



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:24 AM UTC

PDB ID : 8CEO / pdb_00008ceo
EMDB ID : EMD-16611
Title : Yeast RNA polymerase II transcription pre-initiation complex with core Mediator and the +1 nucleosome
Authors : Wang, H.; Cramer, P.
Deposited on : 2023-02-02
Resolution : 3.60 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:

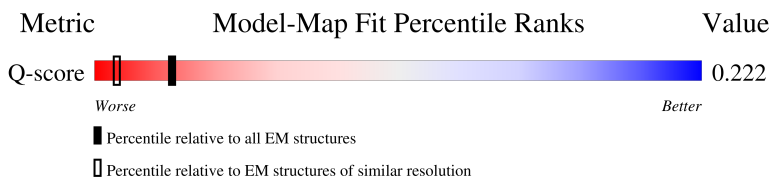
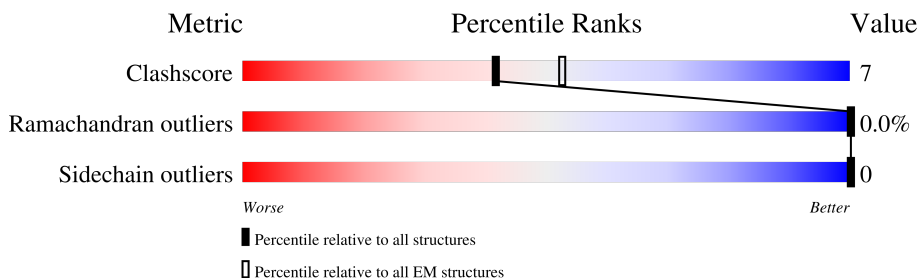
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.60 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	12797 (3.10 - 4.10)

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	1082	
43	m	220	
44	n	140	
45	o	127	
46	p	566	
47	r	135	
47	v	135	
48	s	102	
48	w	102	
49	t	129	
49	x	129	
50	u	125	
50	y	125	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 113584 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 IIIH 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 TFB1 isoform 1.

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 RNA polymerase II transcription factor B subunit 2.

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 IIIH 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 IIIH 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.

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	209	Total	C	N	O	P	0	0
			4263	2035	761	1259	208		

- 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	209	Total	C	N	O	P	0	0
			4300	2045	802	1245	208		

- Molecule 27 is a protein called TOA1 isoform 1.

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	172	Total	C	N	O	S	0	0
			1407	895	240	269	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 a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	97	Total	C	N	O	S	0	0
			801	506	155	138	2		
47	v	98	Total	C	N	O	S	0	0
			810	512	157	139	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	102	ALA	GLY	conflict	UNP P84233
r	110	ALA	CYS	engineered mutation	UNP P84233
v	102	ALA	GLY	conflict	UNP P84233
v	110	ALA	CYS	engineered mutation	UNP P84233

- Molecule 48 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
48	w	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

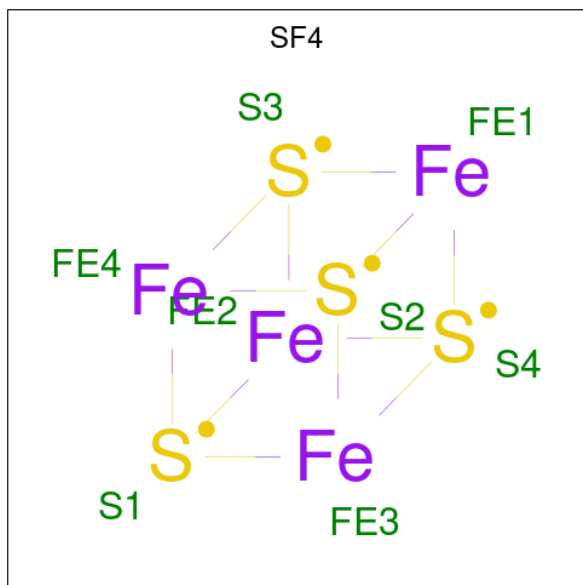
- Molecule 49 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	109	Total	C	N	O		0	0
			843	531	167	145			
49	x	106	Total	C	N	O		0	0
			818	516	160	142			

- Molecule 50 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	97	Total	C	N	O	S	0	0
			767	481	142	142	2		
50	y	95	Total	C	N	O	S	0	0
			745	469	134	140	2		

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
51	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	2	Total	Zn	0
			2	2	
52	4	1	Total	Zn	0
			1	1	
52	6	4	Total	Zn	0
			4	4	
52	A	2	Total	Zn	0
			2	2	
52	B	1	Total	Zn	0
			1	1	
52	C	1	Total	Zn	0
			1	1	
52	I	2	Total	Zn	0
			2	2	

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

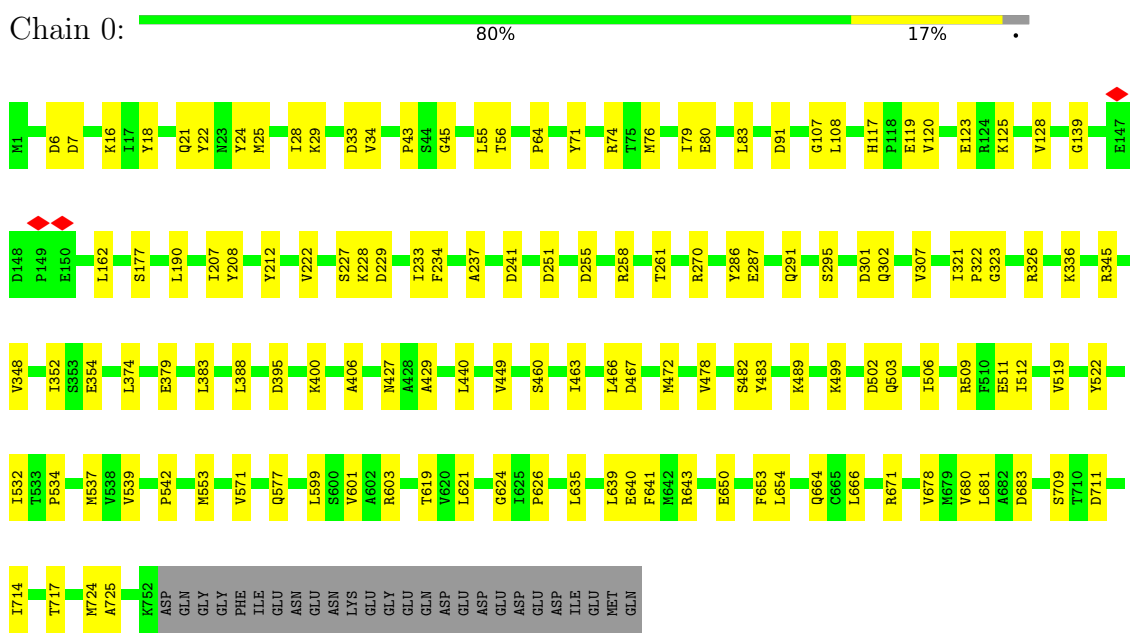
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

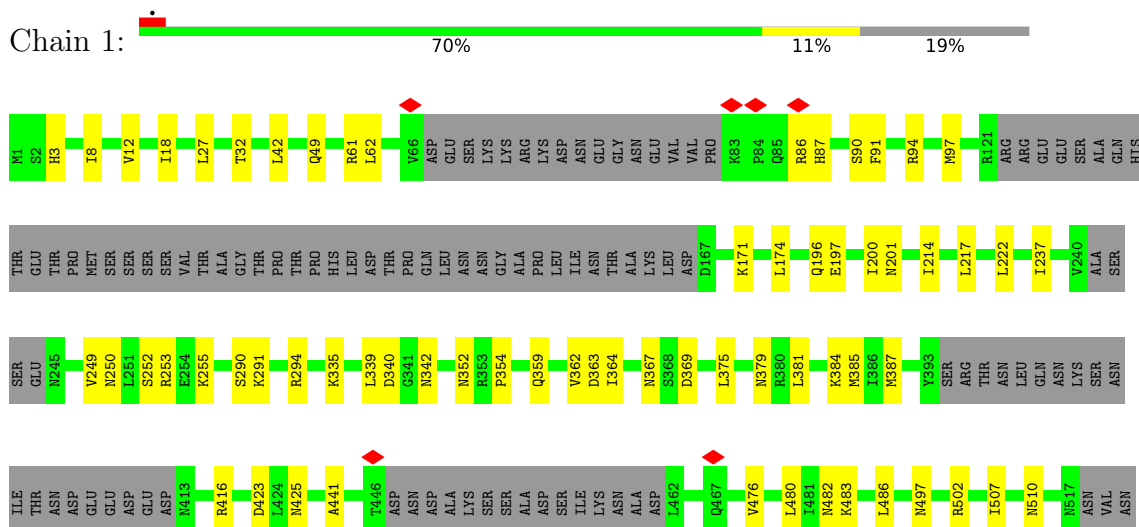
3 Residue-property plots

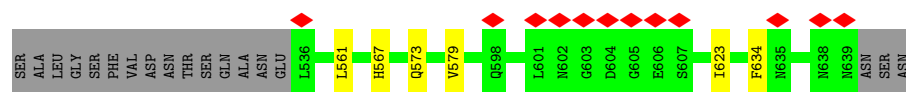
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD



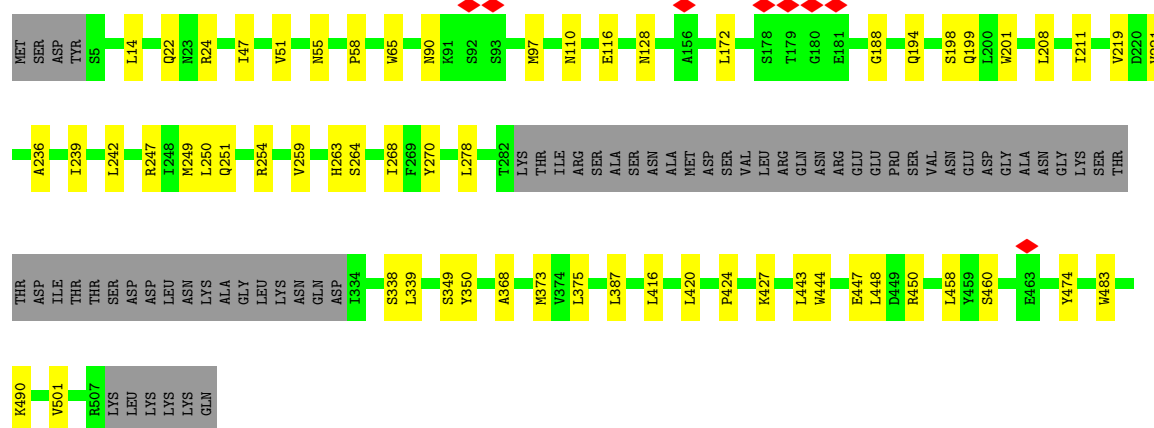
- Molecule 2: TFB1 isoform 1





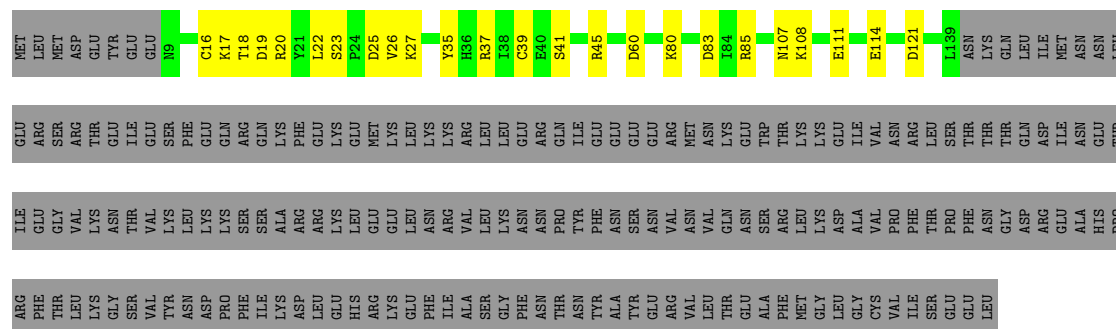
• Molecule 3: RNA polymerase II transcription factor B subunit 2

Chain 2: 76% 12% 12%



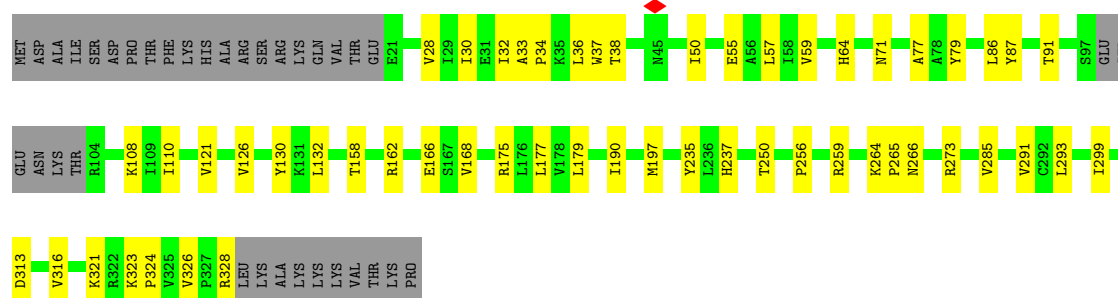
• Molecule 4: RNA polymerase II transcription factor B subunit 3

Chain 3: 33% 7% 59%



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

Chain 4: 73% 16% 11%



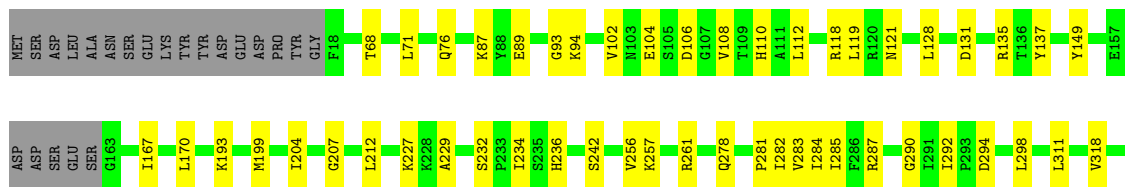
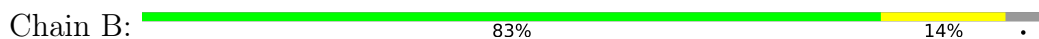
• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

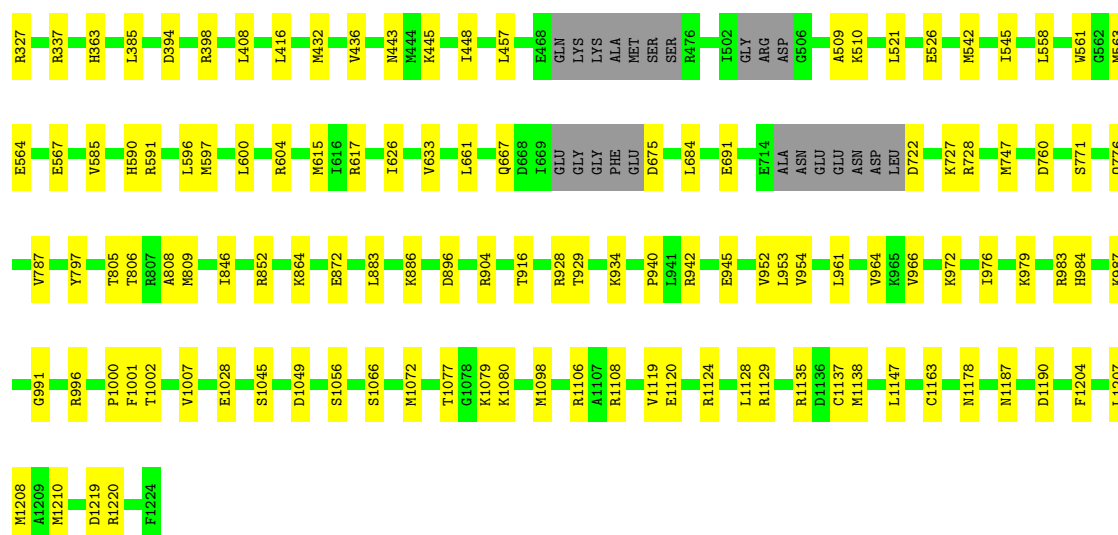
Amino Acid	Relative Abundance (%)
MET	100
A2	85
R5	75
D13	65
K17	55
D29	45
I30	35
V31	25
L32	15
L35	10
D36	5
D37	5
L40	5
L41	5
M66	5
ASP	5
GLU	5
GIU	5
GLU	5
ASN	5
GLN	5

[illegible]

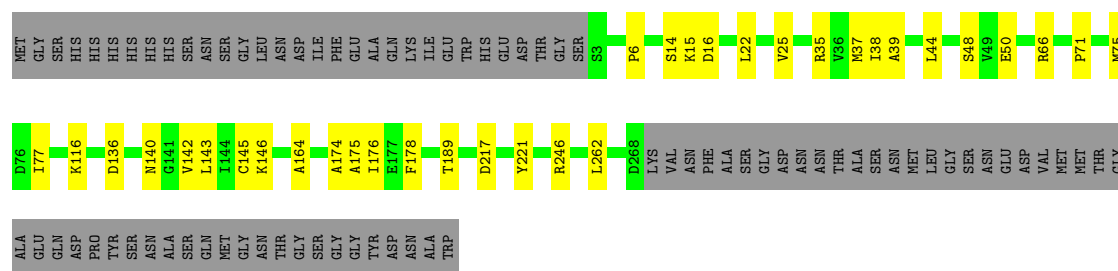
ARG	PHE	S679	R519	I362	GLN	GLN	A150	THR	MET
LYS	GLY	Q682	L527	E367	GLN	LEU	Q154	GLY	THR
SER	GLY	N528	F529	K372	GLN	GLY	L157	GLY	VAL
ALA	GLY	Q685	L530	R380	THR	THR	I160	ARG	PRO
VAL	ARG	G688	L535	S381	ALA	ALA	I164	GLY	GLY
ARG	GLY	R689	A538	I383	GLY	GLY	K174	GLY	THR
GLU	GLY	R692	E542	L386	PRO	ALA	Y181	SER	SER
GLY	SER	A703	K546	G389	THR	THR	A182	GLY	GLY
LEU	SER	L708	V552	T393	ASN	ASN	V184	ARG	LYS
LEU	GLY	K711	F565	I397	VAL	HIS	S185	HIS	ILE
ALA	LEU	D712	F566	T398	ASN	THR	T190	ALA	PRO
GLY	GLY	M716	Q567	R405	PRO	ALA	D198	ASP	ASP
GLY	GLY	K721	E568	V409	ASN	ASP	K202	ASP	MET
GLU	GLY	R722	B571	Q423	VAL	VAL	I209	SER	GLY
MET	ASP	H735	A574	W427	GLU	GLU	I213	GLY	GLY
ALA	ALA	H738	M583	F438	ALA	ALA	K214	MET	GLY
TYR	TYR	N747	C591	T439	ILE	ILE	I223	ASP	ASP
MET	GLU	L748	Q592	S440	GLY	GLY	I236	GLN	GLY
ASP	ASN	A751	K443	R443	ASP	ASP	T237	ASP	ASP
GLY	GLY	L760	R601	Q447	GLU	GLU	Q238	THR	ASP
LEU	GLY	N767	G602	V460	ARG	ARG	I241	ALA	ALA
GLY	GLY	H830	I606	V454	GLU	GLU	E235	THR	GLY
HIS	ALA	L832	F626	T456	GLU	ASN	T236	ASN	ILE
P831	ALA	ASP	S609	R499	ASP	ASP	Q238	SER	ASP
L832	GLY	GLY	N622	R500	ASP	ASP	I241	ILE	ASN
Y837	ILE	GLY	P625	I486	ILE	ASP	A102	TYR	ASP
TYR	GLU	VAL	F626	V490	ALA	ASP	D103	ASP	ASP
ASN	ASP	ASP	I627	A495	V313	PRO	G252	ASN	ASN
LEU	LEU	ASP	R636	I496	Q331	ARG	G111	GLU	GLY
LYS	ALA	ASP	F636	N497	ILE	ILE	R114	THR	THR
LYS	ASN	ASN	I652	F498	D334	ASP	R124	SER	SER
GLY	SER	VAL	L654	R499	F335	SER	H127	GLY	GLY
GLY	VAL	GLY	T660	R500	V337	HIS	L132	GLY	GLY
ARG	ARG	ARG	I505	I505	E340	VAL	W133	GLY	ARG
GLY	GLY	GLY	I671	T514	R344	GLN	I134	ARG	ASP
SER	SER	ASN	Q672	A515	D351	PRO	D138	THR	THR
ASN	GLY	GLY	I673	T516	ASP	GLY	I141	GLY	GLY
HIS	HIS	HIS	Q572	N497	L356	VAL	F150	MET	MET

Chain A: 74% 13% 13%

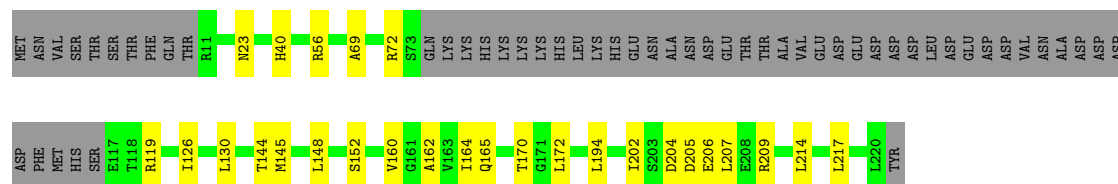




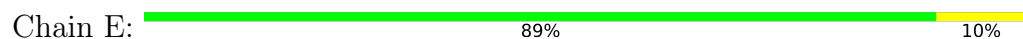
- Molecule 11: DNA-directed RNA polymerase II subunit RPB3



- Molecule 12: DNA-directed RNA polymerase II subunit RPB4

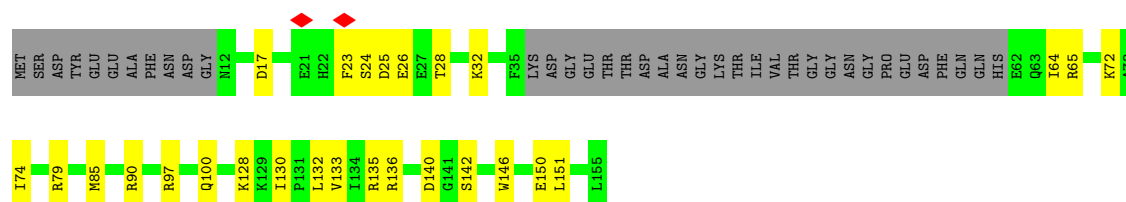


- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1



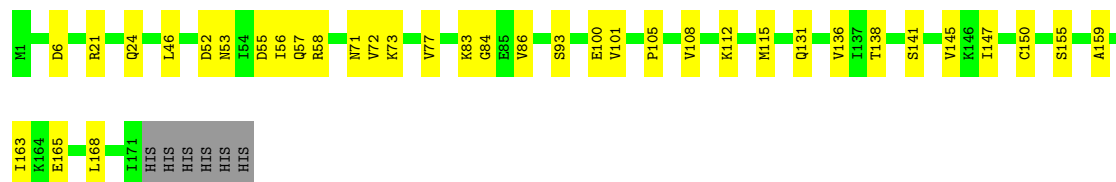
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2





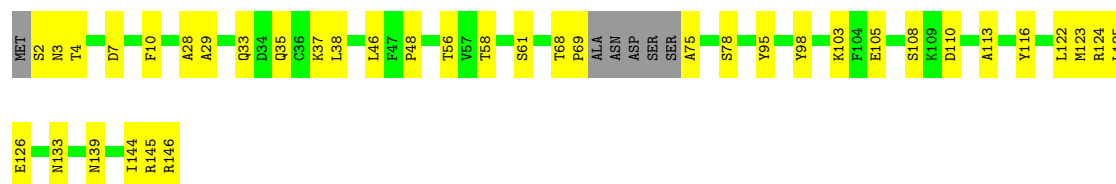
- Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G: 76% 20% .



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

Chain H: 70% 26% .



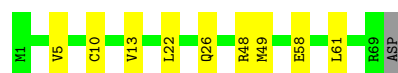
- Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I: 75% 20% 5% .



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

Chain J: 86% 13% .



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

Chain K: 88% 8% .



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

Chain L:  51% 13% 36%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN ALA LEU ASP ALA ALA ALA GLY THR SER GLN ARG ALA THR ALA T26 Y29 I30 C31 C34 V46 L56 L64 F65 Q66 F67 F68 A69 R70

• Molecule 21: Transcription initiation factor IIB

Chain M:  74% 14% 12%

MET MET THR ARG GLU SER ILE ASP LYS PRO THR ASN ALA GLY ARG R14 I20 V21 L22 E26 R37 E40 V43 V44 I213 I212 V51 R215 D58 ARG SER GLU TRP ARG THR PHE SER ASP ASP HIS ASN ASP GLY ASP PRO SER R78 L92 A113 M117 K121 I133 A140 E160 M172 C180 R181 V185 A186 R187 T188 E191 L195 K199 E202 K205 N212 I213 R215 S231 G232 A233 Q234 S244 T259 I269 P274 V280 S281 N285 Q303 G312 Y313 L316 L323 V324 P326 Q327 P340 G341 V342 GLU LYS LYS LYS HIS HIS HIS HIS

• Molecule 22: Nontemplate DNA (209-MER)

Chain N:  33% 84% 16%

A-73 G-65 A-59 T-58 T-42 G-39 A-38 T-26 G-25 C-15 A-14 T-13 A-12 A1 T2 A3 T8 T9 C10 T11 G12 C13 G14 G17 T18 G19 T20 T21 G22 G23 T24 C25 G26 T27 A30 C31 A32 G33 C34 T35 C36 T37 C40 A41 C42 C43 G44 C45 T46 T47 A48 A49 A50 C51 G52 C53 A54 C55 G56 T57 A58 C59 C68 C69 C70 G89 G90 C100 T104 C105 T106 C107 C108 A109 G110 G111 C112 A113 C114 G115 G116 T117 T118 C119 T123 A124 T125 A126 T127 A128 C129 A130 T131 C132 G133 A134 T135

• Molecule 23: TATA-binding protein

Chain O:  62% 14% 25%

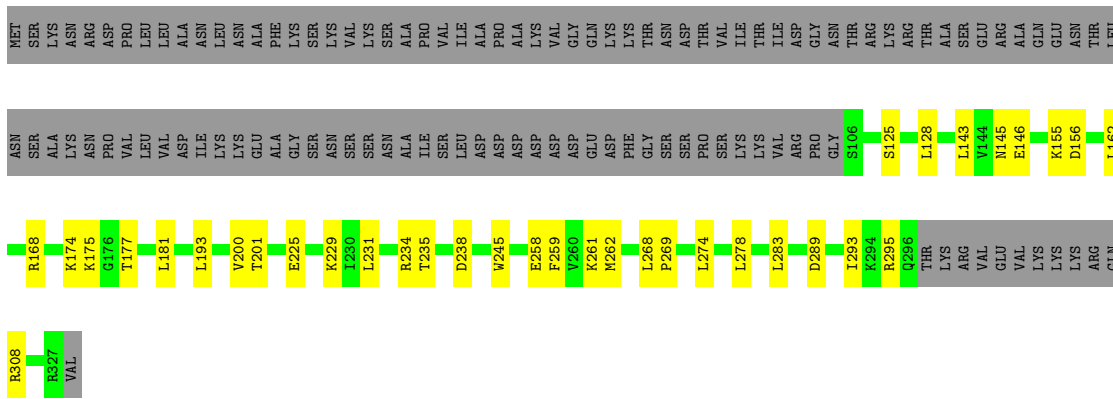
MET ALA ASP GLU ARG GLU LEU LYS GLU PHE THR ASN ALA ASP PRO ASN THR ARG GLN VAL TRP GLU ASN GLN ASN ARG ASP GLY THR ALA THR PHE GLN SER GLY ASP ILE ARG ALA PRO GLU SER THR LYS ASP ALA L204 L205 V208 V213 L214 I230 L234 V74 T75 L76 L82 V85 H88 K97 R105 I106 R107 E108 P109 M121 Y139 I143 I146 G147 F148 A149 A150 I157 Q158 N159 I160 L172 G180 S183 S184 Y185 L193 M197 L204 L205 V208 V213 L214 I230 L234 W240

