



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:15 PM UTC

PDB ID : 7NVR / pdb_00007nvr
EMDB ID : EMD-12610
Title : Human Mediator with RNA Polymerase II Pre-initiation complex
Authors : Rengachari, S.; Schilbach, S.; Aibara, S.; Cramer, P.
Deposited on : 2021-03-15
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

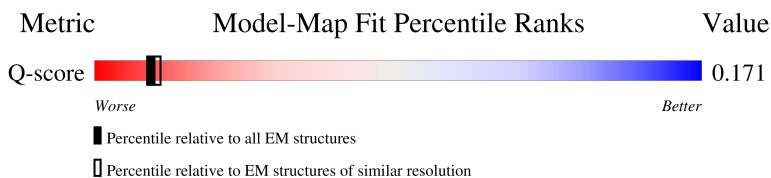
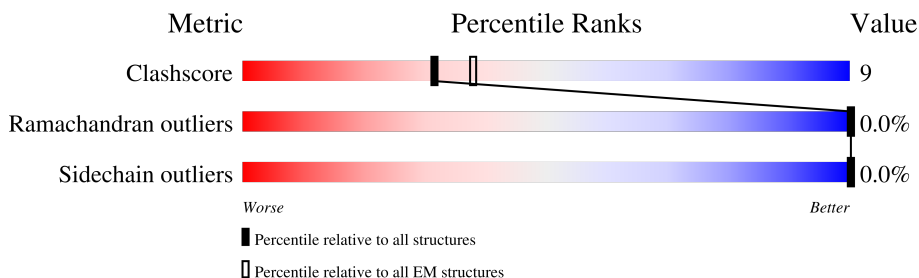
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	2937 (4.00 - 5.00)

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	760	
2	1	548	
3	2	462	
4	3	309	

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Mol	Chain	Length	Quality of chain
5	4	308	
6	5	71	
7	6	395	
8	7	782	
9	8	346	
10	9	323	
11	A	1970	
12	B	1174	
13	C	275	
14	D	142	
15	E	210	
16	F	127	
17	G	172	
18	H	150	
19	I	125	
20	J	67	
21	K	117	
22	L	58	
23	M	316	
24	N	106	
25	O	339	
26	Q	517	
27	R	249	
28	T	106	
29	U	376	

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Mol	Chain	Length	Quality of chain
30	V	109	
31	W	439	
32	X	291	
33	Y	19	
34	Z	8	
35	a	246	
36	b	268	
37	c	117	
38	d	651	
39	e	208	
40	f	212	
41	g	200	
42	h	270	
43	i	233	
44	j	146	
45	k	135	
46	l	1454	
47	m	244	
48	n	144	
49	o	131	
50	p	311	
51	q	178	
52	r	20	
53	s	178	
54	v	22	

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Mol	Chain	Length	Quality of chain
55	w	16	 100%
56	x	11	 100%
57	y	18	 89%11%
58	z	23	 100%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 96126 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 TFIIF basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 3 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	390	Total	C	N	O	S	0	0
			3158	2050	545	551	12		

- Molecule 4 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	214	Total	C	N	O	S	0	0
			1737	1092	299	334	12		

- Molecule 5 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	S	0	0
			523	337	83	100	3		

- Molecule 7 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	298	Total	C	N	O	S	0	0
			2376	1537	404	423	12		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	281	Total	C	N	O	S	0	0
			2293	1465	394	416	18		

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

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

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

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

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

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

- Molecule 14 is a protein called RPOL4c domain-containing protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called RNA_pol_L_2 domain-containing protein.

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

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

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

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

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

- Molecule 24 is a DNA chain called NT.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	64	Total	C	N	O	P	0	0
			1318	624	243	388	63		

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

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

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

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

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

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

- Molecule 28 is a DNA chain called TEMPLATE.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	64	Total	C	N	O	P	0	0
			1303	616	245	378	64		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

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

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

- Molecule 33 is a protein called Unassigned peptide, likely TFIIIE-beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Y	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 34 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	143	Total	C	N	O	S	0	0
			1167	754	198	210	5		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	136	Total	C	N	O	S	0	0
			1046	657	179	207	3		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	109	Total	C	N	O	S	0	0
			858	524	159	171	4		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	439	Total	C	N	O	S	0	0
			3510	2232	627	637	14		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	167	Total	C	N	O	S	0	0
			1353	868	233	238	14		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	186	Total	C	N	O	S	0	0
			1448	924	238	270	16		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	130	Total	C	N	O	S	0	0
			1063	656	181	222	4		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	138	Total	C	N	O	S	0	0
			1114	696	195	219	4		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	113	Total	C	N	O	S	0	0
			960	614	170	170	6		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	72	Total	C	N	O	S	0	0
			596	375	108	109	4		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	133	Total	C	N	O	S	0	0
			1088	690	188	206	4		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	501	Total	C	N	O	S	0	0
			4031	2591	694	722	24		

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	84	Total	C	N	O	S	0	0
			655	417	113	121	4		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	132	Total	C	N	O	S	0	0
			1005	621	170	210	4		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	91	Total	C	N	O	S	0	0
			804	535	132	133	4		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	154	Total	C	N	O	S	0	0
			1262	813	218	222	9		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	69	Total	C	N	O	S	0	0
			591	373	111	106	1		

- Molecule 52 is a protein called unassigned peptide (MED29 or MED30).

Mol	Chain	Residues	Atoms				AltConf	Trace
52	r	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	44	Total	C	N	O	S	0	0
			369	227	72	67	3		

- Molecule 54 is a protein called unassigned peptide (MED14).

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 55 is a protein called unassigned peptide (MED6).

Mol	Chain	Residues	Atoms				AltConf	Trace
55	w	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 56 is a protein called unassigned peptide (MED17).

Mol	Chain	Residues	Atoms				AltConf	Trace
56	x	11	Total	C	N	O	0	0
			55	33	11	11		

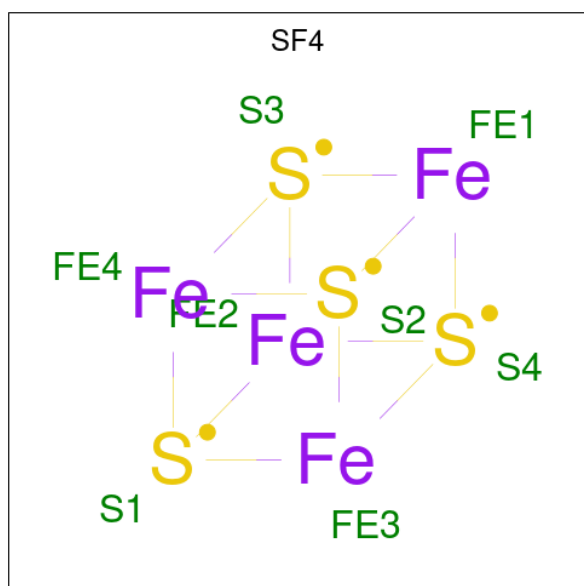
- Molecule 57 is a protein called unassigned peptide (MED29 or MED30).

Mol	Chain	Residues	Atoms				AltConf	Trace
57	y	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 58 is a protein called unassigned peptide (MED29 or MED30).

Mol	Chain	Residues	Atoms				AltConf	Trace
58	z	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
59	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	3	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
60	4	2	Total 2	Zn 2	0
60	6	3	Total 3	Zn 3	0
60	A	2	Total 2	Zn 2	0
60	B	1	Total 1	Zn 1	0
60	C	1	Total 1	Zn 1	0
60	I	2	Total 2	Zn 2	0
60	J	1	Total 1	Zn 1	0
60	L	1	Total 1	Zn 1	0
60	M	1	Total 1	Zn 1	0
60	W	1	Total 1	Zn 1	0
60	p	1	Total 1	Zn 1	0

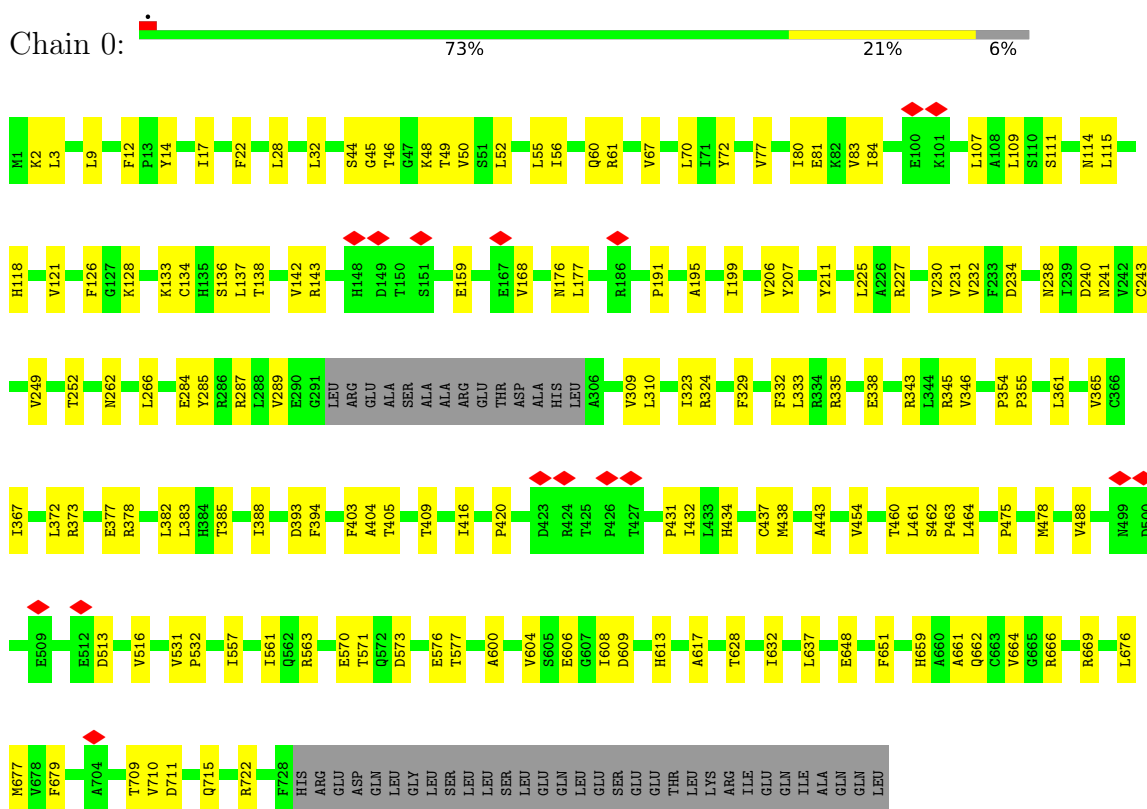
- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

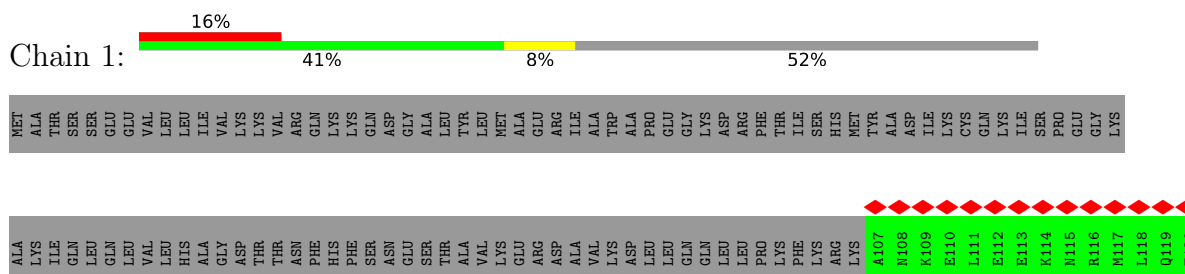
3 Residue-property plots

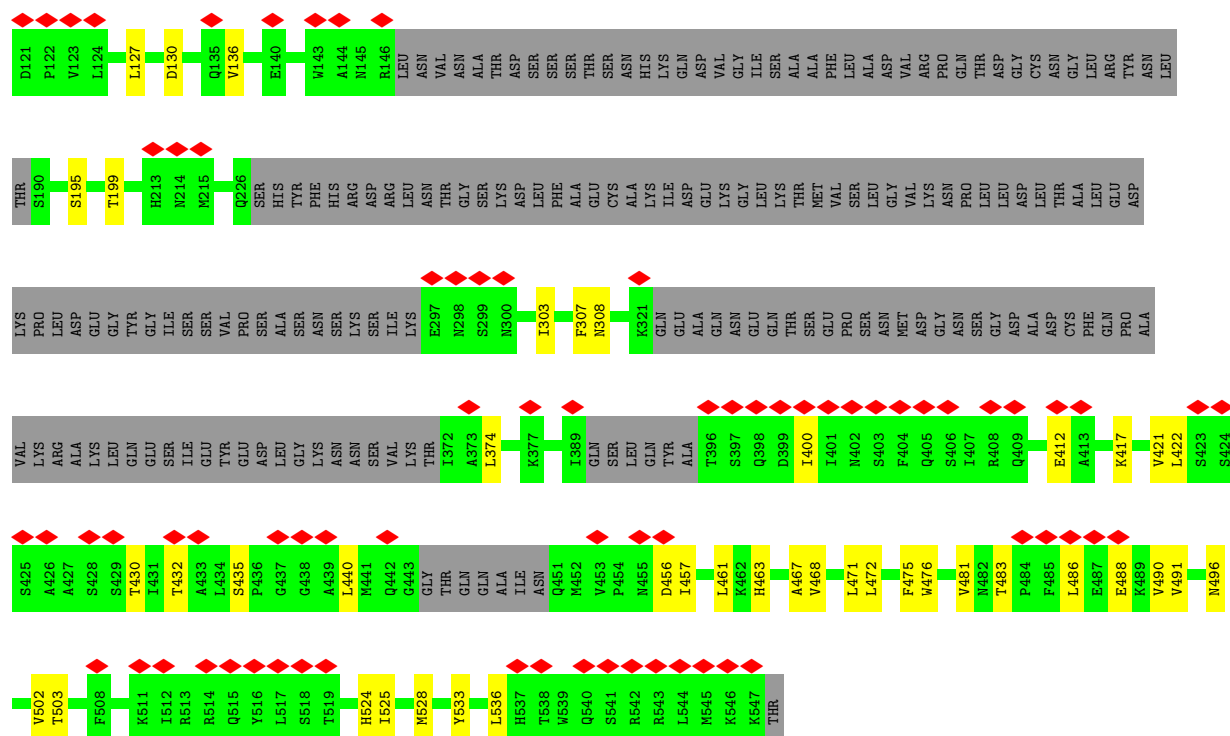
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TFIIH basal transcription factor complex helicase XPD subunit

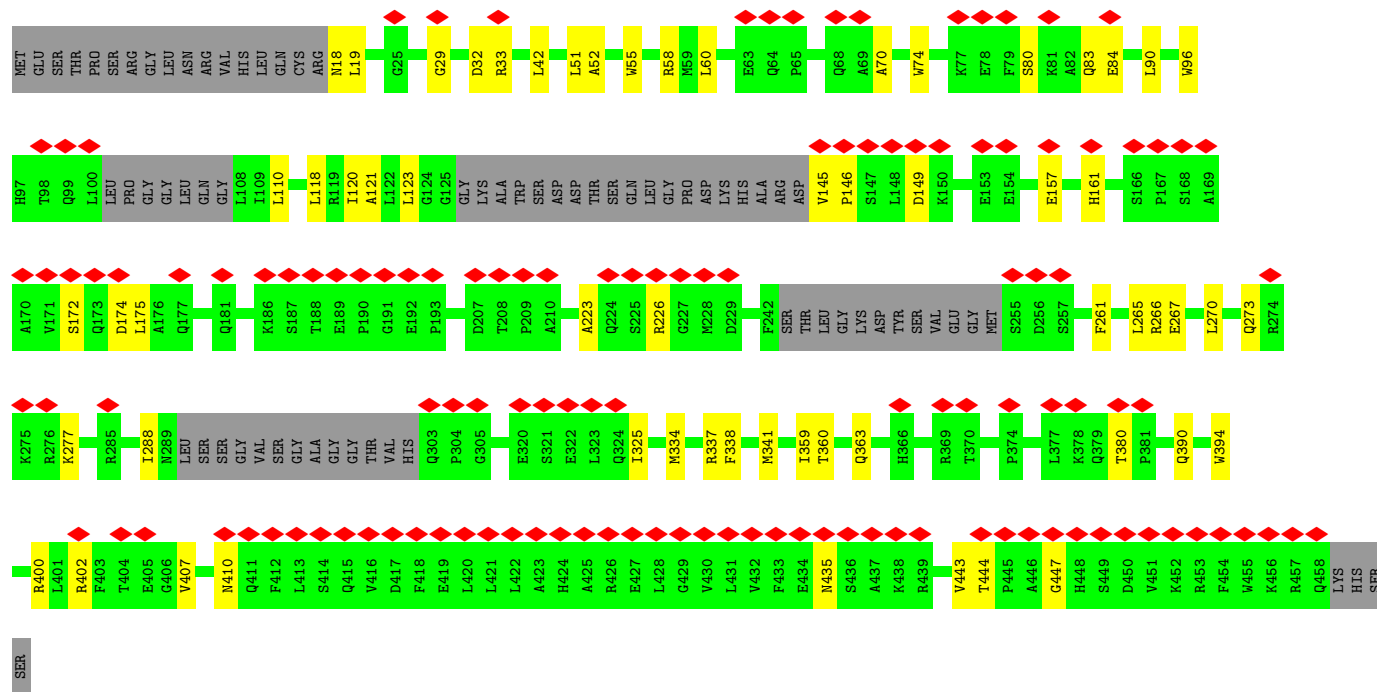


- Molecule 2: General transcription factor IIH subunit 1





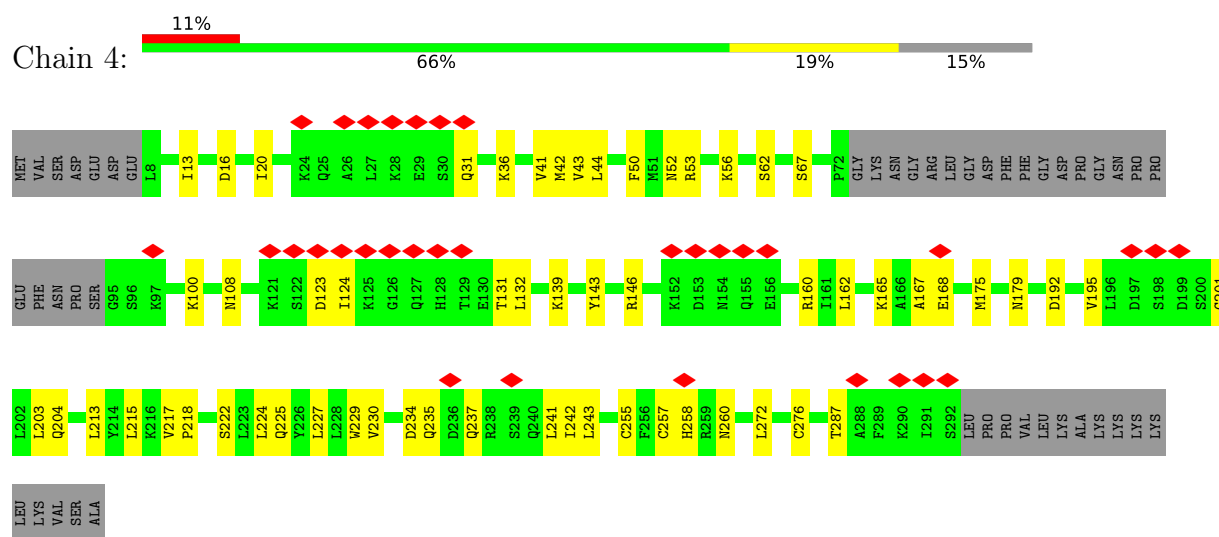
• Molecule 3: General transcription factor IIH subunit 4



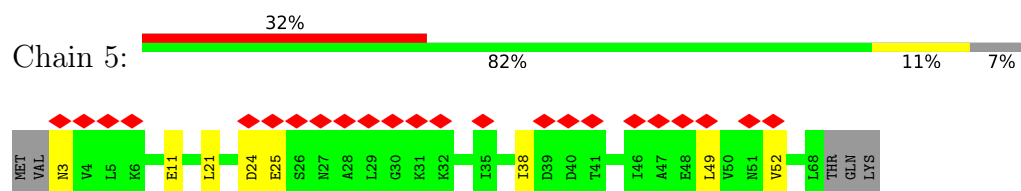
• Molecule 4: CDK-activating kinase assembly factor MAT1



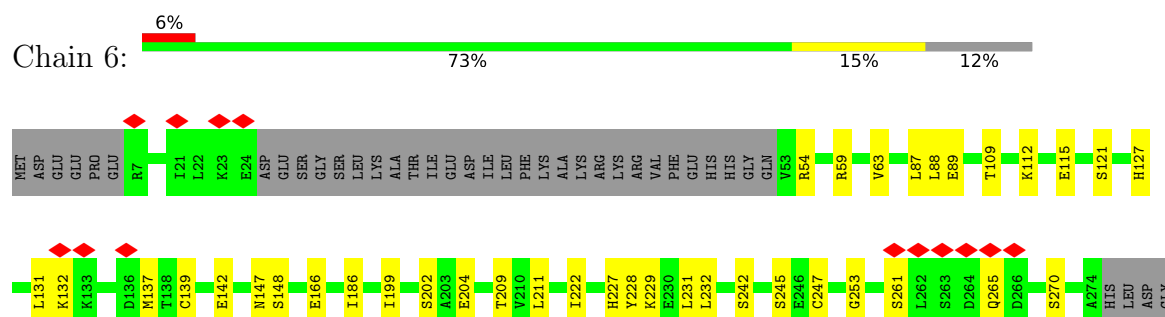
- Molecule 5: General transcription factor IIH subunit 3

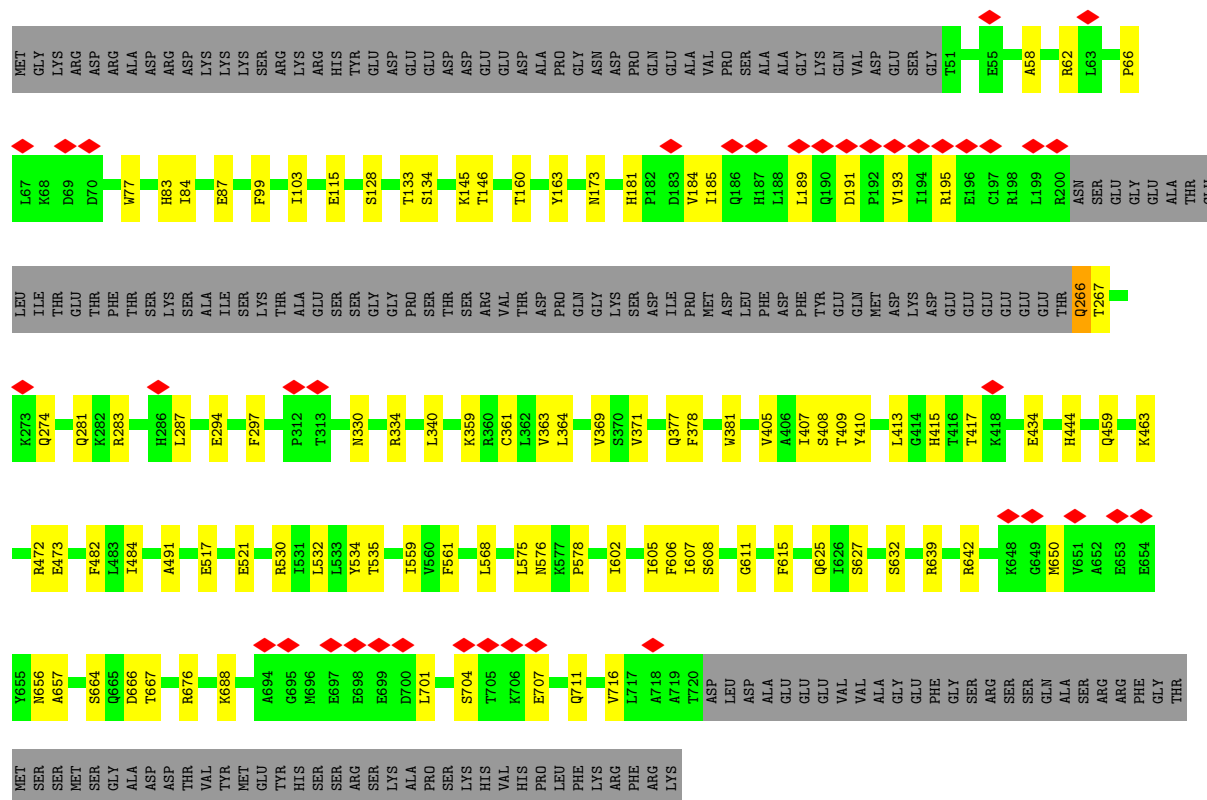


- Molecule 6: General transcription factor IIH subunit 5

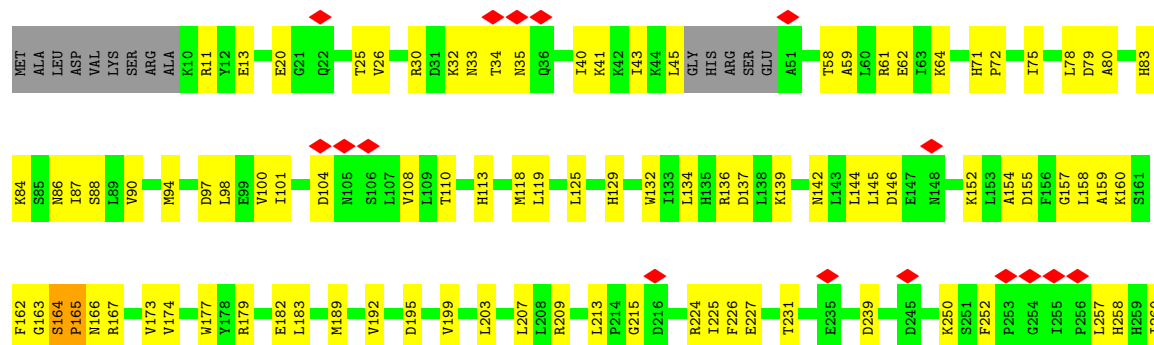


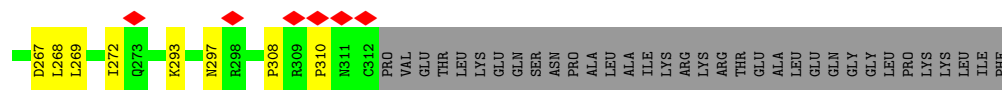
- Molecule 7: General transcription factor IIH subunit 2



