



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:57 AM UTC

PDB ID : 8CEN / pdb_00008cen
EMDB ID : EMD-16610
Title : Yeast RNA polymerase II transcription pre-initiation complex with core Mediator
Authors : Wang, H.; Schilbach, S.; Cramer, P.
Deposited on : 2023-02-02
Resolution : 3.00 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:

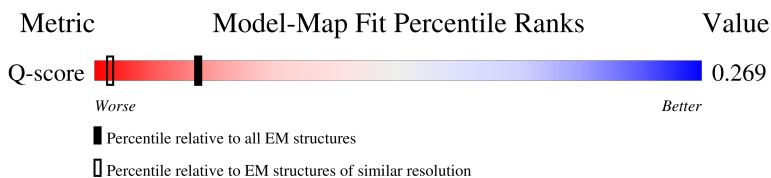
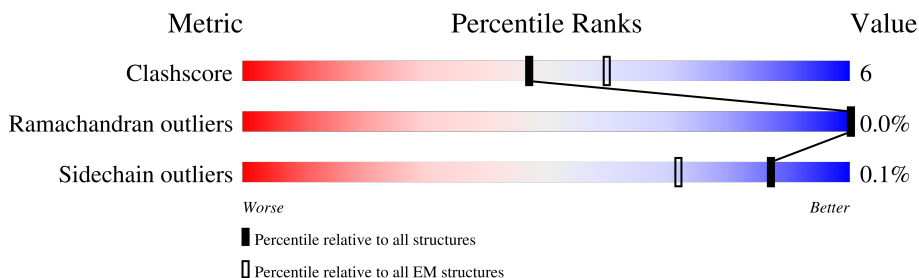
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.00 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	14081 (2.50 - 3.50)

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	778	
2	1	642	
3	2	513	
4	3	321	

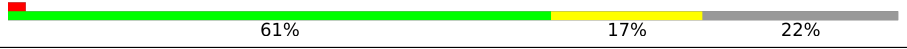
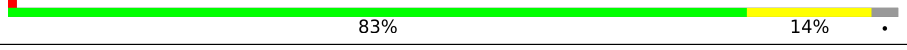
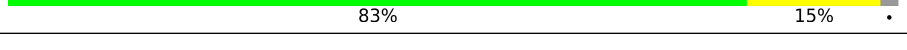
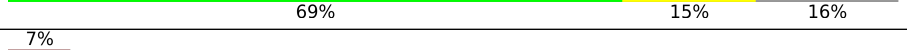
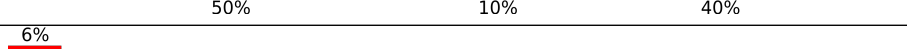
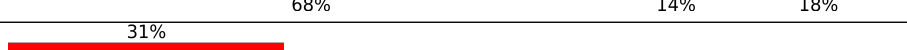
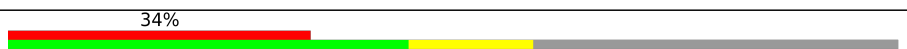
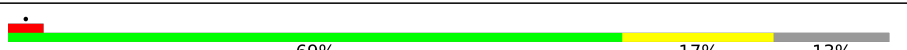
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Mol	Chain	Length	Quality of chain
5	4	338	
6	5	72	
7	6	461	
8	7	843	
9	A	1733	
10	B	1224	
11	C	347	
12	D	221	
13	E	215	
14	F	155	
15	G	177	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	352	
22	N	209	
23	O	240	
24	Q	735	
25	R	400	
26	T	209	
27	U	286	
28	V	122	
29	W	492	

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Mol	Chain	Length	Quality of chain
30	X	328	
31	a	295	
32	b	223	
33	c	115	
34	d	687	
35	e	307	
36	f	210	
37	g	121	
38	h	284	
39	i	222	
40	j	149	
41	k	157	
42	l	745	
43	m	220	
44	n	140	
45	o	127	
46	p	566	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 101943 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 XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	522	Total	C	N	O	S	0	0
			4214	2660	734	798	22		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	452	Total	C	N	O	S	0	0
			3647	2354	600	677	16		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	302	Total	C	N	O	S	0	0
			2338	1492	390	442	14		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	383	Total	C	N	O	S	0	0
			3019	1915	523	552	29		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	615	Total	C	N	O	S	0	0
			4954	3153	860	914	27		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1508	Total	C	N	O	S	0	0
			11815	7442	2042	2269	62		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1180	Total	C	N	O	S	0	0
			9404	5946	1643	1760	55		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	266	Total	C	N	O	S	0	0
			2092	1315	348	416	13		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	initiating methionine	UNP P16370
C	-27	GLY	-	expression tag	UNP P16370
C	-26	SER	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	HIS	-	expression tag	UNP P16370
C	-19	SER	-	expression tag	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	ASN	-	expression tag	UNP P16370
C	-17	SER	-	expression tag	UNP P16370
C	-16	GLY	-	expression tag	UNP P16370
C	-15	LEU	-	expression tag	UNP P16370
C	-14	ASN	-	expression tag	UNP P16370
C	-13	ASP	-	expression tag	UNP P16370
C	-12	ILE	-	expression tag	UNP P16370
C	-11	PHE	-	expression tag	UNP P16370
C	-10	GLU	-	expression tag	UNP P16370
C	-9	ALA	-	expression tag	UNP P16370
C	-8	GLN	-	expression tag	UNP P16370
C	-7	LYS	-	expression tag	UNP P16370
C	-6	ILE	-	expression tag	UNP P16370
C	-5	GLU	-	expression tag	UNP P16370
C	-4	TRP	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	GLU	-	expression tag	UNP P16370
C	-1	ASP	-	expression tag	UNP P16370
C	0	THR	-	expression tag	UNP P16370
C	1	GLY	-	expression tag	UNP P16370
C	2	SER	-	expression tag	UNP P16370
C	3	SER	-	expression tag	UNP P16370

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	167	Total	C	N	O	S	0	0
			1343	829	242	270	2		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	118	Total	C	N	O	S	0	0
			983	623	164	193	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	HIS	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	310	Total	C	N	O	S	0	0
			2379	1504	408	449	18		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	346	LYS	-	expression tag	UNP P29055
M	347	HIS	-	expression tag	UNP P29055
M	348	HIS	-	expression tag	UNP P29055
M	349	HIS	-	expression tag	UNP P29055
M	350	HIS	-	expression tag	UNP P29055
M	351	HIS	-	expression tag	UNP P29055
M	352	HIS	-	expression tag	UNP P29055

- Molecule 22 is a DNA chain called NONTEMPLATE DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	73	Total	C	N	O	P	0	0
			1495	717	270	436	72		

- Molecule 23 is a protein called TATA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 24 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	221	Total	C	N	O	S	0	0
			1871	1179	346	339	7		

- Molecule 25 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	268	Total	C	N	O	S	0	0
			2230	1409	392	419	10		

- Molecule 26 is a DNA chain called TEMPLATE DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	73	Total	C	N	O	P	0	0
			1495	716	268	438	73		

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	304	Total	C	N	O	S	0	0
			2473	1558	431	477	7		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	483	ALA	-	expression tag	UNP P36100
W	484	ALA	-	expression tag	UNP P36100
W	485	ALA	-	expression tag	UNP P36100
W	486	LEU	-	expression tag	UNP P36100
W	487	GLU	-	expression tag	UNP P36100
W	488	HIS	-	expression tag	UNP P36100
W	489	HIS	-	expression tag	UNP P36100
W	490	HIS	-	expression tag	UNP P36100
W	491	HIS	-	expression tag	UNP P36100
W	492	HIS	-	expression tag	UNP P36100

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	211	Total	C	N	O	S	0	0
			1708	1089	293	320	6		

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	178	Total	C	N	O	S	0	0
			1495	970	240	278	7		

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	173	Total	C	N	O	S	0	0
			1414	900	241	270	3		

- Molecule 33 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	111	Total	C	N	O	S	0	0
			902	566	154	178	4		

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	501	Total	C	N	O	S	0	0
			4063	2613	684	752	14		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	256	Total	C	N	O	S	0	0
			2017	1280	336	390	11		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	206	Total	C	N	O	S	0	0
			1578	998	266	309	5		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	102	Total	C	N	O	S	0	0
			815	512	134	164	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	171	Total	C	N	O	S	0	0
			1394	884	234	271	5		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	181	Total	C	N	O	S	0	0
			1512	973	253	280	6		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	102	Total	C	N	O	S	0	0
			852	533	156	162	1		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	157	Total	C	N	O	S	0	0
			1259	777	222	257	3		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	535	Total	C	N	O	S	0	0
			4385	2846	759	763	17		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	130	Total	C	N	O	S	0	0
			1068	672	185	209	2		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	136	Total	C	N	O	S	0	0
			1095	685	185	220	5		

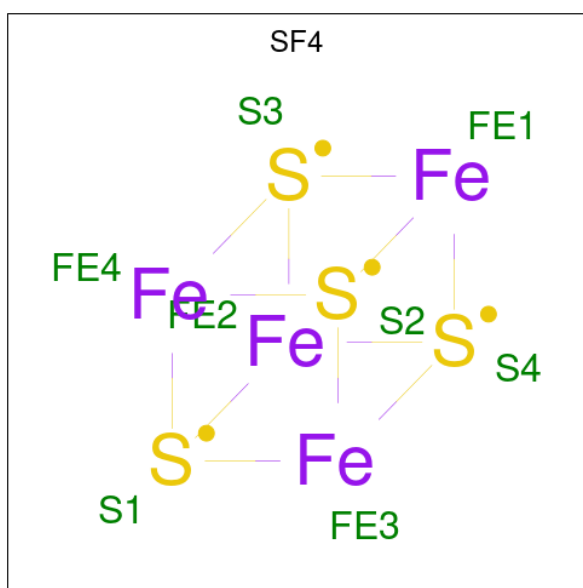
- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	110	Total	C	N	O	S	0	0
			922	607	143	166	6		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	225	Total	C	N	O	S	0	0
			1863	1193	298	366	6		

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
47	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	3	2	Total	Zn	0
			2	2	
48	4	1	Total	Zn	0
			1	1	
48	6	4	Total	Zn	0
			4	4	
48	A	2	Total	Zn	0
			2	2	

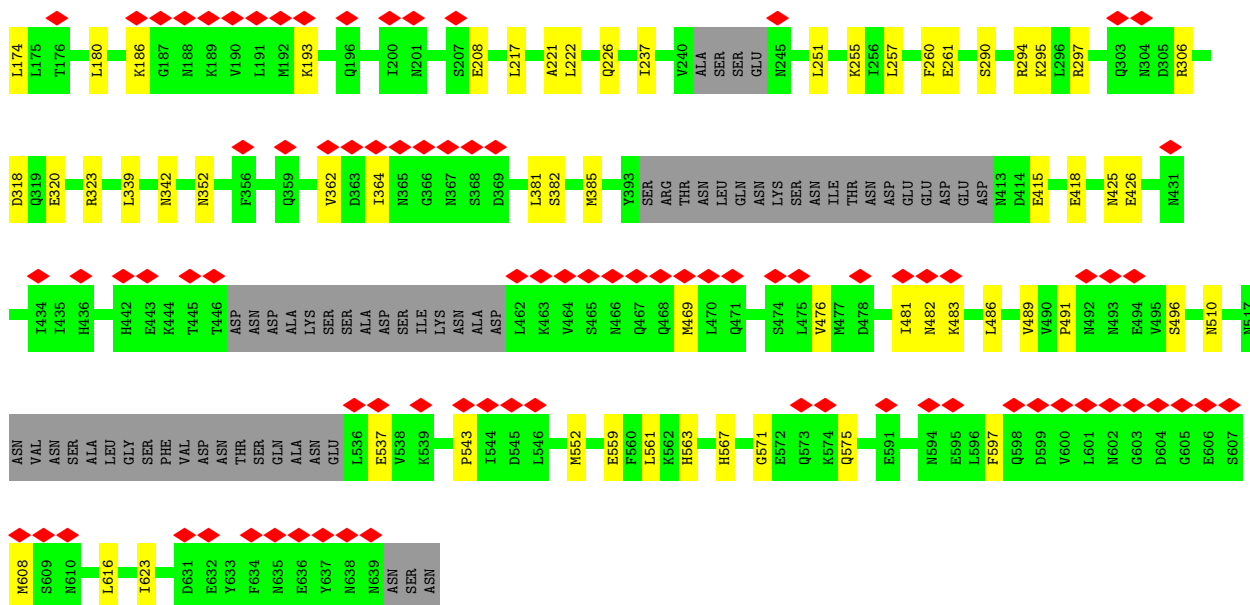
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Mol	Chain	Residues	Atoms		AltConf
48	B	1	Total 1	Zn 1	0
48	C	1	Total 1	Zn 1	0
48	I	2	Total 2	Zn 2	0
48	J	1	Total 1	Zn 1	0
48	L	1	Total 1	Zn 1	0
48	M	1	Total 1	Zn 1	0
48	W	1	Total 1	Zn 1	0

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

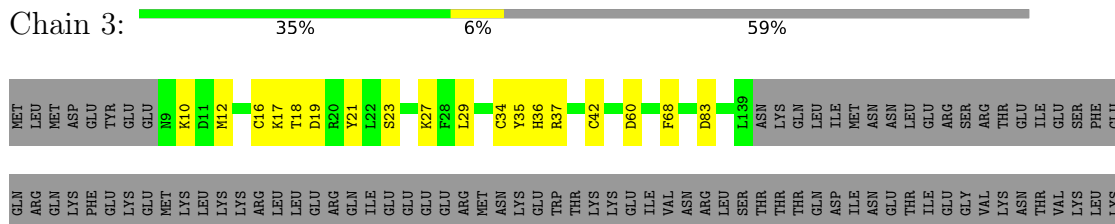
Mol	Chain	Residues	Atoms		AltConf
49	A	1	Total 1	Mg 1	0

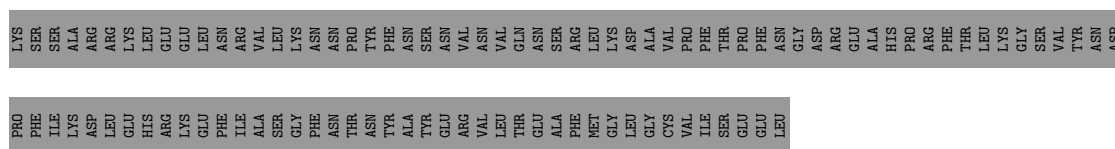


- Molecule 3: General transcription and DNA repair factor IIH subunit TFB2

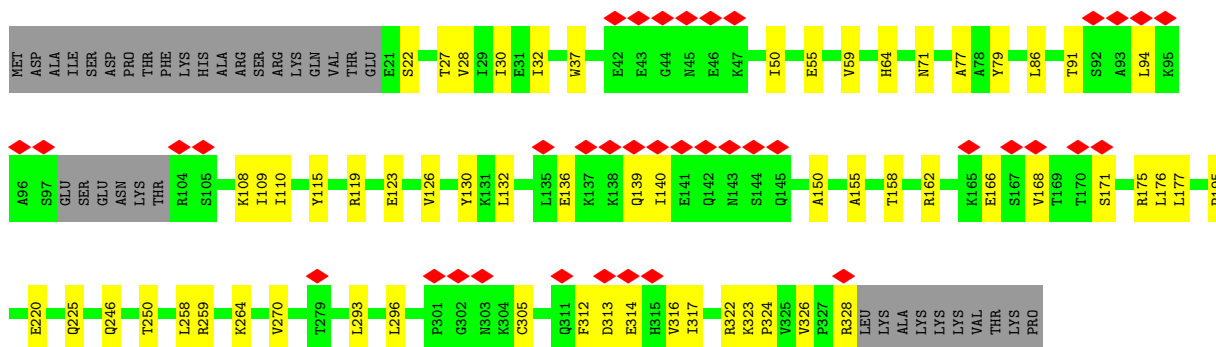


- Molecule 4: RNA polymerase II transcription factor B subunit 3

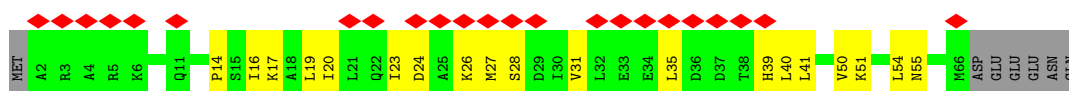




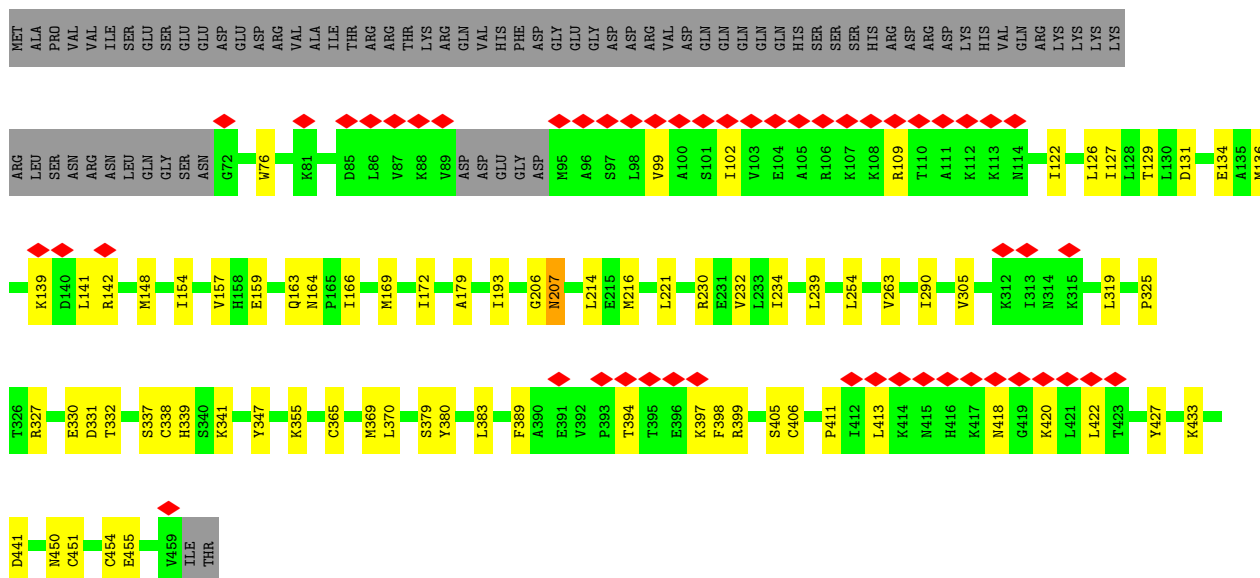
• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4



• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5



• Molecule 7: General transcription and DNA repair factor IIH subunit SSL1



• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

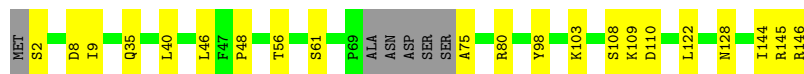




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M1152	Q952	I729	F557	R398	ASP	
C1163	L953	R730	W561		LEU	
M1178	N957	I743	E567	Q415	ALA	
	L961	M747	V570	L420	ASN	
M1187	K962	F757	Q573	L424	SER	
I1189	F963	D760	H590	I428	LYS	
D1190	V966	R766	L596	F429	TVR	
H1195	1976	Q770	L600	N443	ASP	
L1207	K979	S771	L603	K444	GLU	
M1208	F980	V787	R604	K445	ASP	
R1220	H984	T805	D608	L446	PRO	
F1224	G987	M809	M615	A447	TVR	
	G988	V825	R617	I448	GLY	
	G991	M839	M616	I453	F18	
	R996	B848	K652	L457	E21	
P1000	F1001	Q862	G656	L461	F38	
T1002	L1010	E863	R664	V633	L69	
	R1020	M868	S869	Y634	I70	
I1050	S1056	E872	L893	G656	L71	
S1066	M1072	Q1093	R1096	L894	L84	
	R1106	L1114	R1124	P501	K87	
	L1124	R1133	E1134	L502	T98	
	M1133	D1136	A937	GLY	V102	
	E1135	A937	S938	ASP	N103	
	L1147	R1147	R722	R476	L112	
				GLU	L119	
				GLY	R120	
				PHE	N121	
				GLU	L122	
				D675	L128	
				D895	Y137	
				R904	F138	
				I911	A139	
				I912	Y149	
				T916	F157	
				E924	ASP	
				R928	ASP	
				T929	SER	
				GLU	GLU	
				GLU	SER	
				D936	GLU	
				A937	SER	
				S938	G163	
				R930	F168	

- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  82% 14% .



- Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I:  76% 19% 5%



- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  84% 14% .



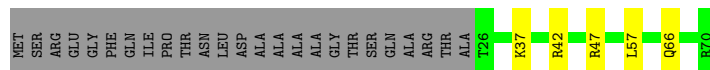
- Molecule 19: DNA-directed RNA polymerase II subunit RPB11

Chain K:  80% 16% .



- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  57% 7% 36%

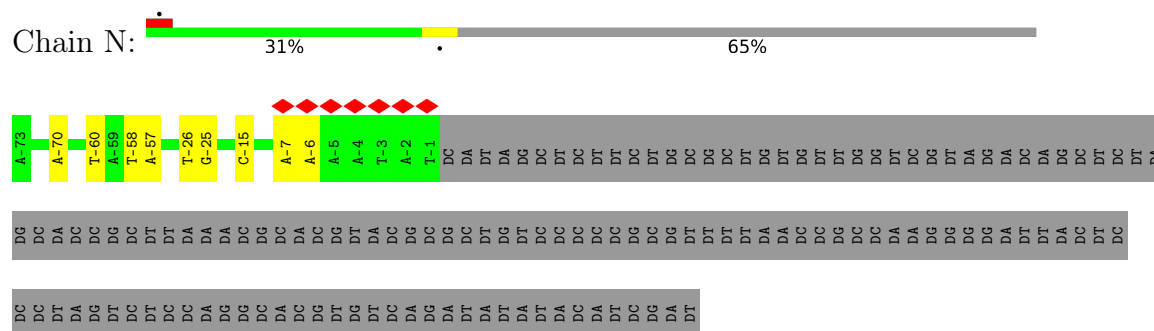


- Molecule 21: Transcription initiation factor IIB

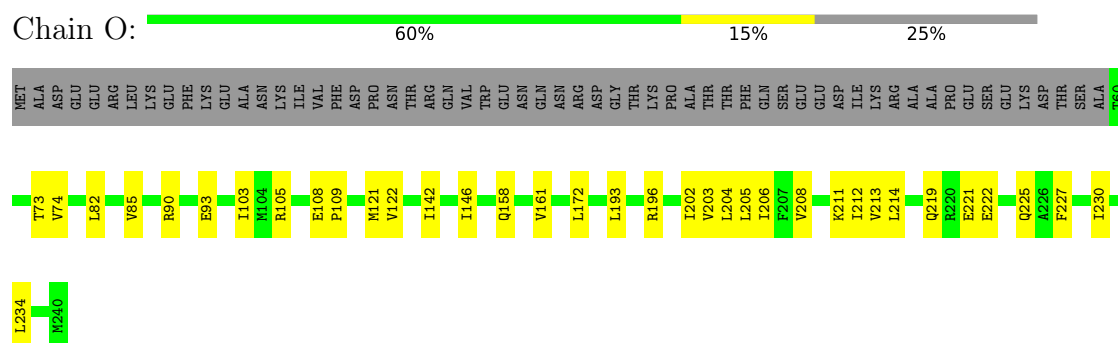
Chain M:  73% 15% 12%



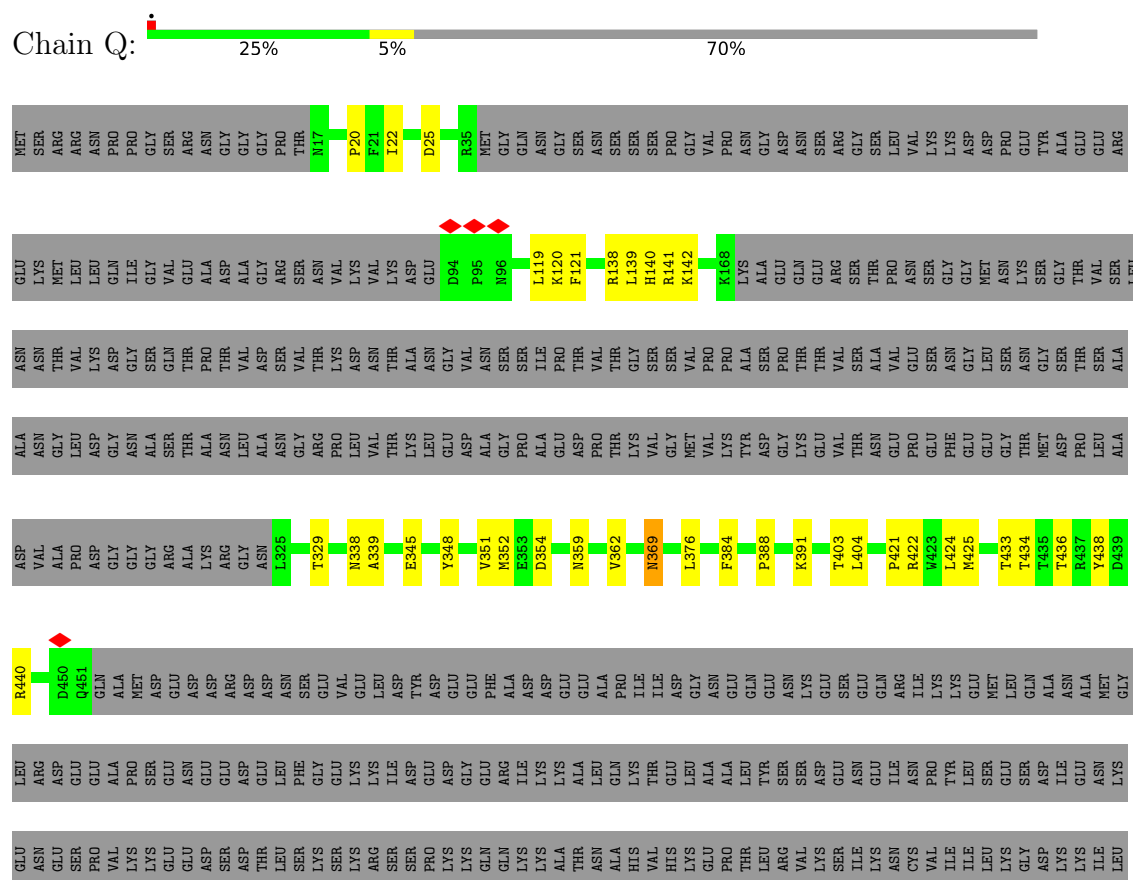
- Molecule 22: NONTEMPLATE DNA (209-MER)



