



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 12:32 AM UTC

PDB ID : 8BYQ / pdb_00008byq
EMDB ID : EMD-16331
Title : RNA polymerase II pre-initiation complex with the proximal +1 nucleosome (PIC-Nuc10W)
Authors : Abril-Garrido, J.; Dienemann, C.; Grabbe, F.; Velychko, T.; Lidschreiber, M.; Wang, H.; Cramer, P.
Deposited on : 2022-12-14
Resolution : 4.10 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:

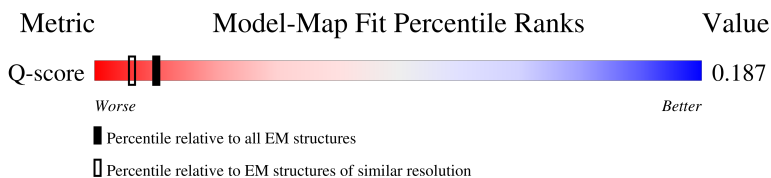
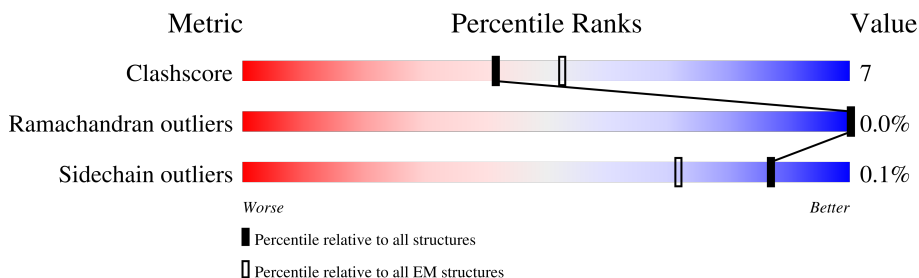
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	0	782	 66% 17% 16%
2	1	760	 75% 25%
3	2	548	 67% 7% 26%
4	3	462	 80% 18% .

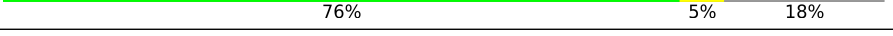
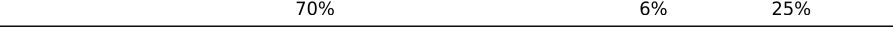
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Mol	Chain	Length	Quality of chain
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	8	346	
10	9	323	
11	A	1970	
12	B	1174	
13	C	275	
14	D	142	
15	E	210	
16	F	127	
17	G	172	
18	H	150	
19	I	125	
20	J	67	
21	K	117	
22	L	58	
23	M	316	
24	N	210	
25	O	339	
26	Q	517	
27	R	249	
28	T	210	
29	U	376	

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Mol	Chain	Length	Quality of chain
30	V	109	
31	W	196	
32	X	291	
33	a	136	
33	e	136	
34	b	103	
34	f	103	
35	c	130	
35	g	130	
36	d	126	
36	h	126	

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 85971 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 General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	653	Total	C	N	O	S	0	0
			5189	3303	899	957	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	760	Total	C	N	O	S	0	0
			6034	3853	1053	1099	29		

- Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	408	Total	C	N	O	S	0	0
			2643	1646	486	503	8		

- Molecule 4 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	452	Total	C	N	O	S	0	0
			3589	2307	631	637	14		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	366	Total	C	N	O	S	0	0
			2710	1702	476	506	26		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	263	Total	C	N	O	S	0	0
			2064	1322	344	379	19		

- Molecule 7 is a protein called General transcription factor IIIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	273	Total	C	N	O	S	0	0
			2233	1397	391	432	13		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	298	Total	C	N	O	S	0	0
			2370	1531	404	424	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 14 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 22 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 24 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	198	Total	C	N	O	P	0	0
			4051	1921	746	1187	197		

- Molecule 25 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 26 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 27 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 28 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	198	Total	C	N	O	P	0	0
			4061	1924	755	1185	197		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 30 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 31 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 32 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 33 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
33	e	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	103	ALA	GLY	engineered mutation	UNP P84233
e	103	ALA	GLY	engineered mutation	UNP P84233

- Molecule 34 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
34	f	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

- Molecule 35 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	109	Total	C	N	O		0	0
			843	531	167	145			
35	g	106	Total	C	N	O		0	0
			818	516	160	142			

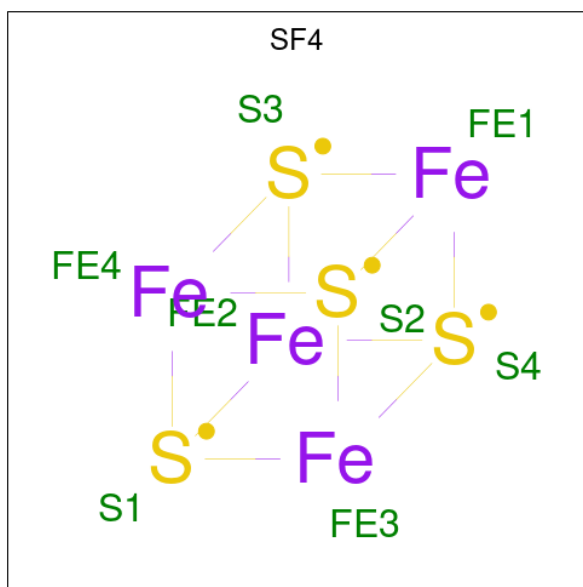
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	conflict	UNP P06897
g	100	ARG	GLY	conflict	UNP P06897

- Molecule 36 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
36	h	95	Total	C	N	O	S	0	0
			744	468	134	140	2		

- Molecule 37 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	4	3	Total	Zn	0
			3	3	
38	5	1	Total	Zn	0
			1	1	
38	7	2	Total	Zn	0
			2	2	
38	A	2	Total	Zn	0
			2	2	
38	B	1	Total	Zn	0
			1	1	
38	C	1	Total	Zn	0
			1	1	
38	I	2	Total	Zn	0
			2	2	

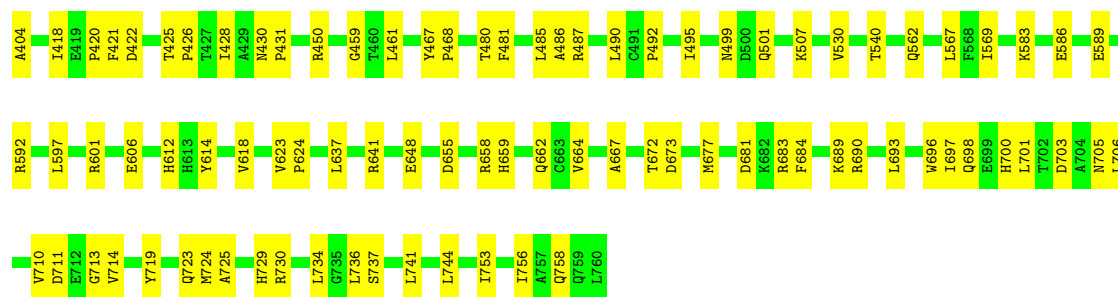
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Mol	Chain	Residues	Atoms		AltConf
38	J	1	Total 1	Zn 1	0
38	L	1	Total 1	Zn 1	0
38	M	1	Total 1	Zn 1	0
38	W	1	Total 1	Zn 1	0

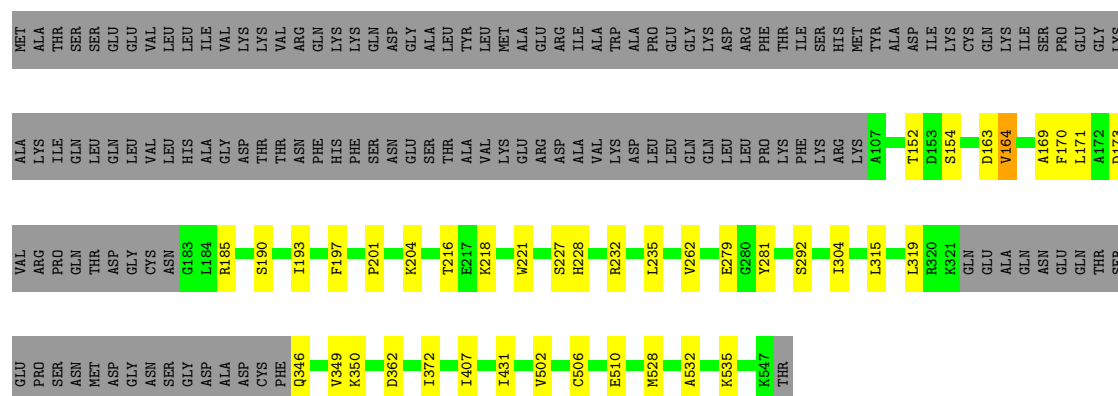
- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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



• Molecule 3: General transcription factor IIH subunit 1

Chain 2: 67% 7% 26%



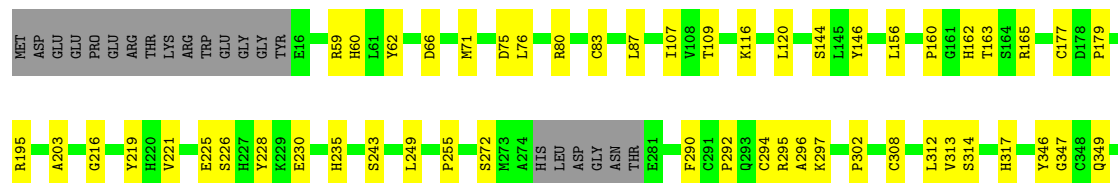
• Molecule 4: General transcription factor IIH subunit 4

Chain 3: 80% 18%



• Molecule 5: General transcription factor IIH subunit 2

Chain 4: 78% 14% 7%



[illegible]

Chain A: 61% 12% 28%

Sequence Logo: MET, GLY, HIS, GLY, VAL, GLY, GLN, PRO, PRO, SER, GLY, ASP, S11, Q22, L31, M34, I41, G55, D59, H61, C71, Q72, T73, C74, H84, F85, G86, H87, E88, L89, L90, H95, M122, K127, R140, D146, K149, E155, GLY, GLY, GLU, GLU, MET, ASP, LYS, LYS.

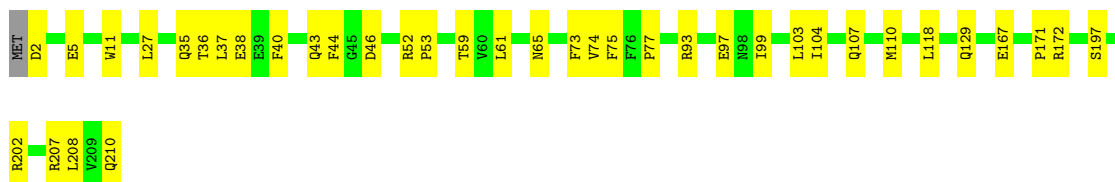
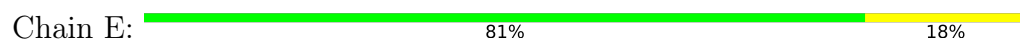
Amino Acid Sequence:

PRO	GLN	ALA	ILE	GLU	V1141	L909	I672	R483	K317	PHE
SER	SER	ALA	PRO	GLU	F1142	L909	I672	N485	R334	GLY
PRO	PRO	ASP	LEU	GLU	L1143	D937	L680		P335	VAL
THR	THR	ALA	GLY	VAL	Q1146	F956	I687	V488	L336	GLN
SER	TYR	SER	ALA	VAL	S1147	F956	I687		K337	PRO
PRO	SER	GLY	ALA	ASP	D1150	M959	I706	P491	Q341	GLU
PRO	PRO	GLY	THR	GLY	H1163	R967	V713	D495	V350	SER
THR	THR	GLY	PRO	THR	R1167	G973	T728	D496	L354	GLY
SER	THR	GLY	MET	GLY	G1300	G973	T728	D497	LEU	ASP
THR	TYR	SER	PHE	GLY	I1301	G973	T728			
PRO	PRO	ALA	PHE	GLY	T1170	P980	T736	M501	THR	
THR	THR	ALA	GLY	GLY	C981	P980	T736	L503	LYS	
TYR	TYR	THR	SER	THR	T1173	R985	Q740	M502	LYS	
SER	SER	SER	ALA	ALA	D1178	R986	R743	L525	GLY	
PRO	PRO	THR	PRO	PRO		R987	R743	V526	HIS	
SER	THR	THR	SER	SER	W1192	W988	F766	N531	G192	
PRO	PRO	GLY	MET	GLY	W1210	K992	A774	R532	W202	
THR	THR	GLY	GLY	GLY	L1211	K992	K775	P533	LYS	
PRO	PRO	GLY	ILE	GLY	L1216	H1005	I781	V534	VAL	
THR	THR	GLY	GLY	GLY	D1217	P1006	I781	M535	ASN	
ASN	ASN	PRO	PRO	PRO	R1218	I1007	V787	L542	GLU	
PRO	PRO	GLY	ALA	ALA	K1219	I1022	V787		ASP	
SER	PRO	PRO	MET	THR	H1220	I1022	G801	T549	SER	
THR	THR	SER	PRO	PRO	M1221	M1036	F802	L564	GLN	
SER	PRO	PRO	THR	THR			K803		GLY	
PRO	PRO	TYR	ASN	ASN	T1227	F1058	H804	M570	K212	
THR	THR	ILE	GLN	GLN	M1228	M1228	R805		D230	
SER	TYR	GLY	GLY	GLY	E1229	F1076	P817	P577	F234	
PRO	PRO	SER	ALA	ALA	Q1230	G1088	P808	A575		
THR	THR	PRO	THR	THR	M1242	G1088	I811	L579	P414	
GLY	GLY	GLY	ALA	GLY	C1245	A1099	P817	P584	R421	
PRO	PRO	ALA	TYR	TYR	I1246	M1102	P817	L585	R241	
THR	THR	MET	GLY	GLY	F1247		T634	V586	D425	
ALA	SER	SER	ALA	ALA	C1430		T634		R244	
PRO	PRO	PRO	TRP	TRP	N1248	H1105	E845	K589	P245	
SER	PRO	SER	SER	SER	D1249	THR	E845	H606	L246	
PRO	PRO	TYR	PRO	PRO	D1250	PHE	PHE		W247	
SER	SER	TYR	SER	SER		HIS	HIS		R430	
VAL	VAL	THR	VAL	VAL	K1254	TYR	I865	P617	V250	
GLY	GLY	SER	GLY	GLY	L1255	ALA	E869	V618	T251	
THR	THR	SER	SER	SER	V1256	GLY	S870	L621	V252	
PRO	PRO	PRO	GLY	GLY	L1257	VAL	V871		L253	
THR	THR	ALA	THR	THR	R1258	SER	M872	H465	P254	
PRO	PRO	THR	MET	MET	I1259	ALA	V873	C641	V255	
SER	SER	GLU	PRO	PRO	K1115	K1115		M467		
PRO	PRO									

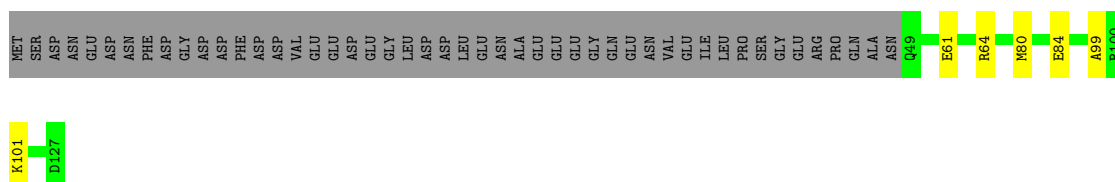




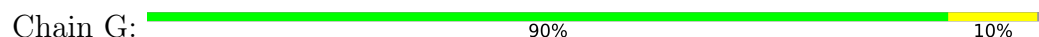
- Molecule 15: DNA-directed RNA polymerase II subunit E



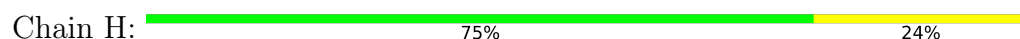
- Molecule 16: DNA-directed RNA polymerase II subunit F



- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 19: DNA-directed RNA polymerase II subunit RPB9



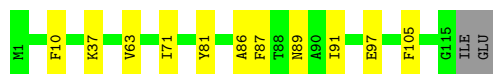
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  76% 19% .



- Molecule 21: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  89% 9% .



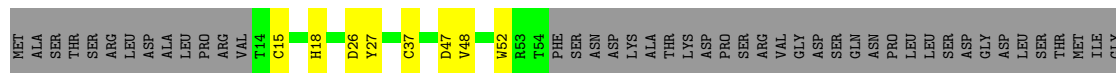
- Molecule 22: RNA polymerase II subunit K

Chain L:  55% 21% 24%



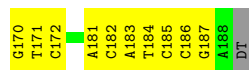
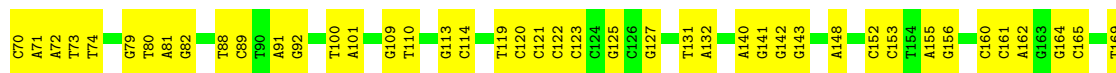
- Molecule 23: Transcription initiation factor IIB

Chain M:  70% 9% 20%

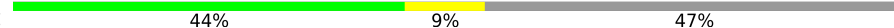


- Molecule 24: Non-template DNA

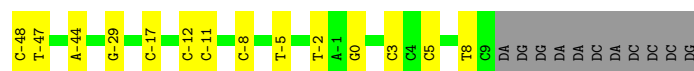
Chain N:  53% 41% 6%



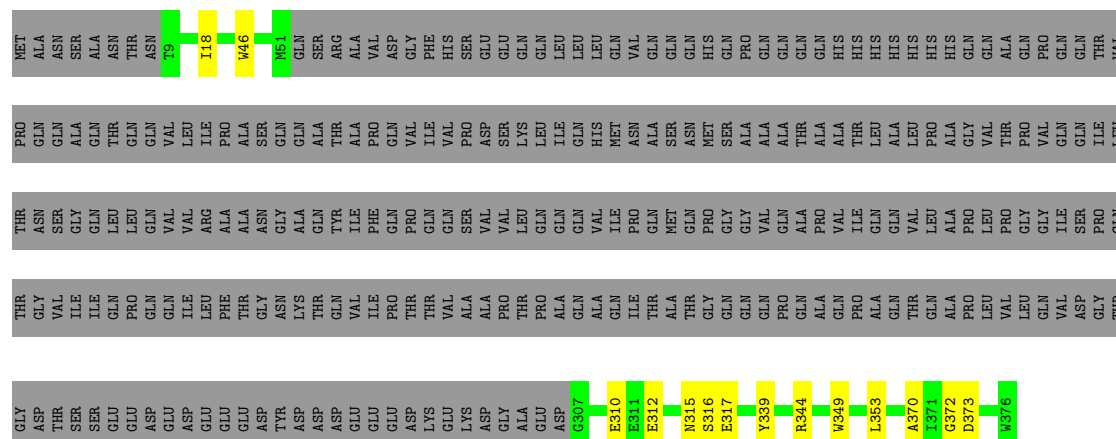
- Molecule 25: TATA-box-binding protein

Chain O:  44% 9% 47%

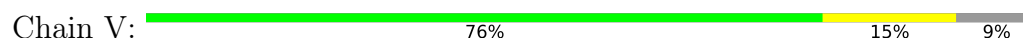




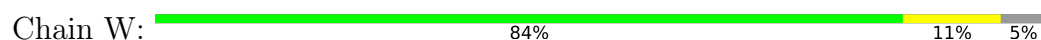
• Molecule 29: Transcription initiation factor IIA subunit 1



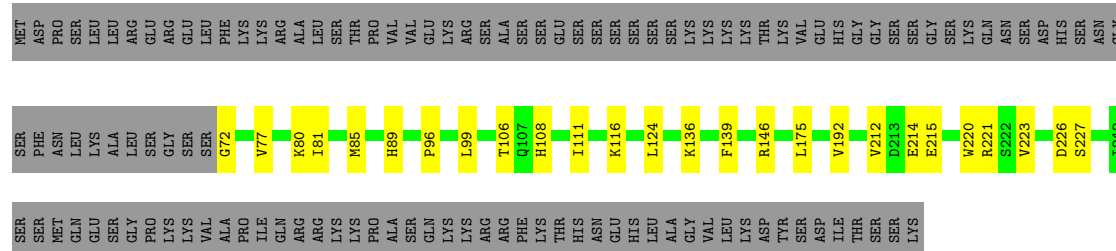
• Molecule 30: Transcription initiation factor IIA subunit 2



