



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:11 AM UTC

PDB ID : 7FIK / pdb_00007fik
EMDB ID : EMD-31600
Title : The cryo-EM structure of the CR subunit from *X. laevis* NPC
Authors : Shi, Y.; Huang, G.; Zhan, X.
Deposited on : 2021-07-31
Resolution : 3.70 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:

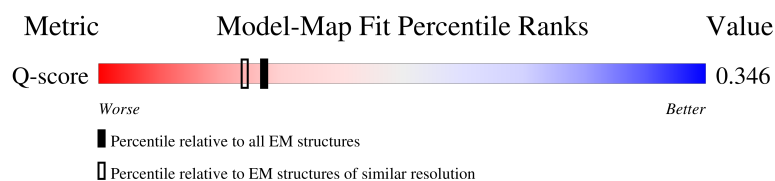
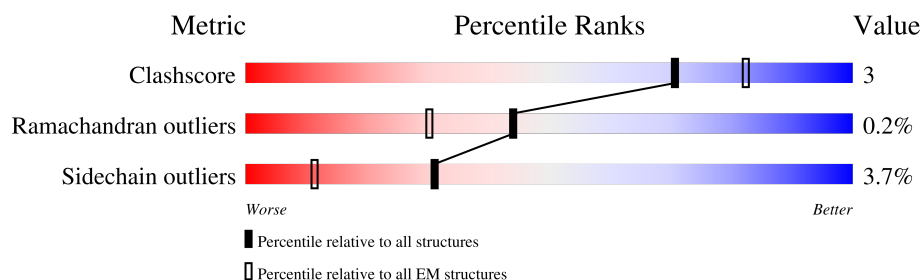
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2011	 86% 11%
1	a	2011	 82% 14%
2	B	653	 79% 11% 8%
2	b	653	 78% 13% 9%

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Mol	Chain	Length	Quality of chain
3	C	375	
3	c	375	
4	D	360	
4	d	360	
5	E	1435	
5	e	1435	
6	F	326	
6	f	326	
7	G	1742	
7	g	1742	
8	H	320	
8	h	320	
9	I	916	
9	i	916	
10	J	1140	
11	K	2905	
11	L	2905	
11	M	2905	
11	N	2905	
11	O	2905	
12	P	820	
12	S	820	
12	p	820	
12	s	820	
13	W	1388	

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Mol	Chain	Length	Quality of chain
14	X	161	83% 100%
15	Y	728	38% 45% 53%
16	j	1140	90% 90% 10%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 116163 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 MGC83295 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1795	Total	C	N	O	S	0	0
			9238	5541	1851	1841	5		
1	a	1725	Total	C	N	O	S	0	0
			8811	5278	1770	1757	6		

- Molecule 2 is a protein called Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	598	Total	C	N	O	S	0	0
			4799	3051	833	878	37		
2	b	595	Total	C	N	O	S	0	0
			4549	2894	793	829	33		

- Molecule 3 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2557	1590	461	488	18		
3	c	309	Total	C	N	O	S	0	0
			2445	1518	443	468	16		

- Molecule 4 is a protein called Nucleoporin SEH1-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	316	Total	C	N	O	S	0	0
			2473	1550	443	463	17		
4	d	312	Total	C	N	O	S	0	0
			2435	1531	435	451	18		

- Molecule 5 is a protein called outer Nup160.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1310	Total	C	N	O	S	0	0
			7891	4857	1495	1522	17		
5	e	1247	Total	C	N	O	S	0	0
			8134	5074	1497	1533	30		

- Molecule 6 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	326	Total	C	N	O		0	0
			1607	954	326	327			
6	f	322	Total	C	N	O	S	0	0
			2524	1612	436	461	15		

- Molecule 7 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	567	Total	C	N	O	S	0	0
			4209	2659	769	764	17		
7	g	603	Total	C	N	O	S	0	0
			4770	3022	868	856	24		

- Molecule 8 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	288	Total	C	N	O	S	0	0
			2235	1417	383	423	12		
8	h	288	Total	C	N	O	S	0	0
			2259	1429	385	433	12		

- Molecule 9 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	729	Total	C	N	O	0	0
			3626	2168	729	729		
9	i	673	Total	C	N	O	0	0
			3347	2001	673	673		

- Molecule 10 is a protein called nuclear pore complex protein Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	1015	Total	C	N	O	0	0
			5029	2999	1015	1015		

- Molecule 11 is a protein called Nup358 complex, clamps.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	697	Total	C	N	O	0	0
			3460	2066	697	697		
11	L	679	Total	C	N	O	0	0
			3372	2014	679	679		
11	M	654	Total	C	N	O	0	0
			3246	1938	654	654		
11	N	701	Total	C	N	O	0	0
			3480	2078	701	701		
11	O	683	Total	C	N	O	0	0
			3391	2025	683	683		

- Molecule 12 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	593	Total	C	N	O		0	0
			2945	1759	593	593			
12	S	52	Total	C	N	O	S	0	0
			432	272	77	81	2		
12	s	52	Total	C	N	O	S	0	0
			432	272	77	81	2		
12	p	456	Total	C	N	O		0	0
			2267	1355	456	456			

- Molecule 13 is a protein called Nup155-prov protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	324	Total	C	N	O	S	0	0
			2636	1688	447	485	16		

- Molecule 14 is a protein called Nup98.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	161	Total	C	N	O	0	0
			794	472	161	161		

- Molecule 15 is a protein called Nucleoporin Nup88A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	339	Total	C	N	O	0	0
			1676	998	339	339		

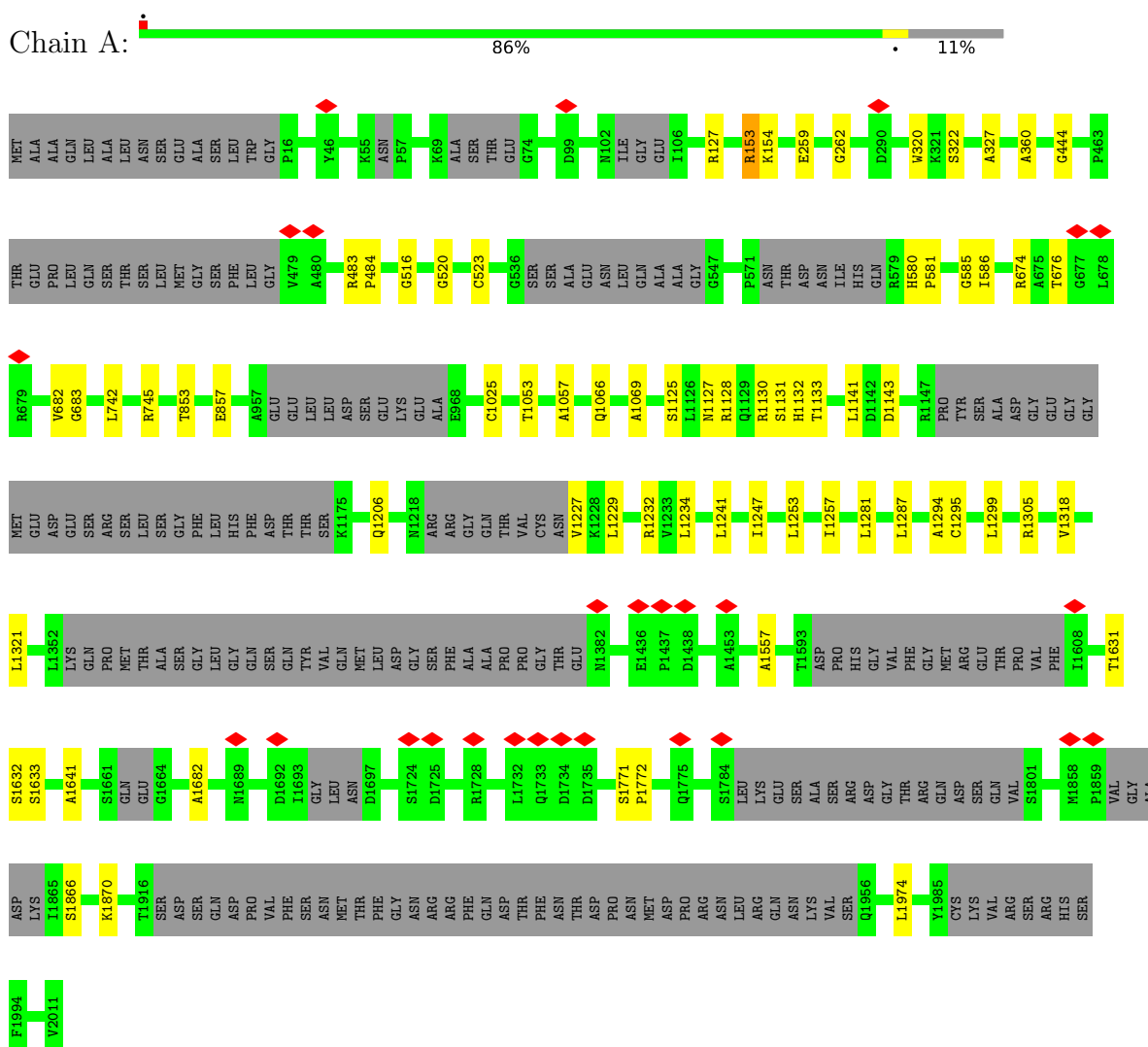
- Molecule 16 is a protein called outer Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	j	1028	5094	3038	1028	1028	0	0

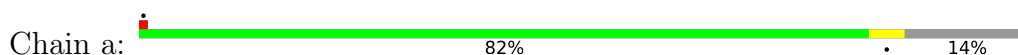
3 Residue-property plots

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.