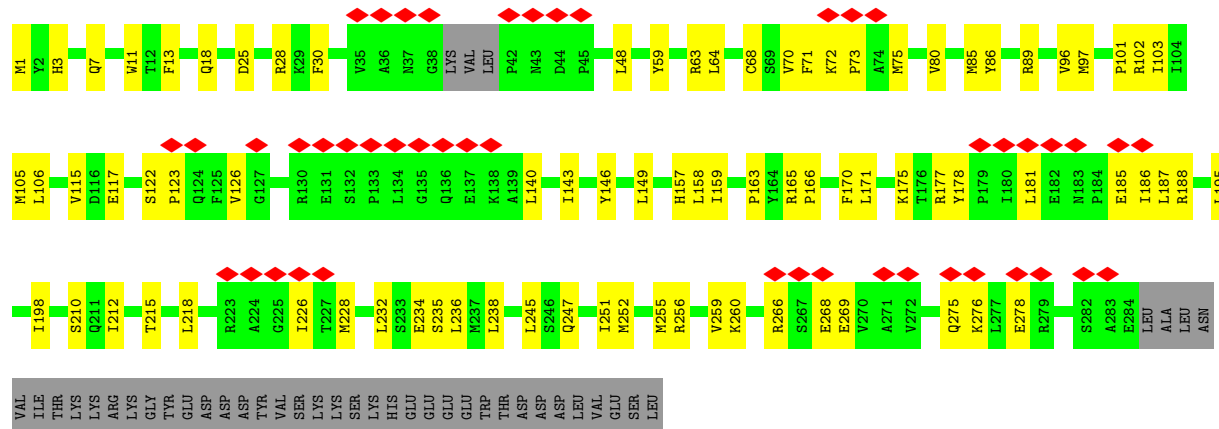


Chain 8: 6% 57% 28% 14%

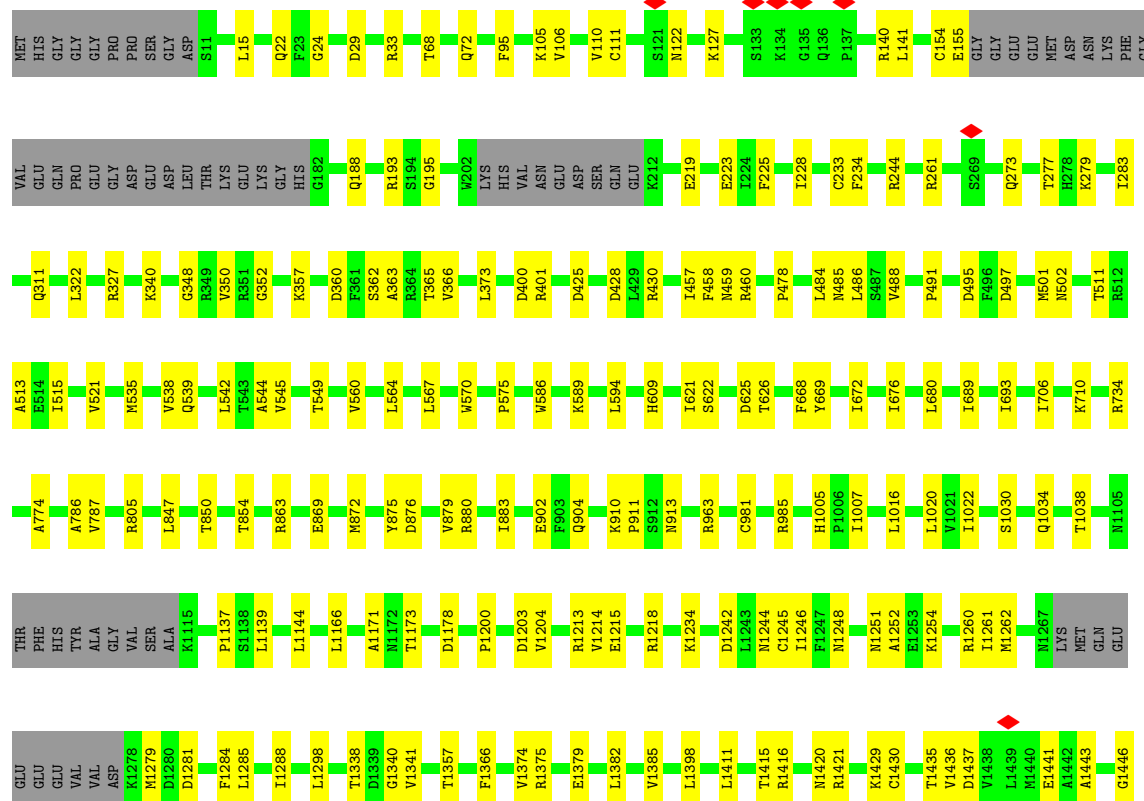


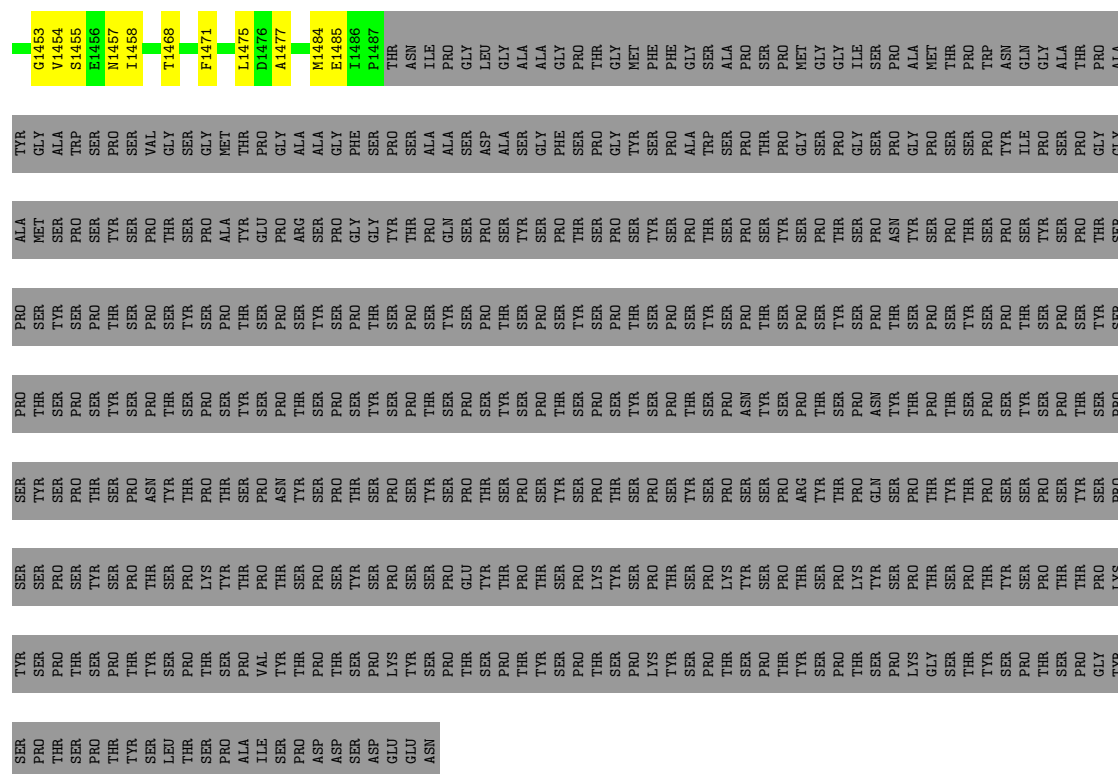


• Molecule 10: Cyclin-H

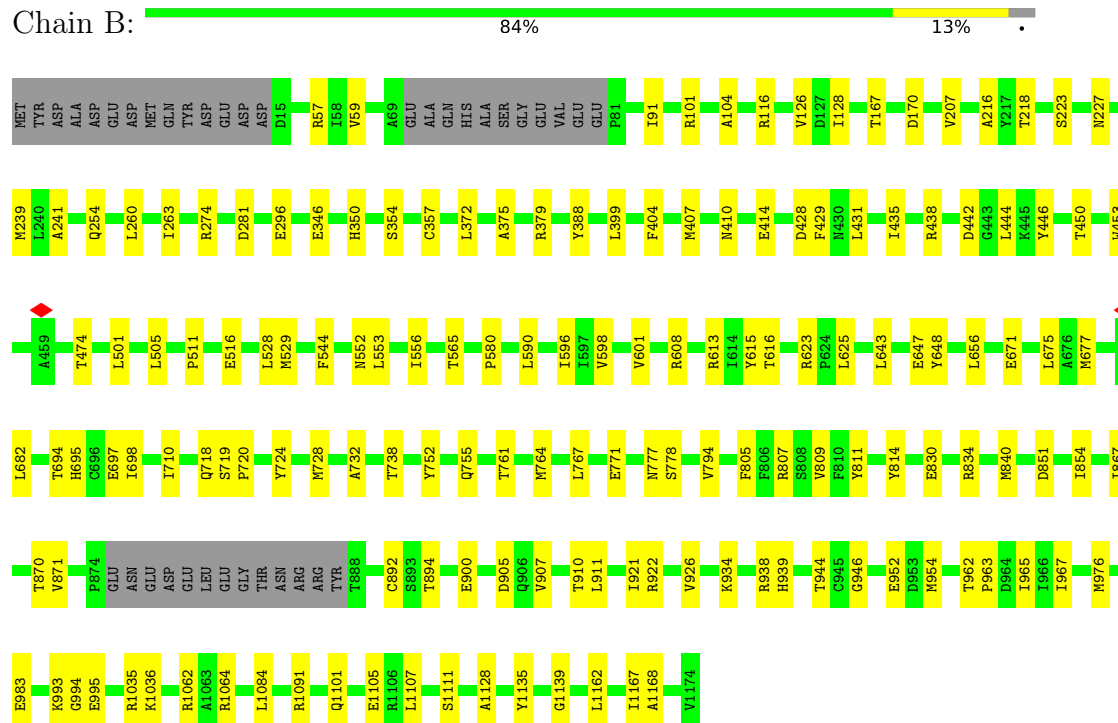


• Molecule 11: DNA-directed RNA polymerase subunit

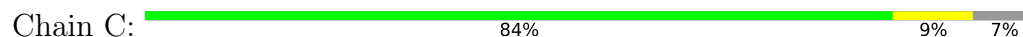


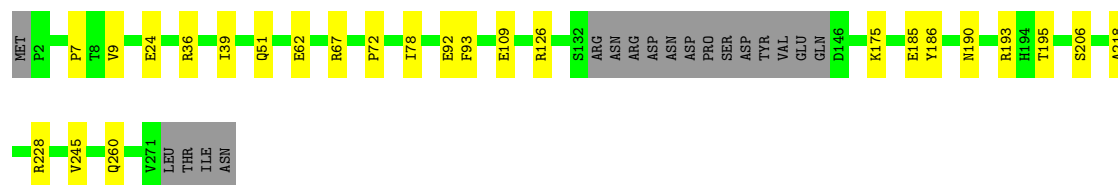


- Molecule 12: DNA-directed RNA polymerase subunit beta

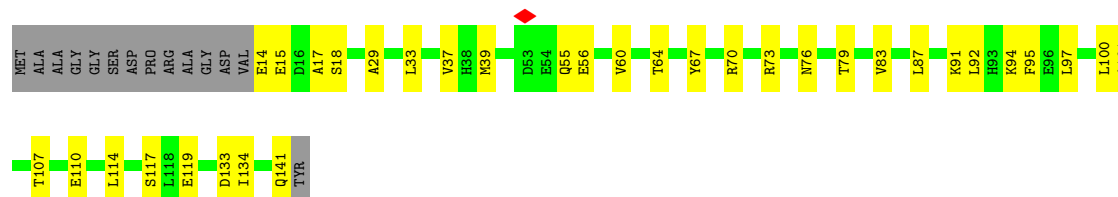


- Molecule 13: DNA-directed RNA polymerase II subunit RPB3





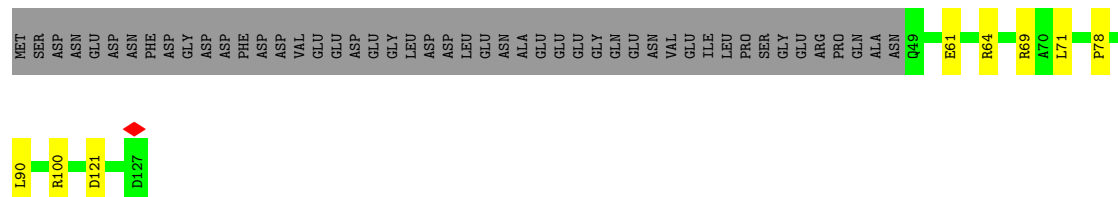
- Molecule 14: RPOL4c domain-containing protein



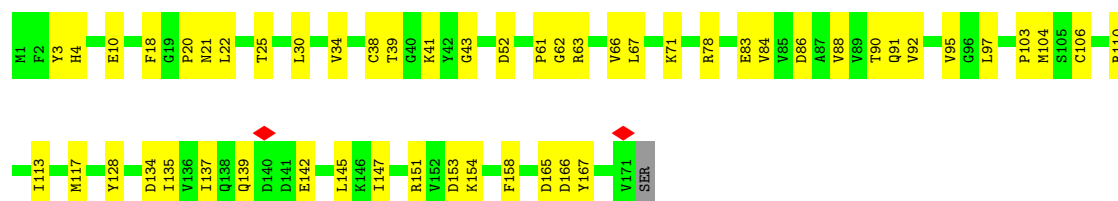
- Molecule 15: DNA-directed RNA polymerase II subunit E



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



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

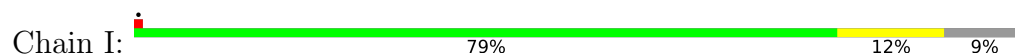


- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3

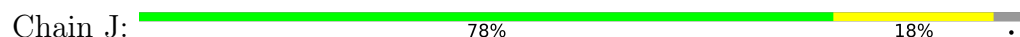




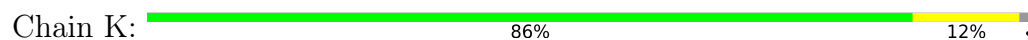
- Molecule 19: DNA-directed RNA polymerase II subunit RPB9



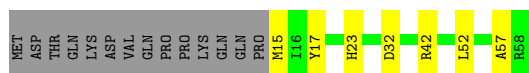
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 21: RNA_pol_L_2 domain-containing protein



- Molecule 22: RNA polymerase II subunit K

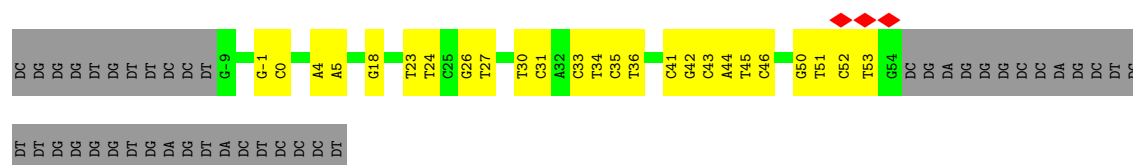


- Molecule 23: Transcription initiation factor IIB



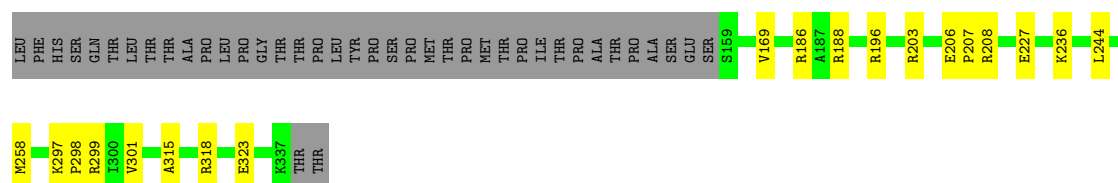
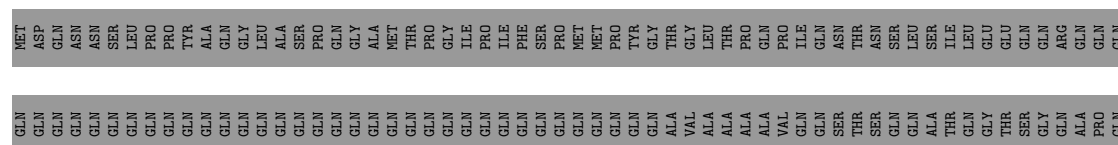
- Molecule 24: NT





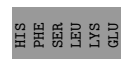
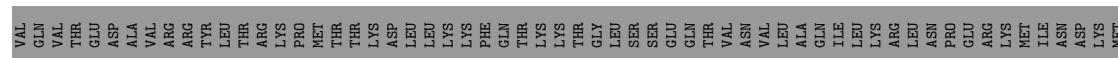
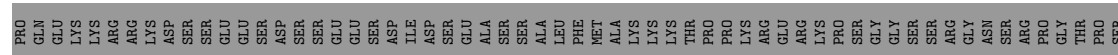
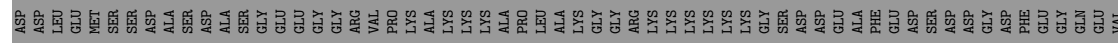
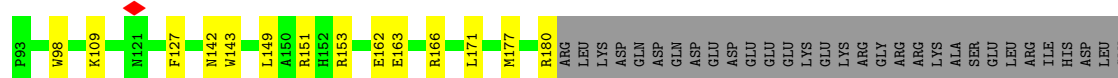
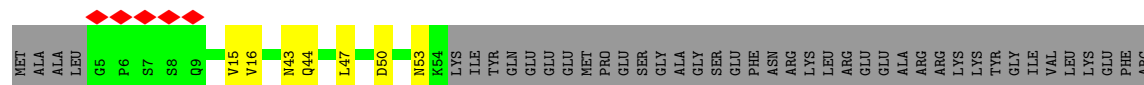
• Molecule 25: TATA-box-binding protein

Chain O: 47% 6% 47%



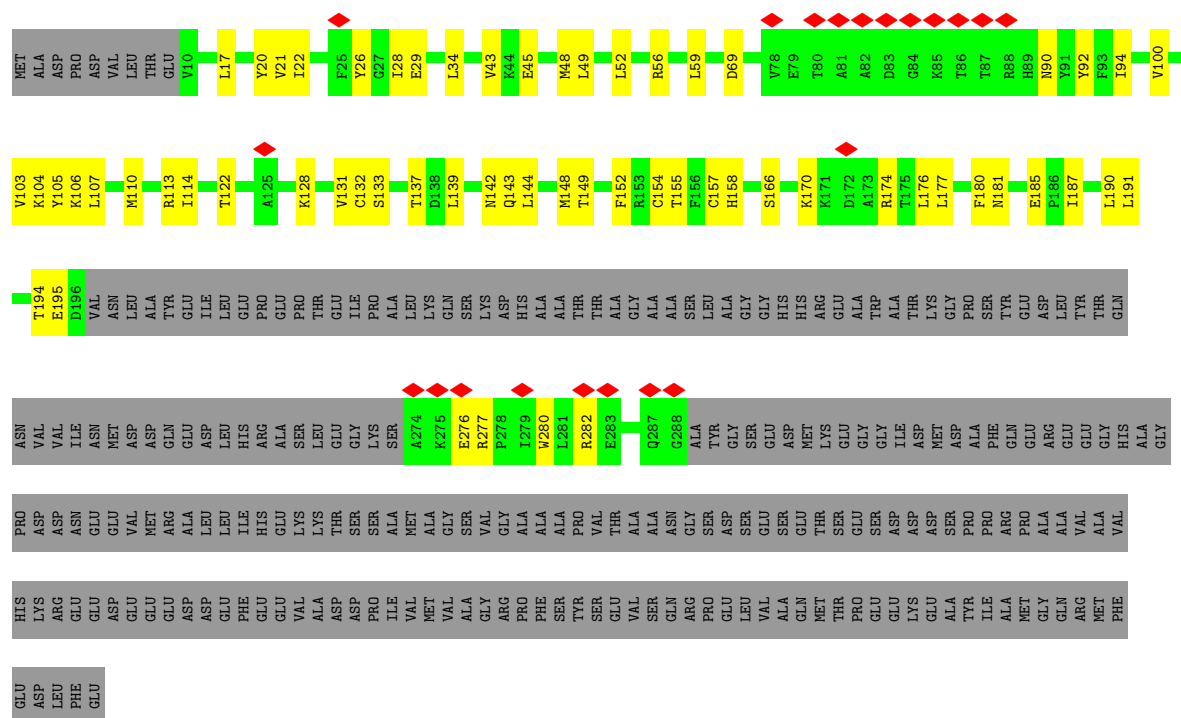
• Molecule 26: General transcription factor IIF subunit 1

Chain Q: 23% 0% 73%

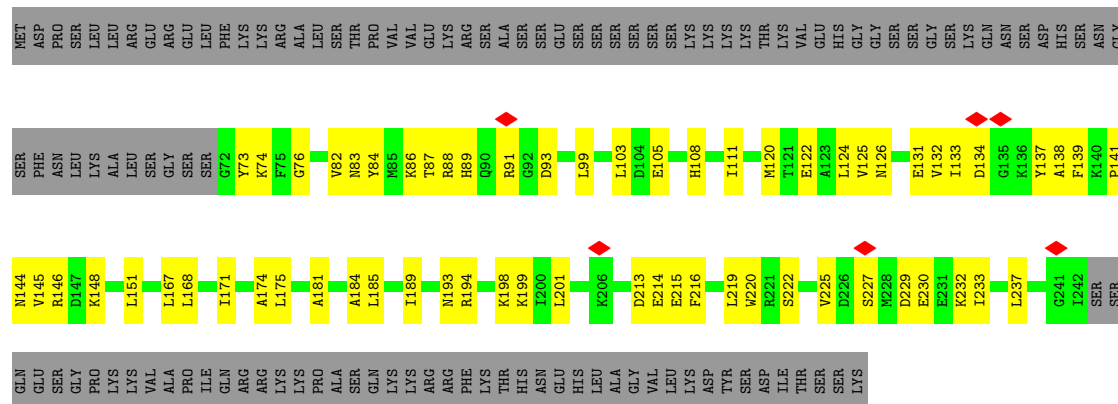


• Molecule 27: General transcription factor IIF subunit 2

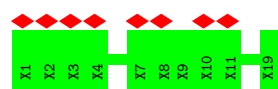
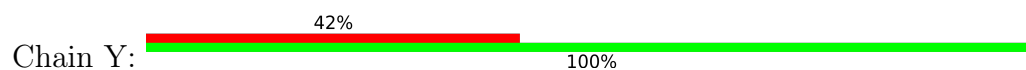
Chain R: 79% 10% 11%



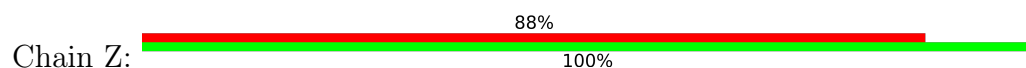
• Molecule 32: Transcription initiation factor IIE subunit beta

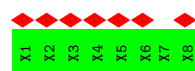


• Molecule 33: Unassigned peptide, likely TFIIE-beta



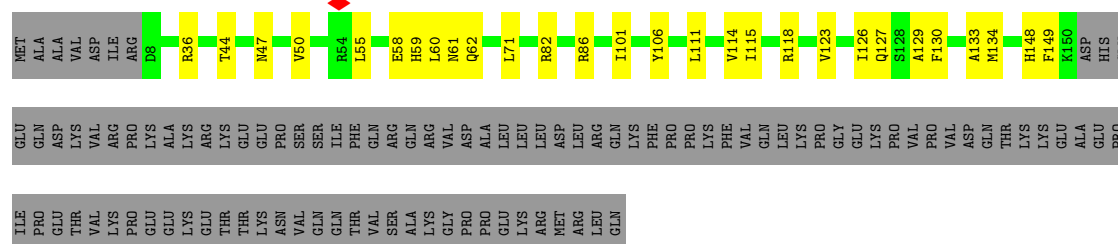
• Molecule 34: Unassigned peptide, likely XPB





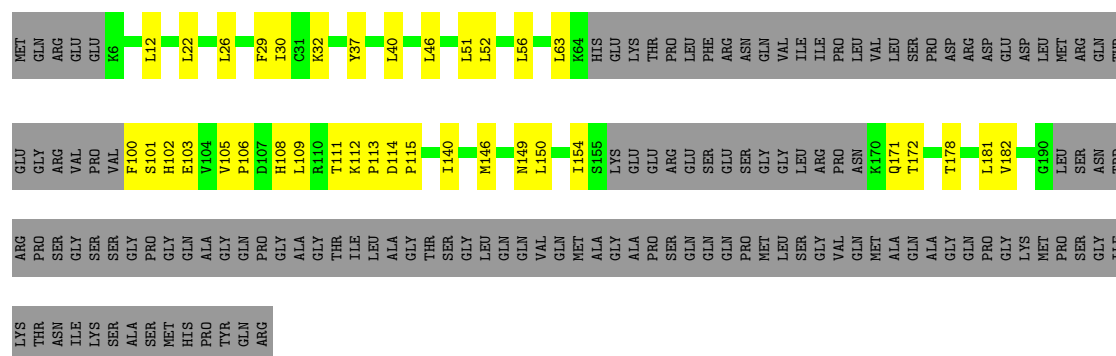
• Molecule 35: Mediator of RNA polymerase II transcription subunit 6

Chain a: 47% 11% 42%



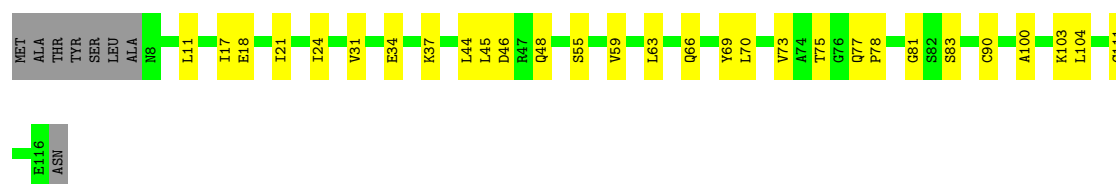
• Molecule 36: Mediator of RNA polymerase II transcription subunit 8

Chain b: 37% 13% 49%



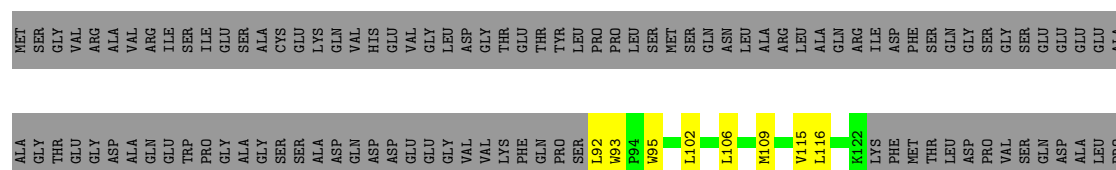
• Molecule 37: Mediator of RNA polymerase II transcription subunit 11

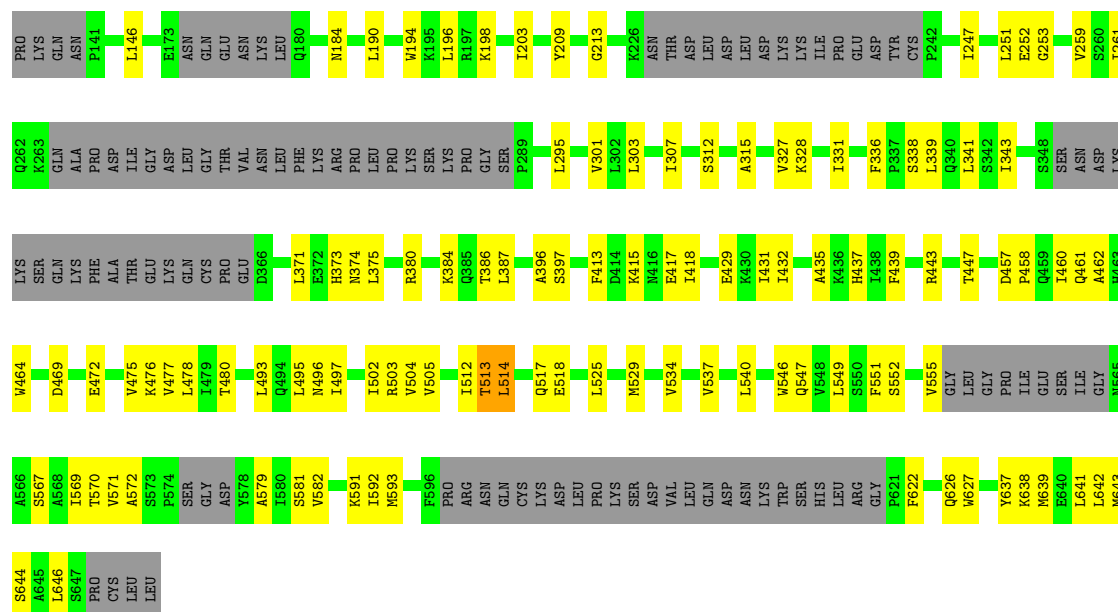
Chain c: 68% 25% 7%



• Molecule 38: Mediator of RNA polymerase II transcription subunit 17

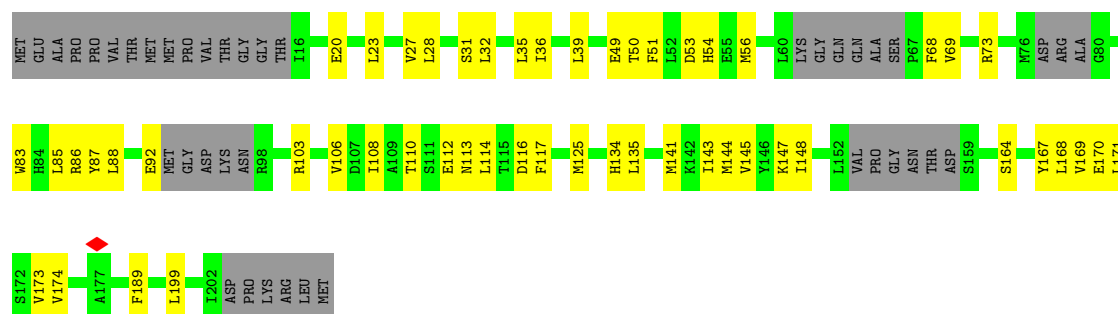
Chain d: 49% 18% 33%





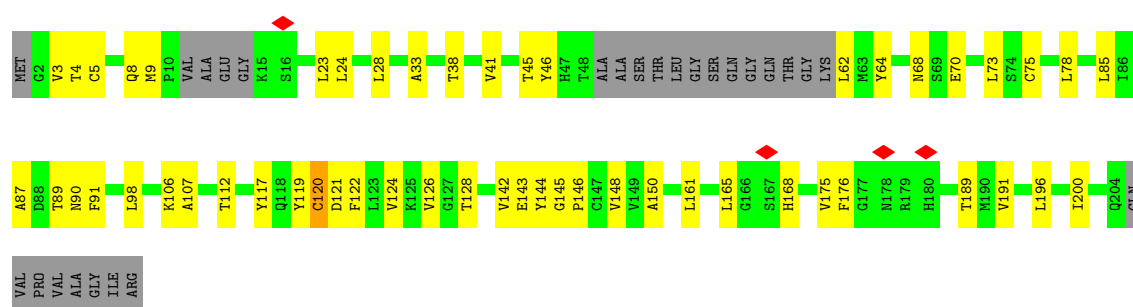
• Molecule 39: Mediator of RNA polymerase II transcription subunit 18

Chain e: 55% 25% 20%



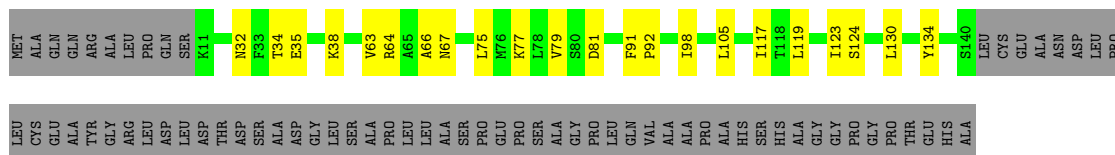
• Molecule 40: Mediator of RNA polymerase II transcription subunit 20

Chain f: 63% 25% 12%

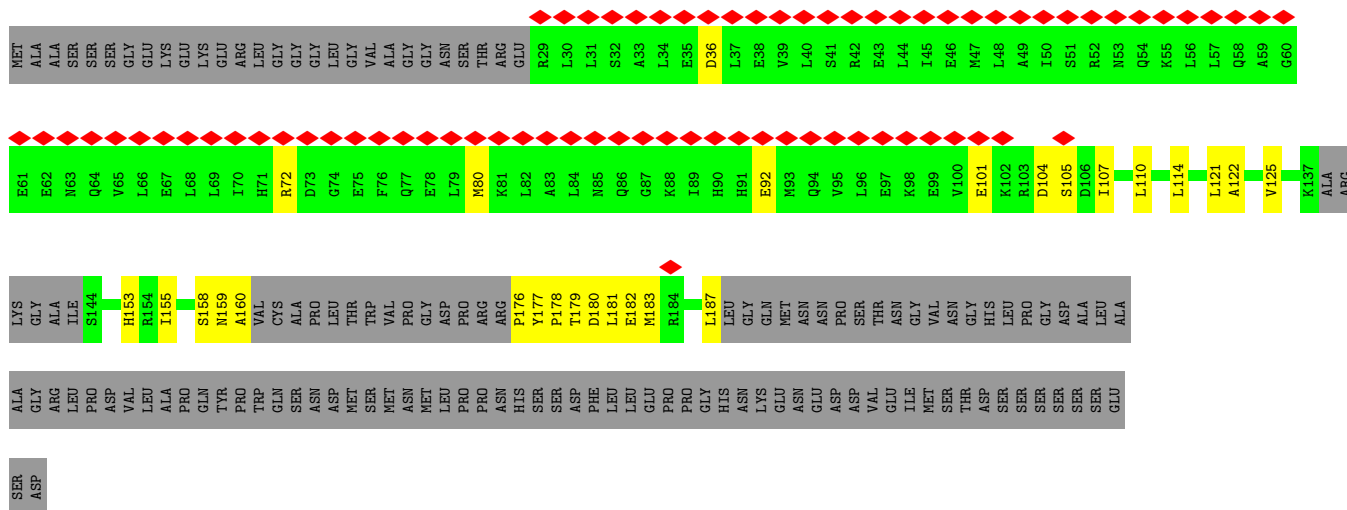
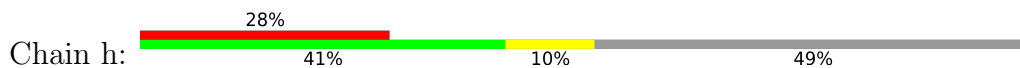


• Molecule 41: Mediator of RNA polymerase II transcription subunit 22

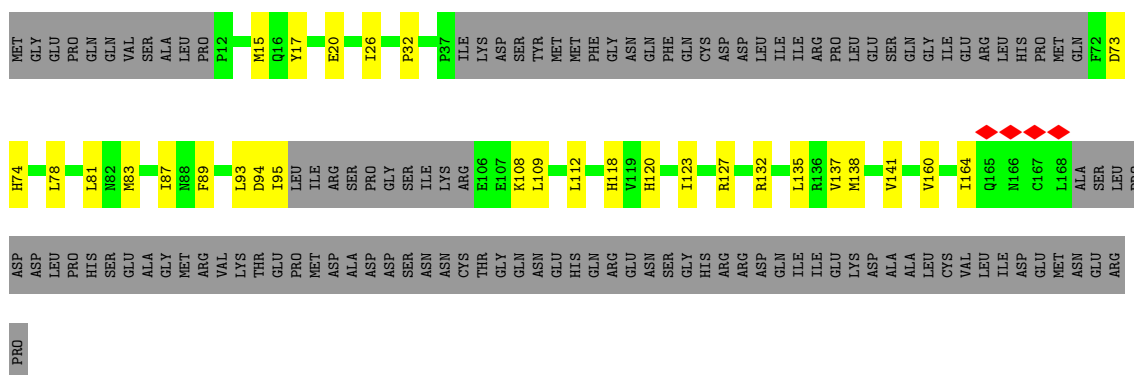
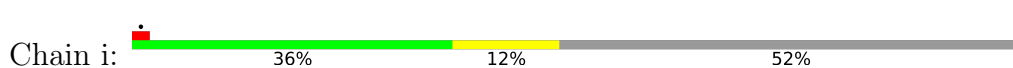
Chain g: 54% 11% 35%



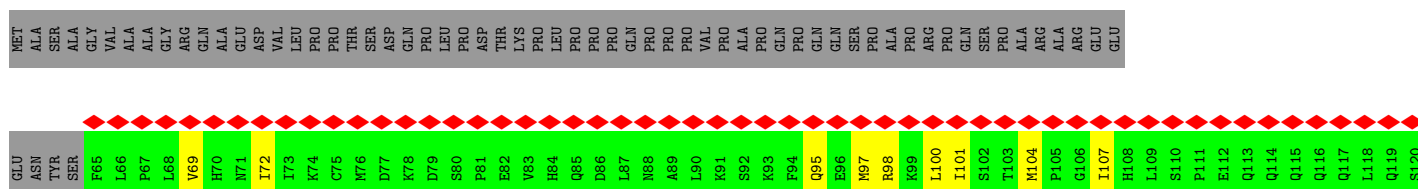
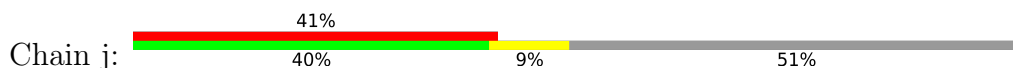
• Molecule 42: Mediator of RNA polymerase II transcription subunit 4



• Molecule 43: Mediator of RNA polymerase II transcription subunit 7



• Molecule 44: Mediator of RNA polymerase II transcription subunit 9

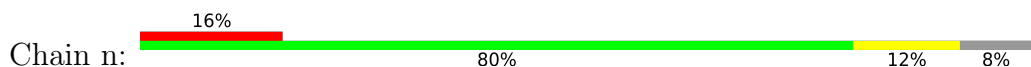


[illegible]

- Molecule 47: Mediator of RNA polymerase II transcription subunit 19

[illegible]

- Molecule 48: Mediator of RNA polymerase II transcription subunit 21

[illegible]

HIS
SER
GLN
SER
LEU
PRO
ASP
SER

- Molecule 49: Mediator of RNA polymerase II transcription subunit 31

Chain o:  56% 13% 31%

MET ALA ALA VAL MET THR THR ASP ASP GLY ASN R15 R16 R17 E23 C27 L28 L34 A47 F48 V49 N50 Y51 L52 K53 Y54 K65 K68 H74 M75 L76 L79 W105 GLN HIS TYR SER ARG LYS ARG MET ARG LEU GLN GLN ALA LEU ALA

GLU
GLN
GLN
GLN
GLN
ASN
THR
SER
GLY
LYS

- Molecule 50: Mediator of RNA polymerase II transcription subunit 27

Chain p:  34% 15% 50%

MET ALA ASP VAL ILE ASN VAL SER VAL VAL ASN ASN LEU LEU GLU PHE SER SER GLN ALA ILE SER ALA ILE SER ARG SER SER VAL SER ARG VAL PHE ASP CYS LEU LYS ASP GLY MET ARG ASN LYS THR LYS GLU THR LEU GLN GLY ARG GLU LYS ALA PHE ILE ARG HIS PHE GLN ASP TYR LEU

HIS SER VAL ASN ARG LEU ASN GLU LEU GLU ARG LEU SER ASN VAL GLY LYS PRO SER GLU ASN HIS PRO LEU HIS ASN VAL SER GLY LEU LEU SER LEU ASP PRO VAL GLN ASP LYS THR PRO LEU TYR SER GLN LEU LEU ALA GLN TYR LYS TRP TRP ASN LYS LEU GLN ASP TYR HIS

ALA GLY LEU ALA SER GLY LEU LEU ASN ASN GLN GLN SER LEU LYS ARG SER ALA ASN GLN MET GLY VAL SER VAL ALA LYS ARG ARG HIS PRO THR THR VAL L157 I166 I178 T186 L190 L191 L192 T193 K199 V200 I201 M204 R205 S206 L207 F208 I209 D210

R211 V221 I230 W231 V238 V242 T243 D244 H245 A249 L250 Y253 V263 W269 L270 Y273 L276 F277 C281 Q282 L288 Q289 L292 P293 P294 T295 W296 R297 T301 L302 E303 A304 F305 H306 D307 T308 C309 R310 GLN

- Molecule 51: Mediator of RNA polymerase II transcription subunit 28

Chain q:  32% 7% 61%

MET ALA PRO LEU GLY MET PHE ASP SER GLY GLN PRO PRO GLY PRO PRO GLN ALA PRO PRO GLY LEU PRO GLY ALA PRO ARG PRO SER SER SER THR LEU VAL ASP GLU LEU LEU ASP LEU SER SER PHE GLU ALA CYS PHE ALA SER LEU VAL

SER GLN ASP TYR VAL ASN GLY THR SER GLN GLU ILE ARG THR GLY VAL ASP CYS ILE Q82 R99 L100 S103 V104 Q105 K106 P107 V115 H132 L136 L143 N147 H150 LYS PRO ALA ASP ILE PRO GLN SER LEU ALA TYR LEU GLN ALA

SER
ALA
ILE
PRO
ALA
PRO
LEU
PRO
THR

- Molecule 52: unassigned peptide (MED29 or MED30)

Chain r:  80% 20%

X1 X7 X8 X11 X12 X20

- Molecule 53: Mediator of RNA polymerase II transcription subunit 30

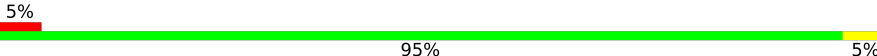
Chain s:  17% 8% 75%

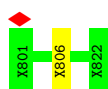
MET SER THR PRO LEU ALA ALA SER MET MET ALA PRO GLY PRO PHE ALA GLY PRO GLN ALA ALA GLN GLN GLN ALA ALA ARG ARG VAL VAL PHE ASN THR ALA SER LEU CYS ARG ILE GLY GLN GLU THR THR VAL ASN ASN CYS ASP ILE VAL MET TYR THR PRO MET MET GLU ILE PHE GLN GLN LEU LEU ARG ASN MET VAL GLU LEU

PRO ASN VAL THR TYR HIS THR GLY THR TYR GLN ASP ARG LEU THR LYS LEU GLN ASP ASN ASN LEU ARG GLN GLN LEU SER VAL VAL PHE ARG LYS LEU ARG LEU CYS VAL TYR ASP LYS CYS ASN THR THR ASN ASN CYS GLY GLY MET ASP THR PRO ILE PRO VAL PHE GLN GLN ILE PRO TYR VAL VAL GLU

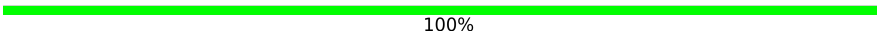
ASP GLY SER LYS ASN ASP ASP ARG ALA GLY THR PRO PRO ARG PHE A134 I141 I155 I188 M159 D160 Q161 L162 R163 I166 W167 M172 L173 A174 M175 R176 N177

- Molecule 54: unassigned peptide (MED14)

Chain v:  5% 95% 5%

 X801 X806 X822

- Molecule 55: unassigned peptide (MED6)

Chain w:  100%

There are no outlier residues recorded for this chain.