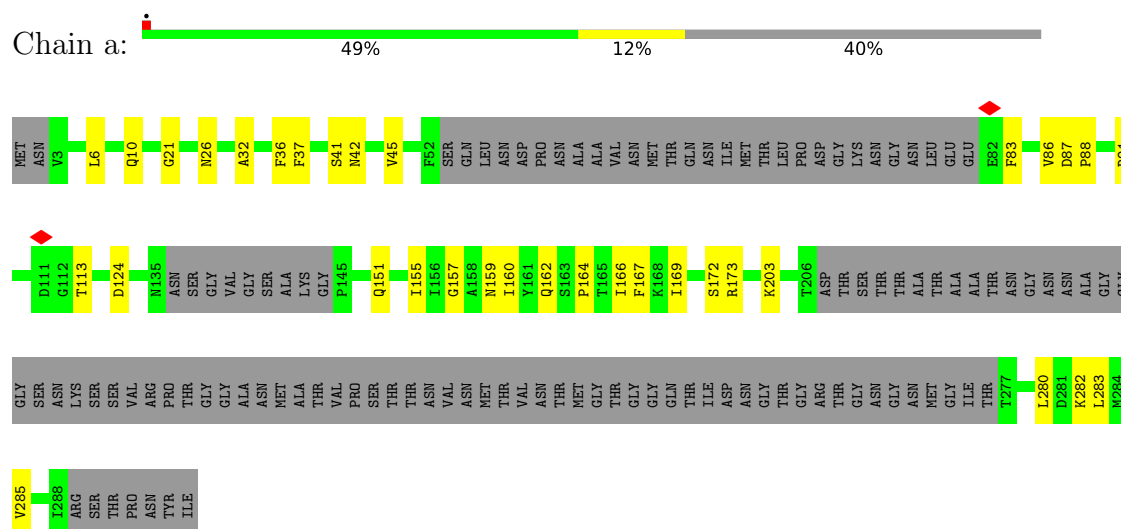
• Molecule 23: TATA-binding protein



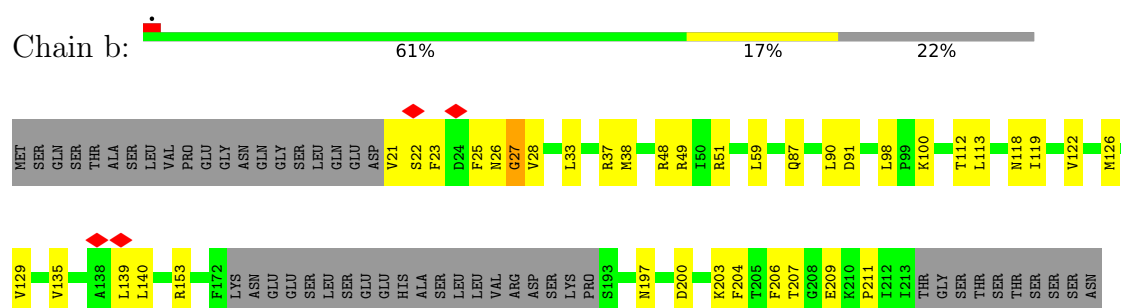
• Molecule 24: Transcription initiation factor IIF subunit alpha



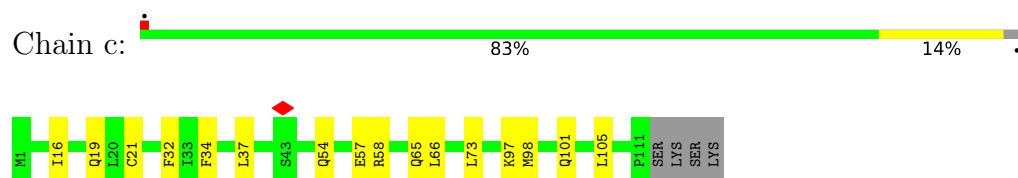
- Molecule 31: Mediator of RNA polymerase II transcription subunit 6



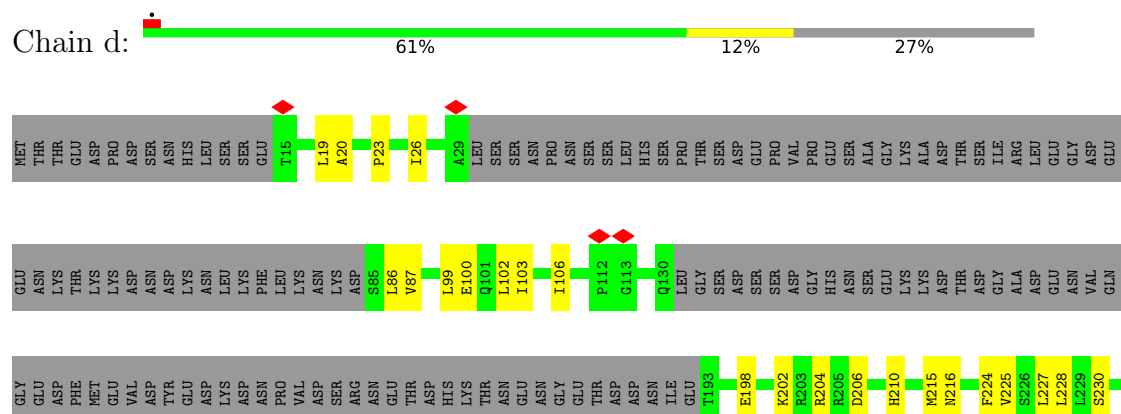
- Molecule 32: Mediator of RNA polymerase II transcription subunit 8

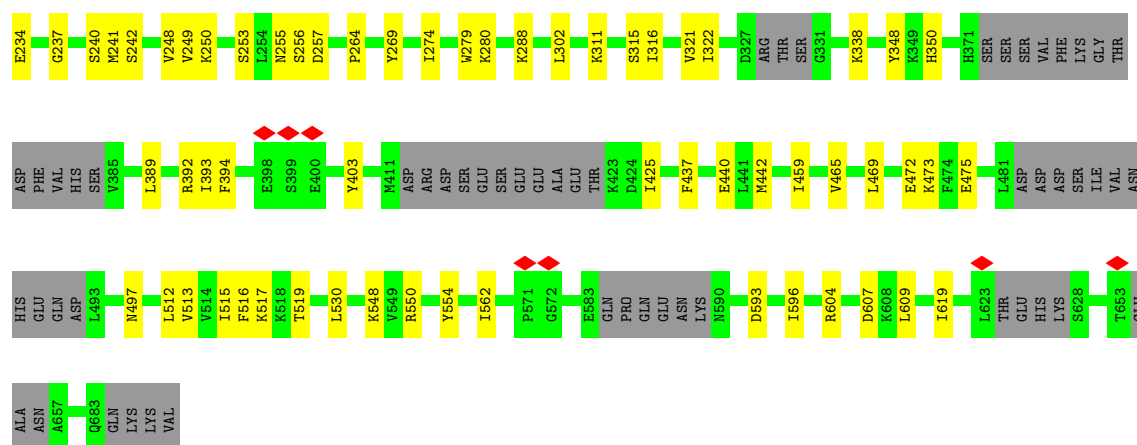


- Molecule 33: Mediator of RNA polymerase II transcription subunit 11

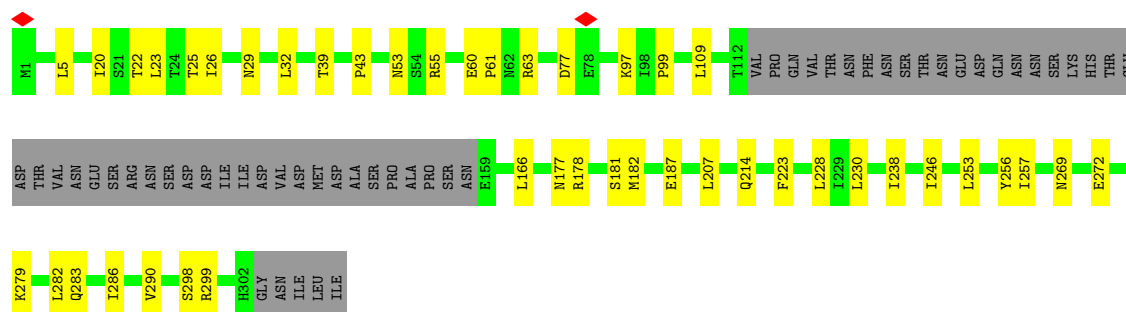


- Molecule 34: Mediator of RNA polymerase II transcription subunit 17

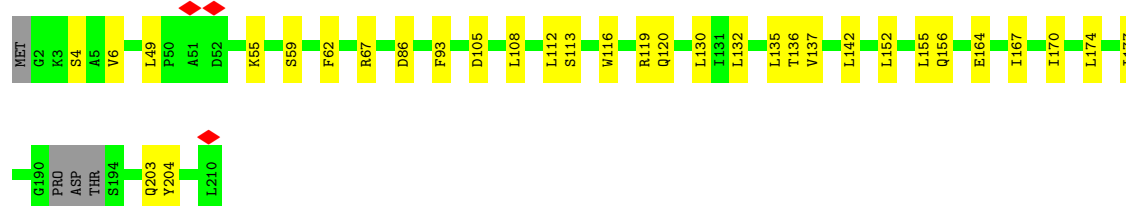
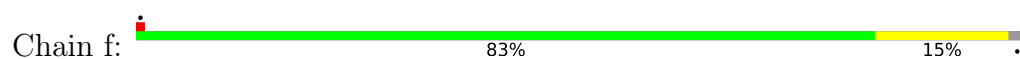




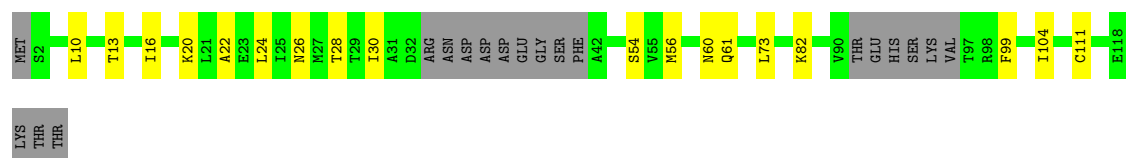
• Molecule 35: Mediator of RNA polymerase II transcription subunit 18



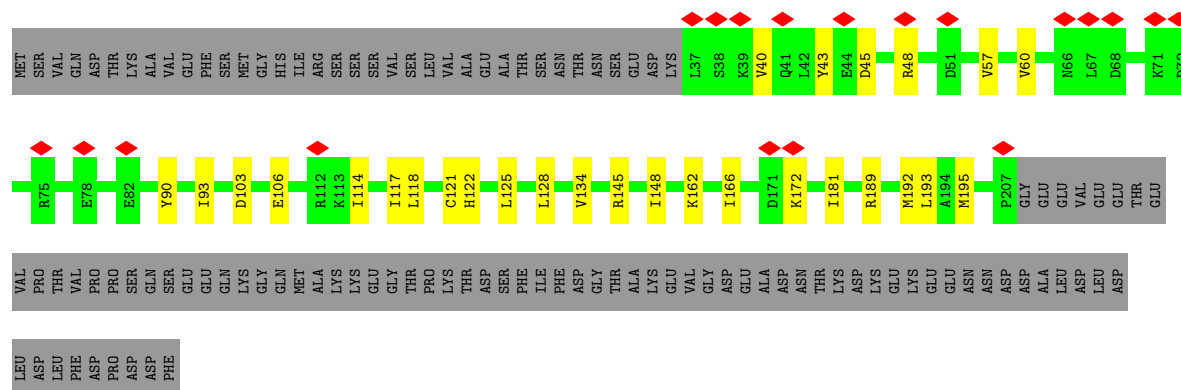
• Molecule 36: Mediator of RNA polymerase II transcription subunit 20



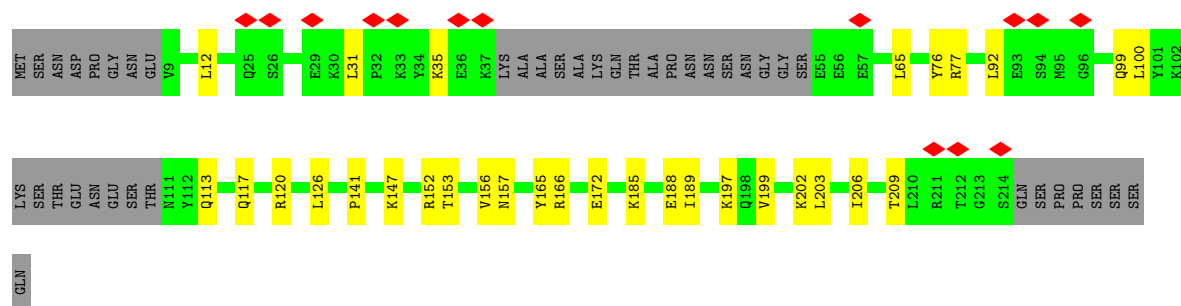
• Molecule 37: Mediator of RNA polymerase II transcription subunit 22



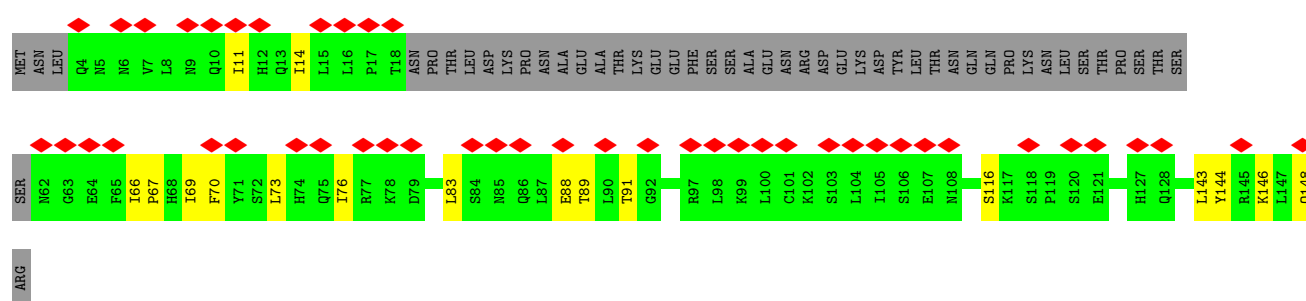
• Molecule 38: Mediator of RNA polymerase II transcription subunit 4



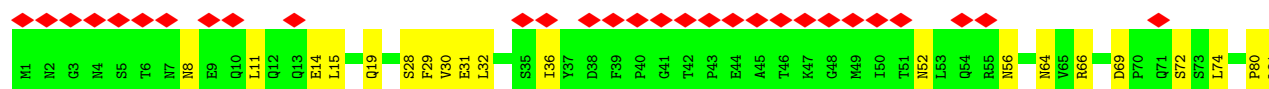
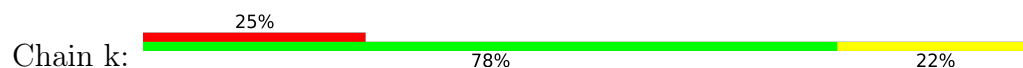
• Molecule 39: Mediator of RNA polymerase II transcription subunit 7

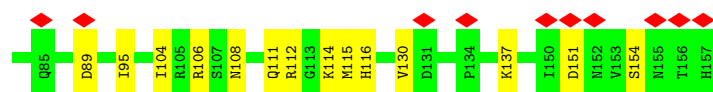


• Molecule 40: Mediator of RNA polymerase II transcription subunit 9

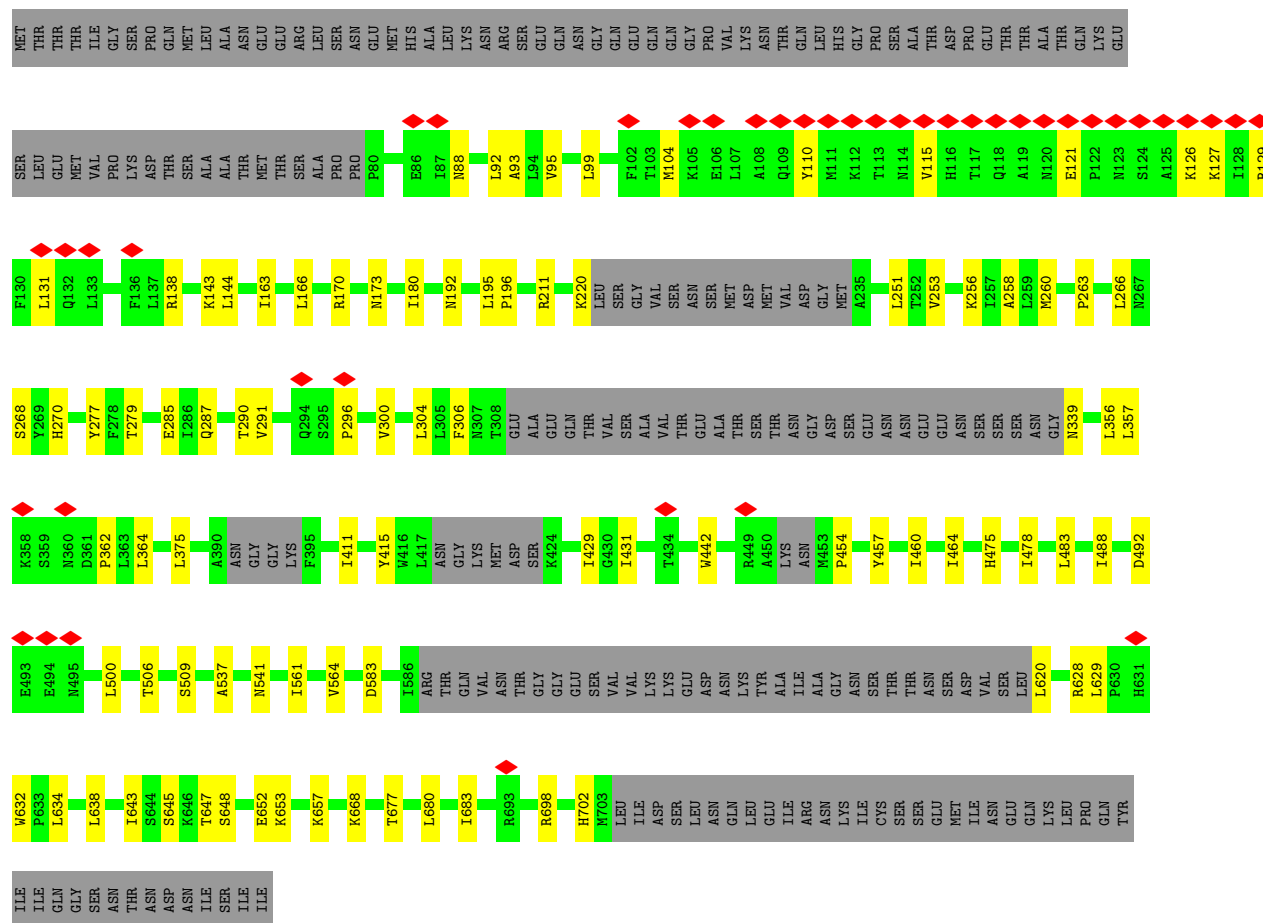


• Molecule 41: Mediator of RNA polymerase II transcription subunit 10

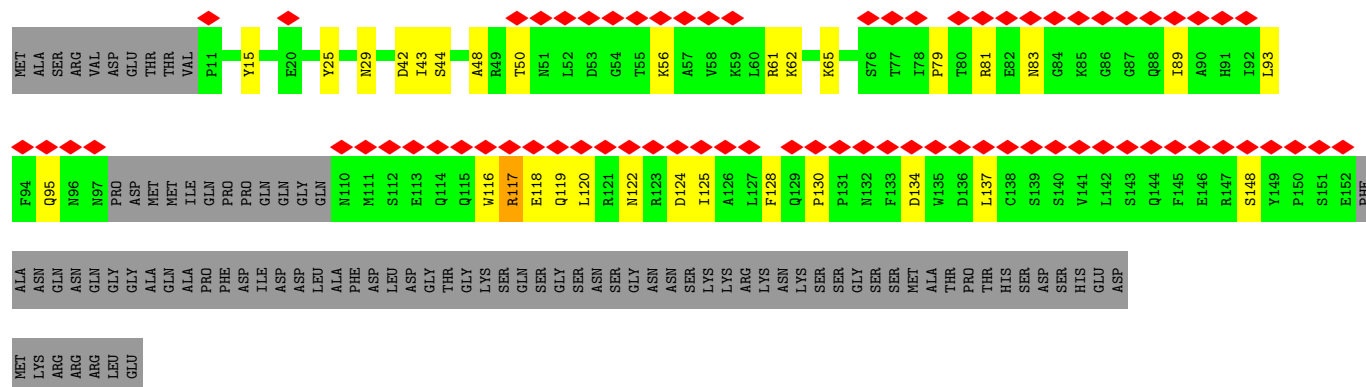




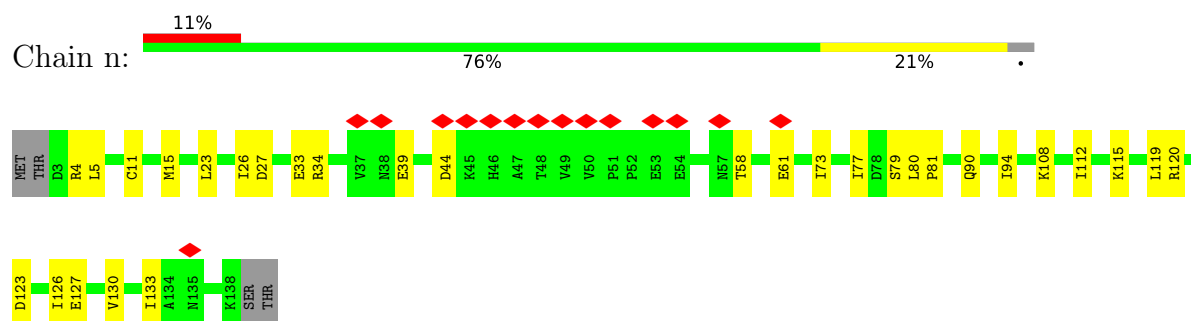
• Molecule 42: Mediator of RNA polymerase II transcription subunit 14



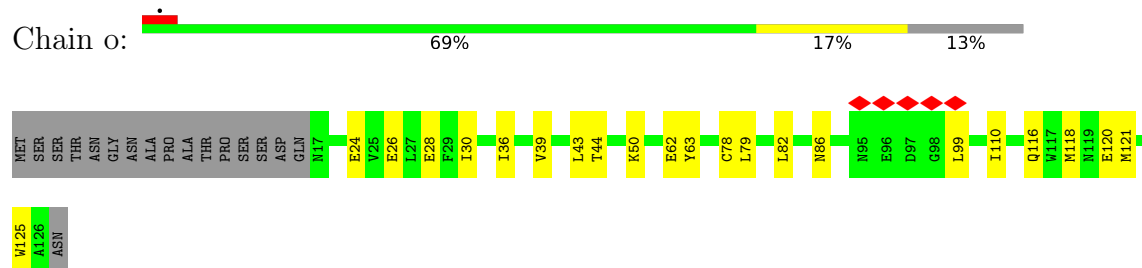
• Molecule 43: Mediator of RNA polymerase II transcription subunit 19



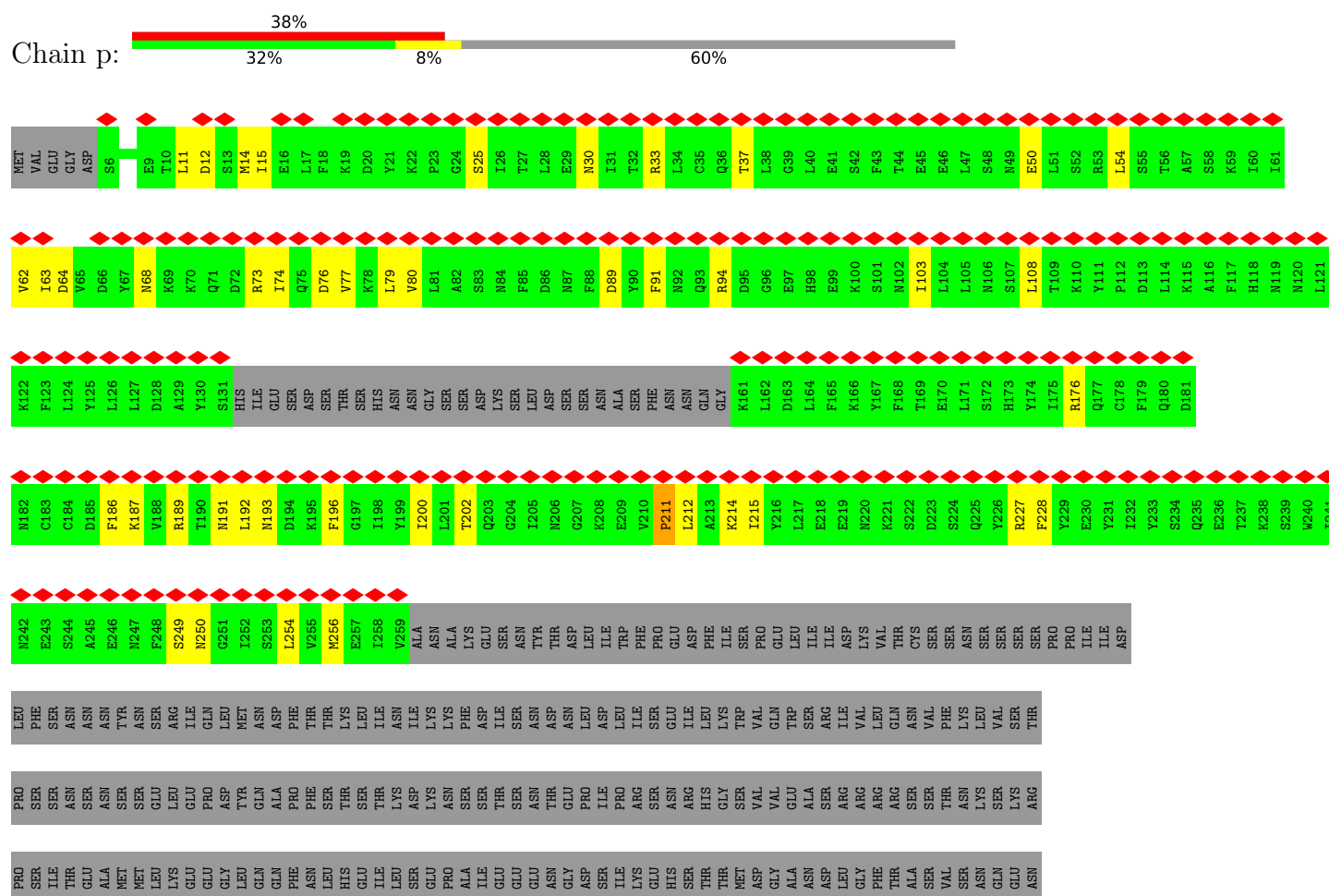
- Molecule 44: Mediator of RNA polymerase II transcription subunit 21