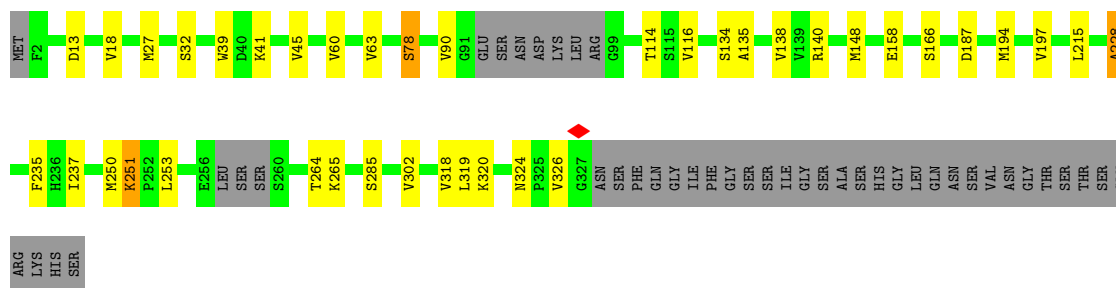
- Molecule 1: MGC83295 protein



- Molecule 1: MGC83295 protein

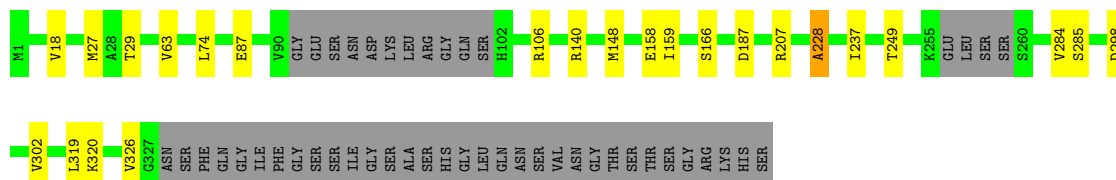






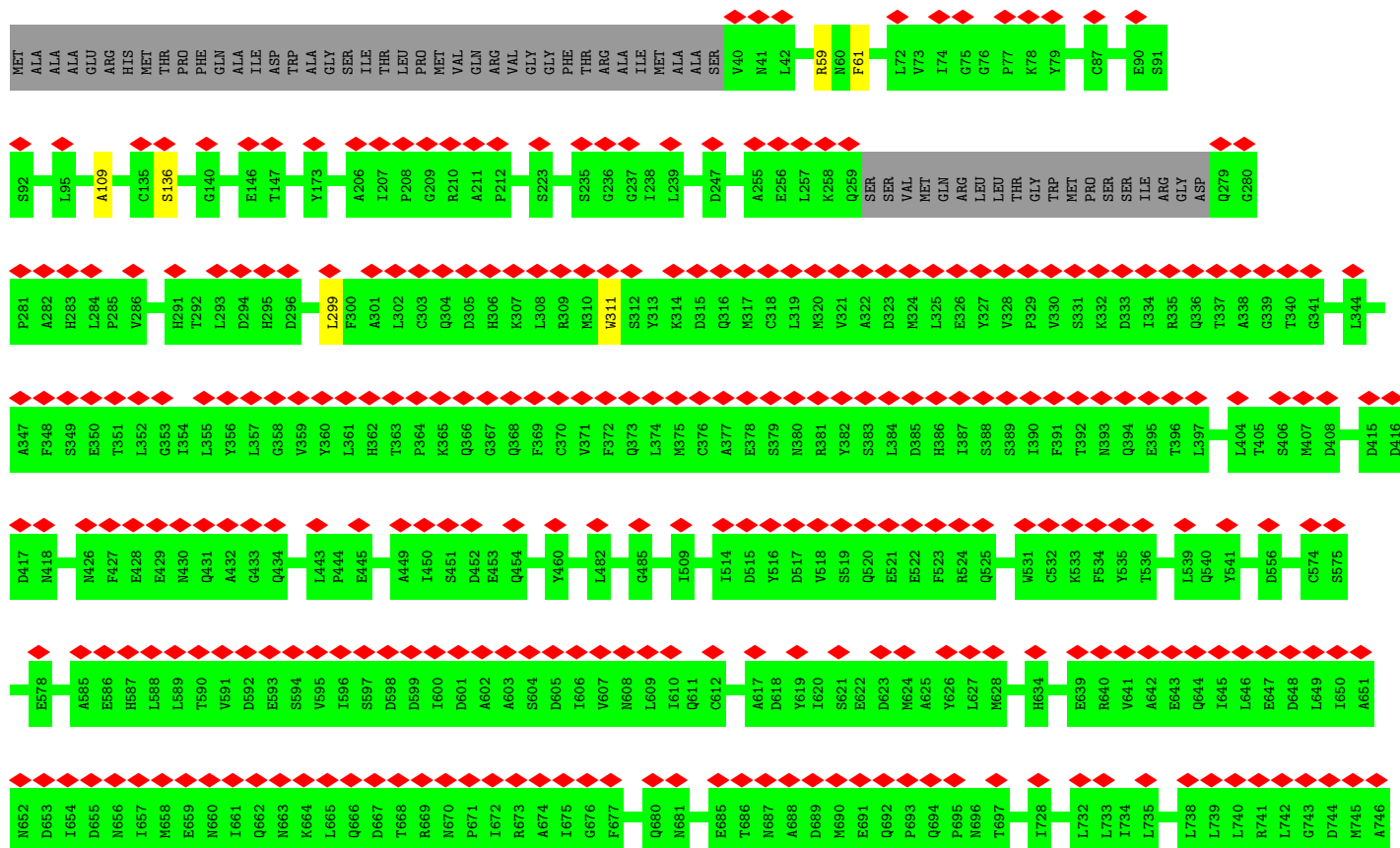
• Molecule 4: Nucleoporin SEH1-B

Chain d: 80% 6% 13%



• Molecule 5: outer Nup160

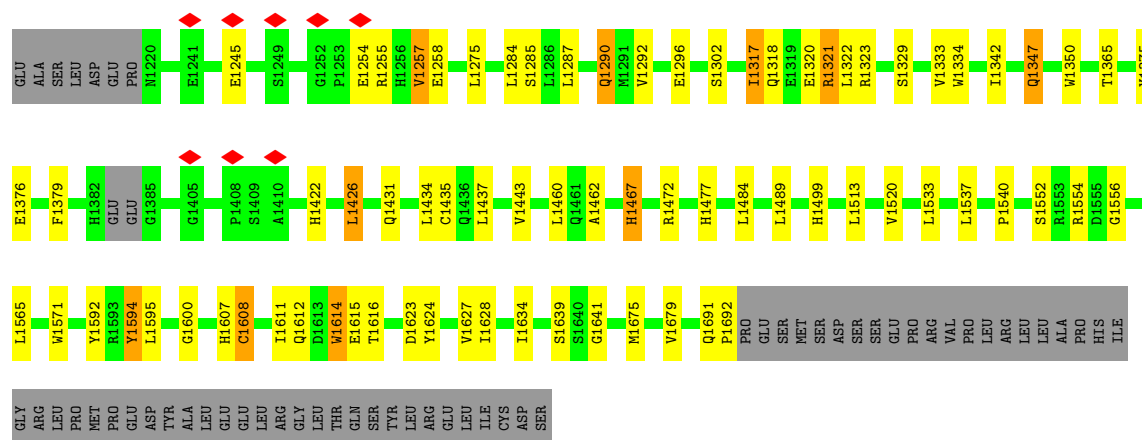
Chain E: 24% 83% 7% 9%





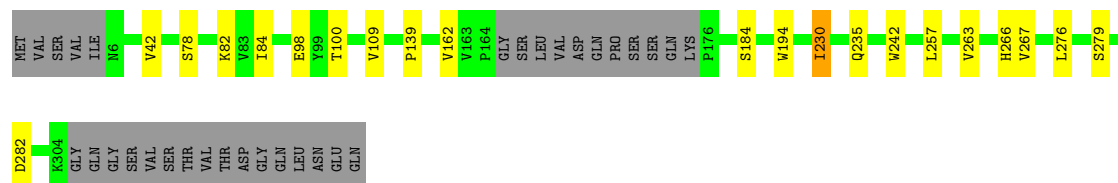