• Molecule 31: General transcription factor IIE subunit 1

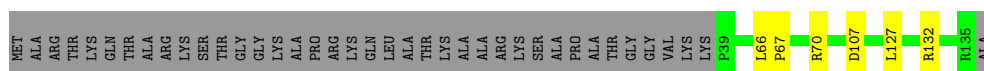


• Molecule 32: Transcription initiation factor IIE subunit beta

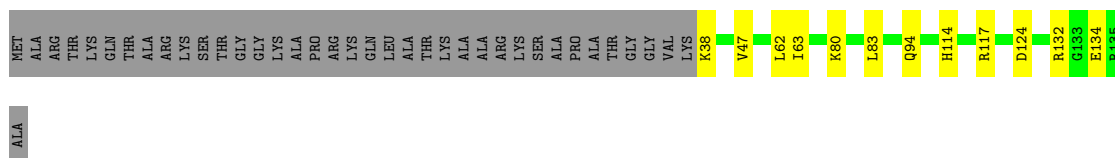


• Molecule 33: Histone H3.2





- Molecule 33: Histone H3.2



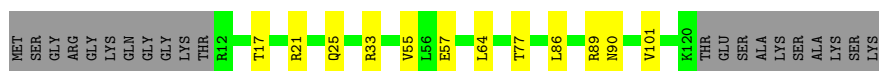
- Molecule 34: Histone H4



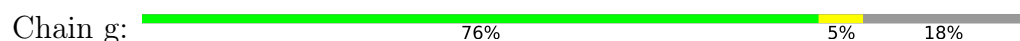
- Molecule 34: Histone H4



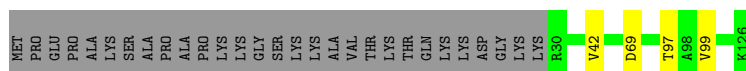
- Molecule 35: Histone H2A type 1



- Molecule 35: Histone H2A type 1

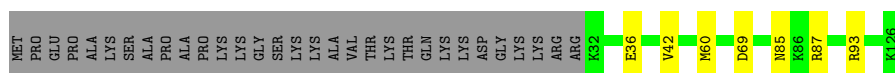


- Molecule 36: Histone H2B 1.1



- Molecule 36: Histone H2B 1.1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101994	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	21.074	Depositor
Minimum map value	-5.711	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, MG, SF4

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	0	0.15	0/5294	0.52	0/7158
2	1	0.21	0/6158	0.59	0/8342
3	2	0.32	0/2683	0.59	0/3672
4	3	0.13	0/3672	0.51	0/4979
5	4	0.15	0/2764	0.54	0/3754
6	5	0.16	0/2101	0.59	0/2843
7	6	0.13	0/528	0.43	0/713
8	7	0.17	0/2269	0.54	0/3053
9	8	0.17	0/2429	0.59	0/3295
10	9	0.16	0/2384	0.51	0/3220
11	A	0.31	0/11479	0.55	0/15496
12	B	0.38	0/9257	0.58	0/12493
13	C	0.36	0/2102	0.58	0/2857
14	D	0.13	0/1064	0.41	0/1428
15	E	0.24	0/1752	0.47	0/2366
16	F	0.31	0/646	0.55	0/871
17	G	0.18	0/1382	0.48	0/1874
18	H	0.29	0/1207	0.53	0/1628
19	I	0.20	0/949	0.48	0/1284
20	J	0.41	0/516	0.66	0/696
21	K	0.34	0/939	0.52	0/1271
22	L	0.35	0/378	0.74	0/500
23	M	0.26	0/1983	0.49	0/2679
24	N	0.32	0/4543	0.67	0/7009
25	O	0.18	0/1448	0.47	0/1948
26	Q	0.13	0/1167	0.40	0/1576
27	R	0.17	0/1817	0.41	0/2445
28	T	0.30	0/4557	0.63	0/7033
29	U	0.14	0/945	0.41	0/1274
30	V	0.14	0/816	0.41	0/1105
31	W	0.15	0/1560	0.47	0/2097
32	X	0.13	0/1427	0.42	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.11	0/814	0.45	0/1092
33	e	0.12	0/823	0.41	0/1104
34	b	0.10	0/660	0.40	0/883
34	f	0.13	0/660	0.44	0/883
35	c	0.10	0/853	0.37	0/1149
35	g	0.11	0/828	0.41	0/1117
36	d	0.16	0/777	0.46	0/1041
36	h	0.18	0/755	0.43	0/1013
All	All	0.25	0/88386	0.54	0/121157

