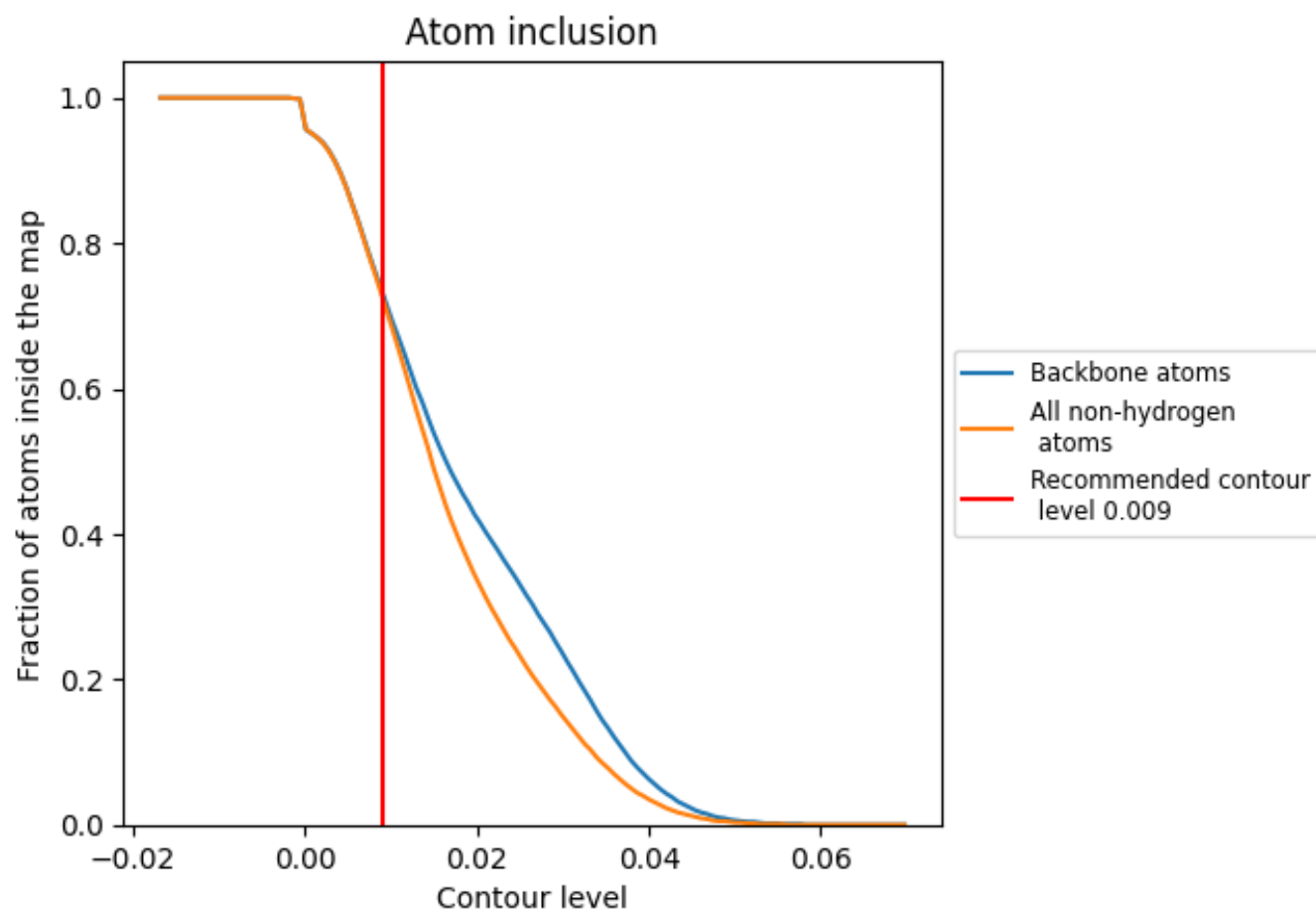
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.1080
A	 0.9780	 0.2370
B	 0.9740	 0.2300
C	 0.9820	 0.2070
D	 0.9710	 0.1310
E	 0.9790	 0.2060
F	 0.9790	 0.2550
G	 0.9550	 0.1360
H	 0.9620	 0.2270
I	 0.9880	 0.1830
J	 0.9590	 0.2350
K	 0.9810	 0.1810
L	 0.9500	 0.2180
M	 0.7290	 0.0200
N	 0.8450	 0.0450
O	 0.2110	 0.0120
P	 0.9670	 0.1610
Q	 0.0610	 0.0020
R	 0.1610	 0.0020
S	 0.8360	 0.1210
T	 0.8510	 0.0670
U	 0.5840	 0.0550
V	 0.3340	 0.0030
W	 0.1150	 -0.0060
X	 0.0120	 0.0150
Y	 0.4280	 0.0100
Z	 0.6410	 0.0500
a	 0.9340	 0.0090
b	 0.9310	 -0.0040
c	 0.9240	 0.0290
d	 0.8770	 -0.0020
e	 0.9920	 0.0310
f	 0.9780	 0.0520
g	 0.9520	 0.0280
h	 0.9090	 0.0590
k	 0.9420	 -0.0310