- Molecule 45: Mediator of RNA polymerase II transcription subunit 31



- Molecule 46: Mediator of RNA polymerase II transcription subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186599	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.009	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: SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.17	0/6209	0.44	0/8384
2	1	0.17	0/4277	0.43	1/5755 (0.0%)
3	2	0.19	0/3717	0.46	0/5028
4	3	0.14	0/1109	0.37	0/1492
5	4	0.17	0/2377	0.43	0/3216
6	5	0.20	0/520	0.48	0/701
7	6	0.17	0/3082	0.43	0/4165
8	7	0.16	0/5059	0.40	1/6841 (0.0%)
9	A	0.18	0/12048	0.42	0/16321
10	B	0.18	0/9589	0.41	0/12934
11	C	0.17	0/2130	0.39	0/2887
12	D	0.19	0/1351	0.50	0/1811
13	E	0.16	0/1788	0.42	0/2406
14	F	0.17	0/1001	0.40	0/1347
15	G	0.16	0/1367	0.40	0/1844
16	H	0.15	0/1139	0.36	0/1544
17	I	0.15	0/962	0.48	0/1295
18	J	0.19	0/578	0.42	0/775
19	K	0.17	0/942	0.38	0/1272
20	L	0.15	0/361	0.43	0/478
21	M	0.17	0/2408	0.44	0/3241
22	N	0.22	0/1677	0.40	0/2587
23	O	0.16	0/1449	0.41	0/1952
24	Q	0.16	0/1907	0.41	0/2556
25	R	0.15	0/2270	0.39	0/3052
26	T	0.21	0/1676	0.39	0/2584
27	U	0.21	0/898	0.54	0/1212
28	V	0.19	0/822	0.47	0/1109
29	W	0.19	0/2513	0.50	0/3388
30	X	0.17	0/1739	0.47	1/2339 (0.0%)
31	a	0.19	0/1531	0.49	0/2072
32	b	0.21	0/1443	0.48	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.20	0/913	0.54	0/1228
34	d	0.18	0/4118	0.44	0/5532
35	e	0.14	0/2054	0.40	0/2782
36	f	0.17	0/1602	0.44	0/2169
37	g	0.19	0/818	0.49	0/1104
38	h	0.23	0/1415	0.58	0/1907
39	i	0.18	0/1543	0.44	1/2084 (0.0%)
40	j	0.22	0/865	0.57	0/1166
41	k	0.27	0/1277	0.66	1/1727 (0.1%)
42	l	0.19	0/4468	0.47	0/6048
43	m	0.23	0/1093	0.65	5/1481 (0.3%)
44	n	0.21	0/1106	0.48	0/1488
45	o	0.18	0/949	0.41	0/1294
46	p	0.32	1/1898 (0.1%)	0.68	4/2559 (0.2%)
All	All	0.18	1/104058 (0.0%)	0.45	14/141114 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	p	211	PRO	CG-CD	-10.29	1.15	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	p	211	PRO	N-CD-CG	-16.42	78.57	103.20
46	p	211	PRO	CA-CB-CG	-14.28	77.37	104.50
8	7	106	PRO	CA-N-CD	-8.41	100.23	112.00
41	k	80	PRO	CA-N-CD	-7.78	101.10	112.00
46	p	211	PRO	N-CA-CB	-6.71	97.45	103.36
43	m	118	GLU	N-CA-CB	5.67	119.03	110.30
46	p	211	PRO	CA-N-CD	-5.62	104.14	112.00
30	X	223	GLN	N-CA-CB	5.43	119.41	110.39
39	i	152	ARG	CA-CB-CG	5.34	124.78	114.10
2	1	261	GLU	N-CA-CB	5.28	118.06	110.20
43	m	118	GLU	CA-C-N	-5.19	111.47	121.58
43	m	118	GLU	C-N-CA	-5.19	111.47	121.58
43	m	117	ARG	CA-C-N	-5.07	112.06	120.68
43	m	117	ARG	C-N-CA	-5.07	112.06	120.68

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	6091	0	6155	86	0
2	1	4214	0	4288	48	0
3	2	3647	0	3732	43	0
4	3	1089	0	1069	12	0
5	4	2338	0	2404	41	0
6	5	514	0	541	13	0
7	6	3019	0	3040	51	0
8	7	4954	0	4946	68	0
9	A	11815	0	11816	162	0
10	B	9404	0	9398	115	0
11	C	2092	0	2050	36	0
12	D	1343	0	1366	15	0
13	E	1752	0	1776	15	0
14	F	983	0	968	16	0
15	G	1339	0	1357	23	0
16	H	1120	0	1086	14	0
17	I	944	0	899	16	0
18	J	569	0	585	7	0
19	K	924	0	934	15	0
20	L	359	0	381	6	0
21	M	2379	0	2488	32	0
22	N	1495	0	828	7	0
23	O	1422	0	1500	25	0
24	Q	1871	0	1883	27	0
25	R	2230	0	2254	36	0
26	T	1495	0	827	6	0
27	U	885	0	866	14	0
28	V	815	0	822	22	0
29	W	2473	0	2476	40	0
30	X	1708	0	1761	17	0
31	a	1495	0	1476	22	0
32	b	1414	0	1413	36	0
33	c	902	0	918	12	0
34	d	4063	0	4247	58	0
35	e	2017	0	2024	31	0
36	f	1578	0	1595	21	0
37	g	815	0	839	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	1394	0	1420	22	0
39	i	1512	0	1544	26	0
40	j	852	0	857	12	0
41	k	1259	0	1241	27	0
42	l	4385	0	4612	60	0
43	m	1068	0	1021	23	0
44	n	1095	0	1116	24	0
45	o	922	0	907	15	0
46	p	1863	0	1819	32	0
47	0	8	0	0	0	0
48	3	2	0	0	0	0
48	4	1	0	0	0	0
48	6	4	0	0	0	0
48	A	2	0	0	0	0
48	B	1	0	0	0	0
48	C	1	0	0	0	0
48	I	2	0	0	0	0
48	J	1	0	0	0	0
48	L	1	0	0	0	0
48	M	1	0	0	0	0
48	W	1	0	0	0	0
49	A	1	0	0	0	0
All	All	101943	0	101545	1227	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 6.