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5189	0	5164	93	0
2	1	6034	0	6002	135	0
3	2	2643	0	2044	32	0
4	3	3589	0	3621	61	0
5	4	2710	0	2538	36	0
6	5	2064	0	2099	39	0
7	6	522	0	528	8	0
8	7	2233	0	2210	30	0
9	8	2370	0	2391	28	0
10	9	2334	0	2357	8	0
11	A	11274	0	11406	149	0
12	B	9076	0	9116	105	0
13	C	2059	0	2008	31	0
14	D	1050	0	1033	11	0
15	E	1721	0	1737	24	0
16	F	636	0	665	6	0
17	G	1351	0	1358	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	1186	0	1147	22	0
19	I	928	0	859	15	0
20	J	507	0	523	11	0
21	K	920	0	942	9	0
22	L	373	0	379	11	0
23	M	1953	0	1990	23	0
24	N	4051	0	2222	69	0
25	O	1422	0	1514	23	0
26	Q	1138	0	1103	14	0
27	R	1788	0	1819	29	0
28	T	4061	0	2221	49	0
29	U	930	0	888	12	0
30	V	806	0	818	9	0
31	W	1535	0	1539	17	0
32	X	1403	0	1428	19	0
33	a	802	0	841	4	0
33	e	811	0	853	8	0
34	b	653	0	696	7	0
34	f	653	0	696	11	0
35	c	843	0	908	10	0
35	g	818	0	877	5	0
36	d	766	0	797	4	0
36	h	744	0	771	8	0
37	1	8	0	0	0	0
38	4	3	0	0	0	0
38	5	1	0	0	0	0
38	7	2	0	0	0	0
38	A	2	0	0	0	0
38	B	1	0	0	0	0
38	C	1	0	0	0	0
38	I	2	0	0	0	0
38	J	1	0	0	0	0
38	L	1	0	0	0	0
38	M	1	0	0	0	0
38	W	1	0	0	0	0
39	A	1	0	0	0	0
All	All	85971	0	82108	1044	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1044) 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)
11:A:74:CYS:SG	11:A:84:HIS:CE1	2.49	1.04
12:B:905:ASP:OD1	12:B:924:ARG:NH1	2.11	0.84
12:B:953:ASP:OD1	13:C:36:ARG:NH2	2.13	0.82
15:E:46:ASP:O	15:E:52:ARG:NH1	2.14	0.81
5:4:349:GLN:O	6:5:146:ARG:NH2	2.13	0.80
12:B:933:ASP:OD2	12:B:1050:ARG:NH2	2.15	0.79
24:N:29:DC:O2	28:T:-29:DG:N2	2.17	0.76
24:N:17:DG:N2	28:T:-17:DC:O2	2.14	0.76
15:E:77:PRO:O	15:E:107:GLN:NE2	2.16	0.74
1:0:636:GLU:HG2	1:0:639:ARG:HH22	1.53	0.74
2:1:22:PHE:HB3	2:1:753:ILE:HG21	1.66	0.74
24:N:-5:DG:O6	28:T:5:DC:N4	2.18	0.74
24:N:-5:DG:N1	28:T:5:DC:N3	2.34	0.74
1:0:46:VAL:HG21	1:0:155:PHE:HB2	1.70	0.74
2:1:690:ARG:O	2:1:698:GLN:NE2	2.22	0.72
2:1:56:ILE:HG21	2:1:70:LEU:HD22	1.69	0.72
2:1:237:HIS:CE1	2:1:662:GLN:HB2	2.24	0.71
12:B:60:GLU:OE2	27:R:140:ARG:NH1	2.23	0.71
22:L:32:ASP:OD2	22:L:37:ARG:NH2	2.18	0.71
1:0:628:SER:O	1:0:676:ARG:NH2	2.24	0.71
11:A:428:ASP:OD2	11:A:430:ARG:NH1	2.22	0.71
11:A:535:MET:O	11:A:669:TYR:OH	2.08	0.71
12:B:513:GLU:OE2	12:B:525:ASN:ND2	2.24	0.70
11:A:889:LEU:O	11:A:890:ARG:NH1	2.24	0.70
12:B:812:ARG:NH1	12:B:900:GLU:OE2	2.25	0.70
24:N:11:DG:H2"	24:N:12:DG:N7	2.07	0.70
2:1:319:VAL:HG11	2:1:324:ARG:HH21	1.55	0.70
11:A:1434:GLU:HG2	11:A:1437:ASP:HB2	1.71	0.69
11:A:1036:ASN:OD1	15:E:202:ARG:NH1	2.25	0.69
12:B:294:ASP:OD2	12:B:379:ARG:NH1	2.24	0.69
25:O:206:GLU:OE1	25:O:236:LYS:NZ	2.24	0.69
2:1:145:GLN:HA	2:1:148:HIS:CE1	2.27	0.69
1:0:668:GLN:NE2	7:6:67:SER:O	2.26	0.68
11:A:71:CYS:SG	11:A:74:CYS:HB2	2.32	0.68
11:A:465:HIS:ND1	11:A:467:MET:HE2	2.07	0.68
13:C:37:VAL:HG13	13:C:41:GLU:HB2	1.75	0.68
4:3:7:ARG:NH1	7:6:51:ASN:O	2.26	0.68
12:B:505:LEU:HD22	12:B:509:VAL:HB	1.75	0.68
23:M:18:HIS:CE1	23:M:37:CYS:HB2	2.29	0.68
9:8:264:ALA:HB1	9:8:268:LEU:HD22	1.73	0.67
27:R:175:ARG:HE	27:R:209:PRO:HA	1.59	0.67
11:A:497:ASP:O	12:B:942:LYS:HE2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:176:ARG:HD2	9:8:179:ARG:HH21	1.59	0.67
2:1:592:ARG:NH1	5:4:177:CYS:SG	2.67	0.67
6:5:160:ARG:NH1	6:5:233:PRO:O	2.24	0.67
5:4:294:CYS:HB3	5:4:308:CYS:SG	2.34	0.66
12:B:1035:ARG:NH1	12:B:1036:LYS:O	2.28	0.66
2:1:237:HIS:HE1	2:1:662:GLN:HB2	1.59	0.66
24:N:74:DT:OP1	35:c:21:ARG:NH2	2.28	0.66
18:H:130:ASN:HA	18:H:133:HIS:CE1	2.31	0.66
12:B:643:LEU:HD11	12:B:656:LEU:HD11	1.77	0.66
12:B:910:THR:HG22	22:L:43:ILE:HA	1.77	0.66
35:g:33:ARG:NH2	36:h:36:GLU:OE1	2.24	0.65
24:N:17:DG:N1	28:T:-17:DC:N3	2.36	0.65
13:C:180:ALA:O	20:J:42:ARG:NH2	2.29	0.65
4:3:438:LYS:HE3	4:3:440:LEU:HD11	1.79	0.65
12:B:677:MET:H	12:B:682:LEU:HG	1.61	0.65
12:B:1059:ILE:O	12:B:1080:ARG:NH2	2.30	0.65
1:0:189:LEU:HB3	8:7:188:GLU:HA	1.80	0.64
4:3:7:ARG:HD2	7:6:51:ASN:HA	1.79	0.64
1:0:300:ASP:OD2	1:0:303:ASN:ND2	2.22	0.64
27:R:175:ARG:HH21	27:R:209:PRO:HA	1.63	0.64
4:3:322:GLU:OE2	4:3:337:ARG:NH2	2.24	0.63
19:I:20:CYS:SG	19:I:22:ASN:ND2	2.70	0.63
2:1:421:PHE:HA	2:1:430:ASN:H	1.62	0.63
13:C:60:HIS:CE1	13:C:63:PHE:HB2	2.33	0.63
33:a:107:ASP:OD2	33:a:132:ARG:NH1	2.31	0.63
2:1:606:GLU:HG2	2:1:662:GLN:HE22	1.63	0.62
2:1:20:GLU:HA	2:1:756:ILE:HG21	1.80	0.62
25:O:204:ILE:HD12	25:O:207:PRO:HG2	1.79	0.62
2:1:378:ARG:NH1	2:1:382:LEU:HB2	2.14	0.62
15:E:44:PHE:CB	15:E:52:ARG:HG3	2.30	0.62
2:1:343:ARG:HG2	2:1:357:PHE:CE2	2.35	0.62
6:5:233:PRO:HG2	6:5:238:ARG:NH1	2.14	0.62
25:O:318:ARG:NH1	25:O:322:TYR:OH	2.30	0.61
4:3:101:LEU:HB2	4:3:105:LEU:HB2	1.83	0.61
11:A:264:VAL:O	11:A:272:ASN:N	2.31	0.61
14:D:87:LEU:HB3	14:D:97:LEU:HD22	1.82	0.61
18:H:58:LEU:HD11	18:H:143:LEU:HD11	1.82	0.61
30:V:64:THR:HB	30:V:75:VAL:HB	1.82	0.61
24:N:29:DC:N3	28:T:-29:DG:N1	2.44	0.61
14:D:44:ARG:NH1	14:D:47:GLN:OE1	2.34	0.61
30:V:16:GLN:NE2	30:V:20:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:38:ILE:HG21	6:5:115:ILE:HD13	1.82	0.61
12:B:385:ARG:NE	12:B:492:ASP:OD1	2.24	0.61
19:I:41:ASN:HA	26:Q:177:MET:HE2	1.83	0.60
1:0:562:ALA:HB2	1:0:626:ILE:HD12	1.82	0.60
15:E:46:ASP:HB3	15:E:52:ARG:HB3	1.83	0.60
11:A:1483:GLY:HA3	16:F:80:MET:HA	1.83	0.60
11:A:988:TRP:HE1	11:A:992:LYS:HE3	1.67	0.60
23:M:120:GLU:HG3	23:M:124:MET:HE2	1.83	0.60
24:N:79:DG:H2''	24:N:80:DT:C6	2.37	0.60
4:3:65:PRO:HB2	4:3:107:GLY:HA3	1.82	0.60
4:3:400:ARG:NH1	7:6:13:ASP:OD2	2.31	0.60
31:W:88:ARG:NH1	31:W:90:ASN:OD1	2.33	0.60
2:1:287:ARG:NH1	2:1:293:ARG:O	2.35	0.60
1:0:198:ARG:NH1	8:7:188:GLU:OE1	2.30	0.60
9:8:179:ARG:HD2	9:8:184:LEU:CD2	2.31	0.60
24:N:45:DC:H2''	24:N:46:DG:C8	2.36	0.60
11:A:244:ARG:HB2	11:A:247:TRP:CD2	2.36	0.59
11:A:1468:THR:HG22	16:F:64:ARG:HD2	1.83	0.59
2:1:601:ARG:NH2	2:1:624:PRO:O	2.24	0.59
11:A:1178:ASP:OD1	11:A:1260:ARG:NH2	2.33	0.59
6:5:160:ARG:HH11	6:5:238:ARG:NH2	1.99	0.59
7:6:9:LEU:HD11	7:6:42:HIS:HB3	1.83	0.59
15:E:2:ASP:N	15:E:5:GLU:OE2	2.35	0.59
8:7:85:ARG:NH2	8:7:143:GLU:OE2	2.36	0.59
2:1:237:HIS:HB2	2:1:658:ARG:HD2	1.84	0.59
3:2:372:ILE:HD11	5:4:243:SER:HB3	1.83	0.59
6:5:233:PRO:HG2	6:5:238:ARG:HH11	1.67	0.59
2:1:623:VAL:HB	2:1:683:ARG:HH11	1.67	0.59
4:3:361:ALA:HB1	4:3:391:ILE:HG22	1.84	0.59
12:B:593:GLN:NE2	12:B:595:ASP:OD2	2.35	0.59
12:B:601:VAL:HG22	12:B:616:THR:HG23	1.84	0.59
21:K:81:TYR:OH	21:K:89:ASN:OD1	2.20	0.59
11:A:460:ARG:HB2	11:A:501:MET:HE3	1.85	0.58
1:0:54:ASP:OD2	4:3:337:ARG:NH1	2.35	0.58
1:0:74:ARG:NH1	1:0:142:LYS:O	2.35	0.58
5:4:146:TYR:HB3	5:4:179:PRO:HD2	1.84	0.58
8:7:8:ARG:NH1	8:7:48:GLU:OE2	2.34	0.58
24:N:131:DT:H2''	24:N:132:DA:C8	2.38	0.58
29:U:344:ARG:HD3	29:U:349:TRP:CE2	2.38	0.58
13:C:183:ALA:HB3	13:C:232:ASN:HB3	1.86	0.58
12:B:110:PRO:HG2	12:B:163:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:934:LYS:HG2	12:B:944:THR:HG22	1.84	0.58
11:A:805:ARG:NH2	12:B:671:GLU:O	2.36	0.58
2:1:52:LEU:HD21	2:1:232:VAL:HG11	1.86	0.58
2:1:683:ARG:HD3	2:1:689:LYS:NZ	2.19	0.58
6:5:191:ILE:O	6:5:212:GLY:HA3	2.04	0.58
29:U:372:GLY:HA3	30:V:58:PHE:CZ	2.38	0.57
28:T:-44:DA:OP1	33:e:38:LYS:NZ	2.31	0.57
1:0:531:ILE:HA	1:0:534:TYR:CE2	2.39	0.57
12:B:721:ARG:NH1	12:B:940:GLY:O	2.38	0.57
1:0:517:GLU:OE2	1:0:706:LYS:NZ	2.30	0.57
1:0:624:ILE:HG12	1:0:660:TYR:HB2	1.87	0.57
2:1:378:ARG:HH12	2:1:382:LEU:HB2	1.69	0.57
25:O:297:LYS:HB3	25:O:298:PRO:HD3	1.86	0.57
4:3:37:HIS:HB3	4:3:40:THR:HG23	1.86	0.57
4:3:248:ASP:OD2	4:3:280:ARG:NH1	2.31	0.57
12:B:453:TRP:NE1	12:B:466:VAL:HB	2.20	0.57
30:V:66:ARG:HB2	30:V:73:THR:HB	1.86	0.57
2:1:379:LEU:HD11	2:1:394:PHE:HZ	1.70	0.57
1:0:642:ARG:O	1:0:645:ARG:NH2	2.36	0.57
2:1:161:PHE:CD1	2:1:165:GLY:HA3	2.40	0.57
11:A:365:THR:HG22	11:A:482:PHE:CE2	2.40	0.57
18:H:118:TYR:HB2	18:H:121:LEU:HB2	1.86	0.57
22:L:17:TYR:HB3	22:L:44:MET:HB3	1.86	0.57
2:1:583:LYS:HD2	3:2:315:LEU:HD23	1.87	0.57
11:A:1005:HIS:HD2	11:A:1006:PRO:HD2	1.70	0.57
1:0:398:ASP:OD1	1:0:425:ARG:NH1	2.37	0.57
9:8:104:ASP:OD1	9:8:105:ASN:N	2.37	0.57
28:T:-133:DT:H2"	28:T:-132:DT:C6	2.39	0.57
1:0:123:LEU:O	1:0:127:VAL:HG23	2.05	0.56
24:N:142:DG:H2"	24:N:143:DG:C8	2.40	0.56
4:3:40:THR:HG22	4:3:238:PHE:HD2	1.69	0.56
8:7:113:VAL:HG12	8:7:115:LEU:H	1.69	0.56
28:T:-54:DG:H2"	28:T:-53:DG:C8	2.40	0.56
5:4:249:LEU:HG	6:5:266:TYR:HB3	1.86	0.56
2:1:269:THR:OG1	2:1:272:ARG:NH2	2.36	0.56
4:3:151:TYR:CZ	4:3:269:GLY:HA2	2.40	0.56
13:C:240:ARG:NE	13:C:242:GLU:OE2	2.33	0.56
15:E:172:ARG:NH1	15:E:210:GLN:OE1	2.38	0.56
19:I:69:ILE:HG22	19:I:71:ASP:H	1.71	0.56
2:1:1:MET:HG3	2:1:741:LEU:HD13	1.88	0.56
2:1:297:ALA:O	2:1:301:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:78:ILE:HG21	13:C:127:VAL:HG22	1.88	0.56
25:O:283:TYR:CZ	25:O:285:PRO:HG3	2.40	0.56
4:3:32:ASP:OD1	4:3:111:ASN:ND2	2.39	0.56
11:A:1211:LEU:HD11	11:A:1258:ARG:HB3	1.87	0.56
11:A:1146:GLN:O	11:A:1150:ASP:N	2.39	0.55
2:1:370:LYS:HB3	2:1:371:PRO:HD3	1.88	0.55
20:J:9:THR:OG1	20:J:47:ARG:NH2	2.39	0.55
24:N:63:DG:N2	28:T:-62:DT:O2	2.39	0.55
26:Q:119:THR:HB	26:Q:122:THR:HB	1.88	0.55
11:A:1170:THR:HA	11:A:1216:LEU:HA	1.87	0.55
12:B:1119:CYS:HB2	12:B:1137:CYS:SG	2.47	0.55
28:T:-112:DG:H2''	28:T:-111:DT:C5	2.42	0.55
2:1:270:VAL:HA	2:1:273:ILE:HG22	1.88	0.55
31:W:110:MET:HE1	32:X:220:TRP:HA	1.89	0.55
15:E:11:TRP:HB2	15:E:40:PHE:CD2	2.42	0.55
1:0:127:VAL:HG22	1:0:160:THR:HG23	1.87	0.55
12:B:387:HIS:NE2	12:B:671:GLU:OE2	2.39	0.55
24:N:59:DC:H2''	24:N:60:DC:C6	2.41	0.55
2:1:269:THR:HA	2:1:272:ARG:NE	2.22	0.55
2:1:318:ALA:HB3	2:1:374:PHE:CZ	2.42	0.55
11:A:531:ASN:OD1	11:A:1394:ASN:ND2	2.40	0.55
24:N:46:DG:H2''	24:N:47:DA:C8	2.41	0.55
1:0:360:ARG:NH2	1:0:434:GLU:H	2.05	0.55
24:N:81:DA:H2''	24:N:82:DG:C8	2.42	0.55
31:W:77:ARG:HD3	31:W:91:TYR:CE1	2.42	0.55
32:X:77:VAL:O	32:X:81:ILE:HG12	2.07	0.55
8:7:74:ILE:HG23	8:7:109:LEU:HD23	1.89	0.54
19:I:27:LYS:N	19:I:36:LEU:O	2.40	0.54
5:4:60:HIS:CE1	5:4:163:THR:HG21	2.43	0.54
11:A:481:THR:O	11:A:483:ARG:NH1	2.40	0.54
12:B:743:ARG:O	12:B:922:ARG:NH1	2.41	0.54
28:T:-57:DA:H2''	28:T:-56:DC:C6	2.42	0.54
2:1:725:ALA:HB1	5:4:221:VAL:HG21	1.88	0.54
4:3:325:ILE:HG23	4:3:334:MET:HE1	1.90	0.54
11:A:1245:CYS:HB3	11:A:1257:LEU:HD21	1.90	0.54
2:1:362:ALA:HA	2:1:366:CYS:HA	1.90	0.54
18:H:49:PRO:O	18:H:147:LYS:NZ	2.26	0.54
14:D:59:GLU:OE1	14:D:59:GLU:N	2.39	0.54
4:3:42:LEU:HD13	6:5:50:PHE:CE1	2.43	0.54
11:A:659:GLU:OE2	11:A:985:ARG:NH1	2.35	0.54
25:O:186:ARG:NH1	25:O:244:LEU:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:69:LYS:NZ	2:1:202:ALA:O	2.38	0.54
13:C:260:GLN:HB2	21:K:91:ILE:HG21	1.89	0.54
32:X:85:MET:HG2	32:X:139:PHE:CE1	2.43	0.54
34:b:60:LYS:NZ	34:b:64:GLU:OE2	2.31	0.54
12:B:388:TYR:CZ	12:B:505:LEU:HD21	2.43	0.53
11:A:408:ARG:NH1	11:A:414:PRO:O	2.40	0.53
19:I:84:HIS:ND1	19:I:125:GLU:OE2	2.34	0.53
18:H:102:ASP:OD2	18:H:110:THR:OG1	2.17	0.53
5:4:75:ASP:OD2	5:4:80:ARG:NH2	2.37	0.53
11:A:479:TRP:HB2	11:A:483:ARG:NH2	2.23	0.53
13:C:44:ILE:HG21	13:C:178:PRO:HB3	1.90	0.53
16:F:84:GLU:N	16:F:84:GLU:OE1	2.42	0.53
32:X:89:HIS:HB2	32:X:139:PHE:CE1	2.43	0.53
6:5:232:LEU:N	6:5:233:PRO:HD2	2.24	0.53
31:W:154:CYS:O	31:W:158:HIS:N	2.40	0.53
5:4:156:LEU:HB3	5:4:165:ARG:HD2	1.90	0.53
12:B:971:ALA:O	12:B:975:ARG:HD3	2.08	0.53
18:H:10:PHE:CE2	18:H:32:SER:HB3	2.43	0.53
19:I:99:SER:HB3	19:I:107:ALA:HB1	1.90	0.53
31:W:106:LYS:HE3	32:X:223:VAL:HB	1.90	0.53
5:4:160:PRO:HB2	5:4:162:HIS:CE1	2.44	0.53
11:A:1005:HIS:CD2	11:A:1006:PRO:HD2	2.44	0.53
12:B:812:ARG:CZ	12:B:897:ARG:HH22	2.22	0.53
4:3:404:THR:O	7:6:9:LEU:N	2.42	0.53
11:A:430:ARG:HH22	23:M:26:ASP:CG	2.17	0.53
12:B:724:TYR:HB3	12:B:728:MET:HE3	1.91	0.53
14:D:41:LEU:HD12	14:D:68:THR:HG21	1.91	0.53
28:T:-133:DT:H2"	28:T:-132:DT:C5	2.44	0.53
31:W:110:MET:O	31:W:114:ILE:N	2.27	0.53
2:1:486:ALA:HB2	2:1:736:LEU:HB2	1.91	0.53
2:1:681:ASP:HB3	2:1:684:PHE:CD2	2.43	0.53
12:B:926:VAL:HG21	13:C:62:GLU:HG3	1.91	0.53
1:0:97:GLN:HE22	1:0:109:ARG:HE	1.58	0.52
2:1:237:HIS:CD2	2:1:658:ARG:HD2	2.44	0.52
4:3:251:VAL:O	4:3:279:ARG:NH1	2.42	0.52
6:5:270:VAL:HG21	6:5:287:THR:HG21	1.89	0.52
11:A:86:GLY:O	11:A:255:VAL:N	2.29	0.52
12:B:1108:PHE:CE1	12:B:1113:PRO:HA	2.44	0.52
29:U:349:TRP:O	29:U:373:ASP:HA	2.09	0.52
34:f:60:LYS:NZ	34:f:64:GLU:OE2	2.31	0.52
13:C:101:PHE:CE2	13:C:122:SER:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:113:VAL:N	4:3:310:GLU:OE2	2.40	0.52
8:7:108:ASN:OD1	8:7:112:ASN:ND2	2.39	0.52
11:A:122:ASN:O	11:A:127:LYS:NZ	2.39	0.52
19:I:15:ARG:HB3	19:I:24:LEU:HD12	1.91	0.52
6:5:268:CYS:SG	6:5:270:VAL:HB	2.50	0.52
12:B:399:LEU:HB3	12:B:453:TRP:CZ3	2.44	0.52
2:1:372:LEU:HD11	2:1:404:ALA:HB1	1.90	0.52
2:1:623:VAL:HB	2:1:683:ARG:NH1	2.24	0.52
4:3:38:PRO:HA	4:3:117:ASN:HB3	1.92	0.52
12:B:771:GLU:O	20:J:55:LEU:HD21	2.10	0.52
14:D:14:GLU:N	14:D:14:GLU:OE1	2.43	0.52
25:O:170:SER:HA	25:O:255:ILE:HA	1.92	0.52
35:g:64:LEU:HD11	36:h:42:VAL:HG13	1.90	0.52
2:1:284:GLU:OE1	2:1:287:ARG:NE	2.42	0.52
3:2:152:THR:C	3:2:154:SER:N	2.67	0.52
13:C:193:ARG:NH2	13:C:218:ALA:O	2.35	0.52
24:N:171:DT:H2"	24:N:172:DC:C5	2.44	0.52
2:1:95:GLU:O	2:1:99:GLY:N	2.43	0.52
3:2:197:PHE:CE2	3:2:204:LYS:HG3	2.45	0.52
11:A:1246:ILE:O	11:A:1258:ARG:N	2.24	0.52
27:R:87:SER:O	27:R:113:ARG:NH2	2.38	0.52
28:T:-48:DC:H2"	28:T:-47:DT:C6	2.45	0.52
34:b:99:TYR:OH	36:h:69:ASP:OD2	2.23	0.52
3:2:506:CYS:O	3:2:510:GLU:N	2.43	0.52
26:Q:18:VAL:O	27:R:35:SER:OG	2.21	0.52
1:0:188:LEU:HD12	1:0:287:LEU:HD23	1.91	0.52
2:1:480:THR:O	2:1:758:GLN:N	2.29	0.52
9:8:172:GLN:C	9:8:179:ARG:HH12	2.18	0.52
18:H:112:LEU:HB2	18:H:132:LEU:HD12	1.90	0.52
11:A:253:LEU:HD21	11:A:317:MET:HE1	1.92	0.52
27:R:58:LEU:HD11	27:R:62:LEU:HD23	1.92	0.52
13:C:60:HIS:NE2	13:C:63:PHE:HB2	2.25	0.51
25:O:174:LEU:HD12	25:O:178:LEU:HD11	1.91	0.51
28:T:-173:DT:H2"	28:T:-172:DG:C5	2.44	0.51
1:0:59:LYS:HB3	1:0:61:TYR:CZ	2.45	0.51
1:0:564:ASN:ND2	1:0:723:ASP:O	2.35	0.51
23:M:264:ALA:HB2	23:M:313:LEU:HD21	1.90	0.51
24:N:80:DT:H2"	24:N:81:DA:N7	2.25	0.51
1:0:35:GLN:HA	1:0:285:ILE:HD13	1.92	0.51
1:0:60:ASP:HA	4:3:337:ARG:HB2	1.93	0.51
1:0:101:VAL:HG22	1:0:109:ARG:HH21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:101:TYR:HE2	6:5:104:LEU:HB2	1.74	0.51
13:C:9:VAL:HG11	21:K:105:PHE:CD2	2.46	0.51
20:J:6:ARG:HD3	20:J:13:ILE:HD13	1.91	0.51
33:a:127:LEU:HD22	33:e:114:HIS:CG	2.45	0.51
34:f:40:ARG:NH1	34:f:44:VAL:O	2.42	0.51
6:5:165:LYS:HE3	6:5:200:SER:HB2	1.93	0.51
11:A:1141:VAL:HA	11:A:1357:THR:HG23	1.93	0.51
31:W:110:MET:SD	32:X:223:VAL:HG21	2.50	0.51
9:8:71:HIS:CG	9:8:72:PRO:HD2	2.46	0.51
25:O:239:ARG:NH2	29:U:315:ASN:OD1	2.43	0.51
34:b:32:LYS:HE3	34:b:52:TYR:CE2	2.45	0.51
9:8:176:ARG:CD	9:8:179:ARG:HH21	2.21	0.51
11:A:410:ASN:HD22	11:A:430:ARG:HB3	1.75	0.51
24:N:92:DG:N2	28:T:-91:DT:O2	2.44	0.51
27:R:179:ASP:OD1	27:R:179:ASP:N	2.38	0.51
31:W:137:THR:HG22	31:W:139:LEU:H	1.76	0.51
3:2:216:THR:HG22	3:2:218:LYS:H	1.75	0.51
12:B:387:HIS:CD2	12:B:504:THR:HG21	2.44	0.51
12:B:792:ASP:CG	12:B:975:ARG:HH22	2.19	0.51
35:c:101:VAL:HG11	34:f:99:TYR:CE2	2.46	0.51
24:N:-8:DA:H61	28:T:8:DT:H3	1.59	0.51
26:Q:26:TYR:HA	27:R:97:THR:HG22	1.92	0.51
2:1:195:ALA:O	2:1:199:ILE:HG13	2.11	0.50
2:1:196:ARG:HA	2:1:199:ILE:HD12	1.92	0.50
3:2:193:ILE:HB	3:2:221:TRP:CZ2	2.46	0.50
12:B:121:SER:HB3	12:B:151:LYS:HB3	1.93	0.50
12:B:248:LYS:HE2	26:Q:171:LEU:HD22	1.93	0.50
19:I:17:CYS:HB2	19:I:39:CYS:SG	2.51	0.50
31:W:42:CYS:SG	31:W:91:TYR:HB3	2.51	0.50
11:A:1120:GLY:H	11:A:1385:VAL:HG23	1.76	0.50
2:1:329:PHE:CE2	2:1:378:ARG:HG3	2.46	0.50
2:1:703:ASP:HA	2:1:706:LEU:HD13	1.94	0.50
7:6:28:ALA:O	7:6:56:ARG:NH1	2.44	0.50
24:N:127:DG:O6	28:T:-128:DA:N6	2.44	0.50
31:W:176:LEU:HD13	32:X:215:GLU:HG2	1.92	0.50
2:1:422:ASP:OD2	2:1:430:ASN:ND2	2.45	0.50
11:A:34:MET:HA	12:B:1138:ARG:HB3	1.94	0.50
11:A:871:VAL:HB	11:A:1088:GLY:HA3	1.93	0.50
13:C:172:GLU:OE2	22:L:58:ARG:NH2	2.43	0.50
23:M:128:ILE:HG23	23:M:183:VAL:HG11	1.94	0.50
1:0:68:LYS:HB3	1:0:145:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:310:LEU:HD11	1:0:352:THR:HG23	1.92	0.50
1:0:591:GLN:OE1	1:0:595:ASN:ND2	2.45	0.50
2:1:104:PHE:H	2:1:172:ALA:HB1	1.77	0.50
17:G:119:PHE:HB2	17:G:128:TYR:CE2	2.46	0.50
18:H:95:LYS:HD3	18:H:138:ASP:HA	1.92	0.50
24:N:123:DC:H5''	34:f:48:SER:HA	1.94	0.50
26:Q:44:GLN:HE22	26:Q:46:ARG:HG3	1.76	0.50
10:9:266:ARG:NH2	10:9:269:GLU:OE1	2.39	0.50
13:C:263:LEU:HD22	21:K:87:PHE:HD2	1.77	0.50
36:d:69:ASP:OD2	34:f:99:TYR:OH	2.29	0.50
2:1:655:ASP:O	2:1:659:HIS:ND1	2.35	0.50
5:4:76:LEU:HD13	5:4:83:CYS:SG	2.52	0.50
12:B:42:GLN:H	12:B:42:GLN:CD	2.20	0.50
35:c:25:GLN:N	35:c:57:GLU:OE1	2.45	0.50