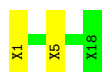
- Molecule 56: unassigned peptide (MED17)

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: unassigned peptide (MED29 or MED30)

Chain y:  89% 11%

 X1 X5 X18

- Molecule 58: unassigned peptide (MED29 or MED30)

Chain z:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25967	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 ($e^-/\text{\AA}^2$)	58.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	40.088	Depositor
Minimum map value	-17.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	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: MG, ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.12	0/5875	0.30	0/7955
2	1	0.14	0/2210	0.30	0/2975
3	2	0.15	0/3230	0.31	0/4376
4	3	0.24	0/1769	0.37	0/2385
5	4	0.17	0/2103	0.36	0/2846
6	5	0.11	0/529	0.25	0/714
7	6	0.11	0/2793	0.27	0/3780
8	7	0.12	0/4994	0.28	0/6745
9	8	0.34	0/2434	0.56	2/3300 (0.1%)
10	9	0.33	0/2342	0.46	0/3159
11	A	0.11	0/11479	0.27	0/15496
12	B	0.12	0/9257	0.28	0/12493
13	C	0.11	0/2102	0.28	0/2857
14	D	0.09	0/1064	0.21	0/1428
15	E	0.11	0/1752	0.27	0/2366
16	F	0.11	0/646	0.26	0/871
17	G	0.11	0/1382	0.23	0/1874
18	H	0.10	0/1207	0.28	0/1628
19	I	0.11	0/949	0.29	0/1284
20	J	0.12	0/516	0.25	0/696
21	K	0.11	0/939	0.23	0/1271
22	L	0.12	0/378	0.27	0/500
23	M	0.12	0/1983	0.27	0/2679
24	N	0.18	0/1478	0.42	0/2283
25	O	0.13	0/1448	0.28	0/1948
26	Q	0.10	0/1167	0.27	0/1576
27	R	0.12	0/1817	0.27	0/2445
28	T	0.18	0/1461	0.41	0/2249
29	U	0.12	0/945	0.30	0/1274
30	V	0.13	0/816	0.29	0/1105
31	W	0.23	0/1686	0.44	0/2266
32	X	0.22	0/1427	0.44	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	a	0.10	0/1200	0.29	0/1634
36	b	0.16	0/1058	0.47	1/1427 (0.1%)
37	c	0.12	0/864	0.33	0/1161
38	d	0.15	0/3573	0.36	0/4812
39	e	0.13	0/1377	0.32	0/1846
40	f	0.15	0/1478	0.46	3/1996 (0.2%)
41	g	0.10	0/1072	0.24	0/1440
42	h	0.11	0/1121	0.27	0/1496
43	i	0.13	0/979	0.34	0/1315
44	j	0.11	0/605	0.30	0/810
45	k	0.09	0/1107	0.26	0/1487
46	l	0.11	0/4102	0.29	0/5537
47	m	0.12	0/671	0.30	0/908
48	n	0.09	0/1016	0.26	0/1381
49	o	0.10	0/829	0.25	0/1119
50	p	0.16	0/1294	0.36	0/1756
51	q	0.10	0/599	0.27	0/803
53	s	0.11	0/370	0.26	0/491
All	All	0.15	0/97493	0.32	6/132159 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
38	d	0	1
46	l	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	102	HIS	N-CA-C	10.57	122.80	111.28
9	8	164	SER	CA-C-N	7.40	129.09	119.84
9	8	164	SER	C-N-CA	7.40	129.09	119.84
40	f	120	CYS	CA-C-N	6.65	134.16	123.93
40	f	120	CYS	C-N-CA	6.65	134.16	123.93
40	f	148	VAL	CG1-CB-CG2	5.04	121.88	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	d	513	THR	Peptide
46	l	443	LEU	Peptide