• Molecule 24: Transcription initiation factor IIF subunit alpha

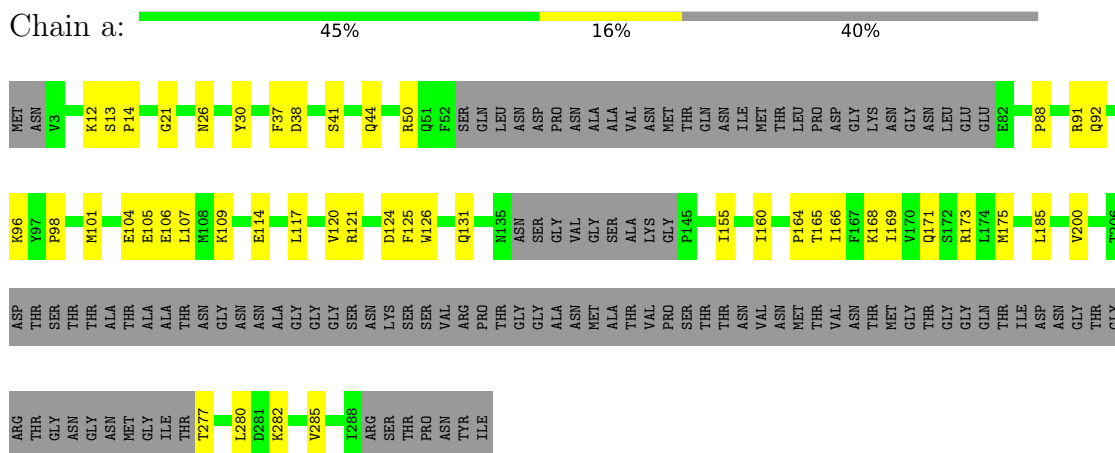
Chain Q:  24% 6% 70%

MET SER ARG ASN PRO PRO GLY SER ASN ASN GLY GLY PRO THR M17 D25 R35 MET GLY GLN ASN GLY SER ASN F148 SER SER SER PRO GLY VAL PRO ASN GLY ASP ASN SER ARG GLY SER LEU VAL LYS LYS ASP ASP PRO GLU THR ALA GLU ARG GLU ARG LYS MET LEU

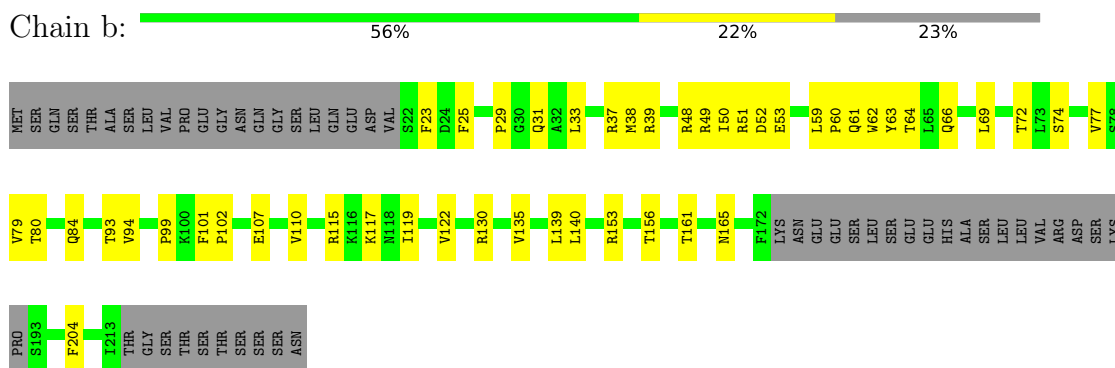




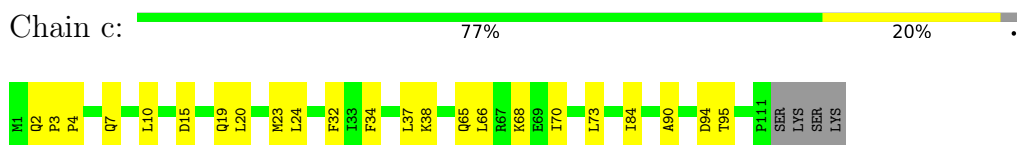
- Molecule 31: Mediator of RNA polymerase II transcription subunit 6



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

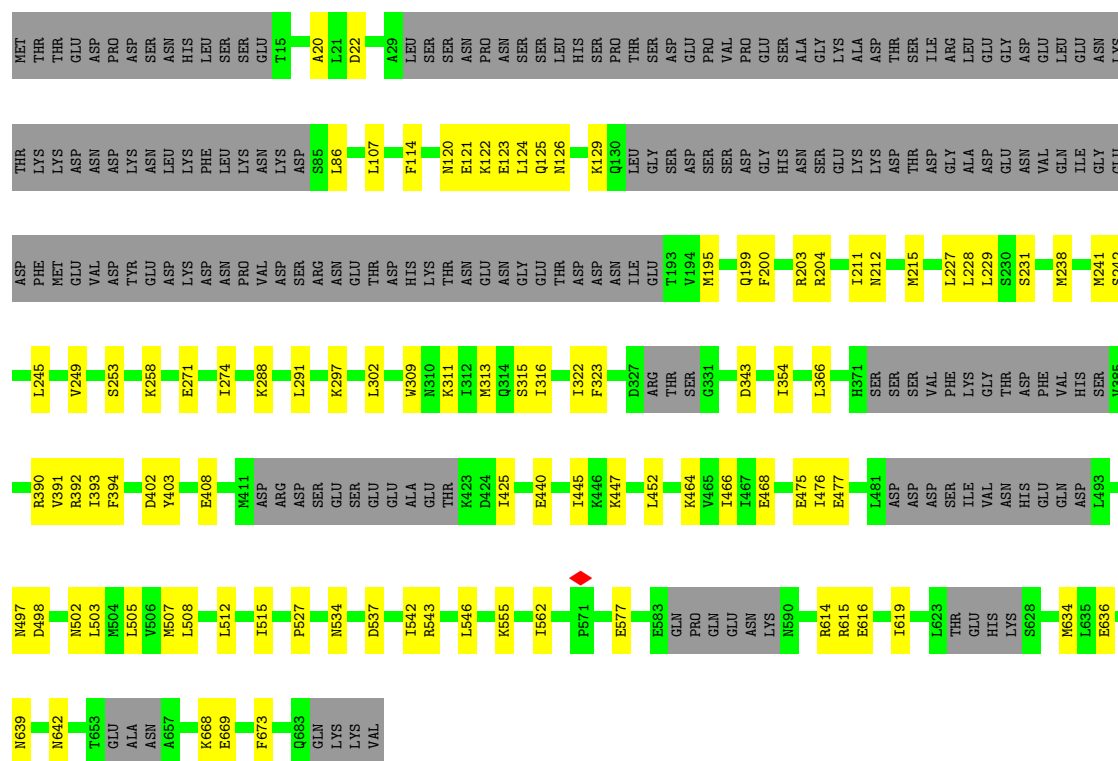


- Molecule 33: Mediator of RNA polymerase II transcription subunit 11



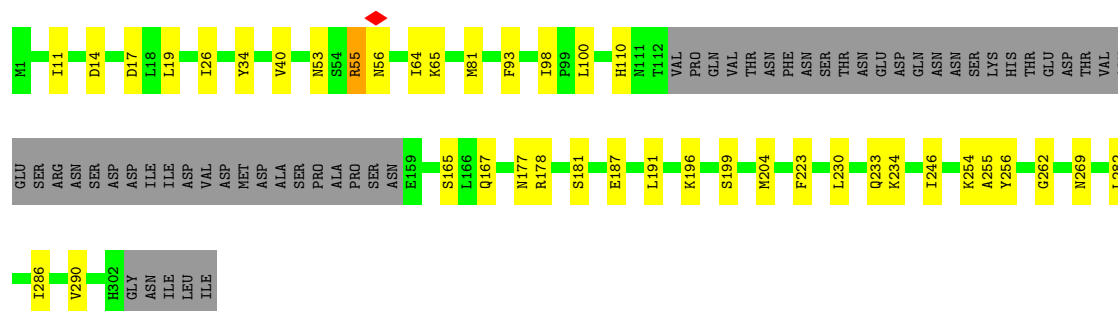
- Molecule 34: Mediator of RNA polymerase II transcription subunit 17

Chain d:  59% 14% 27%



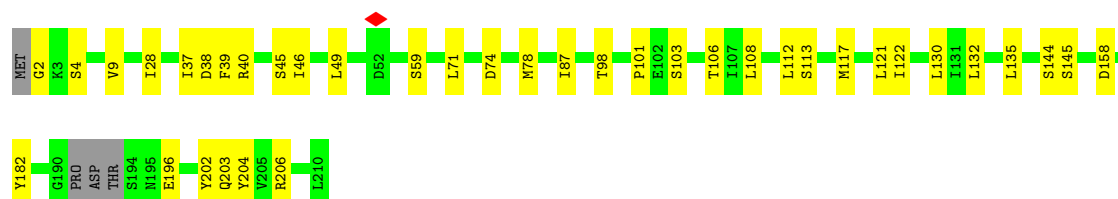
• Molecule 35: Mediator of RNA polymerase II transcription subunit 18

Chain e:  70% 13% 17%



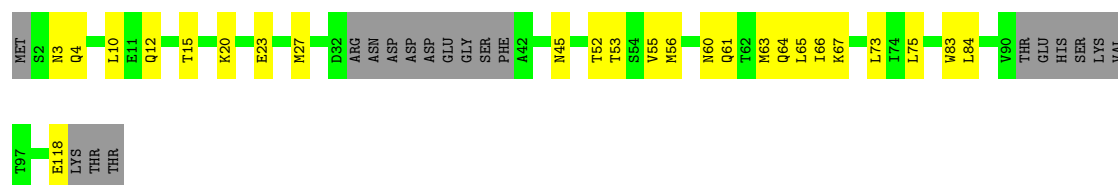
• Molecule 36: Mediator of RNA polymerase II transcription subunit 20

Chain f:  80% 18%



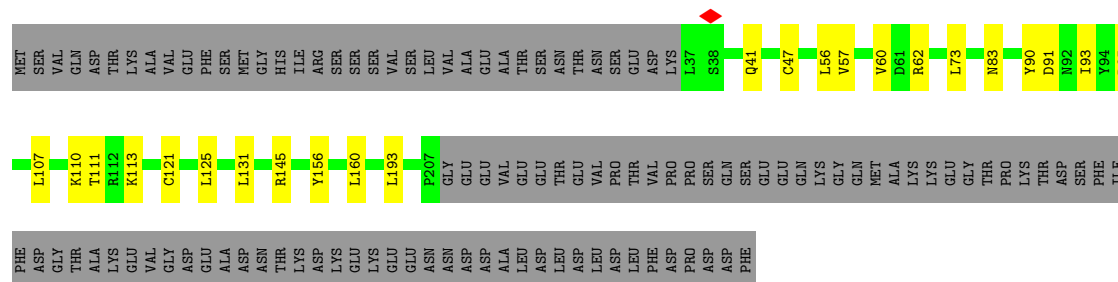
• Molecule 37: Mediator of RNA polymerase II transcription subunit 22

Chain g: 



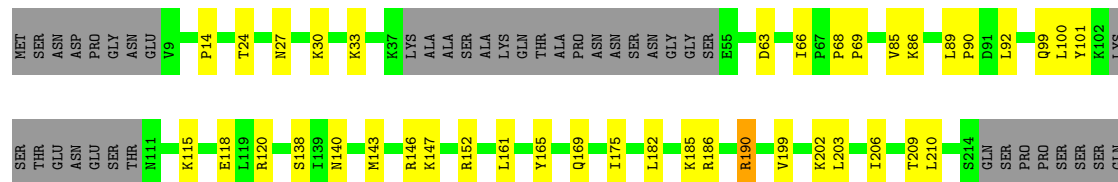
- Molecule 38: Mediator of RNA polymerase II transcription subunit 4

Chain h: 

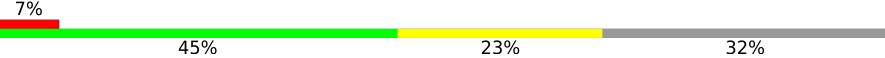


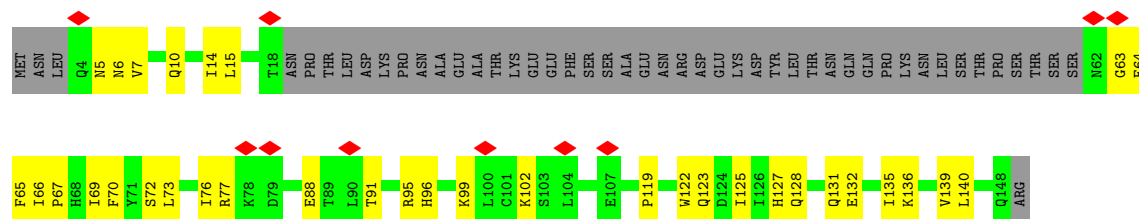
- Molecule 39: Mediator of RNA polymerase II transcription subunit 7

Chain i: 



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

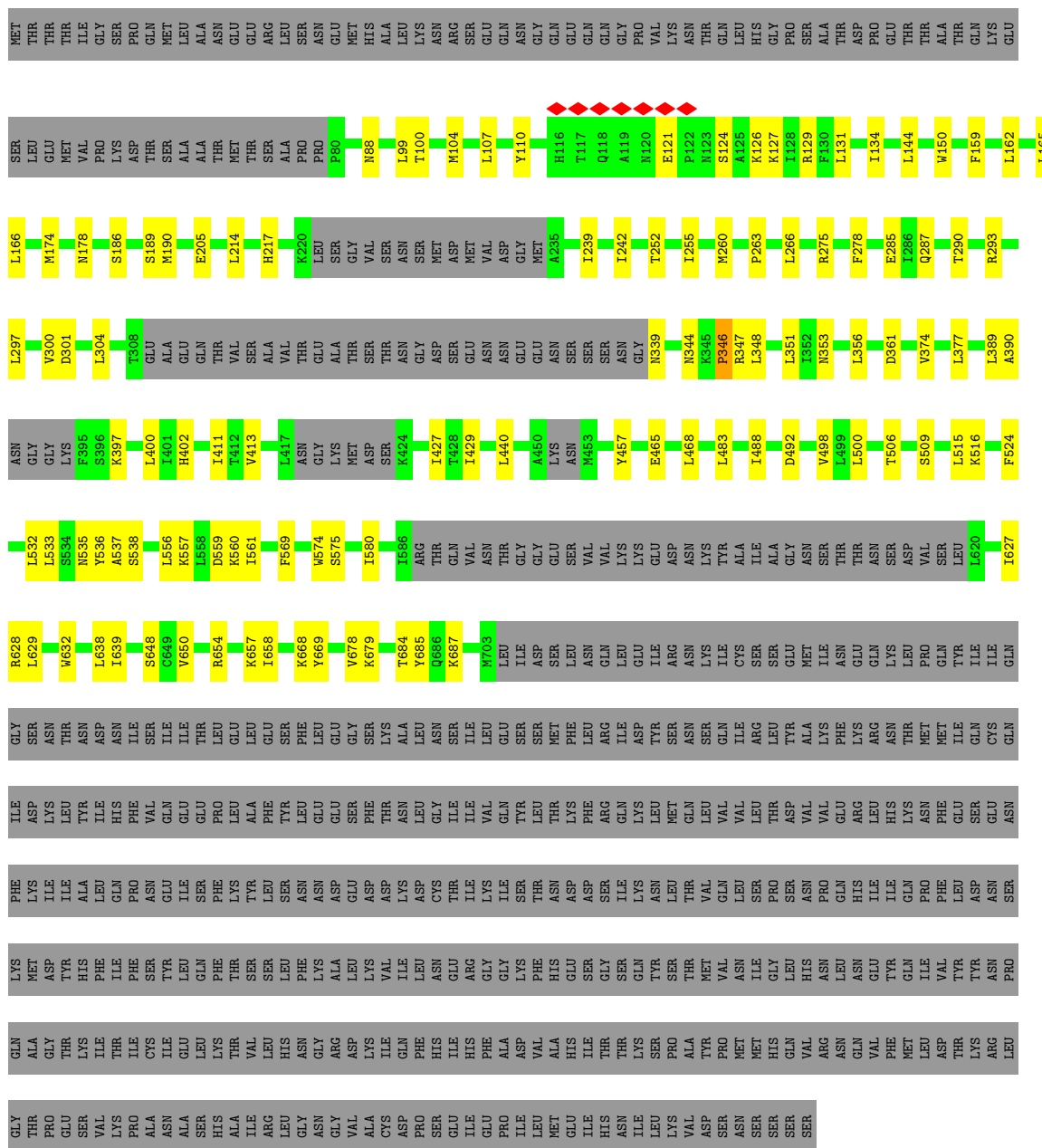
Chain j: 



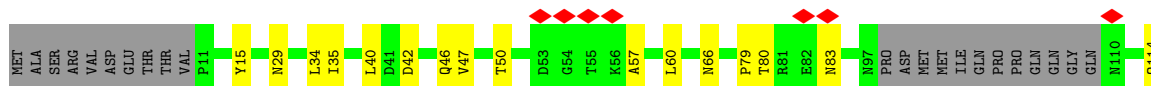
- Molecule 41: Mediator of RNA polymerase II transcription subunit 10

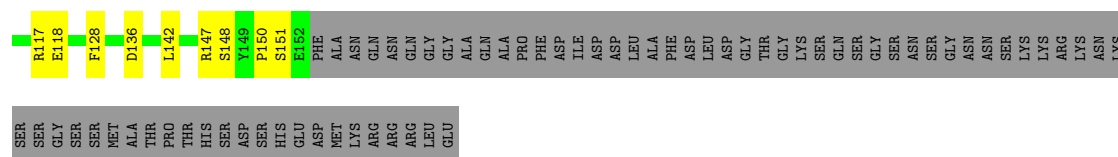
Chain k: 



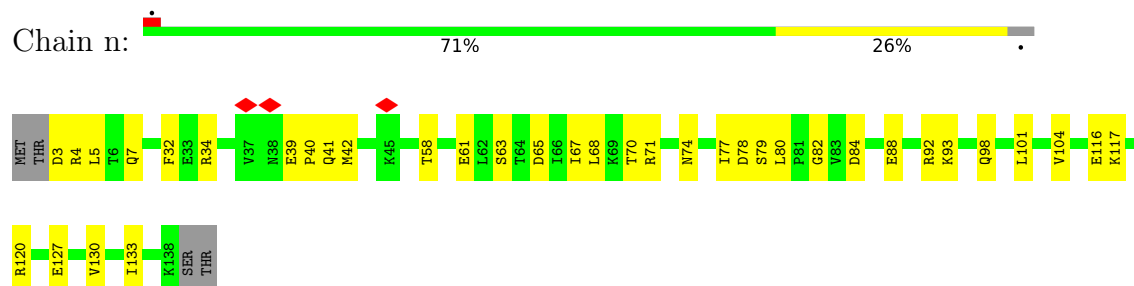


- Molecule 43: Mediator of RNA polymerase II transcription subunit 19

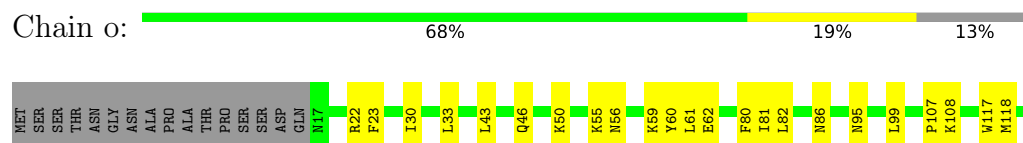




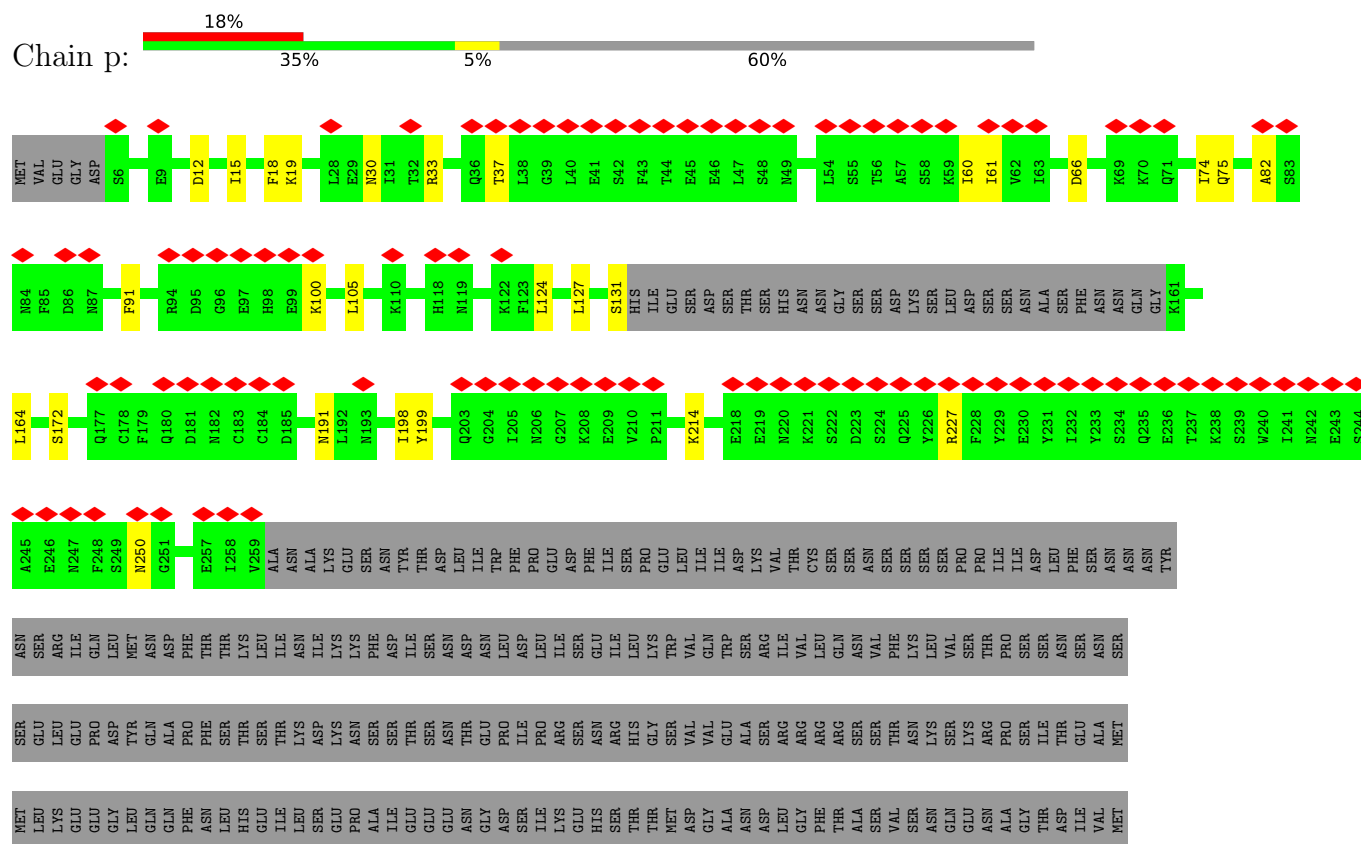
• Molecule 44: Mediator of RNA polymerase II transcription subunit 21



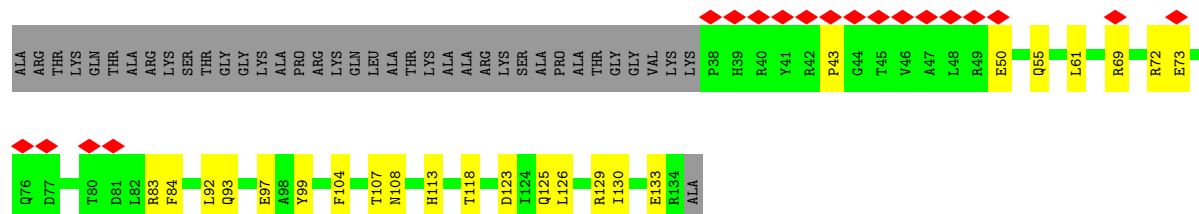
• Molecule 45: Mediator of RNA polymerase II transcription subunit 31



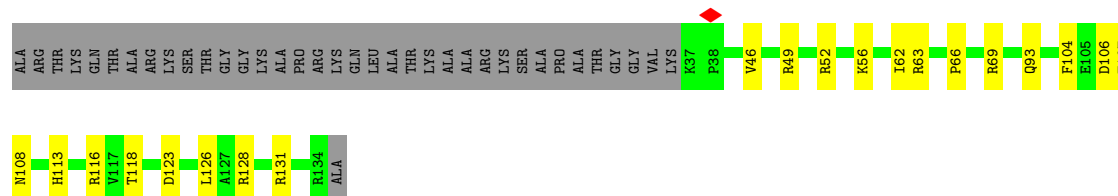
• Molecule 46: Mediator of RNA polymerase II transcription subunit 1



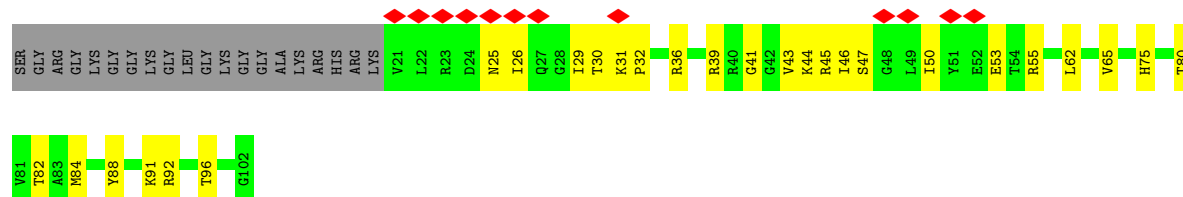
- Molecule 47: Histone H3.2



- Molecule 47: Histone H3.2



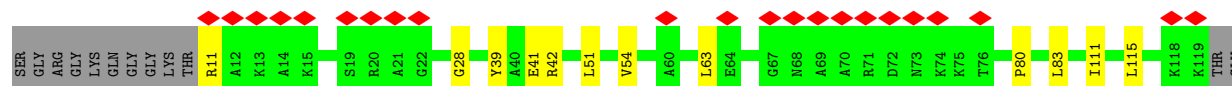
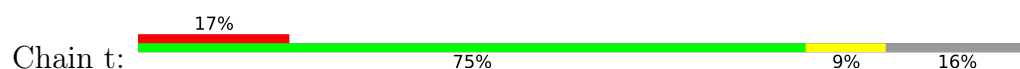
- Molecule 48: Histone H4



- Molecule 48: Histone H4



- Molecule 49: Histone H2A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50715	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	0.234	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.16	0/6209	0.34	0/8384
2	1	0.14	0/4277	0.33	0/5755
3	2	0.17	0/3717	0.42	0/5028
4	3	0.13	0/1109	0.36	0/1492
5	4	0.16	0/2377	0.35	0/3216
6	5	0.20	0/520	0.51	0/701
7	6	0.16	0/3082	0.39	0/4165
8	7	0.16	0/5059	0.35	0/6841
9	A	0.20	0/12048	0.37	0/16321
10	B	0.22	0/9589	0.36	0/12934
11	C	0.23	0/2130	0.36	0/2887
12	D	0.14	0/1351	0.37	0/1811
13	E	0.19	0/1788	0.45	2/2406 (0.1%)
14	F	0.22	0/1001	0.44	0/1347
15	G	0.18	0/1367	0.44	0/1844
16	H	0.20	0/1139	0.40	0/1544
17	I	0.19	0/962	0.43	0/1295
18	J	0.25	0/578	0.43	0/775
19	K	0.23	0/942	0.44	0/1272
20	L	0.23	0/361	0.49	0/478
21	M	0.17	0/2408	0.42	0/3241
22	N	0.23	0/4776	0.41	0/7366
23	O	0.21	0/1449	0.45	0/1952
24	Q	0.17	0/1907	0.37	0/2556
25	R	0.15	0/2270	0.37	0/3052
26	T	0.22	0/4830	0.37	0/7457
27	U	0.17	0/898	0.47	0/1212
28	V	0.17	0/822	0.45	0/1109
29	W	0.13	0/2513	0.34	0/3388
30	X	0.13	0/1739	0.37	0/2339
31	a	0.16	0/1531	0.45	0/2072
32	b	0.18	0/1436	0.50	0/1947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.20	0/913	0.46	0/1228
34	d	0.17	0/4118	0.42	0/5532
35	e	0.17	0/2054	0.41	1/2782 (0.0%)
36	f	0.18	0/1602	0.36	0/2169
37	g	0.20	0/818	0.48	0/1104
38	h	0.23	0/1415	0.62	0/1907
39	i	0.17	0/1543	0.45	1/2084 (0.0%)
40	j	0.24	0/865	0.71	0/1166
41	k	0.19	0/1277	0.48	0/1727
42	l	0.18	0/4468	0.49	3/6048 (0.0%)
43	m	0.15	0/1093	0.40	0/1481
44	n	0.21	0/1106	0.61	0/1488
45	o	0.19	0/949	0.48	0/1294
46	p	0.15	0/1898	0.40	0/2559
47	r	0.20	0/813	0.51	0/1091
47	v	0.18	0/822	0.44	0/1103
48	s	0.23	0/660	0.59	0/883
48	w	0.21	0/645	0.53	0/862
49	t	0.22	0/853	0.53	0/1149
49	x	0.18	0/828	0.45	0/1117
50	u	0.20	0/778	0.50	0/1043
50	y	0.20	0/756	0.54	0/1015
All	All	0.19	0/116459	0.41	7/159019 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	l	346	PRO	CA-N-CD	-11.55	95.84	112.00
42	l	346	PRO	N-CA-C	6.33	122.98	114.18
35	e	55	ARG	CA-CB-CG	6.29	126.69	114.10
42	l	346	PRO	N-CD-CG	-5.39	95.11	103.20
39	i	190	ARG	CB-CG-CD	5.21	123.28	111.30
13	E	101	GLN	N-CA-CB	5.19	118.30	110.30
13	E	102	GLU	N-CA-CB	5.00	118.56	110.40