11:A:549:THR:O	11:A:589:LYS:NZ	2.44	0.49
11:A:1128:ILE:HG13	11:A:1129:ASN:N	2.27	0.49
12:B:255:ARG:HE	12:B:307:GLU:CD	2.19	0.49
12:B:777:ASN:O	20:J:47:ARG:NH1	2.43	0.49
17:G:39:THR:HG23	17:G:42:TYR:H	1.77	0.49
1:0:184:VAL:HG13	1:0:289:TYR:CE1	2.47	0.49
2:1:118:HIS:CD2	2:1:137:LEU:HD13	2.47	0.49
2:1:192:TYR:OH	2:1:196:ARG:NH2	2.35	0.49
11:A:279:LYS:HA	11:A:279:LYS:HE2	1.95	0.49
11:A:458:PHE:HE2	11:A:484:LEU:HD11	1.77	0.49
6:5:255:CYS:SG	6:5:262:ILE:HD11	2.52	0.49
11:A:146:ASP:HA	11:A:149:LYS:HE2	1.94	0.49
11:A:364:ARG:HD2	11:A:502:ASN:OD1	2.12	0.49
12:B:411:LEU:HD12	12:B:439:ILE:HD12	1.94	0.49
22:L:41:TYR:CE2	22:L:43:ILE:HB	2.46	0.49
28:T:-188:DT:H2''	28:T:-187:DC:H5'	1.94	0.49
33:e:62:LEU:HD13	34:f:37:ARG:HB3	1.95	0.49
5:4:87:LEU:HD11	5:4:225:GLU:HG3	1.94	0.49
11:A:653:VAL:HG11	11:A:669:TYR:OH	2.12	0.49
11:A:1178:ASP:CG	11:A:1260:ARG:HH22	2.17	0.49
24:N:68:DC:H2''	24:N:69:DT:C5	2.47	0.49
2:1:361:LEU:O	2:1:366:CYS:N	2.46	0.49
8:7:193:PRO:HG2	8:7:196:LEU:HB2	1.94	0.49
9:8:122:LEU:HD12	9:8:295:PHE:CZ	2.47	0.49
11:A:801:GLY:HA3	12:B:503:ASN:HB2	1.95	0.49
12:B:236:TRP:HB2	12:B:259:THR:HB	1.95	0.49
13:C:7:PRO:HA	13:C:24:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:206:GLU:HB3	25:O:207:PRO:HD3	1.95	0.49
25:O:235:ARG:NH2	29:U:316:SER:OG	2.42	0.49
11:A:1099:ALA:HA	11:A:1102:MET:SD	2.53	0.49
12:B:1066:PRO:HG2	12:B:1077:GLY:HA3	1.95	0.49
24:N:73:DT:H5''	35:c:17:THR:HA	1.93	0.49
24:N:170:DG:H2''	24:N:171:DT:C5	2.47	0.49
35:c:55:VAL:HG21	36:d:99:VAL:HG21	1.95	0.49
6:5:192:ASP:OD2	6:5:238:ARG:NH2	2.46	0.49
10:9:33:LYS:NZ	17:G:21:ASN:OD1	2.46	0.49
17:G:4:HIS:CE1	17:G:73:LYS:HD2	2.48	0.49
18:H:97:TYR:CZ	18:H:115:TYR:HB3	2.47	0.49
20:J:8:PHE:CD2	20:J:48:MET:HE1	2.47	0.49
23:M:48:VAL:HG23	23:M:52:TRP:CE3	2.47	0.49
3:2:502:VAL:O	3:2:506:CYS:N	2.43	0.49
8:7:268:ARG:HG3	8:7:272:LEU:HD23	1.93	0.49
11:A:369:PRO:HB3	11:A:496:PHE:CE2	2.47	0.49
11:A:811:ILE:HD12	19:I:79:PRO:HB3	1.95	0.49
12:B:198:GLU:OE2	12:B:391:LYS:NZ	2.32	0.49
1:0:371:VAL:HG13	1:0:407:ILE:HB	1.94	0.49
2:1:3:LEU:HD13	2:1:744:LEU:HD13	1.94	0.49
2:1:729:HIS:CG	2:1:730:ARG:H	2.31	0.49
11:A:395:THR:HG22	11:A:396:PRO:HD2	1.95	0.49
1:0:377:GLN:HA	1:0:380:MET:HG2	1.95	0.49
2:1:379:LEU:HD11	2:1:394:PHE:CZ	2.47	0.49
6:5:12:VAL:HG21	6:5:144:ILE:HD11	1.95	0.49
13:C:60:HIS:CD2	13:C:62:GLU:HG2	2.48	0.49
27:R:230:LYS:HE2	28:T:-17:DC:H5''	1.94	0.49
2:1:345:ARG:HG3	8:7:1:MET:HE3	1.95	0.48
2:1:693:LEU:O	2:1:698:GLN:NE2	2.45	0.48
13:C:60:HIS:HD2	13:C:62:GLU:HG2	1.78	0.48
4:3:52:ALA:HB2	4:3:86:SER:HB2	1.96	0.48
9:8:83:HIS:CD2	9:8:84:LYS:HG2	2.49	0.48
11:A:1227:THR:H	11:A:1230:GLN:NE2	2.10	0.48
22:L:41:TYR:OH	22:L:43:ILE:HD12	2.13	0.48
24:N:184:DT:H2''	24:N:185:DC:C6	2.48	0.48
25:O:305:PHE:CZ	28:T:-2:DT:H1'	2.49	0.48
2:1:161:PHE:CE1	2:1:194:LEU:HA	2.48	0.48
8:7:284:ALA:HB2	9:8:239:ASP:OD1	2.13	0.48
11:A:901:VAL:HA	11:A:980:PRO:HA	1.96	0.48
11:A:1218:ARG:NH1	11:A:1250:ASP:OD1	2.45	0.48
12:B:1112:ASP:OD1	12:B:1112:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:203:VAL:HG21	27:R:210:VAL:HG22	1.95	0.48
31:W:151:THR:OG1	31:W:160:GLU:OE2	2.19	0.48
1:0:444:HIS:HA	1:0:472:ARG:NE	2.28	0.48
24:N:148:DA:N6	28:T:-149:DG:O6	2.47	0.48
30:V:67:PHE:CZ	30:V:70:ASN:HA	2.48	0.48
2:1:42:MET:O	2:1:459:GLY:N	2.45	0.48
2:1:280:ARG:O	2:1:284:GLU:HG2	2.14	0.48
2:1:562:GLN:NE2	2:1:567:LEU:HB2	2.28	0.48
3:2:163:ASP:O	3:2:164:VAL:C	2.55	0.48
5:4:62:TYR:OH	5:4:120:LEU:HB2	2.14	0.48
11:A:22:GLN:NE2	11:A:1446:GLY:O	2.47	0.48
10:9:86:TYR:OH	10:9:158:LEU:O	2.26	0.48
11:A:365:THR:HG22	11:A:482:PHE:CD2	2.48	0.48
11:A:400:ASP:OD1	11:A:401:ARG:N	2.46	0.48
11:A:937:ASP:OD1	11:A:937:ASP:N	2.45	0.48
12:B:715:ASP:N	12:B:715:ASP:OD1	2.46	0.48
14:D:112:LYS:HD2	14:D:119:GLU:HG3	1.96	0.48
17:G:144:ARG:NH2	17:G:167:TYR:HB3	2.28	0.48
24:N:181:DA:H2"	24:N:182:DC:C6	2.48	0.48
1:0:413:LEU:HD11	1:0:457:ILE:HG21	1.96	0.48
1:0:503:ALA:HB2	1:0:646:ALA:HA	1.95	0.48
4:3:42:LEU:HD13	6:5:50:PHE:CZ	2.49	0.48
8:7:271:TYR:CG	10:9:176:THR:HG22	2.49	0.48
9:8:74:ILE:HG23	9:8:156:PHE:CZ	2.49	0.48
18:H:71:ASP:OD2	18:H:142:TYR:OH	2.16	0.48
1:0:413:LEU:HD13	1:0:430:LEU:HD23	1.95	0.48
4:3:384:PRO:HD2	4:3:387:ILE:HD12	1.96	0.48
11:A:845:GLU:OE2	12:B:500:GLN:HG2	2.14	0.48
23:M:248:ARG:NH1	28:T:0:DG:H5"	2.28	0.48
1:0:622:VAL:HG13	1:0:658:PHE:HB2	1.94	0.48
1:0:644:LEU:O	1:0:645:ARG:NH1	2.39	0.48
24:N:164:DG:N2	28:T:-163:DC:O2	2.46	0.48
24:N:185:DC:N4	28:T:-186:DG:O6	2.47	0.48
34:b:45:LYS:HD2	35:g:116:LEU:HB3	1.96	0.48
34:b:83:THR:HG22	34:b:85:MET:H	1.79	0.48
1:0:169:VAL:N	1:0:176:PHE:O	2.46	0.48
2:1:165:GLY:HA2	2:1:189:TRP:CH2	2.49	0.48
2:1:209:TYR:OH	2:1:234:ASP:HB3	2.14	0.48
10:9:265:PRO:HA	10:9:266:ARG:NH1	2.29	0.48
33:e:117:ARG:HH22	33:e:124:ASP:CG	2.22	0.48
4:3:55:TRP:CZ2	4:3:75:VAL:HG23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:347:THR:HG23	4:3:350:SER:H	1.79	0.47
11:A:804:HIS:CE1	19:I:100:HIS:CD2	3.02	0.47
24:N:21:DC:N4	24:N:22:DG:O6	2.47	0.47
24:N:141:DG:H2''	24:N:142:DG:C8	2.49	0.47
24:N:169:DT:H2''	24:N:170:DG:C8	2.49	0.47
3:2:201:PRO:HA	3:2:204:LYS:HB3	1.96	0.47
9:8:118:MET:HA	9:8:121:THR:HG22	1.96	0.47
25:O:239:ARG:NE	29:U:317:GLU:O	2.47	0.47
11:A:1217:ASP:OD2	11:A:1219:LYS:NZ	2.44	0.47
29:U:353:LEU:HD12	29:U:370:ALA:HB3	1.96	0.47
1:0:62:ARG:HG2	4:3:338:PHE:C	2.39	0.47
3:2:528:MET:HG2	5:4:295:ARG:HB2	1.95	0.47
5:4:249:LEU:HD22	6:5:289:PHE:CE2	2.49	0.47
9:8:129:HIS:CE1	9:8:192:VAL:HG13	2.49	0.47
12:B:972:ILE:HG21	12:B:981:LEU:HD11	1.96	0.47
18:H:14:ASP:HB2	18:H:29:HIS:HB2	1.96	0.47
4:3:300:THR:HB	4:3:303:GLN:O	2.15	0.47
25:O:267:PRO:HG2	25:O:337:LYS:HB3	1.97	0.47
27:R:192:GLU:OE1	32:X:72:GLY:N	2.47	0.47
1:0:446:ILE:O	1:0:472:ARG:NH2	2.48	0.47
2:1:569:ILE:HG23	2:1:597:LEU:HD11	1.97	0.47
10:9:195:LEU:HA	10:9:198:ILE:HG22	1.97	0.47
12:B:136:GLY:O	12:B:137:GLU:HG3	2.15	0.47
12:B:355:ASP:N	12:B:355:ASP:OD1	2.47	0.47
12:B:836:THR:HB	12:B:889:LYS:HE2	1.96	0.47
15:E:104:ILE:O	15:E:129:GLN:HA	2.15	0.47
24:N:-8:DA:N6	28:T:8:DT:H3	2.12	0.47
1:0:444:HIS:HA	1:0:472:ARG:HE	1.79	0.47
12:B:873:LEU:HD21	12:B:890:ARG:HB2	1.96	0.47
2:1:569:ILE:HG21	3:2:304:ILE:HG12	1.96	0.47
28:T:-82:DC:H2''	28:T:-81:DT:C6	2.49	0.47
32:X:111:ILE:O	32:X:116:LYS:NZ	2.48	0.47
1:0:197:CYS:HB3	1:0:272:VAL:HG13	1.96	0.47
3:2:228:HIS:NE2	3:2:235:LEU:O	2.47	0.47
11:A:1139:LEU:HB2	11:A:1338:THR:OG1	2.15	0.47
12:B:565:THR:HG21	12:B:580:PRO:HG3	1.97	0.47
12:B:711:ILE:HG12	12:B:725:GLN:HG2	1.96	0.47
18:H:102:ASP:OD1	18:H:110:THR:N	2.48	0.47
21:K:81:TYR:CE2	21:K:86:ALA:HB2	2.50	0.47
2:1:641:ARG:HH21	2:1:648:GLU:CD	2.20	0.47
3:2:279:GLU:C	3:2:281:TYR:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:255:CYS:SG	6:5:276:CYS:HB2	2.55	0.47
11:A:892:GLY:C	11:A:894:ASP:H	2.23	0.47
12:B:785:TYR:O	12:B:786:THR:HG22	2.15	0.47
24:N:91:DA:H1'	24:N:92:DG:C8	2.49	0.47
29:U:339:TYR:HA	29:U:353:LEU:HA	1.97	0.47
32:X:214:GLU:OE2	32:X:221:ARG:NH2	2.46	0.47
2:1:118:HIS:HA	2:1:157:PHE:CE1	2.48	0.46
14:D:70:ARG:NE	17:G:142:GLU:OE2	2.46	0.46
15:E:52:ARG:HD3	15:E:53:PRO:HD3	1.96	0.46
15:E:93:ARG:NE	15:E:97:GLU:OE2	2.32	0.46
1:0:703:PHE:CZ	1:0:712:LEU:HD22	2.50	0.46
2:1:135:HIS:CD2	2:1:391:LEU:HD11	2.51	0.46
2:1:618:VAL:O	2:1:677:MET:HA	2.15	0.46
11:A:668:PHE:CE1	11:A:672:ILE:HD11	2.50	0.46
12:B:529:MET:HE1	12:B:698:ILE:HD12	1.97	0.46
24:N:7:DA:H1'	25:O:214:PHE:CZ	2.51	0.46
24:N:183:DA:H2''	24:N:184:DT:C6	2.50	0.46
28:T:-144:DC:H2''	28:T:-143:DC:C6	2.49	0.46
2:1:41:GLU:HG2	2:1:459:GLY:HA2	1.98	0.46
2:1:43:PRO:HG3	2:1:696:TRP:CD2	2.50	0.46
2:1:499:ASN:HD21	2:1:711:ASP:H	1.63	0.46
11:A:395:THR:CG2	11:A:396:PRO:HD2	2.46	0.46
28:T:-58:DC:OP1	35:c:77:THR:N	2.43	0.46
28:T:-5:DT:OP1	29:U:344:ARG:NH2	2.37	0.46
36:h:60:MET:HE3	36:h:60:MET:O	2.15	0.46
1:0:295:TYR:OH	1:0:300:ASP:OD2	2.15	0.46
8:7:24:ASN:ND2	8:7:57:ASN:O	2.47	0.46
11:A:87:HIS:NE2	11:A:89:GLU:OE2	2.48	0.46
11:A:740:GLN:O	11:A:743:ARG:HG2	2.15	0.46
14:D:108:ALA:HB1	14:D:127:LEU:HD23	1.97	0.46
15:E:73:PHE:CE2	15:E:99:ILE:HG13	2.50	0.46
23:M:131:PRO:HD2	23:M:134:ILE:HD12	1.98	0.46
2:1:5:VAL:HA	2:1:22:PHE:CZ	2.51	0.46
1:0:357:VAL:HG12	1:0:359:LYS:HB2	1.98	0.46
1:0:611:GLY:HA2	1:0:617:LEU:HD11	1.96	0.46
2:1:490:LEU:HD21	2:1:697:ILE:HG23	1.98	0.46
2:1:530:VAL:HG21	2:1:714:VAL:HG13	1.98	0.46
11:A:350:VAL:HA	11:A:354:LEU:HD12	1.98	0.46
11:A:668:PHE:CZ	11:A:672:ILE:HD11	2.50	0.46
13:C:149:LEU:HD21	13:C:152:LYS:HE3	1.98	0.46
24:N:121:DC:H2''	24:N:122:DC:C5	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:186:DC:H2''	24:N:187:DG:C8	2.50	0.46
32:X:146:ARG:HA	32:X:175:LEU:HB2	1.98	0.46
2:1:378:ARG:HH22	2:1:382:LEU:HD13	1.80	0.46
5:4:226:SER:O	5:4:230:GLU:HG3	2.15	0.46
11:A:59:ASP:CG	11:A:61:ARG:HE	2.22	0.46
11:A:465:HIS:CE1	11:A:467:MET:HB2	2.50	0.46
11:A:1242:ASP:HA	11:A:1262:MET:HE3	1.98	0.46
12:B:841:ARG:CZ	23:M:27:TYR:HD2	2.28	0.46
13:C:190:ASN:ND2	13:C:195:THR:O	2.43	0.46
24:N:109:DG:H2''	24:N:110:DT:C6	2.51	0.46
2:1:344:LEU:HG	2:1:431:PRO:HB2	1.98	0.46
5:4:109:THR:CG2	5:4:144:SER:H	2.28	0.46
6:5:177:PHE:CE2	6:5:181:ILE:HD11	2.50	0.46
13:C:84:TYR:CZ	13:C:167:LYS:HE2	2.51	0.46
2:1:223:LYS:HG2	2:1:450:ARG:HG2	1.97	0.46
11:A:90:LEU:HD12	11:A:250:VAL:O	2.15	0.46
11:A:239:GLU:HG3	11:A:241:ARG:HG2	1.98	0.46
11:A:1210:TRP:CE2	11:A:1282:ASP:HB3	2.51	0.46
12:B:117:ASN:HA	12:B:189:GLY:HA3	1.97	0.46
16:F:99:ALA:O	16:F:101:LYS:HE3	2.15	0.46
25:O:239:ARG:HG3	25:O:239:ARG:HH11	1.81	0.46
1:0:195:ARG:NH2	8:7:188:GLU:O	2.49	0.46
2:1:729:HIS:CG	2:1:730:ARG:N	2.84	0.46
3:2:228:HIS:HA	3:2:232:ARG:HA	1.98	0.46
8:7:152:GLU:HA	8:7:155:ARG:HD2	1.98	0.46
11:A:334:ARG:NH1	11:A:336:LEU:HA	2.31	0.46
11:A:496:PHE:CD2	12:B:791:GLU:HB2	2.50	0.46
15:E:110:MET:SD	15:E:118:LEU:HD11	2.56	0.46
19:I:24:LEU:HB3	19:I:37:TYR:HB3	1.98	0.46
23:M:15:CYS:HB3	23:M:18:HIS:O	2.15	0.46
23:M:157:ASP:OD2	23:M:185:ARG:NE	2.43	0.46
2:1:349:VAL:HA	2:1:418:ILE:O	2.16	0.45
5:4:367:PHE:HB3	5:4:371:CYS:HB2	1.98	0.45
11:A:579:ILE:O	11:A:584:PRO:HA	2.16	0.45
11:A:1211:LEU:HD13	11:A:1258:ARG:NH1	2.31	0.45
11:A:1308:TYR:HB2	11:A:1337:GLU:OE2	2.16	0.45
11:A:1371:ILE:HG12	11:A:1409:GLY:HA2	1.98	0.45
12:B:584:MET:HG3	12:B:605:ARG:HD2	1.98	0.45
28:T:-186:DG:H2''	28:T:-185:DG:C8	2.50	0.45
28:T:-164:DC:H2''	28:T:-163:DC:C5	2.51	0.45
1:0:628:SER:N	1:0:669:GLU:OE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:719:TYR:O	2:1:723:GLN:HG2	2.16	0.45
4:3:110:LEU:HB2	4:3:115:ARG:CZ	2.46	0.45
6:5:31:GLN:O	6:5:36:LYS:HE3	2.17	0.45
11:A:909:LEU:HD12	11:A:967:ARG:HD3	1.98	0.45
28:T:-184:DA:H2''	28:T:-183:DT:H5'	1.98	0.45
28:T:-99:DA:OP2	33:a:70:ARG:NH1	2.43	0.45
3:2:190:SER:O	3:2:193:ILE:HG22	2.16	0.45
11:A:618:TYR:O	11:A:621:ILE:O	2.34	0.45
12:B:453:TRP:N	12:B:453:TRP:CD1	2.84	0.45
28:T:-122:DG:H2''	28:T:-121:DG:C8	2.51	0.45
1:0:202:SER:HB3	8:7:177:ARG:CD	2.47	0.45
4:3:151:TYR:OH	4:3:266:ARG:O	2.34	0.45
5:4:87:LEU:HD12	5:4:228:TYR:CD2	2.52	0.45
11:A:1430:CYS:HB3	11:A:1435:THR:HG23	1.99	0.45
12:B:56:GLN:NE2	12:B:60:GLU:HG3	2.31	0.45
20:J:14:VAL:HB	20:J:49:LEU:HD11	1.99	0.45
2:1:485:LEU:HA	2:1:737:SER:HB2	1.98	0.45
2:1:612:HIS:H	2:1:673:ASP:CG	2.24	0.45
5:4:302:PRO:HB3	5:4:313:VAL:HA	1.98	0.45
11:A:1318:LYS:HE2	11:A:1332:GLN:OE1	2.16	0.45
12:B:455:ASP:HB3	12:B:458:LYS:HG2	1.98	0.45
19:I:100:HIS:CD2	19:I:100:HIS:O	2.69	0.45
27:R:194:HIS:HB3	27:R:197:TYR:CZ	2.51	0.45
29:U:18:ILE:HD11	29:U:46:TRP:CZ3	2.51	0.45
2:1:105:LEU:HD23	2:1:202:ALA:HA	1.99	0.45
3:2:279:GLU:C	3:2:281:TYR:N	2.74	0.45
11:A:956:PHE:HA	11:A:959:MET:HE3	1.99	0.45
18:H:95:LYS:HE2	18:H:140:ARG:CZ	2.46	0.45
1:0:97:GLN:HE22	1:0:109:ARG:NE	2.15	0.45
4:3:134:SER:HB3	4:3:280:ARG:HH22	1.81	0.45
5:4:314:SER:HB3	5:4:317:HIS:CD2	2.51	0.45
5:4:360:CYS:HB3	5:4:363:CYS:SG	2.56	0.45
11:A:379:GLY:HA2	11:A:475:ARG:O	2.17	0.45
24:N:0:DC:H5'	24:N:0:DC:C6	2.50	0.45
26:Q:173:HIS:O	26:Q:176:ILE:HG22	2.17	0.45
28:T:-82:DC:H2''	28:T:-81:DT:C5	2.52	0.45
32:X:77:VAL:HG12	32:X:108:HIS:CE1	2.52	0.45
1:0:392:PHE:CD1	1:0:398:ASP:HB2	2.51	0.45
2:1:20:GLU:HB3	2:1:42:MET:HE1	1.99	0.45
2:1:118:HIS:CD2	2:1:120:GLU:HB2	2.52	0.45
2:1:487:ARG:CZ	2:1:724:MET:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:67:PRO:HG2	4:3:70:ALA:HB3	1.99	0.45
4:3:329:ALA:HB2	4:3:334:MET:SD	2.56	0.45
9:8:40:ILE:HG12	9:8:90:VAL:HG22	1.99	0.45
12:B:167:THR:HG23	12:B:170:ASP:H	1.81	0.45
1:0:203:GLU:H	8:7:177:ARG:HE	1.65	0.45
6:5:145:HIS:CE1	6:5:149:LYS:HE3	2.51	0.45
11:A:654:HIS:NE2	11:A:658:LEU:HD11	2.31	0.45
11:A:1192:TRP:CZ3	11:A:1246:ILE:HG22	2.52	0.45
12:B:271:ILE:HD12	12:B:311:ILE:HD12	1.99	0.45
18:H:37:MET:SD	18:H:127:GLY:HA3	2.57	0.45
25:O:228:GLU:CD	25:O:231:ARG:HH22	2.23	0.45
1:0:509:GLU:HA	1:0:661:SER:O	2.17	0.45
2:1:143:ARG:HD3	2:1:158:TYR:CE1	2.52	0.45
4:3:53:LYS:HE3	4:3:53:LYS:HB2	1.83	0.45
6:5:24:LYS:O	6:5:28:LYS:N	2.47	0.45
9:8:241:CYS:HA	9:8:246:TYR:CD1	2.52	0.45
11:A:337:LYS:HA	11:A:341:GLN:OE1	2.17	0.45
21:K:63:VAL:HG12	21:K:71:ILE:HG22	1.99	0.45
23:M:127:ARG:HD3	27:R:153:TYR:CE1	2.52	0.45
23:M:193:ARG:NH2	24:N:2:DA:OP2	2.41	0.45
29:U:339:TYR:HB3	30:V:97:ALA:HB1	1.99	0.45
31:W:120:ASP:HA	31:W:123:ASN:ND2	2.31	0.45
3:2:407:ILE:HD11	6:5:34:LEU:HD22	2.00	0.44
8:7:99:LEU:O	8:7:103:GLU:HG2	2.17	0.44
11:A:606:HIS:ND1	11:A:641:CYS:SG	2.85	0.44
11:A:865:ILE:O	11:A:869:GLU:HB2	2.16	0.44
11:A:1411:LEU:O	11:A:1421:ARG:NH2	2.50	0.44
24:N:125:DG:H3'	33:e:47:VAL:HG21	1.99	0.44
24:N:160:DC:H2''	24:N:161:DC:C6	2.52	0.44
34:b:76:HIS:HB2	36:d:97:THR:HG21	1.99	0.44
2:1:145:GLN:HB3	2:1:152:LEU:CD1	2.48	0.44
2:1:641:ARG:NH2	2:1:648:GLU:OE2	2.40	0.44
4:3:64:GLN:C	4:3:109:ILE:HD11	2.42	0.44
5:4:203:ALA:O	5:4:219:TYR:OH	2.32	0.44
11:A:893:GLU:OE1	15:E:197:SER:OG	2.29	0.44
12:B:198:GLU:HA	12:B:393:LEU:HD23	1.99	0.44
18:H:75:TYR:CZ	18:H:77:PRO:HB3	2.52	0.44
28:T:-150:DA:H3'	36:h:87:ARG:NH1	2.32	0.44
35:c:89:ARG:NH2	35:c:101:VAL:O	2.50	0.44
2:1:244:ILE:O	2:1:248:SER:N	2.49	0.44
6:5:96:SER:OG	6:5:109:GLU:OE1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:250:LYS:HE3	9:8:252:PHE:CE1	2.52	0.44
11:A:244:ARG:HB3	11:A:246:GLU:CD	2.41	0.44
11:A:526:VAL:HA	11:A:533:PRO:HA	1.98	0.44
12:B:954:MET:HE1	12:B:966:ILE:HG13	1.99	0.44
17:G:30:LEU:O	17:G:34:VAL:HG22	2.18	0.44
1:0:105:GLU:HG3	1:0:122:SER:HB3	1.99	0.44
4:3:352:GLN:NE2	4:3:394:TRP:O	2.47	0.44
11:A:872:MET:HG2	11:A:873:VAL:N	2.33	0.44
24:N:140:DA:H2''	24:N:141:DG:C8	2.52	0.44
26:Q:46:ARG:NH1	27:R:3:GLU:OE2	2.50	0.44
26:Q:111:LYS:O	26:Q:146:PHE:HA	2.17	0.44
26:Q:180:ARG:O	26:Q:180:ARG:NE	2.51	0.44
27:R:41:GLY:HA3	27:R:56:PHE:CZ	2.52	0.44
1:0:186:GLN:O	1:0:190:GLN:HG2	2.18	0.44
11:A:617:PRO:O	18:H:124:ARG:NH2	2.49	0.44
17:G:132:ASP:OD1	17:G:132:ASP:N	2.50	0.44
17:G:15:PRO:HA	17:G:18:PHE:CE1	2.52	0.44
11:A:1228:MET:HE3	11:A:1228:MET:HA	1.99	0.44
15:E:59:THR:HG22	15:E:75:PHE:HA	1.99	0.44
2:1:72:TYR:O	2:1:206:VAL:HA	2.18	0.44
2:1:146:TYR:CD1	2:1:150:THR:HA	2.52	0.44
2:1:540:THR:HG23	2:1:624:PRO:HA	1.98	0.44
6:5:96:SER:N	6:5:106:SER:HB2	2.33	0.44
24:N:164:DG:H2''	24:N:165:DC:C6	2.53	0.44
28:T:-174:DC:H2''	28:T:-173:DT:C6	2.52	0.44
1:0:203:GLU:N	8:7:177:ARG:HE	2.15	0.44
1:0:364:LEU:HB3	1:0:410:TYR:CE2	2.53	0.44
2:1:637:LEU:HD22	2:1:648:GLU:HA	1.99	0.44
4:3:52:ALA:HB1	4:3:90:LEU:HD21	2.00	0.44
11:A:96:HIS:HE1	11:A:1440:MET:HE1	1.82	0.44
24:N:89:DC:OP2	24:N:89:DC:H2'	2.18	0.44
26:Q:13:GLU:HA	27:R:44:ARG:HA	2.00	0.44
28:T:-143:DC:H2''	28:T:-142:DC:C5	2.53	0.44
1:0:559:ILE:HG13	1:0:620:ALA:HB2	1.99	0.43
2:1:110:SER:OG	2:1:114:ASN:HB2	2.17	0.43
24:N:120:DC:H2''	24:N:121:DC:C5	2.53	0.43
27:R:175:ARG:NE	27:R:209:PRO:HA	2.30	0.43
1:0:167:LYS:HG2	1:0:292:LEU:HB3	2.00	0.43
1:0:198:ARG:HD3	8:7:188:GLU:OE1	2.17	0.43
1:0:365:GLY:O	1:0:409:THR:HA	2.18	0.43
3:2:262:VAL:HA	3:2:350:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:374:PRO:HA	4:3:377:LEU:HG	2.00	0.43
12:B:818:GLU:HG2	12:B:917:LYS:HB3	2.00	0.43
19:I:96:PHE:HB3	19:I:112:TYR:CD2	2.53	0.43
27:R:23:VAL:HA	27:R:116:CYS:HB3	2.00	0.43
30:V:47:ALA:CB	30:V:51:ARG:HH21	2.32	0.43
33:e:80:LYS:HB3	33:e:83:LEU:HD11	1.99	0.43
1:0:628:SER:HB3	1:0:669:GLU:CG	2.48	0.43
4:3:251:VAL:HG13	4:3:254:MET:SD	2.57	0.43
4:3:373:HIS:CG	4:3:374:PRO:HD2	2.53	0.43
9:8:72:PRO:O	9:8:152:LYS:NZ	2.45	0.43
11:A:1163:HIS:CD2	11:A:1302:GLU:HA	2.53	0.43
15:E:74:VAL:HA	15:E:103:LEU:O	2.17	0.43
34:f:78:LYS:HE3	36:h:93:ARG:CZ	2.48	0.43
2:1:589:GLU:OE2	2:1:614:TYR:OH	2.18	0.43
4:3:308:VAL:HB	4:3:316:TYR:HB2	2.00	0.43
8:7:43:ALA:HB1	8:7:55:LYS:HA	2.01	0.43
12:B:85:LEU:HB2	12:B:131:THR:OG1	2.19	0.43
12:B:758:LEU:HD23	12:B:758:LEU:HA	1.87	0.43