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	5751	0	5794	103	0
2	1	2167	0	2175	34	0
3	2	3158	0	3213	49	0
4	3	1737	0	1709	47	0
5	4	2066	0	2098	58	0
6	5	523	0	530	9	0
7	6	2732	0	2698	46	0
8	7	4890	0	4949	65	0
9	8	2376	0	2402	87	0
10	9	2293	0	2315	71	0
11	A	11274	0	11406	155	0
12	B	9076	0	9116	123	0
13	C	2059	0	2007	20	0
14	D	1050	0	1033	32	0
15	E	1721	0	1737	16	0
16	F	636	0	665	9	0
17	G	1351	0	1358	83	0
18	H	1186	0	1147	6	0
19	I	928	0	859	11	0
20	J	507	0	523	13	0
21	K	920	0	942	14	0
22	L	373	0	378	7	0
23	M	1953	0	1987	22	0
24	N	1318	0	721	16	0
25	O	1422	0	1514	16	0
26	Q	1138	0	1103	15	0
27	R	1788	0	1819	19	0
28	T	1303	0	714	9	0
29	U	930	0	888	11	0
30	V	806	0	818	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	W	1659	0	1665	95	0
32	X	1403	0	1428	65	0
33	Y	95	0	24	0	0
34	Z	40	0	10	0	0
35	a	1167	0	1141	27	0
36	b	1046	0	1060	53	0
37	c	858	0	864	20	0
38	d	3510	0	3583	134	0
39	e	1353	0	1367	53	0
40	f	1448	0	1427	42	0
41	g	1063	0	1051	26	0
42	h	1114	0	1147	25	0
43	i	960	0	980	21	0
44	j	596	0	618	13	0
45	k	1088	0	1094	11	0
46	l	4031	0	4141	102	0
47	m	655	0	662	20	0
48	n	1005	0	986	15	0
49	o	804	0	791	15	0
50	p	1262	0	1270	47	0
51	q	591	0	608	8	0
52	r	100	0	22	2	0
53	s	369	0	388	16	0
54	v	110	0	25	1	0
55	w	80	0	18	0	0
56	x	55	0	13	0	0
57	y	90	0	20	1	0
58	z	115	0	25	0	0
59	0	8	0	0	0	0
60	3	2	0	0	0	0
60	4	2	0	0	0	0
60	6	3	0	0	0	0
60	A	2	0	0	0	0
60	B	1	0	0	0	0
60	C	1	0	0	0	0
60	I	2	0	0	0	0
60	J	1	0	0	0	0
60	L	1	0	0	0	0
60	M	1	0	0	0	0
60	W	1	0	0	0	0
60	p	1	0	0	0	0
61	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	96126	0	95046	1656	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1656) 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)
17:G:158:PHE:CD2	31:W:142:ASN:ND2	1.81	1.43
17:G:158:PHE:CE2	31:W:142:ASN:ND2	1.81	1.40
4:3:287:TYR:OH	9:8:165:PRO:HG3	1.18	1.30
4:3:287:TYR:OH	9:8:165:PRO:CG	1.98	1.12
11:A:1477:ALA:CB	17:G:22:LEU:HD11	1.80	1.10
11:A:1477:ALA:HB1	17:G:22:LEU:HD11	1.31	1.05
5:4:255:CYS:SG	5:4:258:HIS:ND1	2.31	1.03
31:W:113:ARG:NH1	32:X:222:SER:OG	1.92	1.02
4:3:8:ARG:O	31:W:181:ASN:ND2	1.93	1.01
11:A:1485:GLU:OE1	17:G:20:PRO:HD2	1.60	1.00
42:h:158:SER:OG	49:o:68:LYS:O	1.83	0.96
31:W:17:LEU:HD22	31:W:194:THR:HG21	1.50	0.94
17:G:158:PHE:HE1	31:W:143:GLN:NE2	1.66	0.92
17:G:158:PHE:HE1	31:W:143:GLN:HE21	0.98	0.92
4:3:54:ARG:HH22	17:G:166:ASP:CG	1.77	0.91
17:G:158:PHE:CE1	31:W:143:GLN:NE2	2.39	0.91
46:l:234:LEU:HD21	46:l:296:LEU:HD23	1.51	0.91
5:4:255:CYS:HG	5:4:258:HIS:HD1	1.20	0.90
9:8:108:VAL:HG12	35:a:55:LEU:HD13	1.53	0.89
36:b:171:GLN:O	36:b:172:THR:HG22	1.72	0.89
11:A:1005:HIS:CD2	11:A:1007:ILE:HG22	2.08	0.88
31:W:105:TYR:CE2	32:X:233:ILE:HG23	2.08	0.88
46:l:497:LYS:NZ	46:l:559:ASN:O	2.06	0.87
17:G:158:PHE:CE2	31:W:142:ASN:HB3	2.09	0.87
3:2:120:ILE:O	5:4:100:LYS:NZ	2.07	0.86
5:4:62:SER:OG	5:4:132:LEU:O	1.95	0.85
1:0:571:THR:OG1	1:0:573:ASP:OD1	1.94	0.85
32:X:230:GLU:HA	32:X:233:ILE:HD13	1.58	0.85
36:b:103:GLU:O	36:b:106:PRO:HD2	1.76	0.85
17:G:158:PHE:CE2	31:W:142:ASN:CG	2.54	0.85
38:d:504:VAL:HG12	38:d:514:LEU:HD11	1.57	0.84
11:A:1485:GLU:OE2	17:G:20:PRO:CG	2.25	0.84
17:G:41:LYS:O	17:G:78:ARG:NH2	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:397:SER:OG	39:e:86:ARG:NH2	2.11	0.83
17:G:158:PHE:CE2	31:W:142:ASN:CB	2.62	0.83
31:W:105:TYR:OH	32:X:233:ILE:O	1.94	0.82
25:O:206:GLU:OE1	25:O:236:LYS:NZ	2.13	0.82
36:b:103:GLU:C	36:b:106:PRO:HD2	2.05	0.82
41:g:130:LEU:HD21	53:s:155:LEU:HD11	1.61	0.82
4:3:55:LYS:HD3	17:G:165:ASP:HA	1.63	0.81
46:l:128:LEU:O	46:l:132:THR:OG1	1.97	0.81
11:A:1485:GLU:CD	17:G:20:PRO:HD2	2.05	0.81
17:G:154:LYS:NZ	31:W:143:GLN:HB3	1.96	0.81
43:i:109:LEU:HD13	46:l:132:THR:HG22	1.61	0.81
4:3:295:ARG:HD2	9:8:163:GLY:HA3	1.62	0.81
9:8:94:MET:HE3	9:8:152:LYS:HD2	1.61	0.81
11:A:911:PRO:O	11:A:963:ARG:NH2	2.14	0.81
21:K:81:TYR:OH	21:K:89:ASN:OD1	1.98	0.81
8:7:266:GLN:N	8:7:266:GLN:HE21	1.79	0.80
35:a:58:GLU:O	35:a:62:GLN:NE2	2.14	0.80
12:B:1064:ARG:NH2	23:M:43:ASP:OD1	2.14	0.80
11:A:535:MET:O	11:A:669:TYR:OH	1.98	0.80
36:b:12:LEU:HD11	38:d:116:LEU:HD11	1.62	0.80
2:1:430:THR:OG1	5:4:222:SER:OG	2.00	0.79
4:3:85:ARG:NH2	4:3:143:GLU:OE1	2.16	0.79
46:l:416:LEU:HD23	46:l:438:LEU:HD13	1.65	0.79
36:b:100:PHE:CD1	36:b:101:SER:N	2.51	0.79
11:A:902:GLU:OE2	11:A:985:ARG:NH2	2.16	0.79
10:9:126:VAL:HG11	10:9:140:LEU:HB2	1.63	0.79
25:O:188:ARG:NH2	29:U:321:SER:OG	2.16	0.79
5:4:56:LYS:NZ	5:4:143:TYR:OH	2.17	0.78
11:A:22:GLN:NE2	11:A:1446:GLY:O	2.17	0.78
17:G:154:LYS:HZ3	31:W:143:GLN:HB3	1.49	0.77
15:E:79:GLU:OE2	15:E:86:THR:OG1	2.00	0.77
38:d:540:LEU:HD12	38:d:639:MET:HE3	1.66	0.77
38:d:503:ARG:NH2	50:p:244:ASP:OD1	2.18	0.77
46:l:60:HIS:HB2	47:m:137:LEU:HD13	1.65	0.77
14:D:94:LYS:NZ	17:G:3:TYR:OH	2.17	0.77
2:1:503:THR:HG1	2:1:533:TYR:HH	1.19	0.76
11:A:1173:THR:OG1	19:I:56:ASN:OD1	2.03	0.76
1:0:722:ARG:NH2	7:6:202:SER:OG	2.18	0.76
40:f:9:MET:HE1	40:f:168:HIS:HB2	1.67	0.76
11:A:1242:ASP:HA	11:A:1262:MET:HE2	1.68	0.76
32:X:120:MET:HA	32:X:124:LEU:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:126:ILE:HD13	36:b:52:LEU:HD21	1.68	0.76
17:G:95:VAL:HG11	31:W:152:PHE:CZ	2.21	0.75
1:0:711:ASP:OD1	1:0:715:GLN:NE2	2.19	0.75
8:7:371:VAL:HG23	8:7:407:ILE:HG22	1.68	0.75
18:H:2:ALA:O	18:H:84:ARG:NH2	2.20	0.75
28:T:-3:DA:OP1	29:U:346:LYS:NZ	2.20	0.75
41:g:35:GLU:OE2	41:g:64:ARG:NH1	2.20	0.75
46:l:153:ALA:HB1	46:l:156:TYR:CD2	2.22	0.74
35:a:118:ARG:NH2	36:b:108:HIS:O	2.19	0.74
46:l:559:ASN:OD1	46:l:560:LYS:N	2.19	0.74
21:K:77:THR:OG1	21:K:81:TYR:O	2.04	0.74
43:i:32:PRO:O	49:o:54:TYR:OH	2.04	0.74
12:B:59:VAL:HG21	12:B:91:ILE:HD11	1.70	0.74
17:G:95:VAL:HG11	31:W:152:PHE:CE1	2.22	0.73
14:D:67:TYR:OH	17:G:86:ASP:OD1	2.06	0.73
11:A:279:LYS:O	11:A:283:ILE:HD12	1.87	0.73
14:D:87:LEU:HD11	14:D:100:LEU:HD11	1.70	0.73
7:6:109:THR:HG1	7:6:148:SER:HG	1.28	0.73
50:p:288:LEU:HD22	50:p:306:HIS:CB	2.18	0.73
4:3:307:GLN:NE2	10:9:247:GLN:OE1	2.21	0.73
17:G:158:PHE:HE2	31:W:142:ASN:CB	2.01	0.73
31:W:105:TYR:HE2	32:X:233:ILE:HA	1.54	0.73
11:A:869:GLU:OE1	11:A:1455:SER:OG	2.07	0.72
11:A:1005:HIS:HD2	11:A:1007:ILE:HG22	1.50	0.72
6:5:24:ASP:OD1	6:5:25:GLU:N	2.22	0.72
32:X:84:TYR:OH	32:X:105:GLU:OE1	2.04	0.72
31:W:17:LEU:HD22	31:W:194:THR:CG2	2.19	0.72
50:p:281:CYS:HB2	50:p:305:PHE:HA	1.70	0.72
5:4:160:ARG:NH2	5:4:234:ASP:OD1	2.23	0.71
5:4:272:LEU:O	5:4:272:LEU:HD23	1.90	0.71
17:G:158:PHE:HE2	31:W:142:ASN:HB3	1.53	0.71
43:i:15:MET:SD	43:i:17:TYR:N	2.63	0.71
4:3:120:LYS:O	4:3:124:ILE:HD12	1.91	0.71
31:W:20:TYR:CD2	31:W:190:LEU:HD11	2.26	0.71
1:0:571:THR:OG1	1:0:576:GLU:OE1	2.08	0.71
11:A:1485:GLU:CD	17:G:20:PRO:CD	2.64	0.71
1:0:231:VAL:HG13	1:0:454:VAL:HG23	1.70	0.71
3:2:29:GLY:O	3:2:33:ARG:NE	2.24	0.70
8:7:191:ASP:O	8:7:195:ARG:NH1	2.25	0.70
43:i:26:ILE:HD12	49:o:50:ASN:HB3	1.73	0.70
12:B:254:GLN:N	12:B:254:GLN:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1485:GLU:OE2	17:G:20:PRO:HG3	1.91	0.70
2:1:195:SER:O	2:1:199:THR:OG1	2.06	0.70
11:A:322:LEU:O	11:A:327:ARG:NH2	2.23	0.70
32:X:82:VAL:HG12	32:X:86:LYS:NZ	2.06	0.70
42:h:114:LEU:HD21	48:n:118:ILE:HB	1.72	0.70
4:3:307:GLN:CG	10:9:251:ILE:HD11	2.21	0.70
5:4:67:SER:O	5:4:139:LYS:NZ	2.24	0.70
1:0:252:THR:HG22	1:0:432:ILE:HG22	1.74	0.70
23:M:19:PRO:HG3	39:e:92:GLU:CD	2.17	0.70
31:W:100:VAL:HG22	31:W:104:LYS:HD3	1.71	0.70
46:l:658:ARG:NH2	54:v:806:UNK:O	2.25	0.70
42:h:121:LEU:HD11	48:n:111:GLY:HA3	1.74	0.70
2:1:468:VAL:HG21	2:1:525:ILE:HD11	1.74	0.69
46:l:212:LEU:HD23	46:l:212:LEU:O	1.92	0.69
8:7:611:GLY:O	8:7:642:ARG:NH2	2.25	0.69
9:8:43:ILE:HD13	9:8:87:ILE:HG13	1.73	0.69
38:d:315:ALA:HB2	38:d:331:ILE:HD11	1.74	0.69
23:M:23:LEU:HD12	23:M:32:MET:HE2	1.74	0.69
9:8:125:LEU:HD21	9:8:195:ASP:HB3	1.75	0.69
11:A:1248:ASN:ND2	11:A:1254:LYS:O	2.26	0.69
16:F:100:ARG:NH2	16:F:121:ASP:O	2.26	0.69
17:G:154:LYS:HZ3	31:W:143:GLN:CG	2.06	0.69
31:W:105:TYR:OH	32:X:237:LEU:HG	1.93	0.69
38:d:537:VAL:HG22	38:d:639:MET:SD	2.33	0.68
11:A:1475:LEU:CD2	17:G:18:PHE:CZ	2.76	0.68
9:8:40:ILE:HG12	9:8:90:VAL:HG22	1.76	0.68
12:B:777:ASN:O	20:J:47:ARG:NH1	2.27	0.68
17:G:21:ASN:O	17:G:25:THR:OG1	2.05	0.68
17:G:97:LEU:HD23	17:G:113:ILE:HD11	1.75	0.68
11:A:373:LEU:O	11:A:485:ASN:ND2	2.25	0.68
46:l:509:ILE:HD11	46:l:641:LEU:CD2	2.24	0.68
1:0:637:LEU:HD11	1:0:648:GLU:HA	1.74	0.68
13:C:193:ARG:NH2	13:C:218:ALA:O	2.25	0.68
46:l:312:THR:HG21	46:l:337:LEU:HD11	1.75	0.68
38:d:374:ASN:HD21	53:s:175:MET:HG2	1.59	0.68
9:8:226:PHE:HB3	9:8:231:THR:HG22	1.76	0.68
10:9:238:LEU:HB3	10:9:245:LEU:HB2	1.75	0.68
3:2:400:ARG:NH2	8:7:666:ASP:OD2	2.27	0.67
7:6:88:LEU:CD2	7:6:131:LEU:HD21	2.25	0.67
14:D:18:SER:O	14:D:117:SER:OG	2.09	0.67
32:X:89:HIS:CE1	32:X:139:PHE:HB3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:72:TYR:OH	1:0:234:ASP:OD2	2.12	0.67
31:W:34:LEU:HD11	31:W:94:ILE:HD12	1.76	0.67
9:8:158:LEU:HD12	9:8:173:VAL:HB	1.76	0.67
40:f:121:ASP:OD2	50:p:238:VAL:HG23	1.95	0.67
11:A:430:ARG:NH2	23:M:26:ASP:OD1	2.28	0.67
12:B:814:TYR:OH	12:B:900:GLU:OE1	2.13	0.67
23:M:128:ILE:HG23	23:M:183:VAL:HG11	1.77	0.67
13:C:109:GLU:OE1	13:C:109:GLU:N	2.28	0.67
1:0:60:GLN:OE1	1:0:61:ARG:NH1	2.28	0.66
5:4:43:VAL:HG11	5:4:224:LEU:HD21	1.78	0.66
8:7:701:LEU:O	8:7:704:SER:OG	2.14	0.66
9:8:113:HIS:CD2	9:8:308:PRO:HD3	2.30	0.66
29:U:20:ASP:OD2	30:V:51:ARG:NH2	2.27	0.66
3:2:60:LEU:HD13	3:2:118:LEU:HD23	1.76	0.66
27:R:214:LYS:NZ	28:T:-14:DC:OP2	2.23	0.66
11:A:805:ARG:NH2	12:B:671:GLU:O	2.28	0.66
18:H:91:VAL:HG22	18:H:144:LEU:CD2	2.26	0.66
4:3:106:VAL:O	4:3:110:THR:HG23	1.95	0.66
10:9:218:LEU:HD12	10:9:252:MET:HE1	1.78	0.66
50:p:242:VAL:HG23	50:p:295:THR:HG23	1.78	0.66
11:A:1475:LEU:HD22	17:G:18:PHE:CZ	2.31	0.66
35:a:148:HIS:ND1	35:a:148:HIS:O	2.28	0.66
39:e:145:VAL:HG22	39:e:169:VAL:HG12	1.76	0.66
1:0:238:ASN:ND2	1:0:662:GLN:OE1	2.29	0.66
46:l:470:LEU:HD12	46:l:470:LEU:O	1.95	0.66
17:G:154:LYS:HZ3	31:W:143:GLN:CB	2.09	0.66
38:d:259:VAL:HG22	38:d:343:ILE:HG23	1.77	0.66
51:q:147:ASN:O	51:q:150:HIS:ND1	2.29	0.66
4:3:14:TYR:OH	31:W:185:GLU:OE2	2.12	0.65
12:B:354:SER:HG	12:B:357:CYS:HG	1.44	0.65
12:B:926:VAL:HG21	13:C:62:GLU:HG3	1.78	0.65
32:X:229:ASP:O	32:X:233:ILE:HD12	1.95	0.65
11:A:513:ALA:HB2	16:F:90:LEU:HD21	1.78	0.65
10:9:177:ARG:NH2	10:9:235:SER:O	2.30	0.65
11:A:140:ARG:NH1	11:A:234:PHE:O	2.30	0.65
11:A:589:LYS:NZ	11:A:625:ASP:OD2	2.23	0.65
14:D:87:LEU:HB3	14:D:97:LEU:HD22	1.78	0.65
17:G:151:ARG:HD2	31:W:139:LEU:HD11	1.77	0.65
11:A:122:ASN:O	11:A:127:LYS:NZ	2.30	0.65
12:B:116:ARG:HG2	12:B:910:THR:HG21	1.79	0.65
38:d:190:LEU:HD22	38:d:196:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:145:VAL:HG13	32:X:175:LEU:HB2	1.79	0.65
3:2:172:SER:OG	3:2:174:ASP:OD1	2.15	0.65
38:d:339:LEU:HD11	38:d:439:PHE:CD2	2.31	0.65
44:j:104:MET:HE3	44:j:107:ILE:HD13	1.79	0.65
4:3:54:ARG:NH2	17:G:166:ASP:CG	2.54	0.64
31:W:276:GLU:OE2	31:W:282:ARG:NH1	2.30	0.64
32:X:82:VAL:HG12	32:X:86:LYS:HZ2	1.62	0.64
35:a:111:LEU:O	35:a:111:LEU:HD23	1.98	0.64
11:A:1475:LEU:HD22	17:G:66:VAL:HG21	1.80	0.64
32:X:189:ILE:HD11	32:X:201:LEU:HD13	1.79	0.64
3:2:410:ASN:O	6:5:3:ASN:N	2.30	0.64
40:f:45:THR:HG22	40:f:106:LYS:HE3	1.80	0.64
1:0:382:LEU:O	1:0:385:THR:OG1	2.11	0.64
11:A:1477:ALA:CA	17:G:22:LEU:HD11	2.28	0.64
42:h:153:HIS:ND1	42:h:153:HIS:O	2.31	0.64
14:D:14:GLU:OE1	14:D:14:GLU:N	2.31	0.64
19:I:60:HIS:ND1	19:I:60:HIS:O	2.30	0.64
43:i:20:GLU:OE1	49:o:17:ARG:NH1	2.31	0.64
10:9:175:LYS:NZ	10:9:185:GLU:OE2	2.29	0.64
12:B:910:THR:HG22	12:B:911:LEU:H	1.63	0.64
39:e:143:ILE:HD11	39:e:189:PHE:CE2	2.32	0.64
8:7:287:LEU:O	8:7:287:LEU:HD23	1.98	0.64
14:D:29:ALA:HB3	17:G:3:TYR:CE2	2.33	0.64
38:d:582:VAL:HG11	38:d:591:LYS:HE3	1.79	0.64
5:4:168:GLU:OE1	5:4:168:GLU:N	2.31	0.64
7:6:377:ASP:O	7:6:380:HIS:NE2	2.30	0.64
12:B:677:MET:H	12:B:682:LEU:HD22	1.62	0.64
25:O:297:LYS:NZ	25:O:323:GLU:OE2	2.31	0.63
8:7:517:GLU:O	8:7:521:GLU:OE1	2.16	0.63
1:0:2:LYS:HB3	1:0:9:LEU:HD11	1.81	0.63
5:4:16:ASP:OD1	5:4:131:THR:OG1	2.15	0.63
8:7:330:ASN:OD1	8:7:334:ARG:NH2	2.31	0.63
25:O:186:ARG:NH1	25:O:244:LEU:O	2.31	0.63
31:W:113:ARG:NH1	32:X:219:LEU:O	2.31	0.63
11:A:1375:ARG:NH1	11:A:1379:GLU:OE1	2.31	0.63
12:B:101:ARG:NH2	23:M:171:GLU:O	2.32	0.63
12:B:529:MET:HE1	12:B:698:ILE:HD12	1.79	0.63
12:B:407:MET:HE1	12:B:444:LEU:HG	1.80	0.63
13:C:24:GLU:OE2	13:C:228:ARG:NH1	2.32	0.63
23:M:273:GLU:O	23:M:277:ILE:HD12	1.98	0.63
36:b:12:LEU:HD11	38:d:116:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:i:78:LEU:HD22	48:m:73:ILE:HD13	1.79	0.63
44:j:104:MET:HE3	44:j:107:ILE:HG21	1.80	0.63
1:0:335:ARG:NH1	4:3:71:GLU:OE2	2.32	0.63
6:5:49:LEU:HD12	6:5:52:VAL:CG1	2.29	0.63
8:7:266:GLN:HG2	8:7:267:THR:HG23	1.80	0.63
9:8:30:ARG:HH21	9:8:35:ASN:HB2	1.63	0.63
24:N:18:DG:H1	28:T:-18:DC:H42	1.47	0.63
36:b:101:SER:HB3	36:b:105:VAL:HG23	1.80	0.62
39:e:27:VAL:HG21	39:e:35:LEU:HD22	1.81	0.62
3:2:55:TRP:CZ2	3:2:83:GLN:NE2	2.66	0.62
3:2:172:SER:OG	3:2:267:GLU:OE2	2.13	0.62
1:0:343:ARG:O	1:0:346:VAL:HG12	1.99	0.62
15:E:29:THR:HG23	15:E:32:GLU:H	1.65	0.62
2:1:432:THR:O	2:1:435:SER:OG	2.10	0.62
8:7:371:VAL:HG23	8:7:407:ILE:CG2	2.30	0.62
7:6:112:LYS:O	7:6:147:ASN:ND2	2.32	0.62
10:9:215:THR:HA	10:9:252:MET:HE3	1.82	0.62
13:C:9:VAL:HG11	21:K:105:PHE:CD1	2.34	0.62
7:6:137:MET:SD	7:6:139:CYS:N	2.68	0.62
15:E:9:ARG:O	15:E:13:ILE:HD12	1.99	0.62
8:7:473:GLU:N	8:7:473:GLU:OE1	2.33	0.62
9:8:132:TRP:CD1	10:9:1:MET:HE3	2.35	0.62
14:D:29:ALA:HB3	17:G:3:TYR:CZ	2.35	0.62
14:D:119:GLU:OE1	14:D:119:GLU:N	2.33	0.62
38:d:464:TRP:CZ3	38:d:475:VAL:HG22	2.34	0.62
50:p:193:THR:HG22	50:p:199:LYS:HG2	1.81	0.62
2:1:130:ASP:OD2	2:1:463:HIS:NE2	2.33	0.61
11:A:1471:PHE:O	16:F:64:ARG:NH1	2.33	0.61
39:e:110:THR:HG21	39:e:114:LEU:HD12	1.82	0.61
41:g:119:LEU:HD12	51:q:143:LEU:HD21	1.82	0.61
4:3:265:MET:SD	4:3:268:ARG:NE	2.73	0.61
7:6:379:LEU:HD22	7:6:381:CYS:O	1.99	0.61
15:E:168:ASN:OD1	15:E:172:ARG:NH2	2.33	0.61
40:f:120:CYS:O	40:f:121:ASP:OD1	2.17	0.61
7:6:87:LEU:HD22	7:6:232:LEU:HD12	1.82	0.61
13:C:78:ILE:HD11	13:C:126:ARG:HB3	1.82	0.61
38:d:209:TYR:O	38:d:213:GLY:N	2.32	0.61
45:k:51:ILE:HB	46:l:59:LEU:HD21	1.81	0.61
1:0:44:SER:OG	1:0:46:THR:O	2.16	0.61
47:m:127:LEU:HA	47:m:130:LEU:HD12	1.82	0.61
50:p:204:MET:HB3	50:p:209:ILE:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:p:295:THR:O	50:p:295:THR:HG22	2.01	0.61
38:d:371:LEU:HD21	38:d:435:ALA:HB2	1.83	0.61
50:p:288:LEU:HD22	50:p:306:HIS:HB3	1.82	0.61
9:8:213:LEU:HD13	9:8:225:ILE:HG12	1.83	0.61
38:d:374:ASN:ND2	53:s:175:MET:HG2	2.16	0.61
38:d:570:THR:HG23	38:d:581:SER:HB3	1.82	0.61
9:8:134:LEU:HD11	9:8:192:VAL:HA	1.81	0.61
36:b:12:LEU:CD1	38:d:116:LEU:HD11	2.30	0.61
49:o:52:LEU:HD13	49:o:79:LEU:CD1	2.31	0.61
9:8:79:ASP:OD2	9:8:80:ALA:N	2.33	0.61
10:9:86:TYR:OH	10:9:158:LEU:O	2.18	0.61
12:B:57:ARG:NE	12:B:227:ASN:O	2.34	0.61
11:A:29:ASP:OD2	11:A:33:ARG:NH2	2.34	0.60
48:n:26:LEU:HD21	48:n:55:ALA:HB2	1.82	0.60
1:0:405:THR:O	1:0:409:THR:OG1	2.16	0.60
31:W:176:LEU:HD11	32:X:215:GLU:HG3	1.82	0.60
3:2:265:LEU:CD1	3:2:270:LEU:HD12	2.31	0.60
8:7:266:GLN:N	8:7:266:GLN:NE2	2.50	0.60
24:N:5:DA:C2	25:O:169:VAL:HG21	2.36	0.60
2:1:422:LEU:HD22	5:4:225:GLN:HE22	1.66	0.60
7:6:88:LEU:HD22	7:6:131:LEU:HD21	1.84	0.60
10:9:25:ASP:OD1	10:9:28:ARG:NH2	2.35	0.60
27:R:80:GLU:OE2	27:R:81:HIS:N	2.35	0.60
7:6:242:SER:O	7:6:245:SER:OG	2.17	0.60
9:8:258:HIS:HB3	9:8:269:LEU:HD21	1.83	0.60
10:9:48:LEU:HD23	10:9:276:LYS:HE3	1.84	0.60
10:9:68:CYS:HB3	10:9:80:VAL:HG22	1.84	0.60
20:J:8:PHE:CD2	20:J:48:MET:HE1	2.36	0.60
1:0:513:ASP:OD1	1:0:516:VAL:N	2.29	0.60
7:6:357:VAL:HG13	7:6:366:VAL:HG23	1.83	0.60
14:D:29:ALA:HB1	17:G:4:HIS:O	2.01	0.60
37:c:77:GLN:HB3	37:c:78:PRO:HD3	1.84	0.60
1:0:609:ASP:OD1	1:0:669:ARG:NH2	2.34	0.60
1:0:664:VAL:HG22	1:0:677:MET:HG2	1.83	0.60
14:D:70:ARG:NH2	17:G:142:GLU:OE2	2.35	0.60
46:l:57:PHE:CE2	47:m:130:LEU:HD13	2.37	0.60
8:7:189:LEU:O	8:7:195:ARG:NH1	2.33	0.59
24:N:5:DA:OP1	25:O:299:ARG:NH2	2.35	0.59
1:0:628:THR:HG22	1:0:628:THR:O	2.02	0.59
8:7:415:HIS:NE2	8:7:417:THR:OG1	2.35	0.59
11:A:1475:LEU:HD21	17:G:18:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:794:VAL:HG13	12:B:965:ILE:HG23	1.82	0.59
17:G:151:ARG:HB3	31:W:139:LEU:HD21	1.83	0.59
31:W:69:ASP:HA	32:X:225:VAL:HG23	1.83	0.59
38:d:512:ILE:HG23	46:l:510:LYS:NZ	2.18	0.59
51:q:100:LEU:O	51:q:104:VAL:HG23	2.02	0.59
1:0:372:LEU:HD11	1:0:404:ALA:HB1	1.84	0.59
12:B:274:ARG:NH2	12:B:281:ASP:OD1	2.36	0.59
17:G:10:GLU:HG2	17:G:67:LEU:HD12	1.84	0.59
31:W:154:CYS:HB2	31:W:157:CYS:SG	2.42	0.59
1:0:461:LEU:HD23	1:0:464:LEU:CD2	2.31	0.59
8:7:707:GLU:O	8:7:711:GLN:OE1	2.19	0.59
38:d:540:LEU:HB3	38:d:643:MET:HE1	1.84	0.59
9:8:118:MET:HE2	9:8:203:LEU:HD22	1.84	0.59
11:A:261:ARG:HD2	11:A:261:ARG:O	2.02	0.59
13:C:9:VAL:HG11	21:K:105:PHE:HD1	1.68	0.59
23:M:248:ARG:NH2	23:M:287:GLN:OE1	2.36	0.59
31:W:105:TYR:HE2	32:X:233:ILE:CA	2.15	0.59
38:d:547:GLN:O	38:d:572:ALA:N	2.35	0.59
5:4:195:VAL:HG12	5:4:203:LEU:HD23	1.85	0.59
38:d:339:LEU:HD21	38:d:439:PHE:HB3	1.84	0.59
1:0:462:SER:OG	1:0:463:PRO:HD2	2.02	0.59
7:6:345:CYS:O	7:6:349:GLN:N	2.36	0.59
32:X:144:ASN:HB3	32:X:174:ALA:HB1	1.84	0.59
39:e:68:PHE:CE1	40:f:98:LEU:HD13	2.37	0.59
45:k:120:ASP:OD2	45:k:123:LYS:NZ	2.36	0.59
9:8:137:ASP:OD2	9:8:139:LYS:NZ	2.35	0.59
9:8:267:ASP:OD2	9:8:297:ASN:ND2	2.31	0.59
38:d:591:LYS:HB2	38:d:627:TRP:HH2	1.68	0.59
50:p:269:TRP:CZ2	50:p:273:TYR:OH	2.53	0.59
1:0:262:ASN:O	1:0:266:LEU:HD23	2.03	0.58
4:3:35:VAL:HG13	4:3:58:PHE:CE2	2.38	0.58
10:9:198:ILE:HD11	10:9:255:MET:SD	2.43	0.58
3:2:18:ASN:OD1	3:2:19:LEU:N	2.35	0.58
11:A:1245:CYS:O	11:A:1246:ILE:HD13	2.03	0.58
17:G:154:LYS:HD2	31:W:143:GLN:OE1	2.03	0.58
38:d:493:LEU:HD13	38:d:504:VAL:CG2	2.32	0.58
38:d:551:PHE:CE2	38:d:569:ILE:HD12	2.38	0.58
42:h:36:ASP:OD2	42:h:72:ARG:NE	2.35	0.58
31:W:144:LEU:HD22	31:W:155:THR:H	1.68	0.58
32:X:141:PRO:O	32:X:146:ARG:NH1	2.36	0.58
35:a:61:ASN:O	35:a:86:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:126:SER:O	47:m:129:SER:N	2.36	0.58
50:p:166:ILE:CG2	50:p:178:ILE:HG21	2.33	0.58
2:1:422:LEU:HD22	5:4:225:GLN:NE2	2.19	0.58
8:7:281:GLN:NE2	8:7:482:PHE:O	2.37	0.58
11:A:1453:GLY:O	11:A:1457:ASN:ND2	2.36	0.58
42:h:183:MET:O	42:h:187:LEU:HG	2.02	0.58
12:B:407:MET:HE1	12:B:444:LEU:CD2	2.33	0.58
32:X:122:GLU:OE2	32:X:126:ASN:OD1	2.22	0.58
37:c:81:GLY:HA3	41:g:98:ILE:HD13	1.86	0.58
46:l:438:LEU:O	46:l:438:LEU:HD23	2.03	0.58
36:b:103:GLU:CA	36:b:106:PRO:HD2	2.34	0.58
46:l:315:LEU:HD21	46:l:320:TRP:CE3	2.39	0.58
1:0:240:ASP:OD1	1:0:241:ASN:N	2.37	0.58
9:8:26:VAL:HG22	9:8:41:LYS:HG3	1.84	0.58
11:A:111:CYS:SG	11:A:188:GLN:NE2	2.77	0.58
12:B:867:ILE:HB	12:B:894:THR:HG22	1.85	0.58
40:f:73:LEU:O	40:f:89:THR:N	2.37	0.57
46:l:444:GLU:HB2	46:l:445:PRO:CD	2.34	0.57
2:1:471:LEU:HD12	2:1:472:LEU:HD22	1.84	0.57
4:3:40:VAL:HG21	31:W:122:THR:OG1	2.04	0.57
4:3:54:ARG:NH2	17:G:166:ASP:OD2	2.35	0.57
12:B:223:SER:HG	12:B:350:HIS:CE1	2.19	0.57
31:W:114:ILE:HG23	31:W:177:LEU:HD22	1.86	0.57
38:d:203:ILE:O	38:d:203:ILE:HG22	2.04	0.57
46:l:359:ILE:HD13	46:l:392:ILE:HD13	1.86	0.57
2:1:417:LYS:HA	2:1:421:VAL:HG23	1.85	0.57
11:A:1030:SER:OG	15:E:162:ARG:NE	2.34	0.57
17:G:38:CYS:SG	17:G:39:THR:N	2.78	0.57
31:W:132:CYS:O	31:W:133:SER:OG	2.18	0.57
39:e:68:PHE:CZ	40:f:98:LEU:HD22	2.39	0.57
9:8:108:VAL:CG1	35:a:55:LEU:HD13	2.30	0.57
30:V:62:LEU:HA	30:V:76:LEU:HD23	1.87	0.57
4:3:295:ARG:HH11	9:8:164:SER:H	1.53	0.57
5:4:52:ASN:OD1	5:4:53:ARG:N	2.37	0.57
20:J:64:PRO:O	22:L:23:HIS:NE2	2.37	0.57
30:V:29:THR:HG23	30:V:32:LEU:H	1.69	0.57
32:X:83:ASN:O	32:X:87:THR:HG23	2.05	0.57
40:f:5:CYS:SG	40:f:161:LEU:HD21	2.44	0.57
46:l:60:HIS:CB	47:m:137:LEU:HD13	2.34	0.57
11:A:668:PHE:CE1	11:A:672:ILE:HD11	2.40	0.57
17:G:166:ASP:OD1	17:G:167:TYR:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:58:ARG:HD2	5:4:229:TRP:CE3	2.39	0.57
36:b:26:LEU:O	36:b:30:ILE:HD12	2.03	0.57
31:W:17:LEU:CD2	31:W:194:THR:HG21	2.27	0.57
32:X:167:LEU:HD23	32:X:198:LYS:HD3	1.86	0.57
35:a:130:PHE:CE2	35:a:134:MET:HE3	2.40	0.57
41:g:124:SER:OG	50:p:205:ARG:NH1	2.38	0.57
8:7:625:GLN:OE1	8:7:639:ARG:NH1	2.36	0.57
18:H:102:ASP:OD2	18:H:110:THR:OG1	2.21	0.57
26:Q:142:ASN:OD1	26:Q:143:TRP:N	2.37	0.57
38:d:413:PHE:HB3	38:d:417:GLU:OE2	2.03	0.57
44:j:131:LEU:HD13	48:n:124:ASP:HB3	1.86	0.57
50:p:301:THR:HG23	50:p:303:GLU:HG2	1.87	0.57
5:4:241:LEU:HD23	5:4:243:LEU:HD11	1.86	0.57
12:B:910:THR:HG22	12:B:911:LEU:N	2.18	0.57
13:C:7:PRO:O	21:K:104:ARG:NH1	2.37	0.57
36:b:108:HIS:HB3	38:d:115:VAL:HG22	1.86	0.57
46:l:200:ARG:CZ	46:l:217:VAL:HG21	2.34	0.57
46:l:638:ASN:OD1	46:l:639:LYS:N	2.38	0.57
12:B:851:ASP:OD2	22:L:17:TYR:OH	2.19	0.56
7:6:261:SER:OG	7:6:265:GLN:O	2.23	0.56
10:9:85:MET:HE3	10:9:89:ARG:HE	1.69	0.56
11:A:193:ARG:NH1	11:A:195:GLY:O	2.38	0.56
38:d:190:LEU:CD2	38:d:196:LEU:HD11	2.35	0.56
45:k:111:GLN:O	45:k:114:SER:OG	2.24	0.56
17:G:158:PHE:CZ	31:W:142:ASN:HB3	2.39	0.56
46:l:535:LYS:N	46:l:553:GLU:OE1	2.38	0.56
5:4:215:LEU:HD22	5:4:230:VAL:HG21	1.86	0.56
8:7:444:HIS:O	8:7:472:ARG:NH1	2.39	0.56
11:A:223:GLU:OE2	32:X:232:LYS:NZ	2.38	0.56
14:D:100:LEU:HD12	14:D:101:ALA:N	2.20	0.56
35:a:149:PHE:CG	38:d:95:TRP:HZ2	2.24	0.56
36:b:140:ILE:HD13	38:d:146:LEU:HD22	1.87	0.56
43:i:135:LEU:HA	43:i:138:MET:SD	2.46	0.56
12:B:346:GLU:OE1	12:B:346:GLU:N	2.38	0.56
12:B:764:MET:HE1	12:B:938:ARG:NH1	2.21	0.56
12:B:934:LYS:HG3	12:B:944:THR:HG22	1.87	0.56
12:B:938:ARG:NH2	12:B:983:GLU:OE2	2.38	0.56
38:d:429:GLU:HA	38:d:432:ILE:HG22	1.88	0.56
1:0:664:VAL:HG21	1:0:679:PHE:CE1	2.40	0.56
2:1:456:ASP:OD1	2:1:457:ILE:HD12	2.06	0.56
11:A:1279:MET:HA	26:Q:171:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:643:LEU:HD11	12:B:656:LEU:HD11	1.87	0.56
37:c:69:TYR:O	37:c:73:VAL:HG22	2.05	0.56
12:B:694:THR:HG22	12:B:695:HIS:CE1	2.41	0.56
18:H:33:GLU:OE2	18:H:55:LYS:NZ	2.38	0.56
8:7:361:CYS:SG	8:7:405:VAL:HG13	2.46	0.56
12:B:755:GLN:HE22	20:J:48:MET:HE2	1.70	0.56
11:A:1411:LEU:O	11:A:1421:ARG:NH2	2.39	0.56
31:W:105:TYR:CZ	32:X:233:ILE:HG23	2.39	0.56
37:c:83:SER:HB3	41:g:98:ILE:HG23	1.87	0.56
38:d:540:LEU:CD1	38:d:639:MET:HE3	2.35	0.56
10:9:72:LYS:HB3	10:9:73:PRO:HD3	1.86	0.55
11:A:357:LYS:NZ	12:B:1107:LEU:O	2.33	0.55
38:d:261:ILE:HD11	38:d:339:LEU:HD23	1.88	0.55
39:e:143:ILE:HD11	39:e:189:PHE:HE2	1.71	0.55
4:3:292:ALA:HB2	9:8:165:PRO:HG3	1.87	0.55
9:8:58:THR:HG23	9:8:157:GLY:HA3	1.87	0.55
11:A:1234:LYS:NZ	11:A:1298:LEU:O	2.39	0.55
14:D:133:ASP:OD1	14:D:134:ILE:N	2.39	0.55
31:W:22:ILE:HD11	31:W:26:TYR:CD2	2.41	0.55
32:X:108:HIS:O	32:X:111:ILE:HG22	2.06	0.55
38:d:551:PHE:HE2	38:d:569:ILE:HD12	1.71	0.55
4:3:307:GLN:HG3	10:9:251:ILE:HD11	1.88	0.55
17:G:154:LYS:NZ	31:W:143:GLN:CB	2.66	0.55
38:d:331:ILE:HG23	38:d:331:ILE:O	2.07	0.55
45:k:16:VAL:HG11	47:m:112:LEU:HD22	1.88	0.55
45:k:93:GLU:O	45:k:97:GLY:N	2.34	0.55
1:0:420:PRO:HA	1:0:431:PRO:HB3	1.89	0.55
5:4:242:ILE:C	5:4:243:LEU:HD12	2.31	0.55
12:B:91:ILE:HD13	12:B:126:VAL:HG12	1.87	0.55
50:p:207:LEU:CD1	50:p:263:VAL:HG21	2.36	0.55
1:0:114:ASN:HD22	1:0:114:ASN:C	2.15	0.55
7:6:59:ARG:NH2	7:6:166:GLU:OE1	2.39	0.55
9:8:144:LEU:HG	9:8:154:ALA:HB2	1.88	0.55
46:l:192:LEU:HD13	46:l:220:GLY:HA2	1.89	0.55
1:0:17:ILE:HD11	1:0:22:PHE:CZ	2.42	0.55
8:7:664:SER:O	8:7:667:THR:OG1	2.25	0.55
9:8:164:SER:HB3	10:9:165:ARG:NH1	2.22	0.55
17:G:154:LYS:NZ	31:W:143:GLN:CG	2.68	0.55
32:X:99:LEU:HD22	32:X:120:MET:HE2	1.88	0.55
36:b:103:GLU:O	36:b:106:PRO:CD	2.51	0.55
24:N:5:DA:H2	25:O:169:VAL:HG21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:181:LEU:HD21	39:e:148:ILE:CD1	2.35	0.55
8:7:87:GLU:OE2	8:7:145:LYS:NZ	2.39	0.55
11:A:261:ARG:NH1	11:A:277:THR:OG1	2.40	0.55
38:d:591:LYS:HB2	38:d:627:TRP:CH2	2.41	0.55
39:e:106:VAL:HG23	39:e:106:VAL:O	2.07	0.55
38:d:327:VAL:HG12	38:d:328:LYS:N	2.21	0.55
50:p:207:LEU:HD11	50:p:263:VAL:HG21	1.88	0.55
9:8:165:PRO:C	9:8:167:ARG:H	2.15	0.54
11:A:362:SER:HB2	12:B:1084:LEU:HD12	1.89	0.54
26:Q:109:LYS:O	26:Q:149:LEU:N	2.38	0.54
36:b:140:ILE:CD1	38:d:146:LEU:HD22	2.36	0.54
1:0:133:LYS:O	1:0:137:LEU:HD23	2.08	0.54
1:0:606:GLU:O	1:0:666:ARG:NH2	2.40	0.54
2:1:486:LEU:O	2:1:490:VAL:HG23	2.07	0.54
4:3:292:ALA:HB2	9:8:165:PRO:CG	2.37	0.54
11:A:350:VAL:HG12	11:A:1435:THR:HG21	1.89	0.54
11:A:621:ILE:HG23	11:A:621:ILE:O	2.06	0.54
11:A:850:THR:O	11:A:854:THR:HG23	2.07	0.54
5:4:44:LEU:HD21	5:4:162:LEU:HD13	1.89	0.54
10:9:64:LEU:HB2	10:9:105:MET:HG3	1.89	0.54
14:D:29:ALA:O	14:D:94:LYS:NZ	2.39	0.54
30:V:16:GLN:NE2	30:V:20:ASP:OD2	2.40	0.54
38:d:336:PHE:HB2	38:d:339:LEU:HD13	1.90	0.54
42:h:114:LEU:HD22	48:n:115:LEU:HA	1.90	0.54
1:0:309:VAL:O	1:0:309:VAL:HG12	2.06	0.54
8:7:377:GLN:OE1	8:7:381:TRP:NE1	2.40	0.54
11:A:734:ARG:NE	19:I:107:ALA:O	2.40	0.54
8:7:83:HIS:ND1	8:7:115:GLU:OE2	2.40	0.54
14:D:110:GLU:O	14:D:114:LEU:HD23	2.07	0.54
31:W:106:LYS:O	31:W:110:MET:HG2	2.08	0.54
38:d:380:ARG:O	38:d:384:LYS:N	2.35	0.54
1:0:80:ILE:HD11	1:0:206:VAL:HB	1.90	0.54
23:M:173:VAL:O	23:M:175:ARG:NH1	2.40	0.54
46:l:509:ILE:HD11	46:l:641:LEU:HD23	1.88	0.54
9:8:78:LEU:N	9:8:90:VAL:O	2.40	0.54
12:B:752:TYR:HE1	12:B:809:VAL:HG23	1.73	0.54
29:U:15:ARG:HA	29:U:18:ILE:HD12	1.89	0.54
3:2:42:LEU:HD13	5:4:50:PHE:CE1	2.42	0.54
11:A:233:CYS:SG	11:A:244:ARG:NH1	2.81	0.54
11:A:521:VAL:HG13	11:A:535:MET:HE1	1.90	0.54
12:B:501:LEU:HD12	12:B:505:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:289:VAL:HG22	1:0:324:ARG:NH1	2.23	0.54
11:A:1485:GLU:OE2	17:G:20:PRO:HG2	2.05	0.54
38:d:497:ILE:HD13	38:d:502:ILE:HG23	1.90	0.54
39:e:20:GLU:HG2	39:e:174:VAL:HG12	1.89	0.54
11:A:1484:MET:N	11:A:1484:MET:SD	2.80	0.54
38:d:327:VAL:HG12	38:d:328:LYS:H	1.73	0.54
46:l:82:LYS:HB2	47:m:159:LEU:HD13	1.89	0.54
3:2:80:SER:O	3:2:84:GLU:OE1	2.25	0.53
12:B:718:GLN:HG2	12:B:720:PRO:HD2	1.90	0.53
23:M:133:ASN:OD1	23:M:134:ILE:N	2.41	0.53
31:W:113:ARG:CZ	32:X:222:SER:OG	2.54	0.53
1:0:437:CYS:SG	1:0:438:MET:N	2.81	0.53
35:a:47:ASN:OD1	35:a:60:LEU:HD21	2.07	0.53
41:g:130:LEU:HD21	53:s:155:LEU:CD1	2.37	0.53
3:2:265:LEU:HD12	3:2:270:LEU:HD12	1.90	0.53
4:3:255:THR:HG22	10:9:3:HIS:CE1	2.44	0.53
26:Q:163:GLU:OE1	26:Q:163:GLU:N	2.40	0.53
31:W:148:MET:SD	31:W:149:THR:N	2.81	0.53
31:W:277:ARG:O	31:W:282:ARG:NH1	2.42	0.53
38:d:496:ASN:N	38:d:503:ARG:O	2.36	0.53
38:d:512:ILE:HG23	46:l:510:LYS:HZ1	1.74	0.53
8:7:632:SER:OG	8:7:676:ARG:NH2	2.41	0.53
12:B:260:LEU:HB2	12:B:263:ILE:HD12	1.89	0.53
40:f:75:CYS:N	40:f:87:ALA:O	2.41	0.53
46:l:320:TRP:HB3	46:l:324:VAL:HG12	1.90	0.53
12:B:128:ILE:HG21	12:B:431:LEU:HD21	1.90	0.53
17:G:154:LYS:HZ3	31:W:143:GLN:CD	2.16	0.53
1:0:28:LEU:HD22	1:0:55:LEU:HD23	1.91	0.53
5:4:195:VAL:CG1	5:4:203:LEU:HD23	2.38	0.53
7:6:109:THR:OG1	7:6:148:SER:OG	2.05	0.53
12:B:410:ASN:O	12:B:414:GLU:OE1	2.26	0.53
17:G:92:VAL:HG23	17:G:139:GLN:HG2	1.89	0.53
23:M:222:LEU:CD2	23:M:277:ILE:HD13	2.38	0.53
39:e:88:LEU:HD12	39:e:103:ARG:CG	2.38	0.53
52:r:8:UNK:O	52:r:12:UNK:N	2.41	0.53
8:7:568:LEU:HD11	8:7:606:PHE:HB3	1.91	0.53
12:B:552:ASN:OD1	12:B:553:LEU:N	2.42	0.53
38:d:375:LEU:HG	38:d:431:ILE:HD12	1.89	0.53
38:d:493:LEU:HD13	38:d:504:VAL:HG23	1.89	0.53
7:6:337:GLU:O	7:6:340:ASN:ND2	2.38	0.53
9:8:258:HIS:O	35:a:36:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:613:ARG:NH1	12:B:615:TYR:OH	2.41	0.53
46:l:416:LEU:HD22	46:l:463:PHE:CE2	2.43	0.53
1:0:365:VAL:O	1:0:365:VAL:HG22	2.08	0.53
5:4:44:LEU:HD22	5:4:227:LEU:HB3	1.90	0.53
25:O:208:ARG:NH2	29:U:346:LYS:O	2.41	0.53
36:b:181:LEU:HD23	36:b:181:LEU:C	2.34	0.53
42:h:104:ASP:HA	42:h:107:ILE:HD12	1.90	0.53
11:A:459:ASN:OD1	11:A:460:ARG:N	2.42	0.53
12:B:752:TYR:CE2	12:B:807:ARG:HG2	2.43	0.53
13:C:175:LYS:NZ	22:L:57:ALA:O	2.42	0.53
36:b:150:LEU:HD21	37:c:45:LEU:HB3	1.90	0.53
44:j:104:MET:CE	44:j:107:ILE:HG21	2.39	0.53
3:2:32:ASP:OD1	3:2:33:ARG:N	2.42	0.52
3:2:58:ARG:NH1	5:4:229:TRP:CZ3	2.77	0.52
8:7:463:LYS:O	8:7:484:ILE:HG23	2.09	0.52
11:A:425:ASP:HB2	23:M:39:LEU:HD11	1.90	0.52
17:G:52:ASP:N	17:G:71:LYS:O	2.43	0.52
1:0:393:ASP:OD1	1:0:394:PHE:N	2.42	0.52
5:4:258:HIS:HE1	5:4:276:CYS:SG	2.31	0.52
39:e:28:LEU:O	39:e:31:SER:OG	2.25	0.52
40:f:78:LEU:HD21	40:f:191:VAL:HG22	1.91	0.52
7:6:87:LEU:HD11	7:6:229:LYS:HG2	1.91	0.52
9:8:110:THR:OG1	9:8:113:HIS:ND1	2.30	0.52
18:H:91:VAL:HG22	18:H:144:LEU:HD23	1.92	0.52
39:e:27:VAL:HG21	39:e:35:LEU:CD2	2.39	0.52
39:e:32:LEU:CD1	39:e:167:TYR:CD2	2.92	0.52
42:h:101:GLU:O	42:h:105:SER:N	2.38	0.52
1:0:115:LEU:HD13	1:0:191:PRO:HB2	1.92	0.52
35:a:106:TYR:CE1	36:b:109:LEU:HD13	2.45	0.52
35:a:114:VAL:HG13	35:a:115:ILE:H	1.73	0.52
46:l:509:ILE:HD11	46:l:641:LEU:HD22	1.92	0.52
8:7:363:VAL:HG21	8:7:378:PHE:HE2	1.75	0.52
19:I:69:ILE:HG22	19:I:71:ASP:H	1.74	0.52
50:p:191:LEU:HD11	50:p:221:VAL:HG11	1.91	0.52
12:B:474:THR:OG1	12:B:732:ALA:O	2.24	0.52
36:b:103:GLU:HA	36:b:106:PRO:HD2	1.92	0.52
40:f:4:THR:HG21	40:f:189:THR:HG23	1.90	0.52
1:0:709:THR:HG22	1:0:710:VAL:N	2.25	0.52
8:7:181:HIS:O	8:7:184:VAL:HG12	2.10	0.52
9:8:213:LEU:HA	9:8:224:ARG:HD2	1.92	0.52
12:B:939:HIS:NE2	12:B:983:GLU:OE1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:222:LEU:HD21	23:M:277:ILE:HD13	1.92	0.52
32:X:89:HIS:CE1	32:X:139:PHE:CB	2.93	0.52
36:b:178:THR:O	36:b:182:VAL:HG23	2.10	0.52
8:7:340:LEU:HD23	8:7:491:ALA:HB2	1.91	0.52
10:9:7:GLN:HG3	10:9:89:ARG:NH2	2.25	0.52
38:d:374:ASN:HD22	38:d:374:ASN:C	2.14	0.52
1:0:488:VAL:O	1:0:488:VAL:HG23	2.09	0.52
4:3:287:TYR:OH	9:8:165:PRO:CB	2.57	0.52
7:6:54:ARG:NH2	7:6:245:SER:O	2.43	0.52
7:6:88:LEU:HD23	7:6:131:LEU:HD21	1.91	0.52
11:A:904:GLN:NE2	11:A:981:CYS:O	2.42	0.52
15:E:111:THR:HG23	15:E:114:ALA:H	1.74	0.52
38:d:513:THR:C	38:d:514:LEU:HD12	2.35	0.52
41:g:63:VAL:O	41:g:67:ASN:N	2.43	0.52
42:h:181:LEU:HD21	49:o:23:GLU:OE1	2.10	0.52
43:i:112:LEU:HD13	46:l:136:LEU:HD11	1.92	0.52
46:l:444:GLU:HB2	46:l:445:PRO:HD3	1.91	0.52
30:V:57:ASN:OD1	30:V:58:PHE:N	2.43	0.52
38:d:312:SER:OG	46:l:319:ARG:HD2	2.10	0.52
39:e:147:LYS:HB3	39:e:167:TYR:CD1	2.45	0.52
45:k:132:HIS:O	45:k:134:PRO:HD3	2.10	0.52
11:A:1016:LEU:O	11:A:1020:LEU:HG	2.10	0.51
26:Q:43:ASN:OD1	26:Q:44:GLN:N	2.43	0.51
38:d:198:LYS:HE2	38:d:203:ILE:HG23	1.92	0.51
46:l:153:ALA:HB1	46:l:156:TYR:HD2	1.72	0.51
48:n:82:THR:HG22	48:n:84:ALA:H	1.75	0.51
3:2:338:PHE:N	3:2:341:MET:O	2.43	0.51
10:9:85:MET:O	10:9:89:ARG:HG3	2.11	0.51
17:G:39:THR:O	17:G:43:GLY:N	2.42	0.51
19:I:29:ASP:O	19:I:33:ARG:N	2.40	0.51
31:W:103:VAL:O	31:W:107:LEU:HG	2.10	0.51
46:l:259:THR:OG1	46:l:271:ILE:HG21	2.10	0.51
46:l:545:LEU:HD22	46:l:653:PRO:HD3	1.91	0.51
47:m:128:ARG:NH2	47:m:132:GLU:OE2	2.42	0.51
10:9:275:GLN:O	10:9:278:GLU:HG3	2.10	0.51
12:B:905:ASP:N	12:B:922:ARG:O	2.42	0.51
21:K:63:VAL:HG23	21:K:63:VAL:O	2.10	0.51
35:a:114:VAL:HG13	35:a:115:ILE:N	2.25	0.51
2:1:412:GLU:OE1	2:1:412:GLU:N	2.44	0.51
3:2:390:GLN:HE21	3:2:394:TRP:NE1	2.09	0.51
9:8:207:LEU:HD11	9:8:268:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:485:ASN:O	11:A:488:VAL:HG22	2.10	0.51
25:O:206:GLU:HB3	25:O:207:PRO:HD3	1.91	0.51
37:c:17:ILE:HG21	37:c:63:LEU:CD2	2.40	0.51
39:e:116:ASP:OD1	39:e:117:PHE:N	2.44	0.51
57:y:1:UNK:O	57:y:5:UNK:N	2.44	0.51
9:8:268:LEU:O	9:8:272:ILE:HG12	2.11	0.51
11:A:1139:LEU:HD13	11:A:1341:VAL:HA	1.91	0.51
11:A:1284:PHE:CE2	11:A:1288:ILE:HD11	2.46	0.51
11:A:1382:LEU:HD23	11:A:1398:LEU:HD13	1.93	0.51
25:O:196:ARG:NH1	28:T:-7:DT:O3'	2.43	0.51
38:d:513:THR:O	38:d:514:LEU:CD1	2.58	0.51
43:i:93:LEU:HD12	43:i:94:ASP:N	2.26	0.51
46:l:395:LEU:HD12	46:l:395:LEU:O	2.09	0.51
2:1:127:LEU:HD12	2:1:467:ALA:HA	1.91	0.51
9:8:75:ILE:HA	9:8:152:LYS:HD3	1.92	0.51
13:C:51:GLN:NE2	22:L:52:LEU:HD13	2.26	0.51
23:M:107:MET:O	23:M:112:ARG:NH2	2.43	0.51
39:e:23:LEU:HG	39:e:199:LEU:HD13	1.91	0.51
40:f:38:THR:HG23	40:f:38:THR:O	2.10	0.51
1:0:377:GLU:OE1	1:0:377:GLU:N	2.44	0.51
10:9:59:TYR:CZ	10:9:63:ARG:HD2	2.46	0.51
10:9:181:LEU:HD13	10:9:226:ILE:HG21	1.92	0.51
11:A:863:ARG:NH2	11:A:1415:THR:OG1	2.44	0.51
12:B:809:VAL:HG11	12:B:811:TYR:CE2	2.46	0.51
12:B:834:ARG:HG2	12:B:840:MET:HE2	1.93	0.51
26:Q:162:GLU:OE1	26:Q:162:GLU:N	2.43	0.51
31:W:170:LYS:O	31:W:174:ARG:HD3	2.10	0.51
1:0:3:LEU:O	1:0:9:LEU:HD12	2.11	0.51
3:2:266:ARG:HE	3:2:277:LYS:HZ2	1.58	0.51
9:8:174:VAL:O	9:8:179:ARG:NH2	2.31	0.51
1:0:126:PHE:CE2	1:0:128:LYS:HB2	2.46	0.51
4:3:304:LEU:HD11	10:9:170:PHE:HZ	1.76	0.51
31:W:49:LEU:HD22	31:W:56:ARG:HD3	1.93	0.51
32:X:193:ASN:OD1	32:X:194:ARG:N	2.43	0.51
36:b:146:MET:SD	37:c:37:LYS:NZ	2.83	0.51
38:d:92:LEU:HD22	38:d:93:TRP:H	1.76	0.51
12:B:625:LEU:HD13	12:B:675:LEU:HD21	1.91	0.51
35:a:115:ILE:HG21	36:b:63:LEU:CD1	2.41	0.51
36:b:100:PHE:CG	36:b:101:SER:N	2.77	0.51
40:f:41:VAL:HG22	40:f:68:ASN:OD1	2.11	0.51
7:6:204:GLU:OE1	7:6:209:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:228:ILE:HG23	27:R:229:HIS:N	2.26	0.50
39:e:56:MET:HG2	39:e:125:MET:HE2	1.92	0.50
1:0:118:HIS:HB3	1:0:121:VAL:HG22	1.94	0.50
8:7:369:VAL:HG11	8:7:615:PHE:HA	1.93	0.50
9:8:108:VAL:HG11	35:a:59:HIS:HB3	1.93	0.50
31:W:180:PHE:HA	32:X:216:PHE:CZ	2.46	0.50
32:X:124:LEU:HD13	32:X:137:TYR:CD1	2.47	0.50
9:8:167:ARG:HH21	9:8:167:ARG:HG2	1.74	0.50
1:0:637:LEU:HD13	1:0:651:PHE:CD2	2.47	0.50
21:K:105:PHE:CE2	21:K:109:ILE:HD11	2.45	0.50
44:j:101:ILE:HG23	44:j:104:MET:HE2	1.94	0.50
2:1:136:VAL:HG11	2:1:502:VAL:HG12	1.92	0.50
2:1:471:LEU:HD13	2:1:475:PHE:HE2	1.75	0.50
3:2:402:ARG:NH1	6:5:11:GLU:OE2	2.44	0.50
8:7:274:GLN:OE1	8:7:459:GLN:NE2	2.44	0.50
12:B:601:VAL:HG22	12:B:616:THR:HG23	1.93	0.50
32:X:131:GLU:N	32:X:138:ALA:O	2.42	0.50
38:d:546:TRP:HE3	38:d:571:VAL:HG12	1.77	0.50
46:l:359:ILE:HD11	46:l:392:ILE:HG21	1.94	0.50
2:1:471:LEU:HD13	2:1:475:PHE:CE2	2.47	0.50
17:G:97:LEU:HD21	17:G:128:TYR:CE1	2.46	0.50
35:a:71:LEU:HD13	35:a:82:ARG:HH11	1.76	0.50
36:b:22:LEU:HD21	36:b:56:LEU:HD12	1.94	0.50
42:h:155:ILE:HG21	49:o:65:LYS:O	2.12	0.50
10:9:234:GLU:C	10:9:236:LEU:H	2.20	0.50
12:B:907:VAL:HG22	12:B:921:ILE:HG12	1.94	0.50
24:N:4:DA:H5'	25:O:301:VAL:HG21	1.94	0.50
31:W:20:TYR:HB3	31:W:190:LEU:HD13	1.94	0.50
31:W:114:ILE:CG2	31:W:177:LEU:HD22	2.42	0.50
35:a:71:LEU:HD13	35:a:82:ARG:HD2	1.94	0.50
40:f:24:LEU:HD23	40:f:126:VAL:HG21	1.94	0.50
46:l:312:THR:CG2	46:l:337:LEU:HD11	2.41	0.50
50:p:242:VAL:CG2	50:p:295:THR:HG23	2.42	0.50
3:2:435:ASN:ND2	6:5:38:ILE:O	2.45	0.50
5:4:165:LYS:NZ	5:4:167:ALA:O	2.38	0.50
31:W:17:LEU:HD13	31:W:194:THR:OG1	2.12	0.50
31:W:137:THR:CG2	31:W:139:LEU:HD13	2.41	0.50
38:d:198:LYS:HG2	38:d:203:ILE:HA	1.92	0.50
44:j:97:MET:O	44:j:100:LEU:N	2.44	0.50
46:l:66:LEU:O	46:l:70:THR:HG23	2.12	0.50
46:l:93:ARG:NH2	47:m:113:PRO:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:67:ARG:NH2	20:J:2:ILE:HG23	2.27	0.49
30:V:73:THR:HG22	30:V:73:THR:O	2.12	0.49
39:e:49:GLU:OE1	39:e:49:GLU:N	2.45	0.49
2:1:374:LEU:HD12	2:1:374:LEU:O	2.13	0.49
9:8:20:GLU:HG3	9:8:25:THR:HG22	1.94	0.49
11:A:1382:LEU:HD23	11:A:1398:LEU:CD1	2.42	0.49
12:B:296:GLU:OE2	19:I:103:ARG:NH2	2.44	0.49
12:B:528:LEU:HD21	12:B:767:LEU:HD21	1.93	0.49
35:a:106:TYR:HE1	36:b:109:LEU:HD13	1.77	0.49
38:d:386:THR:C	38:d:387:LEU:HD23	2.37	0.49
47:m:126:SER:O	47:m:130:LEU:HG	2.12	0.49
50:p:253:TYR:HE2	50:p:269:TRP:HB2	1.76	0.49
1:0:284:GLU:HA	1:0:287:ARG:HG2	1.94	0.49
2:1:481:VAL:HG23	2:1:483:THR:HG23	1.94	0.49
11:A:1173:THR:HG22	11:A:1214:VAL:HG23	1.94	0.49
1:0:284:GLU:HG2	1:0:385:THR:HG21	1.94	0.49
7:6:87:LEU:HD11	7:6:229:LYS:CG	2.42	0.49
38:d:537:VAL:HG21	38:d:582:VAL:HG21	1.94	0.49
46:l:557:VAL:HB	46:l:558:PRO:CD	2.42	0.49
52:r:7:UNK:O	52:r:11:UNK:N	2.45	0.49
12:B:738:THR:HG21	20:J:58:LYS:HG3	1.93	0.49
12:B:962:THR:O	20:J:9:THR:HG23	2.12	0.49
17:G:83:GLU:OE2	17:G:147:ILE:HD12	2.13	0.49
31:W:131:VAL:HB	31:W:157:CYS:HB2	1.94	0.49
36:b:37:TYR:O	38:d:95:TRP:CZ3	2.66	0.49
40:f:3:VAL:O	40:f:144:TYR:N	2.39	0.49
50:p:201:ILE:HG21	50:p:230:ILE:HG13	1.95	0.49
8:7:363:VAL:HG21	8:7:378:PHE:CE2	2.47	0.49
11:A:539:GLN:HA	11:A:774:ALA:HB1	1.93	0.49
11:A:1218:ARG:NH2	11:A:1252:ALA:O	2.46	0.49
14:D:73:ARG:O	14:D:141:GLN:NE2	2.44	0.49
38:d:315:ALA:CB	38:d:331:ILE:HD11	2.43	0.49
38:d:571:VAL:O	38:d:579:ALA:HB1	2.13	0.49
42:h:121:LEU:HD13	48:n:108:VAL:HA	1.95	0.49
1:0:243:CYS:SG	1:0:443:ALA:HB3	2.53	0.49
5:4:255:CYS:SG	5:4:258:HIS:CE1	3.03	0.49
11:A:360:ASP:OD1	12:B:1062:ARG:NE	2.43	0.49
38:d:525:LEU:O	38:d:529:MET:HE2	2.12	0.49
39:e:56:MET:HE1	39:e:83:TRP:HZ3	1.78	0.49
46:l:57:PHE:CD2	47:m:130:LEU:HD13	2.48	0.49
46:l:516:SER:HA	46:l:540:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:88:ARG:NH2	32:X:93:ASP:OD2	2.45	0.49
38:d:261:ILE:CD1	38:d:339:LEU:HD23	2.42	0.49
38:d:386:THR:HG22	38:d:387:LEU:N	2.27	0.49
50:p:288:LEU:HG	50:p:289:GLN:N	2.28	0.49
3:2:174:ASP:OD1	3:2:175:LEU:N	2.45	0.49
8:7:578:PRO:HG3	8:7:602:ILE:HD11	1.94	0.49
12:B:1035:ARG:NH1	12:B:1036:LYS:O	2.44	0.49
39:e:141:MET:HA	39:e:173:VAL:HG22	1.95	0.49
11:A:1178:ASP:OD2	11:A:1260:ARG:NH2	2.46	0.49
14:D:114:LEU:CD1	17:G:84:VAL:HG21	2.43	0.49
17:G:134:ASP:OD1	17:G:135:ILE:N	2.46	0.49
24:N:52:DC:H4'	24:N:53:DT:OP1	2.13	0.49
31:W:191:LEU:O	31:W:195:GLU:OE1	2.29	0.49
32:X:181:ALA:O	32:X:185:LEU:HD23	2.13	0.49
43:i:160:VAL:O	43:i:164:ILE:N	2.39	0.49
4:3:258:PRO:HG2	4:3:301:PHE:CG	2.47	0.48
4:3:303:GLY:O	10:9:210:SER:HB2	2.13	0.48
12:B:167:THR:HG23	12:B:170:ASP:H	1.78	0.48
29:U:18:ILE:HD11	29:U:46:TRP:CZ3	2.48	0.48
38:d:626:GLN:OE1	38:d:626:GLN:N	2.45	0.48
39:e:85:LEU:HD11	39:e:108:ILE:HG12	1.95	0.48
39:e:88:LEU:HD12	39:e:103:ARG:HG3	1.94	0.48
40:f:175:VAL:O	40:f:175:VAL:HG22	2.12	0.48
43:i:83:MET:SD	43:i:87:ILE:HD11	2.52	0.48
1:0:134:CYS:O	1:0:138:THR:HG22	2.12	0.48
1:0:310:LEU:HG	1:0:409:THR:HG21	1.95	0.48
2:1:524:HIS:ND1	7:6:270:SER:OG	2.39	0.48
7:6:121:SER:OG	7:6:127:HIS:NE2	2.39	0.48
7:6:285:THR:O	7:6:297:LYS:NZ	2.45	0.48
9:8:61:ARG:HD3	9:8:159:ALA:H	1.78	0.48
11:A:1242:ASP:O	11:A:1262:MET:N	2.46	0.48
31:W:128:LYS:HZ1	31:W:166:SER:N	2.12	0.48
39:e:53:ASP:OD1	39:e:73:ARG:NH2	2.44	0.48
1:0:81:GLU:O	1:0:84:ILE:HG22	2.13	0.48
4:3:275:VAL:HG21	4:3:293:CYS:HB2	1.95	0.48
8:7:575:LEU:O	8:7:576:ASN:OD1	2.32	0.48
9:8:64:LYS:NZ	10:9:117:GLU:OE2	2.43	0.48
11:A:95:PHE:N	11:A:311:GLN:OE1	2.43	0.48
12:B:404:PHE:HA	12:B:407:MET:HE3	1.94	0.48
32:X:148:LYS:HD2	32:X:184:ALA:HB3	1.95	0.48
38:d:534:VAL:HG21	38:d:567:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:650:MET:SD	8:7:656:ASN:ND2	2.82	0.48
25:O:227:GLU:OE1	25:O:318:ARG:NH2	2.46	0.48
31:W:43:VAL:HB	31:W:48:MET:HE3	1.94	0.48
31:W:105:TYR:CE2	32:X:233:ILE:CG2	2.90	0.48
2:1:503:THR:OG1	2:1:533:TYR:OH	2.01	0.48
10:9:195:LEU:HA	10:9:198:ILE:HG22	1.94	0.48
38:d:591:LYS:HD3	38:d:627:TRP:CH2	2.49	0.48
50:p:249:ALA:CB	50:p:269:TRP:CZ2	2.97	0.48
7:6:63:VAL:HG11	7:6:88:LEU:HD11	1.95	0.48
9:8:59:ALA:HB1	9:8:87:ILE:HD11	1.94	0.48
11:A:1415:THR:HG22	11:A:1416:ARG:N	2.29	0.48
12:B:501:LEU:HD11	12:B:511:PRO:HA	1.95	0.48
14:D:55:GLN:NE2	14:D:56:GLU:O	2.46	0.48
15:E:25:GLY:O	15:E:65:ASN:ND2	2.47	0.48
16:F:64:ARG:HH21	17:G:61:PRO:HG3	1.79	0.48
36:b:181:LEU:HD12	39:e:164:SER:CB	2.44	0.48
38:d:472:GLU:OE1	50:p:211:ARG:NH1	2.47	0.48
38:d:478:LEU:HG	38:d:480:THR:HG23	1.95	0.48
39:e:39:LEU:CD1	39:e:143:ILE:HG21	2.42	0.48
46:l:315:LEU:HD21	46:l:320:TRP:HE3	1.77	0.48
1:0:722:ARG:NH1	7:6:222:ILE:O	2.46	0.48
12:B:892:CYS:SG	23:M:53:ARG:NE	2.87	0.48
17:G:30:LEU:O	17:G:34:VAL:HG22	2.14	0.48
25:O:203:ARG:NE	30:V:65:TYR:OH	2.46	0.48
27:R:43:LEU:HD12	27:R:55:SER:O	2.13	0.48
36:b:172:THR:OG1	39:e:31:SER:HB3	2.13	0.48
41:g:34:THR:O	41:g:38:LYS:N	2.38	0.48
1:0:136:SER:O	1:0:142:VAL:HG21	2.13	0.48
2:1:440:LEU:HD11	5:4:218:PRO:CD	2.43	0.48
5:4:13:ILE:HD13	5:4:41:VAL:HG13	1.94	0.48
9:8:142:ASN:ND2	9:8:155:ASP:OD1	2.47	0.48
11:A:350:VAL:CG1	11:A:1435:THR:HG21	2.43	0.48
11:A:1251:ASN:OD1	11:A:1252:ALA:N	2.46	0.48
38:d:184:ASN:C	38:d:184:ASN:HD22	2.21	0.48
51:q:132:HIS:O	51:q:136:LEU:HD23	2.14	0.48
1:0:115:LEU:HD12	1:0:115:LEU:O	2.13	0.48
10:9:186:ILE:H	10:9:186:ILE:HD12	1.79	0.48
11:A:225:PHE:HA	11:A:228:ILE:HD12	1.96	0.48
11:A:348:GLY:O	11:A:352:GLY:N	2.46	0.48
11:A:363:ALA:O	12:B:1084:LEU:HD11	2.13	0.48
11:A:1144:LEU:H	11:A:1144:LEU:HD23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:92:GLU:O	13:C:93:PHE:CG	2.67	0.48
20:J:6:ARG:HD3	20:J:13:ILE:HD13	1.96	0.48
37:c:100:ALA:O	37:c:104:LEU:HD23	2.14	0.48
40:f:9:MET:SD	40:f:165:LEU:HD12	2.54	0.48
2:1:488:GLU:O	2:1:491:VAL:HG22	2.14	0.48
3:2:360:THR:HG22	3:2:363:GLN:OE1	2.13	0.48
9:8:97:ASP:HA	9:8:144:LEU:HA	1.94	0.48