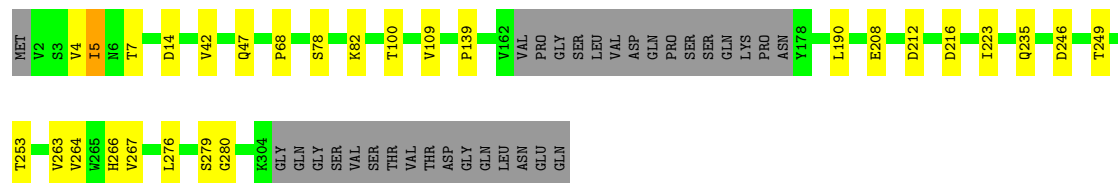
• Molecule 8: Protein SEC13 homolog

Chain H: 83% 6% 10%



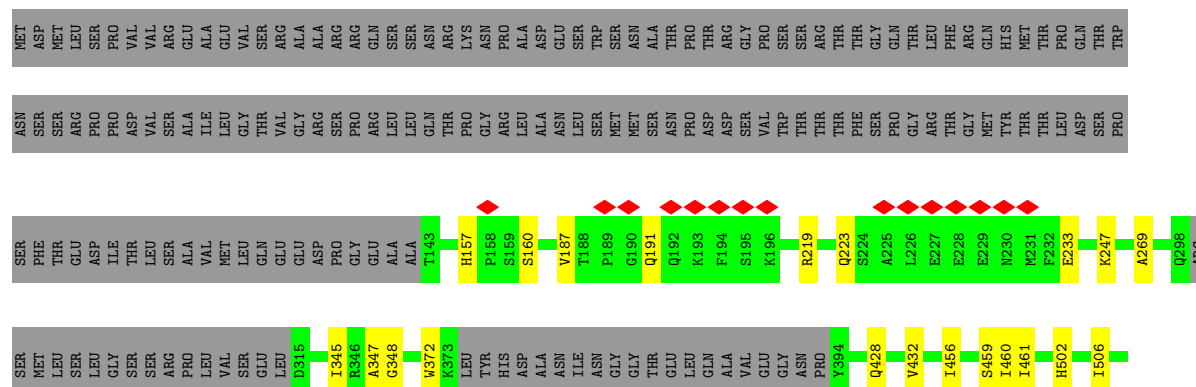
• Molecule 8: Protein SEC13 homolog

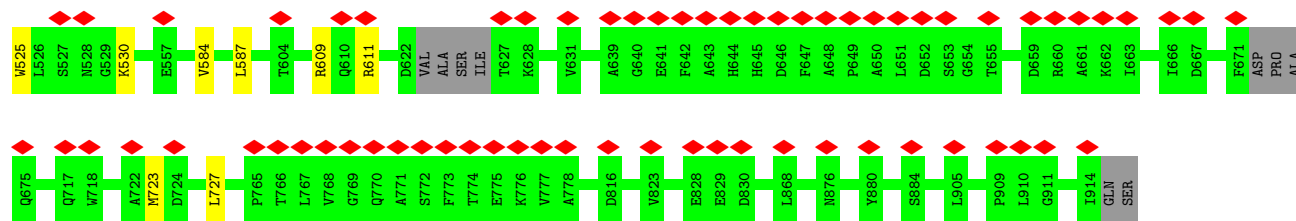
Chain h: 81% 8% 10%



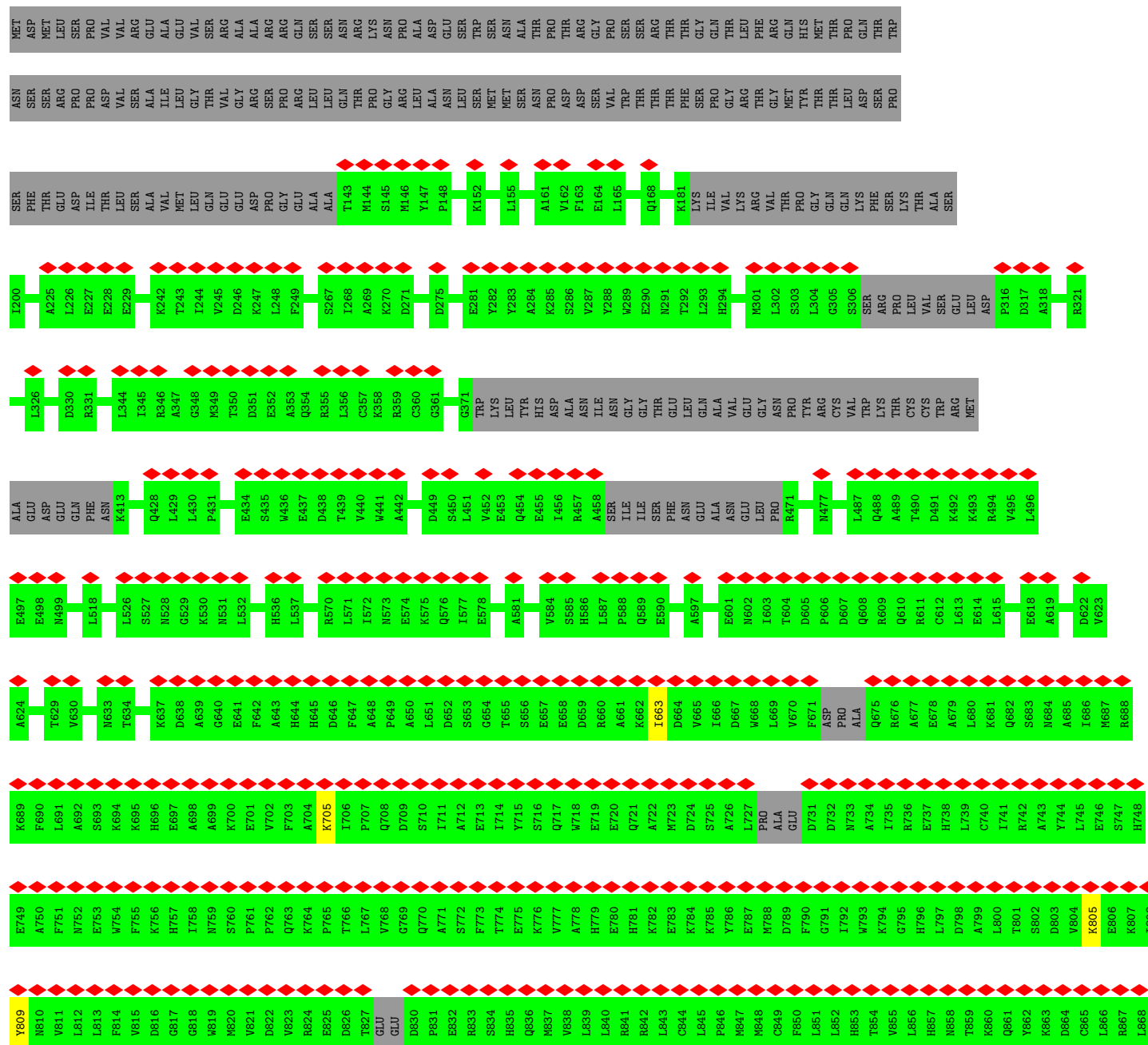
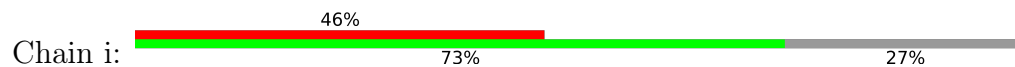
• Molecule 9: Nuclear pore complex protein