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	90	0
2	1	4214	0	4288	52	0
3	2	3647	0	3732	38	0
4	3	1089	0	1069	19	0
5	4	2338	0	2404	40	0
6	5	514	0	541	10	0
7	6	3019	0	3040	47	0
8	7	4954	0	4946	81	0
9	A	11815	0	11816	156	0
10	B	9404	0	9398	112	0
11	C	2092	0	2050	28	0
12	D	1343	0	1366	18	0
13	E	1752	0	1776	12	0
14	F	983	0	968	22	0
15	G	1339	0	1357	23	0
16	H	1120	0	1086	27	0
17	I	944	0	899	15	0
18	J	569	0	585	6	0
19	K	924	0	934	7	0
20	L	359	0	381	7	0
21	M	2379	0	2488	38	0
22	N	4263	0	2359	37	0
23	O	1422	0	1500	25	0
24	Q	1871	0	1883	36	0
25	R	2230	0	2254	35	0
26	T	4300	0	2352	29	0
27	U	885	0	866	23	0
28	V	815	0	822	18	0
29	W	2473	0	2476	35	0
30	X	1708	0	1761	25	0
31	a	1495	0	1476	29	0
32	b	1407	0	1404	42	0
33	c	902	0	918	18	0
34	d	4063	0	4247	71	0
35	e	2017	0	2024	31	0
36	f	1578	0	1595	23	0
37	g	815	0	839	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	1394	0	1420	18	0
39	i	1512	0	1544	34	0
40	j	852	0	857	23	0
41	k	1259	0	1241	32	0
42	l	4385	0	4612	76	0
43	m	1068	0	1021	25	0
44	n	1095	0	1116	31	0
45	o	922	0	907	18	0
46	p	1863	0	1819	17	0
47	r	801	0	841	23	0
47	v	810	0	853	16	0
48	s	653	0	696	27	0
48	w	638	0	676	13	0
49	t	843	0	908	12	0
49	x	818	0	877	16	0
50	u	767	0	799	15	0
50	y	745	0	773	15	0
51	0	8	0	0	0	0
52	3	2	0	0	0	0
52	4	1	0	0	0	0
52	6	4	0	0	0	0
52	A	2	0	0	0	0
52	B	1	0	0	0	0
52	C	1	0	0	0	0
52	I	2	0	0	0	0
52	J	1	0	0	0	0
52	L	1	0	0	0	0
52	M	1	0	0	0	0
52	W	1	0	0	0	0
53	A	1	0	0	0	0
All	All	113584	0	111015	1429	0