All (1227) 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)
4:3:16:CYS:HB3	4:3:42:CYS:SG	2.04	0.95
7:6:338:CYS:SG	7:6:339:HIS:CE1	2.75	0.79
29:W:127:CYS:HB3	29:W:152:CYS:SG	2.26	0.76
3:2:458:LEU:HD21	3:2:490:LYS:HD3	1.70	0.74
16:H:2:SER:N	16:H:61:SER:HG	1.86	0.74
2:1:102:MET:HE1	2:1:306:ARG:HD3	1.70	0.73
31:a:88:PRO:HB2	32:b:21:VAL:HG11	1.69	0.73
31:a:86:VAL:HG23	31:a:91:ARG:HE	1.53	0.73
38:h:125:LEU:HD12	39:i:199:VAL:HG21	1.70	0.72
27:U:267:VAL:O	27:U:273:ASP:HA	1.90	0.72
12:D:148:LEU:O	12:D:152:SER:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:260:CYS:HB2	27:U:281:VAL:HB	1.72	0.71
31:a:167:PHE:HB2	32:b:90:LEU:HB3	1.72	0.71
9:A:1444:MET:HE1	14:F:135:ARG:HB2	1.71	0.71
1:0:111:ARG:O	1:0:115:CYS:HB2	1.91	0.70
46:p:214:LYS:O	46:p:256:MET:HA	1.90	0.70
17:I:5:ARG:HG3	17:I:14:LEU:HD12	1.73	0.69
8:7:561:MET:HG2	8:7:584:ASN:HD22	1.57	0.69
3:2:165:ASN:HA	3:2:168:LYS:HG2	1.74	0.69
2:1:186:LYS:NZ	29:W:354:GLU:OE1	2.24	0.69
9:A:469:ARG:NH2	10:B:991:GLY:O	2.24	0.68
3:2:458:LEU:HD11	3:2:490:LYS:HB3	1.75	0.68
10:B:71:LEU:HD11	24:Q:329:THR:HB	1.75	0.68
24:Q:421:PRO:HG2	24:Q:424:LEU:HB2	1.75	0.68
3:2:146:ILE:HD11	3:2:163:VAL:HG21	1.73	0.68
27:U:247:LEU:HA	28:V:116:CYS:H	1.57	0.68
9:A:597:LEU:HD21	16:H:103:LYS:HG2	1.76	0.67
9:A:397:ASN:HB2	35:e:55:ARG:HH12	1.60	0.67
34:d:315:SER:HB2	34:d:425:ILE:HG12	1.77	0.67
2:1:237:ILE:HD11	2:1:255:LYS:HD3	1.77	0.67
9:A:1140:HIS:HE2	9:A:1272:THR:HG1	1.39	0.67
9:A:1373:ASP:O	9:A:1377:THR:HB	1.94	0.66
17:I:28:GLU:HG3	17:I:35:VAL:HG22	1.77	0.66
9:A:1591:TYR:HA	38:h:189:ARG:HE	1.58	0.66
34:d:20:ALA:HB2	38:h:145:ARG:HE	1.59	0.66
30:X:291:ALA:HA	30:X:295:ARG:HD3	1.76	0.66
43:m:89:ILE:O	43:m:93:LEU:HB2	1.96	0.66
2:1:174:LEU:HD12	2:1:217:LEU:HB3	1.77	0.66
9:A:420:ARG:HD2	35:e:60:GLU:HG2	1.78	0.66
10:B:868:MET:SD	21:M:182:ARG:NH1	2.69	0.66
34:d:198:GLU:OE1	34:d:202:LYS:NZ	2.29	0.66
46:p:73:ARG:HE	46:p:74:ILE:H	1.42	0.66
5:4:136:GLU:HA	5:4:139:GLN:HG2	1.76	0.65
9:A:1192:LEU:HD11	9:A:1239:ARG:HB3	1.78	0.65
23:O:93:GLU:HB2	23:O:103:ILE:HB	1.77	0.65
5:4:270:VAL:O	7:6:327:ARG:NH2	2.29	0.65
2:1:8:ILE:HB	2:1:90:SER:HB2	1.77	0.65
41:k:72:SER:HB2	41:k:74:LEU:HD23	1.78	0.65
1:0:534:PRO:HA	7:6:239:LEU:HB3	1.79	0.64
34:d:459:ILE:HG22	34:d:465:VAL:HG12	1.78	0.64
15:G:101:VAL:HG11	15:G:145:VAL:HG11	1.78	0.64
8:7:610:ASP:OD1	8:7:686:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:92:HIS:HB3	9:A:95:PHE:HB2	1.80	0.64
11:C:39:ALA:HA	11:C:164:ALA:HB3	1.79	0.64
23:O:90:ARG:NH2	28:V:68:THR:OG1	2.29	0.64
31:a:151:GLN:OE1	31:a:162:GLN:NE2	2.31	0.63
1:0:624:GLY:HA2	1:0:683:ASP:HB2	1.80	0.63
9:A:1029:ARG:O	9:A:1033:GLN:HB3	1.98	0.63
12:D:126:ILE:HD12	12:D:145:MET:HB3	1.81	0.63
7:6:330:GLU:HG3	7:6:332:THR:H	1.64	0.63
24:Q:121:PHE:HB2	25:R:131:ASN:HB3	1.80	0.63
32:b:153:ARG:NH1	37:g:30:ILE:O	2.31	0.63
41:k:116:HIS:ND1	44:n:33:GLU:OE2	2.32	0.63
29:W:108:ARG:NH2	30:X:262:MET:O	2.31	0.63
35:e:166:LEU:O	35:e:187:GLU:HA	1.99	0.62
24:Q:376:LEU:HB2	25:R:69:TRP:HB2	1.81	0.62
42:l:698:ARG:O	42:l:702:HIS:ND1	2.30	0.62
1:0:295:SER:O	1:0:299:LEU:HB2	1.99	0.62
1:0:307:VAL:HG22	1:0:400:LYS:HG2	1.82	0.62
35:e:53:ASN:HB2	36:f:113:SER:HB2	1.82	0.62
45:o:36:ILE:HA	45:o:39:VAL:HG22	1.81	0.62
2:1:339:LEU:HD23	2:1:342:ASN:HD22	1.64	0.62
9:A:107:CYS:SG	9:A:171:GLN:NE2	2.72	0.62
46:p:228:PHE:HB3	46:p:249:SER:HB3	1.82	0.62
29:W:108:ARG:HH22	30:X:262:MET:HG3	1.65	0.62
42:l:411:ILE:HB	42:l:429:ILE:HB	1.82	0.62
7:6:157:VAL:HG22	7:6:169:MET:HE1	1.80	0.62
31:a:155:ILE:HD12	31:a:160:ILE:HG12	1.80	0.62
1:0:271:ILE:HG12	1:0:328:ALA:HB1	1.82	0.62
15:G:84:GLY:N	15:G:147:ILE:O	2.29	0.62
6:5:17:LYS:HG3	6:5:40:LEU:HD21	1.82	0.61
9:A:909:ASP:HB3	9:A:912:LEU:HG	1.80	0.61
42:l:263:PRO:HG3	42:l:364:LEU:HD23	1.81	0.61
10:B:996:ARG:NH1	11:C:174:ALA:O	2.33	0.61
1:0:505:ALA:HB1	1:0:684:ARG:HD2	1.82	0.61
7:6:131:ASP:HB3	7:6:136:MET:HE2	1.83	0.61
9:A:911:SER:HB3	40:j:89:THR:HG23	1.82	0.61
1:0:460:SER:HB3	1:0:463:ILE:HB	1.82	0.61
9:A:326:ARG:HG3	9:A:1406:VAL:HG21	1.82	0.61
9:A:243:PRO:HB2	9:A:245:PRO:HD2	1.81	0.61
32:b:100:LYS:NZ	34:d:253:SER:OG	2.32	0.61
38:h:118:LEU:HD11	39:i:206:ILE:HD13	1.82	0.61
9:A:840:ARG:NH1	9:A:1384:VAL:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:144:TYR:O	40:j:148:GLN:NE2	2.34	0.61
6:5:51:LYS:O	6:5:55:ASN:ND2	2.34	0.60
11:C:142:VAL:HG11	18:J:5:VAL:HG13	1.82	0.60
24:Q:141:ARG:NH1	24:Q:348:TYR:O	2.33	0.60
9:A:226:GLU:HG2	9:A:227:VAL:HG23	1.82	0.60
10:B:1189:ILE:HD12	15:G:41:LYS:HG3	1.82	0.60
27:U:246:CYS:SG	27:U:247:LEU:N	2.69	0.60
24:Q:433:THR:HG22	24:Q:434:THR:HG23	1.84	0.60
29:W:6:ASP:OD2	29:W:205:ARG:NH1	2.35	0.60
45:o:62:GLU:OE2	45:o:86:ASN:ND2	2.34	0.60
10:B:542:MET:HE2	10:B:747:MET:HG3	1.84	0.60
10:B:904:ARG:NH2	20:L:66:GLN:O	2.34	0.60
11:C:33:LEU:HG	11:C:37:MET:HE2	1.84	0.60
28:V:86:THR:HG22	28:V:105:VAL:HG22	1.83	0.60
32:b:25:PHE:HE1	32:b:98:LEU:HD11	1.64	0.60
46:p:187:LYS:HE3	46:p:189:ARG:HH12	1.66	0.60
41:k:64:ASN:ND2	43:m:124:ASP:OD2	2.35	0.60
10:B:1056:SER:HB3	10:B:1066:SER:HB2	1.83	0.60
10:B:604:ARG:NH2	10:B:691:GLU:OE2	2.33	0.60
2:1:320:GLU:OE2	2:1:323:ARG:NH2	2.35	0.60
3:2:369:ARG:HG3	3:2:374:VAL:HG12	1.84	0.60
9:A:362:ASP:HB3	9:A:508:PRO:HD3	1.84	0.60
25:R:43:ASN:HB2	25:R:205:VAL:HG23	1.84	0.60
9:A:896:ARG:HD3	9:A:1030:ARG:HH11	1.67	0.59
9:A:1675:TYR:HD2	42:l:170:ARG:HD2	1.67	0.59
1:0:633:ARG:HH21	1:0:636:LYS:HE2	1.66	0.59
11:C:250:THR:HA	11:C:253:LYS:HE2	1.83	0.59
36:f:136:THR:HB	36:f:156:GLN:HB2	1.84	0.59
22:N:-15:DC:H5	26:T:15:DG:H1	1.48	0.59
3:2:201:TRP:NE1	3:2:278:LEU:O	2.35	0.59
24:Q:119:LEU:HD23	25:R:133:TYR:HB2	1.84	0.59
27:U:245:LEU:HD12	28:V:9:LEU:HB3	1.84	0.59
1:0:666:LEU:HD11	1:0:681:LEU:HD21	1.85	0.59
10:B:872:GLU:HG2	10:B:916:THR:HG22	1.84	0.59
34:d:279:TRP:CD1	37:g:54:SER:HG	2.19	0.59
1:0:83:LEU:HD11	1:0:107:GLY:HA3	1.85	0.59
5:4:64:HIS:O	5:4:71:ASN:ND2	2.31	0.59
28:V:8:GLU:HB2	28:V:11:ARG:HH22	1.67	0.59
32:b:26:ASN:C	32:b:28:VAL:H	2.11	0.59
46:p:73:ARG:NH1	46:p:108:LEU:O	2.36	0.59
7:6:76:TRP:HE1	8:7:367:GLU:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1163:CYS:HB2	10:B:1187:ASN:HD21	1.67	0.59
9:A:875:ALA:HB2	9:A:1366:ARG:HD2	1.84	0.59
46:p:186:PHE:HB3	46:p:200:ILE:HD11	1.85	0.59
45:o:116:GLN:NE2	45:o:120:GLU:OE2	2.36	0.58
3:2:387:LEU:HB3	3:2:448:LEU:HD22	1.84	0.58
9:A:840:ARG:NH1	9:A:1106:ASN:OD1	2.34	0.58
9:A:1671:THR:HG22	42:l:163:ILE:HD12	1.85	0.58
42:l:375:LEU:HD23	42:l:431:ILE:HG12	1.86	0.58
9:A:1329:THR:HG22	9:A:1331:SER:H	1.67	0.58
11:C:143:LEU:HD21	11:C:146:LYS:HE3	1.85	0.58
33:c:21:CYS:HB2	34:d:302:LEU:HD12	1.86	0.58
32:b:21:VAL:HG23	32:b:23:PHE:H	1.69	0.58
1:0:56:THR:HG21	1:0:233:ILE:HD11	1.84	0.58
10:B:526:GLU:HG3	10:B:771:SER:HB3	1.85	0.58
9:A:404:TYR:HB2	9:A:433:GLU:HB3	1.85	0.58
28:V:66:LEU:HA	28:V:80:VAL:HA	1.85	0.58
36:f:155:LEU:HD11	36:f:170:ILE:HG13	1.85	0.58
44:n:4:ARG:NH1	44:n:79:SER:O	2.36	0.58
29:W:141:ASN:HB3	29:W:148:LEU:HD23	1.85	0.58
30:X:317:MET:HB2	30:X:320:ILE:HB	1.85	0.58
1:0:573:THR:HG22	1:0:575:ASP:H	1.68	0.58
2:1:27:LEU:HD23	2:1:42:LEU:HD11	1.86	0.58
10:B:979:LYS:HD3	10:B:987:LYS:HD2	1.85	0.58
21:M:329:ILE:HD12	21:M:336:LEU:HD23	1.84	0.58
21:M:195:LEU:HB3	21:M:196:ILE:HD12	1.86	0.58
42:l:628:ARG:HH21	42:l:634:LEU:HA	1.69	0.58
9:A:451:HIS:O	9:A:454:SER:OG	2.21	0.57
12:D:66:ARG:NH2	15:G:35:GLU:OE1	2.37	0.57
27:U:239:PRO:O	27:U:271:ARG:NH2	2.37	0.57
33:c:54:GLN:HA	33:c:57:GLU:HG2	1.86	0.57
39:i:166:ARG:HG3	42:l:195:LEU:HB3	1.86	0.57
42:l:304:LEU:O	42:l:339:ASN:ND2	2.37	0.57
1:0:532:ILE:HD13	1:0:714:ILE:HG23	1.86	0.57
2:1:476:VAL:HG21	5:4:50:ILE:HD12	1.86	0.57
6:5:50:VAL:O	6:5:54:LEU:HB2	2.04	0.57
46:p:103:ILE:HG21	46:p:196:PHE:HE1	1.68	0.57
3:2:274:LEU:HA	3:2:277:MET:HG3	1.87	0.57
10:B:1133:MET:HA	10:B:1136:ASP:HB2	1.86	0.57
24:Q:404:LEU:HD13	24:Q:425:MET:HE1	1.85	0.57
41:k:114:LYS:NZ	44:n:27:ASP:OD1	2.36	0.57
18:J:21:TYR:HB2	18:J:39:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:28:TYR:HA	13:E:64:PRO:HA	1.86	0.57
1:0:258:ARG:HH11	1:0:262:ARG:HH21	1.52	0.57
9:A:997:LEU:O	9:A:1011:GLN:NE2	2.36	0.57
9:A:1030:ARG:NH2	9:A:1035:TYR:OH	2.37	0.57
10:B:728:ARG:NH1	10:B:760:ASP:OD2	2.37	0.57
8:7:227:ILE:O	8:7:348:ARG:NH2	2.37	0.57
19:K:21:ILE:HG12	19:K:33:ILE:HG12	1.87	0.57
39:i:113:GLN:O	39:i:117:GLN:NE2	2.37	0.57
42:l:253:VAL:HG12	42:l:290:THR:HG22	1.87	0.57
1:0:83:LEU:HD13	1:0:177:SER:HA	1.85	0.57
1:0:611:ASP:OD2	1:0:671:ARG:NH1	2.37	0.57
10:B:287:ARG:NH1	10:B:292:ILE:O	2.37	0.57
3:2:193:LEU:HD11	3:2:395:GLN:HB2	1.87	0.57
8:7:601:ARG:NH1	8:7:603:ASP:OD2	2.39	0.56
2:1:193:LYS:HE3	2:1:552:MET:HB3	1.87	0.56
3:2:50:MET:HE3	3:2:100:LEU:HB2	1.87	0.56
9:A:1199:ARG:NH2	9:A:1233:ASP:O	2.39	0.56
11:C:48:SER:HB3	11:C:158:VAL:HB	1.88	0.56
13:E:100:ILE:HG23	13:E:105:PHE:HB2	1.87	0.56
29:W:73:ARG:HB3	29:W:83:GLU:HA	1.86	0.56
1:0:48:LYS:NZ	1:0:235:ASP:OD1	2.37	0.56
42:l:629:LEU:HB3	42:l:632:TRP:HE1	1.69	0.56
7:6:134:GLU:HG3	7:6:206:GLY:H	1.70	0.56
8:7:111:GLY:O	8:7:114:ARG:NH2	2.39	0.56
21:M:33:LYS:HG3	21:M:46:ALA:HB3	1.88	0.56
34:d:604:ARG:HA	34:d:607:ASP:HB2	1.87	0.56
5:4:293:LEU:HD11	7:6:122:ILE:HG21	1.87	0.56
10:B:87:LYS:HB3	10:B:137:TYR:HB2	1.88	0.56
16:H:75:ALA:N	16:H:98:TYR:HH	2.02	0.56
22:N:-58:DT:H4'	23:O:158:GLN:HB3	1.87	0.56
25:R:43:ASN:ND2	25:R:202:ILE:O	2.39	0.56
29:W:96:ASP:HA	29:W:99:LYS:HD3	1.88	0.56
1:0:314:GLN:HE22	1:0:448:PRO:HB3	1.70	0.56
21:M:281:SER:O	21:M:285:ASN:ND2	2.34	0.56
32:b:206:PHE:HD2	35:e:298:SER:HB3	1.71	0.56
38:h:122:HIS:NE2	44:n:123:ASP:OD1	2.38	0.56
10:B:1135:ARG:HG3	10:B:1147:LEU:HD11	1.88	0.56
33:c:98:MET:HB2	34:d:513:VAL:HG11	1.86	0.56
1:0:295:SER:HB3	1:0:379:GLU:HG3	1.88	0.56
10:B:848:ARG:HH22	10:B:996:ARG:HE	1.54	0.56
23:O:105:ARG:NH1	28:V:69:TYR:OH	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:269:ILE:O	27:U:272:ASN:HB2	2.05	0.56
4:3:21:TYR:OH	29:W:99:LYS:NZ	2.39	0.56
9:A:378:GLU:OE2	9:A:387:ARG:NH2	2.37	0.56
10:B:883:LEU:HD11	10:B:928:ARG:HD3	1.86	0.56
16:H:2:SER:N	16:H:61:SER:OG	2.39	0.56
5:4:30:ILE:HG12	5:4:32:ILE:HG23	1.88	0.55
24:Q:436:THR:HG22	24:Q:438:TYR:H	1.70	0.55
44:n:58:THR:HA	44:n:61:GLU:HG2	1.88	0.55
2:1:251:LEU:HA	2:1:255:LYS:HD2	1.88	0.55
2:1:571:GLY:HA3	5:4:322:ARG:HD3	1.88	0.55
9:A:590:ARG:NH2	9:A:621:THR:OG1	2.39	0.55
24:Q:440:ARG:NH1	25:R:198:ARG:O	2.39	0.55
38:h:166:ILE:HG21	38:h:172:LYS:HG2	1.88	0.55
43:m:130:PRO:HG3	43:m:134:ASP:HA	1.87	0.55
1:0:310:PRO:HB3	1:0:404:THR:HG23	1.88	0.55
1:0:573:THR:O	1:0:579:THR:OG1	2.23	0.55
9:A:1397:LEU:HB2	9:A:1426:GLU:HG3	1.89	0.55
7:6:394:THR:HG21	7:6:422:LEU:HD12	1.88	0.55
9:A:427:GLN:OE1	35:e:177:ASN:ND2	2.39	0.55
3:2:14:LEU:O	3:2:22:GLN:NE2	2.39	0.55
42:l:270:HIS:HB3	42:l:277:TYR:HB2	1.87	0.55
8:7:133:TRP:HB2	8:7:142:ILE:HB	1.89	0.55
31:a:164:PRO:HG2	31:a:169:ILE:HD11	1.88	0.55
42:l:211:ARG:HH11	42:l:220:LYS:HD2	1.70	0.55
1:0:321:ILE:O	1:0:326:ARG:NH2	2.40	0.55
8:7:386:LEU:HD23	8:7:538:ALA:HB2	1.89	0.55
9:A:1648:SER:HB2	9:A:1651:SER:HB2	1.88	0.55
1:0:678:VAL:HG11	1:0:717:THR:HG23	1.89	0.55
2:1:561:LEU:HD13	2:1:623:ILE:HG22	1.87	0.55
8:7:132:LEU:HB2	8:7:201:SER:HA	1.89	0.55
10:B:805:THR:OG1	10:B:809:MET:SD	2.59	0.55
24:Q:139:LEU:HD13	24:Q:352:MET:HB2	1.89	0.55
2:1:543:PRO:HD2	2:1:608:MET:HE1	1.89	0.55
7:6:139:LYS:O	7:6:142:ARG:NH1	2.40	0.55
8:7:660:THR:O	8:7:689:ARG:NH2	2.40	0.55
9:A:463:ILE:HD13	9:A:469:ARG:HG3	1.89	0.55
11:C:116:LYS:HD3	11:C:140:ASN:HA	1.88	0.55
23:O:196:ARG:HG2	23:O:203:VAL:HG22	1.89	0.55
41:k:14:GLU:HG2	41:k:66:ARG:HH21	1.71	0.55
9:A:147:VAL:HG13	9:A:149:GLU:HG2	1.89	0.55
9:A:402:ALA:HA	9:A:434:ARG:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1149:ALA:HB3	9:A:1196:GLU:HB3	1.89	0.55
10:B:398:ARG:HD3	10:B:509:ALA:HB2	1.89	0.55
25:R:90:GLN:HE21	25:R:92:LEU:HD21	1.71	0.55
32:b:203:LYS:O	32:b:207:THR:OG1	2.23	0.55
35:e:39:THR:HG21	35:e:109:LEU:HD21	1.89	0.55
9:A:179:LEU:HD23	9:A:297:GLN:HG3	1.90	0.54
1:0:111:ARG:NH1	1:0:130:ASP:OD1	2.40	0.54
1:0:125:LYS:HB2	1:0:128:VAL:HG22	1.89	0.54
1:0:725:ALA:HB1	7:6:290:ILE:HG13	1.88	0.54
19:K:44:ASN:OD1	19:K:47:ARG:NH2	2.40	0.54
32:b:197:ASN:HB3	32:b:200:ASP:HB2	1.90	0.54
9:A:1588:SER:HB3	39:i:12:LEU:HD12	1.89	0.54
32:b:26:ASN:O	32:b:28:VAL:N	2.40	0.54
9:A:562:THR:O	9:A:576:GLN:NE2	2.41	0.54
9:A:1168:GLU:HA	9:A:1171:GLN:HG3	1.88	0.54
5:4:162:ARG:NH1	7:6:406:CYS:O	2.41	0.54
32:b:37:ARG:NH1	34:d:240:SER:OG	2.39	0.54
39:i:188:GLU:OE1	44:n:108:LYS:NZ	2.40	0.54
8:7:409:VAL:HG22	8:7:486:ILE:HB	1.90	0.54
10:B:1050:ILE:HD13	24:Q:20:PRO:HA	1.88	0.54
9:A:1573:THR:HG22	32:b:48:ARG:HE	1.71	0.54
8:7:440:SER:O	8:7:443:LYS:NZ	2.41	0.54
9:A:881:GLN:NE2	9:A:958:VAL:O	2.35	0.54
41:k:29:PHE:HA	41:k:32:LEU:HD23	1.90	0.54
46:p:11:LEU:HA	46:p:14:MET:HE2	1.89	0.54
7:6:221:LEU:HD13	7:6:230:ARG:HB3	1.90	0.54
8:7:514:THR:HG21	8:7:517:LEU:HD13	1.90	0.54
24:Q:351:VAL:HG22	24:Q:362:VAL:HG22	1.89	0.54
24:Q:369:ASN:C	24:Q:369:ASN:HD22	2.16	0.54
32:b:22:SER:O	32:b:23:PHE:HB2	2.08	0.54
42:l:287:GLN:O	42:l:300:VAL:HB	2.08	0.54
10:B:805:THR:HG23	24:Q:22:ILE:HD12	1.90	0.54
25:R:80:LYS:NZ	25:R:113:ASN:OD1	2.41	0.54
25:R:279:LYS:HB2	25:R:282:ARG:HH21	1.72	0.54
32:b:26:ASN:C	32:b:28:VAL:N	2.66	0.54
8:7:517:LEU:HD23	8:7:534:LYS:HE2	1.89	0.53
9:A:40:THR:HG22	9:A:53:LEU:HB2	1.89	0.53
17:I:74:GLU:OE1	17:I:81:ARG:NH1	2.41	0.53
21:M:186:ALA:O	21:M:241:ARG:NH2	2.40	0.53
21:M:286:ILE:HG23	21:M:291:ILE:HB	1.90	0.53
32:b:27:GLY:HA3	34:d:257:ASP:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:19:ASP:OD2	17:I:24:ARG:NH1	2.42	0.53
21:M:259:THR:HG23	21:M:323:LEU:HB3	1.90	0.53
31:a:42:ASN:HA	31:a:45:VAL:HG22	1.88	0.53
34:d:394:PHE:HB3	34:d:403:TYR:HB3	1.89	0.53
10:B:542:MET:HE1	10:B:743:ILE:HB	1.90	0.53
43:m:125:ILE:HA	43:m:128:PHE:HD2	1.73	0.53
46:p:91:PHE:O	46:p:191:ASN:ND2	2.39	0.53
11:C:11:ARG:NH2	11:C:19:ASP:OD1	2.42	0.53
15:G:108:VAL:HG22	15:G:159:ALA:HB3	1.91	0.53
36:f:62:PHE:O	36:f:67:ARG:HA	2.08	0.53
8:7:164:ILE:HD11	8:7:174:LYS:HB2	1.90	0.53
10:B:1187:ASN:HD22	10:B:1190:ASP:HB3	1.72	0.53
14:F:128:LYS:HD2	14:F:149:GLU:HA	1.91	0.53
17:I:19:ASP:HB3	17:I:24:ARG:H	1.74	0.53
21:M:316:LEU:HD22	21:M:323:LEU:HD11	1.89	0.53
10:B:443:ASN:HB3	10:B:446:LEU:HD12	1.89	0.53
13:E:169:ARG:HH12	14:F:65:ARG:NH1	2.07	0.53
17:I:101:PHE:HE1	17:I:112:SER:HB3	1.73	0.53
25:R:138:GLN:HG2	25:R:211:LYS:HD3	1.90	0.53
35:e:282:LEU:HD13	35:e:286:ILE:HD11	1.91	0.53
41:k:108:ASN:OD1	41:k:112:ARG:NH2	2.42	0.53
9:A:397:ASN:H	35:e:55:ARG:HH22	1.56	0.53
23:O:82:LEU:HA	23:O:85:VAL:HG12	1.91	0.53
29:W:120:ASN:HA	29:W:161:SER:HB3	1.89	0.53
1:0:15:PRO:HG3	2:1:426:GLU:HG2	1.91	0.53
5:4:166:GLU:HG2	5:4:168:VAL:HG13	1.91	0.53
7:6:126:LEU:O	7:6:169:MET:HA	2.09	0.53
7:6:397:LYS:NZ	7:6:398:PHE:O	2.41	0.53
9:A:346:ASP:OD1	10:B:1106:ARG:NE	2.38	0.53
30:X:289:ASP:HB2	30:X:293:ILE:HD12	1.91	0.53
34:d:23:PRO:HB2	34:d:86:LEU:HD11	1.91	0.53
4:3:34:CYS:SG	4:3:36:HIS:CE1	2.78	0.53
29:W:61:LEU:HB3	29:W:67:ILE:HG12	1.91	0.53
34:d:86:LEU:HD12	34:d:87:VAL:HG23	1.91	0.53
40:j:73:LEU:HA	40:j:76:ILE:HG12	1.91	0.53
43:m:44:SER:O	43:m:48:ALA:HB2	2.09	0.53
3:2:194:GLN:HG3	3:2:198:SER:HB3	1.91	0.52
10:B:706:GLN:HE22	10:B:730:ARG:HD3	1.73	0.52
21:M:23:THR:HG22	21:M:32:PRO:HG3	1.90	0.52
28:V:108:VAL:HG11	28:V:111:LEU:HB2	1.90	0.52
3:2:239:ILE:HG13	3:2:242:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:347:TYR:O	7:6:355:LYS:HA	2.09	0.52
9:A:1399:ARG:HB3	9:A:1408:ILE:HD13	1.91	0.52
41:k:89:ASP:HA	43:m:81:ARG:HG2	1.91	0.52
6:5:20:ILE:HA	6:5:23:ILE:HG22	1.91	0.52
10:B:102:VAL:HG21	10:B:122:LEU:HD13	1.91	0.52
11:C:6:PRO:O	19:K:104:ASN:ND2	2.42	0.52
21:M:207:LEU:HG	21:M:211:LYS:HE2	1.91	0.52
45:o:118:MET:HA	45:o:121:MET:HG2	1.90	0.52
6:5:26:LYS:HE3	6:5:27:MET:HE2	1.90	0.52
21:M:188:THR:H	21:M:191:GLU:HG3	1.75	0.52
29:W:193:ARG:NH2	30:X:286:ALA:O	2.41	0.52
39:i:117:GLN:OE1	39:i:120:ARG:NH1	2.42	0.52
1:0:374:LEU:HD22	1:0:406:ALA:HB1	1.91	0.52
8:7:592:GLN:NE2	8:7:747:ASN:O	2.43	0.52
21:M:180:CYS:HB3	21:M:186:ALA:HA	1.92	0.52
34:d:392:ARG:HB2	34:d:475:GLU:HB2	1.91	0.52
46:p:25:SER:O	46:p:30:ASN:ND2	2.42	0.52
3:2:110:ASN:ND2	3:2:116:GLU:OE2	2.42	0.52
6:5:16:ILE:HD13	6:5:19:LEU:HD12	1.91	0.52
13:E:126:SER:OG	13:E:127:ILE:N	2.42	0.52
23:O:202:ILE:HD11	23:O:222:GLU:HB3	1.92	0.52
9:A:1386:ARG:NH2	9:A:1403:GLU:OE1	2.43	0.52
10:B:166:PHE:HZ	10:B:169:ARG:HG3	1.74	0.52
8:7:230:ASN:ND2	8:7:478:THR:O	2.36	0.52
9:A:295:LEU:HD22	21:M:113:ALA:HB1	1.91	0.52
29:W:21:TYR:OH	29:W:64:ASP:OD2	2.24	0.52
34:d:103:ILE:HD13	34:d:106:ILE:HD12	1.90	0.52
1:0:223:SER:O	1:0:452:ARG:NH2	2.43	0.52
2:1:226:GLN:NE2	7:6:179:ALA:O	2.35	0.52
8:7:682:GLN:HG2	8:7:722:ARG:HH22	1.75	0.52
9:A:156:ASP:OD1	9:A:156:ASP:N	2.43	0.52
9:A:446:ARG:HG3	9:A:487:MET:HG2	1.91	0.52
10:B:912:ILE:HB	10:B:939:THR:HB	1.92	0.52
24:Q:345:GLU:OE1	24:Q:391:LYS:NZ	2.42	0.52
33:c:19:GLN:OE1	33:c:58:ARG:NH1	2.41	0.52
4:3:29:LEU:HD12	4:3:68:PHE:HB3	1.92	0.51
27:U:5:GLU:OE2	28:V:56:THR:OG1	2.28	0.51
5:4:155:ALA:HA	7:6:405:SER:HB2	1.93	0.51
12:D:155:ARG:HD2	12:D:220:LEU:HD12	1.92	0.51
27:U:248:TYR:N	28:V:116:CYS:O	2.43	0.51
33:c:73:LEU:HD21	37:g:82:LYS:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:208:GLU:OE1	2:1:567:HIS:NE2	2.43	0.51
4:3:16:CYS:SG	4:3:18:THR:OG1	2.62	0.51
10:B:722:ASP:OD1	10:B:722:ASP:N	2.43	0.51
11:C:46:ILE:HG13	11:C:72:LEU:HD11	1.91	0.51
35:e:77:ASP:OD2	35:e:97:LYS:NZ	2.43	0.51
8:7:438:PHE:HB3	8:7:455:SER:HB2	1.91	0.51
10:B:957:ASN:HD21	10:B:961:LEU:HB2	1.75	0.51
21:M:279:VAL:HG21	21:M:304:VAL:HG21	1.92	0.51
41:k:66:ARG:HA	41:k:69:ASP:HB2	1.92	0.51
42:l:268:SER:OG	42:l:279:THR:O	2.27	0.51
2:1:510:ASN:ND2	5:4:264:LYS:O	2.44	0.51
5:4:313:ASP:HB3	5:4:316:VAL:HG12	1.93	0.51
9:A:427:GLN:HG2	35:e:178:ARG:HH21	1.75	0.51
32:b:59:LEU:HD21	34:d:204:ARG:HD3	1.92	0.51
34:d:23:PRO:HA	34:d:26:ILE:HD11	1.93	0.51
35:e:181:SER:HB3	35:e:290:VAL:HG13	1.92	0.51
6:5:35:LEU:HD22	6:5:39:HIS:HB2	1.93	0.51
8:7:356:LEU:HD11	8:7:398:THR:HG23	1.91	0.51
9:A:148:CYS:O	9:A:164:ARG:NH1	2.42	0.51
9:A:439:ASN:HA	9:A:459:ARG:HB3	1.93	0.51
11:C:36:VAL:HG13	11:C:40:GLU:HB2	1.91	0.51
15:G:132:SER:OG	15:G:135:ASP:OD1	2.28	0.51
29:W:141:ASN:O	29:W:144:ARG:NH1	2.41	0.51
41:k:81:LEU:HD22	42:l:88:ASN:HB3	1.92	0.51
42:l:99:LEU:HD23	42:l:144:LEU:HD22	1.91	0.51
3:2:391:ILE:HA	3:2:395:GLN:HE21	1.76	0.51
9:A:744:LYS:HG3	9:A:748:MET:HE2	1.93	0.51
8:7:552:VAL:HG21	8:7:687:LEU:HD11	1.92	0.51
9:A:173:THR:OG1	9:A:184:SER:OG	2.28	0.51
3:2:173:MET:HE1	3:2:184:ILE:HG13	1.91	0.51
34:d:280:LYS:HB3	37:g:28:THR:HG23	1.93	0.51
36:f:152:LEU:HD21	36:f:204:TYR:HE2	1.76	0.51
38:h:45:ASP:O	38:h:48:ARG:NH1	2.43	0.51
1:0:16:LYS:NZ	2:1:425:ASN:O	2.42	0.50
8:7:738:HIS:HB3	29:W:298:THR:HB	1.92	0.50
10:B:214:ALA:HB3	10:B:498:THR:HG22	1.93	0.50
21:M:35:VAL:HG23	21:M:46:ALA:HB2	1.92	0.50
29:W:92:PRO:HB2	30:X:287:SER:HB2	1.93	0.50
41:k:30:VAL:HG12	42:l:138:ARG:HH12	1.76	0.50
42:l:121:GLU:HB3	42:l:129:ARG:HH22	1.76	0.50
9:A:544:ASP:N	9:A:544:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1290:LYS:HE3	9:A:1298:TYR:HB3	1.93	0.50
10:B:137:TYR:HB3	10:B:149:TYR:HB3	1.92	0.50
11:C:179:GLU:HG2	11:C:206:ASN:HD22	1.75	0.50
16:H:48:PRO:O	16:H:146:ARG:NH2	2.44	0.50
24:Q:338:ASN:OD1	24:Q:339:ALA:N	2.44	0.50
6:5:14:PRO:HB3	8:7:563:ALA:HB2	1.92	0.50
9:A:1444:MET:HG3	15:G:60:ARG:HA	1.94	0.50
10:B:522:VAL:HG21	10:B:537:LYS:HD2	1.92	0.50
10:B:928:ARG:NH1	10:B:929:THR:O	2.44	0.50
32:b:200:ASP:HB3	32:b:211:PRO:HB3	1.93	0.50
35:e:5:LEU:O	35:e:256:TYR:HA	2.11	0.50
36:f:108:LEU:HA	36:f:112:LEU:HB2	1.92	0.50
3:2:14:LEU:HD23	3:2:17:ILE:HD12	1.93	0.50
6:5:24:ASP:O	6:5:28:SER:HA	2.11	0.50
9:A:108:MET:H	9:A:171:GLN:HE21	1.58	0.50
9:A:130:ASP:OD1	9:A:130:ASP:N	2.44	0.50
11:C:258:ILE:HG13	19:K:42:LEU:HD21	1.93	0.50
29:W:74:GLU:OE2	29:W:84:ARG:NE	2.45	0.50
35:e:214:GLN:HG3	35:e:238:ILE:HB	1.94	0.50
38:h:193:LEU:N	45:o:28:GLU:OE1	2.40	0.50
5:4:32:ILE:HA	5:4:37:TRP:HE1	1.76	0.50
10:B:445:LYS:NZ	25:R:265:HIS:O	2.45	0.50
34:d:394:PHE:HB2	34:d:473:LYS:HB3	1.93	0.50
39:i:153:THR:HA	39:i:156:VAL:HG22	1.92	0.50
46:p:73:ARG:HH21	46:p:74:ILE:HG12	1.77	0.50
1:0:429:ALA:HB2	2:1:364:ILE:HG13	1.93	0.50
9:A:8:SER:HB3	10:B:1178:ASN:HD21	1.77	0.50
14:F:64:ILE:HG23	14:F:65:ARG:HG3	1.93	0.50
25:R:240:ARG:HA	25:R:243:ILE:HD12	1.92	0.50
29:W:127:CYS:SG	29:W:129:THR:OG1	2.64	0.50
36:f:174:LEU:HA	36:f:177:ILE:HG22	1.93	0.50
1:0:120:VAL:HG23	1:0:123:GLU:HG3	1.92	0.50
9:A:242:PRO:HD2	9:A:266:LEU:HD11	1.94	0.50
9:A:511:ILE:HA	9:A:521:MET:HE3	1.93	0.50
10:B:216:GLU:OE1	10:B:500:THR:OG1	2.29	0.50
10:B:1152:MET:HE1	10:B:1195:HIS:HB3	1.94	0.50
11:C:84:ARG:O	36:f:120:GLN:NE2	2.42	0.50
14:F:67:LYS:O	14:F:72:LYS:NZ	2.45	0.50
16:H:56:THR:HB	16:H:145:ARG:HG2	1.94	0.50
24:Q:376:LEU:HB3	24:Q:384:PHE:HD2	1.77	0.50
34:d:440:GLU:HG2	34:d:516:PHE:HZ	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:550:ARG:NH2	34:d:554:TYR:OH	2.44	0.50
41:k:28:SER:OG	41:k:52:ASN:OD1	2.28	0.50
43:m:61:ARG:HD2	43:m:65:LYS:HD3	1.94	0.50
1:0:666:LEU:HD22	1:0:679:MET:HB3	1.94	0.50
8:7:231:ARG:HH21	8:7:233:PHE:HZ	1.60	0.50
9:A:860:LEU:HD21	9:A:1394:THR:HA	1.94	0.50
9:A:1114:PRO:HB2	9:A:1311:VAL:HG23	1.94	0.50
10:B:604:ARG:NH2	10:B:697:GLU:OE2	2.40	0.50
14:F:85:MET:HE1	14:F:148:VAL:HG13	1.93	0.50
24:Q:141:ARG:NH1	24:Q:345:GLU:O	2.45	0.50
1:0:288:LYS:HD2	1:0:298:ILE:HG12	1.94	0.50
10:B:864:LYS:HA	10:B:961:LEU:HD13	1.93	0.50
14:F:65:ARG:NE	14:F:71:GLU:O	2.36	0.50
42:l:258:ALA:HB1	44:n:133:ILE:HD11	1.93	0.50
1:0:570:LEU:HD21	2:1:382:SER:HB2	1.92	0.49
3:2:250:LEU:HD12	3:2:259:VAL:HG11	1.93	0.49
15:G:1:MET:N	15:G:80:LYS:O	2.45	0.49
21:M:22:LEU:HD21	21:M:43:VAL:HG11	1.94	0.49
23:O:108:GLU:HG3	23:O:109:PRO:HD3	1.93	0.49
23:O:230:ILE:HG13	23:O:234:LEU:HD13	1.94	0.49
28:V:61:THR:OG1	28:V:86:THR:OG1	2.28	0.49
34:d:206:ASP:O	34:d:210:HIS:ND1	2.34	0.49
38:h:90:TYR:HA	38:h:93:ILE:HG22	1.94	0.49
1:0:138:ASN:O	1:0:302:GLN:NE2	2.44	0.49
1:0:427:ASN:ND2	2:1:362:VAL:O	2.45	0.49
8:7:642:ASN:ND2	30:X:322:LYS:O	2.41	0.49
9:A:596:THR:OG1	9:A:598:LEU:O	2.24	0.49
37:g:24:LEU:HD12	37:g:61:GLN:HB3	1.94	0.49
38:h:162:LYS:HA	42:l:196:PRO:HG2	1.94	0.49
8:7:664:LEU:HD12	8:7:689:ARG:HD2	1.94	0.49
8:7:672:GLN:OE1	8:7:686:ARG:NH1	2.44	0.49
9:A:1169:ILE:O	9:A:1173:HIS:ND1	2.31	0.49
2:1:290:SER:O	2:1:294:ARG:NH1	2.46	0.49
8:7:490:VAL:HG12	8:7:514:THR:HB	1.94	0.49
9:A:1399:ARG:NH2	9:A:1417:GLU:OE1	2.46	0.49
9:A:1640:TYR:OH	31:a:124:ASP:OD2	2.18	0.49
10:B:184:ALA:HB1	10:B:188:ASP:HB3	1.94	0.49
27:U:45:LYS:HA	27:U:48:GLU:HG2	1.93	0.49
32:b:119:ILE:HG13	32:b:122:VAL:H	1.75	0.49
34:d:469:LEU:HB3	34:d:472:GLU:H	1.77	0.49
46:p:227:ARG:NH1	46:p:250:ASN:OD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:605:ILE:HA	8:7:669:CYS:O	2.12	0.49
9:A:157:ASP:OD1	9:A:160:GLN:NE2	2.45	0.49
15:G:52:ASP:OD1	15:G:52:ASP:N	2.46	0.49
42:l:92:LEU:HA	42:l:95:VAL:HG12	1.94	0.49
1:0:18:TYR:HB2	1:0:21:GLN:HG3	1.95	0.49
9:A:853:ASP:OD2	9:A:857:ARG:NH2	2.45	0.49
9:A:946:VAL:HG22	13:E:201:LYS:HD2	1.94	0.49
9:A:1409:LEU:HD13	10:B:1207:LEU:HD21	1.94	0.49
10:B:326:ASP:HB2	24:Q:403:THR:HG21	1.92	0.49
35:e:63:ARG:NH1	35:e:299:ARG:O	2.45	0.49
36:f:4:SER:O	36:f:203:GLN:NE2	2.43	0.49
2:1:49:GLN:HB2	2:1:61:ARG:HB3	1.93	0.49
5:4:323:LYS:HG3	5:4:324:PRO:HD2	1.94	0.49
10:B:415:GLN:OE1	10:B:476:ARG:NH2	2.46	0.49
35:e:228:LEU:HD12	35:e:257:ILE:HD11	1.94	0.49
42:l:620:LEU:HB2	42:l:643:ILE:HD11	1.94	0.49
3:2:100:LEU:HD23	3:2:105:LYS:HD3	1.94	0.49
7:6:159:GLU:OE2	7:6:163:GLN:NE2	2.39	0.49
8:7:552:VAL:HG12	8:7:703:ALA:HB3	1.95	0.49
11:C:258:ILE:HD12	19:K:19:LEU:HD21	1.95	0.49
22:N:-60:DT:H4'	23:O:203:VAL:HG11	1.93	0.49
25:R:310:TYR:O	25:R:313:TRP:NE1	2.44	0.49
30:X:132:THR:HA	30:X:135:ILE:HG22	1.95	0.49
36:f:164:GLU:HA	36:f:167:ILE:HG22	1.95	0.49
38:h:114:ILE:HA	38:h:117:ILE:HG12	1.94	0.49
46:p:202:THR:HG22	46:p:212:LEU:HD11	1.94	0.49
3:2:131:SER:HA	3:2:135:LEU:HB2	1.95	0.49
7:6:325:PRO:HB2	7:6:347:TYR:HB3	1.93	0.49
9:A:1668:TYR:OH	9:A:1672:SER:O	2.30	0.49
10:B:895:ASP:O	20:L:42:ARG:NH2	2.45	0.49
10:B:952:VAL:HG22	10:B:966:VAL:HG22	1.95	0.49
35:e:77:ASP:HB3	35:e:99:PRO:HG3	1.95	0.49
37:g:99:PHE:HB3	37:g:104:ILE:HD11	1.95	0.49
42:l:356:LEU:HD23	42:l:362:PRO:HB3	1.95	0.49
9:A:512:VAL:HA	9:A:519:PRO:HA	1.94	0.48
25:R:273:ASP:OD1	25:R:273:ASP:N	2.46	0.48
34:d:321:VAL:HG13	34:d:338:LYS:HB3	1.95	0.48
42:l:638:LEU:HD21	42:l:653:LYS:HG3	1.94	0.48
10:B:102:VAL:HB	10:B:112:LEU:HD22	1.94	0.48
33:c:97:LYS:O	33:c:101:GLN:HG2	2.13	0.48
1:0:7:ASP:OD1	1:0:7:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:114:LEU:HD22	1:0:192:PRO:HB2	1.94	0.48
25:R:330:LYS:HE2	25:R:334:ASP:HB3	1.94	0.48
1:0:496:ILE:HG12	1:0:681:LEU:HD12	1.96	0.48
4:3:17:LYS:HB3	29:W:176:MET:HG3	1.95	0.48
10:B:608:ASP:OD1	25:R:245:LYS:NZ	2.47	0.48
11:C:66:ARG:NH2	11:C:143:LEU:O	2.38	0.48
18:J:48:ARG:NH1	18:J:49:MET:SD	2.87	0.48
41:k:111:GLN:OE1	42:l:173:ASN:ND2	2.45	0.48
46:p:76:ASP:OD1	46:p:77:VAL:N	2.45	0.48
2:1:57:LYS:HG3	2:1:59:MET:HE3	1.94	0.48
7:6:109:ARG:NH2	7:6:441:ASP:OD2	2.46	0.48
7:6:331:ASP:OD1	7:6:331:ASP:N	2.45	0.48
10:B:373:ARG:NE	10:B:567:GLU:OE2	2.41	0.48
35:e:29:ASN:ND2	35:e:223:PHE:O	2.46	0.48
38:h:57:VAL:HA	38:h:60:VAL:HG12	1.95	0.48
1:0:539:VAL:HG22	1:0:621:LEU:HB3	1.95	0.48
3:2:207:TYR:HE2	3:2:249:MET:HE2	1.78	0.48
16:H:108:SER:OG	16:H:110:ASP:OD1	2.29	0.48
23:O:219:GLN:HG2	23:O:221:GLU:H	1.78	0.48
28:V:11:ARG:NH1	28:V:45:ASP:OD2	2.47	0.48
29:W:159:ASP:O	29:W:163:LYS:NZ	2.46	0.48
41:k:130:VAL:HG13	41:k:137:LYS:HG2	1.95	0.48
7:6:141:LEU:HB3	7:6:148:MET:SD	2.54	0.48
8:7:836:MET:SD	9:A:1244:ARG:NH1	2.86	0.48
9:A:914:GLU:OE2	9:A:977:LYS:NZ	2.46	0.48
9:A:1227:ILE:HD11	9:A:1239:ARG:HD3	1.94	0.48
39:i:203:LEU:HA	39:i:206:ILE:HG12	1.95	0.48
8:7:352:LEU:HB3	8:7:354:ILE:HG22	1.95	0.48
10:B:128:LEU:HD11	10:B:170:LEU:HB2	1.94	0.48
10:B:884:ARG:NH2	10:B:924:GLU:OE1	2.47	0.48
12:D:158:GLU:OE1	32:b:49:ARG:NH2	2.47	0.48
3:2:150:MET:HE1	3:2:191:PHE:CD2	2.48	0.48
8:7:223:VAL:HG23	8:7:337:VAL:HA	1.95	0.48
9:A:208:LEU:HD13	9:A:235:ILE:HB	1.95	0.48
12:D:194:LEU:HD22	15:G:86:VAL:HG11	1.95	0.48
14:F:82:THR:O	14:F:136:ARG:NH1	2.40	0.48
19:K:21:ILE:HD12	19:K:84:LYS:HE3	1.96	0.48
33:c:105:LEU:HD21	37:g:111:CYS:HB2	1.96	0.48
40:j:143:LEU:HA	40:j:146:LYS:HE3	1.96	0.48
42:l:110:TYR:OH	42:l:126:LYS:O	2.31	0.48
1:0:45:GLY:HA2	1:0:671:ARG:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:519:VAL:HG11	1:0:553:MET:HE2	1.96	0.48
3:2:176:VAL:HG22	3:2:178:SER:H	1.78	0.48
5:4:246:GLN:OE1	5:4:250:THR:OG1	2.31	0.48
22:N:-70:DA:H61	26:T:70:DT:H3	1.62	0.48
38:h:181:ILE:HD11	45:o:125:TRP:CG	2.49	0.48
38:h:192:MET:HA	38:h:195:MET:HG2	1.96	0.48
21:M:187:ARG:HE	25:R:268:MET:HG3	1.79	0.47
34:d:548:LYS:HZ1	34:d:609:LEU:HD12	1.77	0.47
36:f:132:LEU:HD12	36:f:135:LEU:HD22	1.96	0.47
42:l:492:ASP:HB2	42:l:500:LEU:HD23	1.96	0.47
10:B:103:ASN:HD21	21:M:141:GLU:HG2	1.79	0.47
10:B:229:ALA:O	10:B:261:ARG:NH1	2.47	0.47
25:R:347:PHE:HB3	26:T:46:DT:H4'	1.96	0.47
11:C:19:ASP:OD2	11:C:231:ASN:ND2	2.47	0.47
22:N:-26:DT:H2''	22:N:-25:DG:C8	2.49	0.47
30:X:183:THR:OG1	30:X:209:ASP:OD2	2.32	0.47
31:a:280:LEU:HA	31:a:283:LEU:HD12	1.97	0.47
41:k:8:ASN:HA	41:k:11:LEU:HD23	1.96	0.47
42:l:645:SER:OG	42:l:647:THR:O	2.33	0.47
45:o:26:GLU:OE1	45:o:63:TYR:OH	2.27	0.47
1:0:499:LYS:HD2	1:0:503:GLN:HG3	1.96	0.47
3:2:165:ASN:O	3:2:169:HIS:ND1	2.36	0.47
7:6:380:TYR:HD1	7:6:383:LEU:HD12	1.79	0.47
8:7:393:THR:O	8:7:397:ILE:HG12	2.14	0.47
11:C:88:CYS:O	36:f:119:ARG:NH1	2.47	0.47
36:f:130:LEU:HB2	36:f:137:VAL:HG23	1.96	0.47
39:i:141:PRO:HD3	41:k:115:MET:HE1	1.96	0.47
42:l:483:LEU:HD22	42:l:488:ILE:HD11	1.95	0.47
2:1:567:HIS:ND1	2:1:575:GLN:OE1	2.46	0.47
8:7:383:ILE:HD11	8:7:527:LEU:HB3	1.96	0.47
9:A:455:MET:HE1	10:B:1134:GLU:HB3	1.95	0.47
10:B:770:GLN:HE22	10:B:1093:GLN:HE22	1.61	0.47
10:B:951:GLN:HE21	20:L:57:LEU:HD22	1.79	0.47
16:H:80:ARG:HG2	19:K:57:LEU:HD22	1.97	0.47
27:U:243:LEU:O	27:U:268:THR:HB	2.14	0.47
5:4:22:SER:OG	5:4:171:SER:O	2.32	0.47
5:4:77:ALA:HB2	5:4:86:LEU:HD11	1.96	0.47
5:4:305:CYS:HB2	5:4:312:PHE:CZ	2.50	0.47
7:6:399:ARG:NH1	7:6:433:LYS:O	2.48	0.47
14:F:65:ARG:HD3	14:F:72:LYS:HA	1.96	0.47
25:R:64:SER:O	25:R:217:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:148:LEU:HA	30:X:151:LEU:HD23	1.96	0.47
34:d:99:LEU:HD12	34:d:102:LEU:HD23	1.97	0.47
40:j:88:GLU:HA	40:j:91:THR:HG22	1.95	0.47
41:k:15:LEU:O	41:k:19:GLN:HG2	2.15	0.47
9:A:1128:GLN:HE22	9:A:1132:LYS:HE2	1.79	0.47
23:O:172:LEU:HD13	23:O:208:VAL:HG12	1.96	0.47
25:R:291:SER:HB2	25:R:325:PRO:HD3	1.97	0.47
2:1:491:PRO:HB2	2:1:496:SER:HB3	1.97	0.47
32:b:135:VAL:HG13	34:d:274:ILE:HD11	1.97	0.47
46:p:50:GLU:O	46:p:68:ASN:ND2	2.48	0.47
2:1:469:MET:HE3	5:4:140:ILE:HD11	1.97	0.47
5:4:293:LEU:HD12	7:6:383:LEU:HD11	1.97	0.47
10:B:69:LEU:HD21	10:B:429:PHE:HB2	1.97	0.47