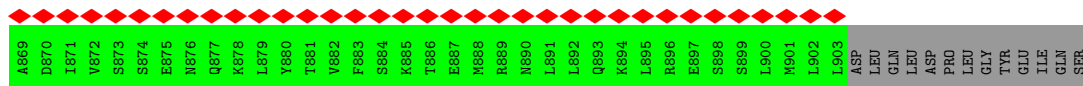
Chain I: 9% 76% 20%



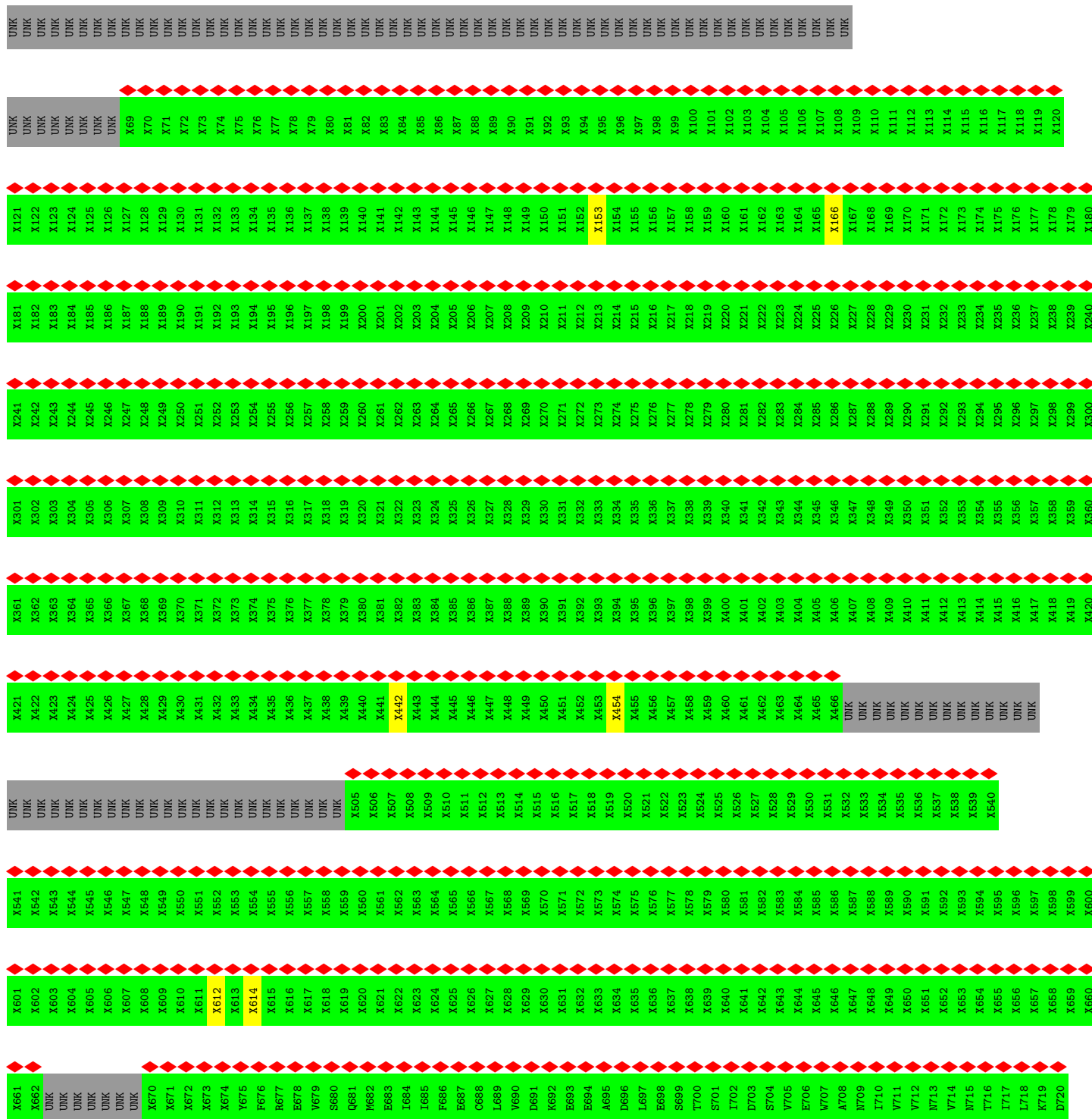
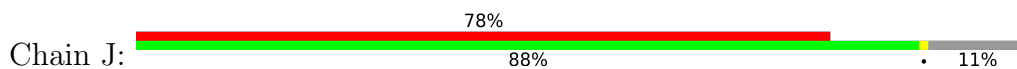


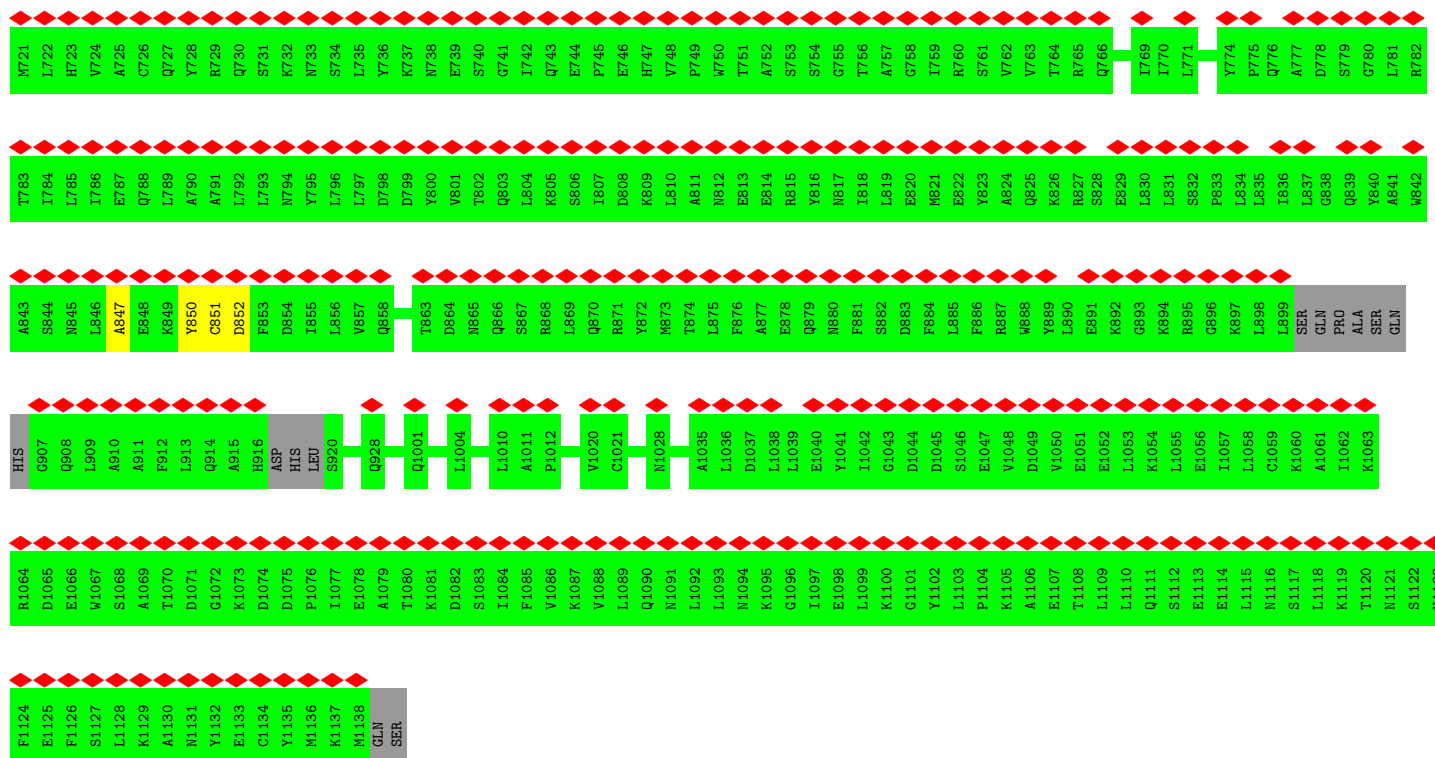
• Molecule 9: Nuclear pore complex protein