14:D:131:LEU:O	14:D:135:GLN:HG2	2.19	0.43
22:L:19:CYS:HB3	22:L:22:CYS:SG	2.58	0.43
30:V:80:GLU:OE2	30:V:89:LYS:HE2	2.19	0.43
1:0:360:ARG:HB2	1:0:435:TRP:CZ3	2.53	0.43
2:1:77:VAL:N	2:1:78:PRO:HD2	2.34	0.43
2:1:507:LYS:HA	2:1:683:ARG:NH2	2.34	0.43
4:3:315:LEU:HD11	4:3:346:VAL:HG13	2.00	0.43
10:9:28:ARG:NH2	16:F:80:MET:O	2.49	0.43
13:C:4:ALA:HB1	21:K:97:GLU:HB2	2.00	0.43
13:C:242:GLU:HG2	13:C:243:THR:N	2.33	0.43
18:H:40:ILE:HD12	18:H:124:ARG:HD2	2.01	0.43
20:J:47:ARG:HD2	20:J:47:ARG:C	2.44	0.43
5:4:66:ASP:O	5:4:71:MET:HG3	2.18	0.43
5:4:109:THR:HG22	5:4:144:SER:H	1.83	0.43
5:4:347:GLY:HA2	6:5:139:LYS:HG2	1.99	0.43
17:G:18:PHE:N	17:G:18:PHE:CD1	2.87	0.43
17:G:119:PHE:HB2	17:G:128:TYR:CZ	2.54	0.43
25:O:295:MET:CG	25:O:298:PRO:HD2	2.49	0.43
28:T:-55:DC:N4	28:T:-54:DG:O6	2.51	0.43
34:f:22:VAL:HG13	34:f:23:LEU:N	2.33	0.43
9:8:99:GLU:OE2	9:8:103:LYS:NZ	2.42	0.43
11:A:577:PRO:HB3	11:A:586:TRP:CE2	2.54	0.43
15:E:36:THR:OG1	15:E:38:GLU:OE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:152:DC:H2''	24:N:153:DC:C5	2.54	0.43
34:f:77:ALA:HB2	36:h:85:ASN:HD21	1.83	0.43
1:0:168:LEU:O	1:0:293:ALA:HA	2.18	0.43
1:0:328:PHE:HB2	2:1:501:GLN:HG3	2.01	0.43
2:1:623:VAL:N	2:1:681:ASP:OD2	2.49	0.43
4:3:35:TYR:O	4:3:117:ASN:ND2	2.52	0.43
8:7:35:VAL:HG22	8:7:58:PHE:CD2	2.53	0.43
11:A:909:LEU:HD21	11:A:973:GLY:HA2	2.01	0.43
12:B:1069:ILE:CG2	23:M:47:ASP:HB2	2.48	0.43
19:I:96:PHE:HA	19:I:111:TYR:O	2.18	0.43
24:N:48:DG:H1'	24:N:49:DA:C8	2.54	0.43
25:O:192:TYR:HB2	25:O:200:VAL:HG22	2.00	0.43
1:0:168:LEU:HB2	1:0:291:LEU:HB3	2.01	0.43
3:2:431:ILE:HD12	4:3:62:LEU:HD21	1.99	0.43
5:4:255:PRO:HB3	5:4:292:PRO:HD3	2.00	0.43
6:5:230:VAL:O	6:5:238:ARG:NH1	2.52	0.43
24:N:100:DT:H2''	24:N:101:DA:C8	2.53	0.43
33:a:66:LEU:HB3	33:a:67:PRO:HD3	2.00	0.43
1:0:528:LYS:HD2	1:0:725:GLU:HG2	2.00	0.43
18:H:96:VAL:HG22	18:H:116:VAL:HG22	2.00	0.43
24:N:36:DT:H2'	24:N:37:DC:C6	2.54	0.43
24:N:70:DC:H2''	24:N:71:DA:C8	2.54	0.43
1:0:517:GLU:H	1:0:517:GLU:CD	2.28	0.42
1:0:584:THR:HG23	1:0:588:GLU:CD	2.44	0.42
3:2:532:ALA:O	3:2:535:LYS:HG2	2.19	0.42
9:8:213:LEU:HD13	9:8:225:ILE:HG12	2.01	0.42
10:9:64:LEU:HD13	10:9:105:MET:HG3	2.00	0.42
11:A:334:ARG:NH1	11:A:335:PRO:O	2.52	0.42
24:N:72:DA:OP1	35:c:33:ARG:NH1	2.47	0.42
31:W:106:LYS:O	31:W:110:MET:HG2	2.19	0.42
2:1:237:HIS:HB3	2:1:461:LEU:HD21	2.01	0.42
2:1:425:THR:N	2:1:426:PRO:HD3	2.34	0.42
11:A:140:ARG:NH1	11:A:234:PHE:O	2.41	0.42
12:B:433:LEU:O	23:M:127:ARG:NH2	2.52	0.42
21:K:10:PHE:HA	21:K:37:LYS:HB3	2.01	0.42
23:M:137:ARG:NE	23:M:171:GLU:OE2	2.49	0.42
24:N:131:DT:H2''	24:N:132:DA:N7	2.34	0.42
2:1:87:LEU:HD12	2:1:90:LEU:HD23	2.00	0.42
2:1:165:GLY:HA2	2:1:189:TRP:CZ3	2.53	0.42
2:1:492:PRO:HD2	2:1:700:HIS:HB2	2.01	0.42
2:1:637:LEU:O	2:1:641:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:672:THR:OG1	3:2:362:ASP:OD1	2.28	0.42
3:2:171:LEU:C	3:2:173:ASP:H	2.27	0.42
4:3:55:TRP:CE3	4:3:96:TRP:HH2	2.37	0.42
8:7:263:LEU:HD11	8:7:290:SER:HB2	2.00	0.42
11:A:261:ARG:HD2	11:A:261:ARG:O	2.19	0.42
11:A:362:SER:HA	11:A:503:LEU:O	2.19	0.42
11:A:485:ASN:O	11:A:488:VAL:HG22	2.19	0.42
11:A:564:LEU:HD13	11:A:570:TRP:CZ2	2.54	0.42
11:A:728:THR:HG23	11:A:736:THR:HG23	2.01	0.42
12:B:938:ARG:HH21	12:B:983:GLU:CD	2.27	0.42
15:E:11:TRP:CE3	15:E:37:LEU:HB2	2.54	0.42
15:E:171:PRO:HB2	15:E:207:ARG:HG2	2.01	0.42
18:H:28:LEU:N	18:H:41:LEU:O	2.51	0.42
2:1:340:VAL:O	2:1:344:LEU:N	2.49	0.42
3:2:185:ARG:O	3:2:218:LYS:HD2	2.19	0.42
6:5:101:TYR:CE2	6:5:104:LEU:HB2	2.55	0.42
12:B:770:ARG:NH2	12:B:771:GLU:OE2	2.52	0.42
13:C:169:PHE:CD1	13:C:171:LYS:HB3	2.54	0.42
24:N:113:DG:C5	24:N:114:DC:C4	3.08	0.42
2:1:121:VAL:HG13	2:1:130:VAL:HA	2.00	0.42
2:1:124:LEU:HB3	2:1:129:ASP:HB2	2.02	0.42
2:1:490:LEU:HD23	2:1:492:PRO:HD3	2.02	0.42
5:4:272:SER:HA	5:4:297:LYS:O	2.19	0.42
11:A:60:PRO:HB2	11:A:72:GLN:OE1	2.19	0.42
11:A:491:PRO:HD3	11:A:535:MET:HB3	2.00	0.42
11:A:1263:ASN:O	11:A:1267:ASN:N	2.48	0.42
12:B:214:LYS:HE2	12:B:215:TYR:CZ	2.54	0.42
18:H:10:PHE:HB2	18:H:56:PHE:CE1	2.55	0.42
23:M:227:GLN:HG2	23:M:228:VAL:N	2.35	0.42
25:O:199:ALA:HB2	25:O:214:PHE:CE2	2.54	0.42
25:O:295:MET:HG3	25:O:298:PRO:HD2	2.02	0.42
35:c:86:LEU:O	35:c:90:ASN:ND2	2.51	0.42
1:0:202:SER:HB3	8:7:177:ARG:HD3	2.01	0.42
2:1:583:LYS:HB3	3:2:315:LEU:HD23	2.02	0.42
4:3:156:TRP:CE3	4:3:268:PHE:HE1	2.37	0.42
11:A:246:GLU:HG2	11:A:247:TRP:CD1	2.54	0.42
11:A:1192:TRP:HZ3	11:A:1246:ILE:HG22	1.85	0.42
12:B:755:GLN:HE22	20:J:48:MET:HE2	1.84	0.42
12:B:1028:LEU:HD13	12:B:1041:ILE:HB	2.01	0.42
1:0:203:GLU:HG2	8:7:177:ARG:NH2	2.34	0.42
1:0:509:GLU:OE1	1:0:673:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:565:VAL:HG22	1:0:727:GLU:OE2	2.19	0.42
5:4:346:TYR:CG	5:4:347:GLY:N	2.87	0.42
9:8:135:HIS:NE2	9:8:155:ASP:O	2.51	0.42
9:8:219:LEU:O	9:8:223:THR:HG23	2.20	0.42
11:A:230:ASP:N	11:A:230:ASP:OD1	2.53	0.42
14:D:45:LYS:HG2	14:D:61:PHE:CE1	2.54	0.42
27:R:206:THR:HG21	27:R:213:LEU:HD13	2.02	0.42
35:g:25:GLN:N	35:g:57:GLU:OE1	2.50	0.42
2:1:322:SER:HB3	8:7:99:LEU:HB3	2.02	0.42
4:3:224:GLN:HG3	4:3:230:LEU:HG	2.02	0.42
12:B:794:VAL:HG13	12:B:965:ILE:HG23	2.01	0.42
27:R:54:VAL:HB	27:R:83:PHE:HB2	2.02	0.42
35:c:64:LEU:HD11	36:d:42:VAL:HG13	2.02	0.42
1:0:67:LEU:HD13	4:3:339:PRO:HB2	2.02	0.42
2:1:24:TYR:HA	2:1:481:PHE:CZ	2.54	0.42
2:1:348:HIS:HA	2:1:420:PRO:HG3	2.00	0.42
4:3:349:GLU:O	4:3:353:GLN:HG2	2.20	0.42
8:7:78:VAL:HG13	8:7:82:TYR:HD2	1.85	0.42
9:8:134:LEU:HG	9:8:162:PHE:CD1	2.55	0.42
11:A:495:ASP:OD1	11:A:495:ASP:O	2.38	0.42
11:A:687:ILE:HD11	11:A:766:PHE:CD2	2.55	0.42
11:A:766:PHE:HB3	11:A:781:ILE:HG12	2.02	0.42
12:B:100:GLU:OE1	22:L:42:ARG:NH1	2.49	0.42
12:B:343:LEU:O	12:B:361:LYS:NZ	2.47	0.42
17:G:118:GLU:HG3	17:G:129:LYS:O	2.20	0.42
28:T:-12:DC:H4'	28:T:-11:DC:OP1	2.20	0.42
34:b:32:LYS:HB3	34:b:33:PRO:HD3	2.02	0.42
1:0:306:ILE:HG22	1:0:306:ILE:O	2.19	0.42
2:1:121:VAL:CG1	2:1:130:VAL:HG13	2.50	0.42
2:1:283:ASP:HA	2:1:286:ARG:HD2	2.01	0.42
2:1:421:PHE:CD1	2:1:426:PRO:HA	2.55	0.42
2:1:428:ILE:HD12	3:2:292:SER:HA	2.02	0.42
2:1:480:THR:N	2:1:758:GLN:O	2.34	0.42
3:2:431:ILE:HG12	4:3:58:ARG:NH2	2.34	0.42
4:3:51:LEU:HD13	4:3:83:GLN:HA	2.02	0.42
4:3:241:SER:HA	4:3:288:ILE:HA	2.01	0.42
8:7:117:ASN:O	8:7:121:LYS:HG3	2.20	0.42
11:A:981:CYS:HB3	11:A:986:MET:HE1	2.02	0.42
12:B:796:MET:O	12:B:948:GLN:HA	2.20	0.42
12:B:847:LYS:HB3	12:B:854:ILE:HD12	2.01	0.42
13:C:56:SER:HB2	13:C:158:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:167:GLU:O	15:E:208:LEU:HD22	2.20	0.42
17:G:15:PRO:HA	17:G:18:PHE:CZ	2.54	0.42
24:N:38:DT:H2''	24:N:39:DT:H71	2.02	0.42
24:N:88:DT:H2''	24:N:89:DC:C6	2.54	0.42
26:Q:93:PRO:HA	26:Q:96:GLN:CD	2.44	0.42
27:R:220:ILE:HG13	27:R:221:GLY:H	1.85	0.42
1:0:305:ASP:OD1	1:0:359:LYS:NZ	2.49	0.41
2:1:467:TYR:N	2:1:468:PRO:HD2	2.35	0.41
5:4:360:CYS:O	5:4:364:GLN:HA	2.20	0.41
11:A:421:ARG:HB2	11:A:425:ASP:OD1	2.20	0.41
12:B:435:ILE:O	23:M:127:ARG:NH1	2.38	0.41
24:N:123:DC:H4'	34:f:46:ARG:CZ	2.50	0.41
27:R:175:ARG:HE	27:R:209:PRO:CA	2.30	0.41
33:e:63:ILE:O	33:e:94:GLN:NE2	2.53	0.41
1:0:161:VAL:HG23	1:0:162:SER:N	2.35	0.41
11:A:41:ILE:HG23	11:A:55:GLY:O	2.20	0.41
11:A:713:VAL:HG11	11:A:817:PRO:HD3	2.02	0.41
11:A:1139:LEU:HD13	11:A:1341:VAL:HA	2.03	0.41
12:B:908:MET:HB3	22:L:45:TYR:CE1	2.55	0.41
12:B:939:HIS:NE2	12:B:983:GLU:OE1	2.50	0.41
26:Q:124:TYR:OH	27:R:22:LYS:HE2	2.19	0.41
28:T:-78:DG:H2''	28:T:-77:DA:C8	2.55	0.41
31:W:25:PHE:CE1	32:X:212:VAL:HG11	2.55	0.41
32:X:99:LEU:HD13	32:X:124:LEU:HD11	2.02	0.41
1:0:541:PHE:CG	1:0:703:PHE:HE2	2.38	0.41
3:2:152:THR:C	3:2:154:SER:H	2.28	0.41
5:4:290:PHE:HA	5:4:296:ALA:O	2.20	0.41
6:5:195:VAL:HG11	6:5:214:TYR:CE1	2.55	0.41
8:7:132:VAL:O	8:7:136:ASN:HB2	2.20	0.41
9:8:125:LEU:HD21	9:8:138:LEU:HD11	2.01	0.41
11:A:458:PHE:CE2	11:A:484:LEU:HD11	2.54	0.41
11:A:542:LEU:HD12	11:A:542:LEU:HA	1.77	0.41
12:B:544:PHE:CE1	12:B:548:TRP:CD1	3.08	0.41
17:G:4:HIS:NE2	17:G:73:LYS:HB3	2.35	0.41
24:N:66:DC:H2''	24:N:67:DG:C8	2.56	0.41
24:N:161:DC:H2''	24:N:162:DA:C5	2.56	0.41
34:f:49:GLY:HA2	34:f:52:TYR:CE2	2.55	0.41
36:h:42:VAL:HG21	36:h:60:MET:HE1	2.02	0.41
1:0:77:TRP:CE2	1:0:145:LYS:HD2	2.55	0.41
1:0:126:ALA:HB1	1:0:131:LEU:HD12	2.02	0.41
1:0:296:ASP:OD2	1:0:299:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:216:MET:HE3	4:3:268:PHE:CE2	2.56	0.41
6:5:145:HIS:NE2	6:5:149:LYS:HE3	2.36	0.41
11:A:1005:HIS:ND1	11:A:1007:ILE:HG22	2.36	0.41
11:A:1173:THR:HG23	19:I:56:ASN:OD1	2.20	0.41
11:A:1248:ASN:ND2	11:A:1254:LYS:O	2.44	0.41
11:A:1471:PHE:CZ	16:F:61:GLU:HA	2.55	0.41
12:B:564:ALA:HB2	12:B:578:LYS:HE2	2.02	0.41
12:B:1060:HIS:HB2	12:B:1080:ARG:HB2	2.02	0.41
23:M:130:LEU:HD22	23:M:134:ILE:HD13	2.02	0.41
2:1:495:ILE:HD11	2:1:713:GLY:HA3	2.02	0.41
2:1:618:VAL:HG21	2:1:667:ALA:HB2	2.03	0.41
4:3:55:TRP:HE3	4:3:96:TRP:HH2	1.68	0.41
9:8:16:ASP:O	9:8:28:LYS:N	2.54	0.41
9:8:179:ARG:HG2	9:8:183:LEU:HB2	2.03	0.41
11:A:478:PRO:O	11:A:479:TRP:CG	2.73	0.41
11:A:802:PHE:CE1	11:A:808:PRO:HD3	2.54	0.41
12:B:552:ASN:OD1	12:B:553:LEU:N	2.54	0.41
22:L:32:ASP:OD1	22:L:32:ASP:N	2.53	0.41
1:0:636:GLU:HG2	1:0:639:ARG:NH2	2.28	0.41
2:1:145:GLN:HB3	2:1:152:LEU:HD13	2.03	0.41
2:1:701:LEU:HD12	2:1:705:ASN:OD1	2.21	0.41
6:5:258:HIS:HE1	6:5:260:ASN:CG	2.28	0.41
12:B:502:HIS:CE1	12:B:504:THR:HG23	2.56	0.41
12:B:1122:CYS:HB3	12:B:1140:CYS:SG	2.60	0.41
14:D:96:GLU:HG3	14:D:121:ARG:NH1	2.35	0.41
15:E:46:ASP:CB	15:E:52:ARG:HB3	2.50	0.41
24:N:-4:DG:O6	28:T:3:DC:N4	2.54	0.41
27:R:140:ARG:O	27:R:141:LEU:HD23	2.21	0.41
31:W:42:CYS:SG	31:W:75:ARG:NH1	2.91	0.41
2:1:112:ARG:HH21	2:1:193:PHE:HZ	1.67	0.41
4:3:51:LEU:HB3	4:3:83:GLN:NE2	2.35	0.41
5:4:107:ILE:HA	5:4:116:LYS:HA	2.03	0.41
11:A:373:LEU:HD23	11:A:373:LEU:HA	1.90	0.41
11:A:1163:HIS:HA	11:A:1300:GLY:HA3	2.02	0.41
12:B:146:LYS:HB3	27:R:149:VAL:HG21	2.03	0.41
12:B:1069:ILE:HG23	23:M:47:ASP:HB2	2.02	0.41
13:C:5:ASN:HB2	21:K:97:GLU:OE2	2.21	0.41
18:H:35:PHE:HB2	18:H:37:MET:HG2	2.01	0.41
28:T:-162:DT:H2"	28:T:-161:DG:C8	2.56	0.41
32:X:96:PRO:HB2	32:X:136:LYS:HE2	2.02	0.41
35:g:63:ILE:HD13	35:g:94:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:561:PHE:CZ	1:0:609:LYS:HA	2.56	0.41
2:1:499:ASN:OD1	2:1:710:VAL:HB	2.21	0.41
5:4:255:PRO:HG3	5:4:312:LEU:HD13	2.02	0.41
9:8:143:LEU:HD12	9:8:151:LEU:HD21	2.02	0.41
11:A:890:ARG:HA	11:A:890:ARG:HD3	1.82	0.41
25:O:187:ALA:HB3	25:O:190:ALA:HB2	2.02	0.41
25:O:297:LYS:CB	25:O:298:PRO:HD3	2.51	0.41
27:R:58:LEU:HD23	27:R:63:ALA:HB2	2.03	0.41
28:T:-134:DG:H2''	28:T:-133:DT:C5	2.56	0.41
30:V:82:ARG:NH1	30:V:83:GLU:O	2.54	0.41
31:W:54:PHE:CZ	32:X:192:VAL:HG11	2.56	0.41
32:X:80:LYS:HE2	32:X:106:THR:HB	2.03	0.41
1:0:167:LYS:HG2	1:0:292:LEU:HD23	2.02	0.41
2:1:586:GLU:OE1	3:2:319:LEU:HD21	2.21	0.41
2:1:664:VAL:HG13	2:1:677:MET:HE1	2.03	0.41
3:2:346:GLN:HB3	3:2:349:VAL:HG23	2.02	0.41
3:2:431:ILE:HG12	4:3:58:ARG:CZ	2.51	0.41
4:3:134:SER:HB3	4:3:280:ARG:NH2	2.36	0.41
5:4:59:ARG:NH2	5:4:235:HIS:O	2.40	0.41
6:5:102:GLU:O	6:5:106:SER:OG	2.37	0.41
6:5:160:ARG:NH1	6:5:238:ARG:NH2	2.66	0.41
6:5:258:HIS:CE1	6:5:260:ASN:CG	2.99	0.41
7:6:36:GLN:HE21	7:6:38:ILE:HG22	1.86	0.41
9:8:179:ARG:HD2	9:8:184:LEU:HD21	2.01	0.41
11:A:525:ILE:O	11:A:534:VAL:N	2.41	0.41
11:A:1143:LEU:HD13	11:A:1147:SER:HB2	2.02	0.41
12:B:764:MET:HE1	12:B:938:ARG:NH1	2.36	0.41
12:B:917:LYS:HE3	22:L:34:ILE:HD11	2.03	0.41
12:B:968:ASN:OD1	12:B:969:PRO:HD2	2.20	0.41
13:C:118:ARG:HD3	13:C:118:ARG:HA	1.89	0.41
13:C:169:PHE:CE1	13:C:171:LYS:HB3	2.55	0.41
18:H:32:SER:O	18:H:36:LYS:HA	2.21	0.41
24:N:-3:DG:C6	24:N:-2:DG:C6	3.09	0.41
24:N:9:DG:N2	28:T:-8:DC:O2	2.53	0.41
24:N:119:DT:H2''	24:N:120:DC:C5	2.56	0.41
24:N:161:DC:H2''	24:N:162:DA:N7	2.36	0.41
27:R:20:LEU:O	27:R:113:ARG:HA	2.20	0.41
27:R:175:ARG:NH2	27:R:209:PRO:HA	2.31	0.41
31:W:171:LYS:O	31:W:175:THR:HG23	2.20	0.41
1:0:431:LYS:HG2	1:0:457:ILE:HG23	2.03	0.41
4:3:243:SER:HB2	4:3:249:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:680:LEU:HA	11:A:680:LEU:HD12	1.82	0.41
11:A:706:ILE:HD11	11:A:787:VAL:HG21	2.02	0.41
12:B:645:GLU:O	12:B:649:ASN:HB3	2.21	0.41
12:B:970:HIS:C	12:B:973:PRO:HD2	2.46	0.41
24:N:11:DG:H1	28:T:-11:DC:H42	1.68	0.41
24:N:155:DA:H2''	24:N:156:DG:H5'	2.03	0.41
26:Q:53:ASN:ND2	26:Q:96:GLN:OE1	2.54	0.41
32:X:226:ASP:OD1	32:X:227:SER:N	2.54	0.41
1:0:522:TYR:CE1	1:0:530:ARG:HD3	2.56	0.40
3:2:227:SER:OG	3:2:228:HIS:N	2.54	0.40
4:3:220:LEU:HA	4:3:223:ALA:HB2	2.03	0.40
4:3:273:GLN:NE2	4:3:281:TYR:HB3	2.36	0.40
11:A:774:ALA:O	11:A:775:LYS:HE2	2.20	0.40
11:A:987:ILE:HG21	11:A:1058:PHE:CD1	2.57	0.40
1:0:363:VAL:HB	1:0:407:ILE:HG23	2.02	0.40
2:1:16:TYR:CE1	2:1:734:LEU:HD21	2.57	0.40
2:1:490:LEU:CD2	2:1:492:PRO:HD3	2.51	0.40
6:5:177:PHE:CE2	6:5:202:LEU:HB3	2.55	0.40
6:5:243:LEU:HB3	6:5:244:PRO:HD2	2.03	0.40
11:A:31:LEU:HD22	11:A:252:VAL:HG13	2.03	0.40
11:A:368:THR:O	11:A:483:ARG:HA	2.21	0.40
11:A:1022:ILE:HD11	11:A:1076:PHE:CZ	2.57	0.40
12:B:994:GLY:HA2	20:J:50:LEU:HD22	2.03	0.40
15:E:61:LEU:HB2	15:E:73:PHE:CE1	2.56	0.40
23:M:172:GLY:C	23:M:174:PRO:HD3	2.47	0.40
24:N:53:DC:H2''	24:N:54:DC:C6	2.57	0.40
28:T:-181:DT:H2''	28:T:-180:DA:C8	2.57	0.40
28:T:-114:DG:C5	28:T:-113:DC:C4	3.09	0.40
32:X:89:HIS:HB2	32:X:139:PHE:CZ	2.56	0.40
1:0:76:LEU:HB2	1:0:144:SER:HA	2.02	0.40
1:0:366:ASN:HD22	1:0:442:GLU:CD	2.27	0.40
2:1:161:PHE:CZ	2:1:194:LEU:HA	2.56	0.40
2:1:311:PRO:O	2:1:312:ASP:C	2.63	0.40
6:5:32:PHE:HB2	6:5:221:PRO:HG3	2.04	0.40
8:7:108:ASN:HA	8:7:112:ASN:HB2	2.02	0.40
9:8:102:ILE:O	9:8:209:ARG:NH2	2.53	0.40
11:A:525:ILE:HA	11:A:535:MET:HE3	2.04	0.40
11:A:834:THR:HG23	12:B:677:MET:HE3	2.04	0.40
12:B:130:LYS:HB3	12:B:142:THR:HG23	2.04	0.40
12:B:551:GLU:HB3	12:B:556:ILE:HG21	2.02	0.40
13:C:106:ARG:HD3	13:C:158:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:27:LEU:HB2	15:E:65:ASN:OD1	2.21	0.40
20:J:43:TYR:HA	20:J:46:ARG:HD3	2.02	0.40
33:e:132:ARG:NE	33:e:134:GLU:OE2	2.51	0.40
1:0:45:GLN:H	1:0:45:GLN:CD	2.29	0.40
1:0:558:ILE:HD11	1:0:624:ILE:CD1	2.52	0.40
1:0:568:LEU:HB3	1:0:581:TYR:OH	2.21	0.40
2:1:259:CYS:SG	2:1:397:LEU:HA	2.61	0.40
5:4:195:ARG:NH1	5:4:216:GLY:O	2.55	0.40
11:A:1167:ARG:HA	11:A:1170:THR:HG22	2.03	0.40
11:A:1221:MET:HE2	11:A:1255:LEU:HD13	2.03	0.40
12:B:916:TYR:OH	23:M:136:ASP:OD2	2.34	0.40
13:C:47:ILE:HA	13:C:165:ALA:HA	2.02	0.40
23:M:133:ASN:OD1	23:M:134:ILE:N	2.54	0.40
27:R:31:TRP:CD1	27:R:40:VAL:HB	2.57	0.40
2:1:28:LEU:HD23	2:1:32:LEU:HD13	2.04	0.40
4:3:55:TRP:HZ2	4:3:75:VAL:HG23	1.84	0.40
15:E:35:GLN:NE2	15:E:43:GLN:OE1	2.30	0.40
29:U:310:GLU:OE2	29:U:312:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	649/782 (83%)	629 (97%)	20 (3%)	0	100	100
2	1	758/760 (100%)	736 (97%)	22 (3%)	0	100	100
3	2	402/548 (73%)	352 (88%)	47 (12%)	3 (1%)	18	55
4	3	450/462 (97%)	437 (97%)	13 (3%)	0	100	100
5	4	362/395 (92%)	340 (94%)	22 (6%)	0	100	100
6	5	259/308 (84%)	244 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	6	64/71 (90%)	64 (100%)	0	0	100	100
8	7	269/309 (87%)	264 (98%)	5 (2%)	0	100	100
9	8	296/346 (86%)	281 (95%)	15 (5%)	0	100	100
10	9	285/323 (88%)	279 (98%)	6 (2%)	0	100	100
11	A	1413/1970 (72%)	1376 (97%)	37 (3%)	0	100	100
12	B	1130/1174 (96%)	1099 (97%)	31 (3%)	0	100	100
13	C	253/275 (92%)	248 (98%)	5 (2%)	0	100	100
14	D	126/142 (89%)	125 (99%)	1 (1%)	0	100	100
15	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
17	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
18	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
19	I	112/125 (90%)	107 (96%)	5 (4%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
22	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
23	M	248/316 (78%)	242 (98%)	6 (2%)	0	100	100
25	O	177/339 (52%)	176 (99%)	1 (1%)	0	100	100
26	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
27	R	218/249 (88%)	215 (99%)	3 (1%)	0	100	100
29	U	109/376 (29%)	108 (99%)	1 (1%)	0	100	100
30	V	97/109 (89%)	94 (97%)	3 (3%)	0	100	100
31	W	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
32	X	169/291 (58%)	162 (96%)	7 (4%)	0	100	100
33	a	95/136 (70%)	95 (100%)	0	0	100	100
33	e	96/136 (71%)	96 (100%)	0	0	100	100
34	b	80/103 (78%)	80 (100%)	0	0	100	100
34	f	80/103 (78%)	80 (100%)	0	0	100	100
35	c	107/130 (82%)	107 (100%)	0	0	100	100
35	g	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
36	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	h	93/126 (74%)	93 (100%)	0	0	100	100
All	All	9731/12274 (79%)	9439 (97%)	289 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	164	VAL
3	2	170	PHE
3	2	169	ALA