11:C:262:LEU:HD22	19:K:87:LEU:HD23	1.96	0.47
1:0:440:LEU:HD23	1:0:641:PHE:HB2	1.96	0.46
9:A:219:PHE:HB2	9:A:224:PHE:HB2	1.96	0.46
9:A:667:GLY:HA2	9:A:670:ILE:HD12	1.96	0.46
10:B:486:TYR:HB3	10:B:1096:ARG:NH2	2.30	0.46
10:B:839:MET:HE1	10:B:980:PHE:HB2	1.96	0.46
33:c:16:ILE:HD11	33:c:65:GLN:HG3	1.97	0.46
34:d:593:ASP:HB3	34:d:596:ILE:HG22	1.96	0.46
3:2:349:SER:O	3:2:373:MET:HA	2.15	0.46
9:A:1146:VAL:HG12	9:A:1197:LEU:HD22	1.97	0.46
10:B:234:ILE:HD13	10:B:257:LYS:HD2	1.96	0.46
29:W:269:ASP:OD1	29:W:269:ASP:N	2.42	0.46
34:d:348:TYR:CZ	34:d:350:HIS:HB2	2.51	0.46
7:6:154:ILE:HG23	7:6:193:ILE:HD12	1.97	0.46
10:B:557:PHE:CZ	10:B:603:LEU:HD11	2.51	0.46
28:V:40:VAL:HA	28:V:43:THR:HG22	1.97	0.46
36:f:142:LEU:HD21	36:f:152:LEU:HD22	1.97	0.46
38:h:134:VAL:HG11	44:n:112:ILE:HG13	1.96	0.46
5:4:109:ILE:HG21	5:4:126:VAL:HG11	1.97	0.46
8:7:341:TYR:OH	8:7:346:ASP:OD2	2.32	0.46
9:A:1428:VAL:HG13	10:B:1151:LEU:HD13	1.97	0.46
12:D:144:THR:HG21	15:G:46:LEU:HD22	1.98	0.46
18:J:7:CYS:HA	18:J:49:MET:HG3	1.97	0.46
19:K:24:ASP:OD2	19:K:74:ARG:NE	2.44	0.46
29:W:17:VAL:HB	29:W:29:LEU:HD23	1.97	0.46
39:i:76:TYR:HB2	45:o:24:GLU:HG2	1.97	0.46
24:Q:120:LYS:HG3	25:R:132:GLU:HG2	1.98	0.46
28:V:79:ILE:HG12	28:V:112:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:185:ASP:OD1	30:X:185:ASP:N	2.44	0.46
34:d:469:LEU:HD23	34:d:472:GLU:HB2	1.97	0.46
5:4:110:ILE:HD11	5:4:126:VAL:HG21	1.96	0.46
7:6:451:CYS:HB3	7:6:454:CYS:HB2	1.97	0.46
9:A:974:ASP:OD1	9:A:974:ASP:N	2.47	0.46
29:W:65:ARG:HG2	29:W:93:HIS:CE1	2.51	0.46
29:W:92:PRO:HG3	29:W:196:GLU:HA	1.97	0.46
42:l:279:THR:HB	42:l:285:GLU:HG3	1.96	0.46
46:p:215:ILE:HD13	46:p:256:MET:HE2	1.98	0.46
9:A:960:ILE:O	9:A:964:ILE:HG12	2.16	0.46
9:A:1582:PRO:HG3	45:o:44:THR:HB	1.96	0.46
17:I:22:ASN:HB2	17:I:24:ARG:HH11	1.80	0.46
1:0:39:ILE:O	1:0:480:GLN:HA	2.16	0.46
3:2:488:LYS:HG3	3:2:490:LYS:HE2	1.98	0.46
7:6:127:ILE:HB	7:6:232:VAL:HG22	1.97	0.46
7:6:234:ILE:HB	7:6:263:VAL:HG22	1.98	0.46
9:A:251:SER:OG	9:A:257:ARG:NH1	2.47	0.46
34:d:389:LEU:HD13	34:d:442:MET:HE2	1.98	0.46
42:l:657:LYS:HE2	42:l:668:LYS:HD3	1.98	0.46
46:p:187:LYS:HE3	46:p:189:ARG:NH1	2.31	0.46
1:0:133:CYS:O	1:0:137:THR:OG1	2.32	0.46
1:0:534:PRO:HB3	7:6:239:LEU:HD22	1.98	0.46
3:2:358:ALA:O	3:2:361:SER:OG	2.31	0.46
4:3:19:ASP:O	4:3:23:SER:OG	2.30	0.46
7:6:122:ILE:HD12	7:6:379:SER:HB3	1.98	0.46
9:A:261:ASP:OD1	9:A:316:GLN:NE2	2.48	0.46
10:B:193:LYS:HB3	10:B:787:VAL:HG21	1.98	0.46
10:B:357:GLN:O	10:B:374:LYS:NZ	2.49	0.46
11:C:75:MET:O	11:C:246:ARG:NH2	2.44	0.46
29:W:60:ARG:NH2	29:W:64:ASP:OD2	2.49	0.46
33:c:34:PHE:HA	33:c:37:LEU:HG	1.97	0.46
35:e:178:ARG:NH1	35:e:269:ASN:OD1	2.47	0.46
38:h:103:ASP:HA	38:h:106:GLU:HG3	1.97	0.46
8:7:756:ARG:HH12	29:W:306:ARG:HD2	1.81	0.46
9:A:470:LEU:HD12	9:A:474:VAL:HG13	1.97	0.46
9:A:1371:LEU:O	9:A:1375:MET:HG3	2.16	0.46
9:A:1442:ASP:HB2	14:F:135:ARG:HB3	1.98	0.46
21:M:117:ASN:O	21:M:121:LYS:NZ	2.45	0.46
23:O:206:ILE:HD13	23:O:212:ILE:HG23	1.97	0.46
29:W:120:ASN:OD1	29:W:121:GLY:N	2.49	0.46
29:W:124:CYS:HB3	29:W:127:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:16:ILE:O	37:g:20:LYS:HB2	2.15	0.46
40:j:70:PHE:HA	40:j:73:LEU:HG	1.96	0.46
44:n:11:CYS:HB3	44:n:73:ILE:HG12	1.98	0.46
1:0:241:ASP:OD2	1:0:660:ARG:NH1	2.47	0.45
1:0:271:ILE:HG13	1:0:388:LEU:HD21	1.98	0.45
9:A:726:ARG:HD3	9:A:766:GLY:HA3	1.98	0.45
9:A:871:ASP:HB3	13:E:205:SER:HB3	1.98	0.45
10:B:38:PHE:HZ	10:B:541:LEU:HB3	1.81	0.45
10:B:121:ASN:HA	10:B:207:GLY:HA3	1.98	0.45
10:B:667:GLN:NE2	10:B:675:ASP:OD1	2.42	0.45
10:B:1002:THR:HG22	10:B:1072:MET:HG2	1.98	0.45
11:C:217:ASP:OD1	11:C:217:ASP:N	2.47	0.45
35:e:178:ARG:NH1	35:e:272:GLU:OE1	2.43	0.45
39:i:31:LEU:HD22	39:i:65:LEU:HD23	1.99	0.45
39:i:165:TYR:HD2	44:n:5:LEU:HD11	1.80	0.45
41:k:95:ILE:HD11	43:m:62:LYS:HA	1.98	0.45
42:l:143:LYS:NZ	43:m:81:ARG:HH21	2.14	0.45
3:2:29:PRO:HB3	3:2:111:ALA:HB2	1.98	0.45
3:2:458:LEU:HD22	6:5:41:LEU:HD11	1.99	0.45
7:6:99:VAL:HA	7:6:102:ILE:HG22	1.98	0.45
8:7:382:GLY:HA3	8:7:535:LEU:HG	1.97	0.45
10:B:757:PRO:HG2	10:B:984:HIS:CE1	2.51	0.45
15:G:95:SER:O	15:G:130:TYR:OH	2.27	0.45
29:W:41:ASP:HA	29:W:44:LYS:HE3	1.97	0.45
36:f:86:ASP:OD1	36:f:86:ASP:N	2.46	0.45
1:0:90:MET:HE2	1:0:103:PHE:CG	2.51	0.45
1:0:104:ARG:N	1:0:204:ASN:OD1	2.48	0.45
5:4:115:TYR:O	5:4:119:ARG:HB2	2.15	0.45
5:4:296:LEU:HD12	7:6:319:LEU:HD11	1.99	0.45
9:A:605:MET:HE3	9:A:621:THR:HG21	1.98	0.45
17:I:29:CYS:SG	17:I:31:THR:OG1	2.70	0.45
23:O:161:VAL:HA	23:O:214:LEU:O	2.16	0.45
36:f:49:LEU:HD12	36:f:55:LYS:HE3	1.97	0.45
2:1:486:LEU:HD12	5:4:59:VAL:HG23	1.97	0.45
3:2:207:TYR:HA	3:2:210:MET:HG2	1.99	0.45
5:4:91:THR:HA	5:4:94:LEU:HD12	1.97	0.45
9:A:846:GLU:OE2	9:A:1425:SER:OG	2.33	0.45
11:C:44:LEU:HB2	11:C:77:ILE:HD13	1.99	0.45
12:D:160:VAL:O	12:D:164:ILE:HD12	2.17	0.45
13:E:79:TRP:HD1	13:E:96:PHE:HE1	1.64	0.45
43:m:116:TRP:HA	43:m:119:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:439:ASN:OD1	9:A:459:ARG:NH1	2.50	0.45
14:F:25:ASP:O	14:F:28:THR:OG1	2.32	0.45
17:I:17:ARG:HB3	17:I:26:LEU:HB2	1.97	0.45
18:J:41:LEU:HD22	18:J:46:CYS:HB3	1.99	0.45
23:O:142:ILE:O	23:O:146:ILE:HG12	2.17	0.45
24:Q:388:PRO:HB3	25:R:82:ARG:HG2	1.98	0.45
31:a:87:ASP:OD1	31:a:87:ASP:N	2.45	0.45
41:k:36:ILE:HG21	42:l:131:LEU:HB2	1.99	0.45
2:1:295:LYS:NZ	2:1:318:ASP:OD2	2.35	0.45
5:4:220:GLU:OE1	5:4:225:GLN:NE2	2.38	0.45
10:B:298:LEU:HD22	10:B:314:LEU:HD13	1.99	0.45
23:O:103:ILE:HD13	26:T:57:DT:H5'	1.99	0.45
24:Q:25:ASP:OD1	24:Q:25:ASP:N	2.49	0.45
32:b:87:GLN:NE2	32:b:91:ASP:OD2	2.49	0.45
35:e:32:LEU:HD13	36:f:93:PHE:HE1	1.82	0.45
41:k:106:ARG:HH22	44:n:44:ASP:CG	2.24	0.45
1:0:288:LYS:HG2	1:0:293:LEU:HD12	1.99	0.45
4:3:10:LYS:HE2	4:3:10:LYS:HB2	1.86	0.45
8:7:584:ASN:ND2	8:7:710:SER:OG	2.49	0.45
9:A:1143:LEU:HD11	9:A:1216:ILE:HD11	1.98	0.45
9:A:1340:GLY:HA2	13:E:183:PRO:HD2	1.97	0.45
10:B:416:LEU:HD23	10:B:457:LEU:HD23	1.97	0.45
14:F:118:LEU:HG	14:F:122:MET:HE3	1.99	0.45
28:V:11:ARG:HA	28:V:16:GLY:HA3	1.99	0.45
31:a:10:GLN:OE1	31:a:159:ASN:ND2	2.42	0.45
35:e:23:LEU:HD23	35:e:26:ILE:HD12	1.99	0.45
41:k:154:SER:OG	43:m:29:ASN:ND2	2.50	0.45
45:o:30:ILE:HD11	45:o:82:LEU:HD22	1.99	0.45
46:p:215:ILE:HD11	46:p:254:LEU:HD23	1.98	0.45
13:E:86:PRO:HA	13:E:113:GLN:HB2	1.99	0.45
23:O:211:LYS:HD2	26:T:61:DT:H5''	1.98	0.45
1:0:251:ASP:OD2	1:0:436:ARG:NH1	2.50	0.45
8:7:408:ILE:O	8:7:485:ILE:HA	2.16	0.45
9:A:35:ILE:HG21	9:A:53:LEU:HD23	1.99	0.45
25:R:279:LYS:HB3	25:R:282:ARG:HB3	1.99	0.45
25:R:352:ARG:HB2	25:R:355:TYR:HD2	1.82	0.45
36:f:6:VAL:HG22	36:f:203:GLN:HB3	1.98	0.45
42:l:256:LYS:HG3	42:l:260:MET:HE2	1.98	0.45
9:A:1441:PHE:O	14:F:92:ARG:NH1	2.50	0.45
10:B:521:LEU:HD22	10:B:633:VAL:HG12	1.99	0.45
24:Q:354:ASP:CG	24:Q:359:ASN:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:311:LYS:O	34:d:315:SER:HB3	2.17	0.45
42:l:296:PRO:HG2	42:l:357:LEU:HD23	1.98	0.45
1:0:641:PHE:O	1:0:645:ASN:HB2	2.16	0.44
2:1:180:LEU:HD21	2:1:221:ALA:HB2	1.99	0.44
2:1:415:GLU:HA	2:1:418:GLU:HG2	1.98	0.44
5:4:150:ALA:HB1	5:4:195:PRO:HB2	1.98	0.44
9:A:332:LYS:HE3	14:F:23:PHE:HB2	1.99	0.44
10:B:71:LEU:HD13	10:B:429:PHE:HE1	1.82	0.44
29:W:47:LEU:HD23	29:W:49:ILE:HD12	1.99	0.44
45:o:36:ILE:HD11	45:o:118:MET:HB3	1.98	0.44
1:0:195:ILE:O	1:0:199:MET:HG2	2.17	0.44
1:0:197:ARG:HH22	1:0:212:TYR:HE1	1.65	0.44
2:1:486:LEU:HD13	5:4:55:GLU:HB2	1.98	0.44
3:2:418:LYS:HA	3:2:421:GLU:HG2	1.99	0.44
9:A:15:LYS:HB3	10:B:1220:ARG:HE	1.82	0.44
9:A:1151:GLU:HG2	17:I:45:ARG:HD3	1.98	0.44
27:U:245:LEU:HD13	28:V:114:VAL:HB	1.99	0.44
34:d:264:PRO:HB2	34:d:269:TYR:CE1	2.53	0.44
35:e:5:LEU:HD13	35:e:182:MET:HG2	1.99	0.44
35:e:207:LEU:HA	36:f:116:TRP:HE1	1.81	0.44
42:l:180:ILE:HG12	44:n:23:LEU:HB3	2.00	0.44
2:1:381:LEU:HG	2:1:385:MET:HE3	1.98	0.44
7:6:337:SER:OG	7:6:365:CYS:SG	2.68	0.44
7:6:418:ASN:HA	7:6:420:LYS:HE3	1.98	0.44
10:B:617:ARG:NH2	17:I:61:ASP:OD2	2.41	0.44
11:C:22:LEU:HG	11:C:25:VAL:HG11	1.98	0.44
21:M:269:ILE:HG13	21:M:272:LYS:HG3	1.99	0.44
27:U:13:ILE:HD12	28:V:48:VAL:HG22	1.99	0.44
30:X:155:LYS:NZ	30:X:156:ASP:O	2.44	0.44
46:p:54:LEU:O	46:p:64:ASP:HA	2.17	0.44
2:1:482:ASN:OD1	2:1:483:LYS:N	2.49	0.44
3:2:197:ASN:OD1	3:2:198:SER:N	2.48	0.44
8:7:627:ILE:HG23	8:7:636:ARG:HG2	2.00	0.44
43:m:117:ARG:HD3	43:m:120:LEU:HD12	1.98	0.44
46:p:73:ARG:HH22	46:p:108:LEU:HB3	1.82	0.44
2:1:222:LEU:HD13	7:6:216:MET:HA	1.99	0.44
3:2:191:PHE:CZ	3:2:199:GLN:HB3	2.53	0.44
3:2:221:VAL:HG22	3:2:249:MET:HE1	2.00	0.44
8:7:585:PRO:HG3	8:7:756:ARG:HG2	1.99	0.44
9:A:365:GLY:HA3	9:A:469:ARG:HB2	1.99	0.44
9:A:1576:SER:HB3	34:d:216:ASN:HD21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:869:SER:HB2	21:M:224:LYS:HD3	2.00	0.44
11:C:6:PRO:HB2	19:K:101:LEU:HD13	1.99	0.44
11:C:48:SER:OG	20:L:66:GLN:OE1	2.35	0.44
15:G:119:LEU:HD11	15:G:137:ILE:HD12	1.99	0.44
31:a:21:GLY:O	31:a:26:ASN:ND2	2.46	0.44
42:l:104:MET:HE1	43:m:128:PHE:CE1	2.52	0.44
1:0:71:TYR:HB3	1:0:207:ILE:HG12	1.99	0.44
1:0:299:LEU:HG	1:0:305:PRO:HG3	1.99	0.44
2:1:57:LYS:HA	2:1:57:LYS:HD2	1.87	0.44
5:4:79:TYR:HB3	5:4:132:LEU:HD21	1.99	0.44
6:5:31:VAL:HG21	6:5:40:LEU:HD12	2.00	0.44
9:A:348:SER:HA	9:A:489:LEU:O	2.18	0.44
32:b:25:PHE:HE1	32:b:98:LEU:CD1	2.30	0.44
34:d:512:LEU:HA	34:d:515:ILE:HD12	1.98	0.44
41:k:11:LEU:O	41:k:15:LEU:HG	2.18	0.44
10:B:420:LEU:HB3	10:B:453:ILE:HD13	1.98	0.44
18:J:67:GLU:OE2	20:L:37:LYS:NZ	2.46	0.44
19:K:16:GLU:OE2	19:K:37:LYS:NZ	2.48	0.44
35:e:230:LEU:HD21	35:e:253:LEU:HD11	1.99	0.44
40:j:11:ILE:HA	40:j:14:ILE:HG22	1.99	0.44
1:0:43:PRO:HD3	1:0:483:TYR:HB2	1.99	0.44
7:6:325:PRO:HG3	7:6:370:LEU:HB3	2.00	0.44
9:A:420:ARG:O	35:e:299:ARG:NH1	2.48	0.44
23:O:193:LEU:HB3	23:O:206:ILE:HB	2.00	0.44
34:d:393:ILE:HG21	34:d:497:ASN:HD22	1.83	0.44
38:h:125:LEU:HD22	44:n:119:LEU:HD13	2.00	0.44
41:k:28:SER:OG	41:k:56:ASN:ND2	2.51	0.44
1:0:565:LYS:HD2	1:0:565:LYS:HA	1.83	0.44
8:7:393:THR:HG21	8:7:423:GLN:HG3	1.99	0.44
10:B:98:THR:HG22	25:R:255:LEU:HD12	1.99	0.44
10:B:119:LEU:HD13	10:B:953:LEU:HD11	2.00	0.44
10:B:199:MET:SD	10:B:199:MET:N	2.85	0.44
13:E:80:VAL:HG22	13:E:109:ILE:HB	2.00	0.44
19:K:33:ILE:HD13	19:K:87:LEU:HD22	1.98	0.44
39:i:153:THR:O	39:i:157:ASN:ND2	2.41	0.44
40:j:67:PRO:HA	40:j:70:PHE:CE2	2.53	0.44
1:0:561:ASP:OD2	2:1:297:ARG:NH2	2.50	0.43
8:7:385:VAL:HA	8:7:514:THR:O	2.18	0.43
9:A:355:GLY:O	9:A:469:ARG:NH1	2.51	0.43
11:C:35:ARG:NE	19:K:41:THR:OG1	2.37	0.43
29:W:177:ASP:HA	29:W:180:GLN:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:172:GLU:OE2	44:n:90:GLN:NE2	2.45	0.43
42:l:583:ASP:OD1	42:l:583:ASP:N	2.50	0.43
45:o:50:LYS:HG3	45:o:99:LEU:HD23	1.99	0.43
9:A:469:ARG:HH21	10:B:976:ILE:HD13	1.83	0.43
10:B:590:HIS:CD2	10:B:596:LEU:HD22	2.53	0.43
11:C:38:ILE:HG13	11:C:176:ILE:HD12	2.00	0.43
11:C:234:SER:HB2	11:C:240:VAL:HB	1.99	0.43
12:D:40:HIS:CE1	15:G:6:ASP:HB3	2.53	0.43
21:M:44:VAL:HG12	21:M:51:VAL:HG22	2.00	0.43
23:O:221:GLU:O	23:O:225:GLN:NE2	2.46	0.43
34:d:519:THR:HG23	34:d:530:LEU:HD22	2.00	0.43
42:l:652:GLU:OE1	42:l:677:THR:OG1	2.32	0.43
3:2:59:LEU:HD12	3:2:96:LEU:HD22	2.00	0.43
9:A:1202:MET:HE1	9:A:1212:VAL:HG21	2.00	0.43
9:A:1572:PRO:HA	34:d:242:SER:HA	2.01	0.43
10:B:205:ILE:HG13	10:B:461:LEU:HB3	1.99	0.43
28:V:8:GLU:HB2	28:V:11:ARG:HH12	1.84	0.43
28:V:68:THR:HB	28:V:79:ILE:HB	2.01	0.43
42:l:115:VAL:HG22	43:m:137:LEU:HD21	1.99	0.43
42:l:460:ILE:HB	42:l:464:ILE:HD13	2.00	0.43
8:7:487:LEU:HD13	8:7:531:ILE:HD12	2.01	0.43
8:7:495:ALA:HB3	8:7:498:PHE:HB2	2.00	0.43
9:A:568:PRO:HB2	11:C:221:TYR:CZ	2.54	0.43
9:A:1166:ASP:HB2	9:A:1169:ILE:HD12	1.98	0.43
10:B:195:CYS:HB3	10:B:198:ASP:HB2	2.00	0.43
25:R:122:LEU:HD12	25:R:122:LEU:HA	1.90	0.43
34:d:248:VAL:HG12	34:d:249:VAL:HG13	2.00	0.43
38:h:40:VAL:HA	40:j:116:SER:HA	2.01	0.43
3:2:161:GLU:HA	3:2:164:LEU:HB2	2.00	0.43
8:7:671:ILE:HG23	8:7:708:LEU:HD13	2.01	0.43
11:C:71:PRO:HG3	18:J:13:VAL:HG21	2.00	0.43
11:C:226:ASP:N	11:C:226:ASP:OD1	2.52	0.43
34:d:230:SER:HA	34:d:234:GLU:H	1.83	0.43
46:p:192:LEU:HD23	46:p:193:ASN:HB2	1.99	0.43
7:6:355:LYS:HE3	7:6:355:LYS:HB2	1.87	0.43
7:6:389:PHE:HB3	7:6:427:TYR:HB3	2.00	0.43
29:W:17:VAL:HA	29:W:21:TYR:HD1	1.83	0.43
30:X:228:SER:OG	30:X:247:ASN:ND2	2.51	0.43
42:l:127:LYS:NZ	43:m:148:SER:O	2.49	0.43
44:n:34:ARG:HH11	44:n:39:GLU:HG3	1.84	0.43
4:3:35:TYR:OH	4:3:83:ASP:OD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:335:ARG:NH2	10:B:1114:LEU:HD21	2.34	0.43
9:A:353:ILE:HG22	9:A:468:PHE:HB2	2.00	0.43
9:A:1155:ASP:HB2	9:A:1241:ARG:HH12	1.83	0.43
13:E:25:ASP:OD2	13:E:187:TYR:OH	2.30	0.43
24:Q:140:HIS:CE1	24:Q:142:LYS:HB3	2.54	0.43
32:b:51:ARG:NH1	34:d:215:MET:HE1	2.34	0.43
32:b:139:LEU:HG	32:b:140:LEU:HD12	2.00	0.43
43:m:122:ASN:HA	43:m:125:ILE:HD12	2.01	0.43
46:p:94:ARG:HD3	46:p:192:LEU:HA	2.00	0.43
1:0:74:ARG:NH1	1:0:664:GLN:OE1	2.52	0.43
5:4:27:THR:HB	5:4:176:LEU:HD23	2.01	0.43
8:7:327:LYS:HG2	8:7:337:VAL:HG11	2.00	0.43
8:7:589:GLN:HB3	8:7:742:MET:HE1	2.01	0.43
31:a:173:ARG:NH2	32:b:112:THR:O	2.52	0.43
37:g:20:LYS:HD2	37:g:61:GLN:HG3	2.00	0.43
39:i:100:LEU:HB3	43:m:15:TYR:CZ	2.54	0.43
40:j:66:ILE:HA	40:j:69:ILE:HG12	2.00	0.43
43:m:79:PRO:HA	43:m:83:ASN:HD21	1.83	0.43
44:n:77:ILE:HA	44:n:80:LEU:HG	2.01	0.43
1:0:208:TYR:HE1	1:0:213:LEU:HB2	1.84	0.43
9:A:944:ARG:NH2	9:A:1296:GLY:O	2.44	0.43
11:C:14:SER:OG	11:C:15:LYS:N	2.52	0.43
35:e:279:LYS:O	35:e:283:GLN:HG3	2.19	0.43
46:p:73:ARG:NH2	46:p:108:LEU:HB3	2.33	0.43
1:0:571:VAL:HG22	1:0:599:LEU:HD12	2.01	0.43
9:A:483:ASP:HB2	10:B:987:LYS:HE3	2.01	0.43
9:A:905:ASP:OD1	9:A:905:ASP:N	2.49	0.43
9:A:1208:THR:HG23	9:A:1211:GLN:H	1.84	0.43
12:D:56:ARG:HB2	12:D:148:LEU:HB3	2.01	0.43
15:G:107:LYS:NZ	29:W:144:ARG:HH21	2.17	0.43
15:G:112:LYS:HA	15:G:115:MET:HE1	2.01	0.43
16:H:8:ASP:OD1	16:H:9:ILE:N	2.47	0.43
25:R:296:LYS:HA	25:R:299:ILE:HG22	2.01	0.43
29:W:54:LEU:HA	29:W:57:LEU:HD12	2.01	0.43
30:X:214:TRP:HD1	30:X:215:PRO:HD2	1.84	0.43
31:a:6:LEU:HD21	31:a:36:PHE:HA	2.01	0.43
31:a:32:ALA:HA	31:a:37:PHE:CG	2.54	0.43
38:h:40:VAL:HG23	38:h:43:TYR:HB2	2.01	0.43
1:0:73:SER:OG	1:0:78:GLU:OE1	2.37	0.42
2:1:9:PHE:HB3	2:1:29:TRP:CE2	2.54	0.42
9:A:66:LYS:HG3	21:M:20:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:981:LEU:HD11	9:A:1042:PHE:HB2	2.00	0.42
10:B:84:ILE:HA	10:B:139:ALA:O	2.19	0.42
10:B:600:LEU:HB3	10:B:615:MET:SD	2.59	0.42
12:D:172:LEU:HD13	12:D:202:ILE:HD11	2.01	0.42
25:R:68:VAL:HG11	25:R:134:VAL:HG21	2.00	0.42
32:b:122:VAL:O	32:b:126:MET:HG3	2.18	0.42
35:e:20:ILE:HD13	35:e:20:ILE:HA	1.92	0.42
42:l:251:LEU:HD11	44:n:126:ILE:HD11	2.00	0.42
46:p:63:ILE:HG22	46:p:79:LEU:HD22	2.00	0.42
8:7:201:SER:OG	8:7:203:VAL:O	2.30	0.42
8:7:341:TYR:HB3	8:7:379:ALA:HB3	2.01	0.42
9:A:484:GLY:HA3	10:B:979:LYS:HE2	2.00	0.42
28:V:32:ILE:HG13	28:V:36:LEU:HD23	2.01	0.42
28:V:78:PHE:O	28:V:112:ARG:HA	2.19	0.42
32:b:33:LEU:HD21	34:d:228:LEU:HB3	2.01	0.42
32:b:126:MET:HA	32:b:129:VAL:HG22	2.01	0.42
34:d:19:LEU:HD21	44:n:94:ILE:HG23	2.00	0.42
37:g:13:THR:HA	37:g:16:ILE:HG22	2.00	0.42
40:j:73:LEU:HD13	46:p:11:LEU:HB2	2.01	0.42
41:k:74:LEU:HB3	42:l:93:ALA:HB2	2.00	0.42
9:A:483:ASP:HA	10:B:988:GLY:HA2	2.01	0.42
9:A:1596:PRO:HG2	39:i:77:ARG:HD2	2.01	0.42
10:B:570:VAL:HB	10:B:573:GLN:HG2	2.01	0.42
10:B:766:ARG:NH2	10:B:1020:ARG:HG2	2.34	0.42
12:D:69:ALA:HA	12:D:72:ARG:HG2	2.01	0.42
23:O:73:THR:HG22	23:O:122:VAL:HG22	1.99	0.42
23:O:205:LEU:HB2	23:O:213:VAL:HB	2.00	0.42
25:R:333:LEU:O	25:R:337:ALA:HB3	2.19	0.42
33:c:66:LEU:HD23	37:g:10:LEU:HD13	2.00	0.42
39:i:185:LYS:O	39:i:189:ILE:HG12	2.20	0.42
2:1:489:VAL:HG12	5:4:55:GLU:HG3	2.01	0.42
3:2:34:ALA:O	3:2:38:ILE:HG12	2.18	0.42
4:3:12:MET:HE1	4:3:17:LYS:HD3	2.01	0.42
8:7:339:GLU:OE2	8:7:510:LYS:NZ	2.37	0.42
9:A:1442:ASP:OD2	14:F:137:TYR:OH	2.37	0.42
10:B:310:MET:HE3	10:B:310:MET:HB2	1.94	0.42
14:F:136:ARG:HD2	14:F:146:TRP:CD1	2.55	0.42
17:I:15:TYR:HB3	24:Q:422:ARG:HD3	2.02	0.42
20:L:47:ARG:HE	20:L:47:ARG:HB3	1.73	0.42
22:N:-57:DA:H5'	23:O:158:GLN:HG2	2.02	0.42
34:d:250:LYS:O	34:d:253:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:147:LYS:HD2	39:i:147:LYS:HA	1.78	0.42
1:0:540:PHE:HB2	1:0:622:MET:SD	2.59	0.42
7:6:129:THR:HA	7:6:172:ILE:O	2.19	0.42
8:7:758:GLU:O	8:7:762:GLU:HG3	2.19	0.42
9:A:569:LYS:HB3	16:H:46:LEU:HD21	2.02	0.42
16:H:40:LEU:HD21	16:H:144:ILE:HD11	2.02	0.42
29:W:198:THR:OG1	29:W:199:PHE:N	2.52	0.42
39:i:206:ILE:HA	39:i:209:THR:HG22	2.02	0.42
42:l:475:HIS:HA	42:l:478:ILE:HG22	2.01	0.42
45:o:78:CYS:SG	45:o:79:LEU:N	2.92	0.42
46:p:30:ASN:OD1	46:p:33:ARG:NH2	2.50	0.42
46:p:33:ARG:O	46:p:37:THR:HG23	2.20	0.42
46:p:89:ASP:OD1	46:p:89:ASP:N	2.47	0.42
3:2:47:ILE:O	3:2:51:VAL:HG23	2.20	0.42
9:A:265:LYS:HA	9:A:265:LYS:HD2	1.81	0.42
9:A:356:ASP:OD2	19:K:65:HIS:NE2	2.50	0.42
9:A:1611:SER:OG	42:l:192:ASN:OD1	2.37	0.42
16:H:109:LYS:O	40:j:83:LEU:N	2.53	0.42
17:I:78:CYS:SG	17:I:106:CYS:HB3	2.59	0.42
21:M:320:ARG:HB3	21:M:336:LEU:HD12	2.01	0.42
37:g:73:LEU:HD23	37:g:73:LEU:HA	1.88	0.42
1:0:100:GLN:NE2	1:0:173:LYS:O	2.53	0.42
1:0:258:ARG:NH1	1:0:262:ARG:HH21	2.17	0.42
1:0:487:LEU:HD13	1:0:491:SER:H	1.85	0.42
3:2:42:LEU:HD23	5:4:258:LEU:HD12	2.00	0.42
8:7:181:TYR:CZ	8:7:336:PRO:HG3	2.55	0.42
9:A:843:LYS:HD3	9:A:843:LYS:HA	1.89	0.42
10:B:1000:PRO:HB2	10:B:1072:MET:HE2	2.01	0.42
45:o:50:LYS:HG2	45:o:99:LEU:HA	2.00	0.42
1:0:30:LYS:HE2	1:0:30:LYS:HB3	1.88	0.42
2:1:559:GLU:OE2	2:1:563:HIS:NE2	2.52	0.42
8:7:143:LEU:HD22	8:7:157:LEU:HD12	2.01	0.42
10:B:21:GLU:HG3	10:B:656:GLY:HA3	2.01	0.42
29:W:106:VAL:HG22	29:W:176:MET:HE1	2.01	0.42
32:b:113:LEU:HD12	32:b:113:LEU:HA	1.91	0.42
41:k:104:ILE:HD13	42:l:166:LEU:HD13	2.01	0.42
42:l:304:LEU:HD12	42:l:306:PHE:CE1	2.55	0.42
42:l:506:THR:OG1	42:l:509:SER:OG	2.33	0.42
1:0:506:ILE:HD12	1:0:522:TYR:HE1	1.85	0.42
5:4:175:ARG:HD2	5:4:259:ARG:HH21	1.84	0.42
8:7:411:CYS:HG	8:7:420:TRP:CD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:968:GLN:HA	9:A:973:ILE:HG12	2.02	0.42
10:B:281:PRO:HD2	10:B:284:ILE:HD12	2.01	0.42
10:B:1001:PHE:HE2	11:C:178:PHE:HB3	1.85	0.42
17:I:17:ARG:HB3	17:I:26:LEU:O	2.19	0.42
26:T:14:DT:H2'	26:T:15:DG:C8	2.54	0.42
32:b:33:LEU:HG	34:d:225:VAL:HG13	2.02	0.42
35:e:22:THR:O	35:e:25:THR:OG1	2.32	0.42
41:k:151:ASP:OD1	43:m:25:TYR:OH	2.35	0.42
42:l:143:LYS:HZ2	43:m:81:ARG:HH21	1.67	0.42
44:n:120:ARG:HA	44:n:123:ASP:HB2	2.01	0.42
46:p:176:ARG:NH1	46:p:186:PHE:O	2.53	0.42
1:0:53:LEU:HD22	1:0:86:LEU:HD13	2.01	0.42
3:2:263:HIS:ND1	3:2:264:SER:O	2.52	0.42
7:6:164:ASN:ND2	7:6:305:VAL:O	2.44	0.42
8:7:672:GLN:OE1	8:7:722:ARG:NH2	2.52	0.42
11:C:145:CYS:SG	11:C:146:LYS:N	2.92	0.42
21:M:215:ARG:NH2	21:M:226:ASP:OD2	2.53	0.42
23:O:74:VAL:HB	23:O:121:MET:HE2	2.02	0.42
25:R:263:MET:O	25:R:266:THR:OG1	2.33	0.42
28:V:67:ASP:N	28:V:79:ILE:O	2.48	0.42
31:a:203:LYS:HB2	31:a:203:LYS:HE3	1.81	0.42
39:i:166:ARG:NE	42:l:195:LEU:O	2.52	0.42
1:0:708:LEU:HA	1:0:712:MET:HE3	2.02	0.41
8:7:745:ILE:HG21	8:7:748:LEU:HD13	2.02	0.41
9:A:185:TRP:HZ3	9:A:200:ARG:HG2	1.84	0.41
9:A:993:LEU:O	9:A:997:LEU:HG	2.20	0.41
9:A:1002:GLY:O	9:A:1008:GLN:NE2	2.47	0.41
10:B:652:LYS:HE2	10:B:652:LYS:HB3	1.91	0.41
15:G:115:MET:HG3	15:G:163:ILE:HD11	2.02	0.41
25:R:73:LEU:HD22	25:R:77:LEU:HD23	2.02	0.41
38:h:128:LEU:HD12	44:n:115:LYS:HG3	2.02	0.41
39:i:92:LEU:HB2	39:i:99:GLN:HB2	2.00	0.41
2:1:597:PHE:HE1	2:1:616:LEU:HD12	1.84	0.41
4:3:27:LYS:O	4:3:37:ARG:NH1	2.53	0.41
9:A:172:PRO:HG2	9:A:174:ILE:HD11	2.02	0.41
9:A:614:PHE:HB3	16:H:122:LEU:HD21	2.01	0.41
9:A:1641:SER:OG	31:a:157:GLY:O	2.38	0.41
10:B:361:LEU:HD22	10:B:363:HIS:HE1	1.85	0.41
15:G:83:LYS:NZ	15:G:148:GLU:O	2.47	0.41
17:I:103:CYS:SG	17:I:105:SER:OG	2.71	0.41
5:4:28:VAL:HG22	5:4:177:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:326:VAL:O	5:4:328:ARG:NH2	2.53	0.41
7:6:214:LEU:HD22	7:6:254:LEU:HD11	2.02	0.41
7:6:411:PRO:HG2	7:6:413:LEU:HG	2.02	0.41
9:A:62:ASP:HB3	9:A:65:LEU:HD12	2.01	0.41
21:M:233:ALA:HA	21:M:274:PRO:HG3	2.01	0.41
29:W:41:ASP:OD1	29:W:41:ASP:N	2.52	0.41
31:a:172:SER:HB2	32:b:118:ASN:HB3	2.02	0.41
34:d:19:LEU:HB2	38:h:148:ILE:HG22	2.01	0.41
46:p:12:ASP:HA	46:p:15:ILE:HG12	2.01	0.41
4:3:60:ASP:OD1	4:3:60:ASP:N	2.51	0.41
9:A:399:HIS:CE1	9:A:462:VAL:HG21	2.56	0.41
13:E:90:VAL:HG13	13:E:123:LEU:HD21	2.02	0.41
21:M:167:SER:O	21:M:171:ILE:HG12	2.20	0.41
27:U:9:VAL:O	27:U:13:ILE:HG12	2.20	0.41
42:l:561:ILE:HA	42:l:564:VAL:HG12	2.02	0.41
44:n:4:ARG:HG2	44:n:81:PRO:HD3	2.01	0.41
45:o:43:LEU:HD12	45:o:110:ILE:HG13	2.02	0.41
1:0:71:TYR:O	1:0:207:ILE:HA	2.21	0.41
1:0:83:LEU:O	1:0:87:GLU:HG3	2.21	0.41
8:7:350:PRO:HB2	8:7:450:SER:HB3	2.02	0.41
8:7:578:MET:HA	8:7:581:TYR:CE2	2.55	0.41
9:A:781:ASP:HB2	9:A:789:LYS:HD3	2.03	0.41
10:B:936:ASP:OD1	10:B:938:SER:OG	2.33	0.41
15:G:49:LEU:N	15:G:75:ARG:O	2.52	0.41
15:G:57:GLN:OE1	15:G:57:GLN:N	2.54	0.41
34:d:227:LEU:HA	34:d:241:MET:HE2	2.02	0.41
43:m:42:ASP:OD1	43:m:43:ILE:N	2.53	0.41
44:n:23:LEU:HA	44:n:26:ILE:HG22	2.02	0.41
46:p:62:VAL:HB	46:p:80:VAL:HG23	2.03	0.41
9:A:844:ALA:HB2	9:A:1384:VAL:HG13	2.01	0.41
12:D:57:LEU:HD12	12:D:160:VAL:HG11	2.03	0.41
25:R:135:PHE:HB3	25:R:214:ILE:HD13	2.02	0.41
30:X:174:LYS:HG3	30:X:175:LYS:HG2	2.01	0.41
31:a:282:LYS:HA	31:a:285:VAL:HG12	2.03	0.41
34:d:100:GLU:HB3	42:l:291:VAL:HG11	2.01	0.41
5:4:108:LYS:HA	5:4:108:LYS:HD3	1.91	0.41
5:4:158:THR:OG1	7:6:405:SER:O	2.39	0.41
6:5:19:LEU:HG	8:7:566:TYR:HE2	1.86	0.41
9:A:741:ASN:HB3	9:A:744:LYS:HB3	2.03	0.41
10:B:862:GLN:HG2	10:B:963:PHE:HB2	2.02	0.41
12:D:151:PHE:HE1	15:G:142:ARG:HH11	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:132:LYS:HA	21:M:135:MET:HG3	2.03	0.41
24:Q:138:ARG:HG3	24:Q:140:HIS:HD2	1.85	0.41
31:a:83:PHE:O	31:a:91:ARG:NH2	2.53	0.41
32:b:204:PHE:CE2	35:e:246:ILE:HG13	2.56	0.41
33:c:32:PHE:HD1	34:d:288:LYS:HE2	1.86	0.41
35:e:43:PRO:HG3	35:e:61:PRO:HB3	2.02	0.41
3:2:362:LEU:HD23	3:2:391:ILE:HD11	2.03	0.41
7:6:166:ILE:HG23	7:6:369:MET:HE2	2.03	0.41
8:7:138:ASP:N	8:7:138:ASP:OD1	2.54	0.41
9:A:1572:PRO:HB2	9:A:1573:THR:H	1.54	0.41
10:B:347:LYS:HA	10:B:347:LYS:HD3	1.83	0.41
10:B:1124:ARG:NH2	21:M:58:ASP:OD2	2.52	0.41
11:C:66:ARG:O	11:C:70:ILE:HG12	2.21	0.41
15:G:115:MET:HG2	15:G:119:LEU:HD22	2.03	0.41
16:H:35:GLN:OE1	16:H:128:ASN:N	2.49	0.41
25:R:112:ASP:OD1	25:R:113:ASN:N	2.49	0.41
37:g:56:MET:O	37:g:60:ASN:HB3	2.21	0.41
39:i:126:LEU:HD23	44:n:15:MET:HE1	2.01	0.41
41:k:31:GLU:HG3	41:k:52:ASN:ND2	2.36	0.41
44:n:127:GLU:HA	44:n:130:VAL:HG22	2.02	0.41
1:0:116:LEU:HD21	1:0:182:LEU:HD22	2.03	0.41
1:0:162:LEU:HD21	1:0:190:LEU:HB3	2.03	0.41
1:0:438:THR:HG22	2:1:352:ASN:HD21	1.86	0.41
2:1:31:SER:OG	2:1:35:ASP:N	2.54	0.41
5:4:119:ARG:NH1	5:4:123:GLU:HB2	2.36	0.41
5:4:314:GLU:HA	5:4:317:ILE:HG12	2.03	0.41
7:6:450:ASN:HB2	7:6:455:GLU:OE2	2.21	0.41
7:6:450:ASN:N	7:6:450:ASN:OD1	2.53	0.41
8:7:468:HIS:CD2	13:E:91:LYS:HE3	2.55	0.41
8:7:591:CYS:HB3	8:7:622:MET:HE1	2.02	0.41
8:7:748:LEU:HD12	8:7:748:LEU:HA	1.94	0.41
9:A:443:LEU:HD13	9:A:501:LEU:HD11	2.01	0.41
9:A:1244:ARG:NH2	9:A:1249:ASP:OD2	2.53	0.41
9:A:1423:GLY:O	9:A:1427:ASN:ND2	2.50	0.41
10:B:383:ASN:O	10:B:387:LEU:HG	2.21	0.41
10:B:561:TRP:NE1	25:R:240:ARG:HD3	2.36	0.41
12:D:217:LEU:HD21	32:b:38:MET:HE2	2.01	0.41
13:E:19:VAL:HG11	13:E:80:VAL:HG11	2.03	0.41
15:G:81:PRO:HB3	15:G:106:MET:HE1	2.03	0.41
19:K:77:THR:OG1	19:K:81:TYR:O	2.36	0.41
21:M:280:VAL:HG11	21:M:312:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:204:LEU:HG	23:O:214:LEU:HG	2.03	0.41
25:R:122:LEU:HG	25:R:222:CYS:HB3	2.01	0.41
32:b:203:LYS:NZ	32:b:209:GLU:OE1	2.54	0.41
42:l:454:PRO:HB2	42:l:457:TYR:HE1	1.85	0.41
42:l:537:ALA:O	42:l:541:ASN:ND2	2.54	0.41
1:0:105:GLY:HA2	1:0:205:ILE:O	2.21	0.41
1:0:106:LEU:HB2	1:0:203:CYS:SG	2.61	0.41
2:1:257:LEU:HA	2:1:260:PHE:HD2	1.86	0.41
3:2:451:VAL:HG23	6:5:51:LYS:NZ	2.36	0.41
7:6:207:ASN:HD22	7:6:207:ASN:HA	1.61	0.41
10:B:428:ILE:HD11	10:B:448:ILE:HG12	2.03	0.41
10:B:825:VAL:HG22	10:B:1010:LEU:HB3	2.02	0.41
33:c:98:MET:SD	34:d:517:LYS:HE3	2.61	0.41
43:m:50:THR:HG22	43:m:56:LYS:HA	2.02	0.41
43:m:89:ILE:O	43:m:93:LEU:CB	2.66	0.41
1:0:486:THR:O	1:0:673:LYS:NZ	2.50	0.40
2:1:537:GLU:HB3	7:6:341:LYS:HB2	2.02	0.40
8:7:615:LEU:HD22	8:7:655:SER:HB3	2.03	0.40
9:A:94:GLY:HA3	9:A:1410:PHE:CE2	2.55	0.40
9:A:115:LEU:HD21	9:A:145:LYS:HE3	2.02	0.40
9:A:290:GLU:HA	9:A:293:GLU:HG2	2.02	0.40
37:g:22:ALA:O	37:g:26:ASN:HB2	2.21	0.40
42:l:195:LEU:HD12	42:l:195:LEU:HA	1.92	0.40
42:l:263:PRO:HG2	42:l:266:LEU:HD12	2.03	0.40
9:A:22:PHE:HZ	10:B:1208:MET:HE3	1.87	0.40
9:A:1144:LYS:HB2	9:A:1144:LYS:HE2	1.93	0.40
10:B:424:LEU:HD11	10:B:448:ILE:HG23	2.03	0.40
10:B:634:TYR:HA	10:B:694:ASP:HA	2.03	0.40
30:X:163:LEU:HD12	30:X:166:LEU:HD12	2.03	0.40
34:d:255:ASN:ND2	34:d:256:SER:H	2.20	0.40
34:d:562:ILE:HD13	34:d:619:ILE:HD11	2.03	0.40
36:f:59:SER:OG	36:f:105:ASP:OD1	2.24	0.40
37:g:20:LYS:HD2	37:g:61:GLN:HA	2.03	0.40
38:h:121:CYS:HB2	39:i:202:LYS:HE3	2.03	0.40
42:l:680:LEU:HA	42:l:683:ILE:HG22	2.03	0.40
1:0:643:ARG:HD3	1:0:650:GLU:HG2	2.04	0.40
10:B:911:ILE:HG13	10:B:912:ILE:HG13	2.04	0.40
13:E:83:CYS:O	13:E:113:GLN:NE2	2.55	0.40
22:N:-7:DA:H2'	22:N:-6:DA:C8	2.57	0.40
29:W:208:PRO:HA	29:W:209:PRO:HD3	1.88	0.40
34:d:437:PHE:CE1	34:d:512:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:61:ARG:HH11	2:1:86:ARG:HD2	1.87	0.40
8:7:458:SER:O	8:7:462:ASN:HB2	2.21	0.40
8:7:560:PRO:HG2	29:W:303:ALA:HB1	2.04	0.40
9:A:451:HIS:CE1	9:A:453:MET:HB2	2.57	0.40
25:R:313:TRP:O	25:R:349:TYR:N	2.49	0.40
29:W:37:VAL:HG22	29:W:206:LEU:HD13	2.04	0.40
31:a:41:SER:HA	31:a:113:THR:HG23	2.03	0.40
34:d:237:GLY:O	34:d:241:MET:HG3	2.22	0.40
34:d:316:ILE:HG21	34:d:322:ILE:HD11	2.03	0.40
34:d:389:LEU:H	34:d:389:LEU:HD23	1.86	0.40
36:f:152:LEU:HD21	36:f:204:TYR:CE2	2.56	0.40
39:i:197:LYS:HD3	39:i:197:LYS:HA	1.93	0.40
46:p:103:ILE:HD13	46:p:196:PHE:CE1	2.57	0.40
1:0:485:MET:HE3	1:0:485:MET:HB2	1.92	0.40
2:1:481:ILE:HD11	5:4:130:TYR:CE1	2.57	0.40
3:2:207:TYR:CE2	3:2:249:MET:HE2	2.56	0.40
9:A:563:PRO:HG3	9:A:572:TRP:CZ2	2.57	0.40
9:A:693:VAL:HG21	9:A:721:PHE:HE2	1.87	0.40
9:A:991:LYS:O	9:A:995:GLU:HG2	2.21	0.40
9:A:1266:THR:O	9:A:1270:ASN:HB2	2.22	0.40
17:I:19:ASP:OD1	17:I:20:LYS:N	2.54	0.40
21:M:291:ILE:HG22	21:M:293:ILE:HG13	2.04	0.40
23:O:227:PHE:HA	23:O:230:ILE:HG22	2.04	0.40
31:a:166:ILE:HG22	34:d:224:PHE:HZ	1.86	0.40
32:b:25:PHE:CE1	32:b:98:LEU:HD11	2.51	0.40
39:i:31:LEU:HG	39:i:35:LYS:HE3	2.04	0.40
42:l:415:TYR:OH	42:l:442:TRP:NE1	2.53	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	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
2	1	508/642 (79%)	502 (99%)	6 (1%)	0	100	100
3	2	448/513 (87%)	441 (98%)	7 (2%)	0	100	100
4	3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
5	4	298/338 (88%)	289 (97%)	9 (3%)	0	100	100
6	5	63/72 (88%)	60 (95%)	3 (5%)	0	100	100
7	6	379/461 (82%)	366 (97%)	13 (3%)	0	100	100
8	7	609/843 (72%)	585 (96%)	24 (4%)	0	100	100
9	A	1494/1733 (86%)	1443 (97%)	51 (3%)	0	100	100
10	B	1168/1224 (95%)	1130 (97%)	38 (3%)	0	100	100
11	C	264/347 (76%)	257 (97%)	7 (3%)	0	100	100
12	D	163/221 (74%)	159 (98%)	4 (2%)	0	100	100
13	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
14	F	114/155 (74%)	108 (95%)	6 (5%)	0	100	100
15	G	169/177 (96%)	163 (96%)	6 (4%)	0	100	100
16	H	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
17	I	114/122 (93%)	110 (96%)	4 (4%)	0	100	100
18	J	67/70 (96%)	67 (100%)	0	0	100	100
19	K	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
20	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
21	M	306/352 (87%)	295 (96%)	11 (4%)	0	100	100
23	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
24	Q	215/735 (29%)	208 (97%)	7 (3%)	0	100	100
25	R	264/400 (66%)	259 (98%)	5 (2%)	0	100	100
27	U	101/286 (35%)	97 (96%)	4 (4%)	0	100	100
28	V	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
29	W	296/492 (60%)	290 (98%)	6 (2%)	0	100	100
30	X	207/328 (63%)	197 (95%)	10 (5%)	0	100	100
31	a	170/295 (58%)	163 (96%)	7 (4%)	0	100	100
32	b	169/223 (76%)	163 (96%)	5 (3%)	1 (1%)	21	56
33	c	109/115 (95%)	107 (98%)	2 (2%)	0	100	100
34	d	481/687 (70%)	470 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	e	252/307 (82%)	246 (98%)	6 (2%)	0	100	100
36	f	202/210 (96%)	196 (97%)	6 (3%)	0	100	100
37	g	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
38	h	169/284 (60%)	166 (98%)	3 (2%)	0	100	100
39	i	175/222 (79%)	173 (99%)	2 (1%)	0	100	100
40	j	98/149 (66%)	94 (96%)	4 (4%)	0	100	100
41	k	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
42	l	521/745 (70%)	506 (97%)	14 (3%)	1 (0%)	43	76
43	m	126/220 (57%)	122 (97%)	4 (3%)	0	100	100
44	n	134/140 (96%)	132 (98%)	2 (2%)	0	100	100
45	o	108/127 (85%)	107 (99%)	1 (1%)	0	100	100
46	p	221/566 (39%)	210 (95%)	11 (5%)	0	100	100
All	All	12095/16091 (75%)	11739 (97%)	354 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	b	27	GLY
42	l	648	SER