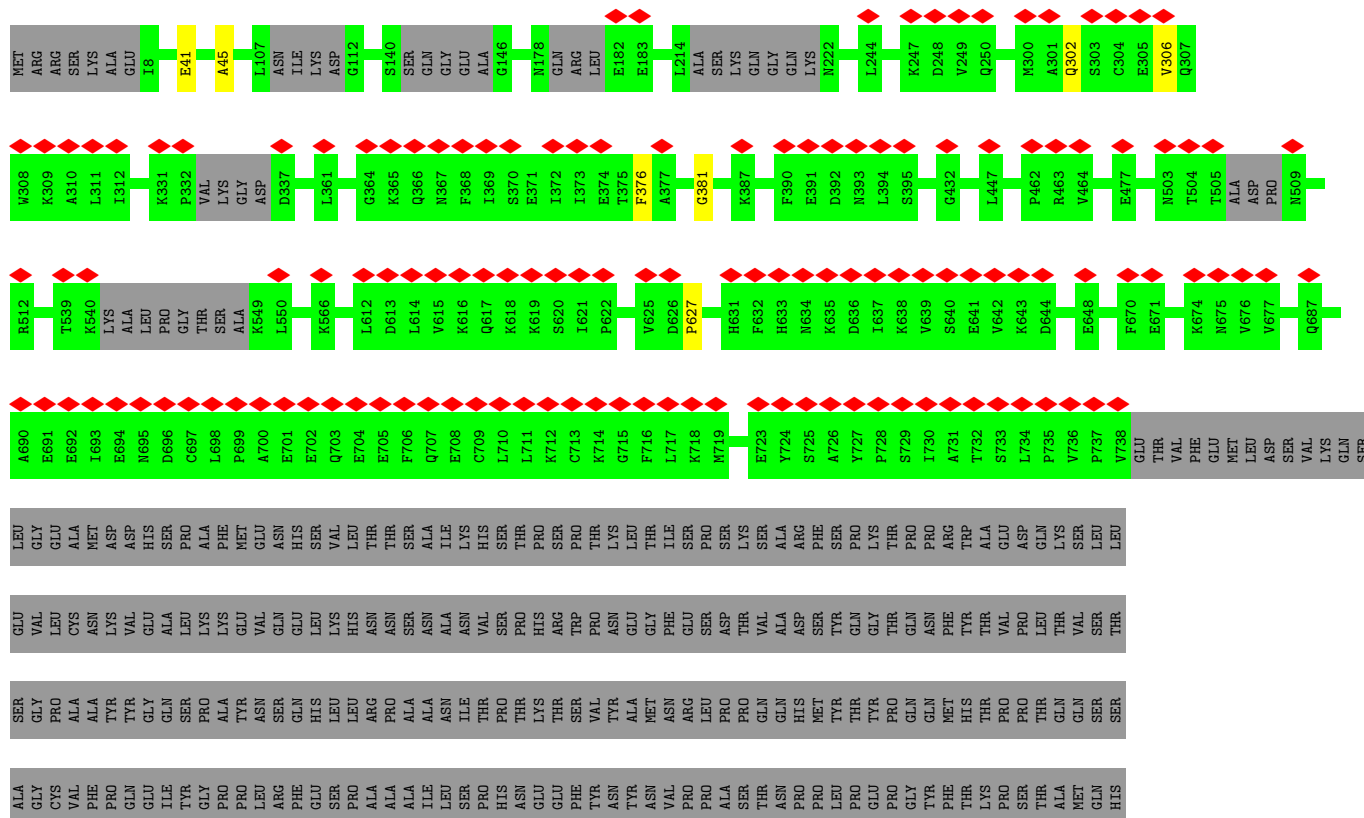


- Molecule 10: nuclear pore complex protein Nup133





• Molecule 11: Nup358 complex, clamps

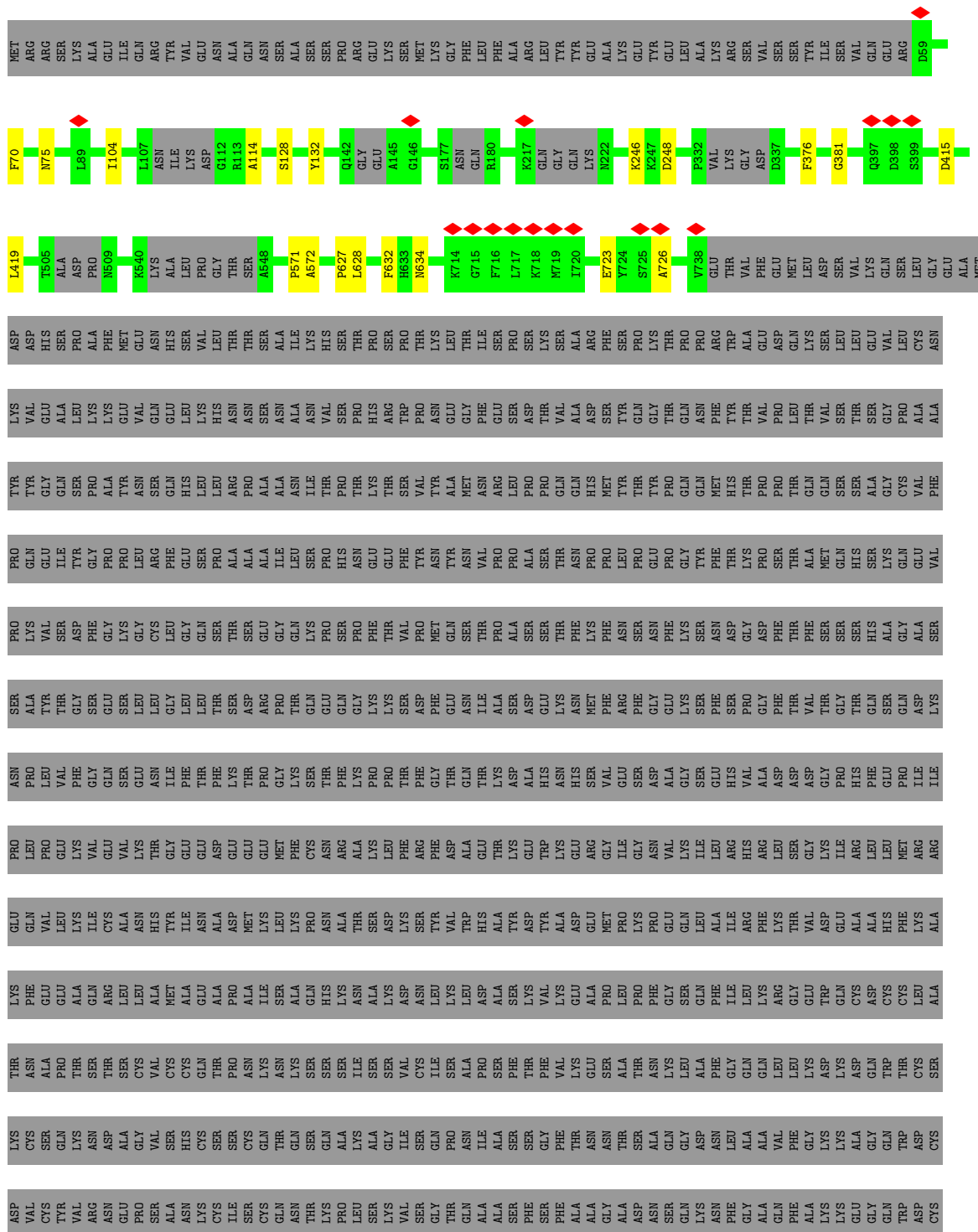














VAL	THR	ALA	THR	ASP	TYR	SER	ASP	GLY	GLU	GLY	LYS	VAL	GLU	GLN	LEU	ALA	VAL	ARG	PHE	LYS	THR	LYS	LEU	LEU	THR	ASP	SER	PHE	GLN	ASN	LYS	PHE	GLU	GLU	CYS	GLN	GLN	ASN	LEU	GLN	GLN	GLU	GLU	ASN	PRO	GLN	THR
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- Molecule 11: Nup358 complex, clamps



K61	A62	H63	R64	F65	L66	G67	Q68	L69	F70	E71	I72	E73	G74	N75	V76	E77	K78	A79	V80	G81	C82	Y83	K84	S85	S86	L87	E88	L89	N90	P91	T92	D95	L96	T97	L98	R99	I100	A101	E102	I103	I104	C105	T106	L107	ASN	ILE	LYS	ASP	G112	R113	A114	E115	Y116	W117	R120	L124
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F125	P126	G127	R133	L134	K135	E136	Q137	L138	L139	S140	S141	Q142	G143	GLU	ALA	GLY	M147	M148	Q149	L150	A156	A160	Y166	L169	K170	L171	V172	D173	L174	F175	L176	S177	M178	GLN	ARG	L181	T198	D199	I200	E201	W202	C203	S204	C205	V206	V207	R208	V209	F210	K211	E212	E213	V213	LEU
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ALA
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D248
V249
S269
A275
M300
K309
A310
L311
L312
A316
A322
P332
VAL
LYS
GLY
ASP
D337
H363
C364
K365
Q366
S370
L373
E374
T375
F376
A377
M378
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S395
M396
Q397
G402

◆ S407 ◆ P414 ◆ D415 ◆ T506
 ALA ASP PRO ASP
 N509 ◆ K540
 LYS ALA
 LEU LEU
 PRO PRO
 GLY GLY
 THR THR
 SER SER
 A548 ◆ P624
 F632
 H633
 N634 ◆ A654
 A666 ◆ A669
 G715 ◆ W738
 GLU THR VAL PHE GLU MET LEU LEU ASP SER VAL VAL GLN SER LEU LEU GLY GLU ALA MET ASP ASP HIS SER PRO ALA