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

All (1429) 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)
20:L:31:CYS:HB3	20:L:34:CYS:SG	2.08	0.93
16:H:75:ALA:N	16:H:98:TYR:HH	1.70	0.89
29:W:127:CYS:HB3	29:W:152:CYS:SG	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:82:GLU:O	41:k:86:TYR:HB2	1.84	0.78
32:b:80:THR:HG21	37:g:52:THR:HG21	1.67	0.76
45:o:55:LYS:HG2	45:o:59:LYS:HZ1	1.50	0.76
16:H:2:SER:N	16:H:61:SER:HG	1.84	0.75
39:i:24:THR:OG1	39:i:27:ASN:ND2	2.20	0.75
34:d:311:LYS:O	34:d:315:SER:HB3	1.87	0.74
44:n:117:LYS:HE2	44:n:120:ARG:HH12	1.52	0.74
35:e:55:ARG:HD2	35:e:56:ASN:H	1.53	0.72
34:d:315:SER:HB2	34:d:425:ILE:HG12	1.71	0.72
17:I:78:CYS:SG	17:I:106:CYS:HB3	2.30	0.72
14:F:65:ARG:HH12	14:F:74:ILE:HG13	1.55	0.71
28:V:78:PHE:HB2	28:V:113:ILE:HB	1.73	0.70
1:0:624:GLY:HA2	1:0:683:ASP:HB2	1.73	0.70
27:U:42:TRP:HA	27:U:45:LYS:HE3	1.75	0.69
3:2:387:LEU:HB3	3:2:448:LEU:HD22	1.75	0.69
23:O:183:SER:HB2	23:O:193:LEU:HD11	1.73	0.69
29:W:124:CYS:HB3	29:W:127:CYS:SG	2.32	0.68
9:A:40:THR:HG22	9:A:53:LEU:HB2	1.76	0.68
14:F:64:ILE:HG23	14:F:65:ARG:HG3	1.76	0.68
27:U:246:CYS:SG	27:U:247:LEU:N	2.67	0.67
41:k:90:GLY:HA3	43:m:80:THR:HG22	1.77	0.67
9:A:1151:GLU:HG2	17:I:45:ARG:HG3	1.76	0.67
49:x:112:GLN:HB2	49:x:115:LEU:HD23	1.75	0.67
8:7:409:VAL:HB	8:7:454:VAL:HG12	1.77	0.67
2:1:94:ARG:HH12	29:W:200:GLU:HB3	1.58	0.67
10:B:1163:CYS:HB2	10:B:1187:ASN:HD21	1.60	0.66
9:A:469:ARG:NH2	10:B:991:GLY:O	2.28	0.66
39:i:152:ARG:HH12	42:l:190:MET:HB2	1.60	0.66
35:e:64:ILE:HD11	35:e:204:MET:HE1	1.76	0.66
6:5:17:LYS:NZ	6:5:36:ASP:O	2.27	0.66
37:g:20:LYS:NZ	37:g:61:GLN:O	2.29	0.66
38:h:91:ASP:OD1	38:h:95:ARG:NH1	2.29	0.66
49:x:32:ARG:HH22	50:y:32:GLU:HG3	1.61	0.66
8:7:711:LYS:HA	8:7:716:MET:HE3	1.78	0.65
29:W:65:ARG:HH21	30:X:268:LEU:HD13	1.60	0.65
37:g:56:MET:O	37:g:60:ASN:HB3	1.96	0.65
42:l:263:PRO:HG2	42:l:266:LEU:HB2	1.79	0.65
1:0:307:VAL:HG22	1:0:400:LYS:HG2	1.79	0.65
8:7:625:PRO:HG2	8:7:652:ILE:HG22	1.79	0.65
27:U:18:VAL:HG21	27:U:39:LYS:HZ1	1.61	0.65
2:1:49:GLN:HB2	2:1:61:ARG:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:48:ARG:NH1	18:J:49:MET:SD	2.70	0.64
39:i:140:ASN:HD22	39:i:143:MET:HE2	1.61	0.64
11:C:262:LEU:HD11	19:K:84:LYS:HG2	1.79	0.64
22:N:-15:DC:H5	26:T:15:DG:H1	1.46	0.64
9:A:1444:MET:HE2	14:F:135:ARG:HB2	1.80	0.64
7:6:136:MET:HE1	7:6:237:GLY:HA3	1.79	0.63
43:m:50:THR:HA	43:m:57:ALA:H	1.62	0.63
23:O:157:ILE:HD12	23:O:160:ILE:HD11	1.81	0.63
9:A:1192:LEU:HD11	9:A:1239:ARG:HB3	1.80	0.63
39:i:120:ARG:NH2	44:n:78:ASP:OD1	2.32	0.62
10:B:542:MET:HG3	10:B:747:MET:HB3	1.80	0.62
1:0:56:THR:HG21	1:0:233:ILE:HD11	1.79	0.62
2:1:252:SER:H	2:1:255:LYS:HD2	1.64	0.62
9:A:107:CYS:SG	9:A:171:GLN:NE2	2.72	0.62
10:B:68:THR:HB	24:Q:334:VAL:HG11	1.82	0.62
35:e:282:LEU:HD13	35:e:286:ILE:HD11	1.82	0.62
39:i:143:MET:HB3	39:i:146:ARG:HH12	1.63	0.62
8:7:133:TRP:HB2	8:7:142:ILE:HB	1.82	0.62
42:l:260:MET:HE1	42:l:361:ASP:HB2	1.82	0.62
1:0:534:PRO:HA	7:6:239:LEU:HB3	1.81	0.62
1:0:326:ARG:NH1	4:3:111:GLU:OE2	2.33	0.62
40:j:70:PHE:HA	40:j:73:LEU:HG	1.82	0.62
27:U:272:ASN:HD22	27:U:273:ASP:N	1.97	0.61
29:W:201:ILE:HG22	29:W:205:ARG:HH12	1.65	0.61
11:C:22:LEU:HG	11:C:25:VAL:HG11	1.81	0.61
32:b:53:GLU:HG3	32:b:60:PRO:HG3	1.82	0.61
34:d:639:ASN:HB3	34:d:642:ASN:HB2	1.82	0.61
14:F:65:ARG:HD3	14:F:72:LYS:HA	1.83	0.61
34:d:452:LEU:HD11	34:d:543:ARG:HG3	1.81	0.61
1:0:25:MET:HG3	1:0:55:LEU:HB2	1.82	0.61
1:0:539:VAL:HG22	1:0:621:LEU:HB3	1.81	0.61
24:Q:130:VAL:HG23	24:Q:131:THR:HG23	1.83	0.61
27:U:260:CYS:HB2	27:U:281:VAL:HB	1.81	0.61
9:A:243:PRO:HB2	9:A:245:PRO:HD2	1.82	0.61
21:M:303:GLN:HE21	25:R:271:ARG:HA	1.65	0.61
22:N:9:DT:H5''	50:u:52:SER:HA	1.83	0.61
41:k:154:SER:OG	43:m:29:ASN:ND2	2.33	0.61
1:0:326:ARG:HH12	4:3:107:ASN:HB3	1.65	0.61
9:A:1613:SER:HB2	42:l:189:SER:HB2	1.83	0.61
15:G:46:LEU:HD21	15:G:105:PRO:HG3	1.83	0.61
21:M:185:VAL:HG22	21:M:187:ARG:HH12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:601:VAL:HG12	1:0:603:ARG:H	1.66	0.60
8:7:606:ILE:HG23	8:7:654:LEU:HD13	1.83	0.60
9:A:291:GLU:HG2	21:M:113:ALA:HB2	1.82	0.60
2:1:174:LEU:HD12	2:1:217:LEU:HB3	1.83	0.60
42:l:411:ILE:HB	42:l:429:ILE:HB	1.83	0.60
17:l:101:PHE:HE1	17:l:112:SER:HB3	1.66	0.60
10:B:71:LEU:HD11	24:Q:329:THR:HB	1.83	0.60
36:f:40:ARG:HB2	36:f:59:SER:HB3	1.82	0.60
42:l:483:LEU:HD22	42:l:488:ILE:HD11	1.83	0.60
16:H:124:ARG:NH1	16:H:126:GLU:OE2	2.35	0.60
32:b:61:GLN:HE21	32:b:64:THR:HG23	1.67	0.60
42:l:124:SER:HB2	43:m:150:PRO:HG2	1.84	0.60
9:A:450:LEU:HD13	9:A:1077:THR:HG21	1.83	0.60
1:0:321:ILE:O	1:0:326:ARG:NH2	2.35	0.60
11:C:39:ALA:HA	11:C:164:ALA:HB3	1.83	0.60
22:N:68:DC:O2	26:T:-67:DG:N2	2.35	0.60
44:n:67:ILE:HG22	44:n:71:ARG:HH11	1.66	0.59
9:A:899:VAL:HG22	9:A:1029:ARG:HH11	1.67	0.59
15:G:46:LEU:HB2	15:G:77:VAL:HG13	1.84	0.59
47:v:108:ASN:ND2	48:w:42:GLY:O	2.35	0.59
31:a:21:GLY:O	31:a:26:ASN:ND2	2.35	0.59
31:a:121:ARG:HB3	31:a:125:PHE:HB3	1.83	0.59
1:0:76:MET:HA	1:0:79:ILE:HD12	1.84	0.59
3:2:90:ASN:HB3	3:2:97:MET:HB3	1.83	0.59
6:5:31:VAL:HG21	6:5:40:LEU:HD12	1.84	0.59
8:7:124:ARG:NH2	8:7:198:ASP:OD1	2.35	0.59
8:7:601:ARG:NH1	8:7:603:ASP:OD2	2.35	0.59
38:h:110:LYS:NZ	39:i:209:THR:OG1	2.36	0.59
8:7:738:HIS:HB3	29:W:298:THR:HB	1.85	0.59
10:B:108:VAL:HG23	21:M:244:SER:HB2	1.85	0.59
10:B:1120:GLU:O	10:B:1124:ARG:NH1	2.35	0.59
13:E:28:TYR:HA	13:E:64:PRO:HA	1.83	0.59
16:H:33:GLN:HB3	16:H:35:GLN:HG3	1.85	0.59
21:M:22:LEU:HD13	21:M:43:VAL:HG11	1.84	0.59
36:f:132:LEU:HB2	36:f:135:LEU:HB3	1.82	0.59
1:0:725:ALA:HB1	7:6:290:ILE:HG13	1.85	0.59
10:B:119:LEU:HD13	10:B:953:LEU:HD11	1.84	0.59
14:F:85:MET:HB2	14:F:151:LEU:HB3	1.85	0.59
42:l:629:LEU:HB3	42:l:632:TRP:HE1	1.67	0.59
21:M:259:THR:HG23	21:M:323:LEU:HB3	1.85	0.59
27:U:272:ASN:HD22	27:U:273:ASP:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:287:ARG:NH1	10:B:292:ILE:O	2.35	0.58
9:A:406:ILE:HB	9:A:431:LYS:HB2	1.84	0.58
17:I:10:CYS:SG	17:I:31:THR:OG1	2.61	0.58
25:R:59:LEU:HD21	25:R:214:ILE:HG12	1.85	0.58
33:c:15:ASP:OD2	33:c:19:GLN:NE2	2.36	0.58
41:k:60:LEU:HD22	42:l:100:THR:HG22	1.85	0.58
9:A:119:ASN:HB3	9:A:122:MET:HG2	1.84	0.58
44:n:65:ASP:HA	44:n:68:LEU:HG	1.84	0.58
29:W:105:VAL:HG13	30:X:262:MET:HE2	1.85	0.58
39:i:152:ARG:HD3	42:l:186:SER:HB3	1.85	0.58
10:B:728:ARG:NH1	10:B:760:ASP:OD2	2.36	0.58
27:U:245:LEU:HD11	28:V:12:ARG:HB2	1.86	0.58
7:6:221:LEU:HD13	7:6:230:ARG:HB3	1.85	0.58
9:A:875:ALA:HB2	9:A:1366:ARG:HD2	1.85	0.58
21:M:215:ARG:NH1	23:O:180:GLY:O	2.37	0.58
42:l:639:ILE:HB	42:l:654:ARG:HB2	1.85	0.58
7:6:330:GLU:HG3	7:6:332:THR:H	1.68	0.58
8:7:552:VAL:HG12	8:7:703:ALA:HB3	1.85	0.58
28:V:66:LEU:HA	28:V:80:VAL:HA	1.85	0.58
45:o:62:GLU:OE2	45:o:86:ASN:ND2	2.36	0.58
10:B:137:TYR:HB3	10:B:149:TYR:HB3	1.86	0.58
22:N:50:DA:H5"	48:s:30:THR:HG21	1.86	0.58
36:f:108:LEU:HA	36:f:112:LEU:HB2	1.84	0.58
42:l:290:THR:HB	42:l:297:LEU:HG	1.85	0.58
8:7:497:MET:HB2	8:7:500:ARG:HE	1.68	0.58
9:A:451:HIS:O	9:A:454:SER:OG	2.22	0.58
48:s:43:VAL:HG21	48:s:46:ILE:HD11	1.86	0.58
4:3:17:LYS:HB3	29:W:176:MET:HG3	1.85	0.57
7:6:338:CYS:SG	7:6:339:HIS:CE1	2.97	0.57
9:A:1199:ARG:NH2	9:A:1233:ASP:O	2.37	0.57
24:Q:151:LEU:HD23	25:R:201:TYR:HB3	1.86	0.57
28:V:8:GLU:HB2	28:V:11:ARG:HH22	1.68	0.57
30:X:289:ASP:O	30:X:295:ARG:NH2	2.37	0.57
2:1:91:PHE:HB2	2:1:97:MET:HE3	1.86	0.57
2:1:250:ASN:HA	29:W:263:ASN:HB2	1.85	0.57
10:B:561:TRP:HE1	25:R:240:ARG:HD3	1.70	0.57
10:B:776:GLN:HE22	14:F:17:ASP:HB2	1.69	0.57
3:2:458:LEU:HD21	3:2:490:LYS:HD3	1.84	0.57
8:7:568:GLU:OE1	8:7:571:ARG:NH1	2.38	0.57
10:B:416:LEU:HD23	10:B:457:LEU:HD23	1.86	0.57
10:B:883:LEU:HD11	10:B:928:ARG:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:253:ARG:HE	29:W:266:THR:HA	1.68	0.57
10:B:1077:THR:HG23	10:B:1079:LYS:H	1.69	0.57
9:A:1397:LEU:HB2	9:A:1426:GLU:HG3	1.87	0.57
24:Q:421:PRO:HG2	24:Q:424:LEU:HB3	1.86	0.57
31:a:165:THR:HA	32:b:94:VAL:HA	1.86	0.57
41:k:52:ASN:O	41:k:56:ASN:ND2	2.38	0.57
21:M:185:VAL:O	21:M:187:ARG:NH1	2.38	0.57
11:C:143:LEU:HD21	11:C:146:LYS:HE3	1.87	0.57
26:T:-106:DA:H5"	49:x:16:THR:HA	1.87	0.57
40:j:136:LYS:HA	40:j:139:VAL:HG12	1.87	0.57
1:0:460:SER:HB3	1:0:463:ILE:HB	1.86	0.56
1:0:678:VAL:HG11	1:0:717:THR:HG23	1.87	0.56
34:d:394:PHE:HB3	34:d:403:TYR:HB3	1.87	0.56
41:k:81:LEU:HD22	42:l:88:ASN:HB3	1.86	0.56
47:r:104:PHE:HA	47:r:107:THR:HG22	1.86	0.56
47:v:62:ILE:O	47:v:93:GLN:NE2	2.38	0.56
1:0:640:GLU:OE1	1:0:643:ARG:NH2	2.38	0.56
8:7:682:GLN:HG2	8:7:722:ARG:HH22	1.70	0.56
8:7:832:LEU:HD21	9:A:1262:LYS:HB3	1.86	0.56
9:A:715:GLU:OE2	9:A:774:ARG:NH1	2.38	0.56
10:B:234:ILE:HD13	10:B:257:LYS:HD2	1.87	0.56
10:B:904:ARG:NH2	20:L:66:GLN:O	2.39	0.56
11:C:142:VAL:HG11	18:J:5:VAL:HG13	1.87	0.56
17:I:29:CYS:HB3	17:I:34:TYR:H	1.70	0.56
41:k:96:TYR:O	41:k:100:PHE:HB2	2.05	0.56
42:l:127:LYS:NZ	43:m:148:SER:O	2.35	0.56
47:r:118:THR:OG1	48:s:45:ARG:NH1	2.37	0.56
42:l:110:TYR:OH	42:l:126:LYS:O	2.24	0.56
1:0:571:VAL:HG22	1:0:599:LEU:HD12	1.87	0.56
2:1:561:LEU:HD13	2:1:623:ILE:HG22	1.88	0.56
24:Q:121:PHE:HB2	25:R:131:ASN:HB3	1.88	0.56
46:p:61:ILE:HD11	46:p:124:LEU:HD23	1.86	0.56
1:0:228:LYS:NZ	43:m:151:SER:O	2.39	0.56
11:C:136:ASP:N	11:C:136:ASP:OD1	2.38	0.56
21:M:140:ALA:HB2	21:M:195:LEU:HD11	1.87	0.56
24:Q:433:THR:HG22	24:Q:434:THR:HG23	1.88	0.56
44:n:34:ARG:NH1	44:n:40:PRO:O	2.37	0.56
50:y:69:ARG:HB3	50:y:98:LEU:HD11	1.87	0.56
1:0:6:ASP:HB2	1:0:29:LYS:HE3	1.88	0.56
9:A:427:GLN:HG3	35:e:177:ASN:HD21	1.71	0.56
9:A:596:THR:OG1	9:A:598:LEU:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:54:DA:N6	26:T:-55:DG:O6	2.39	0.56
36:f:87:ILE:HD11	36:f:101:PRO:HD3	1.88	0.56
42:l:239:ILE:HA	42:l:242:ILE:HG22	1.88	0.56
9:A:346:ASP:OD1	10:B:1106:ARG:NE	2.39	0.56
2:1:573:GLN:HE22	5:4:328:ARG:HH22	1.52	0.56
7:6:394:THR:HG21	7:6:422:LEU:HD12	1.86	0.56
8:7:111:GLY:O	8:7:114:ARG:NH2	2.39	0.56
8:7:679:SER:OG	8:7:722:ARG:NH1	2.38	0.56
21:M:281:SER:O	21:M:285:ASN:ND2	2.33	0.56
35:e:98:ILE:HG22	35:e:100:LEU:H	1.71	0.56
40:j:119:PRO:O	40:j:123:GLN:NE2	2.40	0.56
42:l:390:ALA:HB2	42:l:397:LYS:HE3	1.88	0.56
12:D:119:ARG:HH21	12:D:152:SER:H	1.52	0.55
32:b:130:ARG:HH12	34:d:271:GLU:HG2	1.71	0.55
33:c:32:PHE:HB2	34:d:288:LYS:HG3	1.89	0.55
1:0:108:LEU:HB3	1:0:208:TYR:HB3	1.88	0.55
9:A:350:ARG:HB2	10:B:1128:LEU:HD21	1.87	0.55
40:j:10:GLN:O	40:j:14:ILE:HB	2.07	0.55
1:0:287:GLU:OE1	1:0:291:GLN:NE2	2.40	0.55
34:d:562:ILE:HD13	34:d:619:ILE:HD11	1.89	0.55
47:v:104:PHE:HA	47:v:107:THR:HG22	1.88	0.55
6:5:32:LEU:HB2	6:5:41:LEU:HD22	1.88	0.55
8:7:672:GLN:OE1	8:7:722:ARG:NH2	2.39	0.55
9:A:443:LEU:HB3	9:A:490:HIS:HB2	1.88	0.55
10:B:996:ARG:NH1	11:C:174:ALA:O	2.40	0.55
2:1:497:ASN:OD1	3:2:55:ASN:ND2	2.39	0.55
9:A:184:SER:HB2	9:A:197:PRO:HB2	1.87	0.55
23:O:205:LEU:HB2	23:O:213:VAL:HB	1.88	0.55
32:b:25:PHE:CE1	34:d:231:SER:HB2	2.41	0.55
42:l:214:LEU:HD21	45:o:121:MET:HB3	1.89	0.55
4:3:45:ARG:NH2	29:W:165:ASN:OD1	2.40	0.55
5:4:162:ARG:NH1	7:6:406:CYS:O	2.39	0.55
9:A:147:VAL:HG13	9:A:149:GLU:HG2	1.89	0.55
44:n:98:GLN:HA	44:n:98:GLN:HE21	1.71	0.55
48:s:26:ILE:HG13	48:s:55:ARG:HD3	1.89	0.55
47:v:106:ASP:OD2	47:v:131:ARG:NH1	2.39	0.55
9:A:840:ARG:NH2	9:A:1106:ASN:OD1	2.40	0.55
12:D:162:ALA:HA	12:D:165:GLN:HG3	1.88	0.55
42:l:515:LEU:HD11	42:l:524:PHE:HB3	1.89	0.55
2:1:8:ILE:HB	2:1:90:SER:HB2	1.89	0.55
3:2:208:LEU:HD23	3:2:211:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:972:LYS:HG3	10:B:1098:MET:HE3	1.89	0.55
15:G:165:GLU:HB3	15:G:168:LEU:HD13	1.89	0.55
24:Q:141:ARG:NH1	24:Q:348:TYR:O	2.39	0.55
33:c:65:GLN:HG3	33:c:68:LYS:HZ3	1.72	0.55
38:h:121:CYS:HB2	39:i:202:LYS:HE3	1.89	0.55
42:l:532:LEU:HD11	42:l:560:LYS:HD3	1.89	0.55
9:A:119:ASN:O	9:A:123:ARG:NH1	2.40	0.55
11:C:6:PRO:O	19:K:104:ASN:ND2	2.40	0.55
41:k:106:ARG:NH1	44:n:42:MET:O	2.40	0.55
50:u:38:VAL:HA	50:u:41:VAL:HG12	1.89	0.55
2:1:290:SER:O	2:1:294:ARG:NH1	2.40	0.54
9:A:402:ALA:HA	9:A:434:ARG:HA	1.89	0.54
39:i:186:ARG:HB3	39:i:190:ARG:NH1	2.22	0.54
49:x:68:ASN:OD1	49:x:71:ARG:NH2	2.40	0.54
3:2:443:LEU:HD11	8:7:735:VAL:HG21	1.89	0.54
32:b:115:ARG:NH2	32:b:117:LYS:O	2.38	0.54
34:d:20:ALA:HB2	38:h:145:ARG:HB2	1.90	0.54
47:r:83:ARG:HB2	48:s:80:THR:HG22	1.89	0.54
3:2:251:GLN:OE1	3:2:254:ARG:NH2	2.40	0.54
32:b:37:ARG:HD3	34:d:229:LEU:HD13	1.89	0.54
42:l:252:THR:HG23	42:l:293:ARG:HH22	1.73	0.54
45:o:30:ILE:HD11	45:o:82:LEU:HD22	1.88	0.54
1:0:295:SER:HB3	1:0:379:GLU:HG3	1.88	0.54
1:0:429:ALA:HB2	2:1:364:ILE:HG13	1.88	0.54
9:A:440:ASP:OD1	9:A:498:ARG:NH2	2.36	0.54
16:H:2:SER:N	16:H:61:SER:OG	2.39	0.54
21:M:44:VAL:HG12	21:M:51:VAL:HG12	1.90	0.54
29:W:40:GLU:HG2	29:W:44:LYS:HE2	1.90	0.54
31:a:88:PRO:HA	31:a:91:ARG:HB2	1.88	0.54
40:j:6:ASN:OD1	40:j:7:VAL:N	2.41	0.54
50:y:60:ASN:OD1	50:y:64:ASN:ND2	2.40	0.54
4:3:80:LYS:NZ	4:3:121:ASP:OD1	2.41	0.54
9:A:1580:THR:HG23	45:o:108:LYS:HD3	1.90	0.54
23:O:107:ARG:HE	27:U:286:VAL:HB	1.73	0.54
29:W:159:ASP:O	29:W:163:LYS:NZ	2.41	0.54
40:j:131:GLN:NE2	40:j:132:GLU:OE1	2.41	0.54
42:l:353:ASN:HA	42:l:356:LEU:HD12	1.90	0.54
1:0:532:ILE:HD13	1:0:714:ILE:HG23	1.90	0.54
10:B:864:LYS:HA	10:B:961:LEU:HD13	1.89	0.54
15:G:108:VAL:HG22	15:G:159:ALA:HB3	1.89	0.54
6:5:37:ASP:OD1	6:5:37:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:332:LYS:HG3	14:F:24:SER:HA	1.90	0.54
16:H:133:ASN:O	38:h:62:ARG:NH1	2.40	0.54
17:I:29:CYS:SG	17:I:31:THR:OG1	2.64	0.54
22:N:-26:DT:H2"	22:N:-25:DG:C8	2.43	0.54
34:d:527:PRO:HA	35:e:223:PHE:HB3	1.90	0.54
9:A:1009:ASN:OD1	9:A:1012:ARG:NH2	2.40	0.54
15:G:84:GLY:N	15:G:147:ILE:O	2.40	0.54
15:G:112:LYS:NZ	29:W:122:TYR:OH	2.40	0.54
22:N:90:DG:N2	26:T:-89:DC:O2	2.41	0.54
42:l:304:LEU:O	42:l:339:ASN:ND2	2.40	0.54
3:2:201:TRP:NE1	3:2:278:LEU:O	2.40	0.54
8:7:542:GLU:HG2	8:7:546:LYS:HZ2	1.73	0.54
10:B:526:GLU:HG3	10:B:771:SER:HB3	1.89	0.54
21:M:212:ASN:OD1	21:M:215:ARG:NH2	2.40	0.54
1:0:322:PRO:O	4:3:107:ASN:ND2	2.41	0.54
3:2:221:VAL:HG13	3:2:249:MET:HE3	1.90	0.54
23:O:88:HIS:HB2	23:O:146:ILE:HD11	1.90	0.54
43:m:42:ASP:OD1	43:m:42:ASP:N	2.41	0.54
47:v:128:ARG:HH11	48:w:57:VAL:HG22	1.71	0.54
7:6:333:PRO:HB2	7:6:342:LEU:HD12	1.89	0.53
8:7:495:ALA:HB3	8:7:498:PHE:HB2	1.90	0.53
8:7:660:THR:O	8:7:689:ARG:NH2	2.40	0.53
42:l:174:MET:O	42:l:178:ASN:N	2.42	0.53
3:2:172:LEU:HD12	3:2:188:GLY:HA2	1.90	0.53
7:6:136:MET:HB3	7:6:146:HIS:HB2	1.91	0.53
12:D:202:ILE:HG21	12:D:207:LEU:HD13	1.89	0.53
21:M:188:THR:H	21:M:191:GLU:HG3	1.73	0.53
24:Q:137:VAL:HG23	25:R:59:LEU:HB3	1.89	0.53
13:E:86:PRO:HA	13:E:113:GLN:HB2	1.91	0.53
14:F:97:ARG:NH1	14:F:100:GLN:OE1	2.41	0.53
17:I:5:ARG:HB3	17:I:14:LEU:HD12	1.91	0.53
30:X:225:GLU:OE1	30:X:234:ARG:NH1	2.41	0.53
1:0:16:LYS:NZ	2:1:425:ASN:O	2.36	0.53
1:0:83:LEU:HD13	1:0:177:SER:HA	1.91	0.53
9:A:175:ARG:HH21	9:A:199:LEU:HD13	1.73	0.53
10:B:567:GLU:HG3	24:Q:368:GLY:HA3	1.89	0.53
13:E:62:ALA:HB3	13:E:78:LEU:HB3	1.90	0.53
22:N:51:DC:OP2	48:s:30:THR:OG1	2.27	0.53
31:a:166:ILE:HA	31:a:169:ILE:HD12	1.90	0.53
49:x:51:LEU:HD13	50:y:91:ILE:HD11	1.90	0.53
9:A:16:GLU:HB3	9:A:1418:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:200:ARG:NH1	9:A:201:VAL:O	2.41	0.53
9:A:325:ILE:HB	10:B:1210:MET:HE3	1.90	0.53
24:Q:359:ASN:HB3	24:Q:361:TRP:HE1	1.74	0.53
35:e:53:ASN:HB2	36:f:113:SER:HB2	1.90	0.53
41:k:151:ASP:HB3	41:k:154:SER:HB2	1.91	0.53
1:0:74:ARG:NH1	1:0:664:GLN:OE1	2.40	0.53
9:A:914:GLU:OE2	9:A:977:LYS:NZ	2.42	0.53
17:I:19:ASP:OD2	17:I:24:ARG:NH1	2.41	0.53
22:N:-58:DT:H4'	23:O:158:GLN:HB3	1.91	0.53
22:N:134:DA:H61	26:T:-134:DT:H3	1.56	0.53
24:Q:150:GLN:O	24:Q:437:ARG:NH1	2.42	0.53
14:F:97:ARG:HD3	14:F:130:ILE:HG23	1.89	0.53
33:c:66:LEU:HD23	37:g:10:LEU:HD13	1.91	0.53
34:d:445:ILE:HD11	34:d:508:LEU:HD22	1.89	0.53
9:A:744:LYS:HG3	9:A:748:MET:HE2	1.91	0.53
9:A:1386:ARG:NH2	14:F:32:LYS:O	2.41	0.53
15:G:131:GLN:HG3	15:G:136:VAL:HG12	1.90	0.53
22:N:-59:DA:N3	23:O:159:ASN:ND2	2.53	0.53
28:V:8:GLU:HB2	28:V:11:ARG:HH12	1.73	0.53
40:j:73:LEU:O	40:j:77:ARG:NH1	2.42	0.53
42:l:498:VAL:HG23	42:l:516:LYS:HG2	1.89	0.53
48:w:68:ASP:OD2	48:w:93:GLN:NE2	2.42	0.53
32:b:49:ARG:NH2	32:b:52:ASP:OD2	2.39	0.53
32:b:51:ARG:NH1	34:d:212:ASN:OD1	2.41	0.53
33:c:24:LEU:HD11	34:d:291:LEU:HD22	1.91	0.53
50:y:28:LYS:HE3	50:y:29:THR:H	1.74	0.53
9:A:326:ARG:HG3	9:A:1406:VAL:HG21	1.90	0.53
9:A:473:SER:OG	9:A:650:GLN:NE2	2.42	0.53
9:A:1155:ASP:HB3	9:A:1241:ARG:HH12	1.74	0.53
46:p:74:ILE:HD11	46:p:105:LEU:HA	1.89	0.53
25:R:44:ASP:OD1	25:R:48:ASN:ND2	2.42	0.52
25:R:90:GLN:HE21	25:R:92:LEU:HD21	1.73	0.52
27:U:267:VAL:HG21	28:V:60:LEU:HD22	1.90	0.52
30:X:289:ASP:HB2	30:X:293:ILE:HD12	1.91	0.52
35:e:34:TYR:OH	35:e:233:GLN:OE1	2.26	0.52
42:l:162:LEU:HD23	43:m:40:LEU:HD13	1.90	0.52
49:x:91:GLU:HA	49:x:94:ASN:HB2	1.91	0.52
5:4:166:GLU:HG2	5:4:168:VAL:HG13	1.91	0.52
9:A:1125:ALA:HB1	9:A:1303:GLU:HG3	1.91	0.52
10:B:89:GLU:HB3	10:B:135:ARG:HB2	1.90	0.52
21:M:180:CYS:HB3	21:M:186:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:73:ARG:HB3	29:W:83:GLU:HA	1.91	0.52
31:a:200:VAL:HG13	32:b:62:TRP:HD1	1.75	0.52
34:d:390:ARG:HH22	34:d:392:ARG:HH21	1.56	0.52
35:e:196:LYS:NZ	36:f:74:ASP:O	2.42	0.52
45:o:46:GLN:O	45:o:50:LYS:HB2	2.09	0.52
2:1:363:ASP:OD2	2:1:367:ASN:ND2	2.42	0.52
5:4:32:ILE:HA	5:4:37:TRP:HE1	1.72	0.52
11:C:66:ARG:NH2	11:C:143:LEU:O	2.38	0.52
2:1:32:THR:HG21	29:W:208:PRO:HB2	1.92	0.52
39:i:169:GLN:HG3	44:n:5:LEU:HD13	1.90	0.52
6:5:17:LYS:HG3	6:5:40:LEU:HD21	1.91	0.52
10:B:806:THR:HG22	10:B:808:ALA:H	1.74	0.52
9:A:35:ILE:HG21	9:A:53:LEU:HD23	1.90	0.52
9:A:946:VAL:HG22	13:E:201:LYS:HD2	1.92	0.52
30:X:168:ARG:NH1	30:X:181:LEU:O	2.42	0.52
32:b:135:VAL:HG13	34:d:274:ILE:HD11	1.92	0.52
39:i:85:VAL:HG23	39:i:86:LYS:HG2	1.92	0.52
44:n:77:ILE:HA	44:n:80:LEU:HG	1.92	0.52
47:r:125:GLN:NE2	48:s:53:GLU:OE2	2.42	0.52
8:7:552:VAL:HG21	8:7:687:LEU:HD11	1.91	0.52
32:b:29:PRO:HG2	32:b:33:LEU:HB2	1.91	0.52
41:k:28:SER:OG	41:k:56:ASN:ND2	2.43	0.52
41:k:151:ASP:O	41:k:155:ASN:ND2	2.42	0.52
43:m:46:GLN:HG3	43:m:47:VAL:HG13	1.91	0.52
3:2:450:ARG:NH2	6:5:13:ASP:OD2	2.43	0.52
8:7:568:GLU:HG3	8:7:760:LEU:HD11	1.92	0.52
23:O:204:LEU:HD22	23:O:214:LEU:HG	1.92	0.52
24:Q:155:GLU:HG2	24:Q:441:THR:HG22	1.91	0.52
34:d:124:LEU:HD13	42:l:242:ILE:HG23	1.92	0.52
35:e:93:PHE:O	35:e:234:LYS:NZ	2.43	0.52
8:7:679:SER:HB3	22:N:-14:DA:H5"	1.92	0.52
9:A:362:ASP:HB3	9:A:508:PRO:HD3	1.91	0.52
7:6:389:PHE:HB3	7:6:427:TYR:HB3	1.92	0.52
8:7:514:THR:HG21	8:7:517:LEU:HD13	1.92	0.52
9:A:1399:ARG:HB3	9:A:1408:ILE:HD13	1.92	0.52
30:X:155:LYS:NZ	30:X:156:ASP:O	2.40	0.52
46:p:66:ASP:HB3	46:p:75:GLN:HB2	1.92	0.52
2:1:441:ALA:HB3	5:4:190:ILE:HD12	1.93	0.51
8:7:235:GLU:OE2	8:7:313:VAL:N	2.44	0.51
11:C:44:LEU:HB2	11:C:77:ILE:HD13	1.92	0.51
39:i:175:ILE:HD13	44:n:93:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:275:ARG:HD3	42:l:300:VAL:HG11	1.92	0.51
47:r:99:TYR:OH	47:r:133:GLU:OE2	2.27	0.51
2:1:171:LYS:HG3	2:1:214:ILE:HG13	1.92	0.51
8:7:236:THR:HG22	8:7:238:GLN:H	1.74	0.51
8:7:678:GLY:HA3	8:7:721:LYS:HD2	1.93	0.51
10:B:604:ARG:NH2	10:B:691:GLU:OE2	2.39	0.51
10:B:805:THR:OG1	10:B:809:MET:SD	2.61	0.51
10:B:984:HIS:NE2	10:B:1028:GLU:OE1	2.42	0.51
34:d:199:GLN:OE1	34:d:203:ARG:NH1	2.42	0.51
1:0:125:LYS:HB2	1:0:128:VAL:HG22	1.91	0.51
1:0:709:SER:OG	1:0:711:ASP:OD1	2.29	0.51
5:4:30:ILE:HG12	5:4:32:ILE:HG23	1.92	0.51
9:A:103:CYS:HB3	9:A:108:MET:HE1	1.91	0.51
34:d:311:LYS:O	34:d:315:SER:CB	2.58	0.51
36:f:4:SER:O	36:f:203:GLN:NE2	2.41	0.51
42:l:346:PRO:HD2	42:l:347:ARG:H	1.75	0.51
9:A:444:PHE:HE2	9:A:470:LEU:HD13	1.75	0.51
22:N:17:DG:O5'	50:u:30:ARG:NH2	2.44	0.51
43:m:147:ARG:NH1	43:m:148:SER:H	2.08	0.51
49:x:15:LYS:O	49:x:20:ARG:NH1	2.43	0.51
11:C:14:SER:OG	11:C:15:LYS:N	2.44	0.51
2:1:567:HIS:HB3	2:1:579:VAL:HG22	1.91	0.51
9:A:353:ILE:HG22	9:A:468:PHE:HB2	1.93	0.51
9:A:1442:ASP:HB2	14:F:135:ARG:HB3	1.91	0.51
14:F:65:ARG:NH1	14:F:72:LYS:O	2.44	0.51
25:R:138:GLN:HG2	25:R:211:LYS:HD3	1.92	0.51
29:W:100:TRP:HZ3	29:W:104:GLN:HE21	1.58	0.51
47:r:129:ARG:O	47:r:129:ARG:NH1	2.40	0.51
9:A:425:GLN:NE2	35:e:262:GLY:O	2.38	0.51
46:p:30:ASN:HA	46:p:33:ARG:HE	1.75	0.51
1:0:251:ASP:OD1	2:1:352:ASN:ND2	2.40	0.51
4:3:27:LYS:O	4:3:37:ARG:NH1	2.44	0.51
4:3:39:CYS:SG	4:3:41:SER:OG	2.64	0.51
8:7:409:VAL:HG22	8:7:486:ILE:HB	1.92	0.51
10:B:242:SER:OG	10:B:363:HIS:ND1	2.38	0.51
37:g:53:THR:HA	37:g:56:MET:HG3	1.91	0.51
39:i:66:ILE:O	45:o:22:ARG:NH1	2.38	0.51
42:l:492:ASP:HB2	42:l:500:LEU:HD23	1.92	0.51
2:1:61:ARG:HH11	2:1:86:ARG:HD2	1.75	0.51
5:4:285:VAL:HG11	7:6:351:ASN:HB2	1.93	0.51
7:6:211:GLN:NE2	7:6:246:ASP:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:237:GLY:HA2	7:6:266:LEU:HB2	1.93	0.51
9:A:532:ARG:HG3	9:A:618:GLU:HG2	1.91	0.51
13:E:83:CYS:O	13:E:113:GLN:NE2	2.44	0.51
21:M:316:LEU:HD22	21:M:323:LEU:HD11	1.93	0.51
24:Q:440:ARG:NH1	25:R:198:ARG:O	2.44	0.51
35:e:17:ASP:N	35:e:17:ASP:OD1	2.44	0.51
36:f:103:SER:HB3	36:f:106:THR:HG23	1.92	0.51
1:0:374:LEU:HD22	1:0:406:ALA:HB1	1.91	0.51
2:1:510:ASN:ND2	5:4:264:LYS:O	2.44	0.51
3:2:110:ASN:ND2	3:2:116:GLU:OE2	2.44	0.51
10:B:71:LEU:HD21	10:B:436:VAL:HG11	1.93	0.51
22:N:58:DA:H61	26:T:-58:DT:H3	1.58	0.51
8:7:164:ILE:HD11	8:7:174:LYS:HE2	1.92	0.50
22:N:8:DT:O2	26:T:-7:DG:N2	2.44	0.50
23:O:230:ILE:HG13	23:O:234:LEU:HD13	1.92	0.50
24:Q:139:LEU:HD13	24:Q:352:MET:HB2	1.93	0.50
42:l:575:SER:N	42:l:628:ARG:O	2.45	0.50
27:U:45:LYS:HA	27:U:48:GLU:HG2	1.92	0.50
30:X:231:LEU:HB2	30:X:245:TRP:HB2	1.93	0.50
34:d:392:ARG:HB2	34:d:475:GLU:HB2	1.93	0.50
43:m:136:ASP:N	43:m:136:ASP:OD1	2.42	0.50
2:1:480:LEU:HD23	5:4:130:TYR:HD1	1.77	0.50
28:V:11:ARG:HA	28:V:16:GLY:HA3	1.93	0.50
1:0:34:VAL:HG11	1:0:478:VAL:HG21	1.93	0.50
34:d:403:TYR:OH	34:d:468:GLU:OE2	2.25	0.50
42:l:627:ILE:HD11	42:l:638:LEU:HD22	1.93	0.50
1:0:427:ASN:ND2	2:1:362:VAL:O	2.43	0.50
3:2:194:GLN:O	3:2:199:GLN:NE2	2.44	0.50
13:E:80:VAL:HG22	13:E:109:ILE:HB	1.93	0.50
29:W:61:LEU:HG	29:W:66:LEU:HD12	1.94	0.50
33:c:70:ILE:HD11	37:g:75:LEU:HD21	1.93	0.50
42:l:104:MET:HA	42:l:107:LEU:HB2	1.92	0.50
44:n:42:MET:SD	44:n:42:MET:N	2.84	0.50
49:x:54:VAL:HG21	50:y:95:VAL:HG21	1.94	0.50
5:4:273:ARG:HH21	7:6:326:THR:HG23	1.77	0.50
9:A:597:LEU:HD13	16:H:103:LYS:HG2	1.94	0.50
21:M:117:ASN:O	21:M:121:LYS:NZ	2.45	0.50
26:T:-93:DA:H2"	26:T:-92:DT:H5"	1.93	0.50
33:c:2:GLN:HB2	34:d:313:MET:HE2	1.93	0.50
40:j:125:ILE:HA	40:j:128:GLN:HG3	1.92	0.50
16:H:10:PHE:HB3	16:H:28:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:351:VAL:HG22	24:Q:362:VAL:HG22	1.93	0.50
36:f:2:GLY:N	36:f:196:GLU:OE2	2.45	0.50
49:t:39:TYR:HB3	50:u:75:SER:HB2	1.94	0.50
3:2:424:PRO:O	3:2:427:LYS:NZ	2.41	0.50
7:6:418:ASN:HA	7:6:420:LYS:HE3	1.93	0.50
8:7:519:ARG:NH1	22:N:-15:DC:OP1	2.44	0.50