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	0	558/688 (81%)	558 (100%)	0	100	100
2	1	639/664 (96%)	639 (100%)	0	100	100
3	2	176/484 (36%)	176 (100%)	0	100	100
4	3	384/399 (96%)	384 (100%)	0	100	100
5	4	280/352 (80%)	280 (100%)	0	100	100
6	5	234/272 (86%)	234 (100%)	0	100	100
7	6	59/64 (92%)	59 (100%)	0	100	100
8	7	250/283 (88%)	250 (100%)	0	100	100
9	8	258/299 (86%)	253 (98%)	5 (2%)	50	67
10	9	259/296 (88%)	259 (100%)	0	100	100
11	A	1254/1749 (72%)	1254 (100%)	0	100	100
12	B	994/1027 (97%)	994 (100%)	0	100	100
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/126 (94%)	118 (100%)	0	100	100
15	E	191/192 (100%)	191 (100%)	0	100	100
16	F	69/111 (62%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	G	152/153 (99%)	152 (100%)	0	100	100
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	53 (100%)	0	100	100
21	K	104/106 (98%)	104 (100%)	0	100	100
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	121 (100%)	0	100	100
27	R	196/218 (90%)	196 (100%)	0	100	100
29	U	105/324 (32%)	105 (100%)	0	100	100
30	V	90/98 (92%)	90 (100%)	0	100	100
31	W	169/177 (96%)	169 (100%)	0	100	100
32	X	154/261 (59%)	154 (100%)	0	100	100
33	a	85/111 (77%)	85 (100%)	0	100	100
33	e	86/111 (78%)	86 (100%)	0	100	100
34	b	67/79 (85%)	67 (100%)	0	100	100
34	f	67/79 (85%)	67 (100%)	0	100	100
35	c	86/101 (85%)	86 (100%)	0	100	100
35	g	84/101 (83%)	84 (100%)	0	100	100
36	d	83/106 (78%)	83 (100%)	0	100	100
36	h	81/106 (76%)	81 (100%)	0	100	100
All	All	8382/10752 (78%)	8377 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	8	64	LYS
9	8	96	THR
9	8	97	ASP
9	8	203	LEU
9	8	307	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	112	HIS
1	0	172	HIS
1	0	555	ASN
1	0	625	GLN
2	1	97	GLN
2	1	262	ASN
2	1	384	HIS
2	1	452	GLN
2	1	499	ASN
2	1	522	ASN
2	1	590	ASN
2	1	698	GLN
2	1	700	HIS
3	2	226	GLN
3	2	375	ASN
4	3	10	ASN
4	3	13	HIS
4	3	117	ASN
4	3	410	ASN
5	4	162	HIS
5	4	324	HIS
6	5	48	HIS
6	5	258	HIS
7	6	36	GLN
8	7	200	GLN
9	8	83	HIS
9	8	171	HIS
9	8	258	HIS
10	9	94	ASN
11	A	387	ASN
11	A	459	ASN
11	A	504	HIS
11	A	531	ASN
11	A	599	HIS
11	A	671	ASN
11	A	765	ASN
11	A	792	ASN
11	A	861	GLN
11	A	905	ASN
11	A	1005	HIS
11	A	1093	GLN
11	A	1394	ASN
12	B	98	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	312	GLN
12	B	486	ASN
12	B	631	GLN
12	B	642	GLN
12	B	1120	ASN
12	B	1133	HIS
14	D	38	HIS
14	D	55	GLN
15	E	133	GLN
15	E	189	GLN
17	G	28	GLN
17	G	53	ASN
18	H	29	HIS
19	I	22	ASN
19	I	87	GLN
19	I	91	HIS
19	I	100	HIS
19	I	121	HIS
25	O	229	GLN
25	O	278	GLN
26	Q	10	ASN
26	Q	53	ASN
27	R	152	ASN
30	V	27	GLN
30	V	39	GLN
33	a	69	GLN
33	a	109	ASN
35	c	25	GLN
36	d	48	GLN
36	d	50	HIS
36	d	68	ASN
36	h	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
37	SF4	1	1000	2	0,12,12	-	-	-		