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	684/707 (97%)	684 (100%)	0	100	100
2	1	483/589 (82%)	483 (100%)	0	100	100
3	2	414/468 (88%)	414 (100%)	0	100	100
4	3	125/303 (41%)	125 (100%)	0	100	100
5	4	267/300 (89%)	267 (100%)	0	100	100
6	5	59/66 (89%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	6	346/418 (83%)	345 (100%)	1 (0%)	86	91
8	7	547/737 (74%)	547 (100%)	0	100	100
9	A	1330/1520 (88%)	1330 (100%)	0	100	100
10	B	1024/1061 (96%)	1023 (100%)	1 (0%)	88	93
11	C	234/299 (78%)	234 (100%)	0	100	100
12	D	149/200 (74%)	149 (100%)	0	100	100
13	E	196/197 (100%)	196 (100%)	0	100	100
14	F	108/137 (79%)	108 (100%)	0	100	100
15	G	152/158 (96%)	151 (99%)	1 (1%)	76	86
16	H	123/128 (96%)	123 (100%)	0	100	100
17	I	110/116 (95%)	110 (100%)	0	100	100
18	J	64/65 (98%)	64 (100%)	0	100	100
19	K	99/102 (97%)	99 (100%)	0	100	100
20	L	40/57 (70%)	40 (100%)	0	100	100
21	M	267/306 (87%)	267 (100%)	0	100	100
23	O	153/205 (75%)	153 (100%)	0	100	100
24	Q	204/641 (32%)	203 (100%)	1 (0%)	81	89
25	R	252/363 (69%)	252 (100%)	0	100	100
27	U	99/260 (38%)	99 (100%)	0	100	100
28	V	94/108 (87%)	94 (100%)	0	100	100
29	W	275/436 (63%)	275 (100%)	0	100	100
30	X	193/295 (65%)	193 (100%)	0	100	100
31	a	170/259 (66%)	170 (100%)	0	100	100
32	b	162/207 (78%)	162 (100%)	0	100	100
33	c	104/108 (96%)	104 (100%)	0	100	100
34	d	469/642 (73%)	469 (100%)	0	100	100
35	e	232/280 (83%)	232 (100%)	0	100	100
36	f	174/178 (98%)	174 (100%)	0	100	100
37	g	95/113 (84%)	95 (100%)	0	100	100
38	h	158/258 (61%)	158 (100%)	0	100	100
39	i	174/208 (84%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	100/144 (69%)	100 (100%)	0	100	100
41	k	145/145 (100%)	145 (100%)	0	100	100
42	l	505/688 (73%)	505 (100%)	0	100	100
43	m	119/195 (61%)	118 (99%)	1 (1%)	73	86
44	n	128/132 (97%)	128 (100%)	0	100	100
45	o	103/117 (88%)	103 (100%)	0	100	100
46	p	212/528 (40%)	211 (100%)	1 (0%)	81	89
All	All	11141/14444 (77%)	11135 (100%)	6 (0%)	87	93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	207	ASN
10	B	1178	ASN
15	G	96	GLN
24	Q	369	ASN
43	m	95	GLN
46	p	211	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	23	ASN
1	0	291	GLN
1	0	350	HIS
1	0	480	GLN
1	0	521	ASN
1	0	555	GLN
2	1	85	GLN
2	1	106	GLN
2	1	196	GLN
2	1	273	ASN
2	1	468	GLN
2	1	500	ASN
3	2	75	GLN
3	2	90	ASN
3	2	395	GLN
3	2	431	GLN