11:A:1454:VAL:HG12	11:A:1458:ILE:HD12	1.95	0.48
12:B:388:TYR:CE2	12:B:505:LEU:HD21	2.48	0.48
12:B:718:GLN:OE1	12:B:976:MET:HE3	2.14	0.48
12:B:794:VAL:O	12:B:946:GLY:N	2.42	0.48
40:f:23:LEU:HD23	40:f:23:LEU:C	2.39	0.48
5:4:255:CYS:HG	5:4:258:HIS:CE1	2.33	0.47
9:8:45:LEU:HD11	9:8:86:ASN:HB3	1.96	0.47
9:8:136:ARG:NH1	9:8:160:LYS:HD3	2.29	0.47
12:B:438:ARG:NH2	12:B:442:ASP:OD2	2.47	0.47
12:B:752:TYR:CD2	12:B:807:ARG:HB3	2.49	0.47
14:D:15:GLU:OE2	17:G:78:ARG:NH1	2.47	0.47
25:O:297:LYS:HG2	25:O:298:PRO:HD3	1.96	0.47
26:Q:153:ARG:NH1	26:Q:180:ARG:O	2.47	0.47
31:W:45:GLU:HB2	31:W:90:ASN:HB2	1.95	0.47
40:f:5:CYS:SG	40:f:161:LEU:HD11	2.54	0.47
3:2:261:PHE:O	3:2:265:LEU:HD23	2.14	0.47
8:7:605:ILE:HD12	8:7:607:ILE:HD11	1.96	0.47
10:9:178:TYR:CE1	10:9:228:MET:HG2	2.49	0.47
11:A:33:ARG:NH1	12:B:1139:GLY:O	2.47	0.47
14:D:33:LEU:O	14:D:37:VAL:HG23	2.13	0.47
38:d:549:LEU:HD12	38:d:570:THR:HG22	1.96	0.47
38:d:592:ILE:HG22	38:d:593:MET:N	2.29	0.47
44:j:97:MET:O	44:j:101:ILE:HD12	2.13	0.47
51:q:100:LEU:O	51:q:104:VAL:N	2.47	0.47
7:6:253:GLY:N	7:6:310:LEU:HD21	2.29	0.47
11:A:689:ILE:O	11:A:693:ILE:HG12	2.14	0.47
13:C:260:GLN:HB2	21:K:91:ILE:HG21	1.97	0.47
27:R:58:LEU:HD11	27:R:62:LEU:HD23	1.96	0.47
1:0:617:ALA:HB2	1:0:676:LEU:HD21	1.97	0.47
5:4:146:ARG:NH2	7:6:348:CYS:O	2.46	0.47
10:9:96:VAL:HG13	10:9:101:PRO:CG	2.43	0.47
11:A:1171:ALA:N	11:A:1215:GLU:O	2.47	0.47
12:B:407:MET:HE1	12:B:444:LEU:CG	2.43	0.47
40:f:128:THR:O	40:f:128:THR:HG23	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:548:TYR:HA	46:l:570:PHE:HB2	1.96	0.47
5:4:20:ILE:H	5:4:20:ILE:HD12	1.79	0.47
12:B:598:VAL:CG2	12:B:601:VAL:HG23	2.44	0.47
12:B:952:GLU:OE2	13:C:39:ILE:HG22	2.13	0.47
24:N:45:DT:C2	24:N:46:DC:C5	3.03	0.47
46:l:315:LEU:C	46:l:315:LEU:HD23	2.39	0.47
5:4:235:GLN:O	5:4:235:GLN:NE2	2.47	0.47
8:7:608:SER:OG	28:T:-45:DA:OP1	2.17	0.47
9:8:62:GLU:OE2	9:8:157:GLY:N	2.48	0.47
35:a:44:THR:HG22	35:a:44:THR:O	2.14	0.47
38:d:460:ILE:HD11	38:d:529:MET:HE1	1.97	0.47
40:f:150:ALA:HB3	40:f:176:PHE:CE1	2.50	0.47
50:p:190:LEU:HD13	50:p:192:VAL:HG23	1.97	0.47
1:0:45:GLY:O	1:0:48:LYS:NZ	2.44	0.47
1:0:52:LEU:HD21	1:0:232:VAL:HG11	1.96	0.47
2:1:422:LEU:HD13	5:4:225:GLN:NE2	2.30	0.47
4:3:132:VAL:O	4:3:136:ASN:ND2	2.48	0.47
6:5:38:ILE:HD12	6:5:38:ILE:H	1.80	0.47
7:6:89:GLU:OE2	7:6:132:LYS:NZ	2.42	0.47
10:9:11:TRP:CZ3	10:9:89:ARG:HB3	2.50	0.47
10:9:101:PRO:O	10:9:105:MET:HB2	2.15	0.47
11:A:1477:ALA:HB1	17:G:22:LEU:CD1	2.23	0.47
12:B:1036:LYS:H	13:C:186:TYR:HH	1.61	0.47
14:D:79:THR:HA	36:b:51:LEU:HD22	1.96	0.47
17:G:104:MET:HE1	17:G:106:CYS:HB2	1.96	0.47
23:M:128:ILE:HG23	23:M:183:VAL:CG1	2.44	0.47
36:b:105:VAL:HB	36:b:106:PRO:HD3	1.96	0.47
40:f:85:LEU:C	40:f:85:LEU:HD12	2.40	0.47
46:l:444:GLU:CG	46:l:561:PRO:HG3	2.45	0.47
46:l:444:GLU:CB	46:l:445:PRO:CD	2.93	0.47
1:0:563:ARG:NH2	7:6:142:GLU:OE1	2.48	0.47
3:2:407:VAL:N	3:2:443:VAL:O	2.47	0.47
7:6:357:VAL:CG1	7:6:366:VAL:HG23	2.45	0.47
7:6:382:CYS:HB3	7:6:385:CYS:HB3	1.97	0.47
12:B:596:ILE:O	12:B:596:ILE:HG22	2.15	0.47
40:f:112:THR:HG23	40:f:112:THR:O	2.15	0.47
5:4:123:ASP:OD1	5:4:124:ILE:N	2.45	0.47
17:G:90:THR:OG1	17:G:91:GLN:OE1	2.11	0.47
19:I:69:ILE:O	19:I:72:VAL:HG22	2.15	0.47
38:d:303:LEU:CD2	38:d:307:ILE:HD11	2.45	0.47
38:d:443:ARG:NE	38:d:518:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:503:ARG:HA	38:d:513:THR:O	2.14	0.47
39:e:39:LEU:HD13	39:e:143:ILE:HG21	1.95	0.47
41:g:117:ILE:CD1	53:s:173:LEU:HD13	2.44	0.47
46:l:222:VAL:HG12	46:l:223:LYS:N	2.30	0.47
51:q:99:ARG:O	51:q:103:SER:N	2.40	0.47
4:3:307:GLN:CD	4:3:307:GLN:N	2.72	0.47
9:8:61:ARG:HH11	9:8:158:LEU:HA	1.79	0.47
11:A:609:HIS:ND1	11:A:626:THR:HG23	2.30	0.47
11:A:913:ASN:OD1	11:A:963:ARG:NH1	2.48	0.47
11:A:1468:THR:HG21	12:B:1101:GLN:HG3	1.97	0.47
12:B:354:SER:OG	12:B:357:CYS:SG	2.59	0.47
12:B:910:THR:HG23	22:L:42:ARG:O	2.15	0.47
14:D:83:VAL:O	14:D:87:LEU:HD23	2.15	0.47
35:a:50:VAL:HG13	35:a:55:LEU:HB2	1.96	0.47
38:d:582:VAL:HB	38:d:591:LYS:HG2	1.97	0.47
46:l:57:PHE:CD2	47:m:130:LEU:HB3	2.49	0.47
2:1:456:ASP:OD1	2:1:456:ASP:N	2.47	0.46
5:4:42:MET:SD	5:4:108:ASN:ND2	2.86	0.46
10:9:171:LEU:O	10:9:175:LYS:HG3	2.15	0.46
11:A:542:LEU:O	11:A:545:VAL:HG12	2.14	0.46
46:l:465:LEU:HD12	46:l:465:LEU:O	2.15	0.46
3:2:337:ARG:O	8:7:62:ARG:NH1	2.48	0.46
7:6:87:LEU:HD13	7:6:228:TYR:HD2	1.80	0.46
11:A:484:LEU:HD11	11:A:501:MET:SD	2.55	0.46
11:A:491:PRO:HG3	11:A:535:MET:HE2	1.96	0.46
11:A:1485:GLU:CD	17:G:20:PRO:CG	2.87	0.46
37:c:34:GLU:OE1	37:c:44:LEU:HD21	2.15	0.46
38:d:437:HIS:CD2	38:d:497:ILE:HG22	2.50	0.46
38:d:549:LEU:CG	38:d:572:ALA:HB2	2.44	0.46
43:i:95:ILE:HG13	43:i:108:LYS:NZ	2.30	0.46
46:l:128:LEU:O	46:l:132:THR:N	2.42	0.46
46:l:581:SER:HB2	46:l:582:PRO:CD	2.44	0.46
47:m:134:PRO:N	47:m:135:PRO:CD	2.79	0.46
5:4:192:ASP:OD1	5:4:213:LEU:N	2.45	0.46
7:6:112:LYS:N	7:6:142:GLU:O	2.41	0.46
10:9:146:TYR:HD1	10:9:149:LEU:HD23	1.79	0.46
11:A:875:TYR:OH	16:F:61:GLU:OE2	2.26	0.46
30:V:64:THR:HG22	30:V:65:TYR:N	2.31	0.46
36:b:46:LEU:C	36:b:46:LEU:HD23	2.40	0.46
36:b:172:THR:OG1	39:e:31:SER:CB	2.63	0.46
9:8:104:ASP:O	9:8:209:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:167:ARG:HG2	9:8:167:ARG:NH2	2.30	0.46
10:9:106:LEU:HB3	10:9:143:ILE:HD11	1.96	0.46
36:b:171:GLN:O	36:b:172:THR:CG2	2.56	0.46
2:1:457:ILE:HG22	2:1:461:LEU:HD13	1.98	0.46
18:H:91:VAL:HG22	18:H:144:LEU:HD22	1.98	0.46
31:W:22:ILE:HG12	31:W:34:LEU:HD22	1.97	0.46
50:p:293:PRO:HB2	50:p:294:PRO:HD2	1.98	0.46
11:A:458:PHE:HE2	11:A:484:LEU:HD11	1.80	0.46
12:B:128:ILE:CG2	12:B:431:LEU:HD21	2.46	0.46
29:U:321:SER:OG	29:U:322:ASP:N	2.48	0.46
31:W:20:TYR:HD2	31:W:190:LEU:HD11	1.77	0.46
31:W:137:THR:HG22	31:W:139:LEU:H	1.80	0.46
36:b:22:LEU:HD23	38:d:109:MET:HE3	1.98	0.46
37:c:90:CYS:SG	41:g:105:LEU:HD11	2.56	0.46
12:B:553:LEU:HD23	12:B:556:ILE:HD11	1.98	0.46
17:G:154:LYS:HZ1	31:W:143:GLN:HB3	1.74	0.46
19:I:39:CYS:SG	19:I:42:CYS:HB3	2.56	0.46
19:I:58:ILE:H	19:I:58:ILE:HD12	1.81	0.46
32:X:145:VAL:HG11	32:X:171:ILE:HG23	1.98	0.46
43:i:89:PHE:CZ	43:i:112:LEU:HD11	2.51	0.46
46:l:81:ARG:NH1	47:m:151:GLY:O	2.48	0.46
1:0:28:LEU:O	1:0:32:LEU:HD23	2.16	0.46
1:0:137:LEU:O	1:0:142:VAL:HG11	2.15	0.46
4:3:37:LEU:O	4:3:40:VAL:HG12	2.16	0.46
4:3:264:GLU:HG2	4:3:265:MET:N	2.31	0.46
11:A:15:LEU:HD22	17:G:63:ARG:HD2	1.97	0.46
12:B:724:TYR:HB3	12:B:728:MET:HE3	1.97	0.46
32:X:139:PHE:HZ	32:X:144:ASN:OD1	1.99	0.46
49:o:28:LEU:HD23	49:o:28:LEU:O	2.16	0.46
9:8:134:LEU:HD22	9:8:162:PHE:HB3	1.98	0.46
11:A:1200:PRO:HG2	11:A:1204:VAL:HG22	1.96	0.46
24:N:-1:DG:C4	24:N:0:DC:C5	3.04	0.46
26:Q:163:GLU:O	26:Q:166:ARG:N	2.49	0.46
31:W:105:TYR:CZ	32:X:237:LEU:HG	2.51	0.46
38:d:253:GLY:O	38:d:301:VAL:HG21	2.16	0.46
40:f:28:LEU:HD21	40:f:33:ALA:HB3	1.97	0.46
46:l:57:PHE:CE2	47:m:130:LEU:HD22	2.51	0.46
46:l:240:ASP:HB3	46:l:253:LEU:HD23	1.96	0.46
46:l:560:LYS:N	46:l:561:PRO:CD	2.78	0.46
9:8:177:TRP:CD1	9:8:215:GLY:H	2.34	0.46
10:9:218:LEU:HD11	10:9:232:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:207:VAL:HG11	12:B:375:ALA:CB	2.45	0.46
12:B:830:GLU:OE2	12:B:870:THR:OG1	2.21	0.46
14:D:70:ARG:NH2	17:G:88:VAL:HG22	2.31	0.46
21:K:105:PHE:CD2	21:K:109:ILE:HD11	2.51	0.46
27:R:31:TRP:HD1	27:R:62:LEU:HD21	1.81	0.46
38:d:513:THR:O	38:d:514:LEU:HD13	2.16	0.46
38:d:517:GLN:NE2	46:l:447:GLY:O	2.49	0.46
41:g:130:LEU:O	41:g:130:LEU:HD23	2.15	0.46
46:l:343:GLN:HG3	46:l:354:VAL:HG13	1.97	0.46
1:0:107:LEU:HD12	1:0:195:ALA:HB1	1.99	0.45
3:2:334:MET:HB3	8:7:58:ALA:HB2	1.98	0.45
5:4:44:LEU:HD21	5:4:162:LEU:CD1	2.45	0.45
6:5:49:LEU:HD12	6:5:52:VAL:HG11	1.96	0.45
8:7:294:GLU:OE2	8:7:334:ARG:NH1	2.49	0.45
10:9:256:ARG:O	10:9:260:LYS:HG3	2.17	0.45
11:A:1341:VAL:HG23	11:A:1341:VAL:O	2.17	0.45
12:B:993:LYS:NZ	12:B:995:GLU:OE1	2.44	0.45
13:C:72:PRO:HD3	20:J:13:ILE:HD11	1.97	0.45
17:G:117:MET:HE3	17:G:137:ILE:HD13	1.98	0.45
36:b:154:ILE:HG21	41:g:34:THR:CG2	2.46	0.45
11:A:502:ASN:HB3	12:B:1084:LEU:HD13	1.99	0.45
31:W:144:LEU:HD13	31:W:154:CYS:HA	1.97	0.45
38:d:341:LEU:CD2	38:d:343:ILE:HD11	2.45	0.45
38:d:549:LEU:HG	38:d:572:ALA:HB2	1.97	0.45
41:g:32:ASN:ND2	41:g:67:ASN:OD1	2.49	0.45
44:j:123:GLU:OE2	44:j:126:ARG:NH1	2.50	0.45
1:0:613:HIS:O	1:0:613:HIS:ND1	2.49	0.45
7:6:242:SER:N	7:6:245:SER:OG	2.50	0.45
9:8:13:GLU:OE1	9:8:32:LYS:NZ	2.49	0.45
10:9:255:MET:O	10:9:259:VAL:HG23	2.15	0.45
11:A:24:GLY:O	12:B:1168:ALA:HB3	2.16	0.45
11:A:1261:ILE:HG22	11:A:1262:MET:N	2.31	0.45
12:B:851:ASP:CG	22:L:15:MET:HE2	2.42	0.45
17:G:153:ASP:OD1	17:G:154:LYS:N	2.49	0.45
27:R:194:HIS:ND1	27:R:196:TYR:O	2.49	0.45
29:U:22:ILE:HG22	29:U:39:LEU:HD11	1.99	0.45
31:W:48:MET:HE1	31:W:92:TYR:HB2	1.97	0.45
32:X:213:ASP:OD1	32:X:214:GLU:N	2.50	0.45
44:j:72:ILE:HG21	44:j:97:MET:HB3	1.98	0.45
1:0:77:VAL:HA	1:0:80:ILE:HG22	1.97	0.45
1:0:109:LEU:HD12	1:0:207:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:128:SER:OG	8:7:163:TYR:OH	2.17	0.45
8:7:656:ASN:OD1	8:7:657:ALA:N	2.49	0.45
11:A:869:GLU:OE2	12:B:1091:ARG:NH1	2.47	0.45
17:G:110:ARG:HA	17:G:113:ILE:HD12	1.97	0.45
26:Q:127:PHE:CE2	27:R:21:VAL:HG21	2.51	0.45
27:R:30:GLN:O	27:R:62:LEU:HD11	2.16	0.45
39:e:32:LEU:HD21	39:e:36:ILE:CG1	2.47	0.45
39:e:112:GLU:O	39:e:113:ASN:OD1	2.34	0.45
42:h:107:ILE:HD11	48:n:125:ILE:HG21	1.98	0.45
46:l:57:PHE:CE2	47:m:130:LEU:HB3	2.50	0.45
5:4:13:ILE:HG21	5:4:41:VAL:HG13	1.97	0.45
11:A:910:LYS:N	11:A:911:PRO:HD2	2.32	0.45
12:B:710:ILE:HA	12:B:764:MET:HE2	1.99	0.45
24:N:30:DT:H2''	24:N:31:DC:C6	2.52	0.45
36:b:32:LYS:O	36:b:40:LEU:HD11	2.16	0.45
46:l:375:ASP:N	46:l:375:ASP:OD1	2.48	0.45
46:l:557:VAL:HB	46:l:558:PRO:HD3	1.98	0.45
9:8:34:THR:O	9:8:34:THR:HG22	2.17	0.45
10:9:96:VAL:HG13	10:9:101:PRO:HG3	1.98	0.45
11:A:68:THR:HG23	11:A:68:THR:O	2.16	0.45
11:A:495:ASP:C	11:A:495:ASP:OD1	2.60	0.45
11:A:1034:GLN:HE22	11:A:1038:THR:HG21	1.82	0.45
38:d:627:TRP:HD1	38:d:638:LYS:HD2	1.81	0.45
1:0:361:LEU:O	1:0:365:VAL:HG12	2.16	0.45
5:4:201:GLY:O	5:4:204:GLN:HG2	2.17	0.45
8:7:185:ILE:HG22	8:7:189:LEU:HD13	1.98	0.45
9:8:11:ARG:HH11	9:8:33:ASN:HD22	1.64	0.45
10:9:102:ARG:HG3	10:9:103:ILE:HD12	1.99	0.45
11:A:1203:ASP:OD2	11:A:1244:ASN:ND2	2.44	0.45
28:T:-33:DG:H2'	28:T:-32:DT:H72	1.98	0.45
31:W:105:TYR:CE1	32:X:237:LEU:HG	2.52	0.45
50:p:246:ALA:HA	50:p:269:TRP:CH2	2.52	0.45
1:0:329:PHE:O	1:0:333:LEU:HD23	2.17	0.45
13:C:245:VAL:HG11	21:K:105:PHE:CZ	2.52	0.45
38:d:447:THR:OG1	38:d:518:GLU:OE2	2.35	0.45
40:f:85:LEU:HD12	40:f:85:LEU:O	2.17	0.45
41:g:130:LEU:HD23	41:g:130:LEU:C	2.42	0.45
46:l:60:HIS:NE2	47:m:140:SER:O	2.46	0.45
46:l:169:LEU:N	46:l:170:PRO:CD	2.80	0.45
50:p:294:PRO:HB2	50:p:297:ARG:HH12	1.82	0.45
3:2:444:THR:HG23	3:2:447:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:136:ASN:OD1	4:3:137:LYS:N	2.50	0.45
7:6:199:ILE:CG2	7:6:222:ILE:HD11	2.47	0.45
12:B:694:THR:HG22	12:B:695:HIS:ND1	2.31	0.45
32:X:220:TRP:CD1	32:X:220:TRP:C	2.94	0.45
38:d:373:HIS:ND1	53:s:172:MET:HE3	2.32	0.45
38:d:493:LEU:HD13	38:d:504:VAL:HG21	1.97	0.45
41:g:123:ILE:HG23	53:s:162:LEU:HD12	1.98	0.45
42:h:178:PRO:O	42:h:179:THR:HG22	2.16	0.45
8:7:173:ASN:N	8:7:434:GLU:OE2	2.49	0.45
9:8:189:MET:HE2	9:8:189:MET:HB2	1.76	0.45
31:W:17:LEU:O	31:W:21:VAL:HG22	2.16	0.45
38:d:331:ILE:HG22	38:d:343:ILE:O	2.16	0.45
46:l:443:LEU:HD11	46:l:504:ARG:HH21	1.82	0.45
53:s:176:ARG:O	53:s:177:ASN:C	2.60	0.45
10:9:163:PRO:HA	10:9:166:PRO:HG2	1.99	0.44
11:A:400:ASP:OD1	11:A:401:ARG:N	2.49	0.44
17:G:145:LEU:HD23	17:G:145:LEU:H	1.82	0.44
21:K:37:LYS:N	21:K:69:HIS:O	2.49	0.44
24:N:26:DG:H2'	24:N:27:DT:H72	2.00	0.44
38:d:327:VAL:O	38:d:328:LYS:C	2.60	0.44
38:d:582:VAL:CG1	38:d:591:LYS:HE3	2.47	0.44
42:h:92:GLU:OE1	44:j:122:ARG:NH2	2.50	0.44
42:h:182:GLU:HG2	49:o:27:CYS:SG	2.57	0.44
3:2:157:GLU:O	3:2:161:HIS:ND1	2.51	0.44
5:4:31:GLN:OE1	5:4:36:LYS:NZ	2.42	0.44
16:F:64:ARG:NH2	17:G:61:PRO:HG3	2.32	0.44
23:M:245:VAL:HG23	23:M:245:VAL:O	2.17	0.44
27:R:220:ILE:HG13	27:R:221:GLY:H	1.82	0.44
35:a:101:ILE:HG23	35:a:101:ILE:O	2.15	0.44
12:B:752:TYR:CE1	12:B:809:VAL:HG23	2.52	0.44
14:D:17:ALA:HB1	14:D:95:PHE:CE2	2.52	0.44
14:D:91:LYS:C	14:D:92:LEU:HD22	2.42	0.44
22:L:32:ASP:OD1	22:L:32:ASP:N	2.50	0.44
32:X:73:TYR:O	32:X:74:LYS:HG2	2.18	0.44
37:c:103:LYS:NZ	53:s:161:GLN:O	2.50	0.44
38:d:336:PHE:HD2	38:d:339:LEU:HD22	1.82	0.44
40:f:45:THR:HG23	40:f:64:TYR:CE1	2.53	0.44
41:g:75:LEU:O	41:g:79:VAL:HG12	2.16	0.44
42:h:107:ILE:HA	42:h:110:LEU:HD12	1.98	0.44
45:k:99:ILE:HA	45:k:102:MET:HE2	2.00	0.44
50:p:190:LEU:CD1	50:p:192:VAL:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:460:THR:HB	1:0:661:ALA:HB1	1.98	0.44
11:A:1477:ALA:HA	17:G:22:LEU:HD11	1.99	0.44
12:B:809:VAL:HG11	12:B:811:TYR:CZ	2.52	0.44
39:e:54:HIS:NE2	39:e:56:MET:SD	2.90	0.44
39:e:170:GLU:C	39:e:171:LEU:HD22	2.42	0.44
40:f:196:LEU:HD23	40:f:196:LEU:C	2.41	0.44
1:0:600:ALA:HB1	1:0:659:HIS:HD2	1.82	0.44
2:1:400:ILE:H	2:1:400:ILE:HD12	1.82	0.44
7:6:369:VAL:HG13	7:6:370:ASP:N	2.32	0.44
26:Q:151:ARG:HG2	26:Q:151:ARG:O	2.18	0.44
36:b:154:ILE:HD13	41:g:34:THR:HG22	2.00	0.44
43:i:109:LEU:HD11	46:l:136:LEU:HB2	1.98	0.44
50:p:186:THR:HG23	50:p:186:THR:O	2.16	0.44
8:7:133:THR:HB	8:7:160:THR:HG21	2.00	0.44
11:A:273:GLN:HB3	11:A:277:THR:HG21	2.00	0.44
12:B:738:THR:HG21	20:J:58:LYS:CG	2.48	0.44
12:B:761:THR:H	12:B:764:MET:HE3	1.82	0.44
13:C:190:ASN:ND2	13:C:195:THR:O	2.39	0.44
19:I:104:ALA:O	19:I:105:GLU:HG2	2.18	0.44
31:W:180:PHE:HA	32:X:216:PHE:CE1	2.52	0.44
37:c:66:GLN:O	37:c:70:LEU:HD23	2.18	0.44
38:d:396:ALA:HB2	39:e:51:PHE:CD2	2.53	0.44
46:l:105:TRP:HZ2	46:l:112:VAL:HG21	1.83	0.44
50:p:297:ARG:HD3	50:p:303:GLU:O	2.18	0.44
2:1:472:LEU:HD12	2:1:476:TRP:CD1	2.52	0.44
9:8:165:PRO:C	9:8:167:ARG:N	2.76	0.44
10:9:266:ARG:HB2	10:9:269:GLU:HB3	1.98	0.44
11:A:340:LYS:HE2	11:A:1436:VAL:HG11	1.98	0.44
36:b:181:LEU:HD21	39:e:148:ILE:HD11	1.99	0.44
36:b:182:VAL:HG22	39:e:168:LEU:HD11	2.00	0.44
37:c:75:THR:O	37:c:75:THR:HG22	2.17	0.44
38:d:92:LEU:CD2	38:d:93:TRP:H	2.31	0.44
39:e:68:PHE:CZ	40:f:98:LEU:HD13	2.53	0.44
46:l:168:ARG:HG3	49:o:74:HIS:HB2	1.99	0.44
46:l:216:THR:O	46:l:223:LYS:N	2.51	0.44
8:7:133:THR:HG23	8:7:134:SER:N	2.32	0.44
11:A:622:SER:OG	11:A:626:THR:HG22	2.17	0.44
11:A:1366:PHE:HB2	11:A:1374:VAL:HG21	1.99	0.44
15:E:94:MET:HE1	15:E:127:LEU:HD11	2.00	0.44
24:N:23:DT:H2'	24:N:24:DT:H72	2.00	0.44
31:W:26:TYR:CD1	32:X:220:TRP:CZ2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:106:LYS:HE2	32:X:220:TRP:CZ2	2.53	0.44
37:c:24:ILE:HD11	37:c:55:SER:OG	2.17	0.44
38:d:417:GLU:CD	38:d:418:ILE:N	2.76	0.44
39:e:32:LEU:HD21	39:e:36:ILE:HG13	1.98	0.44
3:2:288:ILE:HD12	3:2:288:ILE:H	1.83	0.44
5:4:257:CYS:SG	5:4:276:CYS:HB2	2.58	0.44
6:5:24:ASP:OD1	6:5:24:ASP:C	2.61	0.44
10:9:11:TRP:HE1	10:9:157:HIS:HD2	1.66	0.44
10:9:235:SER:O	10:9:236:LEU:HD12	2.18	0.44
11:A:1213:ARG:NH2	11:A:1215:GLU:OE2	2.51	0.44
36:b:46:LEU:HD11	41:g:66:ALA:HB1	1.99	0.44
39:e:108:ILE:HG22	40:f:90:ASN:CB	2.48	0.44
41:g:119:LEU:C	41:g:119:LEU:HD23	2.43	0.44
42:h:159:ASN:OD1	42:h:160:ALA:N	2.51	0.44
1:0:285:TYR:O	1:0:289:VAL:HG23	2.17	0.43
1:0:434:HIS:CB	1:0:632:ILE:HD11	2.47	0.43
1:0:475:PRO:HG3	1:0:478:MET:HE2	1.99	0.43
7:6:87:LEU:O	7:6:87:LEU:HD23	2.18	0.43
9:8:224:ARG:HA	9:8:227:GLU:HG2	2.00	0.43
10:9:7:GLN:HG3	10:9:89:ARG:HH21	1.81	0.43
24:N:43:DC:C2	24:N:44:DA:C8	3.06	0.43
35:a:114:VAL:O	35:a:118:ARG:HG2	2.18	0.43
38:d:552:SER:O	38:d:567:SER:OG	2.32	0.43
40:f:119:TYR:O	40:f:120:CYS:C	2.60	0.43
42:h:122:ALA:O	42:h:125:VAL:HG13	2.18	0.43
46:l:139:LEU:O	46:l:143:ALA:HB3	2.17	0.43
50:p:281:CYS:HA	50:p:304:ALA:HB3	1.99	0.43
3:2:325:ILE:H	3:2:325:ILE:HD12	1.82	0.43
11:A:72:GLN:OE1	11:A:72:GLN:N	2.50	0.43
11:A:105:LYS:HD2	11:A:141:LEU:HD22	1.99	0.43
11:A:428:ASP:OD2	11:A:430:ARG:NH1	2.51	0.43
12:B:379:ARG:O	12:B:608:ARG:NH2	2.51	0.43
16:F:71:LEU:HD21	17:G:62:GLY:O	2.18	0.43
23:M:25:GLU:OE1	23:M:46:ILE:HD12	2.18	0.43
37:c:31:VAL:HG22	37:c:48:GLN:HB3	2.00	0.43
41:g:134:TYR:CG	53:s:159:MET:HE1	2.53	0.43
44:j:69:VAL:HG22	44:j:100:LEU:HD13	2.00	0.43
50:p:288:LEU:HD22	50:p:306:HIS:CG	2.53	0.43
51:q:115:VAL:HG22	53:s:141:ILE:HD11	1.99	0.43
4:3:249:GLN:HA	4:3:250:PRO:HD3	1.84	0.43
10:9:218:LEU:HB2	10:9:252:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:786:ALA:O	11:A:787:VAL:HG23	2.18	0.43
12:B:719:SER:OG	12:B:720:PRO:HD3	2.18	0.43
15:E:13:ILE:HD12	15:E:13:ILE:H	1.84	0.43
29:U:332:GLU:OE1	29:U:332:GLU:N	2.49	0.43
31:W:157:CYS:O	31:W:158:HIS:HB2	2.19	0.43
36:b:181:LEU:HD22	39:e:168:LEU:CD1	2.48	0.43
38:d:327:VAL:CG1	38:d:328:LYS:H	2.30	0.43
3:2:52:ALA:HB1	3:2:90:LEU:HD21	1.99	0.43
8:7:99:PHE:CZ	8:7:103:ILE:HD13	2.53	0.43
32:X:122:GLU:O	32:X:125:VAL:HG22	2.18	0.43
37:c:18:GLU:O	37:c:21:ILE:HG22	2.18	0.43
45:k:66:GLU:OE1	45:k:80:TYR:OH	2.19	0.43
45:k:76:ASN:ND2	47:m:102:LYS:O	2.51	0.43
46:l:136:LEU:O	46:l:140:ALA:N	2.36	0.43
46:l:357:VAL:HG23	46:l:374:HIS:CE1	2.53	0.43
8:7:184:VAL:HG13	8:7:185:ILE:N	2.33	0.43
9:8:79:ASP:HB3	9:8:90:VAL:HB	2.00	0.43
10:9:185:GLU:O	10:9:188:ARG:HB3	2.18	0.43
11:A:1382:LEU:O	11:A:1385:VAL:HG22	2.18	0.43
14:D:17:ALA:HB1	14:D:95:PHE:HE2	1.83	0.43
15:E:159:LEU:HD12	15:E:163:TYR:CD2	2.53	0.43
24:N:35:DC:H2'	24:N:36:DT:H72	1.99	0.43
28:T:-5:DT:H72	28:T:-4:DT:C7	2.49	0.43
31:W:22:ILE:CD1	31:W:26:TYR:CD2	3.01	0.43
32:X:133:ILE:O	32:X:134:ASP:OD1	2.35	0.43
37:c:11:LEU:HD23	37:c:11:LEU:C	2.43	0.43
38:d:106:LEU:C	38:d:106:LEU:HD23	2.43	0.43
38:d:194:TRP:CE2	38:d:295:LEU:HD23	2.53	0.43
39:e:50:THR:OG1	39:e:134:HIS:NE2	2.50	0.43
46:l:581:SER:HB2	46:l:582:PRO:HD2	1.99	0.43
50:p:210:ASP:N	50:p:210:ASP:OD1	2.51	0.43
50:p:250:LEU:HD23	50:p:250:LEU:C	2.44	0.43
50:p:294:PRO:HA	50:p:306:HIS:CD2	2.54	0.43
1:0:462:SER:OG	1:0:463:PRO:CD	2.66	0.43
4:3:305:PHE:N	4:3:305:PHE:CD1	2.85	0.43
8:7:128:SER:O	8:7:334:ARG:NH2	2.51	0.43
8:7:408:SER:HB3	8:7:413:LEU:HD11	2.01	0.43
9:8:174:VAL:CG1	9:8:179:ARG:HG3	2.48	0.43
10:9:268:GLU:OE1	10:9:268:GLU:N	2.52	0.43
11:A:706:ILE:O	11:A:710:LYS:HG2	2.19	0.43
12:B:752:TYR:O	20:J:1:MET:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:366:ILE:HD11	30:V:48:LEU:HG	2.00	0.43
31:W:52:LEU:CD1	31:W:59:LEU:HD13	2.49	0.43
38:d:247:ILE:HD11	38:d:252:GLU:HA	2.00	0.43
43:i:81:LEU:HD13	43:i:118:HIS:HB2	2.01	0.43
7:6:291:CYS:SG	7:6:294:CYS:N	2.82	0.43
9:8:94:MET:SD	9:8:146:ASP:HB3	2.58	0.43
32:X:132:VAL:HG22	32:X:137:TYR:CD1	2.53	0.43
36:b:29:PHE:HD2	38:d:102:LEU:HD21	1.84	0.43
38:d:338:SER:C	38:d:339:LEU:HD12	2.44	0.43
39:e:108:ILE:HD12	40:f:91:PHE:HD1	1.84	0.43
1:0:338:GLU:HG2	4:3:68:VAL:HG11	2.00	0.43
4:3:26:CYS:SG	4:3:28:HIS:HB2	2.59	0.43
8:7:532:LEU:O	8:7:532:LEU:HD23	2.19	0.43
9:8:83:HIS:ND1	9:8:84:LYS:N	2.66	0.43
9:8:231:THR:HG23	9:8:252:PHE:H	1.83	0.43
10:9:70:VAL:O	10:9:70:VAL:HG12	2.19	0.43
11:A:495:ASP:OD1	11:A:497:ASP:OD1	2.36	0.43
12:B:854:ILE:O	12:B:907:VAL:HG21	2.18	0.43
12:B:871:VAL:O	12:B:871:VAL:HG13	2.18	0.43
13:C:185:GLU:OE2	13:C:206:SER:OG	2.36	0.43
31:W:26:TYR:HD1	32:X:220:TRP:CZ2	2.37	0.43
31:W:113:ARG:NH1	32:X:219:LEU:HA	2.33	0.43
38:d:194:TRP:CD2	38:d:295:LEU:HD23	2.53	0.43
43:i:127:ARG:NE	46:l:152:PHE:CE1	2.86	0.43
46:l:435:LEU:HB2	46:l:436:PRO:HD2	2.00	0.43
46:l:490:ILE:HB	46:l:491:PRO:HD3	2.01	0.43
46:l:509:ILE:HG22	46:l:509:ILE:O	2.19	0.43
53:s:163:ARG:O	53:s:166:ILE:HG22	2.18	0.43
1:0:345:ARG:NH2	4:3:64:GLU:OE1	2.52	0.43
4:3:55:LYS:CD	17:G:165:ASP:HA	2.41	0.43
4:3:246:TYR:CD1	9:8:119:LEU:HD21	2.54	0.43
8:7:193:VAL:HG11	8:7:283:ARG:CD	2.49	0.43
10:9:7:GLN:HE21	10:9:85:MET:HE2	1.83	0.43
14:D:107:THR:HG23	14:D:110:GLU:H	1.83	0.43
15:E:106:VAL:HG12	15:E:107:GLN:N	2.34	0.43
26:Q:47:LEU:HD11	26:Q:98:TRP:HB3	2.01	0.43
26:Q:153:ARG:O	26:Q:177:MET:HE1	2.19	0.43
27:R:48:THR:OG1	27:R:51:ARG:O	2.33	0.43
35:a:114:VAL:HA	36:b:111:THR:HB	2.01	0.43
38:d:592:ILE:HG21	38:d:622:PHE:CD2	2.54	0.43
45:k:48:LEU:HD12	46:l:59:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:558:PRO:HG2	46:l:561:PRO:CG	2.48	0.43
49:o:47:ALA:O	49:o:51:TYR:N	2.47	0.43
50:p:200:VAL:HG11	50:p:270:LEU:HD21	2.01	0.43
1:0:249:VAL:HG21	1:0:403:PHE:HB2	2.01	0.43
2:1:303:ILE:HG22	2:1:307:PHE:CE2	2.54	0.43
4:3:97:ASP:O	4:3:101:GLU:OE1	2.36	0.43
4:3:116:ASP:OD1	4:3:117:ASN:N	2.51	0.43
9:8:64:LYS:HG3	10:9:159:ILE:HD11	2.01	0.43
10:9:195:LEU:O	10:9:198:ILE:HG22	2.18	0.43
15:E:71:GLN:HB2	15:E:99:ILE:HD12	2.00	0.43
15:E:134:GLU:OE1	15:E:181:ARG:NH2	2.50	0.43
35:a:123:VAL:O	35:a:127:GLN:N	2.43	0.43
38:d:642:LEU:HD23	38:d:642:LEU:C	2.44	0.43
43:i:132:ARG:O	43:i:135:LEU:HB2	2.18	0.43
46:l:392:ILE:O	46:l:392:ILE:HG12	2.19	0.43
47:m:128:ARG:NH1	47:m:129:SER:OG	2.51	0.43
1:0:111:SER:N	1:0:211:TYR:OH	2.52	0.42
1:0:354:PRO:HB2	1:0:355:PRO:HD3	2.00	0.42
3:2:380:THR:O	3:2:380:THR:HG23	2.19	0.42
8:7:193:VAL:HG11	8:7:283:ARG:HD3	2.01	0.42
10:9:181:LEU:HD21	10:9:187:LEU:CD1	2.49	0.42
11:A:575:PRO:HG3	11:A:594:LEU:HD11	2.01	0.42
11:A:1281:ASP:O	11:A:1285:LEU:HD13	2.19	0.42
12:B:218:THR:HG23	12:B:218:THR:O	2.18	0.42
12:B:565:THR:HG21	12:B:580:PRO:HG3	2.01	0.42
12:B:1128:ALA:HB1	12:B:1135:TYR:HD1	1.84	0.42
38:d:339:LEU:HD11	38:d:439:PHE:HD2	1.82	0.42
46:l:178:ILE:HB	46:l:179:PRO:HD3	2.00	0.42
48:n:36:ASN:O	48:n:37:ASN:OD1	2.36	0.42
49:o:28:LEU:HD21	49:o:76:LEU:N	2.34	0.42
50:p:288:LEU:HD23	50:p:292:LEU:HD21	2.01	0.42
1:0:168:VAL:HG13	1:0:168:VAL:O	2.18	0.42
3:2:70:ALA:HB1	3:2:74:TRP:CZ2	2.54	0.42
6:5:21:LEU:O	6:5:24:ASP:OD1	2.38	0.42
9:8:239:ASP:O	9:8:239:ASP:CG	2.62	0.42
10:9:218:LEU:HD23	10:9:218:LEU:HA	1.81	0.42
11:A:511:THR:HG21	12:B:1105:GLU:OE1	2.19	0.42
11:A:872:MET:O	11:A:879:VAL:HA	2.18	0.42
12:B:239:MET:HB2	12:B:372:LEU:HD21	2.01	0.42
17:G:154:LYS:CD	31:W:143:GLN:OE1	2.66	0.42
26:Q:50:ASP:OD1	26:Q:53:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:94:THR:HG22	27:R:109:ILE:HG22	2.00	0.42
38:d:339:LEU:HD21	38:d:439:PHE:CB	2.49	0.42
40:f:106:LYS:HG3	40:f:107:ALA:N	2.33	0.42
1:0:67:VAL:HG23	1:0:67:VAL:O	2.19	0.42
10:9:218:LEU:CD2	10:9:228:MET:HE2	2.49	0.42
12:B:544:PHE:CE1	12:B:590:LEU:HD11	2.54	0.42
12:B:1107:LEU:O	12:B:1111:SER:OG	2.30	0.42
23:M:195:PHE:CZ	23:M:199:LEU:HD11	2.55	0.42
29:U:18:ILE:HD11	29:U:46:TRP:CH2	2.54	0.42
38:d:569:ILE:HG23	38:d:582:VAL:HG22	2.00	0.42
1:0:56:ILE:HG21	1:0:70:LEU:HD22	2.01	0.42
12:B:1162:LEU:HB3	12:B:1167:ILE:HB	2.00	0.42
26:Q:15:VAL:HG12	26:Q:16:VAL:N	2.34	0.42
36:b:114:ASP:HB3	36:b:115:PRO:HD2	2.00	0.42
39:e:135:LEU:HA	39:e:144:MET:HA	2.02	0.42
43:i:120:HIS:HA	43:i:123:ILE:HG12	2.00	0.42
50:p:199:LYS:HD3	50:p:221:VAL:HG21	2.01	0.42
1:0:49:THR:HG23	1:0:50:VAL:N	2.34	0.42
1:0:323:ILE:O	1:0:378:ARG:NH1	2.53	0.42
1:0:332:PHE:CZ	1:0:367:ILE:HG23	2.53	0.42
2:1:422:LEU:HD21	5:4:224:LEU:HB3	2.02	0.42
2:1:496:ASN:HB3	2:1:536:LEU:HD11	2.01	0.42
8:7:532:LEU:CD2	8:7:716:VAL:HG13	2.49	0.42
9:8:101:ILE:HD12	9:8:145:LEU:HD21	2.02	0.42
10:9:195:LEU:HA	10:9:195:LEU:HD12	1.86	0.42
11:A:544:ALA:CB	11:A:680:LEU:HD13	2.50	0.42
11:A:847:LEU:HD21	12:B:720:PRO:HB3	2.02	0.42
32:X:168:LEU:HD22	32:X:199:LYS:HB2	2.01	0.42
37:c:111:CYS:N	53:s:158:ILE:HD11	2.35	0.42
38:d:493:LEU:HD12	38:d:493:LEU:O	2.19	0.42
38:d:641:LEU:HA	38:d:644:SER:OG	2.19	0.42
40:f:33:ALA:HB2	40:f:119:TYR:HB2	2.02	0.42
42:h:180:ASP:OD1	42:h:181:LEU:N	2.51	0.42
49:o:34:LEU:CD1	49:o:75:MET:HE2	2.49	0.42
2:1:374:LEU:HD12	2:1:374:LEU:C	2.45	0.42
3:2:58:ARG:HD2	5:4:229:TRP:CZ3	2.55	0.42
3:2:359:ILE:HG22	3:2:360:THR:N	2.35	0.42
9:8:231:THR:HG21	9:8:250:LYS:O	2.20	0.42
10:9:71:PHE:CG	10:9:75:MET:HE3	2.54	0.42
12:B:399:LEU:HB3	12:B:453:TRP:CZ2	2.55	0.42
12:B:446:TYR:CE1	12:B:450:THR:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:154:LYS:NZ	31:W:143:GLN:HG3	2.33	0.42
38:d:251:LEU:HD12	38:d:251:LEU:N	2.35	0.42
38:d:637:TYR:CZ	38:d:641:LEU:HD11	2.55	0.42
40:f:117:TYR:O	40:f:124:VAL:O	2.37	0.42
50:p:288:LEU:HD11	50:p:308:THR:OG1	2.20	0.42
51:q:106:LYS:CG	51:q:107:PRO:HD3	2.50	0.42
3:2:121:ALA:C	5:4:100:LYS:HZ2	2.28	0.42
5:4:217:VAL:HG23	5:4:217:VAL:O	2.20	0.42
10:9:72:LYS:HA	10:9:72:LYS:HD3	1.83	0.42
11:A:1357:THR:O	15:E:142:HIS:NE2	2.46	0.42
12:B:994:GLY:O	20:J:31:GLU:HB2	2.19	0.42
16:F:71:LEU:CD2	17:G:62:GLY:O	2.67	0.42
27:R:31:TRP:CD1	27:R:62:LEU:HD21	2.55	0.42
32:X:99:LEU:HD12	32:X:124:LEU:HD11	2.01	0.42
32:X:148:LYS:CD	32:X:184:ALA:HB3	2.49	0.42
38:d:555:VAL:HB	46:l:646:ALA:HB3	2.01	0.42
42:h:178:PRO:C	42:h:179:THR:HG22	2.45	0.42
43:i:78:LEU:HD21	48:n:69:ILE:CG2	2.49	0.42
46:l:552:VAL:HG12	46:l:566:TYR:CD1	2.55	0.42
1:0:661:ALA:HA	1:0:664:VAL:HG12	2.02	0.42
3:2:261:PHE:CZ	3:2:265:LEU:HD21	2.54	0.42
8:7:297:PHE:O	8:7:359:LYS:NZ	2.38	0.42
11:A:1430:CYS:O	11:A:1435:THR:OG1	2.38	0.42
12:B:778:SER:HG	12:B:805:PHE:HZ	1.66	0.42
30:V:11:LEU:HD23	30:V:44:ILE:HD12	2.02	0.42
40:f:122:PHE:O	40:f:143:GLU:O	2.37	0.42
46:l:253:LEU:HB2	46:l:282:LEU:HD11	2.02	0.42
50:p:190:LEU:C	50:p:190:LEU:HD12	2.45	0.42
1:0:573:ASP:OD1	1:0:573:ASP:N	2.53	0.42
3:2:51:LEU:HD23	5:4:237:GLN:CD	2.45	0.42
9:8:267:ASP:OD1	9:8:268:LEU:N	2.52	0.42
11:A:668:PHE:CZ	11:A:672:ILE:HD11	2.54	0.42
14:D:64:THR:HG22	17:G:103:PRO:HD3	2.01	0.42
26:Q:44:GLN:HE21	26:Q:44:GLN:HB3	1.74	0.42
32:X:103:LEU:HD22	32:X:108:HIS:CB	2.49	0.42
38:d:184:ASN:O	38:d:184:ASN:ND2	2.52	0.42
39:e:68:PHE:CD1	40:f:98:LEU:HD13	2.55	0.42
39:e:69:VAL:HG13	39:e:69:VAL:O	2.19	0.42
41:g:134:TYR:CD2	53:s:159:MET:HE1	2.54	0.42
42:h:80:MET:HE3	44:j:69:VAL:HG11	2.02	0.42
46:l:400:LEU:HD23	46:l:400:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:524:HIS:NE2	2:1:528:MET:SD	2.93	0.42
5:4:258:HIS:HB2	5:4:260:ASN:OD1	2.20	0.42
8:7:535:THR:HG23	8:7:627:SER:HB2	2.02	0.42
9:8:30:ARG:HE	9:8:35:ASN:HB2	1.85	0.42
9:8:100:VAL:HG23	9:8:310:PRO:HG3	2.01	0.42
9:8:164:SER:HA	9:8:165:PRO:HD3	1.55	0.42
10:9:13:PHE:HD1	10:9:18:GLN:NE2	2.18	0.42
10:9:198:ILE:HD11	10:9:255:MET:HG2	2.02	0.42
11:A:672:ILE:HG23	11:A:676:ILE:HD13	2.02	0.42
11:A:1203:ASP:OD1	11:A:1203:ASP:N	2.51	0.42
27:R:58:LEU:CD1	27:R:62:LEU:HD23	2.49	0.42
31:W:105:TYR:N	31:W:105:TYR:CD1	2.87	0.42
31:W:113:ARG:HH12	32:X:219:LEU:HA	1.84	0.42
36:b:181:LEU:HD21	39:e:148:ILE:HD13	2.00	0.42
40:f:142:VAL:O	40:f:142:VAL:HG12	2.19	0.42
43:i:73:ASP:OD1	43:i:74:HIS:N	2.52	0.42
46:l:444:GLU:CB	46:l:445:PRO:HD3	2.50	0.42
5:4:255:CYS:HB2	5:4:276:CYS:N	2.35	0.41
8:7:409:THR:O	8:7:413:LEU:HD13	2.19	0.41
8:7:559:ILE:HG22	8:7:561:PHE:CE1	2.55	0.41
9:8:182:GLU:HG2	9:8:183:LEU:N	2.33	0.41
12:B:718:GLN:CD	12:B:976:MET:HE3	2.45	0.41
38:d:303:LEU:HD23	38:d:307:ILE:HD11	2.02	0.41
41:g:130:LEU:CD2	53:s:155:LEU:HD11	2.43	0.41
46:l:229:GLU:HG3	46:l:230:PHE:H	1.83	0.41
1:0:143:ARG:NH1	1:0:159:GLU:OE1	2.48	0.41
9:8:164:SER:HB3	10:9:165:ARG:HH12	1.85	0.41
11:A:106:VAL:O	11:A:110:VAL:HG12	2.19	0.41
11:A:883:ILE:O	11:A:883:ILE:HG22	2.19	0.41
12:B:216:ALA:HB2	12:B:241:ALA:HA	2.03	0.41
24:N:41:DC:H2"	24:N:42:DG:H8	1.84	0.41
31:W:17:LEU:HD22	31:W:194:THR:OG1	2.21	0.41
32:X:88:ARG:O	32:X:91:ARG:HB2	2.19	0.41
32:X:145:VAL:HG21	32:X:151:LEU:HB2	2.01	0.41
36:b:181:LEU:HD22	39:e:168:LEU:HD13	2.02	0.41
46:l:162:THR:O	46:l:163:THR:OG1	2.32	0.41
46:l:470:LEU:O	46:l:471:ASP:C	2.62	0.41
1:0:109:LEU:HD11	1:0:199:ILE:HD11	2.01	0.41
1:0:176:ASN:OD1	1:0:177:LEU:N	2.49	0.41
5:4:175:MET:HE3	5:4:179:ASN:CG	2.46	0.41
8:7:688:LYS:NZ	31:W:280:TRP:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:154:CYS:SG	11:A:155:GLU:N	2.92	0.41
11:A:497:ASP:OD1	11:A:497:ASP:C	2.63	0.41
11:A:567:LEU:HB2	11:A:570:TRP:HB2	2.01	0.41
11:A:1437:ASP:O	11:A:1441:GLU:HG2	2.20	0.41
13:C:36:ARG:HD3	21:K:41:THR:OG1	2.20	0.41
19:I:41:ASN:C	19:I:41:ASN:OD1	2.63	0.41
32:X:103:LEU:HD22	32:X:108:HIS:HB3	2.02	0.41
40:f:46:TYR:O	40:f:62:LEU:HB2	2.21	0.41
40:f:161:LEU:O	40:f:165:LEU:HD23	2.20	0.41
46:l:443:LEU:HD11	46:l:504:ARG:NH2	2.35	0.41
50:p:178:ILE:HG12	50:p:192:VAL:HG22	2.02	0.41
50:p:293:PRO:CB	50:p:294:PRO:HD2	2.51	0.41
1:0:225:LEU:O	1:0:227:ARG:NH1	2.54	0.41
5:4:175:MET:HE3	5:4:179:ASN:ND2	2.35	0.41
10:9:30:PHE:CD2	10:9:97:MET:HE3	2.55	0.41
11:A:549:THR:O	11:A:549:THR:HG22	2.19	0.41
11:A:876:ASP:OD2	11:A:880:ARG:NH2	2.54	0.41
11:A:1022:ILE:N	11:A:1034:GLN:OE1	2.45	0.41
12:B:794:VAL:HG22	12:B:967:ILE:HG22	2.02	0.41
38:d:461:GLN:O	38:d:477:VAL:HA	2.20	0.41
38:d:504:VAL:HG12	38:d:514:LEU:CD1	2.40	0.41
42:h:107:ILE:HG23	48:n:122:LEU:HD22	2.02	0.41
46:l:83:ILE:HG13	47:m:159:LEU:HD11	2.01	0.41
46:l:401:LEU:O	46:l:405:VAL:HG12	2.20	0.41
50:p:293:PRO:O	50:p:294:PRO:C	2.63	0.41
1:0:354:PRO:HA	1:0:416:ILE:HD12	2.02	0.41
3:2:60:LEU:HD13	3:2:118:LEU:CD2	2.49	0.41
4:3:13:LYS:HD3	4:3:13:LYS:N	2.36	0.41
9:8:41:LYS:O	9:8:88:SER:HA	2.21	0.41
9:8:64:LYS:HD2	10:9:115:VAL:HG13	2.01	0.41
11:A:1166:LEU:HA	11:A:1298:LEU:HD11	2.02	0.41
11:A:1443:ALA:HB2	12:B:1167:ILE:HG23	2.01	0.41
12:B:529:MET:HE1	12:B:698:ILE:CD1	2.49	0.41
24:N:33:DC:H2'	24:N:34:DT:H71	2.01	0.41
27:R:57:THR:O	27:R:57:THR:HG23	2.21	0.41
38:d:259:VAL:CG1	38:d:371:LEU:HD23	2.51	0.41
38:d:261:ILE:HG23	38:d:261:ILE:O	2.20	0.41
50:p:288:LEU:HD21	50:p:308:THR:HG23	2.01	0.41
1:0:114:ASN:C	1:0:114:ASN:ND2	2.78	0.41
3:2:118:LEU:HD11	5:4:50:PHE:CZ	2.55	0.41
9:8:98:LEU:HD12	9:8:98:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:293:LYS:HA	9:8:293:LYS:HD2	1.89	0.41
11:A:486:LEU:HB3	11:A:538:VAL:HG21	2.03	0.41
11:A:560:VAL:HG21	11:A:586:TRP:HB2	2.02	0.41
12:B:435:ILE:O	23:M:127:ARG:NH1	2.51	0.41
46:l:297:HIS:O	46:l:301:LEU:HD23	2.20	0.41
46:l:538:LEU:O	46:l:552:VAL:HG22	2.21	0.41
1:0:557:ILE:HG22	1:0:561:ILE:HD12	2.01	0.41
10:9:122:SER:N	10:9:123:PRO:HD2	2.36	0.41
14:D:76:ASN:O	14:D:79:THR:OG1	2.38	0.41
25:O:258:MET:N	25:O:315:ALA:O	2.54	0.41
31:W:28:ILE:HG13	31:W:29:GLU:N	2.36	0.41
36:b:112:LYS:HB3	36:b:113:PRO:HD2	2.03	0.41
38:d:462:ALA:HA	38:d:476:LYS:O	2.20	0.41
39:e:87:TYR:C	39:e:88:LEU:HD22	2.46	0.41
39:e:145:VAL:HG12	39:e:167:TYR:HD2	1.86	0.41
44:j:95:GLN:OE1	44:j:98:ARG:NH1	2.54	0.41
45:k:128:ARG:O	45:k:132:HIS:ND1	2.53	0.41
49:o:49:VAL:HA	49:o:52:LEU:HD12	2.03	0.41
50:p:292:LEU:HD23	50:p:292:LEU:H	1.84	0.41
53:s:163:ARG:O	53:s:167:TRP:CD1	2.74	0.41
1:0:373:ARG:O	1:0:405:THR:OG1	2.24	0.41
3:2:146:PRO:HA	3:2:149:ASP:OD2	2.21	0.41
4:3:11:THR:HG23	4:3:12:THR:N	2.35	0.41
9:8:118:MET:HE1	9:8:199:VAL:CG1	2.51	0.41
11:A:219:GLU:OE1	32:X:227:SER:HA	2.20	0.41
11:A:478:PRO:HD2	21:K:67:LEU:HD13	2.03	0.41
12:B:764:MET:HE1	12:B:938:ARG:HH11	1.85	0.41
12:B:771:GLU:O	20:J:55:LEU:HD21	2.21	0.41
14:D:60:VAL:HG22	17:G:103:PRO:HG3	2.02	0.41
38:d:415:LYS:HB2	40:f:70:GLU:HA	2.02	0.41
38:d:443:ARG:NH2	38:d:518:GLU:OE1	2.50	0.41
42:h:176:PRO:O	42:h:177:TYR:CD1	2.74	0.41
48:n:36:ASN:O	48:n:37:ASN:C	2.64	0.41
1:0:72:TYR:HE1	1:0:83:VAL:HG21	1.86	0.41
3:2:58:ARG:CD	5:4:229:TRP:CE3	3.04	0.41
3:2:273:GLN:OE1	3:2:277:LYS:NZ	2.46	0.41
4:3:32:GLU:OE1	4:3:32:GLU:N	2.47	0.41
5:4:42:MET:HE3	5:4:108:ASN:HA	2.02	0.41
7:6:115:GLU:OE1	7:6:115:GLU:N	2.54	0.41
7:6:379:LEU:HD23	7:6:379:LEU:O	2.21	0.41
8:7:364:LEU:HD23	8:7:410:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:71:HIS:CD2	9:8:72:PRO:HD2	2.56	0.41
12:B:428:ASP:OD1	12:B:429:PHE:N	2.52	0.41
12:B:516:GLU:OE1	12:B:516:GLU:N	2.54	0.41
12:B:528:LEU:HD23	12:B:528:LEU:HA	1.95	0.41
12:B:623:ARG:NH2	12:B:697:GLU:OE2	2.45	0.41
15:E:17:ILE:HD11	15:E:135:LEU:HD21	2.03	0.41
16:F:69:ARG:NH2	16:F:78:PRO:O	2.53	0.41
23:M:296:ALA:N	23:M:297:PRO:HD2	2.36	0.41
27:R:192:GLU:OE2	32:X:76:GLY:N	2.53	0.41
27:R:224:ASN:ND2	27:R:234:GLU:OE2	2.53	0.41
28:T:-22:DC:H2''	28:T:-21:DG:C8	2.56	0.41
30:V:44:ILE:O	30:V:48:LEU:HD13	2.21	0.41
31:W:17:LEU:HD22	31:W:194:THR:CB	2.50	0.41
35:a:129:ALA:O	35:a:133:ALA:N	2.51	0.41
38:d:549:LEU:HD21	38:d:572:ALA:HB2	2.03	0.41
38:d:627:TRP:CD1	38:d:638:LYS:HB3	2.56	0.41
38:d:646:LEU:HD23	38:d:646:LEU:C	2.45	0.41
39:e:85:LEU:HD23	39:e:114:LEU:HD11	2.03	0.41
43:i:137:VAL:O	43:i:141:VAL:HG23	2.21	0.41
46:l:518:GLU:O	46:l:519:THR:C	2.63	0.41
1:0:383:LEU:HD21	1:0:388:ILE:HD11	2.02	0.41
3:2:55:TRP:HZ2	3:2:83:GLN:NE2	2.19	0.41
7:6:333:GLU:HG2	7:6:333:GLU:O	2.21	0.41
9:8:160:LYS:NZ	10:9:117:GLU:HG3	2.36	0.41
24:N:50:DG:H2'	24:N:51:DT:H72	2.03	0.41
36:b:22:LEU:O	36:b:26:LEU:HD13	2.21	0.41
46:l:67:MET:O	46:l:70:THR:OG1	2.38	0.41
50:p:245:HIS:ND1	50:p:295:THR:O	2.54	0.41
1:0:195:ALA:O	1:0:199:ILE:HG12	2.21	0.40
8:7:530:ARG:O	8:7:534:TYR:CD2	2.75	0.40
11:A:457:ILE:HD11	11:A:515:ILE:HG23	2.03	0.40
11:A:564:LEU:HD23	11:A:567:LEU:HD12	2.04	0.40
11:A:1338:THR:OG1	11:A:1340:GLY:O	2.36	0.40
11:A:1430:CYS:SG	11:A:1435:THR:HG23	2.61	0.40
11:A:1436:VAL:HG13	11:A:1437:ASP:N	2.36	0.40
12:B:647:GLU:O	12:B:648:TYR:CG	2.74	0.40
21:K:64:PRO:HG3	21:K:72:ILE:HD12	2.02	0.40
31:W:187:ILE:H	31:W:187:ILE:HD12	1.87	0.40
37:c:17:ILE:HG23	37:c:59:VAL:HG23	2.03	0.40
38:d:464:TRP:CH2	38:d:475:VAL:HG22	2.56	0.40
38:d:475:VAL:HG12	38:d:476:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:113:ASN:OD1	39:e:113:ASN:C	2.65	0.40
46:l:465:LEU:O	46:l:475:LEU:HD21	2.20	0.40
46:l:478:MET:CE	46:l:489:ILE:HD12	2.50	0.40
49:o:23:GLU:OE1	49:o:23:GLU:HA	2.21	0.40
1:0:12:PHE:CE2	1:0:14:TYR:HB2	2.56	0.40
1:0:56:ILE:HD12	1:0:230:VAL:HG11	2.02	0.40
3:2:145:VAL:HB	3:2:146:PRO:HD3	2.04	0.40
3:2:223:ALA:HA	3:2:226:ARG:HG2	2.02	0.40
5:4:272:LEU:CD2	7:6:318:LEU:HD12	2.51	0.40
11:A:544:ALA:HB2	11:A:680:LEU:HD13	2.03	0.40
11:A:1137:PRO:HB2	11:A:1341:VAL:HG13	2.03	0.40
12:B:104:ALA:HB1	23:M:220:SER:OG	2.21	0.40
14:D:87:LEU:HD11	14:D:100:LEU:CD1	2.47	0.40
17:G:153:ASP:OD2	31:W:143:GLN:HG3	2.21	0.40
25:O:203:ARG:NH1	28:T:-5:DT:OP1	2.54	0.40
36:b:26:LEU:O	36:b:29:PHE:N	2.53	0.40
38:d:184:ASN:C	38:d:184:ASN:ND2	2.78	0.40
38:d:457:ASP:HB2	38:d:458:PRO:CD	2.51	0.40
38:d:505:VAL:O	38:d:505:VAL:HG23	2.21	0.40
41:g:77:LYS:O	41:g:81:ASP:N	2.50	0.40
42:h:107:ILE:HD11	48:n:125:ILE:HD13	2.03	0.40
48:n:80:GLU:HG3	48:n:85:LEU:HD23	2.03	0.40
50:p:276:LEU:HD23	50:p:277:PHE:CD1	2.56	0.40
1:0:531:VAL:HG12	1:0:532:PRO:O	2.22	0.40
9:8:58:THR:HG23	9:8:157:GLY:CA	2.51	0.40
10:9:11:TRP:HE1	10:9:157:HIS:CD2	2.39	0.40
10:9:198:ILE:HD13	10:9:212:ILE:HG23	2.03	0.40
15:E:205:THR:HG22	15:E:206:TYR:N	2.36	0.40
27:R:123:ASN:OD1	27:R:123:ASN:N	2.54	0.40
31:W:21:VAL:HG23	31:W:22:ILE:N	2.36	0.40
32:X:229:ASP:C	32:X:233:ILE:HD12	2.47	0.40
38:d:327:VAL:CG1	38:d:328:LYS:N	2.83	0.40
40:f:8:GLN:OE1	40:f:200:ILE:HD11	2.21	0.40
1:0:576:GLU:OE2	2:1:308:ASN:ND2	2.49	0.40
3:2:96:TRP:HB3	3:2:110:LEU:HD23	2.03	0.40
5:4:287:THR:OG1	7:6:247:CYS:SG	2.78	0.40
7:6:186:ILE:HG12	7:6:211:LEU:HD12	2.03	0.40
8:7:66:PRO:O	8:7:146:THR:OG1	2.37	0.40
8:7:340:LEU:CD2	8:7:491:ALA:HB2	2.51	0.40
11:A:365:THR:OG1	11:A:366:VAL:N	2.55	0.40
14:D:39:MET:HA	14:D:39:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:188:PHE:CZ	32:X:83:ASN:OD1	2.74	0.40
31:W:137:THR:HG22	31:W:139:LEU:HD13	2.03	0.40
36:b:149:ASN:ND2	37:c:46:ASP:OD1	2.54	0.40
38:d:495:LEU:HD11	38:d:502:ILE:HG21	2.03	0.40
46:l:166:TYR:N	46:l:167:PRO:CD	2.85	0.40
1:0:570:GLU:OE1	1:0:577:THR:HG23	2.22	0.40
1:0:604:VAL:O	1:0:608:ILE:HG22	2.21	0.40
3:2:123:LEU:N	5:4:100:LYS:HZ1	2.19	0.40
4:3:63:PHE:HB2	4:3:69:ASP:OD1	2.22	0.40
4:3:108:ASN:OD1	4:3:112:ASN:HB3	2.22	0.40
7:6:227:HIS:CE1	7:6:231:LEU:HD11	2.57	0.40
8:7:77:TRP:O	8:7:84:ILE:HG23	2.22	0.40
9:8:61:ARG:HD2	9:8:157:GLY:O	2.21	0.40
9:8:125:LEU:HG	9:8:129:HIS:CE1	2.56	0.40
9:8:257:LEU:HD23	9:8:260:ILE:HD12	2.03	0.40
10:9:218:LEU:HD12	10:9:252:MET:CE	2.49	0.40
11:A:1420:ASN:O	11:A:1429:LYS:NZ	2.53	0.40
12:B:954:MET:HE3	12:B:963:PRO:O	2.22	0.40
32:X:213:ASP:HB3	32:X:216:PHE:CD2	2.56	0.40
36:b:46:LEU:CD1	41:g:66:ALA:HB1	2.52	0.40
38:d:469:ASP:OD2	50:p:231:TRP:NE1	2.46	0.40
40:f:145:GLY:O	40:f:146:PRO:C	2.65	0.40
41:g:91:PHE:N	41:g:92:PRO:HD2	2.37	0.40
46:l:359:ILE:HD11	46:l:370:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	710/760 (93%)	682 (96%)	28 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
3	2	380/462 (82%)	365 (96%)	15 (4%)	0	100	100
4	3	210/309 (68%)	195 (93%)	15 (7%)	0	100	100
5	4	259/308 (84%)	255 (98%)	4 (2%)	0	100	100
6	5	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
7	6	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
8	7	601/782 (77%)	576 (96%)	25 (4%)	0	100	100
9	8	294/346 (85%)	276 (94%)	16 (5%)	2 (1%)	18	55
10	9	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
11	A	1413/1970 (72%)	1374 (97%)	39 (3%)	0	100	100
12	B	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
13	C	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
14	D	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
15	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
17	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
18	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
19	I	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
22	L	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
23	M	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
25	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
26	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
27	R	218/249 (88%)	213 (98%)	5 (2%)	0	100	100
29	U	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
30	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
31	W	198/439 (45%)	197 (100%)	1 (0%)	0	100	100
32	X	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
35	a	141/246 (57%)	132 (94%)	9 (6%)	0	100	100
36	b	130/268 (48%)	115 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	c	107/117 (92%)	95 (89%)	12 (11%)	0	100	100
38	d	421/651 (65%)	384 (91%)	36 (9%)	1 (0%)	43	77
39	e	157/208 (76%)	149 (95%)	8 (5%)	0	100	100
40	f	180/212 (85%)	168 (93%)	12 (7%)	0	100	100
41	g	128/200 (64%)	122 (95%)	6 (5%)	0	100	100
42	h	132/270 (49%)	128 (97%)	4 (3%)	0	100	100
43	i	107/233 (46%)	105 (98%)	2 (2%)	0	100	100
44	j	70/146 (48%)	64 (91%)	6 (9%)	0	100	100
45	k	131/135 (97%)	129 (98%)	2 (2%)	0	100	100
46	l	477/1454 (33%)	453 (95%)	24 (5%)	0	100	100
47	m	82/244 (34%)	75 (92%)	7 (8%)	0	100	100
48	n	130/144 (90%)	122 (94%)	8 (6%)	0	100	100
49	o	89/131 (68%)	88 (99%)	1 (1%)	0	100	100
50	p	152/311 (49%)	139 (91%)	13 (9%)	0	100	100
51	q	67/178 (38%)	65 (97%)	2 (3%)	0	100	100
53	s	42/178 (24%)	41 (98%)	1 (2%)	0	100	100
All	All	11332/16853 (67%)	10884 (96%)	445 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	d	514	LEU
9	8	166	ASN
9	8	165	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	624/664 (94%)	624 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	342/399 (86%)	342 (100%)	0	100	100
4	3	195/283 (69%)	195 (100%)	0	100	100
5	4	234/272 (86%)	234 (100%)	0	100	100
6	5	59/64 (92%)	59 (100%)	0	100	100
7	6	311/352 (88%)	311 (100%)	0	100	100
8	7	536/688 (78%)	535 (100%)	1 (0%)	87	85
9	8	259/299 (87%)	259 (100%)	0	100	100
10	9	256/296 (86%)	256 (100%)	0	100	100
11	A	1254/1749 (72%)	1254 (100%)	0	100	100
12	B	994/1027 (97%)	994 (100%)	0	100	100
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/126 (94%)	118 (100%)	0	100	100
15	E	191/192 (100%)	191 (100%)	0	100	100
16	F	69/111 (62%)	69 (100%)	0	100	100
17	G	152/153 (99%)	152 (100%)	0	100	100
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	53 (100%)	0	100	100
21	K	104/106 (98%)	104 (100%)	0	100	100
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	121 (100%)	0	100	100
27	R	196/218 (90%)	196 (100%)	0	100	100
29	U	105/324 (32%)	105 (100%)	0	100	100
30	V	90/98 (92%)	90 (100%)	0	100	100
31	W	182/373 (49%)	182 (100%)	0	100	100
32	X	154/261 (59%)	154 (100%)	0	100	100
35	a	128/223 (57%)	128 (100%)	0	100	100
36	b	117/225 (52%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	c	92/98 (94%)	92 (100%)	0	100	100
38	d	395/577 (68%)	395 (100%)	0	100	100
39	e	150/183 (82%)	150 (100%)	0	100	100
40	f	161/178 (90%)	161 (100%)	0	100	100
41	g	122/173 (70%)	122 (100%)	0	100	100
42	h	123/230 (54%)	123 (100%)	0	100	100
43	i	109/216 (50%)	109 (100%)	0	100	100
44	j	70/133 (53%)	70 (100%)	0	100	100
45	k	122/124 (98%)	122 (100%)	0	100	100
46	l	454/1271 (36%)	454 (100%)	0	100	100
47	m	76/208 (36%)	76 (100%)	0	100	100
48	n	109/119 (92%)	109 (100%)	0	100	100
49	o	84/115 (73%)	84 (100%)	0	100	100
50	p	143/280 (51%)	143 (100%)	0	100	100
51	q	67/152 (44%)	67 (100%)	0	100	100
53	s	40/155 (26%)	40 (100%)	0	100	100
All	All	10278/14814 (69%)	10277 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	7	266	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	201	HIS
1	0	384	HIS
1	0	519	ASN
1	0	560	ASN
1	0	645	GLN
2	1	420	GLN
2	1	537	HIS
3	2	211	GLN
3	2	218	GLN