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

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

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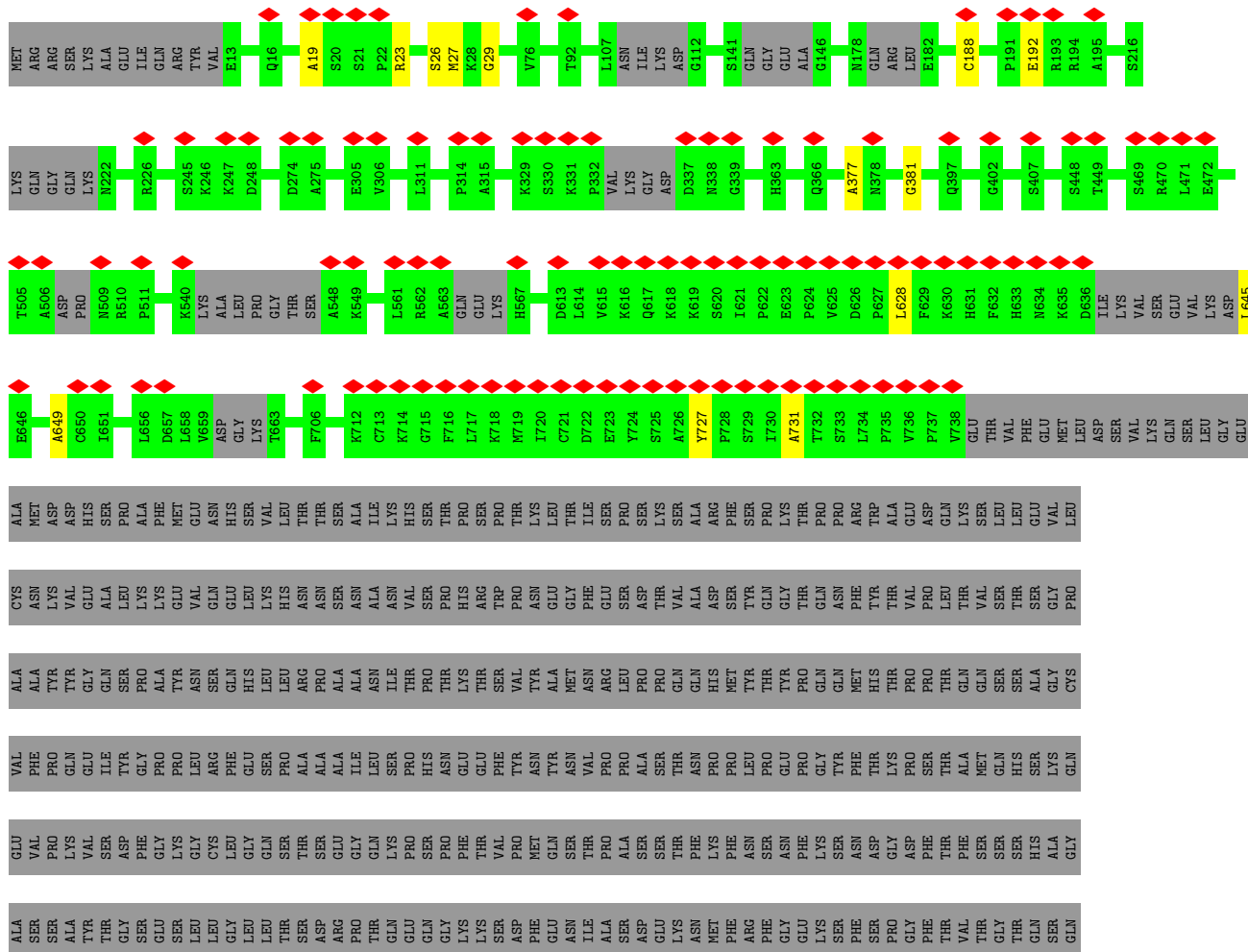
GLU SER LEU LEU LEU LEU LEU THR THR SER SER ASP ARG ARG PRO THR THR GLN GLU GLN GLN GLY GLY LYS LYS SER SER ASP PHE PHE ASN ASN ILE ALA ALA SER SER ASP ASP ARG ARG PHE PHE GLY GLY GLU LYS LYS SER SER PHE PHE PRO GLY GLY PHE THR THR VAL VAL THR GLY THR THR GLN GLN GLN GLN LYS LYS ASP ASP THR THR VAL VAL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

GLN SER GLU ASN PHE THR PHE LYS PRO LYS SER PHE LYS PRO THR PHE GLY THR GLN THR LYS ASP ALA ASN HIS SER VAL GLU SER ASP ALA GLY GLU VAL ASP ALA ASP ASP ASP GLY PRO HIS PHE GLU PRO LEU PRO PRO LYS VAL

GLU	VAL	LYS	THR	GLY	GLU	GLU	ASP	GLU	GLU	GLU	GLU	GLU	MET	PHE	CYS	ASN	ARG	ALA	LYS	LEU	PHE	ARG	PHE	ASP	ALA	GLU	THR	LYS	GLU	TRP	LYS	GLU	ARG	GLY	ILE	GLY	ASN	VAL	LYS	ILE	LEU	ARG	HIS	ARG	LEU	GLY	LYS	ILE	ARG	GLN	VAL	LEU	LYS	THR	TYR
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CYS	ALA	ASN	HIS	TYR	ILE	ASN	ALA	ALA	MET	LYS	LYS	PRO	ASN	ALA	ALA	THR	SER	ASP	LYS	SER	TYR	VAL	TRP	HIS	ALA	ALA	TYR	ASP	TYR	ALA	ALA	ASP	GLU	GLN	LEU	ALA	ALA	ILE	ARG	PHE	LYS	THR	VAL	ASP	GLU	ALA	ALA	HIS	PHE	LYS	LYS	ALA	ALA	ALA	THR	ASN
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[illegible]

- Molecule 12: Nuclear pore complex protein Nup93

Chain P:

[illegible]

- Molecule 12: Nuclear pore complex protein Nup93

Chain S:



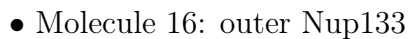
Chain s: 6% • 94%



- Molecule 12: Nuclear pore complex protein Nup93



C362	L302	PRO	ASP	V181	THR	SER
		THR	T242	E182	PHE	VAL
		PRO	L243	M183	VAL	LEU
		ILE	L244	A184	ALA	GLY
		PRO	S245	Y185	GLU	GLY
		GLY	R246	A186	GLU	SER
		LEU	C247	R187	TYR	ARG
		GLN	S248	M188	HIS	GLY
		ASP	G249	Q189	ARG	LEU
		GLY	Q250	M189	ILE	LEU
C363	L303	GLY	Q251	Y190	SER	GLN
		ILE	Q252	Y192	MET	HIS
		GLY	Q253	Y193	VAL	GLN
		PRO	A254	E194	TRP	ARG
		V319	F255	K195	GLU	ALA
		W320	V256	V196	GLU	LEU
		A321	R257	V197	VAL	SER
		L322	Q258	S198	GLN	GLY
		I323	A259	G199	ARG	VAL
		Y324	L260	H200	VAL	THR
C364	L304	C325	M261	L201	HIS	LEU
		C326	V262	Q202	THR	PHE
		M327	L263	P203	LEU	GLU
		R328	E264	S204	ALA	LEU
		C329	Q265	L205	SER	GLU
		G330	S266	V206	GLY	PRO
		D331	V267	D207	VAL	LEU
		L332	K268	L208	ASP	GLN
		M333	N269	C209	ALA	ASP
		A334	Y270	T210	THR	GLN
C365	L305	Q335	T271	E211	PHE	GLN
		Q336	L272	A212	GLY	GLY
		Q337	T273	A213	PHE	GLY
		V338	S274	E214	SER	LEU
		V339	N275	R215	GLU	LEU
		N340	PHE	LEU	THR	ASN
		R341	ALA	ASP	SER	LYS
		A342	ASN	ASP	TYR	LYS
		Q343	LEU	ASP	ILE	ASP
		H344	GLN	K219	SER	ASN
C366	L306	Q345	GLN	N220	GLU	THR
		L346	ALA	V221	GLY	LEU
		G347	GLY	S222	ALA	SER
		D348	LEU	D223	ALA	SER
		F349	GLY	L224	PRO	GLN
		K350	GLY	D225	GLY	ILE
		V351	VAL	W226	SER	GLU
		C352	PRO	V227	ARG	ALA
		L353	THR	M227	LEU	ASN
		M354	GLY	N228	LYS	ARG