9:A:407:ARG:NH2	21:M:26:GLU:OE2	2.45	0.50
10:B:1056:SER:HB3	10:B:1066:SER:HB2	1.93	0.50
22:N:89:DG:N2	26:T:-88:DC:O2	2.44	0.50
1:0:270:ARG:HG3	1:0:388:LEU:HD22	1.94	0.50
7:6:399:ARG:NH1	7:6:433:LYS:O	2.45	0.50
9:A:483:ASP:HB2	10:B:987:LYS:HG3	1.92	0.50
10:B:722:ASP:OD1	10:B:722:ASP:N	2.44	0.50
16:H:48:PRO:O	16:H:146:ARG:NH2	2.42	0.50
29:W:99:LYS:HE2	30:X:283:LEU:HD23	1.93	0.50
34:d:366:LEU:HB2	34:d:425:ILE:HD13	1.93	0.50
48:s:29:ILE:HD11	48:s:55:ARG:HG2	1.94	0.50
9:A:365:GLY:HA3	9:A:469:ARG:HB2	1.94	0.49
9:A:1079:MET:HE2	9:A:1097:GLY:HA2	1.94	0.49
42:l:99:LEU:HD23	42:l:144:LEU:HD22	1.94	0.49
1:0:71:TYR:HB3	1:0:207:ILE:HG12	1.94	0.49
8:7:236:THR:HG21	8:7:241:ILE:HB	1.93	0.49
9:A:544:ASP:N	9:A:544:ASP:OD1	2.43	0.49
10:B:102:VAL:HB	10:B:112:LEU:HD22	1.94	0.49
12:D:162:ALA:HB3	32:b:38:MET:HE3	1.94	0.49
14:F:85:MET:HE3	14:F:90:ARG:HA	1.94	0.49
42:l:427:ILE:HG23	42:l:440:LEU:HD11	1.94	0.49
42:l:650:VAL:HG12	42:l:679:LYS:HA	1.94	0.49
45:o:43:LEU:HD12	45:o:107:PRO:HG3	1.93	0.49
47:r:55:GLN:O	49:x:81:ARG:NH2	2.46	0.49
9:A:261:ASP:HB3	9:A:322:VAL:HG13	1.94	0.49
9:A:884:ASP:OD2	9:A:1030:ARG:NH1	2.42	0.49
9:A:1282:VAL:HG22	9:A:1308:THR:HG23	1.94	0.49
9:A:1324:PRO:HB2	13:E:142:VAL:HG11	1.94	0.49
11:C:38:ILE:HG13	11:C:176:ILE:HD12	1.94	0.49
21:M:181:ARG:NH1	21:M:231:SER:O	2.45	0.49
24:Q:152:THR:HG21	24:Q:357:GLY:HA3	1.93	0.49
32:b:50:ILE:HD11	32:b:72:THR:HG21	1.94	0.49
37:g:20:LYS:HZ3	37:g:64:GLN:HB3	1.77	0.49
1:0:348:VAL:HG21	1:0:352:ILE:HD11	1.94	0.49
1:0:499:LYS:HD2	1:0:503:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:56:ILE:HG12	15:G:72:VAL:HG22	1.94	0.49
16:H:37:LYS:HE3	16:H:126:GLU:HG3	1.94	0.49
29:W:127:CYS:SG	29:W:129:THR:OG1	2.64	0.49
47:r:93:GLN:O	47:r:97:GLU:HG2	2.12	0.49
48:s:82:THR:HG22	48:s:84:MET:H	1.76	0.49
8:7:393:THR:O	8:7:397:ILE:HG12	2.13	0.49
9:A:130:ASP:OD1	9:A:130:ASP:N	2.45	0.49
9:A:882:SER:O	9:A:1025:ARG:NH2	2.39	0.49
22:N:19:DG:H3'	49:t:28:GLY:HA3	1.94	0.49
35:e:165:SER:OG	35:e:187:GLU:OE2	2.30	0.49
42:l:506:THR:OG1	42:l:509:SER:OG	2.28	0.49
50:y:87:THR:H	50:y:90:GLU:HG2	1.77	0.49
1:0:537:MET:HG2	1:0:619:THR:HB	1.95	0.49
7:6:85:ASP:O	7:6:88:LYS:NZ	2.38	0.49
8:7:591:CYS:HB3	8:7:622:MET:HE1	1.94	0.49
13:E:126:SER:OG	13:E:127:ILE:N	2.46	0.49
35:e:230:LEU:HD13	35:e:255:ALA:HB2	1.95	0.49
41:k:18:THR:HG22	41:k:66:ARG:HH21	1.77	0.49
47:v:46:VAL:HA	47:v:49:ARG:HG2	1.93	0.49
2:1:507:ILE:HG13	5:4:265:PRO:HB3	1.94	0.49
6:5:13:ASP:OD1	6:5:13:ASP:N	2.45	0.49
8:7:386:LEU:HD23	8:7:538:ALA:HB2	1.95	0.49
13:E:180:ARG:HH21	13:E:192:ARG:HB2	1.77	0.49
26:T:39:DC:N4	26:T:40:DG:O6	2.45	0.49
46:p:227:ARG:NH1	46:p:250:ASN:OD1	2.43	0.49
5:4:158:THR:OG1	7:6:405:SER:O	2.30	0.49
42:l:217:HIS:H	45:o:117:TRP:HH2	1.61	0.49
42:l:536:TYR:OH	42:l:559:ASP:OD2	2.28	0.49
1:0:472:MET:HE2	1:0:653:PHE:HE1	1.77	0.49
9:A:726:ARG:HD3	9:A:766:GLY:HA3	1.95	0.49
1:0:323:GLY:HA2	1:0:326:ARG:HB2	1.93	0.49
9:A:1383:SER:OG	9:A:1385:THR:OG1	2.28	0.49
12:D:126:ILE:HD12	12:D:145:MET:HB3	1.95	0.49
25:R:306:LEU:HD11	25:R:321:ARG:HG2	1.95	0.49
29:W:62:ARG:HH11	29:W:69:ILE:HG12	1.77	0.49
34:d:120:ASN:HB3	34:d:123:GLU:HB3	1.93	0.49
50:u:76:ARG:NH2	50:u:80:TYR:OH	2.38	0.49
4:3:35:TYR:OH	4:3:83:ASP:OD2	2.30	0.48
5:4:110:ILE:HD11	5:4:126:VAL:HG11	1.95	0.48
8:7:574:ALA:HA	8:7:577:ARG:HH11	1.78	0.48
30:X:200:VAL:HG13	30:X:201:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:124:ASP:OD1	31:a:124:ASP:N	2.45	0.48
44:n:32:PHE:HB2	44:n:41:GLN:HE22	1.77	0.48
46:p:172:SER:HB3	46:p:198:ILE:HD12	1.95	0.48
49:t:54:VAL:HG21	50:u:95:VAL:HG21	1.95	0.48
5:4:91:THR:HG21	7:6:409:ARG:HB2	1.95	0.48
7:6:181:LEU:HD13	7:6:220:LEU:HD11	1.95	0.48
9:A:404:TYR:HB2	9:A:433:GLU:HB2	1.96	0.48
12:D:214:LEU:HD23	12:D:217:LEU:HD12	1.95	0.48
16:H:98:TYR:OH	16:H:139:ASN:ND2	2.46	0.48
8:7:516:THR:HG21	8:7:685:GLN:HG3	1.96	0.48
10:B:942:ARG:HB2	10:B:945:GLU:HB2	1.94	0.48
11:C:217:ASP:OD1	11:C:217:ASP:N	2.45	0.48
15:G:93:SER:OG	15:G:100:GLU:OE1	2.31	0.48
16:H:105:GLU:HB3	16:H:113:ALA:HB3	1.95	0.48
27:U:5:GLU:OE2	28:V:56:THR:OG1	2.29	0.48
28:V:13:SER:O	28:V:17:ASN:ND2	2.47	0.48
34:d:542:ILE:O	34:d:546:LEU:HB3	2.13	0.48
35:e:110:HIS:HA	35:e:199:SER:HB2	1.95	0.48
37:g:20:LYS:HZ1	37:g:65:LEU:N	2.10	0.48
38:h:47:CYS:SG	40:j:102:LYS:NZ	2.86	0.48
1:0:7:ASP:OD1	1:0:7:ASP:N	2.47	0.48
3:2:65:TRP:HZ2	5:4:250:THR:HG22	1.78	0.48
10:B:104:GLU:OE2	10:B:110:HIS:NE2	2.45	0.48
10:B:806:THR:HG23	10:B:1045:SER:HA	1.94	0.48
15:G:57:GLN:NE2	15:G:71:ASN:O	2.46	0.48
22:N:110:DG:N2	26:T:-109:DT:O2	2.47	0.48
23:O:105:ARG:NH2	26:T:58:DA:OP1	2.47	0.48
24:Q:94:ASP:OD2	24:Q:98:TYR:OH	2.30	0.48
29:W:141:ASN:ND2	29:W:146:GLU:OE1	2.46	0.48
36:f:39:PHE:HB3	36:f:122:ILE:HB	1.95	0.48
37:g:12:GLN:HA	37:g:15:THR:HG22	1.94	0.48
47:v:63:ARG:HB2	47:v:66:PRO:HD2	1.96	0.48
5:4:293:LEU:HB3	7:6:376:LEU:HD22	1.95	0.48
8:7:671:ILE:HG23	8:7:708:LEU:HD13	1.95	0.48
9:A:1329:THR:HG22	9:A:1331:SER:H	1.79	0.48
10:B:229:ALA:O	10:B:261:ARG:NH1	2.45	0.48
25:R:352:ARG:HB2	25:R:355:TYR:HD2	1.78	0.48
36:f:9:VAL:HG22	36:f:182:TYR:HB3	1.96	0.48
50:u:76:ARG:O	50:u:79:HIS:N	2.45	0.48
50:y:95:VAL:HG13	50:y:99:LEU:HD13	1.95	0.48
3:2:242:LEU:O	3:2:247:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:291:LEU:HD13	7:6:297:LEU:HD13	1.94	0.48
10:B:667:GLN:NE2	10:B:675:ASP:OD1	2.41	0.48
10:B:952:VAL:HG22	10:B:966:VAL:HG22	1.96	0.48
10:B:1187:ASN:HD22	10:B:1190:ASP:HB3	1.76	0.48
23:O:76:LEU:HB3	23:O:150:ALA:HB1	1.94	0.48
25:R:80:LYS:HE2	25:R:116:ILE:HD13	1.96	0.48
27:U:262:LEU:O	27:U:279:ALA:N	2.47	0.48
34:d:512:LEU:HA	34:d:515:ILE:HD12	1.94	0.48
47:r:123:ASP:OD1	47:v:113:HIS:NE2	2.40	0.48
1:0:577:GLN:NE2	2:1:340:ASP:OD2	2.43	0.48
3:2:339:LEU:HA	3:2:349:SER:HA	1.96	0.48
10:B:1219:ASP:OD1	10:B:1219:ASP:N	2.45	0.48
34:d:616:GLU:HA	34:d:634:MET:HA	1.95	0.48
3:2:373:MET:HE1	8:7:133:TRP:CH2	2.48	0.48
10:B:886:LYS:HE3	10:B:940:PRO:HD3	1.95	0.48
22:N:100:DC:O2	26:T:-99:DG:N2	2.47	0.48
25:R:113:ASN:HB2	25:R:116:ILE:HG12	1.96	0.48
29:W:262:ILE:HD12	29:W:264:ILE:HG12	1.95	0.48
40:j:73:LEU:HD13	46:p:15:ILE:HG22	1.96	0.48
40:j:88:GLU:HA	40:j:91:THR:HG22	1.96	0.48
48:w:47:SER:HB3	48:w:50:ILE:HG12	1.95	0.48
1:0:395:ASP:OD1	1:0:395:ASP:N	2.41	0.48
1:0:534:PRO:HB3	7:6:239:LEU:HD22	1.94	0.48
9:A:397:ASN:HB2	35:e:55:ARG:HH12	1.78	0.48
9:A:614:PHE:HB3	16:H:122:LEU:HD21	1.94	0.48
12:D:56:ARG:HB2	12:D:148:LEU:HB3	1.96	0.48
39:i:203:LEU:HA	39:i:206:ILE:HG12	1.95	0.48
40:j:66:ILE:HA	40:j:69:ILE:HG12	1.95	0.48
42:l:346:PRO:HD2	42:l:347:ARG:N	2.28	0.48
44:n:3:ASP:O	44:n:7:GLN:NE2	2.47	0.48
9:A:1581:SER:OG	32:b:115:ARG:NH2	2.46	0.48
12:D:194:LEU:HD22	15:G:86:VAL:HG11	1.96	0.48
16:H:38:LEU:HD13	16:H:125:LEU:HD13	1.96	0.48
29:W:189:ILE:HD12	29:W:194:ILE:HD11	1.95	0.48
41:k:97:THR:HG23	42:l:150:TRP:HE1	1.78	0.48
45:o:30:ILE:HD13	45:o:61:LEU:HD13	1.95	0.48
22:N:70:DC:O2	26:T:-69:DG:N2	2.46	0.47
25:R:318:LEU:HD23	25:R:333:LEU:HD11	1.94	0.47
44:n:34:ARG:NE	44:n:41:GLN:OE1	2.45	0.47
44:n:98:GLN:HA	44:n:98:GLN:NE2	2.29	0.47
5:4:64:HIS:O	5:4:71:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:748:LEU:HB2	8:7:751:ALA:HB2	1.96	0.47
9:A:1114:PRO:HB2	9:A:1311:VAL:HG23	1.96	0.47
21:M:313:TYR:OH	21:M:340:PRO:O	2.29	0.47
35:e:167:GLN:HG2	35:e:187:GLU:HG2	1.96	0.47
48:s:31:LYS:HG2	48:s:32:PRO:HD3	1.97	0.47
1:0:64:PRO:C	43:m:147:ARG:HH21	2.22	0.47
24:Q:447:ALA:O	24:Q:451:GLN:NE2	2.46	0.47
32:b:84:GLN:HE21	37:g:45:ASN:H	1.61	0.47
35:e:55:ARG:HD2	35:e:56:ASN:N	2.25	0.47
41:k:104:ILE:HG12	42:l:166:LEU:HG	1.95	0.47
47:r:92:LEU:HD12	48:s:62:LEU:HD22	1.96	0.47
9:A:261:ASP:OD1	9:A:316:GLN:NE2	2.46	0.47
10:B:521:LEU:HD22	10:B:633:VAL:HG12	1.97	0.47
30:X:235:THR:OG1	30:X:238:ASP:OD1	2.33	0.47
42:l:684:THR:OG1	42:l:685:TYR:N	2.47	0.47
3:2:236:ALA:HB1	3:2:268:ILE:HB	1.96	0.47
8:7:592:GLN:NE2	8:7:747:ASN:O	2.48	0.47
9:A:202:LEU:HD23	9:A:207:ILE:HD11	1.97	0.47
22:N:111:DG:OP1	50:y:37:TYR:OH	2.29	0.47
31:a:50:ARG:NH1	31:a:106:GLU:OE1	2.48	0.47
41:k:72:SER:O	41:k:76:LYS:NZ	2.47	0.47
44:n:127:GLU:HA	44:n:130:VAL:HG22	1.95	0.47
48:s:75:HIS:HB2	50:u:93:THR:HG21	1.96	0.47
49:t:51:LEU:HD11	50:u:70:ILE:HG21	1.96	0.47
4:3:16:CYS:SG	4:3:18:THR:OG1	2.63	0.47
8:7:423:GLN:OE1	8:7:427:TRP:NE1	2.44	0.47
9:A:1399:ARG:NH2	9:A:1417:GLU:OE1	2.48	0.47
16:H:2:SER:OG	16:H:3:ASN:N	2.47	0.47
24:Q:373:TYR:O	25:R:82:ARG:NH1	2.46	0.47
42:l:255:ILE:HG22	44:n:130:VAL:HG11	1.97	0.47
46:p:127:LEU:HA	46:p:164:LEU:HD23	1.97	0.47
48:s:88:TYR:HA	48:s:91:LYS:HG2	1.95	0.47
1:0:139:GLY:HA3	1:0:302:GLN:HE22	1.79	0.47
1:0:571:VAL:HG11	2:1:375:LEU:HD13	1.96	0.47
1:0:711:ASP:OD1	1:0:711:ASP:N	2.46	0.47
2:1:486:LEU:HD12	5:4:59:VAL:HG23	1.96	0.47
5:4:235:TYR:H	5:4:266:ASN:HB3	1.80	0.47
7:6:77:GLU:OE1	8:7:344:ARG:NH2	2.48	0.47
10:B:1001:PHE:HE2	11:C:178:PHE:HB3	1.80	0.47
15:G:52:ASP:OD1	15:G:53:ASN:N	2.47	0.47
22:N:111:DG:N2	26:T:-110:DC:O2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:-102:DT:H2"	26:T:-101:DA:C8	2.49	0.47
31:a:117:LEU:HD11	31:a:126:TRP:HD1	1.79	0.47
31:a:168:LYS:HA	31:a:171:GLN:HB3	1.97	0.47
41:k:109:GLN:OE1	44:n:34:ARG:NH2	2.41	0.47
42:l:533:LEU:O	42:l:537:ALA:N	2.46	0.47
48:s:39:ARG:HH11	48:s:43:VAL:HG23	1.80	0.47
49:x:57:TYR:HD2	49:x:58:LEU:HD22	1.79	0.47
7:6:398:PHE:HE2	7:6:421:LEU:HD13	1.79	0.47
9:A:914:GLU:OE1	40:j:95:ARG:NH2	2.43	0.47
14:F:79:ARG:NH1	14:F:150:GLU:OE2	2.40	0.47
24:Q:120:LYS:HG3	25:R:132:GLU:HG2	1.97	0.47
24:Q:407:ASP:N	24:Q:407:ASP:OD1	2.45	0.47
25:R:319:LYS:NZ	25:R:324:GLN:O	2.47	0.47
31:a:13:SER:HB2	31:a:30:TYR:HE1	1.78	0.47
32:b:107:GLU:HA	32:b:110:VAL:HG12	1.96	0.47
37:g:3:ASN:OD1	37:g:4:GLN:NE2	2.47	0.47
1:0:91:ASP:OD2	2:1:416:ARG:NH1	2.47	0.47
10:B:443:ASN:ND2	21:M:195:LEU:O	2.48	0.47
10:B:983:ARG:NH2	10:B:1028:GLU:OE2	2.41	0.47
16:H:7:ASP:OD1	16:H:7:ASP:N	2.48	0.47
32:b:51:ARG:HH21	34:d:211:ILE:HG13	1.80	0.47
34:d:577:GLU:HB2	34:d:615:ARG:HD3	1.96	0.47
41:k:101:VAL:HA	41:k:104:ILE:HD12	1.96	0.47
44:n:101:LEU:HA	44:n:104:VAL:HG12	1.97	0.47
4:3:85:ARG:NH1	4:3:114:GLU:OE2	2.44	0.47
8:7:185:SER:OG	8:7:340:GLU:OE2	2.32	0.47
9:A:338:GLY:HA2	10:B:1129:ARG:HH22	1.79	0.47
9:A:512:VAL:HA	9:A:519:PRO:HA	1.97	0.47
11:C:37:MET:HE3	11:C:176:ILE:HD13	1.96	0.47
11:C:48:SER:HB2	20:L:66:GLN:HE21	1.79	0.47
21:M:233:ALA:HA	21:M:274:PRO:HG3	1.96	0.47
38:h:110:LYS:HG3	38:h:113:LYS:HE3	1.97	0.47
39:i:100:LEU:HB3	43:m:15:TYR:CZ	2.50	0.47
41:k:122:ARG:HH12	41:k:148:SER:HB3	1.79	0.47
1:0:24:TYR:CZ	1:0:28:ILE:HD11	2.50	0.46
8:7:566:TYR:OH	8:7:712:ASP:O	2.26	0.46
9:A:156:ASP:OD1	9:A:156:ASP:N	2.45	0.46
23:O:97:LYS:HB3	25:R:290:LYS:HB3	1.97	0.46
23:O:97:LYS:HE3	25:R:290:LYS:HE3	1.97	0.46
28:V:61:THR:OG1	28:V:86:THR:OG1	2.33	0.46
34:d:466:ILE:HG22	34:d:475:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:614:ARG:HG2	34:d:636:GLU:HB2	1.97	0.46
41:k:50:ILE:HG13	43:m:142:LEU:HD11	1.97	0.46
46:p:91:PHE:O	46:p:191:ASN:ND2	2.45	0.46
1:0:571:VAL:O	2:1:379:ASN:ND2	2.39	0.46
2:1:476:VAL:HG21	5:4:50:ILE:HD12	1.97	0.46
8:7:351:ASP:OD1	8:7:405:LYS:NZ	2.39	0.46
9:A:87:ALA:HB2	9:A:277:GLU:HG3	1.97	0.46
9:A:1581:SER:HB3	32:b:119:ILE:HA	1.96	0.46
17:I:103:CYS:SG	17:I:105:SER:OG	2.70	0.46
24:Q:114:MET:HB3	24:Q:114:MET:HE2	1.75	0.46
39:i:115:LYS:HB3	39:i:161:LEU:HD11	1.97	0.46
42:l:159:PHE:HA	42:l:162:LEU:HD12	1.98	0.46
1:0:666:LEU:HD11	1:0:681:LEU:HD21	1.98	0.46
2:1:339:LEU:HD23	2:1:342:ASN:HD22	1.81	0.46
9:A:889:SER:HB3	9:A:1297:GLU:HG2	1.97	0.46
9:A:1648:SER:HB2	9:A:1651:SER:HB2	1.97	0.46
32:b:39:ARG:HB3	32:b:79:VAL:HG22	1.97	0.46
33:c:10:LEU:HD11	34:d:309:TRP:HB3	1.97	0.46
34:d:498:ASP:O	34:d:502:ASN:ND2	2.48	0.46
42:l:348:LEU:HA	42:l:351:LEU:HD23	1.96	0.46
44:n:70:THR:O	44:n:74:ASN:ND2	2.48	0.46
21:M:187:ARG:HB3	21:M:191:GLU:HG3	1.97	0.46
22:N:18:DT:OP1	50:u:30:ARG:NH1	2.48	0.46
34:d:120:ASN:OD1	34:d:121:GLU:N	2.48	0.46
41:k:97:THR:HG22	42:l:159:PHE:HE2	1.81	0.46
44:n:4:ARG:NH1	44:n:79:SER:O	2.49	0.46
1:0:542:PRO:HB3	1:0:626:PRO:HA	1.97	0.46
3:2:239:ILE:HG13	3:2:242:LEU:HD12	1.98	0.46
7:6:325:PRO:HB2	7:6:347:TYR:HB3	1.97	0.46
9:A:484:GLY:HA3	10:B:979:LYS:HE2	1.97	0.46
9:A:590:ARG:NH2	9:A:621:THR:OG1	2.49	0.46
10:B:93:GLY:N	10:B:131:ASP:O	2.43	0.46
31:a:282:LYS:HA	31:a:285:VAL:HG12	1.96	0.46
32:b:93:THR:HG22	34:d:258:LYS:HD2	1.98	0.46
46:p:60:ILE:HA	46:p:82:ALA:HB3	1.96	0.46
5:4:291:VAL:HG13	7:6:119:GLN:HG3	1.98	0.46
8:7:499:ARG:HG3	8:7:530:LEU:HD21	1.97	0.46
9:A:355:GLY:O	9:A:469:ARG:NH1	2.49	0.46
30:X:235:THR:OG1	30:X:238:ASP:O	2.27	0.46
33:c:38:LYS:HD3	33:c:38:LYS:HA	1.71	0.46
41:k:61:TYR:HE1	43:m:128:PHE:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:114:GLN:NE2	43:m:118:GLU:OE2	2.49	0.46
1:0:506:ILE:HD12	1:0:522:TYR:HE1	1.80	0.46
2:1:222:LEU:HD13	7:6:216:MET:HA	1.97	0.46
2:1:502:ARG:NH2	5:4:237:HIS:O	2.46	0.46
5:4:326:VAL:O	5:4:328:ARG:NH2	2.48	0.46
7:6:234:ILE:HB	7:6:263:VAL:HG22	1.97	0.46
27:U:262:LEU:HB2	27:U:279:ALA:HB3	1.97	0.46
29:W:177:ASP:OD1	29:W:177:ASP:N	2.49	0.46
31:a:98:PRO:O	31:a:101:MET:HG3	2.16	0.46
34:d:86:LEU:HD13	42:l:205:GLU:HG2	1.97	0.46
47:r:72:ARG:HH21	47:r:84:PHE:HB2	1.80	0.46
2:1:196:GLN:HA	2:1:200:ILE:HD13	1.98	0.46
3:2:128:ASN:HA	3:2:270:TYR:HE2	1.80	0.46
5:4:299:ILE:HD13	5:4:321:LYS:HE3	1.97	0.46
9:A:397:ASN:H	35:e:55:ARG:HH22	1.64	0.46
11:C:75:MET:O	11:C:246:ARG:NH2	2.49	0.46
11:C:116:LYS:HD3	11:C:140:ASN:HA	1.98	0.46
36:f:46:ILE:HB	36:f:49:LEU:HG	1.97	0.46
47:r:73:GLU:OE2	48:s:25:ASN:ND2	2.48	0.46
1:0:234:PHE:HB3	1:0:237:ALA:HB2	1.98	0.46
8:7:383:ILE:HD11	8:7:527:LEU:HB3	1.97	0.46
9:A:860:LEU:HD21	9:A:1394:THR:HA	1.98	0.46
10:B:1129:ARG:HG2	14:F:23:PHE:CE2	2.51	0.46
12:D:170:THR:HB	12:D:172:LEU:HD13	1.98	0.46
31:a:164:PRO:HG2	31:a:169:ILE:HD11	1.97	0.46
35:e:14:ASP:OD1	35:e:14:ASP:N	2.42	0.46
40:j:132:GLU:HA	40:j:135:ILE:HG22	1.97	0.46
49:t:41:GLU:HG2	49:t:42:ARG:HG3	1.98	0.46
10:B:954:VAL:HG12	10:B:964:VAL:HG12	1.97	0.46
36:f:144:SER:OG	36:f:145:SER:N	2.48	0.46
39:i:165:TYR:OH	44:n:82:GLY:O	2.27	0.46
42:l:569:PHE:HB3	42:l:574:TRP:HB2	1.96	0.46
46:p:19:LYS:HD3	46:p:37:THR:HG21	1.98	0.46
47:v:116:ARG:NH1	47:v:118:THR:O	2.48	0.46
3:2:14:LEU:O	3:2:22:GLN:NE2	2.47	0.45
9:A:417:TYR:OH	21:M:37:ARG:NH1	2.49	0.45
9:A:1409:LEU:HD13	10:B:1207:LEU:HD21	1.97	0.45
16:H:108:SER:OG	16:H:110:ASP:OD1	2.32	0.45
20:L:68:GLU:OE1	20:L:70:ARG:NH1	2.49	0.45
32:b:59:LEU:HD21	34:d:204:ARG:HD3	1.98	0.45
35:e:178:ARG:NH1	35:e:269:ASN:OD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:138:SER:HB3	41:k:118:LEU:HB3	1.97	0.45
3:2:198:SER:HA	3:2:201:TRP:HB2	1.97	0.45
6:5:5:ARG:HE	6:5:41:LEU:HD11	1.81	0.45
8:7:356:LEU:HD11	8:7:398:THR:HG23	1.98	0.45
10:B:727:LYS:HE3	10:B:1049:ASP:HB2	1.99	0.45
12:D:130:LEU:HD11	12:D:145:MET:HG3	1.98	0.45
15:G:150:CYS:HA	15:G:159:ALA:HA	1.98	0.45
17:I:98:VAL:HG21	17:I:113:ASP:HB2	1.98	0.45
38:h:57:VAL:HA	38:h:60:VAL:HG12	1.97	0.45
39:i:206:ILE:HA	39:i:209:THR:HG22	1.99	0.45
42:l:402:HIS:HA	42:l:413:VAL:HG12	1.98	0.45
44:n:88:GLU:OE2	44:n:92:ARG:NH1	2.44	0.45
48:w:39:ARG:NH1	48:w:43:VAL:O	2.49	0.45
1:0:466:LEU:HD11	1:0:482:SER:HB3	1.97	0.45
3:2:263:HIS:ND1	3:2:264:SER:O	2.47	0.45
7:6:141:LEU:HB3	7:6:148:MET:SD	2.56	0.45
7:6:176:ASN:OD1	7:6:205:LYS:NZ	2.44	0.45
9:A:219:PHE:HB2	9:A:224:PHE:HB2	1.98	0.45
10:B:398:ARG:HD3	10:B:509:ALA:HB2	1.97	0.45
11:C:71:PRO:HG3	18:J:13:VAL:HG21	1.99	0.45
34:d:195:MET:HE1	34:d:200:PHE:HB2	1.99	0.45
34:d:302:LEU:HD23	34:d:302:LEU:HA	1.84	0.45
42:l:580:ILE:HD11	42:l:658:ILE:HG21	1.97	0.45
1:0:18:TYR:OH	2:1:423:ASP:OD2	2.34	0.45
1:0:301:ASP:N	1:0:301:ASP:OD1	2.49	0.45
8:7:440:SER:O	8:7:443:LYS:NZ	2.50	0.45
26:T:70:DT:H2''	26:T:71:DG:C8	2.52	0.45
31:a:38:ASP:HB2	31:a:41:SER:HB2	1.98	0.45
50:y:60:ASN:O	50:y:64:ASN:ND2	2.39	0.45
1:0:286:TYR:OH	4:3:111:GLU:OE1	2.30	0.45
9:A:886:ILE:HG13	9:A:944:ARG:HG3	1.97	0.45
10:B:298:LEU:HD13	10:B:311:LEU:HD22	1.97	0.45
17:I:54:GLU:HG3	17:I:55:THR:HG23	1.98	0.45
28:V:61:THR:HB	28:V:63:LYS:HZ3	1.80	0.45
31:a:92:GLN:O	31:a:96:LYS:HB2	2.16	0.45
34:d:390:ARG:NH1	34:d:408:GLU:OE1	2.49	0.45
8:7:132:LEU:HB2	8:7:201:SER:HA	1.99	0.45
8:7:389:GLY:HA3	8:7:692:ARG:HB3	1.97	0.45
23:O:197:MET:HE2	23:O:197:MET:HB3	1.79	0.45
24:Q:103:LEU:HD12	25:R:95:ILE:HD11	1.99	0.45
26:T:-60:DC:H2''	26:T:-59:DG:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:120:ASN:HA	29:W:161:SER:HB3	1.98	0.45
30:X:259:PHE:HA	30:X:262:MET:HG2	1.98	0.45
31:a:114:GLU:N	31:a:131:GLN:O	2.41	0.45
34:d:107:LEU:HB2	34:d:114:PHE:HD2	1.81	0.45
34:d:122:LYS:HA	34:d:125:GLN:HB2	1.99	0.45
38:h:56:LEU:HD21	46:p:18:PHE:HZ	1.82	0.45
41:k:98:ARG:HH12	43:m:60:LEU:H	1.63	0.45
42:l:165:LEU:HD11	43:m:34:LEU:HD13	1.98	0.45
42:l:400:LEU:HD21	42:l:468:LEU:HD21	1.99	0.45
49:t:80:PRO:HD3	50:u:55:ALA:HB2	1.99	0.45
1:0:18:TYR:HB2	1:0:21:GLN:HG3	1.99	0.45
1:0:83:LEU:HD11	1:0:107:GLY:HA3	1.98	0.45
2:1:12:VAL:HG13	29:W:211:ASN:HB3	1.98	0.45
3:2:24:ARG:HE	3:2:219:VAL:HG11	1.82	0.45
9:A:569:LYS:HD2	11:C:221:TYR:HB2	1.99	0.45
9:A:711:ARG:HH21	17:I:95:THR:HG23	1.82	0.45
9:A:905:ASP:OD1	9:A:905:ASP:N	2.47	0.45
31:a:37:PHE:HE2	31:a:44:GLN:HB3	1.81	0.45
37:g:63:MET:HA	37:g:66:ILE:HG12	1.99	0.45
41:k:108:ASN:OD1	41:k:112:ARG:NH2	2.49	0.45
49:x:59:THR:HA	49:x:62:ILE:HG22	1.98	0.45
1:0:295:SER:HA	1:0:383:LEU:HD21	1.98	0.45
1:0:509:ARG:NH1	1:0:511:GLU:OE2	2.44	0.45
8:7:438:PHE:HB3	8:7:455:SER:HB3	1.99	0.45
9:A:62:ASP:HB3	9:A:65:LEU:HB2	1.99	0.45
10:B:363:HIS:HD2	10:B:585:VAL:HG22	1.81	0.45
11:C:262:LEU:HD22	19:K:87:LEU:HD23	1.97	0.45
15:G:101:VAL:HG11	15:G:145:VAL:HG11	1.98	0.45
23:O:108:GLU:OE2	27:U:229:TYR:OH	2.34	0.45
38:h:107:LEU:O	38:h:111:THR:OG1	2.30	0.45
41:k:94:ASP:OD1	41:k:97:THR:OG1	2.35	0.45
42:l:285:GLU:OE2	42:l:287:GLN:NE2	2.45	0.45
42:l:389:LEU:HD12	42:l:465:GLU:HG3	1.99	0.45
1:0:489:LYS:HE2	1:0:724:MET:HG2	1.98	0.45
10:B:87:LYS:HB3	10:B:137:TYR:HB2	1.98	0.45
23:O:82:LEU:HA	23:O:85:VAL:HG12	1.98	0.45
2:1:381:LEU:HG	2:1:385:MET:HE3	1.98	0.45
3:2:444:TRP:HA	3:2:447:GLU:HG2	1.99	0.45
5:4:33:ALA:HB3	5:4:36:LEU:HB2	1.99	0.45
8:7:138:ASP:N	8:7:138:ASP:OD1	2.50	0.45
8:7:382:GLY:HA3	8:7:535:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:515:GLN:HE21	9:A:1075:PRO:HG3	1.81	0.45
10:B:281:PRO:HD2	10:B:284:ILE:HD12	1.99	0.45
10:B:872:GLU:HG2	10:B:916:THR:HG22	1.99	0.45
22:N:26:DG:O6	26:T:-27:DA:N6	2.50	0.45
25:R:73:LEU:HD13	25:R:77:LEU:HG	1.99	0.45
35:e:11:ILE:HG21	35:e:19:LEU:HD22	1.99	0.45
47:r:104:PHE:HB3	48:s:41:GLY:HA3	1.99	0.45
5:4:77:ALA:HB2	5:4:86:LEU:HD11	1.99	0.44
8:7:609:SER:HB3	8:7:673:ILE:HB	1.99	0.44
9:A:981:LEU:HD11	9:A:1042:PHE:HB2	1.99	0.44
10:B:1000:PRO:HB2	10:B:1072:MET:HE2	1.98	0.44
29:W:269:ASP:OD1	29:W:269:ASP:N	2.47	0.44
36:f:132:LEU:HD12	36:f:135:LEU:HD23	1.98	0.44
39:i:63:ASP:O	45:o:22:ARG:NH2	2.48	0.44
45:o:95:ASN:OD1	45:o:99:LEU:N	2.50	0.44
49:x:33:LEU:HA	49:x:36:LYS:HG2	1.98	0.44
1:0:117:HIS:CE1	1:0:119:GLU:HB2	2.51	0.44
1:0:227:SER:OG	1:0:229:ASP:OD1	2.28	0.44
1:0:440:LEU:HD23	1:0:641:PHE:HB2	1.99	0.44
2:1:62:LEU:HB2	2:1:87:HIS:HB2	1.99	0.44
12:D:40:HIS:CE1	15:G:6:ASP:HB3	2.52	0.44
23:O:143:ILE:HG22	23:O:148:PHE:HB2	1.98	0.44
25:R:43:ASN:HB2	25:R:205:VAL:HG22	1.98	0.44
29:W:89:VAL:O	29:W:197:ASN:ND2	2.47	0.44
32:b:33:LEU:HD11	34:d:228:LEU:HD22	1.98	0.44
32:b:61:GLN:HE22	32:b:63:TYR:HB2	1.82	0.44
49:t:63:LEU:HD22	50:u:42:LEU:HD13	2.00	0.44
1:0:45:GLY:HA2	1:0:671:ARG:HA	1.99	0.44
2:1:3:HIS:HB3	2:1:18:ILE:HB	1.99	0.44
8:7:127:HIS:HB2	8:7:202:LYS:HD3	1.98	0.44
8:7:456:THR:HG21	26:T:19:DA:H5"	2.00	0.44
22:N:-65:DG:OP1	27:U:257:ARG:NH1	2.50	0.44
22:N:-25:DG:O6	26:T:24:DA:N6	2.51	0.44
22:N:51:DC:OP2	48:s:31:LYS:NZ	2.50	0.44
31:a:277:THR:HA	31:a:280:LEU:HD23	1.99	0.44
2:1:354:PRO:O	2:1:359:GLN:NE2	2.50	0.44
9:A:66:LYS:HG3	21:M:20:ILE:HG12	1.99	0.44
9:A:929:LEU:HD21	9:A:983:ILE:HG21	1.98	0.44
10:B:896:ASP:OD2	20:L:29:TYR:OH	2.35	0.44
13:E:100:ILE:HG23	13:E:105:PHE:HB2	1.99	0.44
27:U:247:LEU:HD12	28:V:116:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:440:LEU:HB3	42:l:457:TYR:HB2	1.99	0.44
44:n:84:ASP:OD1	44:n:84:ASP:N	2.43	0.44
3:2:483:TRP:HZ3	6:5:35:LEU:HD23	1.82	0.44
5:4:34:PRO:O	5:4:38:THR:OG1	2.28	0.44
9:A:1148:ILE:N	9:A:1196:GLU:O	2.40	0.44
10:B:121:ASN:HA	10:B:207:GLY:HA3	1.99	0.44
10:B:282:ILE:HA	10:B:285:ILE:HD12	1.99	0.44
10:B:290:GLY:HA2	10:B:327:ARG:HD2	1.99	0.44
31:a:105:GLU:O	31:a:109:LYS:NZ	2.50	0.44
35:e:40:VAL:HG22	35:e:65:LYS:HB3	1.99	0.44
39:i:92:LEU:HB2	39:i:99:GLN:HB2	1.99	0.44
42:l:121:GLU:HB3	42:l:129:ARG:HH22	1.81	0.44
50:u:95:VAL:HG13	50:u:99:LEU:HD12	1.99	0.44
1:0:29:LYS:NZ	1:0:33:ASP:OD2	2.50	0.44
1:0:76:MET:HE2	1:0:76:MET:HB3	1.94	0.44
4:3:20:ARG:NH1	4:3:26:VAL:O	2.47	0.44
4:3:60:ASP:N	4:3:60:ASP:OD1	2.48	0.44
5:4:323:LYS:HG3	5:4:324:PRO:HD2	2.00	0.44
9:A:308:ILE:HB	9:A:311:GLN:HB2	1.99	0.44
10:B:232:SER:O	10:B:261:ARG:NH1	2.44	0.44
22:N:90:DG:H3'	48:w:79:LYS:HZ3	1.82	0.44
26:T:-54:DT:H5''	47:r:43:PRO:HA	1.99	0.44
42:l:266:LEU:HD22	42:l:278:PHE:HB3	1.98	0.44
42:l:301:ASP:OD1	42:l:301:ASP:N	2.49	0.44
44:n:58:THR:HA	44:n:61:GLU:HG3	1.99	0.44
46:p:91:PHE:CG	46:p:100:LYS:HG3	2.53	0.44
2:1:27:LEU:HD23	2:1:42:LEU:HD11	2.00	0.44
4:3:108:LYS:HA	4:3:108:LYS:HD3	1.82	0.44
16:H:4:THR:HG23	16:H:58:THR:HG23	2.00	0.44
24:Q:25:ASP:OD1	24:Q:25:ASP:N	2.42	0.44
24:Q:130:VAL:HG12	25:R:61:LEU:HG	1.98	0.44
27:U:246:CYS:SG	27:U:262:LEU:HB3	2.58	0.44
29:W:114:ASP:O	29:W:117:SER:OG	2.31	0.44
30:X:145:ASN:OD1	30:X:146:GLU:N	2.50	0.44
36:f:28:ILE:HD11	36:f:130:LEU:HD13	1.99	0.44
40:j:123:GLN:O	40:j:127:HIS:ND1	2.44	0.44
45:o:118:MET:HA	45:o:121:MET:HG3	2.00	0.44
48:s:92:ARG:HE	50:u:97:LEU:HD12	1.81	0.44
7:6:331:ASP:OD1	7:6:331:ASP:N	2.51	0.44
9:A:115:LEU:HD13	9:A:119:ASN:HD22	1.83	0.44
9:A:337:ARG:HE	9:A:337:ARG:HB3	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:968:GLN:HA	9:A:973:ILE:HG12	1.99	0.44
10:B:564:GLU:OE2	10:B:591:ARG:NH1	2.45	0.44
30:X:143:LEU:HA	30:X:177:THR:HA	2.00	0.44
34:d:227:LEU:HD11	34:d:245:LEU:HD21	1.99	0.44
39:i:182:LEU:HD23	44:n:104:VAL:HG11	1.99	0.44
50:u:48:ASP:OD1	50:u:48:ASP:N	2.44	0.44
47:v:46:VAL:HG23	47:v:49:ARG:HH11	1.82	0.44
3:2:208:LEU:HA	3:2:211:ILE:HG12	1.99	0.44
5:4:175:ARG:HH11	5:4:256:PRO:HD3	1.82	0.44
7:6:134:GLU:HG3	7:6:206:GLY:H	1.83	0.44
8:7:362:ILE:HG12	8:7:367:GLU:HG3	1.99	0.44
8:7:689:ARG:HD3	8:7:692:ARG:HH12	1.82	0.44
9:A:48:ALA:HB3	9:A:56:PRO:HG3	2.00	0.44
22:N:-13:DT:H2'	22:N:-12:DA:C8	2.53	0.44
30:X:193:LEU:HD21	30:X:229:LYS:HD2	1.99	0.44
32:b:102:PRO:HD2	34:d:249:VAL:HG23	1.99	0.44
32:b:139:LEU:HG	32:b:140:LEU:HD12	2.00	0.44
34:d:297:LYS:HE2	34:d:297:LYS:HB3	1.83	0.44
41:k:70:PRO:HD3	43:m:117:ARG:HB3	2.00	0.44
1:0:43:PRO:HD3	1:0:483:TYR:HB2	2.00	0.43