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Mol	Chain	Res	Type
4	3	31	ASN
7	6	176	ASN
7	6	351	ASN
7	6	353	HIS
8	7	347	HIS
8	7	349	ASN
8	7	471	GLN
8	7	553	GLN
8	7	584	ASN
8	7	676	HIS
8	7	702	ASN
9	A	171	GLN
9	A	313	GLN
9	A	390	GLN
9	A	510	GLN
9	A	736	ASN
9	A	760	GLN
9	A	1128	GLN
9	A	1265	ASN
10	B	224	GLN
10	B	366	GLN
10	B	951	GLN
10	B	957	ASN
10	B	1013	ASN
10	B	1040	ASN
10	B	1093	GLN
10	B	1112	GLN
10	B	1177	HIS
10	B	1205	GLN
11	C	73	GLN
11	C	135	GLN
11	C	214	ASN
12	D	157	GLN
12	D	200	ASN
13	E	32	GLN
13	E	101	GLN
13	E	114	ASN
13	E	115	ASN
14	F	22	HIS
16	H	52	GLN
16	H	128	ASN
16	H	133	ASN

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Mol	Chain	Res	Type
17	I	89	GLN
19	K	40	HIS
19	K	112	GLN
21	M	127	GLN
21	M	193	GLN
21	M	234	GLN
23	O	158	GLN
24	Q	140	HIS
24	Q	427	HIS
25	R	43	ASN
25	R	88	HIS
25	R	248	ASN
25	R	265	HIS
27	U	40	ASN
27	U	43	GLN
27	U	280	GLN
29	W	358	ASN
30	X	136	GLN
30	X	265	ASN
31	a	135	ASN
31	a	162	GLN
32	b	85	HIS
32	b	150	GLN
33	c	2	GLN
34	d	255	ASN
34	d	350	HIS
34	d	360	ASN
34	d	646	HIS
34	d	683	GLN
35	e	3	GLN
35	e	29	ASN
35	e	243	ASN
36	f	156	GLN
38	h	92	ASN
39	i	74	GLN
39	i	99	GLN
40	j	4	GLN
40	j	9	ASN
40	j	86	GLN
40	j	148	GLN
41	k	56	ASN
42	l	89	GLN

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Mol	Chain	Res	Type
42	l	175	ASN
42	l	218	ASN
42	l	282	ASN
42	l	458	ASN
42	l	463	ASN
42	l	635	ASN
42	l	666	ASN
43	m	51	ASN
44	n	121	HIS
44	n	135	ASN
45	o	45	GLN
45	o	111	GLN
45	o	113	GLN
46	p	93	GLN
46	p	177	GLN
46	p	235	GLN
46	p	247	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 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	$\# Z > 2$
47	SF4	0	801	1	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
47	SF4	0	801	1	-	-	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1614:PRO	C	1629:THR	N	23.05

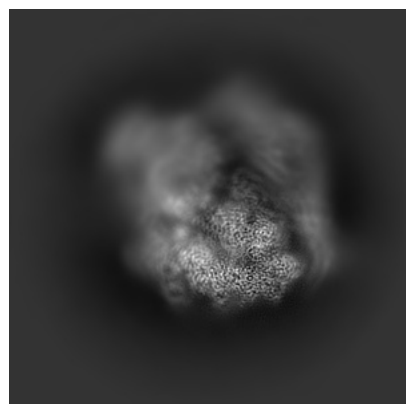
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16610. These allow visual inspection of the internal detail of the map and identification of artifacts.

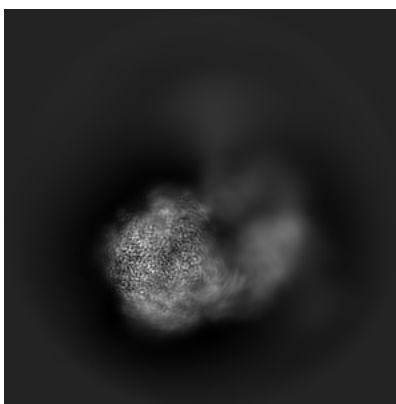
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

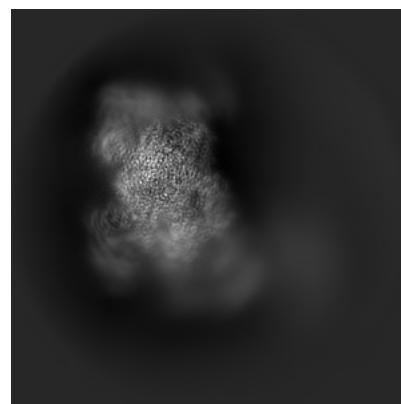
6.1.1 Primary map



X

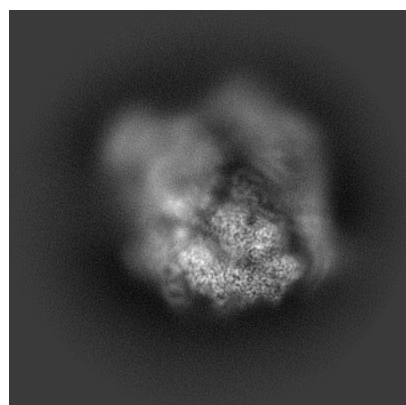


Y

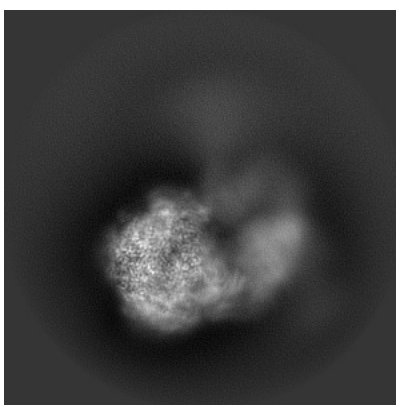


Z

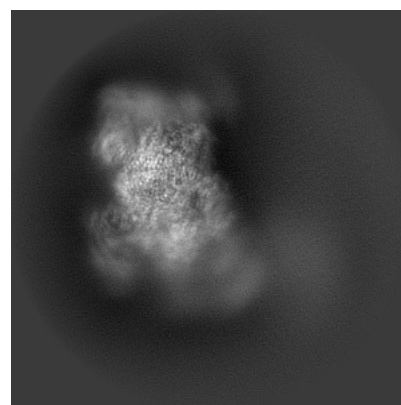
6.1.2 Raw map



X



Y



Z

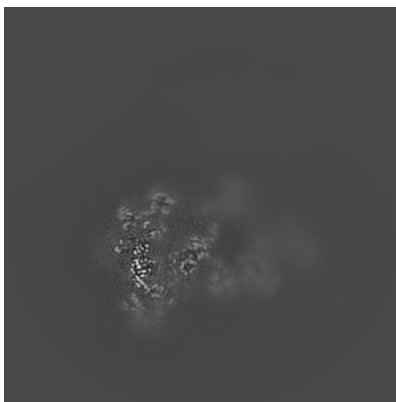
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

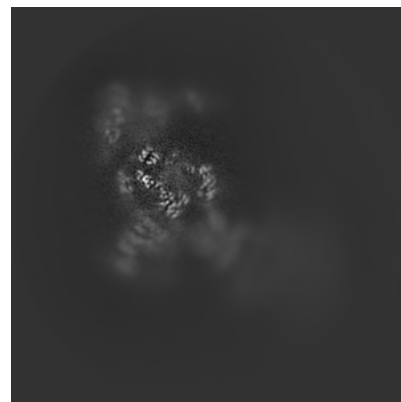
6.2.1 Primary map



X Index: 200

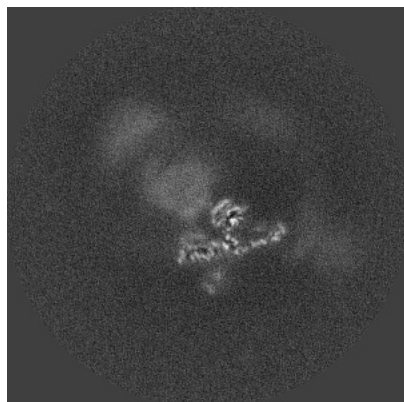


Y Index: 200

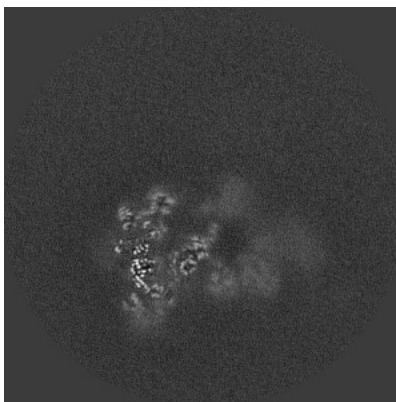


Z Index: 200

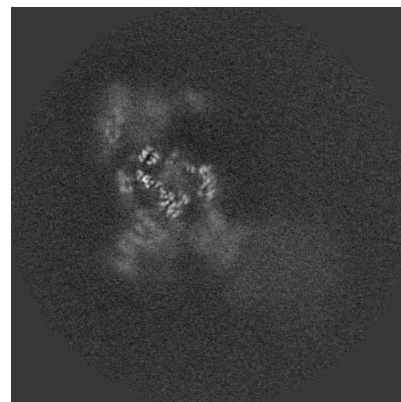
6.2.2 Raw map



X Index: 200



Y Index: 200

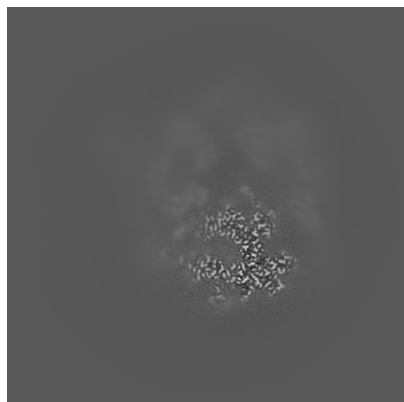


Z Index: 200

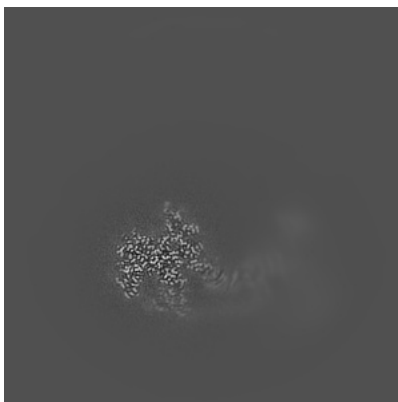
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

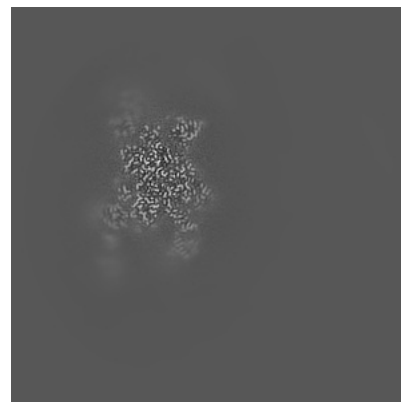
6.3.1 Primary map



X Index: 145

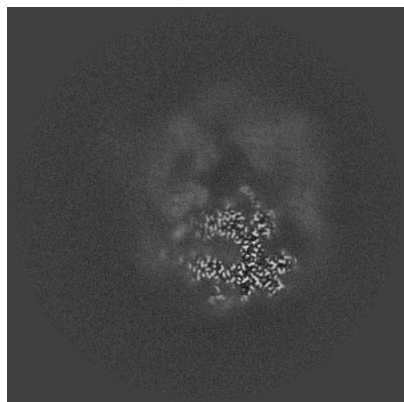


Y Index: 248

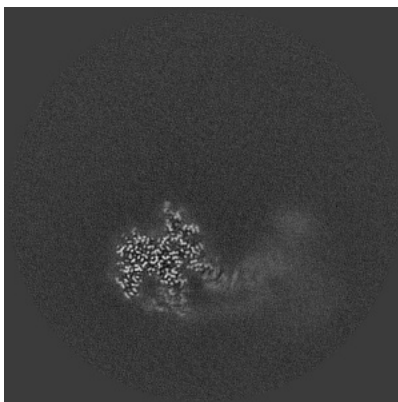


Z Index: 133

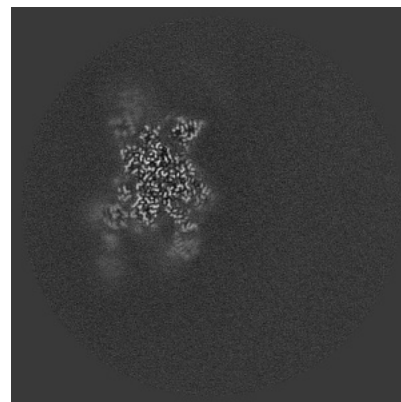
6.3.2 Raw map



X Index: 145



Y Index: 248

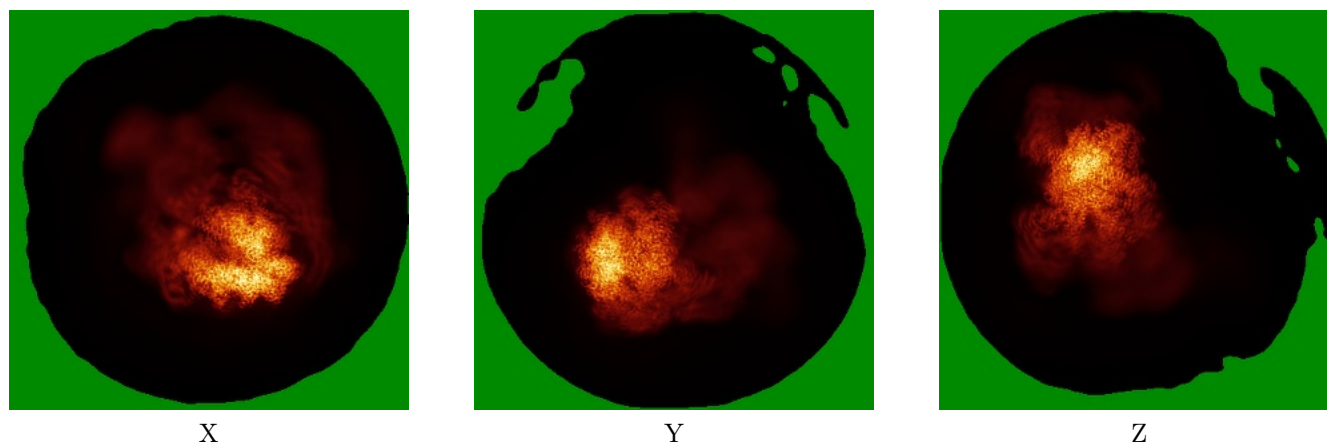


Z Index: 133

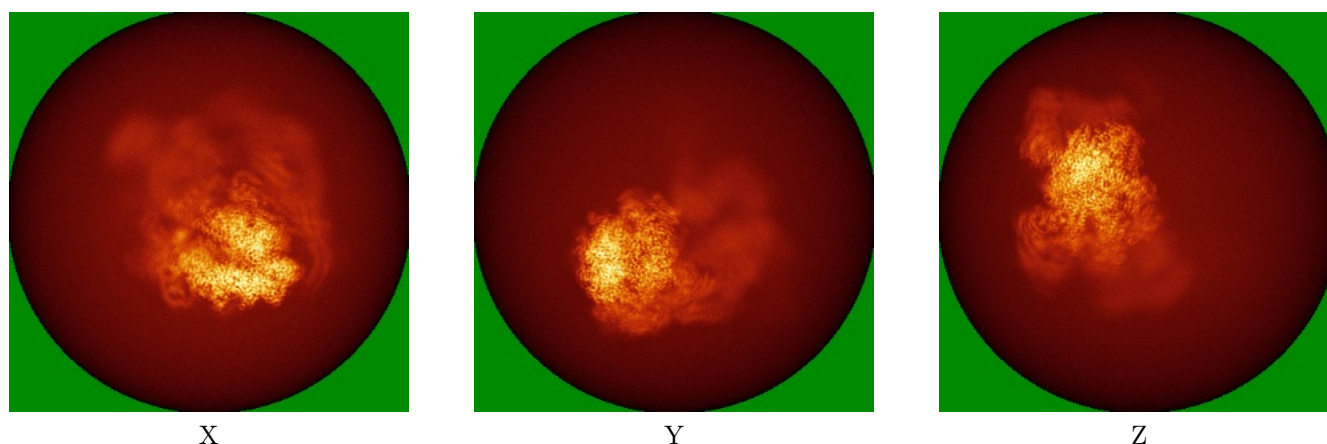
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