K121	N181	G241	D301	T361	G421	SER	D541	L601	R661	M721	L781	A841	Q901
I122	I182	M242	M302	L362	T422	SER	E542	H602	W662	L722	R782	W842	P902
S123	L183	L243	S303	V363	G423	VAL	L543	Q603	C663	H723	T783	A843	A903
H124	H184	S244	R304	T364	R424	LYS	D544	V604	T664	V724	T784	S844	S904
S125	E185	G245	V305	V365	S425	SER	L545	G605	V665	A725	L785	N845	Q905
S126	G186	I246	L306	K366	T426	SER	A546	L606	PRO	C726	L786	L846	H906
S127	T187	G247	R307	D367	L427	ARG	V547	F607	GLN	Q727	E787	A847	Q907
A128	Y188	R248	E308	E368	P428	ALA	N548	S608	ASN	Y728	Q788	E848	Q908
K129	R249	R249	I309	G369	Q429	VAL	Q549	R609	T670	R729	L789	R849	L909
L130	E190	V250	I310	Y370	E430	VAL	I550	L610	A671	Q730	A790	A851	A910
M131	S191	S251	S311	N371	K431	LYS	S551	S611	A672	S731	A791	C851	A911
V132	Y192	T252	D312	I372	I432	ASP	V552	T612	D673	K732	L792	D852	F912
C133	T193	L253	A313	S373	F433	ARG	D553	C613	V674	M733	L793	F853	L913
K134	E194	F254	I314	D374	F434	PRO	L554	Q614	V675	S734	N794	D854	Q914
E135	F195	G255	W315	E375	E435	ASP	L555	T615	F676	L735	Y795	L855	A915
L136	G196	I256	G316	I376	A436	GLN	D556	K616	R677	Y736	L796	L856	H916
P137	S197	L257	S317	T377	Q437	ILE	D557	G617	E678	K737	L797	W857	D917
L138	S198	S258	E318	V378	G438	HIS	Y558	M618	V679	N738	D798	Q858	H918
P139	L199	P259	S319	E379	D439	ASP	P559	L619	S680	E739	D799	L859	L919
L140	C200	A260	D320	V380	N440	ASP	A560	V620	Q681	S740	W800	C860	S920
S141	A201	V261	Y321	T381	I441	K505	S561	A621	M682	G741	Y801	E861	W921
D142	F202	E262	D322	Q382	V442	K507	D562	T622	E683	I742	T802	M862	L922
S143	V203	S263	D323	F383	G443	H508	P563	R623	L684	Q743	Q803	T863	H923
E144	T204	T264	I324	N384	A444	L509	R564	L624	L685	E744	L804	D864	E924
W145	A205	L265	K325	F385	G445	K510	W565	L625	F686	P745	K805	M865	L925
S146	V206	C266	A326	V386	S446	A511	A566	L626	E687	E746	S806	Q866	N926
A147	K207	S267	G327	F387	C447	A512	E567	S627	C688	H747	I807	S867	S927
D148	G208	V268	I328	Q388	E448	F513	S568	E628	L689	V748	D808	R868	Q928
L149	N209	L269	N329	A389	G449	L514	V569	H629	V690	P749	K809	L869	E929
V150	S210	W270	I330	R390	N450	R515	P570	A630	D691	W750	L810	Q870	F930
D151	F211	D271	N331	G391	P451	Y516	E571	E631	K692	T751	A811	R871	E931
I152	I212	K272	Y332	M392	V452	C517	E572	K632	E693	A752	N812	W872	K932
C153	L213	G273	L333	Q393	F453	R518	A573	L633	E694	S753	E813	M873	A933
A154	S214	D274	S334	L394	F454	K519	A574	S634	A695	S754	E814	T874	H934
Q155	S215	C275	L335	C395	I455	D520	G575	A635	D696	G755	R815	L875	A935
T156	E216	F276	N336	Q396	R456	I521	F576	A636	L697	T756	Y816	F876	N936
G157	K217	Y277	Q337	L397	K457	L522	S577	L637	E698	A757	N817	A877	L937
D158	N218	T278	N338	V398	S458	G523	N578	V638	S699	G758	I818	E878	Q938
P159	Q219	L279	C339	V399	G459	A524	T579	L639	T700	I759	L819	Q879	T939
A160	L220	T280	D340	P400	N460	Q525	S580	K640	S701	R760	E820	N880	L940
A161	V221	D281	G341	M401	L461	S526	L581	M641	I702	S761	M821	F881	A941
A162	R222	S282	L342	F402	T462	M527	L582	H642	D703	V762	E822	S882	N942
Q163	L223	S283	V343	S403	V463	V528	L583	H643	S704	W763	E823	D883	M943
S164	T224	I284	I344	S404	V464	D529	L584	A644	V705	T764	A824	F884	E944
V165	P225	N285	L345	Q405	A465	S530	H585	K645	E706	R765	Q825	L885	T945
A166	D226	K286	S346	A406	R466	L531	Q586	L646	W707	Q766	K826	F886	N946
L167	A227	W287	A347	C407	GLU	F532	L587	P647	A708	H767	R827	R887	Y947
M168	S228	D288	A348	Y408	THR	S533	E588	V648	N709	G768	S828	W888	F948
A169	G229	L289	W349	L409	SER	D534	D589	L649	I710	I769	E829	Y889	C949
A170	K230	D290	H350	Y410	VAL	S535	K591	V650	V711	T770	L830	Y891	Q950
T171	M231	D291	P351	T411	PRO	D536	M591	M651	V712	L771	L831	E891	K951
P172	N232	T292	G352	Q412	GLU	M537	K592	S652	N713	K772	S832	K892	K952
E173	Q233	S293	D353	E413	HIS	E538	A593	A653	V714	W773	F833	C893	T953
G174	R234	E294	N354	M414	MET	L594	H594	T654	N715	Y774	L834	K894	L954
S175	V235	S295	P355	I415	GLU	S595	S595	Q655	T716	P775	L835	R895	L955
S176	Q236	Q296	C356	F416	GLU	F596	F596	L656	I717	Q776	T836	C896	Q956
R177	P237	V297	Q357	A417	SER	F597	F597	L657	L718	A777	L837	K897	L957
Y178	Q238	L298	I358	C418	LEU	V598	V598	A658	K719	D778	L838	L898	S958
W179	G239	N299	Y359	S419		D599	D599	D659	D720	S779	L839	L899	K959
P180	Q240	W300	Y360	T420		F600	F600	K660		G780		S900	L960

A961	A962	L963	A964	S965	D966	F967	Q968	E969	D970	V971	L972	Q973	E974	K975	V976	E977	E978	I979	A980	E981	E982	E983	H984	F985	L986	L987	H988	Q989	E990	T991	L992	P993	K994	K995	L996	L997	E998	E999	K1000	Q1001	L1002	D1003	L1004	N1005	A1006	M1007	P1008	V1009	L1010	A1011	P1012	F1013	Q1014	L1015	I1016	Q1017	L1018	Y1019	V1020
C1021	E1022	E1023	N1024	K1025	R1026	A1027	N1028	E1029	N1030	D1031	F1032	M1033	K1034	A1035	L1036	D1037	L1038	L1039	E1040	Y1041	I1042	G1043	D1044	D1045	S1046	E1047	V1048	D1049	V1050	E1051	E1052	L1053	K1054	L1055	E1056	I1057	L1058	C1059	K1060	A1061	I1062	K1063	R1064	D1065	E1066	W1067	S1068	A1069	T1070	D1071	G1072	K1073	D1074	D1075	P1076	I1077	E1078	A1079	T1080
K1081	D1082	S1083	I1084	F1085	V1086	K1087	V1088	L1089	Q1090	M1091	L1092	L1093	N1094	K1095	G1096	I1097	E1098	L1099	K1100	G1101	Y1102	L1103	P1104	K1105	A1106	E1107	T1108	L1109	L1110	Q1111	S1112	E1113	E1114	L1115	M1116	S1117	L1118	K1119	T1120	M1121	S1122	Y1123	F1124	E1125	F1126	S1127	L1128	K1129	A1130	M1131	Y1132	E1133	C1134	Y1135	M1136	K1137	M1138	GLN	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1279270	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 ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.334	Depositor
Minimum map value	-0.334	Depositor
Average map value	0.040	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	710.144, 710.144, 710.144	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.387, 1.387, 1.387	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	0.40	1/9232 (0.0%)	0.64	7/12806 (0.1%)
1	a	0.33	0/8804	0.60	2/12220 (0.0%)
2	B	0.51	0/4893	0.73	5/6602 (0.1%)
2	b	0.54	1/4636 (0.0%)	0.77	7/6272 (0.1%)
3	C	0.37	0/2615	0.83	4/3550 (0.1%)
3	c	0.40	0/2500	0.84	1/3394 (0.0%)
4	D	0.38	0/2536	0.83	7/3442 (0.2%)
4	d	0.39	0/2498	0.79	2/3392 (0.1%)
5	E	0.43	2/7960 (0.0%)	0.67	6/10948 (0.1%)
5	e	0.45	2/8229 (0.0%)	0.70	12/11264 (0.1%)
6	F	0.23	0/1606	0.44	0/2231
6	f	0.37	0/2594	0.77	2/3526 (0.1%)
7	G	0.48	1/4299 (0.0%)	0.78	8/5856 (0.1%)
7	g	0.58	4/4888 (0.1%)	0.86	9/6644 (0.1%)
8	H	0.40	0/2299	0.83	1/3139 (0.0%)
8	h	0.39	0/2322	0.81	3/3169 (0.1%)
9	I	0.21	0/3621	0.49	0/5050
9	i	0.15	0/3339	0.40	0/4651
10	J	0.15	0/2253	0.40	0/3141
11	K	0.21	0/3452	0.48	0/4805
11	L	0.19	0/3362	0.47	0/4677
11	M	0.26	0/3238	0.57	1/4506 (0.0%)
11	N	0.22	0/3471	0.53	0/4830
11	O	0.21	0/3380	0.53	1/4700 (0.0%)
12	P	0.21	0/2939	0.44	2/4093 (0.0%)
12	S	0.48	0/438	0.71	1/586 (0.2%)
12	p	0.64	0/2251	0.62	0/3118
12	s	0.46	0/438	0.66	0/586
13	W	0.56	0/2692	0.80	3/3638 (0.1%)
15	Y	0.57	0/1668	1.09	3/2311 (0.1%)
16	j	0.13	0/5091	0.39	0/7095
All	All	0.39	11/113544 (0.0%)	0.67	87/156242 (0.1%)