9:A:915:SER:OG	9:A:918:GLU:OE2	2.36	0.43
9:A:993:LEU:HD22	9:A:1046:LEU:HD22	2.00	0.43
10:B:193:LYS:HB3	10:B:787:VAL:HG21	2.00	0.43
14:F:136:ARG:HD2	14:F:146:TRP:CD1	2.53	0.43
17:I:22:ASN:HB2	17:I:24:ARG:HH11	1.82	0.43
39:i:89:LEU:HD12	39:i:90:PRO:HD2	1.99	0.43
42:l:131:LEU:HD12	42:l:134:ILE:HD11	2.00	0.43
42:l:165:LEU:HD21	43:m:34:LEU:HB3	2.00	0.43
48:s:62:LEU:HA	48:s:65:VAL:HG12	1.99	0.43
9:A:555:ASP:OD1	9:A:648:ASN:ND2	2.50	0.43
9:A:1121:GLU:HG2	9:A:1122:PRO:HD2	2.00	0.43
10:B:394:ASP:OD1	10:B:394:ASP:N	2.49	0.43
29:W:38:LEU:HD22	29:W:42:ASP:HB3	1.99	0.43
42:l:374:VAL:HA	42:l:377:LEU:HD23	2.00	0.43
45:o:33:LEU:HD23	45:o:81:ILE:HG22	1.99	0.43
48:w:84:MET:HA	48:w:87:VAL:HG12	1.99	0.43
2:1:369:ASP:OD1	2:1:369:ASP:N	2.47	0.43
5:4:175:ARG:HD2	5:4:259:ARG:HH21	1.83	0.43
7:6:397:LYS:NZ	7:6:398:PHE:O	2.45	0.43
8:7:372:LYS:O	8:7:380:ARG:NH2	2.42	0.43
9:A:1169:ILE:HG12	9:A:1227:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:71:LEU:HB2	10:B:432:MET:HE3	2.00	0.43
10:B:287:ARG:NH2	10:B:294:ASP:OD1	2.50	0.43
10:B:846:ILE:O	10:B:852:ARG:NH2	2.40	0.43
21:M:140:ALA:HB1	25:R:268:MET:HE3	2.00	0.43
25:R:258:THR:HB	25:R:261:VAL:HG23	2.00	0.43
33:c:32:PHE:HD1	34:d:288:LYS:HE2	1.83	0.43
37:g:56:MET:O	37:g:60:ASN:CB	2.65	0.43
38:h:193:LEU:HG	39:i:14:PRO:HG2	2.01	0.43
47:r:113:HIS:NE2	47:v:123:ASP:OD1	2.46	0.43
9:A:173:THR:OG1	9:A:184:SER:OG	2.35	0.43
9:A:1195:LEU:HD12	9:A:1238:ILE:HD11	1.99	0.43
10:B:256:VAL:HG12	10:B:385:LEU:HD22	1.99	0.43
10:B:1178:ASN:ND2	15:G:155:SER:OG	2.51	0.43
12:D:69:ALA:HA	12:D:72:ARG:HG2	2.01	0.43
16:H:29:ALA:HA	16:H:37:LYS:HA	1.99	0.43
23:O:172:LEU:HD23	23:O:208:VAL:HG12	2.01	0.43
27:U:247:LEU:HA	28:V:116:CYS:H	1.83	0.43
44:n:34:ARG:HH11	44:n:39:GLU:HG3	1.83	0.43
1:O:120:VAL:HG23	1:O:123:GLU:HG3	1.99	0.43
5:4:87:TYR:CZ	5:4:121:VAL:HG22	2.54	0.43
7:6:129:THR:HB	7:6:234:ILE:HG12	2.01	0.43
9:A:157:ASP:OD1	9:A:160:GLN:NE2	2.48	0.43
9:A:830:LYS:HE2	9:A:830:LYS:HB3	1.92	0.43
10:B:510:LYS:HD2	10:B:510:LYS:HA	1.75	0.43
10:B:1002:THR:HG22	10:B:1072:MET:HG2	1.98	0.43
14:F:133:VAL:HG21	15:G:58:ARG:HD3	2.01	0.43
21:M:199:LYS:HA	21:M:199:LYS:HD2	1.80	0.43
31:a:117:LEU:HD21	31:a:120:VAL:HB	2.00	0.43
33:c:90:ALA:N	34:d:343:ASP:OD2	2.46	0.43
35:e:81:MET:SD	35:e:81:MET:N	2.92	0.43
38:h:56:LEU:HD13	38:h:73:LEU:HD13	2.00	0.43
3:2:194:GLN:HG2	3:2:199:GLN:HG3	2.01	0.43
5:4:28:VAL:HG22	5:4:177:LEU:HD23	2.00	0.43
5:4:313:ASP:HB3	5:4:316:VAL:HG12	2.00	0.43
8:7:150:ALA:O	8:7:154:GLN:N	2.51	0.43
9:A:348:SER:HB2	10:B:1128:LEU:HD22	2.01	0.43
10:B:283:VAL:HG21	10:B:318:VAL:HA	2.00	0.43
12:D:205:ASP:OD1	12:D:206:GLU:N	2.51	0.43
21:M:58:ASP:OD1	21:M:58:ASP:N	2.51	0.43
21:M:160:GLU:HG3	21:M:213:ILE:HG12	1.99	0.43
27:U:37:ASP:OD1	27:U:38:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:174:LYS:HG3	30:X:175:LYS:HG2	2.00	0.43
30:X:278:LEU:HD22	30:X:283:LEU:HB2	1.99	0.43
33:c:73:LEU:HD12	37:g:83:TRP:CD1	2.54	0.43
43:m:66:ASN:OD1	43:m:66:ASN:N	2.52	0.43
3:2:474:TYR:HE2	3:2:501:VAL:HA	1.82	0.43
8:7:181:TYR:CZ	8:7:336:PRO:HG3	2.53	0.43
8:7:223:VAL:HG23	8:7:337:VAL:HA	2.01	0.43
8:7:627:ILE:HD12	8:7:636:ARG:HG2	2.01	0.43
9:A:997:LEU:O	9:A:1011:GLN:NE2	2.41	0.43
10:B:94:LYS:HD3	10:B:94:LYS:HA	1.82	0.43
10:B:445:LYS:NZ	25:R:265:HIS:O	2.51	0.43
24:Q:428:LEU:HG	24:Q:433:THR:HB	2.00	0.43
34:d:22:ASP:OD2	39:i:185:LYS:NZ	2.50	0.43
35:e:187:GLU:HG3	36:f:98:THR:HG23	2.01	0.43
42:l:657:LYS:HE2	42:l:668:LYS:HD3	2.00	0.43
43:m:79:PRO:HA	43:m:83:ASN:HD21	1.83	0.43
46:p:227:ARG:HD3	46:p:227:ARG:HA	1.81	0.43
5:4:293:LEU:HD11	7:6:122:ILE:HG13	2.01	0.43
9:A:1209:MET:HE3	9:A:1209:MET:HB3	1.79	0.43
20:L:46:VAL:HG22	20:L:56:LEU:HD13	2.01	0.43
25:R:273:ASP:OD1	25:R:273:ASP:N	2.46	0.43
30:X:258:GLU:HA	30:X:261:LYS:HE2	2.00	0.43
34:d:391:VAL:HG12	34:d:476:ILE:HG12	2.01	0.43
47:r:108:ASN:ND2	48:s:41:GLY:O	2.52	0.43
7:6:377:ALA:HA	7:6:380:TYR:CE1	2.54	0.43
9:A:15:LYS:O	10:B:1220:ARG:NH1	2.52	0.43
9:A:568:PRO:HD2	16:H:46:LEU:HD23	1.99	0.43
10:B:128:LEU:HD11	10:B:170:LEU:HB2	2.01	0.43
11:C:16:ASP:OD1	11:C:16:ASP:N	2.50	0.43
15:G:115:MET:HG3	15:G:163:ILE:HD11	2.00	0.43
24:Q:399:ASN:HD22	24:Q:437:ARG:HD3	1.84	0.43
33:c:3:PRO:HA	33:c:4:PRO:HD3	1.95	0.43
50:y:77:LEU:HA	50:y:80:TYR:HB2	2.01	0.43
1:0:22:TYR:HA	1:0:25:MET:HE2	2.01	0.43
2:1:384:LYS:HA	2:1:387:MET:HG3	1.99	0.43
3:2:368:ALA:O	3:2:375:LEU:N	2.45	0.43
3:2:460:SER:HB3	3:2:490:LYS:HG2	2.01	0.43
9:A:562:THR:O	9:A:576:GLN:NE2	2.52	0.43
10:B:600:LEU:HB3	10:B:615:MET:SD	2.58	0.43
10:B:996:ARG:HG3	10:B:1007:VAL:HG21	2.00	0.43
21:M:325:ASP:OD2	21:M:327:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:97:LYS:HE2	25:R:291:SER:H	1.84	0.43
27:U:244:MET:HE3	28:V:113:ILE:HG12	2.00	0.43
31:a:173:ARG:NH1	32:b:115:ARG:O	2.52	0.43
31:a:175:MET:HB3	32:b:122:VAL:HG21	2.01	0.43
40:j:63:GLY:HA2	40:j:67:PRO:HG2	2.00	0.43
50:y:28:LYS:HE3	50:y:29:THR:HG22	2.01	0.43
11:C:145:CYS:SG	11:C:146:LYS:N	2.92	0.42
21:M:202:GLU:HA	21:M:205:LYS:HD2	2.00	0.42
22:N:70:DC:H5"	48:w:47:SER:HA	2.01	0.42
33:c:34:PHE:HA	33:c:37:LEU:HG	2.01	0.42
34:d:393:ILE:HG21	34:d:497:ASN:HD22	1.83	0.42
39:i:185:LYS:HA	39:i:185:LYS:HD3	1.73	0.42
42:l:429:ILE:HD13	42:l:440:LEU:HD13	2.01	0.42
1:0:635:LEU:HD21	1:0:654:LEU:HD21	2.00	0.42
2:1:237:ILE:HG23	2:1:249:VAL:HG21	2.01	0.42
10:B:928:ARG:NH1	10:B:929:THR:O	2.50	0.42
11:C:35:ARG:NE	19:K:41:THR:OG1	2.39	0.42
12:D:209:ARG:O	32:b:31:GLN:NE2	2.51	0.42
19:K:63:VAL:HG22	19:K:71:PHE:HB3	2.00	0.42
25:R:43:ASN:ND2	25:R:202:ILE:O	2.52	0.42
38:h:125:LEU:HD12	39:i:199:VAL:HG21	2.01	0.42
39:i:152:ARG:HA	39:i:152:ARG:HD2	1.69	0.42
50:y:86:ILE:HA	50:y:90:GLU:HG3	2.01	0.42
2:1:482:ASN:OD1	2:1:483:LYS:N	2.50	0.42
3:2:338:SER:O	3:2:350:TYR:N	2.44	0.42
5:4:79:TYR:HB3	5:4:132:LEU:HD21	2.01	0.42
10:B:199:MET:SD	10:B:199:MET:N	2.74	0.42
10:B:1135:ARG:HG3	10:B:1147:LEU:HD11	2.00	0.42
12:D:204:ASP:OD1	12:D:205:ASP:N	2.52	0.42
23:O:108:GLU:HG2	23:O:109:PRO:HD3	1.99	0.42
26:T:2:DT:H2"	26:T:3:DA:C8	2.54	0.42
28:V:86:THR:HG22	28:V:105:VAL:HG12	2.01	0.42
32:b:66:GLN:HE22	37:g:67:LYS:HD3	1.83	0.42
34:d:555:LYS:NZ	37:g:118:GLU:OE1	2.52	0.42
39:i:147:LYS:HD2	39:i:147:LYS:HA	1.74	0.42
40:j:15:LEU:HB2	40:j:65:PHE:HZ	1.84	0.42
40:j:72:SER:O	40:j:76:ILE:HG12	2.19	0.42
1:0:162:LEU:HD21	1:0:190:LEU:HB3	2.00	0.42
4:3:19:ASP:O	4:3:23:SER:OG	2.30	0.42
7:6:148:MET:HE3	7:6:148:MET:HB2	1.64	0.42
8:7:164:ILE:HD11	8:7:174:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:148:CYS:O	9:A:164:ARG:NH1	2.43	0.42
17:I:17:ARG:HH21	17:I:28:GLU:HG2	1.85	0.42
22:N:20:DT:O2	49:t:11:ARG:NH2	2.52	0.42
30:X:269:PRO:HD2	30:X:274:LEU:HD21	2.02	0.42
32:b:101:PHE:HB2	34:d:253:SER:HB3	2.02	0.42
35:e:254:LYS:HG2	35:e:256:TYR:HD2	1.84	0.42
36:f:158:ASP:OD1	36:f:158:ASP:N	2.53	0.42
49:x:39:TYR:HB3	50:y:75:SER:HB3	2.02	0.42
10:B:118:ARG:HG3	10:B:204:ILE:HD13	2.02	0.42
13:E:46:TYR:HA	13:E:57:MET:HE1	2.01	0.42
17:I:58:VAL:HG11	17:I:109:ILE:HD11	2.01	0.42
21:M:231:SER:HB3	21:M:234:GLN:HG2	2.01	0.42
26:T:27:DT:H1'	30:X:308:ARG:HH21	1.84	0.42
32:b:51:ARG:HH12	34:d:215:MET:HG2	1.85	0.42
7:6:172:ILE:HD11	7:6:220:LEU:HD12	2.01	0.42
8:7:209:ILE:O	8:7:213:ILE:HG12	2.20	0.42
9:A:70:CYS:SG	9:A:77:CYS:HB2	2.60	0.42
9:A:557:ASP:OD1	9:A:557:ASP:N	2.51	0.42
9:A:569:LYS:HB3	16:H:46:LEU:HD21	2.02	0.42
10:B:597:MET:HG3	10:B:617:ARG:HB2	2.00	0.42
16:H:75:ALA:N	16:H:98:TYR:OH	2.42	0.42
24:Q:369:ASN:OD1	24:Q:369:ASN:N	2.52	0.42
34:d:669:GLU:O	34:d:673:PHE:HB2	2.19	0.42
35:e:181:SER:HB3	35:e:290:VAL:HG13	2.01	0.42
36:f:202:TYR:CZ	36:f:206:ARG:HD3	2.55	0.42
40:j:64:GLU:HG3	40:j:65:PHE:H	1.84	0.42
3:2:47:ILE:O	3:2:51:VAL:HG23	2.20	0.42
4:3:19:ASP:HB2	4:3:22:LEU:HD23	2.01	0.42
8:7:141:ILE:HG21	8:7:157:LEU:HD11	2.01	0.42
9:A:117:GLU:O	9:A:123:ARG:NH1	2.45	0.42
32:b:74:SER:HA	32:b:77:VAL:HG12	2.01	0.42
32:b:77:VAL:HA	32:b:80:THR:HG22	2.01	0.42
33:c:7:GLN:HB2	34:d:313:MET:HE1	2.00	0.42
38:h:95:ARG:CZ	40:j:5:ASN:H	2.33	0.42
39:i:68:PRO:HG2	45:o:23:PHE:HB2	2.02	0.42
41:k:51:THR:HG22	41:k:55:ARG:NE	2.35	0.42
41:k:61:TYR:CE1	43:m:128:PHE:HB3	2.55	0.42
46:p:12:ASP:HA	46:p:15:ILE:HG12	2.02	0.42
48:s:91:LYS:HB3	48:s:96:THR:HA	2.01	0.42
49:t:51:LEU:HD12	49:t:51:LEU:HA	1.80	0.42
48:w:39:ARG:NH1	48:w:44:LYS:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:212:TYR:HD2	1:0:222:VAL:HG21	1.85	0.42
1:0:255:ASP:OD1	1:0:258:ARG:NH2	2.43	0.42
2:1:197:GLU:HA	2:1:201:ASN:HB2	2.02	0.42
5:4:57:LEU:HD13	5:4:179:LEU:HD11	2.00	0.42
8:7:583:MET:HE3	8:7:583:MET:HB3	1.81	0.42
10:B:590:HIS:CD2	10:B:596:LEU:HD22	2.54	0.42
12:D:144:THR:HG21	15:G:46:LEU:HD13	2.01	0.42
14:F:128:LYS:HA	14:F:128:LYS:HD2	1.92	0.42
19:K:37:LYS:HA	19:K:37:LYS:HD3	1.85	0.42
34:d:323:PHE:HZ	34:d:354:ILE:HD12	1.85	0.42
42:l:536:TYR:CG	42:l:556:LEU:HD13	2.55	0.42
43:m:35:ILE:HG23	43:m:40:LEU:HB2	2.01	0.42
47:v:69:ARG:HB3	48:w:25:ASN:HD21	1.83	0.42
1:0:345:ARG:NH2	1:0:354:GLU:OE2	2.53	0.42
7:6:197:LYS:HG2	7:6:200:ARG:HH22	1.85	0.42
11:C:175:ALA:HB2	18:J:10:CYS:HB2	2.02	0.42
12:D:23:ASN:HA	15:G:83:LYS:HG2	2.02	0.42
12:D:160:VAL:O	12:D:164:ILE:HG12	2.19	0.42
22:N:69:DC:O2	26:T:-68:DG:N2	2.53	0.42
30:X:125:SER:HA	30:X:128:LEU:HG	2.02	0.42
36:f:202:TYR:O	36:f:206:ARG:HG2	2.19	0.42
40:j:96:HIS:HA	40:j:99:LYS:HE2	2.01	0.42
8:7:331:GLN:HG2	8:7:529:PHE:HE1	1.84	0.42
8:7:447:GLN:HG3	9:A:159:THR:HG21	2.01	0.42
9:A:1095:THR:HG23	9:A:1100:ARG:HD3	2.00	0.42
18:J:22:LEU:O	18:J:26:GLN:HG3	2.20	0.42
27:U:31:ASP:HB3	27:U:33:GLN:HG3	2.02	0.42
33:c:84:ILE:HD11	35:e:26:ILE:HD11	2.01	0.42
34:d:238:MET:HA	34:d:241:MET:HG2	2.02	0.42
38:h:156:TYR:CZ	38:h:160:LEU:HD11	2.55	0.42
1:0:639:LEU:HD22	1:0:650:GLU:HA	2.02	0.41
7:6:139:LYS:O	7:6:142:ARG:NH1	2.52	0.41
8:7:682:GLN:OE1	8:7:722:ARG:NH1	2.52	0.41
9:A:404:TYR:OH	21:M:40:GLU:OE1	2.32	0.41
10:B:661:LEU:HD11	10:B:684:LEU:HD11	2.02	0.41
15:G:55:ASP:HB3	15:G:73:LYS:HB2	2.01	0.41
21:M:269:ILE:HD13	21:M:316:LEU:HD21	2.01	0.41
37:g:20:LYS:NZ	37:g:64:GLN:HB3	2.34	0.41
47:r:61:LEU:HD11	48:s:36:ARG:HB3	2.02	0.41
48:w:62:LEU:HD23	48:w:62:LEU:HA	1.92	0.41
48:w:82:THR:HG23	48:w:85:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:190:THR:HG23	8:7:213:ILE:HG22	2.02	0.41
8:7:565:PHE:CE1	8:7:760:LEU:HB2	2.55	0.41
9:A:265:LYS:HA	9:A:265:LYS:HD2	1.79	0.41
9:A:563:PRO:HG3	9:A:572:TRP:CZ2	2.55	0.41
9:A:1572:PRO:HA	34:d:242:SER:HA	2.02	0.41
23:O:139:TYR:O	23:O:143:ILE:HG12	2.20	0.41
30:X:238:ASP:OD1	30:X:238:ASP:N	2.53	0.41
36:f:38:ASP:HB2	36:f:121:LEU:HD11	2.01	0.41
39:i:68:PRO:HA	39:i:69:PRO:HD3	1.91	0.41
39:i:210:LEU:HD11	40:j:140:LEU:HD13	2.02	0.41
42:l:100:THR:HB	43:m:128:PHE:HZ	1.85	0.41
45:o:108:LYS:HD2	45:o:108:LYS:HA	1.81	0.41
48:s:44:LYS:HE3	48:s:44:LYS:HB3	1.88	0.41
47:v:62:ILE:HD11	48:w:37:LEU:HD11	2.01	0.41
1:0:336:LYS:HE3	1:0:336:LYS:HB2	1.89	0.41
2:1:237:ILE:HD11	2:1:255:LYS:HD3	2.03	0.41
7:6:411:PRO:HG2	7:6:413:LEU:HG	2.03	0.41
9:A:455:MET:HE3	10:B:1138:MET:SD	2.61	0.41
9:A:1206:ASP:O	9:A:1274:ARG:NH1	2.53	0.41
10:B:167:ILE:HG22	10:B:448:ILE:HG21	2.01	0.41
14:F:25:ASP:O	14:F:28:THR:OG1	2.32	0.41
23:O:185:TYR:HB2	23:O:193:LEU:HD13	2.02	0.41
27:U:45:LYS:HD2	28:V:18:SER:HB3	2.02	0.41
29:W:141:ASN:HB3	29:W:148:LEU:HD23	2.02	0.41
33:c:94:ASP:OD1	33:c:95:THR:N	2.53	0.41
34:d:503:LEU:O	34:d:507:MET:HG2	2.20	0.41
37:g:52:THR:HA	37:g:55:VAL:HG12	2.01	0.41
40:j:122:TRP:CE3	40:j:125:ILE:HD11	2.56	0.41
42:l:214:LEU:HB2	45:o:80:PHE:CE2	2.56	0.41
49:x:17:ARG:NH2	49:x:28:GLY:HA2	2.36	0.41
3:2:58:PRO:HG3	3:2:97:MET:HE1	2.01	0.41
5:4:108:LYS:HA	5:4:108:LYS:HD3	1.86	0.41
8:7:334:ASP:OD1	8:7:334:ASP:N	2.51	0.41
10:B:934:LYS:HE2	10:B:934:LYS:HB2	1.90	0.41
10:B:1080:LYS:HD2	11:C:189:THR:HG23	2.02	0.41
10:B:1204:PHE:O	10:B:1208:MET:HG3	2.21	0.41
15:G:138:THR:O	15:G:141:SER:OG	2.33	0.41
18:J:58:GLU:HA	18:J:61:LEU:HB2	2.02	0.41
21:M:181:ARG:HA	21:M:186:ALA:HB2	2.01	0.41
31:a:185:LEU:HD11	32:b:69:LEU:HD22	2.01	0.41
47:r:113:HIS:CG	47:v:126:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:r:126:LEU:HD22	47:v:113:HIS:CG	2.56	0.41
3:2:250:LEU:HD12	3:2:259:VAL:HG11	2.01	0.41
6:5:29:ASP:OD1	6:5:29:ASP:N	2.46	0.41
8:7:134:ILE:HD12	8:7:205:VAL:HG22	2.01	0.41
8:7:460:VAL:HG11	8:7:505:ILE:HD11	2.02	0.41
8:7:490:VAL:HG12	8:7:514:THR:HB	2.03	0.41
9:A:1445:ILE:HA	14:F:132:LEU:HD23	2.02	0.41
22:N:-42:DT:O4	26:T:41:DA:N6	2.52	0.41
24:Q:142:LYS:HE3	24:Q:142:LYS:HB2	1.88	0.41
29:W:160:ASP:OD1	29:W:160:ASP:N	2.50	0.41
31:a:280:LEU:HB3	42:l:344:ASN:ND2	2.35	0.41
41:k:126:ALA:HB1	41:k:144:ILE:HD11	2.01	0.41
47:r:69:ARG:O	47:r:73:GLU:HG3	2.20	0.41
1:0:234:PHE:HZ	1:0:449:VAL:HG11	1.85	0.41
1:0:241:ASP:OD1	1:0:241:ASP:N	2.54	0.41
3:2:416:LEU:HD23	3:2:420:LEU:HD23	2.03	0.41
8:7:190:THR:HG21	8:7:214:LYS:HD3	2.01	0.41
8:7:672:GLN:OE1	8:7:686:ARG:NH1	2.45	0.41
10:B:278:GLN:OE1	10:B:337:ARG:NE	2.52	0.41
10:B:558:LEU:HD11	10:B:626:ILE:HD12	2.02	0.41
10:B:797:TYR:CE2	10:B:852:ARG:HD2	2.56	0.41
14:F:140:ASP:OD1	14:F:142:SER:OG	2.28	0.41
19:K:24:ASP:OD2	19:K:74:ARG:NE	2.41	0.41
21:M:187:ARG:HE	25:R:268:MET:HG3	1.84	0.41
32:b:49:ARG:O	32:b:53:GLU:HB2	2.21	0.41
34:d:440:GLU:HG3	34:d:512:LEU:HD21	2.03	0.41
36:f:45:SER:HB3	36:f:117:MET:HE3	2.03	0.41
38:h:90:TYR:HD1	38:h:93:ILE:HD11	1.86	0.41
49:x:26:PRO:HD3	50:y:37:TYR:CD2	2.56	0.41
49:x:88:ARG:HA	49:x:88:ARG:HD3	1.80	0.41
1:0:519:VAL:HG11	1:0:553:MET:HG3	2.02	0.41
8:7:160:ILE:HA	8:7:183:ALA:HB2	2.02	0.41
9:A:332:LYS:N	14:F:26:GLU:HG3	2.36	0.41
10:B:106:ASP:N	10:B:106:ASP:OD1	2.46	0.41
10:B:1119:VAL:HB	10:B:1124:ARG:HH12	1.86	0.41
28:V:46:LYS:HA	28:V:46:LYS:HD2	1.82	0.41
34:d:126:ASN:HA	34:d:129:LYS:HB2	2.03	0.41
34:d:668:LYS:H	34:d:668:LYS:HG2	1.53	0.41
41:k:60:LEU:HD23	41:k:60:LEU:HA	1.93	0.41
42:l:657:LYS:HB3	42:l:669:TYR:HB3	2.03	0.41
1:0:502:ASP:OD1	1:0:502:ASP:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:509:ARG:HB2	1:0:512:ILE:HG12	2.03	0.41
1:0:621:LEU:HA	1:0:680:VAL:HG23	2.02	0.41
7:6:402:ASP:OD1	7:6:402:ASP:N	2.53	0.41
10:B:408:LEU:HD23	10:B:545:ILE:HG21	2.02	0.41
16:H:116:TYR:HB2	16:H:123:MET:HE2	2.03	0.41
24:Q:346:GLU:OE2	24:Q:393:TYR:OH	2.30	0.41
34:d:505:LEU:HA	34:d:508:LEU:HD12	2.03	0.41
37:g:23:GLU:O	37:g:27:MET:HG3	2.20	0.41
37:g:73:LEU:HD23	37:g:73:LEU:HA	1.92	0.41
42:l:557:LYS:O	42:l:561:ILE:HG12	2.21	0.41
42:l:678:VAL:HG21	42:l:687:LYS:HE2	2.02	0.41
44:n:67:ILE:HD12	44:n:67:ILE:HG23	1.85	0.41
1:0:724:MET:HE2	1:0:724:MET:HB3	1.90	0.41
3:2:368:ALA:HB3	3:2:375:LEU:HD12	2.02	0.41
8:7:689:ARG:HD3	8:7:689:ARG:HA	1.85	0.41
9:A:504:LEU:O	9:A:510:GLN:NE2	2.54	0.41
9:A:844:ALA:HB2	9:A:1384:VAL:HG13	2.02	0.41
9:A:1258:HIS:CE1	9:A:1262:LYS:HD2	2.56	0.41
10:B:76:GLN:H	24:Q:326:ARG:HH21	1.69	0.41
15:G:21:ARG:O	15:G:24:GLN:HG3	2.21	0.41
21:M:133:ILE:HG13	21:M:172:MET:HE1	2.02	0.41
23:O:74:VAL:HB	23:O:121:MET:HB3	2.03	0.41
23:O:105:ARG:NH1	28:V:69:TYR:OH	2.46	0.41
24:Q:141:ARG:HH12	24:Q:346:GLU:HA	1.85	0.41
24:Q:405:THR:OG1	24:Q:407:ASP:OD1	2.34	0.41
25:R:279:LYS:HB2	25:R:282:ARG:HH21	1.85	0.41
26:T:-26:DC:H2"	26:T:-25:DG:C8	2.56	0.41
27:U:38:LEU:O	27:U:42:TRP:HB2	2.21	0.41
31:a:12:LYS:HG3	31:a:14:PRO:HD3	2.02	0.41
31:a:104:GLU:HA	31:a:107:LEU:HB2	2.03	0.41
32:b:23:PHE:CE1	32:b:99:PRO:HD2	2.56	0.41
32:b:153:ARG:O	32:b:156:THR:OG1	2.31	0.41
34:d:316:ILE:HG13	34:d:322:ILE:HD11	2.02	0.41
34:d:534:ASN:ND2	34:d:537:ASP:OD2	2.54	0.41
36:f:71:LEU:HB2	36:f:78:MET:HB3	2.03	0.41
41:k:96:TYR:O	41:k:100:PHE:CB	2.68	0.41
42:l:166:LEU:HA	42:l:166:LEU:HD23	1.87	0.41
47:r:126:LEU:O	47:r:130:ILE:HG12	2.20	0.41
49:t:63:LEU:HD23	49:t:63:LEU:HA	1.92	0.41
47:v:52:ARG:HG2	47:v:56:LYS:HE2	2.01	0.41
2:1:291:LYS:HA	2:1:294:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:634:PHE:HB2	5:4:326:VAL:HG21	2.03	0.41
9:A:108:MET:H	9:A:171:GLN:HE21	1.68	0.41
9:A:143:LYS:HE3	9:A:143:LYS:HB2	1.96	0.41
9:A:767:GLN:NE2	9:A:768:GLN:O	2.45	0.41
10:B:212:LEU:HA	10:B:212:LEU:HD23	1.80	0.41
16:H:56:THR:HB	16:H:145:ARG:HG2	2.03	0.41
21:M:280:VAL:HG11	21:M:312:GLY:HA3	2.02	0.41
24:Q:148:GLN:HG2	24:Q:399:ASN:ND2	2.36	0.41
24:Q:376:LEU:HB2	25:R:69:TRP:HB2	2.03	0.41
32:b:161:THR:O	32:b:165:ASN:ND2	2.54	0.41
34:d:402:ASP:OD1	34:d:402:ASP:N	2.52	0.41
42:l:535:ASN:O	42:l:538:SER:OG	2.31	0.41
49:t:80:PRO:HA	49:t:83:LEU:HD13	2.03	0.41
1:0:258:ARG:O	1:0:261:THR:OG1	2.38	0.40
5:4:197:MET:HB3	7:6:377:ALA:HB1	2.03	0.40
9:A:185:TRP:O	9:A:198:GLU:N	2.51	0.40
10:B:563:MET:HE2	10:B:563:MET:HB3	2.00	0.40
11:C:77:ILE:HD12	11:C:77:ILE:HA	1.93	0.40
22:N:125:DT:H2'	22:N:126:DA:C8	2.56	0.40
29:W:13:LEU:HA	29:W:16:VAL:HG22	2.02	0.40
31:a:155:ILE:HD12	31:a:160:ILE:HG12	2.03	0.40
34:d:447:LYS:HE2	34:d:447:LYS:HB3	1.94	0.40
34:d:464:LYS:HA	34:d:477:GLU:HA	2.03	0.40
46:p:127:LEU:O	46:p:131:SER:OG	2.39	0.40
7:6:377:ALA:HA	7:6:380:TYR:HE1	1.85	0.40
9:A:242:PRO:HD2	9:A:266:LEU:HD11	2.03	0.40
9:A:264:PHE:HE1	21:M:92:LEU:HD22	1.86	0.40
30:X:278:LEU:HD23	30:X:278:LEU:HA	1.90	0.40
34:d:309:TRP:HZ3	37:g:84:LEU:HD22	1.86	0.40
35:e:191:LEU:HD23	35:e:191:LEU:HA	1.96	0.40
38:h:41:GLN:NE2	38:h:83:ASN:OD1	2.36	0.40
38:h:131:LEU:HB2	44:n:116:GLU:HG3	2.03	0.40
46:p:199:TYR:CZ	46:p:214:LYS:HD3	2.57	0.40
47:r:50:GLU:OE1	48:s:39:ARG:NE	2.54	0.40
9:A:72:GLU:HB3	9:A:76:GLU:HB3	2.02	0.40
13:E:30:ILE:HD13	13:E:30:ILE:HA	1.98	0.40
22:N:-39:DG:H2''	22:N:-38:DA:C8	2.56	0.40
32:b:204:PHE:CE2	35:e:246:ILE:HG13	2.57	0.40
41:k:128:LYS:HE2	44:n:63:SER:HB2	2.04	0.40
45:o:56:ASN:O	45:o:60:TYR:N	2.55	0.40
1:0:80:GLU:HG2	2:1:335:LYS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:467:ASP:N	1:0:467:ASP:OD1	2.52	0.40
4:3:45:ARG:HH12	29:W:114:ASP:HA	1.87	0.40
7:6:355:LYS:HE3	7:6:355:LYS:HB2	1.90	0.40
9:A:944:ARG:NH2	9:A:1296:GLY:O	2.48	0.40
9:A:1573:THR:HG22	32:b:48:ARG:HD3	2.03	0.40
10:B:227:LYS:HG2	10:B:236:HIS:CD2	2.56	0.40
11:C:50:GLU:HG2	20:L:64:LEU:HB3	2.03	0.40
16:H:68:THR:HA	16:H:69:PRO:HD3	1.94	0.40
16:H:95:TYR:HD2	16:H:144:ILE:HD12	1.87	0.40
22:N:50:DA:P	48:s:36:ARG:HH12	2.45	0.40
25:R:73:LEU:HD22	25:R:77:LEU:HD23	2.04	0.40
25:R:85:ASN:O	25:R:88:HIS:NE2	2.55	0.40
33:c:20:LEU:HA	33:c:23:MET:HG2	2.03	0.40
35:e:178:ARG:HA	35:e:178:ARG:HD3	1.87	0.40
48:s:47:SER:HB3	48:s:50:ILE:HB	2.02	0.40
49:t:111:ILE:HG23	49:t:115:LEU:HD22	2.02	0.40
2:1:486:LEU:HD13	5:4:55:GLU:HB2	2.03	0.40
4:3:25:ASP:OD1	4:3:25:ASP:N	2.51	0.40
9:A:433:GLU:OE1	10:B:1108:ARG:NH2	2.51	0.40
9:A:455:MET:HE2	10:B:1137:CYS:HB2	2.02	0.40
9:A:469:ARG:HH21	10:B:976:ILE:HD13	1.87	0.40
9:A:559:VAL:HG12	16:H:78:SER:HB2	2.02	0.40
9:A:1675:TYR:CE2	42:l:166:LEU:HB3	2.57	0.40
9:A:1675:TYR:HE2	42:l:166:LEU:HB3	1.86	0.40
26:T:-29:DC:H2"	26:T:-28:DT:C5	2.57	0.40
30:X:162:LEU:HD23	30:X:162:LEU:HA	1.93	0.40
31:a:98:PRO:O	31:a:101:MET:N	2.52	0.40
36:f:37:ILE:HD13	36:f:204:TYR:HE2	1.87	0.40
39:i:30:LYS:HE3	39:i:33:LYS:HD3	2.02	0.40
39:i:101:TYR:CD2	39:i:118:GLU:HG2	2.56	0.40
44:n:130:VAL:HA	44:n:133:ILE:HG12	2.03	0.40
47:r:50:GLU:CD	48:s:39:ARG:HG3	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	750/778 (96%)	735 (98%)	15 (2%)	0	100	100
2	1	508/642 (79%)	504 (99%)	4 (1%)	0	100	100
3	2	448/513 (87%)	434 (97%)	14 (3%)	0	100	100
4	3	129/321 (40%)	127 (98%)	2 (2%)	0	100	100
5	4	298/338 (88%)	288 (97%)	10 (3%)	0	100	100
6	5	63/72 (88%)	61 (97%)	2 (3%)	0	100	100
7	6	379/461 (82%)	367 (97%)	12 (3%)	0	100	100
8	7	609/843 (72%)	584 (96%)	25 (4%)	0	100	100
9	A	1494/1733 (86%)	1449 (97%)	45 (3%)	0	100	100
10	B	1168/1224 (95%)	1131 (97%)	37 (3%)	0	100	100
11	C	264/347 (76%)	258 (98%)	6 (2%)	0	100	100
12	D	163/221 (74%)	160 (98%)	3 (2%)	0	100	100
13	E	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
14	F	114/155 (74%)	111 (97%)	3 (3%)	0	100	100
15	G	169/177 (96%)	161 (95%)	8 (5%)	0	100	100
16	H	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
17	I	114/122 (93%)	109 (96%)	5 (4%)	0	100	100
18	J	67/70 (96%)	67 (100%)	0	0	100	100
19	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
20	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
21	M	306/352 (87%)	295 (96%)	11 (4%)	0	100	100
23	O	179/240 (75%)	170 (95%)	9 (5%)	0	100	100
24	Q	215/735 (29%)	205 (95%)	10 (5%)	0	100	100
25	R	264/400 (66%)	255 (97%)	9 (3%)	0	100	100
27	U	101/286 (35%)	96 (95%)	5 (5%)	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%)	200 (97%)	7 (3%)	0	100	100
31	a	170/295 (58%)	161 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	b	168/223 (75%)	162 (96%)	6 (4%)	0	100	100
33	c	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
34	d	481/687 (70%)	468 (97%)	13 (3%)	0	100	100
35	e	252/307 (82%)	244 (97%)	8 (3%)	0	100	100
36	f	202/210 (96%)	194 (96%)	8 (4%)	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%)	93 (95%)	5 (5%)	0	100	100
41	k	155/157 (99%)	154 (99%)	1 (1%)	0	100	100
42	l	521/1082 (48%)	503 (96%)	17 (3%)	1 (0%)	43	72
43	m	126/220 (57%)	120 (95%)	6 (5%)	0	100	100
44	n	134/140 (96%)	132 (98%)	2 (2%)	0	100	100
45	o	108/127 (85%)	108 (100%)	0	0	100	100
46	p	221/566 (39%)	207 (94%)	14 (6%)	0	100	100
47	r	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
47	v	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
48	s	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
48	w	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
49	t	107/129 (83%)	103 (96%)	4 (4%)	0	100	100
49	x	104/129 (81%)	104 (100%)	0	0	100	100
50	u	95/125 (76%)	91 (96%)	4 (4%)	0	100	100
50	y	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
All	All	12842/17410 (74%)	12464 (97%)	377 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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
7	6	346/418 (83%)	346 (100%)	0	100	100
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%)	1024 (100%)	0	100	100
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%)	152 (100%)	0	100	100
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%)	204 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	b	161/207 (78%)	161 (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
40	j	100/144 (69%)	100 (100%)	0	100	100
41	k	145/145 (100%)	145 (100%)	0	100	100
42	l	505/1001 (50%)	505 (100%)	0	100	100
43	m	119/195 (61%)	119 (100%)	0	100	100
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%)	212 (100%)	0	100	100
47	r	84/109 (77%)	84 (100%)	0	100	100
47	v	85/109 (78%)	85 (100%)	0	100	100
48	s	67/78 (86%)	67 (100%)	0	100	100
48	w	65/78 (83%)	65 (100%)	0	100	100
49	t	86/101 (85%)	86 (100%)	0	100	100
49	x	84/101 (83%)	84 (100%)	0	100	100
50	u	83/105 (79%)	83 (100%)	0	100	100
50	y	81/105 (77%)	81 (100%)	0	100	100
All	All	11775/15543 (76%)	11775 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	23	ASN
1	0	521	ASN
1	0	645	ASN
1	0	699	GLN