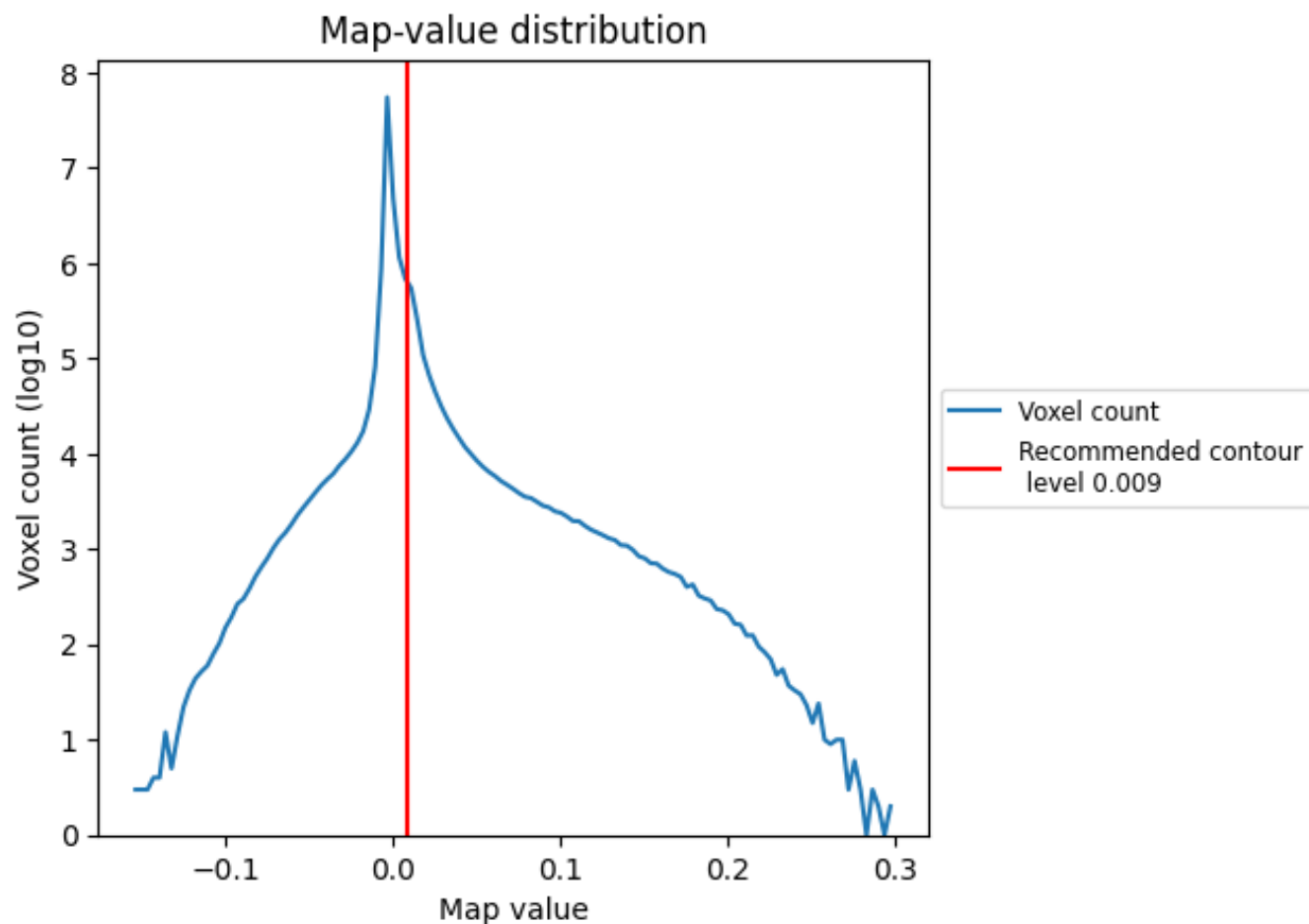
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

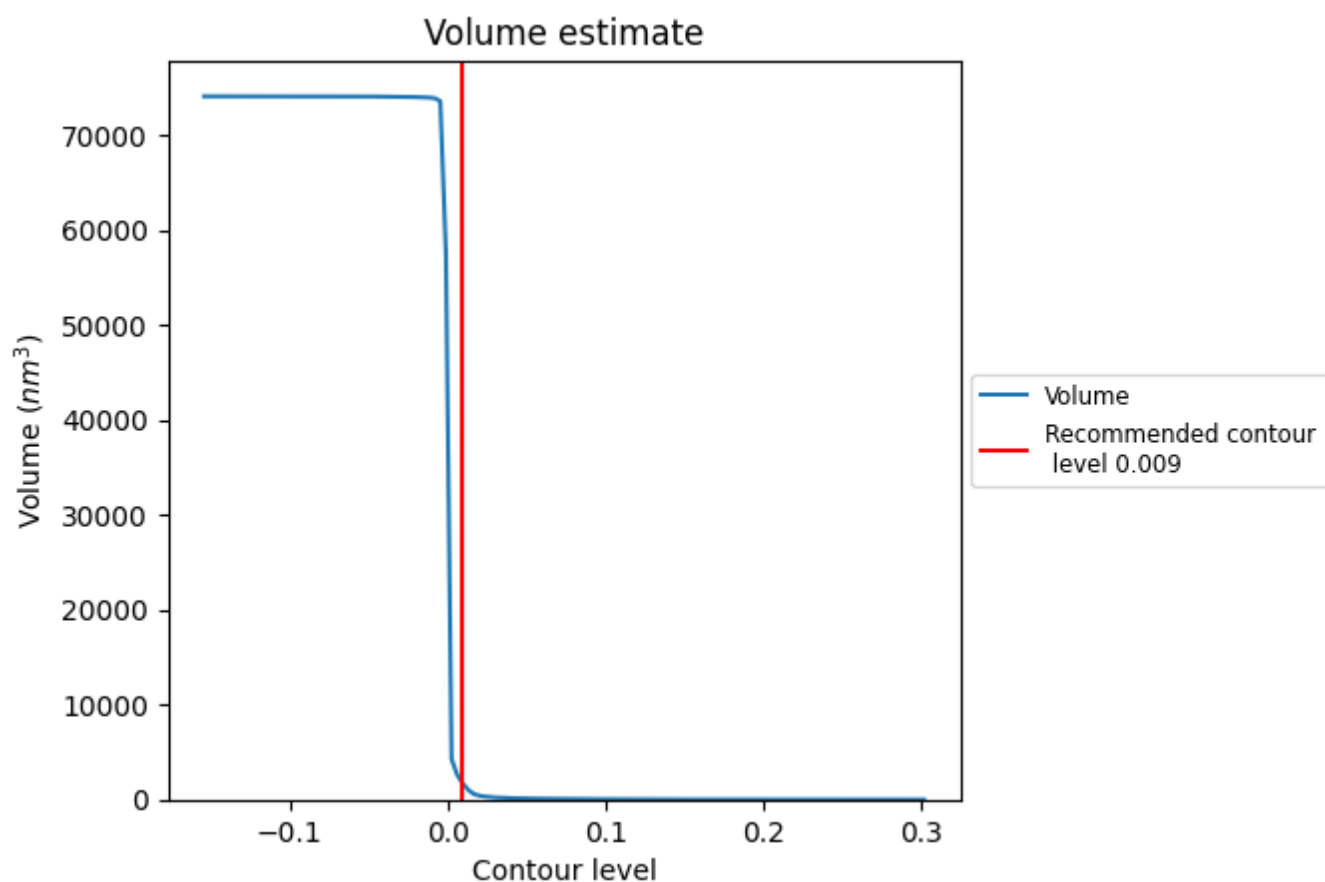
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

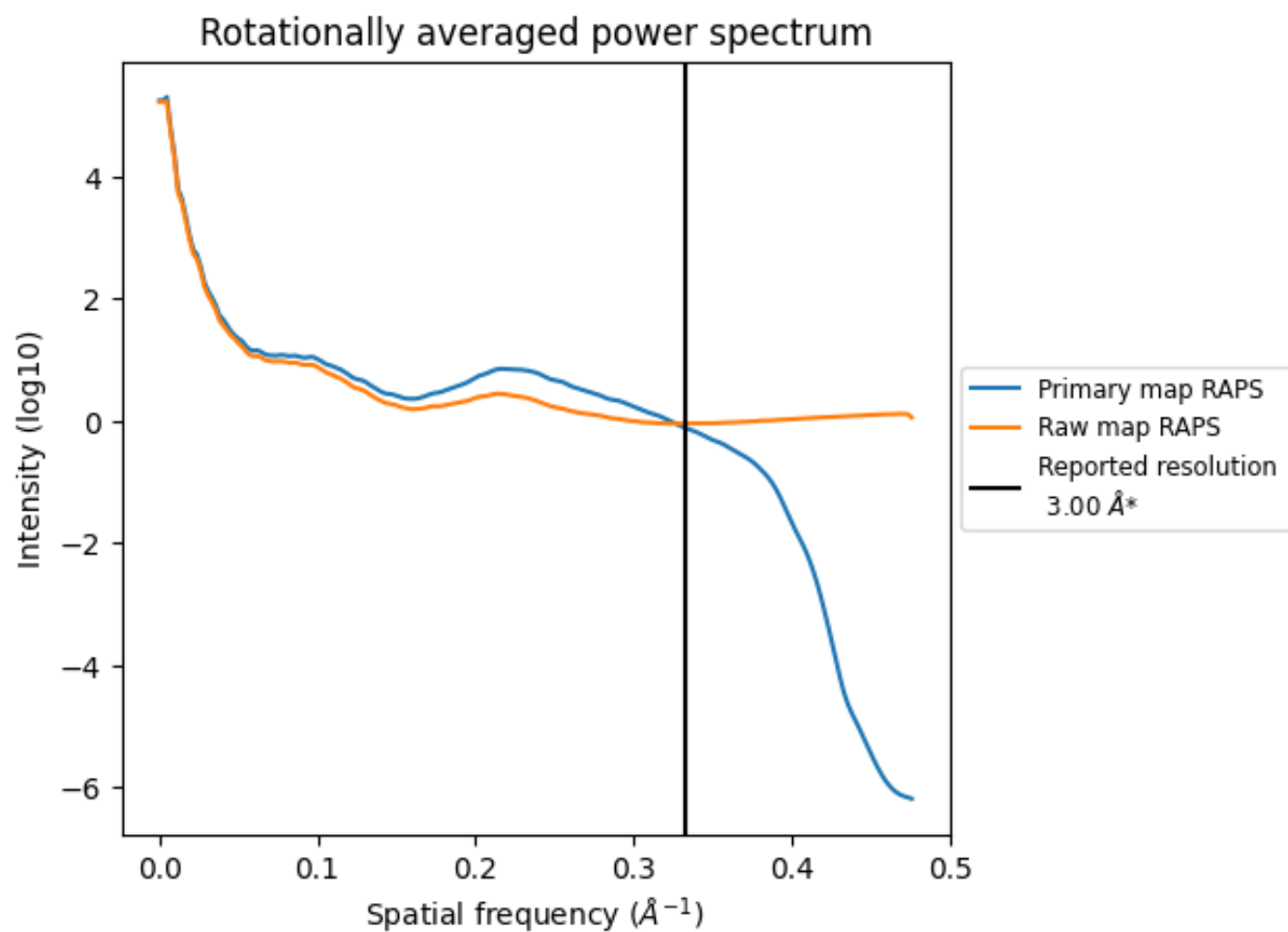
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1864 nm^3 ; this corresponds to an approximate mass of 1684 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 ⓘ

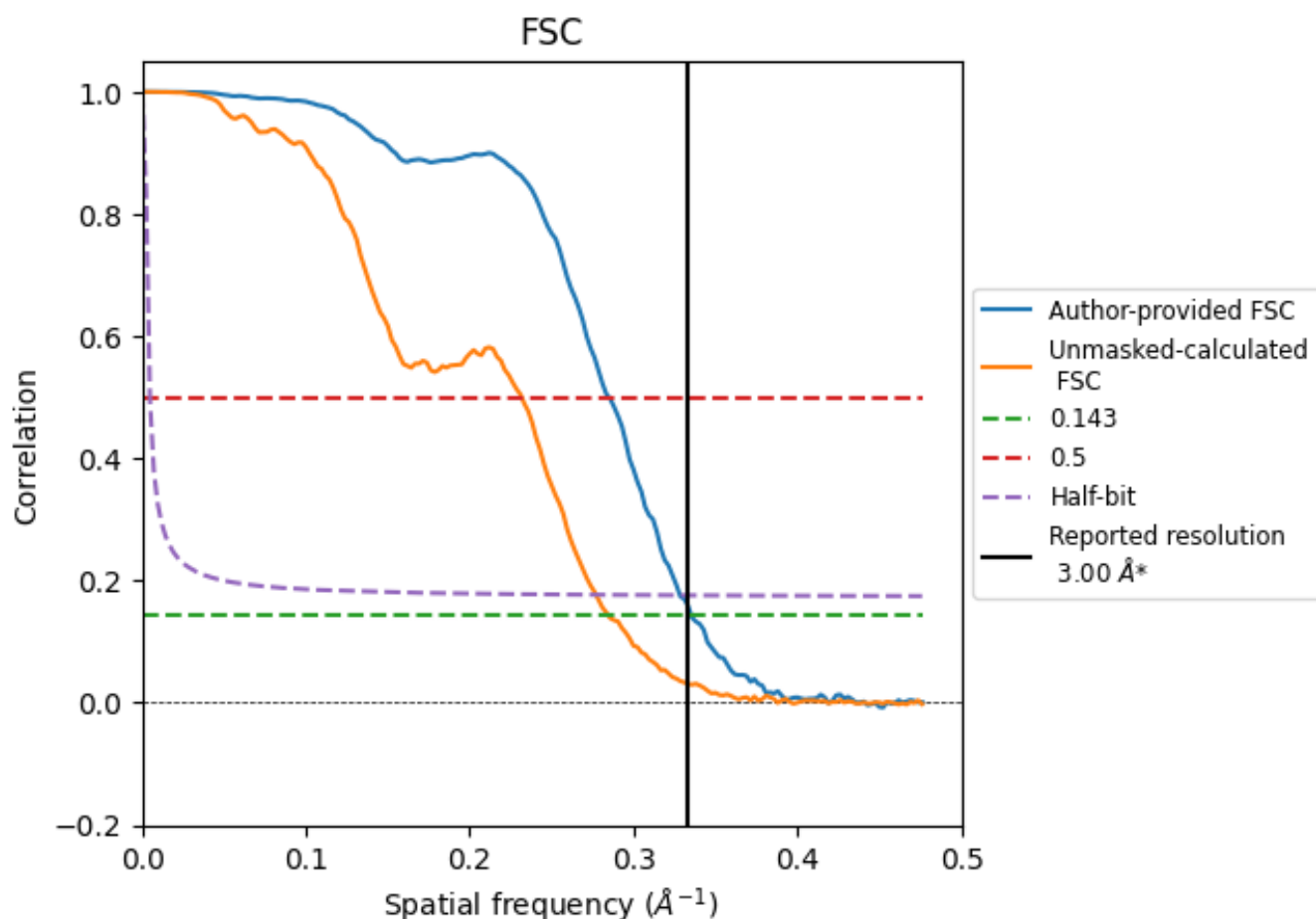


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

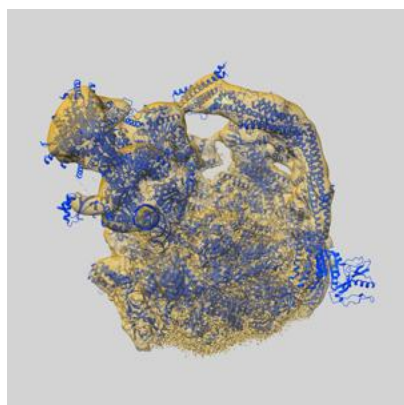
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.51	3.05
Unmasked-calculated*	3.51	4.32	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.0 by more than 10 %

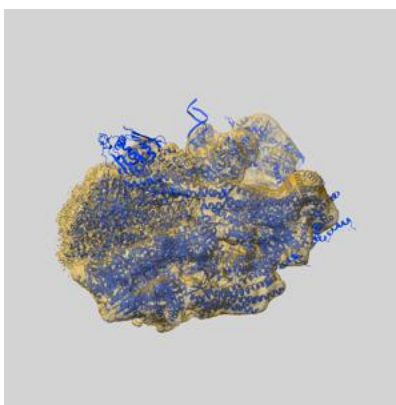
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16610 and PDB model 8CEN. Per-residue inclusion information can be found in section 3 on page 15.

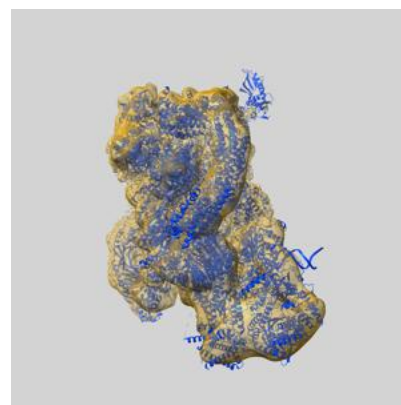
9.1 Map-model overlay [i](#)



X



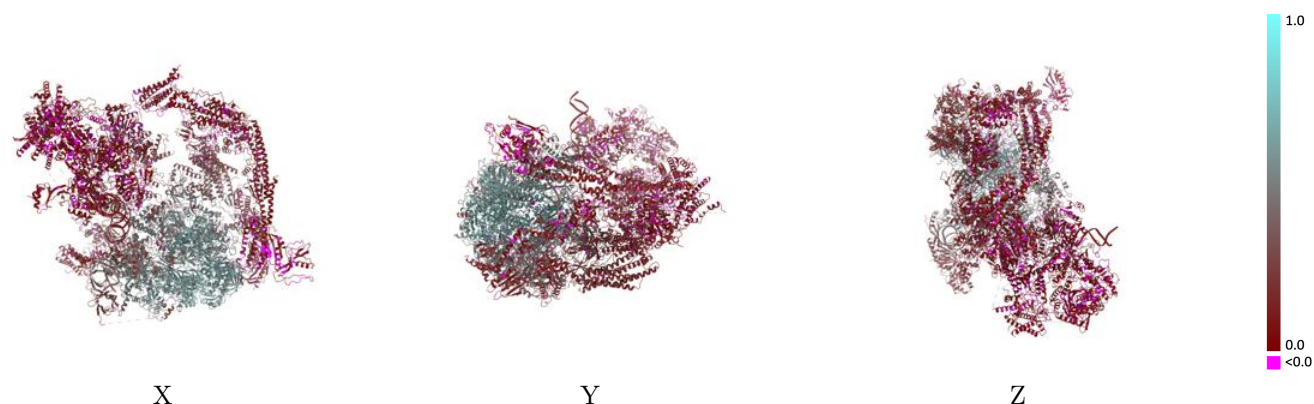
Y



Z

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

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

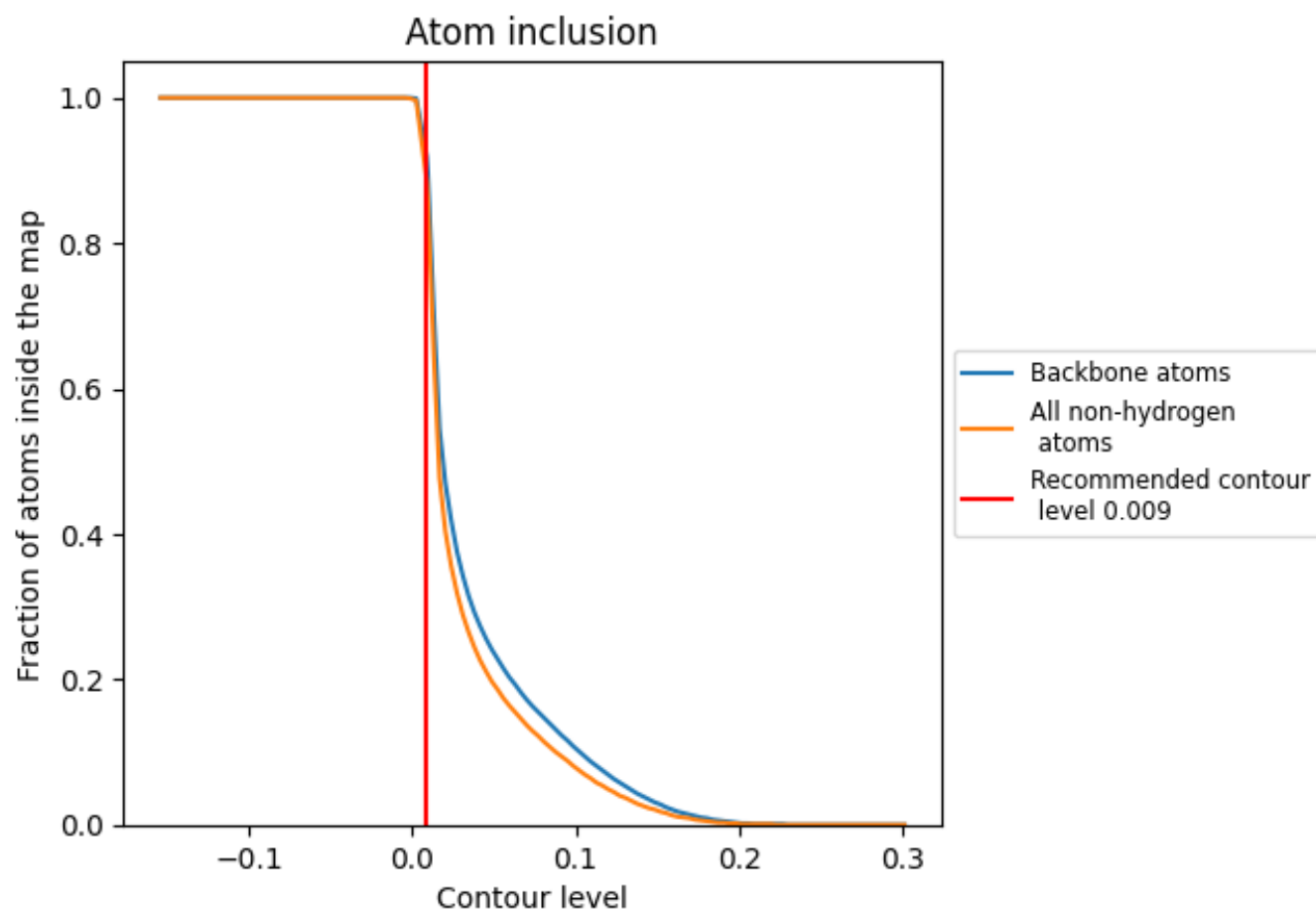


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.2690
0	 0.9110	 0.1000
1	 0.7380	 0.0770
2	 0.7750	 0.0740
3	 0.9280	 0.1710
4	 0.8560	 0.0600
5	 0.6250	 0.0530
6	 0.8420	 0.0690
7	 0.8850	 0.0880
A	 0.9700	 0.5110
B	 0.9810	 0.5560
C	 0.9810	 0.5870
D	 0.9060	 0.2590
E	 0.9770	 0.4580
F	 0.8920	 0.4250
G	 0.9560	 0.3940
H	 0.9770	 0.5400
I	 0.9700	 0.4300
J	 0.9840	 0.5910
K	 0.9860	 0.6000
L	 0.9860	 0.5190
M	 0.9510	 0.4190
N	 0.8850	 0.2060
O	 0.9740	 0.2610
Q	 0.9500	 0.3050
R	 0.9700	 0.2540
T	 0.8720	 0.2020
U	 0.7770	 0.1330
V	 0.8540	 0.1470
W	 0.8560	 0.1750
X	 0.9280	 0.1670
a	 0.9370	 0.1280
b	 0.9230	 0.1850
c	 0.9600	 0.2130
d	 0.9460	 0.1830



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Chain	Atom inclusion	Q-score
e	 0.9380	 0.4110
f	 0.9320	 0.4000
g	 0.9650	 0.1930
h	 0.8090	 0.1300
i	 0.9070	 0.1280
j	 0.4600	 0.0860
k	 0.7230	 0.0910
l	 0.8690	 0.1220
m	 0.4290	 0.0590
n	 0.8320	 0.1050
o	 0.9170	 0.1230
p	 0.0380	 0.0530