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Mol	Chain	Res	Type
3	2	390	GLN
4	3	45	ASN
5	4	9	ASN
7	6	227	HIS
7	6	293	GLN
7	6	317	HIS
7	6	349	GLN
8	7	281	GLN
8	7	498	ASN
8	7	598	HIS
9	8	73	ASN
9	8	129	HIS
9	8	306	GLN
10	9	3	HIS
10	9	142	GLN
11	A	267	GLN
11	A	731	ASN
11	A	905	ASN
11	A	1310	HIS
12	B	90	GLN
12	B	98	HIS
12	B	145	GLN
12	B	420	GLN
12	B	582	GLN
12	B	631	GLN
12	B	790	GLN
12	B	825	GLN
12	B	913	GLN
12	B	1101	GLN
13	C	18	ASN
13	C	66	HIS
13	C	260	GLN
13	C	265	HIS
14	D	38	HIS
15	E	92	GLN
17	G	28	GLN
19	I	98	GLN
21	K	55	GLN
21	K	69	HIS
23	M	116	ASN
25	O	229	GLN
25	O	278	GLN

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Mol	Chain	Res	Type
26	Q	53	ASN
27	R	64	ASN
27	R	152	ASN
30	V	35	GLN
30	V	45	ASN
30	V	70	ASN
30	V	77	ASN
32	X	188	GLN
32	X	217	GLN
35	a	116	ASN
35	a	124	HIS
35	a	140	HIS
36	b	137	GLN
38	d	402	HIS
38	d	437	HIS
43	i	130	GLN
43	i	154	GLN
45	k	59	HIS
46	l	275	HIS
46	l	309	HIS
46	l	411	GLN
48	n	46	GLN
48	n	97	ASN
49	o	32	ASN
49	o	35	ASN