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Mol	Chain	Res	Type
2	1	500	ASN
2	1	573	GLN
2	1	584	ASN
3	2	53	ASN
3	2	90	ASN
3	2	372	ASN
4	3	107	ASN
5	4	81	GLN
5	4	111	ASN
5	4	225	GLN
5	4	311	GLN
7	6	119	GLN
7	6	146	HIS
7	6	202	GLN
7	6	281	ASN
7	6	351	ASN
8	7	349	ASN
8	7	447	GLN
8	7	471	GLN
8	7	598	HIS
9	A	171	GLN
9	A	209	ASN
9	A	339	ASN
9	A	390	GLN
9	A	515	GLN
9	A	611	GLN
9	A	736	ASN
9	A	1265	ASN
9	A	1270	ASN
10	B	383	ASN
10	B	465	ASN
10	B	770	GLN
10	B	776	GLN
10	B	1040	ASN
10	B	1097	HIS
10	B	1178	ASN
10	B	1205	GLN
11	C	123	ASN
11	C	242	GLN
11	C	267	GLN
12	D	157	GLN
12	D	216	ASN

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Mol	Chain	Res	Type
13	E	8	ASN
13	E	115	ASN
16	H	83	GLN
19	K	89	ASN
20	L	66	GLN
21	M	127	GLN
21	M	303	GLN
24	Q	359	ASN
25	R	43	ASN
25	R	98	ASN
25	R	324	GLN
27	U	40	ASN
27	U	272	ASN
28	V	17	ASN
29	W	104	GLN
29	W	263	ASN
30	X	136	GLN
30	X	270	GLN
31	a	43	ASN
31	a	159	ASN
31	a	171	GLN
31	a	195	GLN
32	b	75	GLN
32	b	106	HIS
32	b	150	GLN
32	b	165	ASN
34	d	130	GLN
34	d	314	GLN
34	d	360	ASN
34	d	364	GLN
34	d	595	ASN
34	d	600	ASN
35	e	167	GLN
35	e	197	ASN
36	f	156	GLN
37	g	4	GLN
37	g	43	GLN
37	g	103	GLN
38	h	133	GLN
39	i	27	ASN
39	i	140	ASN
39	i	160	HIS

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Mol	Chain	Res	Type
39	i	163	ASN
40	j	9	ASN
40	j	85	ASN
40	j	86	GLN
41	k	71	GLN
41	k	152	ASN
42	l	167	ASN
42	l	175	ASN
42	l	192	ASN
42	l	273	ASN
42	l	282	ASN
42	l	403	ASN
42	l	458	ASN
42	l	463	ASN
42	l	661	GLN
43	m	29	ASN
44	n	7	GLN
44	n	57	ASN
45	o	46	GLN
46	p	68	ASN
46	p	119	ASN
46	p	177	GLN
46	p	203	GLN
46	p	235	GLN
49	t	112	GLN
50	u	44	GLN
50	u	92	GLN
48	w	27	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
51	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
51	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	22.84

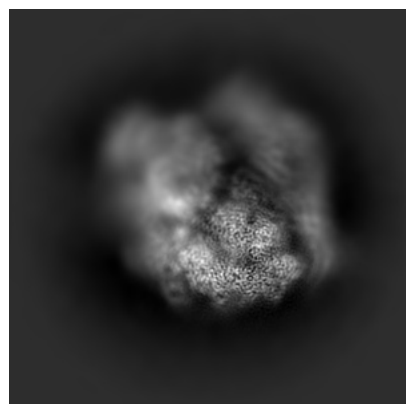
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16611. These allow visual inspection of the internal detail of the map and identification of artifacts.

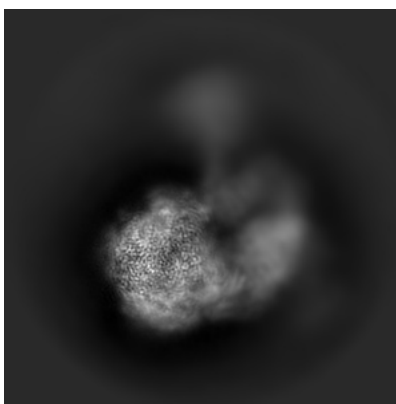
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

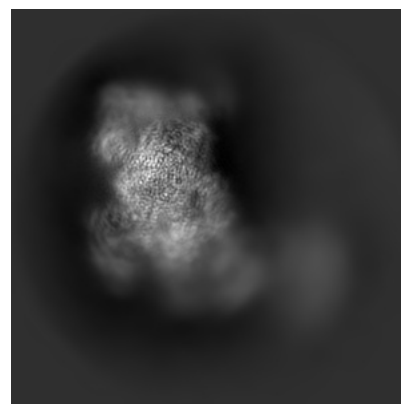
6.1.1 Primary map



X

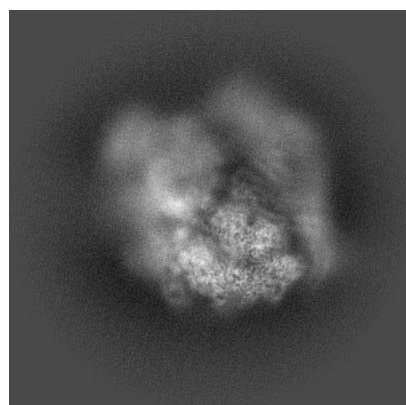


Y

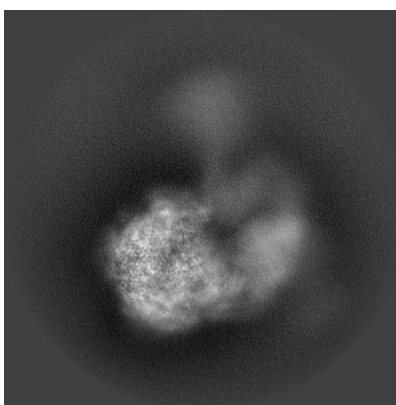


Z

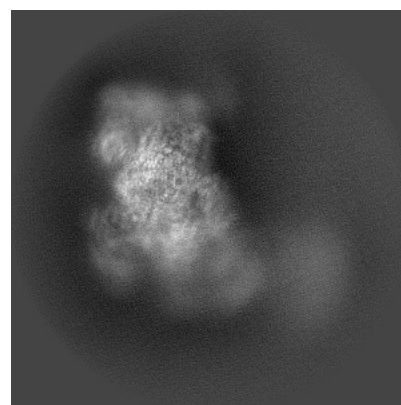
6.1.2 Raw map



X



Y

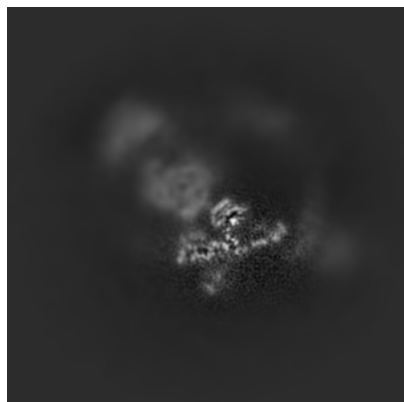


Z

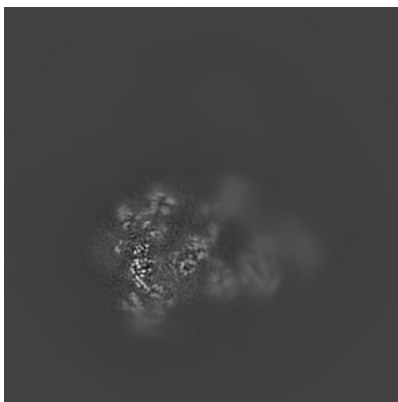
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

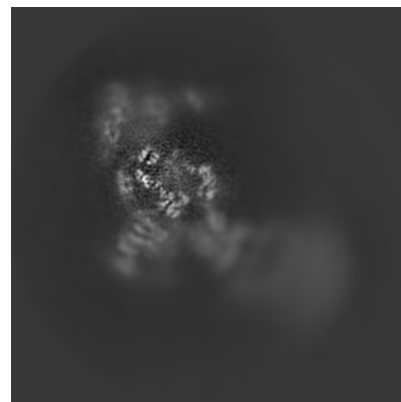
6.2.1 Primary map



X Index: 200

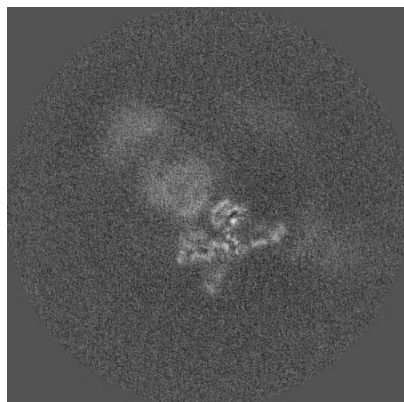


Y Index: 200

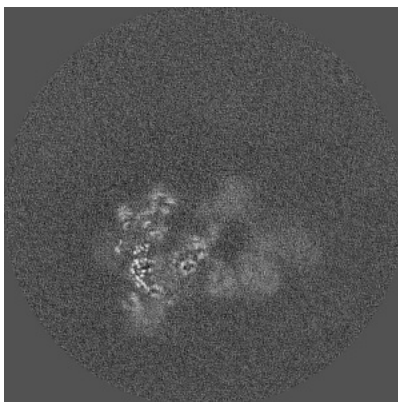


Z Index: 200

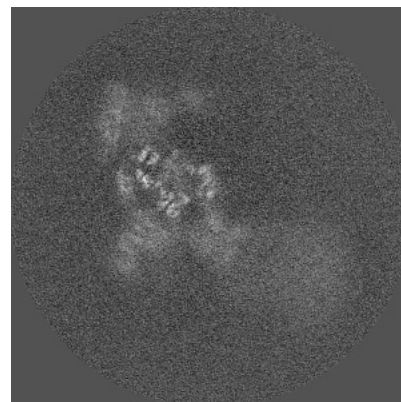
6.2.2 Raw map



X Index: 200



Y Index: 200

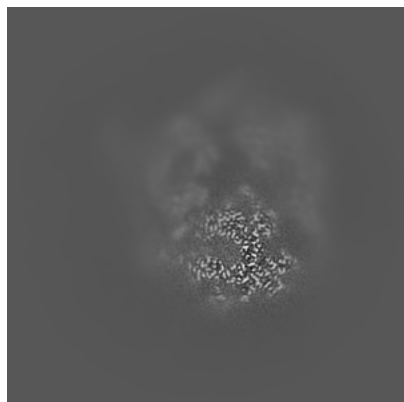


Z Index: 200

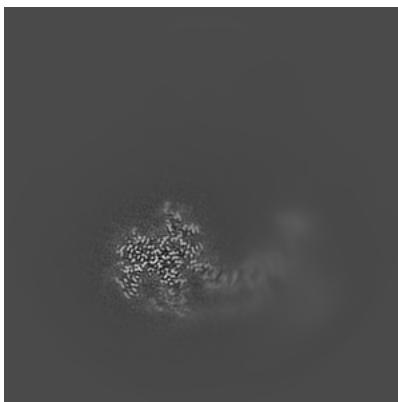
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

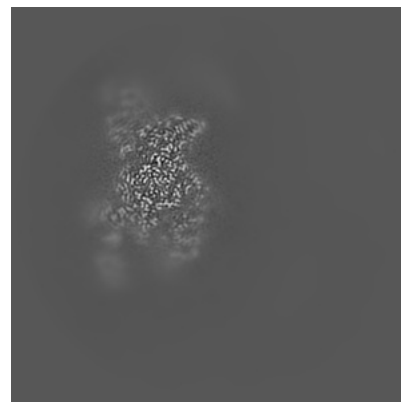
6.3.1 Primary map



X Index: 145

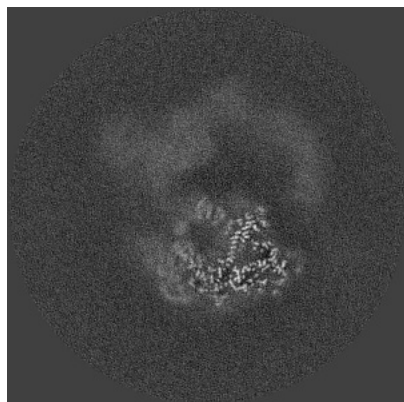


Y Index: 248

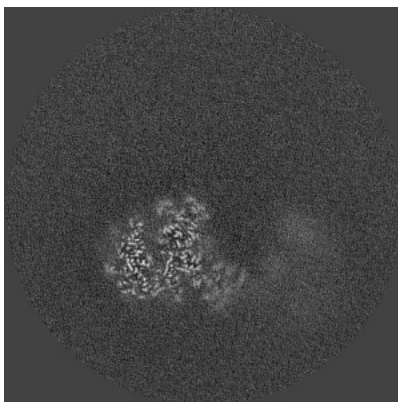


Z Index: 138

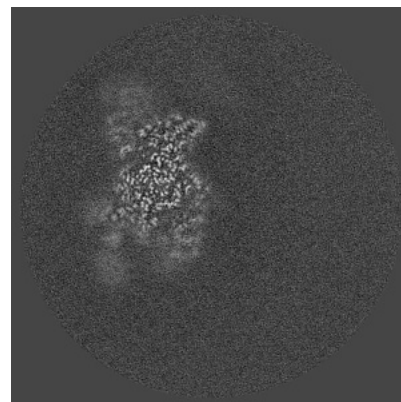
6.3.2 Raw map



X Index: 163



Y Index: 232

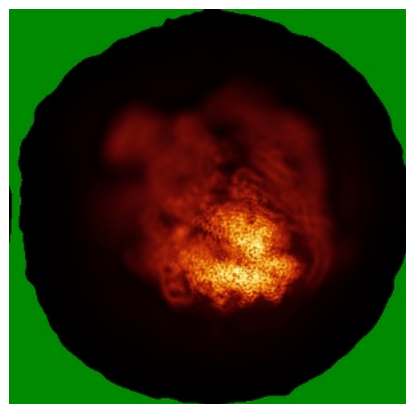


Z Index: 138

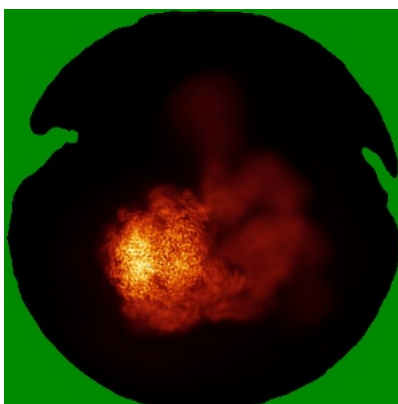
The images above show the largest variance slices of the map in three orthogonal directions.