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
37	SF4	1	1000	2	-	-	0/6/5/5

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 ⓘ

There are no chain breaks in this entry.

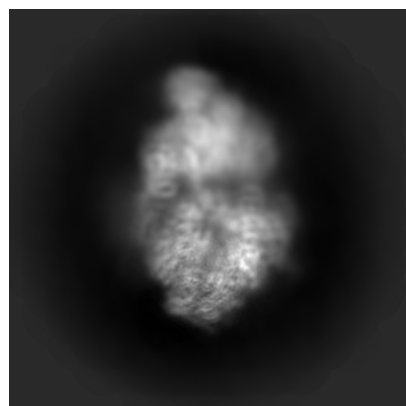
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16331. These allow visual inspection of the internal detail of the map and identification of artifacts.

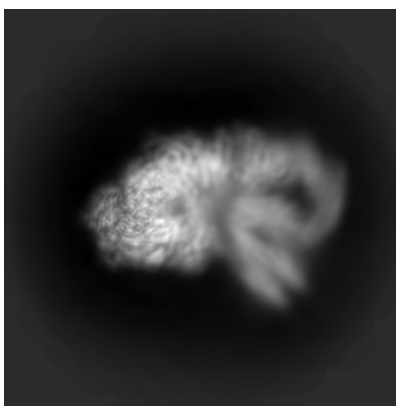
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

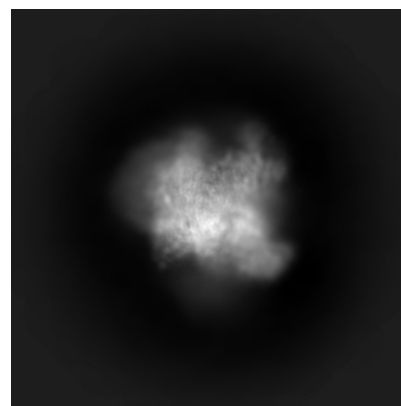
6.1.1 Primary map



X

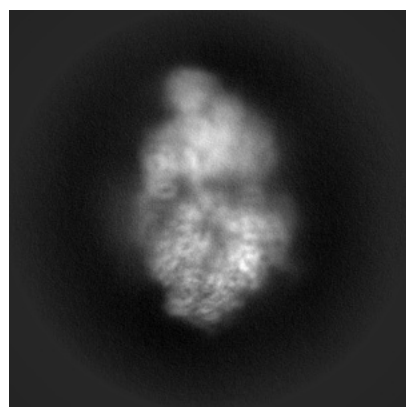


Y

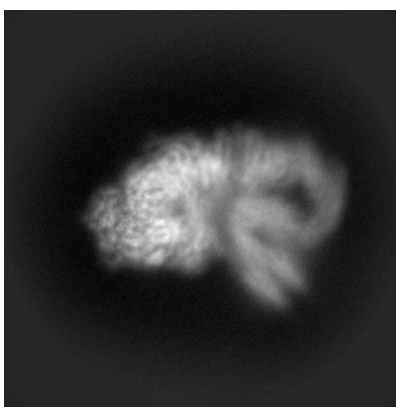


Z

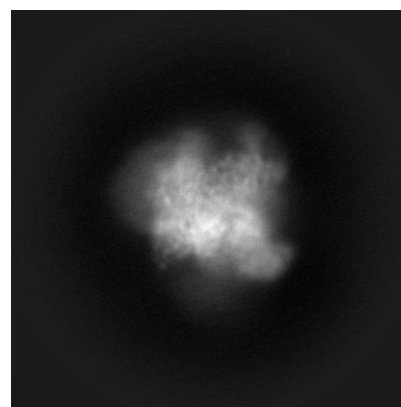
6.1.2 Raw map



X



Y

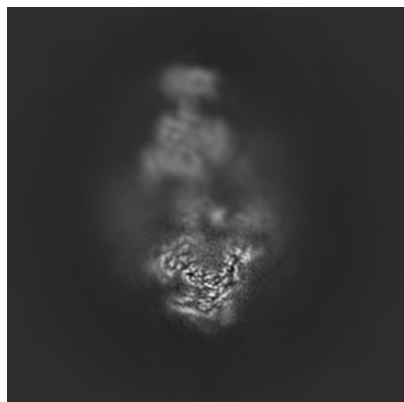


Z

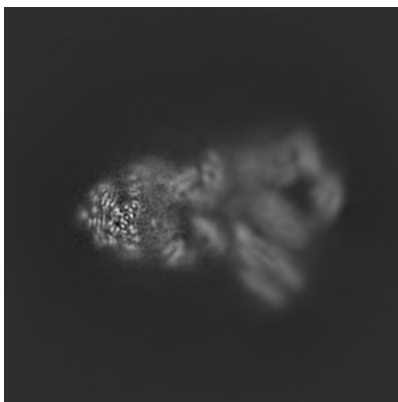
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

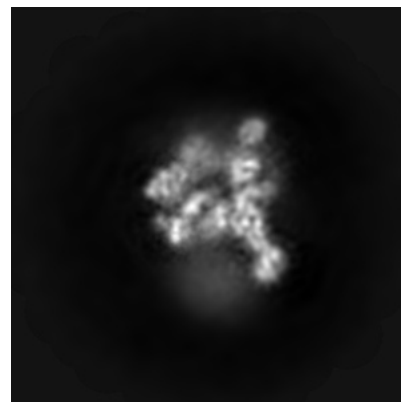
6.2.1 Primary map



X Index: 200

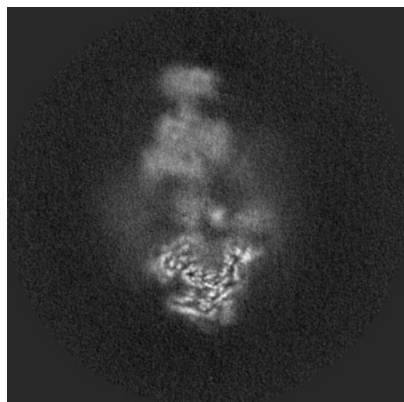


Y Index: 200

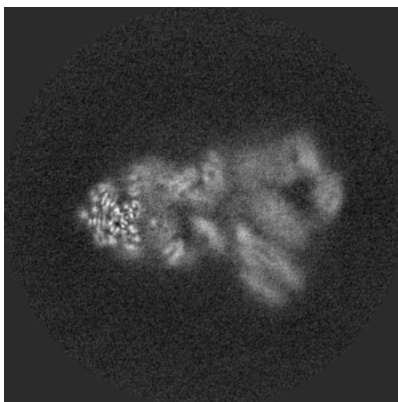


Z Index: 200

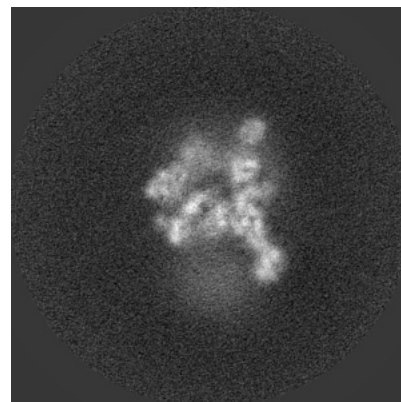
6.2.2 Raw map



X Index: 200



Y Index: 200

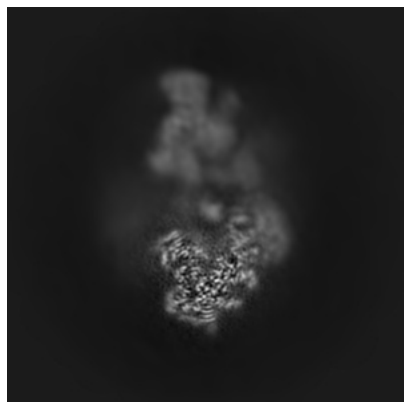


Z Index: 200

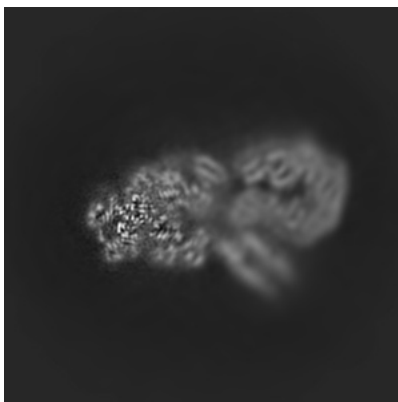
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

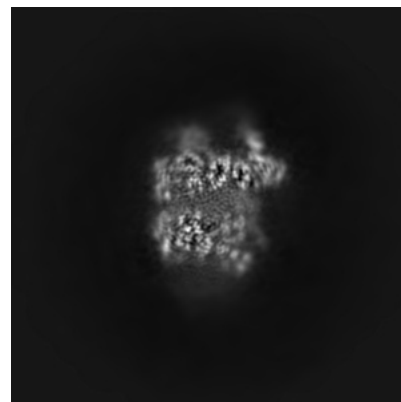
6.3.1 Primary map



X Index: 186

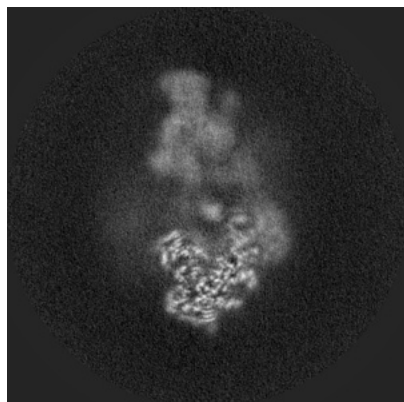


Y Index: 185

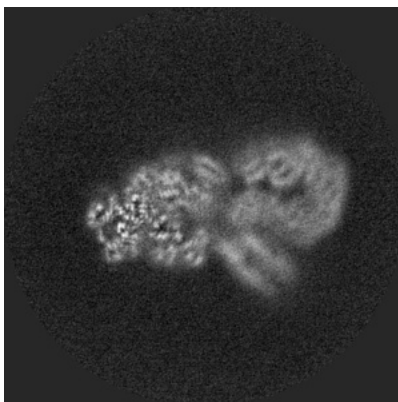


Z Index: 154

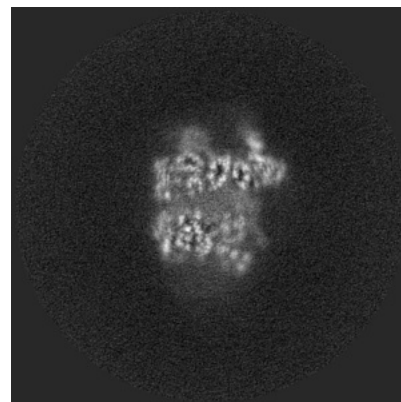
6.3.2 Raw map



X Index: 186



Y Index: 185

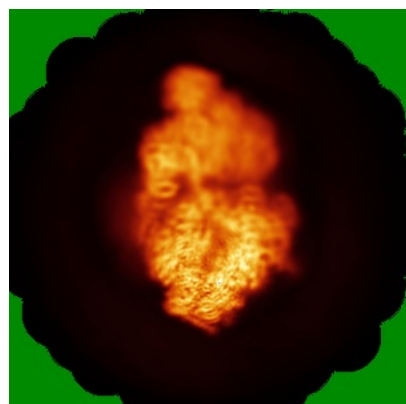


Z Index: 154

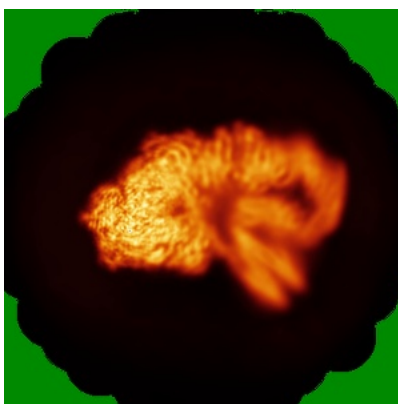
The images above show the largest variance slices of the map in three orthogonal directions.

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

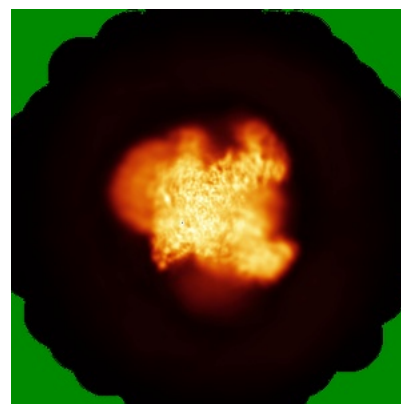
6.4.1 Primary map



X

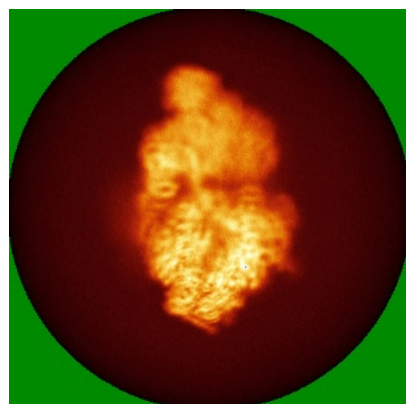


Y

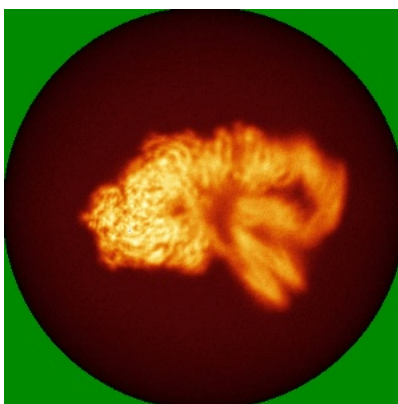


Z

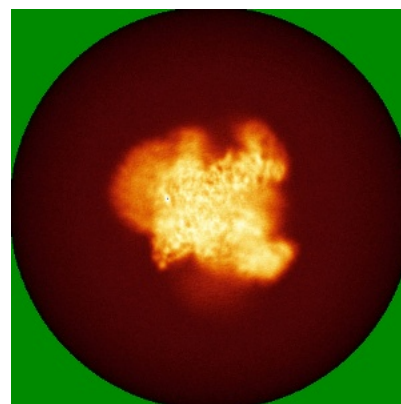
6.4.2 Raw map



X



Y

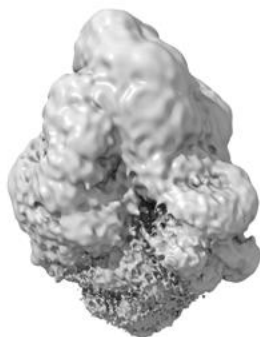


Z

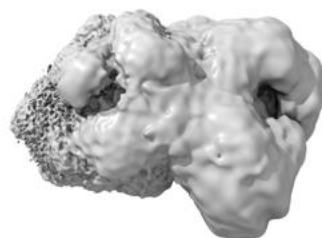
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

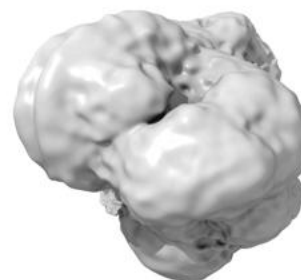
6.5.1 Primary map



X



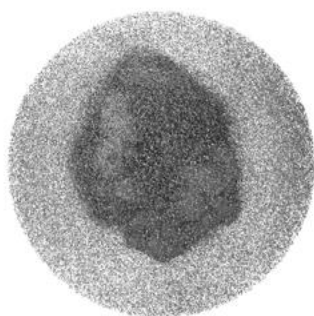
Y



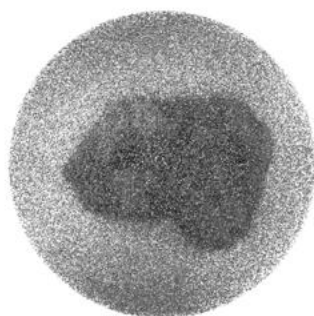
Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

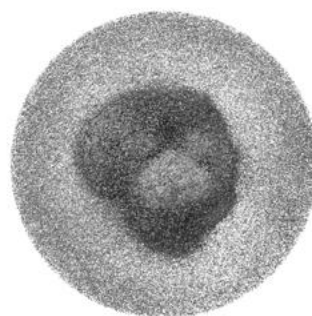
6.5.2 Raw map



X



Y



Z

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

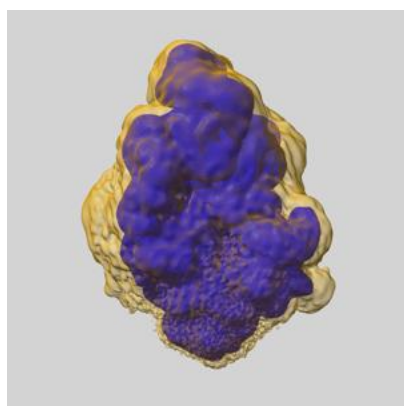
6.6 Mask visualisation [i](#)

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

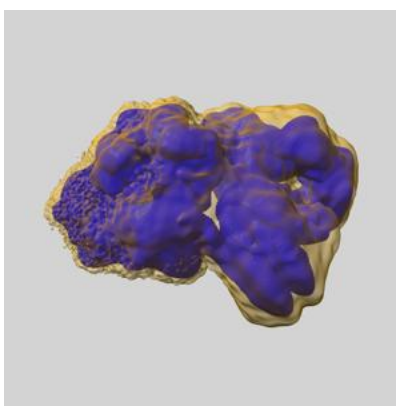
A mask typically either:

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

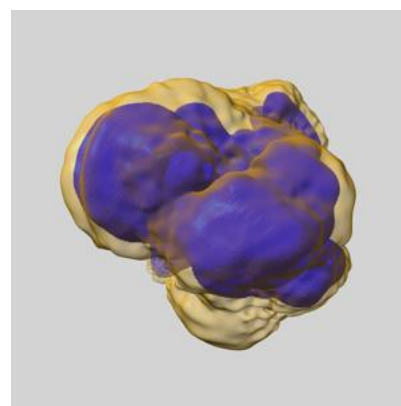
6.6.1 emd_16331_msk_1.map [i](#)



X



Y

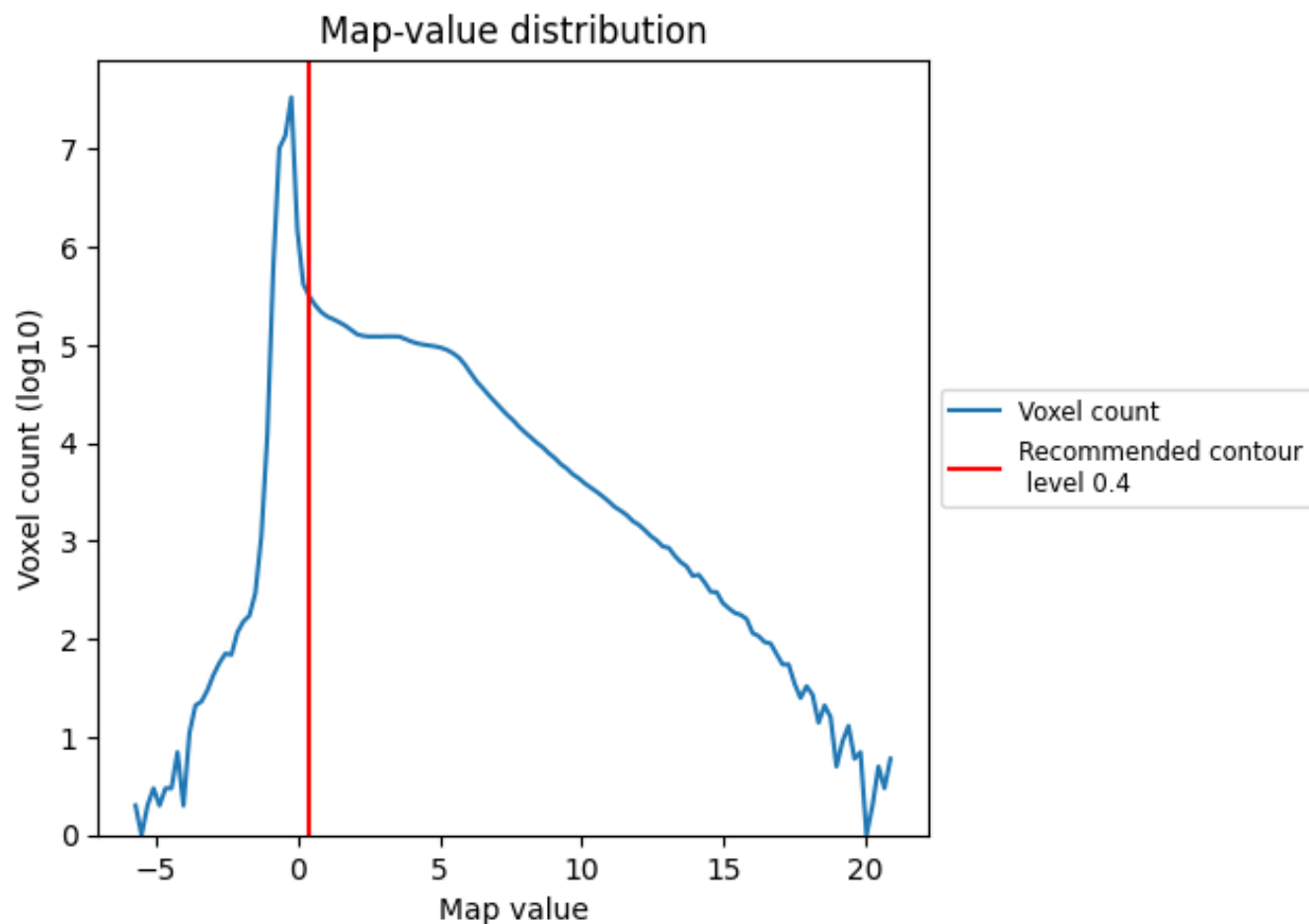


Z

7 Map analysis [i](#)

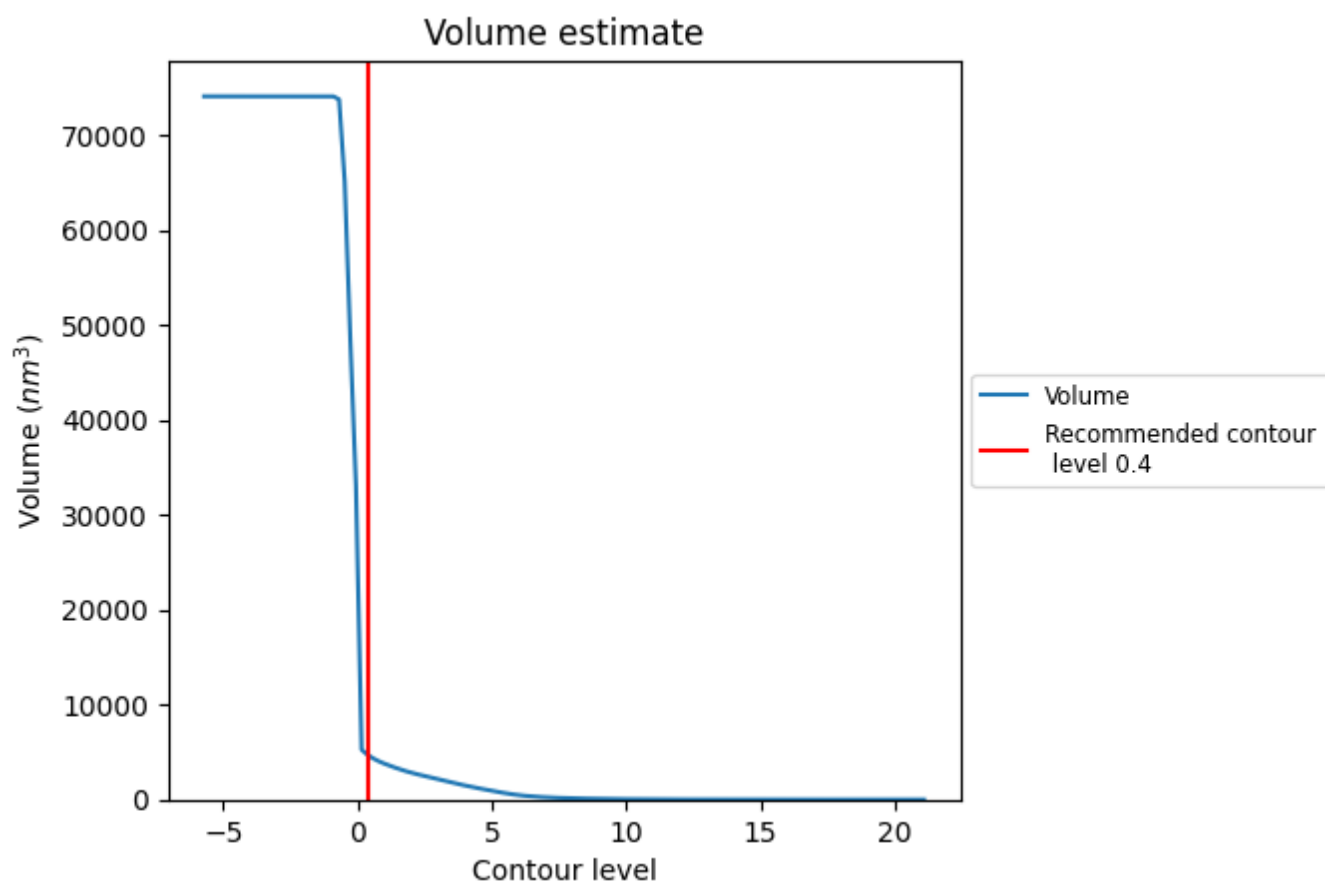
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