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 20 ligands modelled in this entry, 19 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	$\# Z > 2$
59	SF4	0	1000	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
59	SF4	0	1000	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](#)

There are no chain breaks in this entry.

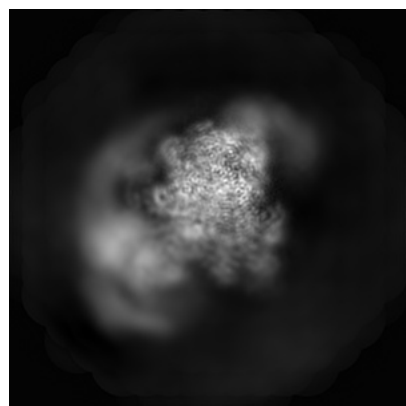
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12610. These allow visual inspection of the internal detail of the map and identification of artifacts.

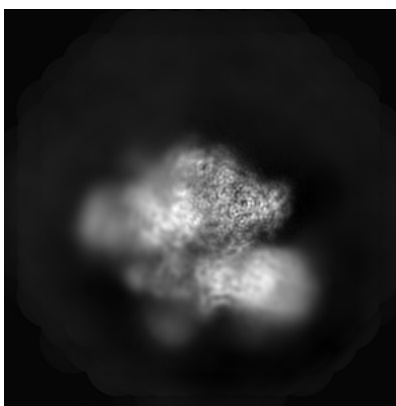
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

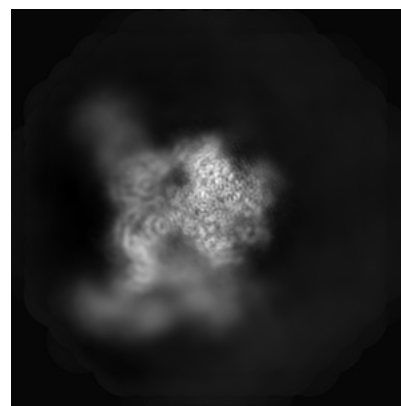
6.1.1 Primary map



X

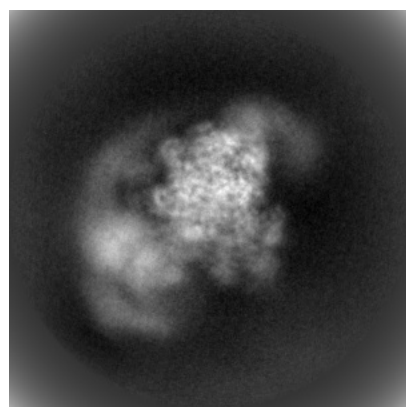


Y

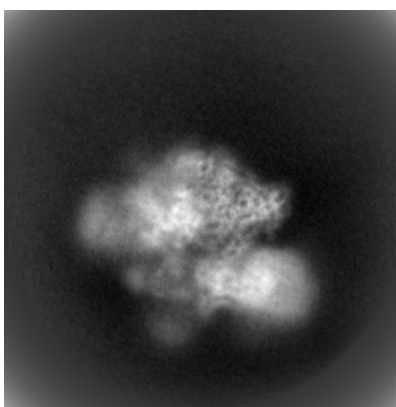


Z

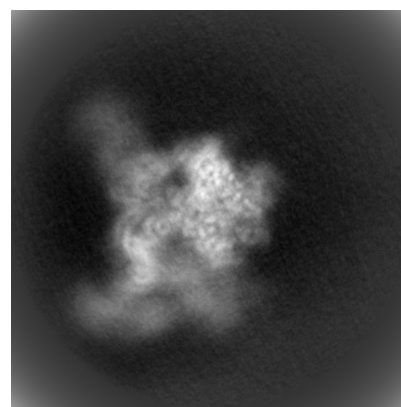
6.1.2 Raw map



X



Y

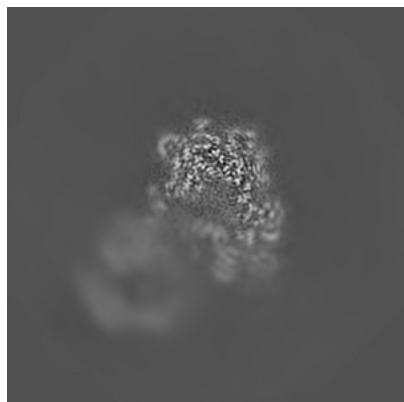


Z

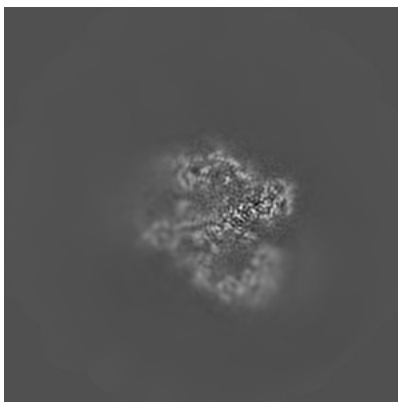
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

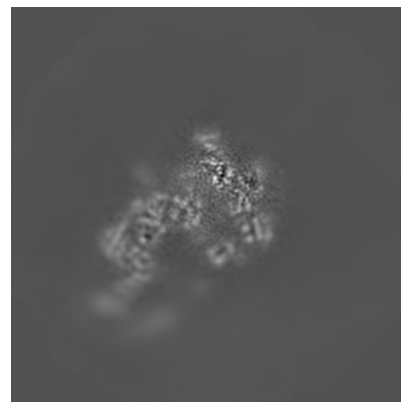
6.2.1 Primary map



X Index: 210

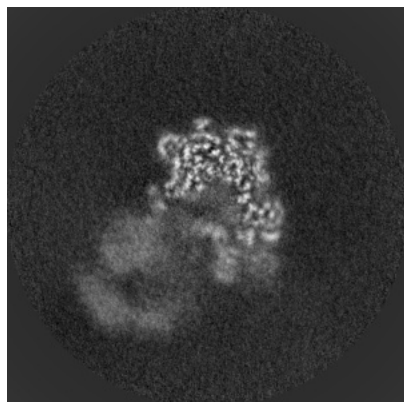


Y Index: 210

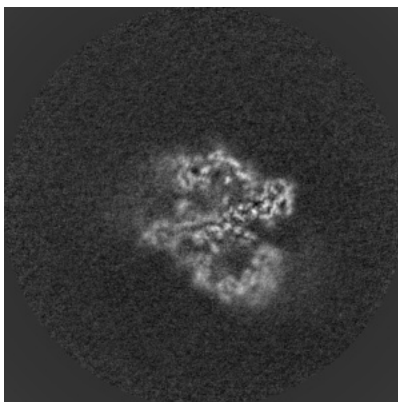


Z Index: 210

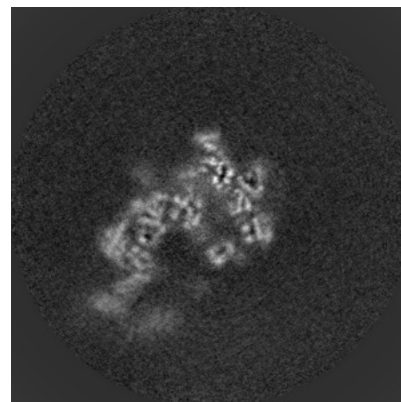
6.2.2 Raw map



X Index: 210



Y Index: 210

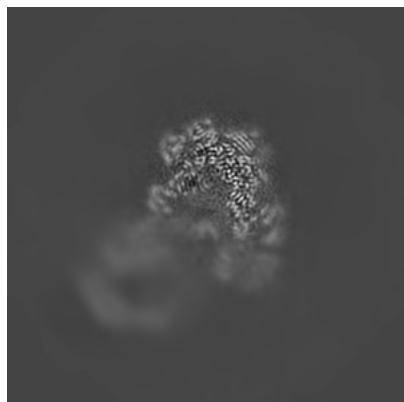


Z Index: 210

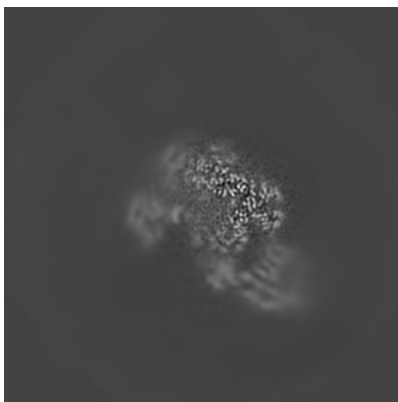
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

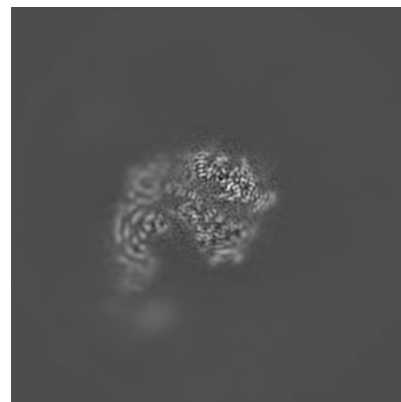
6.3.1 Primary map



X Index: 215

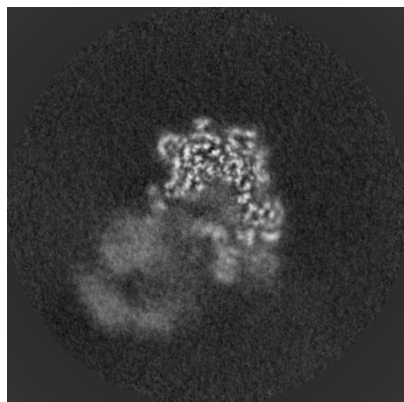


Y Index: 226

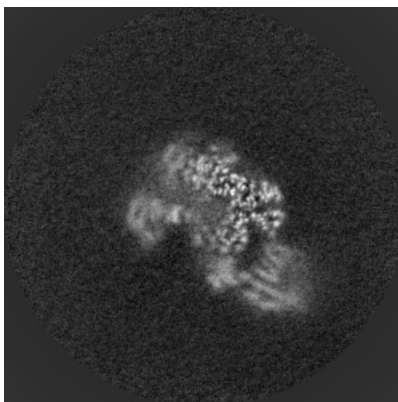


Z Index: 228

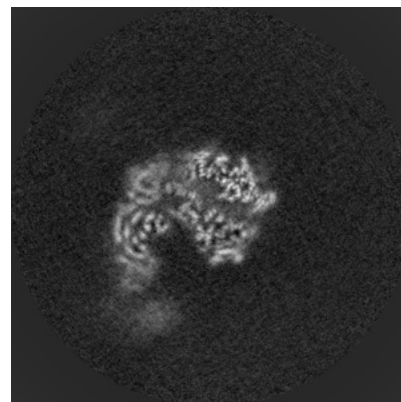
6.3.2 Raw map



X Index: 210



Y Index: 227

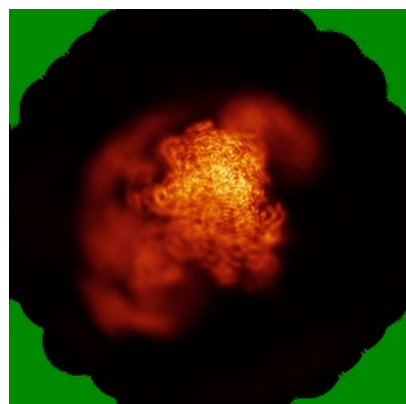


Z Index: 228

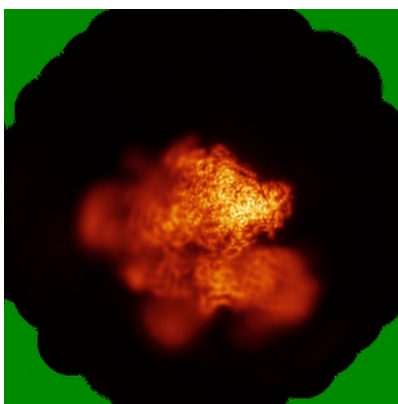
The images above show the largest variance slices of the map in three orthogonal directions.