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

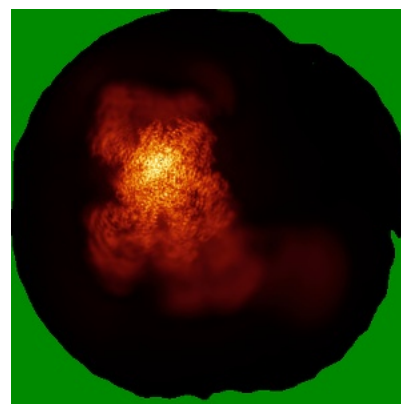
6.4.1 Primary map



X

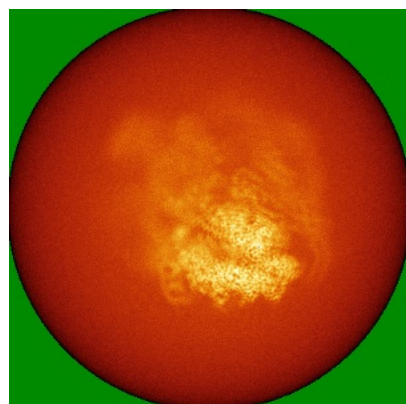


Y

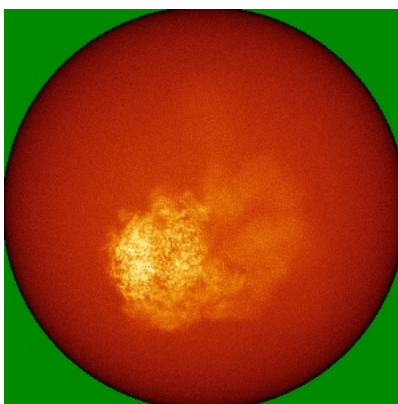


Z

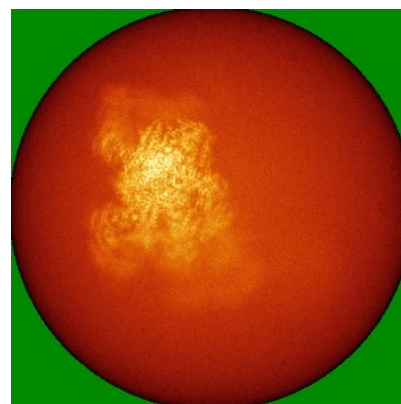
6.4.2 Raw map



X



Y

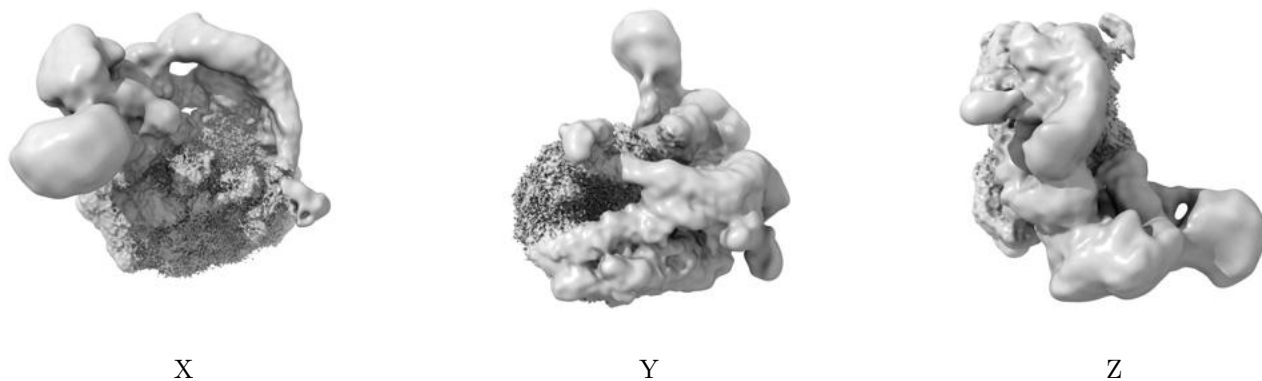


Z

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

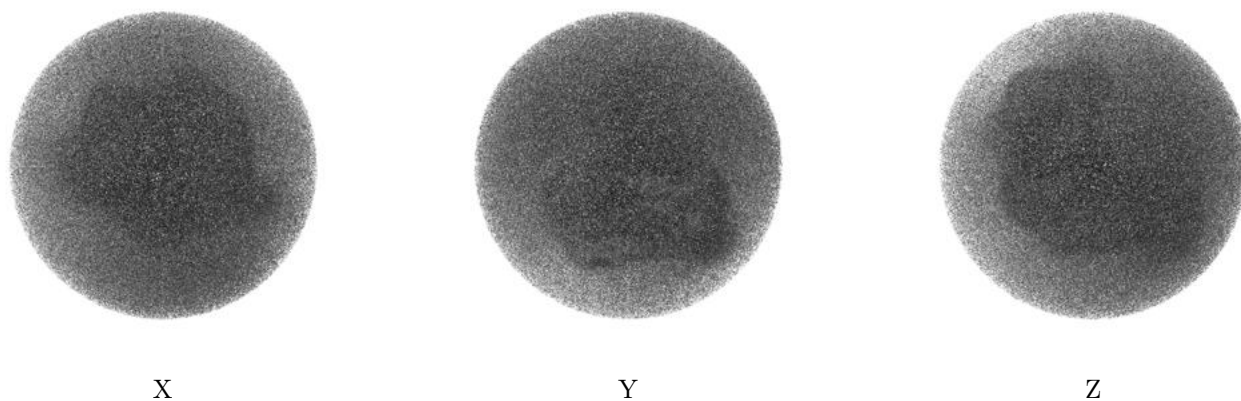
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

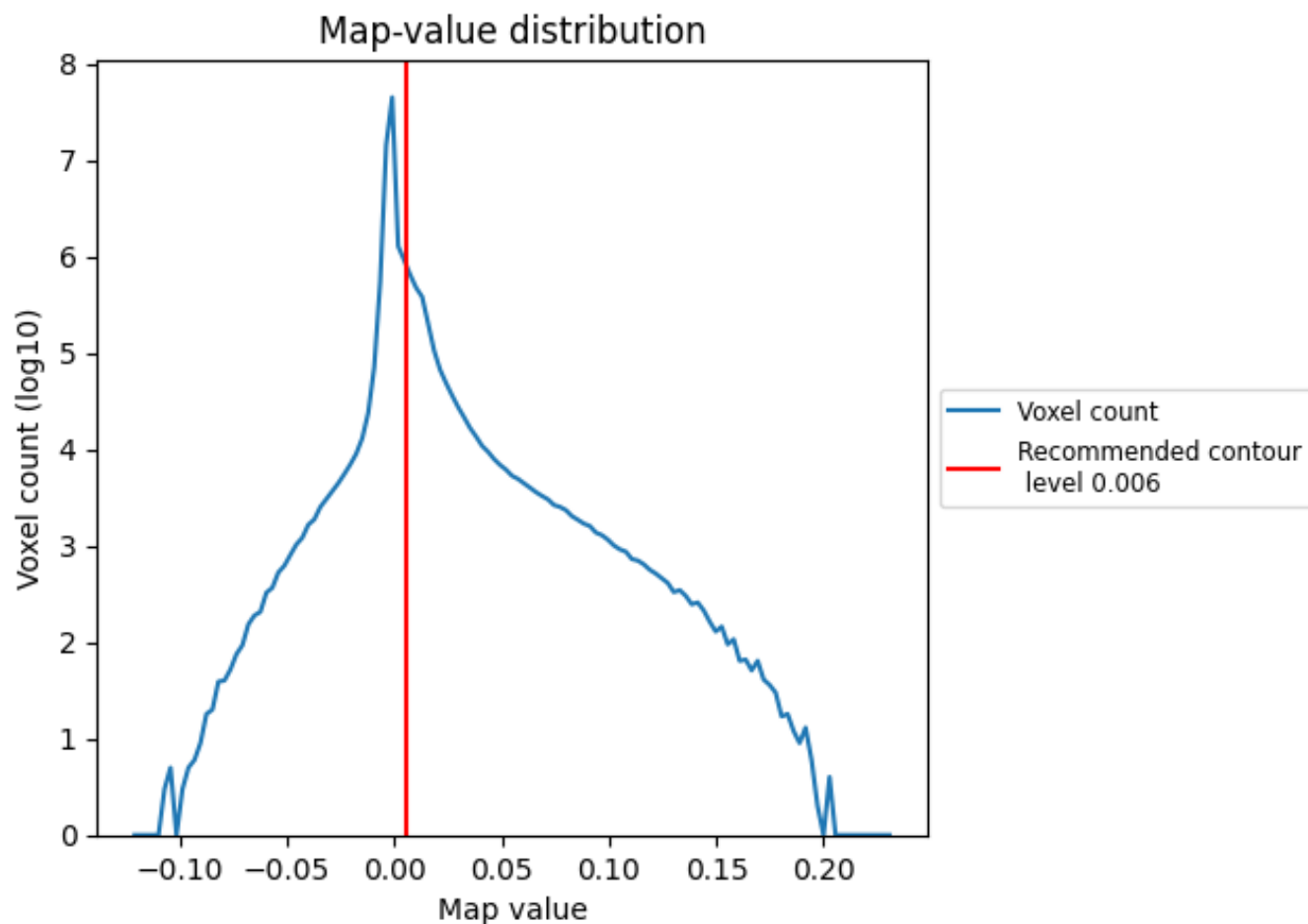
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

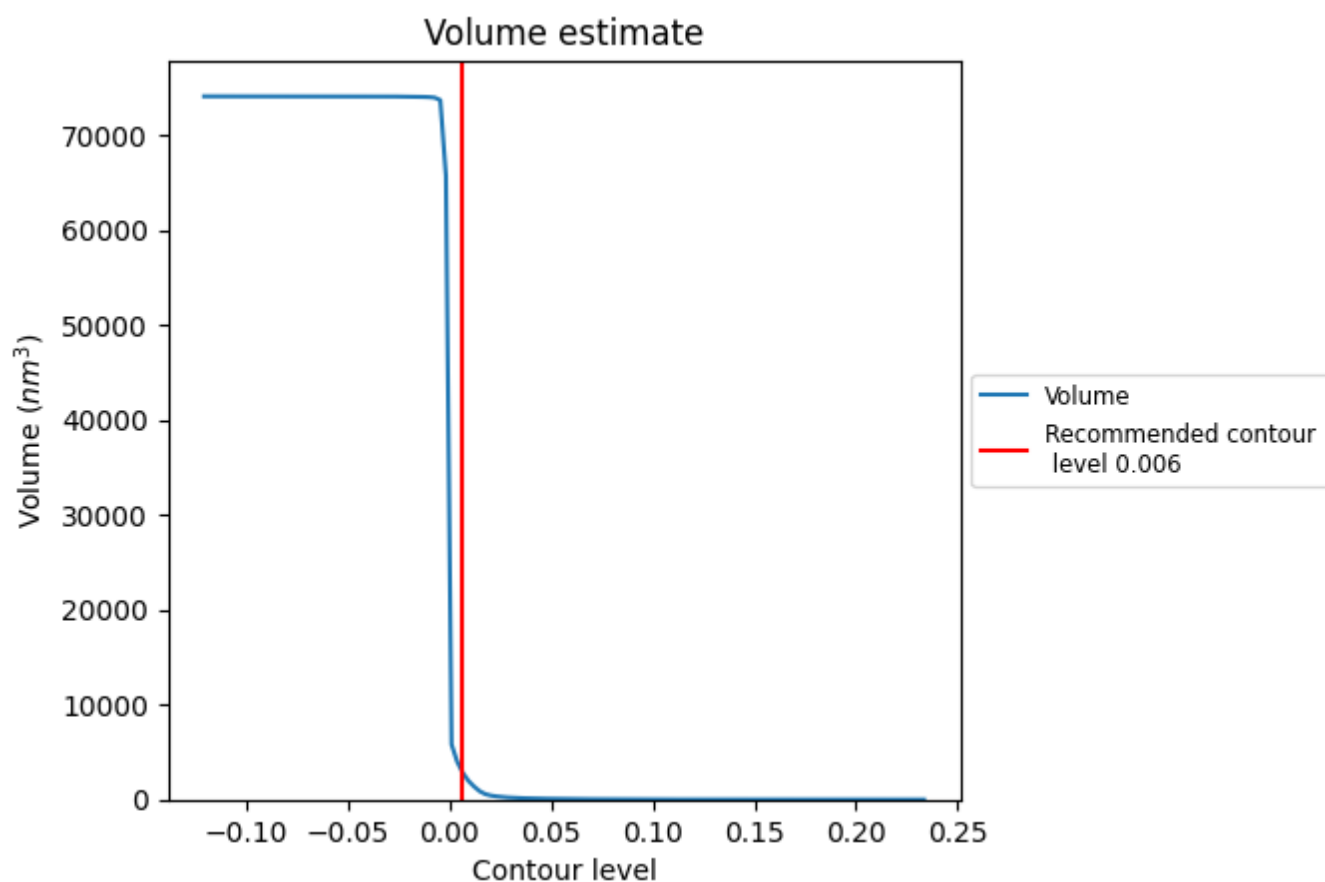
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

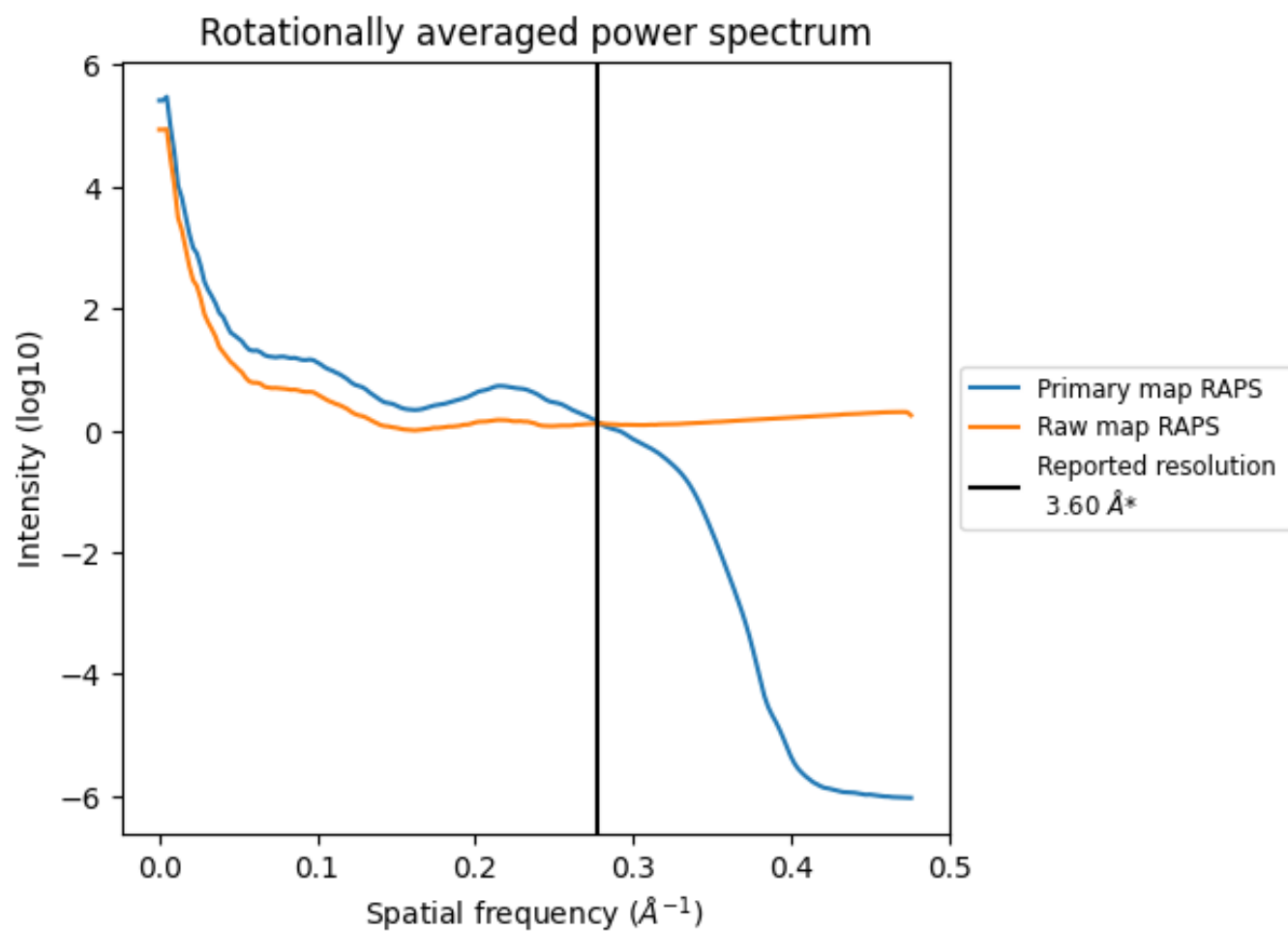
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2978 nm^3 ; this corresponds to an approximate mass of 2690 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 ⓘ

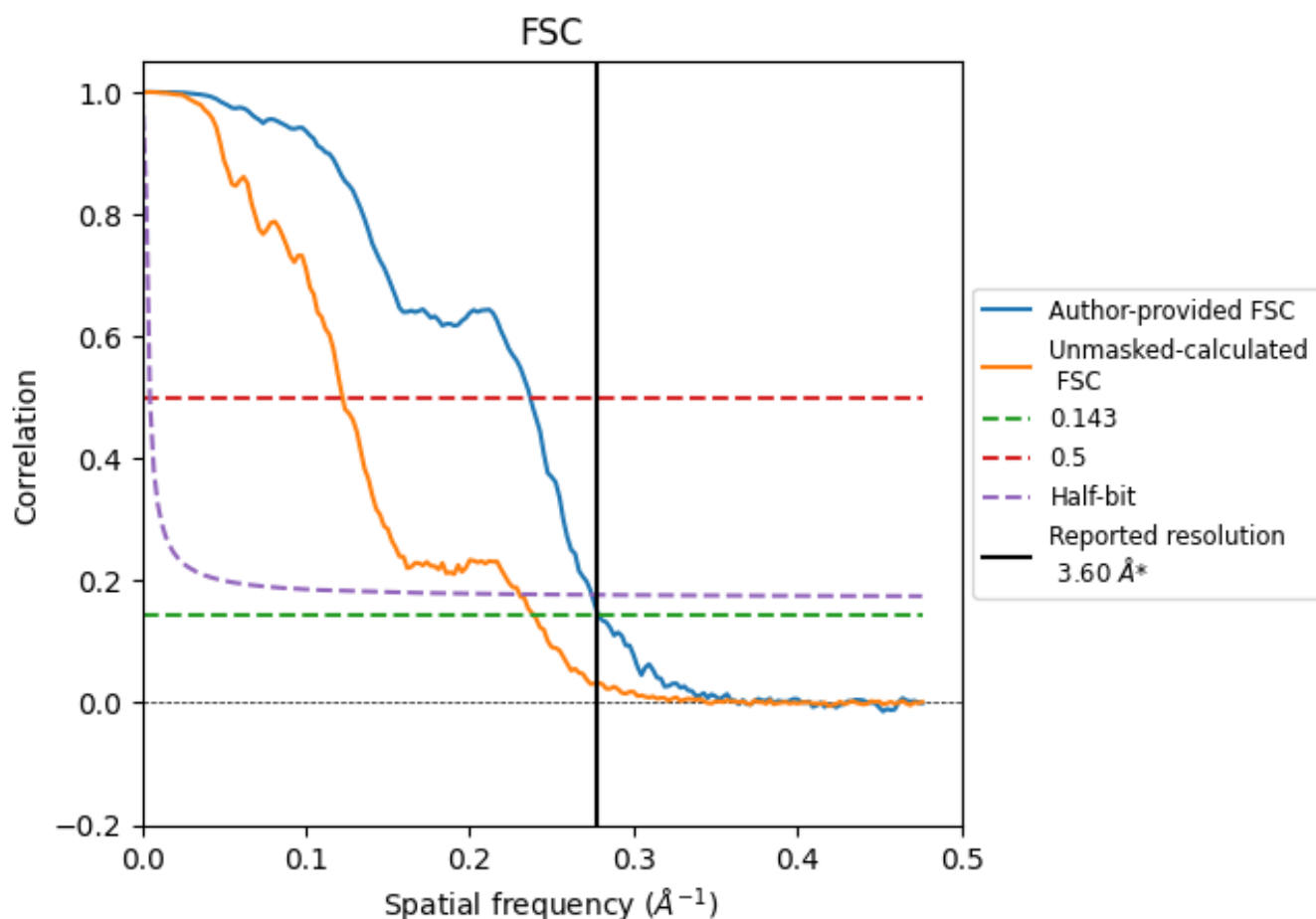


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

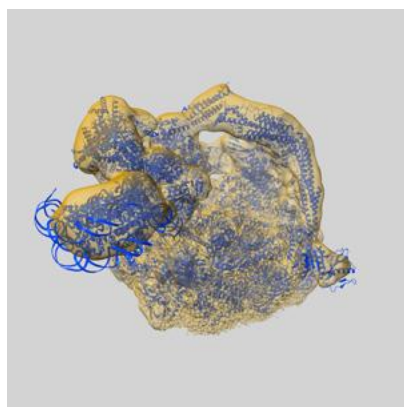
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.22	3.64
Unmasked-calculated*	4.18	8.18	4.34

*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 4.18 differs from the reported value 3.6 by more than 10 %

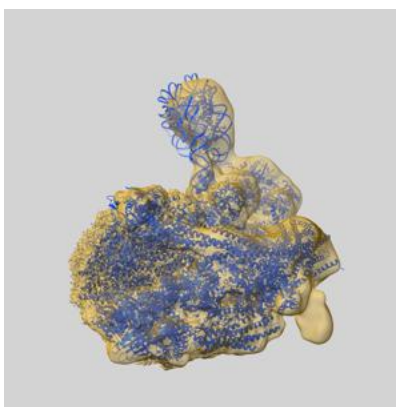
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16611 and PDB model 8CEO. Per-residue inclusion information can be found in section 3 on page 16.

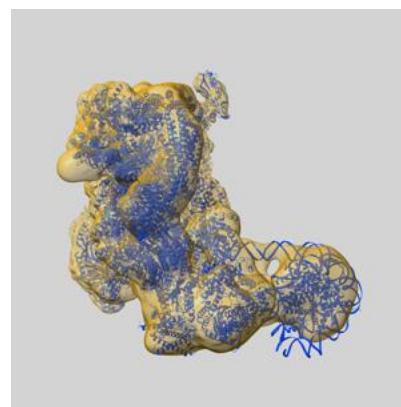
9.1 Map-model overlay [i](#)



X



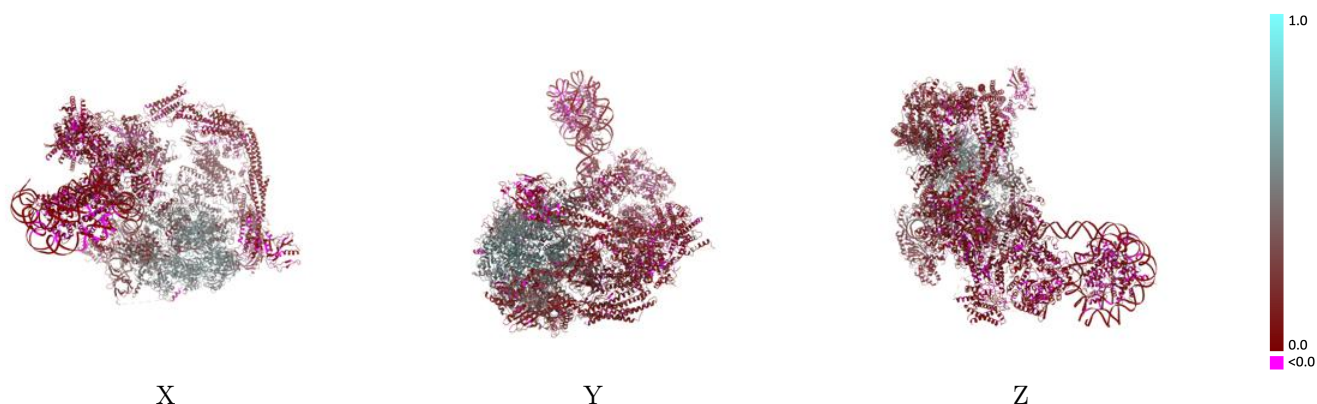
Y



Z

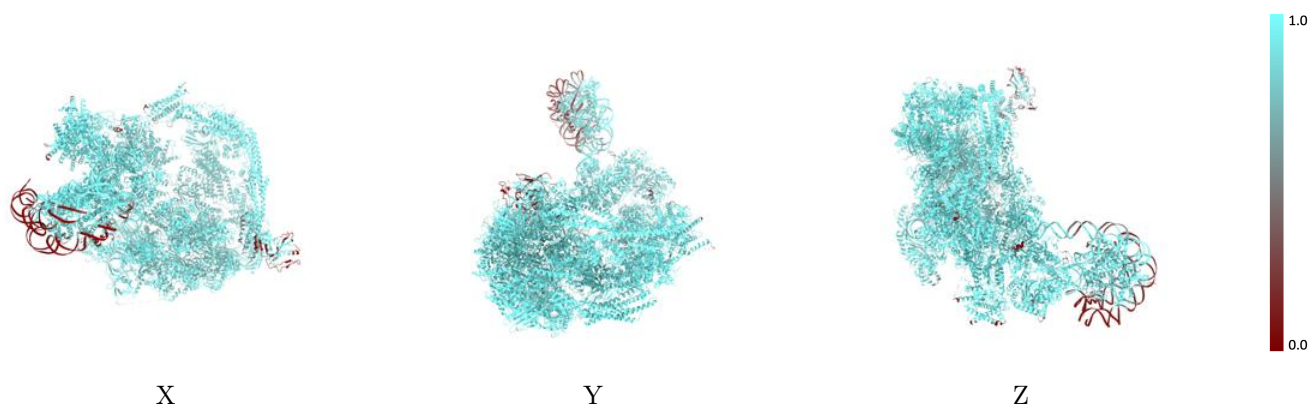
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



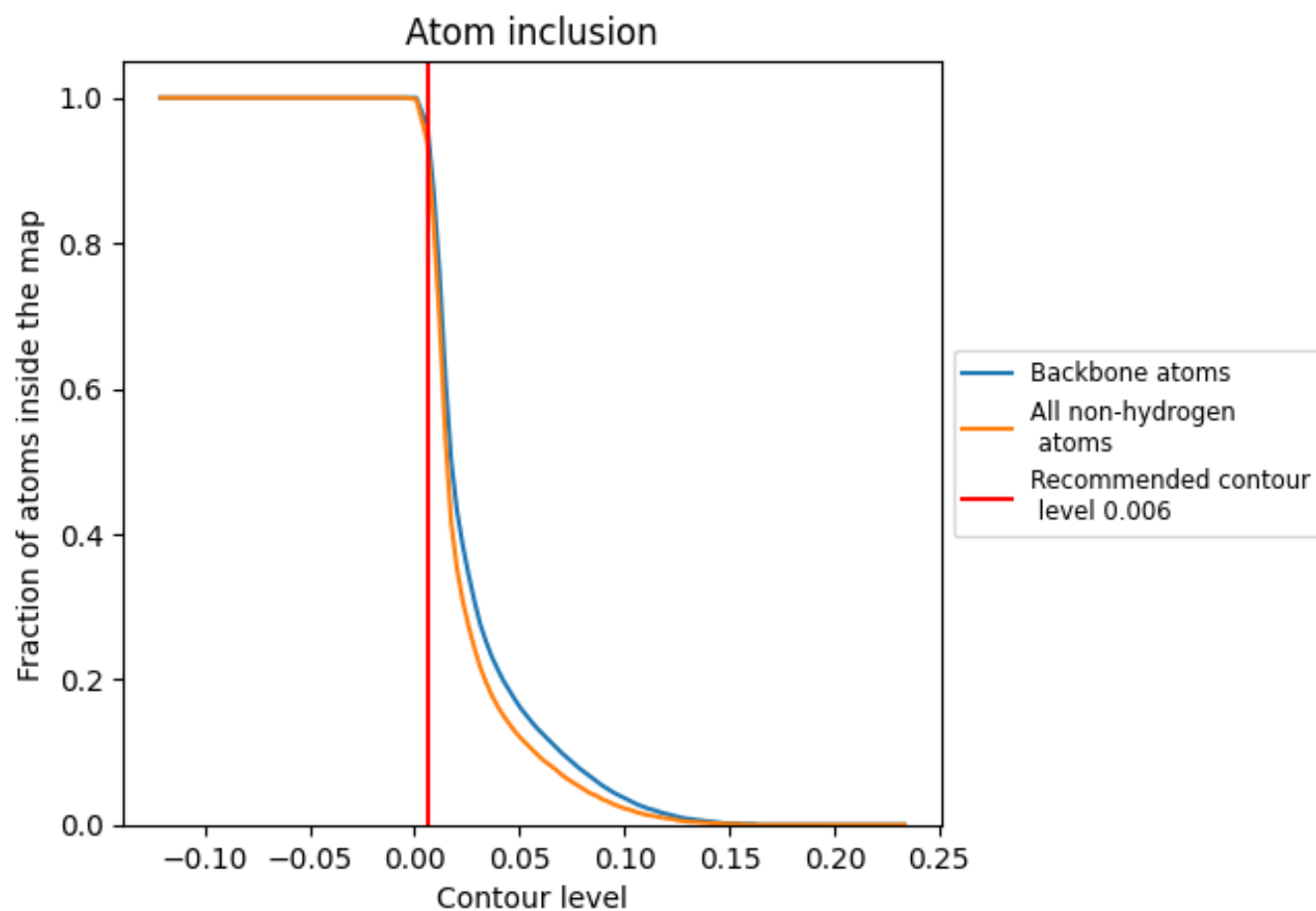
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.2220
0	 0.9880	 0.1100
1	 0.9590	 0.0830
2	 0.9790	 0.0750
3	 0.9880	 0.1710
4	 0.9970	 0.0610
5	 1.0000	 0.0720
6	 0.9640	 0.0820
7	 0.9890	 0.1030
A	 0.9860	 0.4510
B	 0.9850	 0.5000
C	 0.9890	 0.5120
D	 0.9670	 0.1990
E	 0.9900	 0.3850
F	 0.9220	 0.3790
G	 0.9840	 0.3480
H	 0.9780	 0.4460
I	 0.9910	 0.3480
J	 0.9910	 0.5340
K	 0.9770	 0.5050
L	 0.9860	 0.4710
M	 0.9770	 0.3570
N	 0.6520	 0.0940
O	 0.9940	 0.2260
Q	 0.9790	 0.2350
R	 0.9950	 0.2040
T	 0.6500	 0.0970
U	 0.9270	 0.1280
V	 0.9930	 0.1340
W	 0.9690	 0.1600
X	 0.9910	 0.1520
a	 0.9970	 0.1340
b	 0.9870	 0.1620
c	 0.9970	 0.1800
d	 0.9940	 0.1620



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Chain	Atom inclusion	Q-score
e	 0.9620	 0.3730
f	 0.9630	 0.3520
g	 0.9960	 0.1630
h	 0.9550	 0.1030
i	 0.9980	 0.1290
j	 0.8210	 0.1120
k	 0.9450	 0.0840
l	 0.9750	 0.1270
m	 0.9210	 0.0650
n	 0.9680	 0.0960
o	 0.9790	 0.1190
p	 0.5320	 0.0620
r	 0.7950	 0.0260
s	 0.7970	 0.0360
t	 0.7720	 0.0170
u	 0.7470	 0.0230
v	 0.9740	 0.0510
w	 1.0000	 0.0850
x	 0.9280	 0.0490
y	 0.9930	 0.0530