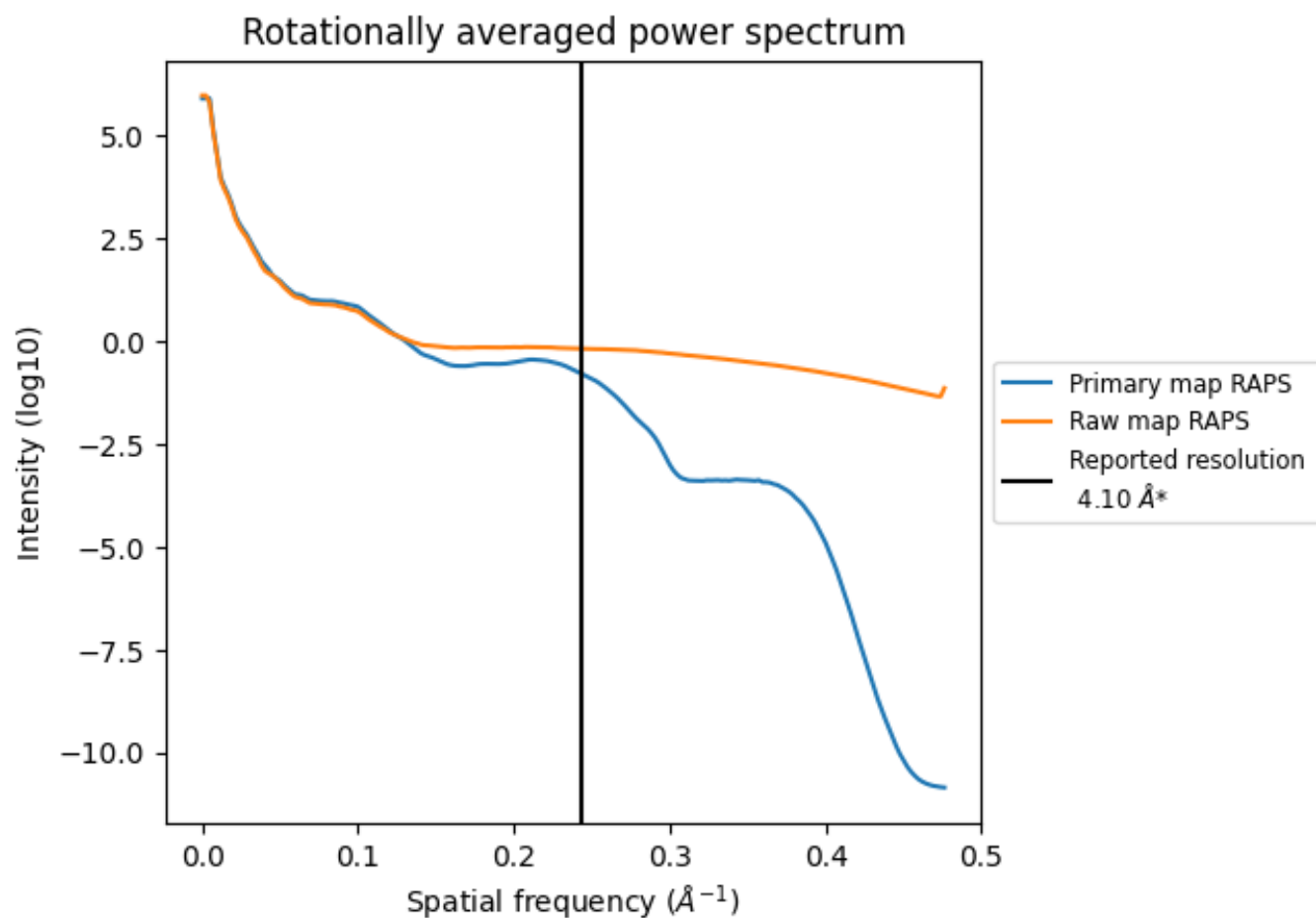
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4663 nm³; this corresponds to an approximate mass of 4212 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 ⓘ

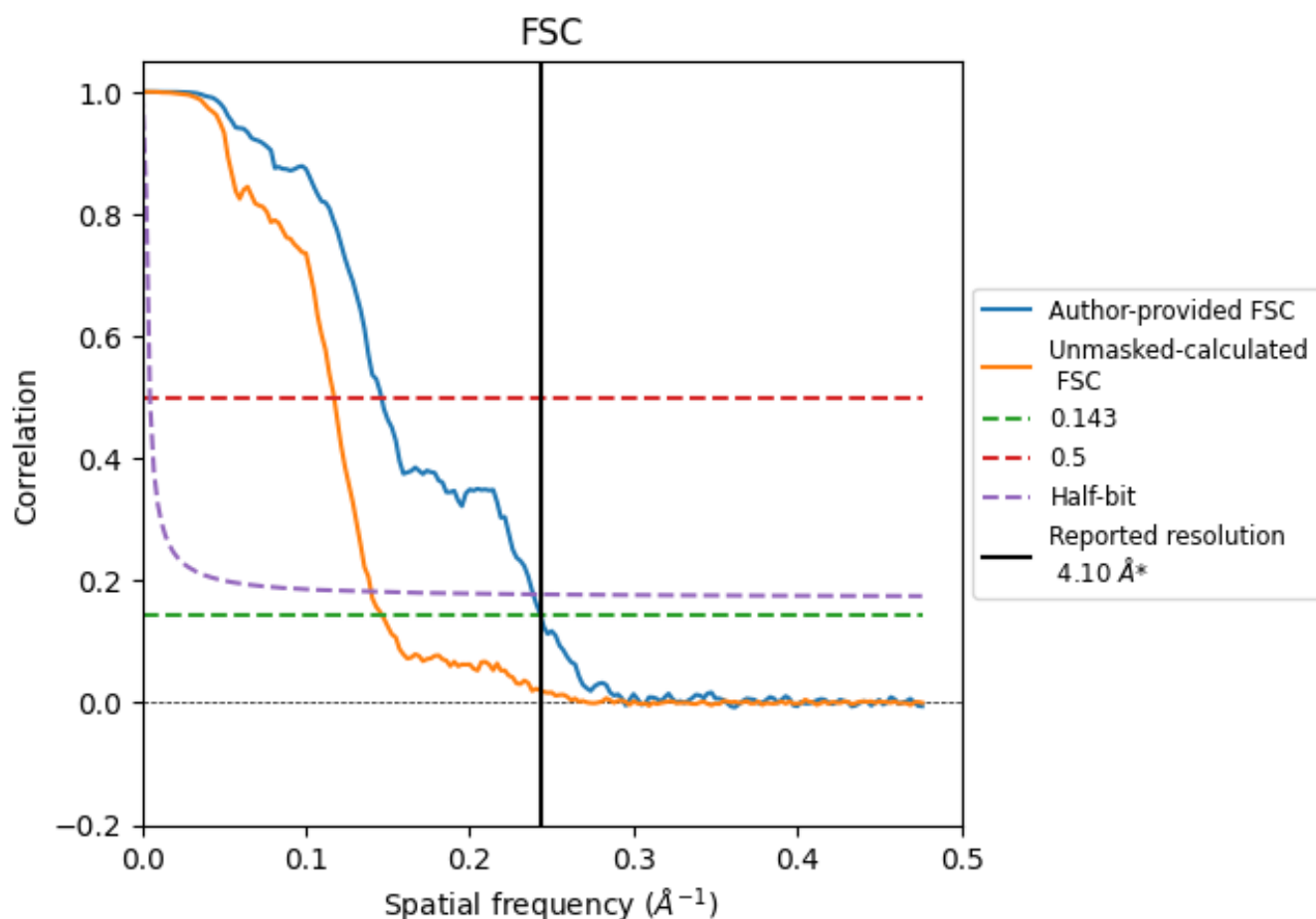


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

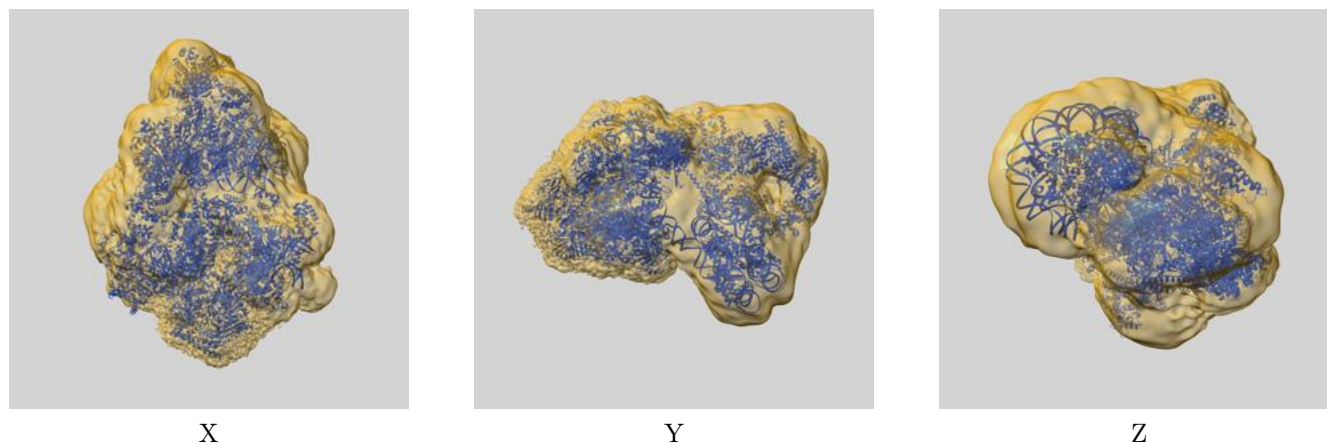
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.11	6.85	4.19
Unmasked-calculated*	6.83	8.54	7.15

*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 6.83 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

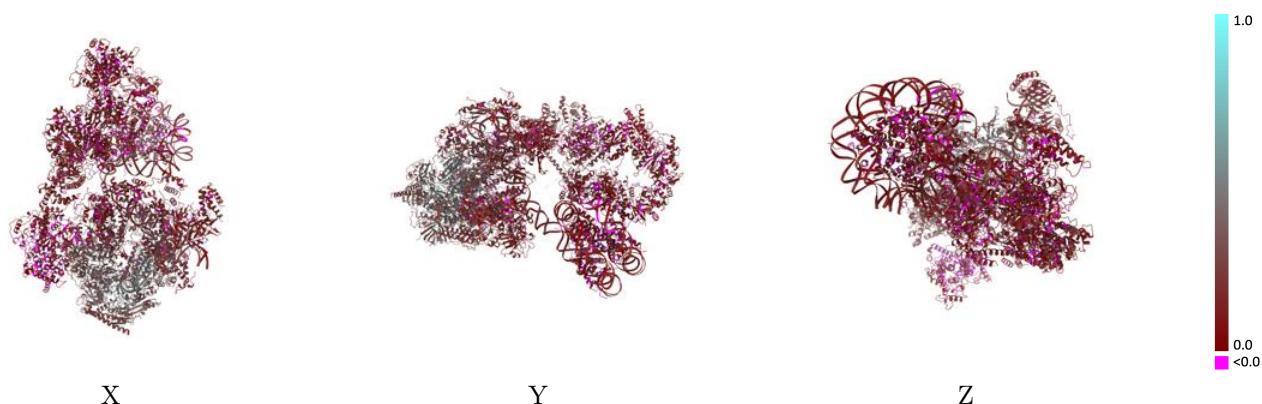
This section contains information regarding the fit between EMDB map EMD-16331 and PDB model 8BYQ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



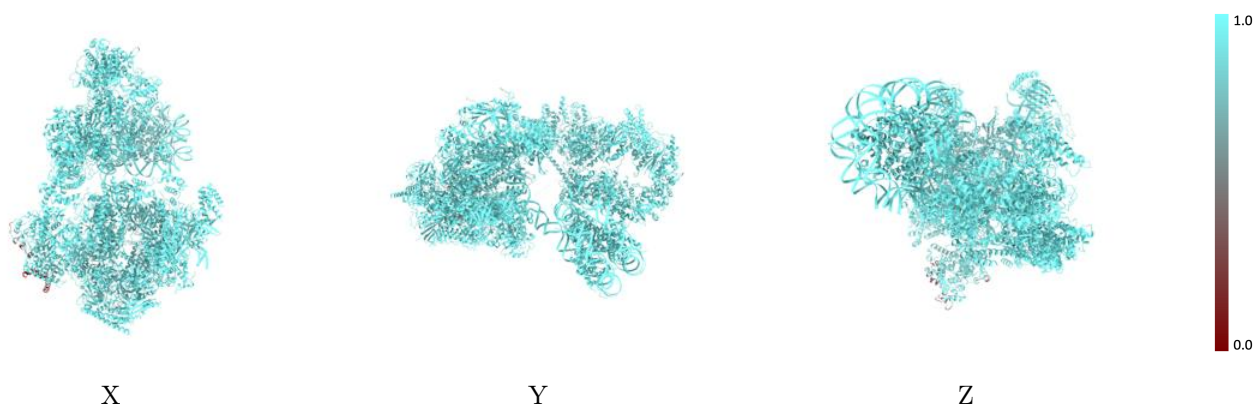
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



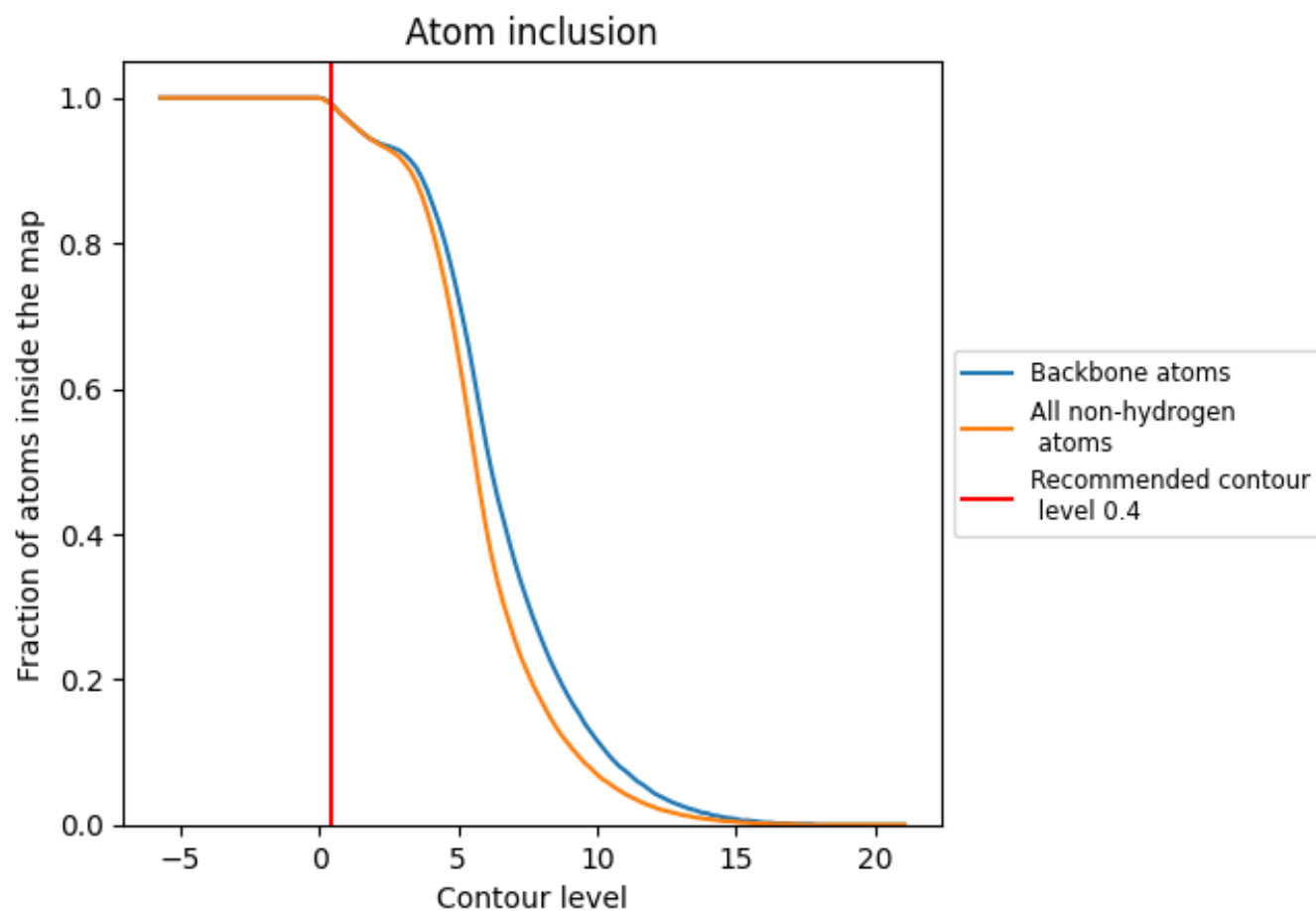
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9920	 0.1870
0	 1.0000	 0.1050
1	 1.0000	 0.1460
2	 1.0000	 0.0750
3	 0.9990	 0.1110
4	 1.0000	 0.1230
5	 1.0000	 0.1010
6	 1.0000	 0.0890
7	 0.9570	 0.1170
8	 0.9540	 0.0540
9	 0.8120	 0.0410
A	 1.0000	 0.2890
B	 1.0000	 0.3560
C	 1.0000	 0.3560
D	 1.0000	 0.1380
E	 1.0000	 0.2410
F	 1.0000	 0.3430
G	 1.0000	 0.1690
H	 1.0000	 0.3070
I	 1.0000	 0.2160
J	 1.0000	 0.3860
K	 1.0000	 0.3430
L	 1.0000	 0.3410
M	 1.0000	 0.2650
N	 1.0000	 0.1450
O	 1.0000	 0.1900
Q	 1.0000	 0.1400
R	 0.9990	 0.1590
T	 1.0000	 0.1470
U	 0.9950	 0.1500
V	 1.0000	 0.1430
W	 1.0000	 0.1230
X	 1.0000	 0.1340
a	 1.0000	 0.0880
b	 1.0000	 0.0830



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Chain	Atom inclusion	Q-score
c	 1.0000	 0.0740
d	 1.0000	 0.0770
e	 1.0000	 0.1130
f	 1.0000	 0.1010
g	 1.0000	 0.0760
h	 1.0000	 0.0900