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

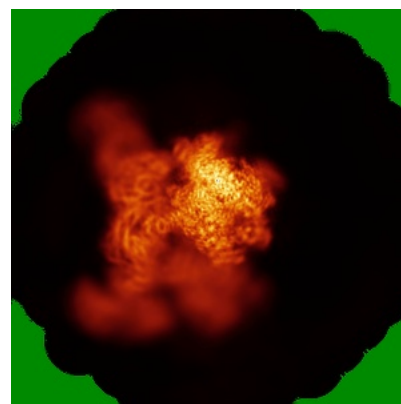
6.4.1 Primary map



X

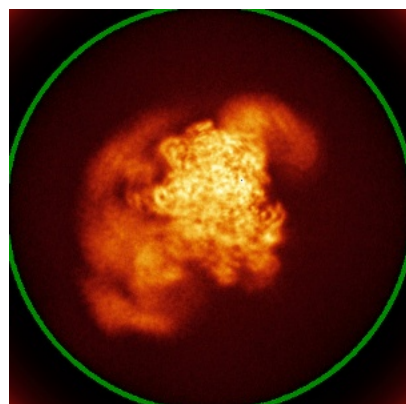


Y

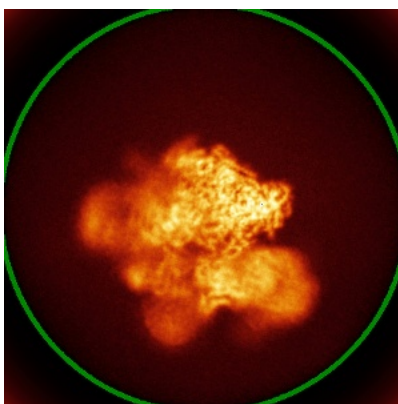


Z

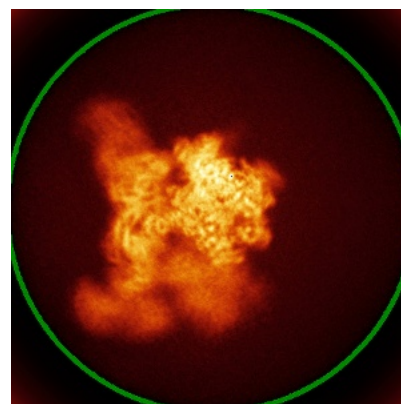
6.4.2 Raw map



X



Y

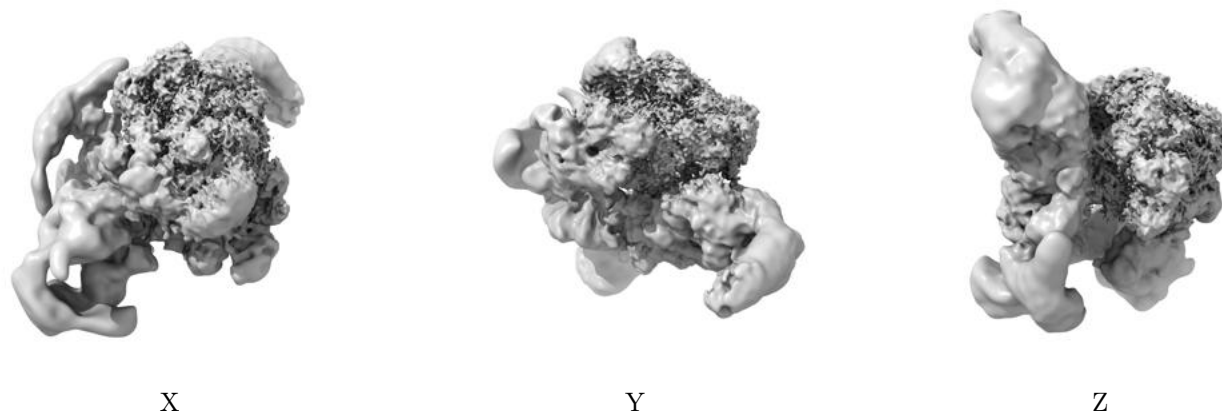


Z

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.

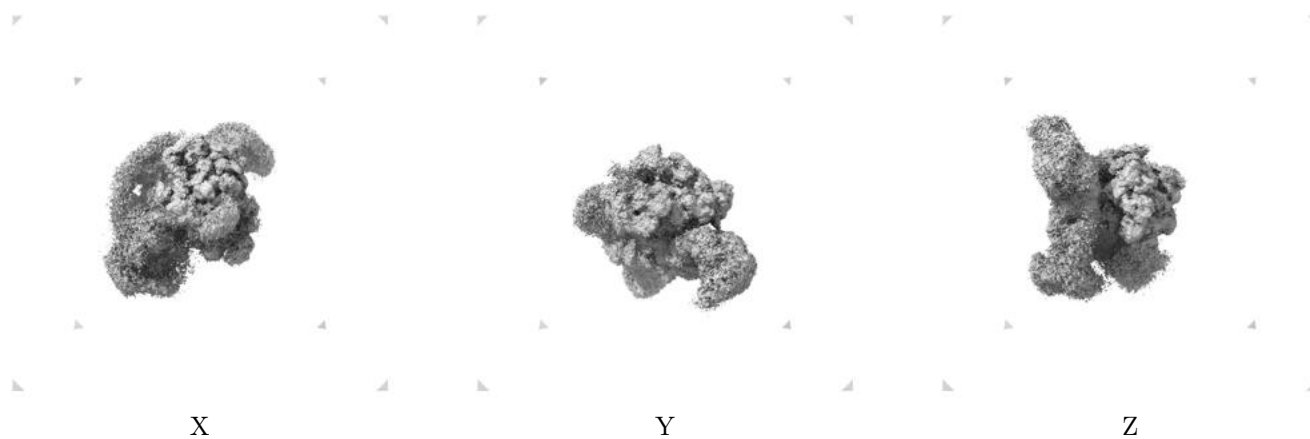
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

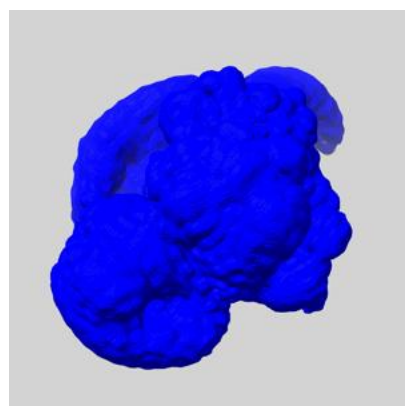
6.6 Mask visualisation [i](#)

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

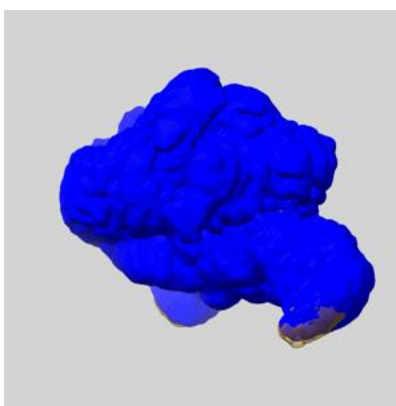
A mask typically either:

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

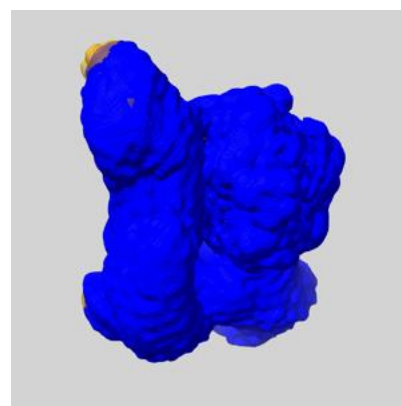
6.6.1 emd_12610_msk_1.map [i](#)



X



Y

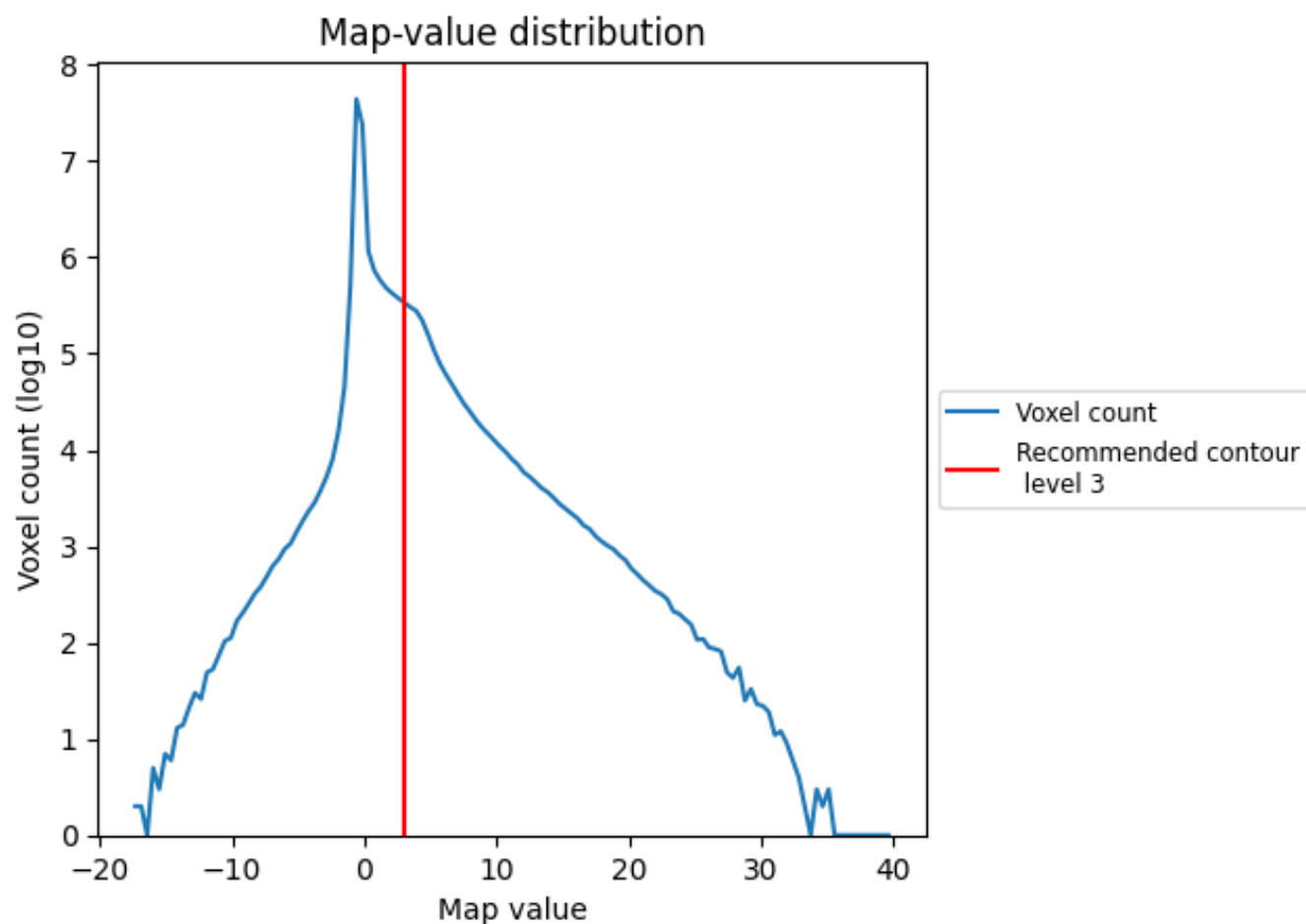


Z

7 Map analysis [i](#)

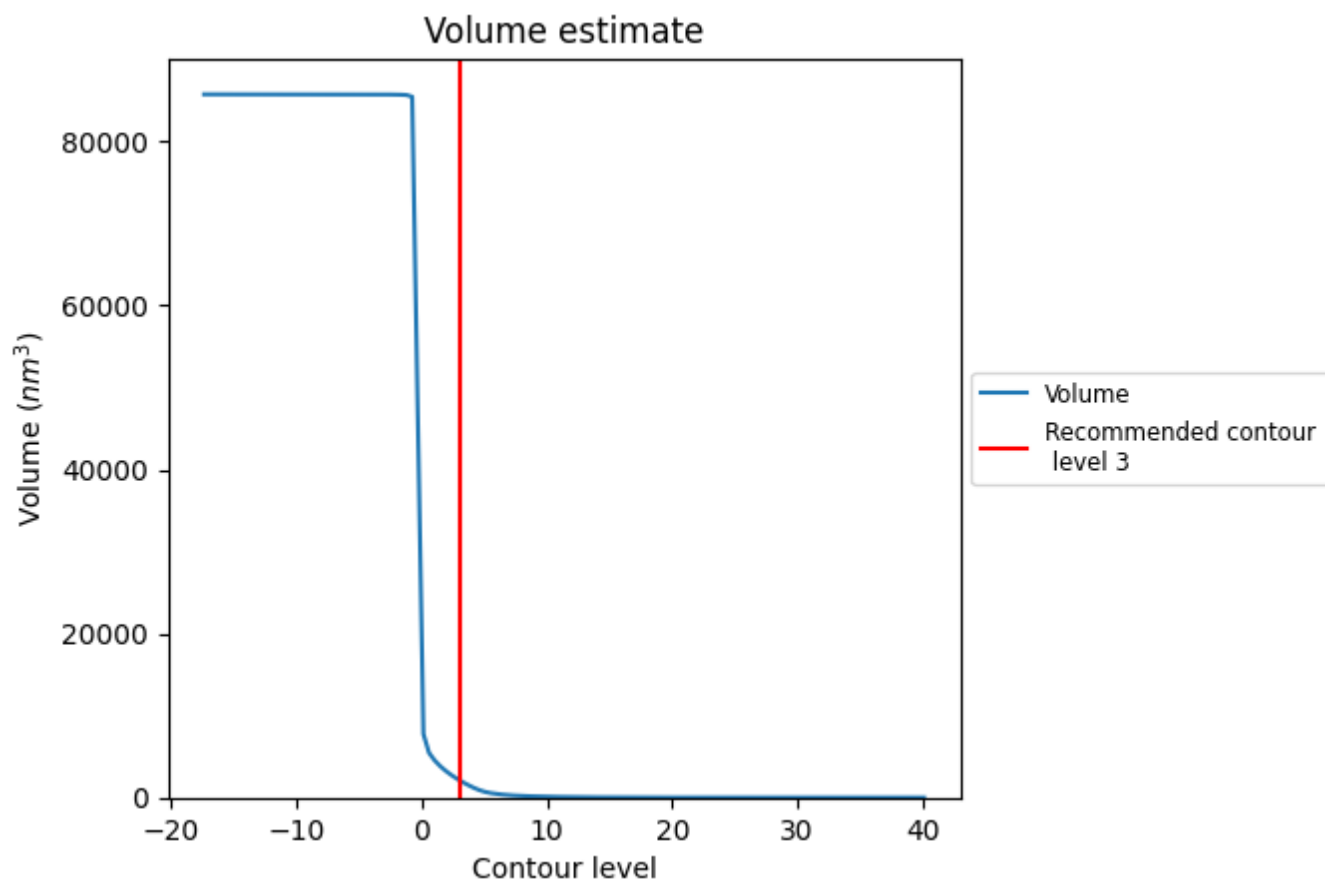
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

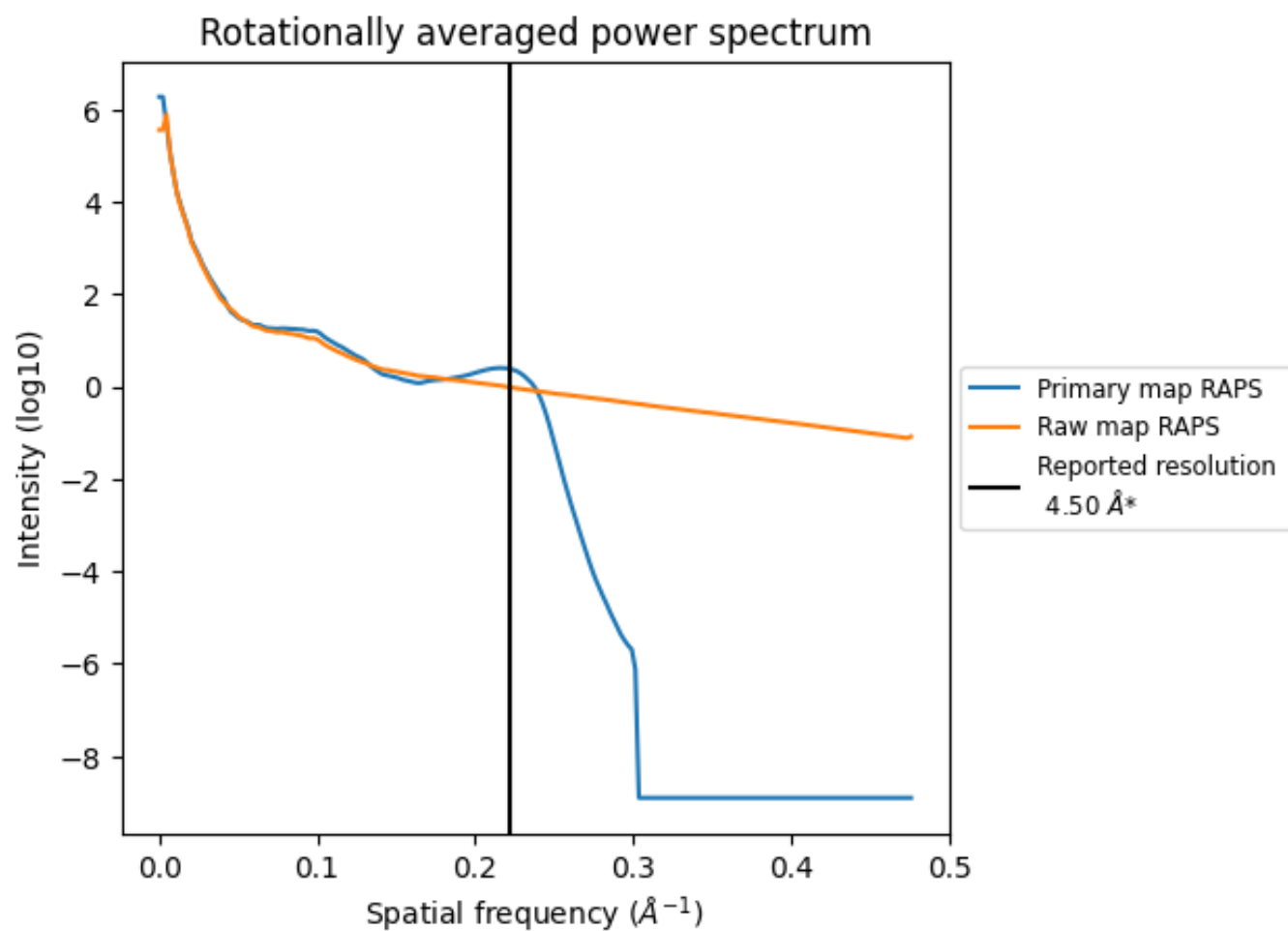
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2146 nm^3 ; this corresponds to an approximate mass of 1939 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 ⓘ

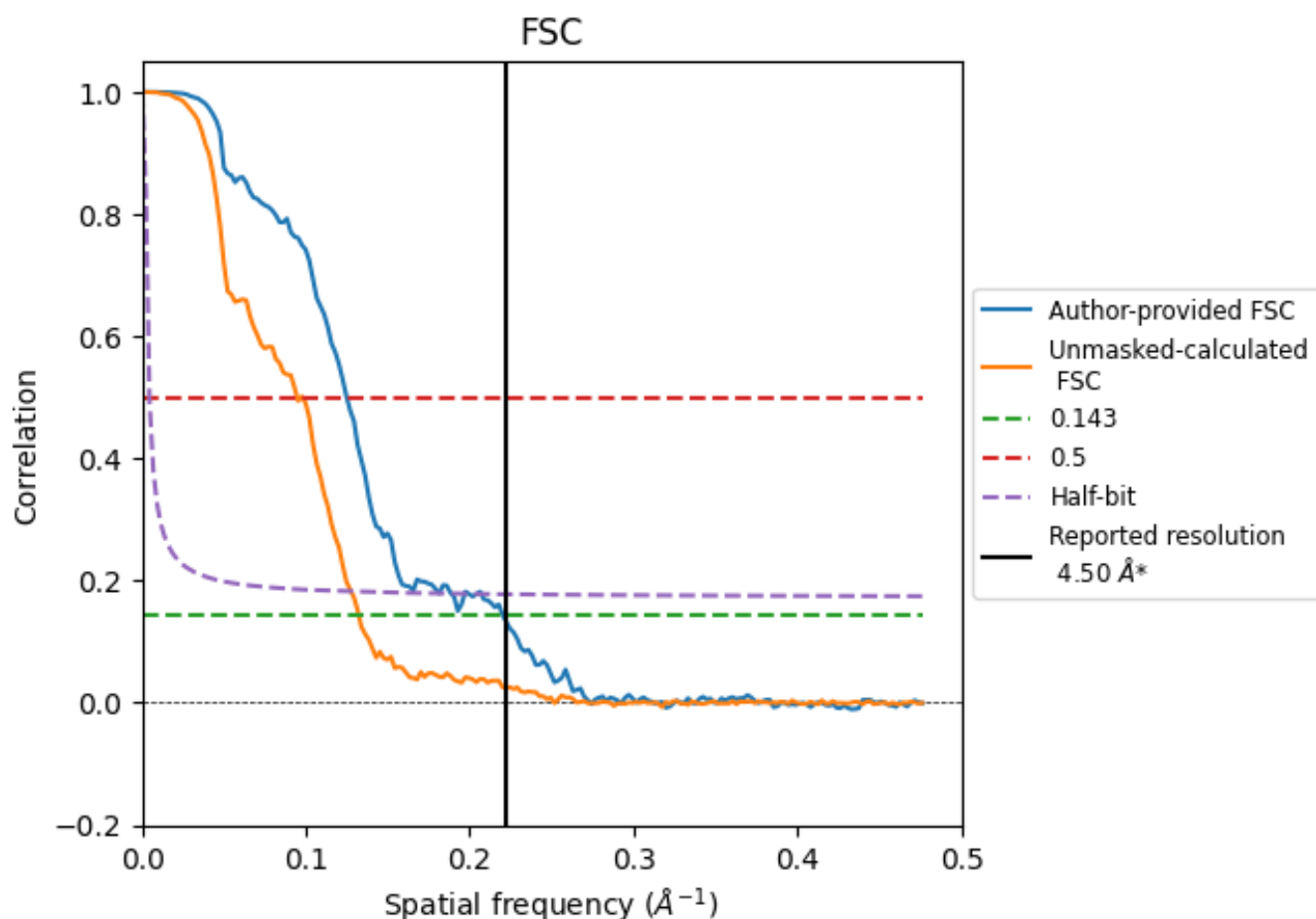


*Reported resolution corresponds to spatial frequency of $0.222 \text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

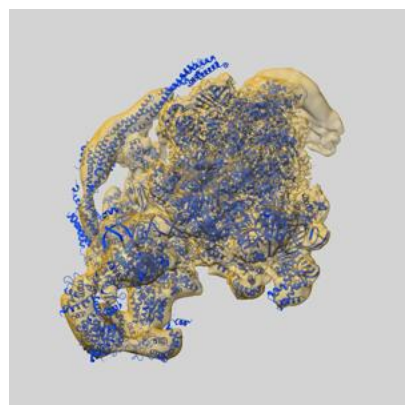
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.54	8.01	5.51
Unmasked-calculated*	7.56	10.57	7.84

*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 7.56 differs from the reported value 4.5 by more than 10 %

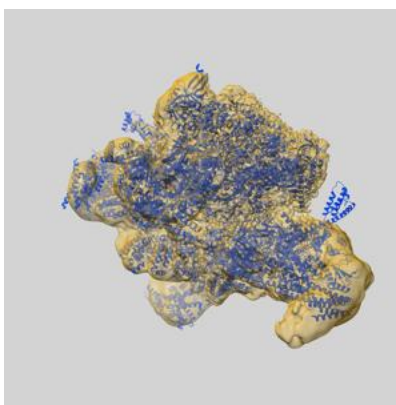
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12610 and PDB model 7NVR. Per-residue inclusion information can be found in section [3](#) on page [16](#).

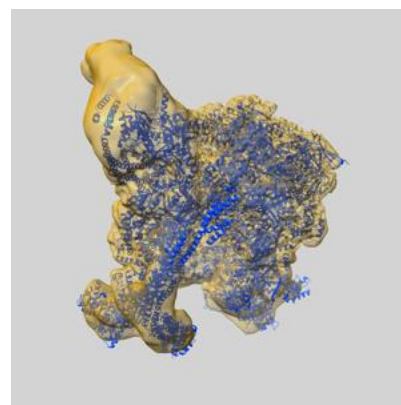
9.1 Map-model overlay [i](#)



X



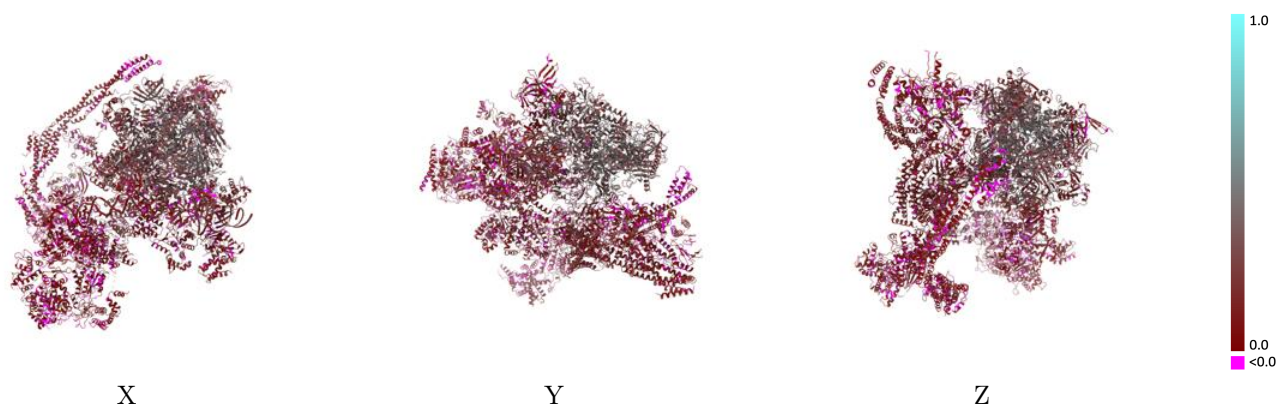
Y



Z

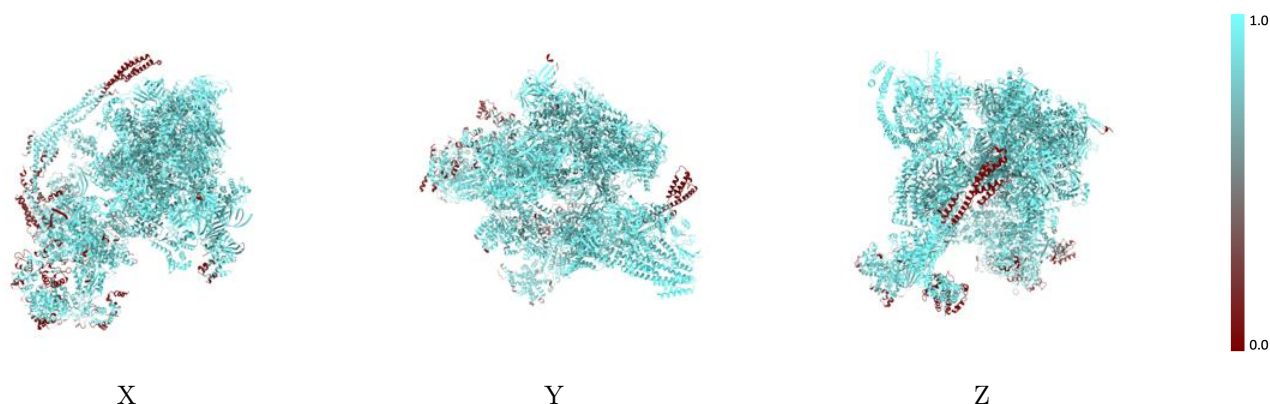
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



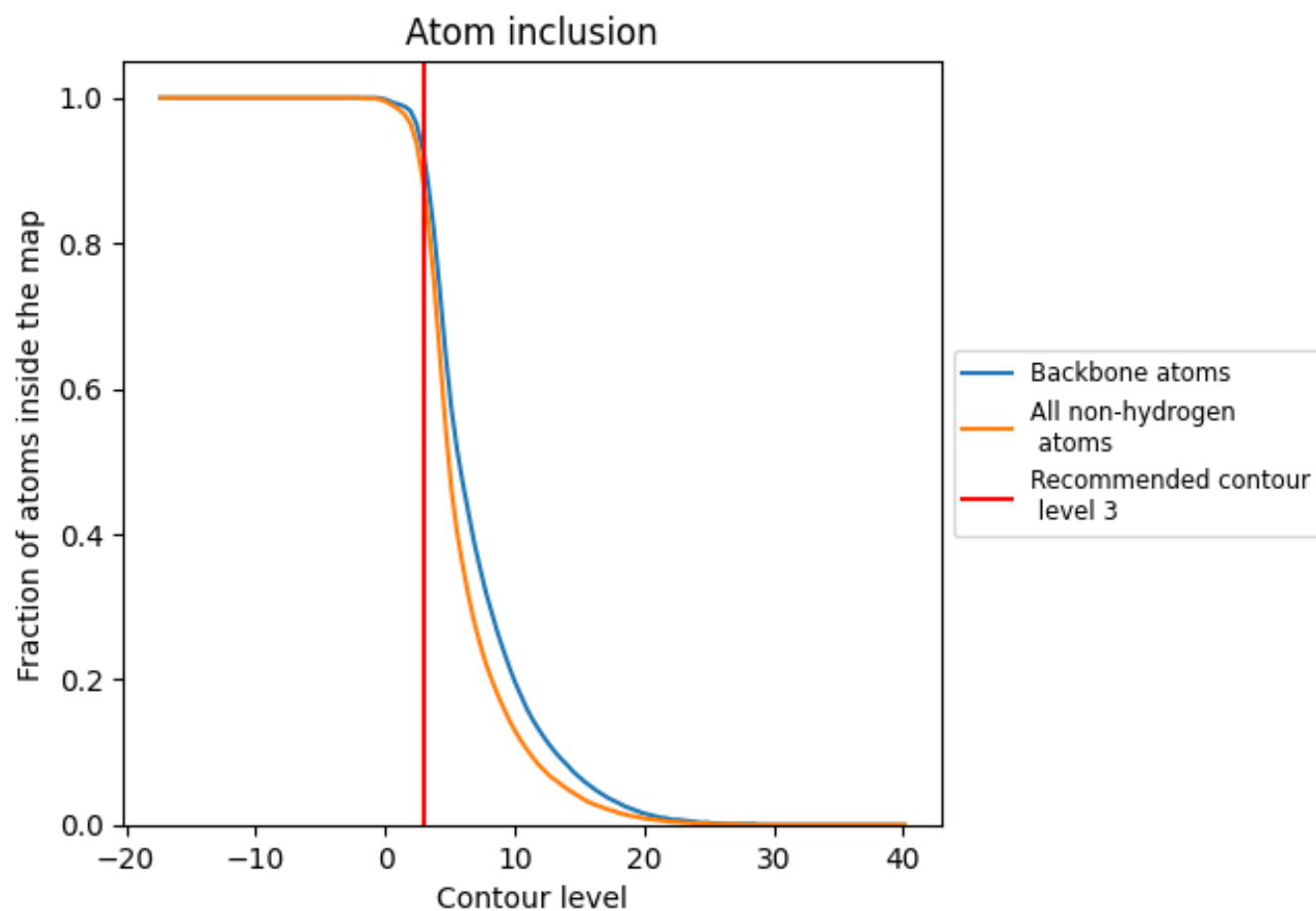
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.1710
0	 0.9490	 0.1120
1	 0.6440	 0.0580
2	 0.6590	 0.0710
3	 0.8920	 0.1210
4	 0.8590	 0.0540
5	 0.5870	 0.0580
6	 0.9050	 0.0660
7	 0.9080	 0.0630
8	 0.8840	 0.0680
9	 0.8380	 0.0620
A	 0.9180	 0.2940
B	 0.9260	 0.3430
C	 0.9410	 0.3380
D	 0.8730	 0.1950
E	 0.9180	 0.2410
F	 0.9030	 0.3430
G	 0.9140	 0.2090
H	 0.9460	 0.3290
I	 0.9630	 0.2520
J	 0.9500	 0.3580
K	 0.9330	 0.3280
L	 0.9380	 0.3080
M	 0.9250	 0.2460
N	 0.9380	 0.1880
O	 0.9710	 0.1590
Q	 0.9330	 0.1300
R	 0.9260	 0.1480
T	 0.9220	 0.1700
U	 0.7690	 0.1300
V	 0.7490	 0.1110
W	 0.8420	 0.1100
X	 0.9520	 0.1410
Y	 0.5370	 0.0390
Z	 0.2500	 0.0870



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Chain	Atom inclusion	Q-score
a	 0.9410	 0.1280
b	 0.9150	 0.1860
c	 0.9530	 0.1710
d	 0.9620	 0.1240
e	 0.9480	 0.1430
f	 0.9410	 0.0990
g	 0.9300	 0.1460
h	 0.4270	 0.0450
i	 0.9550	 0.1140
j	 0.1490	 0.0100
k	 0.4050	 0.0660
l	 0.8780	 0.1070
m	 0.1750	 0.0350
n	 0.8020	 0.0910
o	 0.9710	 0.1060
p	 0.9560	 0.1190
q	 1.0000	 0.1450
r	 1.0000	 0.1280
s	 0.9670	 0.1420
v	 0.9460	 0.0390
w	 1.0000	 0.2650
x	 0.9460	 0.1010
y	 1.0000	 0.1370
z	 1.0000	 0.1300