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
1	A	0	2
1	a	0	2
6	f	0	1
15	Y	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	1614	TRP	C-O	-6.41	1.16	1.24
7	g	1594	TYR	C-O	6.16	1.31	1.24
5	E	1234	LEU	N-CA	6.10	1.53	1.46
7	g	1540	PRO	C-O	5.83	1.29	1.23
5	e	1196	PRO	CA-C	5.58	1.60	1.52
7	g	1600	GLY	C-O	5.55	1.30	1.23
1	A	683	GLY	CA-C	-5.49	1.48	1.51
2	b	407	GLY	C-O	5.38	1.30	1.23
5	E	1088	ASN	C-O	5.21	1.29	1.23
5	e	1196	PRO	C-O	5.17	1.30	1.24
7	G	1418	ASP	C-O	5.16	1.30	1.23

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	GLY	N-CA-C	10.10	119.40	110.21
7	g	1321	ARG	N-CA-C	-9.63	100.73	111.14
5	E	988	ASP	N-CA-C	8.56	123.46	108.56
2	b	427	ASN	N-CA-C	7.87	119.64	111.14
12	S	124	MET	N-CA-C	7.08	118.68	110.97
5	e	884	TYR	N-CA-C	7.06	118.97	111.28
5	e	918	GLU	N-CA-C	6.98	120.30	107.73
5	E	1234	LEU	N-CA-C	6.93	120.31	112.97
7	G	1163	LYS	CA-C-N	-6.86	113.63	120.21
7	G	1163	LYS	C-N-CA	-6.86	113.63	120.21
4	D	78	SER	N-CA-C	6.69	119.62	110.06
7	g	1641	GLY	N-CA-C	6.46	120.49	112.73
4	D	324	ASN	CA-C-N	-6.39	114.04	120.31
4	D	324	ASN	C-N-CA	-6.39	114.04	120.31
7	G	1418	ASP	N-CA-C	6.32	118.95	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	78	SER	N-CA-C	6.27	116.84	108.38
5	e	866	TRP	N-CA-C	-6.25	98.13	109.44
13	W	1155	GLN	N-CA-C	-6.24	104.40	111.14
1	A	1128	ARG	N-CA-C	6.23	120.46	112.86
5	E	1252	GLY	N-CA-C	6.18	121.03	112.57
2	b	569	CYS	N-CA-C	6.17	118.00	111.28
7	g	1163	LYS	CA-C-N	-6.15	113.64	119.85
7	g	1163	LYS	C-N-CA	-6.15	113.64	119.85
7	g	1069	SER	N-CA-C	6.08	118.17	110.33
7	G	1128	LEU	N-CA-C	-6.06	103.26	110.41
7	g	1540	PRO	N-CA-C	6.06	123.62	111.69
5	e	1196	PRO	N-CA-C	6.05	121.50	113.40
3	C	203	ASP	CA-C-N	-6.05	113.74	119.85
3	C	203	ASP	C-N-CA	-6.05	113.74	119.85
11	M	628	LEU	N-CA-C	-5.97	107.82	114.62
7	G	1321	ARG	N-CA-C	-5.90	104.98	111.82
1	A	1974	LEU	N-CA-C	-5.90	105.67	112.92
5	E	1253	GLU	N-CA-C	5.86	117.66	111.28
1	A	1025	CYS	CA-C-N	-5.86	114.59	120.21
1	A	1025	CYS	C-N-CA	-5.86	114.59	120.21
2	b	222	ALA	N-CA-C	5.85	117.46	111.14
12	P	519	GLY	CA-C-N	5.81	128.74	120.49
12	P	519	GLY	C-N-CA	5.81	128.74	120.49
5	e	1316	LEU	CA-C-N	-5.79	114.63	120.31
5	e	1316	LEU	C-N-CA	-5.79	114.63	120.31
5	E	1089	TYR	N-CA-C	5.77	117.57	111.28
5	e	919	GLY	N-CA-C	5.77	119.65	112.73
1	a	344	SER	CB-CA-C	-5.75	109.96	116.63
4	D	251	LYS	CA-C-N	-5.74	114.05	119.85
4	D	251	LYS	C-N-CA	-5.74	114.05	119.85
7	g	1074	TRP	N-CA-C	5.74	119.02	109.96
2	B	365	VAL	N-CA-C	5.72	115.91	110.53
15	Y	295	TYR	CA-C-N	5.58	128.77	120.17
15	Y	295	TYR	C-N-CA	5.58	128.77	120.17
2	B	158	GLY	CA-C-N	-5.57	114.36	119.82
2	B	158	GLY	C-N-CA	-5.57	114.36	119.82
5	e	1195	ASN	O-C-N	-5.54	116.29	121.72
2	b	144	TRP	N-CA-C	-5.51	104.97	110.97
11	O	628	LEU	N-CA-C	-5.50	108.34	114.62
5	E	1025	GLN	N-CA-C	-5.46	104.56	111.11
1	a	60	SER	N-CA-C	5.45	116.55	108.86
4	D	228	ALA	CA-C-N	-5.43	114.17	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	228	ALA	C-N-CA	-5.43	114.17	119.76
3	C	132	THR	N-CA-C	5.41	116.98	111.14
2	b	91	GLY	N-CA-C	5.40	121.17	111.34
6	f	289	GLN	CA-C-N	-5.40	114.36	119.76
6	f	289	GLN	C-N-CA	-5.40	114.36	119.76
2	B	222	ALA	N-CA-C	5.37	117.13	111.28
5	e	1054	HIS	N-CA-C	-5.35	105.34	111.07
5	e	975	ILE	N-CA-C	5.30	115.51	110.42
5	e	798	SER	N-CA-C	-5.30	105.59	111.36
8	h	78	SER	N-CA-C	5.29	116.32	108.60
2	b	645	ILE	N-CA-C	-5.27	105.25	110.62
8	h	253	THR	CA-C-N	-5.23	113.92	120.51
8	h	253	THR	C-N-CA	-5.23	113.92	120.51
13	W	1308	ASP	CA-C-N	-5.21	114.34	120.12
13	W	1308	ASP	C-N-CA	-5.21	114.34	120.12
3	c	136	CYS	N-CA-C	5.21	117.56	108.76
7	G	1435	CYS	N-CA-C	5.20	116.63	111.07
4	d	228	ALA	CA-C-N	-5.19	114.61	119.90
4	d	228	ALA	C-N-CA	-5.19	114.61	119.90
1	A	1057	ALA	N-CA-C	-5.17	107.10	113.41
7	g	1594	TYR	CA-C-N	-5.15	113.37	120.28
7	g	1594	TYR	C-N-CA	-5.15	113.37	120.28
7	G	1252	GLY	CA-C-N	-5.12	114.30	119.83
7	G	1252	GLY	C-N-CA	-5.12	114.30	119.83
5	e	1328	ASP	N-CA-C	5.12	116.94	108.49
2	b	296	ARG	N-CA-C	-5.11	106.88	113.01
2	B	431	GLU	N-CA-C	5.08	116.50	111.07
1	A	682	VAL	N-CA-C	-5.04	107.64	111.62
15	Y	398	GLY	N-CA-C	5.01	117.80	110.63
3	C	256	ALA	CB-CA-C	-5.00	110.79	116.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	THR	Peptide
1	A	1771	SER	Peptide
15	Y	286	TYR	Peptide
1	a	1053	THR	Peptide
1	a	1355	PRO	Peptide
6	f	237	MET	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	A	9238	0	4628	35	0
1	a	8811	0	4324	46	0
2	B	4799	0	4722	51	0
2	b	4549	0	4272	41	0
3	C	2557	0	2454	19	0
3	c	2445	0	2337	17	0
4	D	2473	0	2381	18	0
4	d	2435	0	2340	15	0
5	E	7891	0	5504	81	0
5	e	8134	0	6437	97	0
6	F	1607	0	744	7	0
6	f	2524	0	2439	27	0
7	G	4209	0	3757	47	0
7	g	4770	0	4551	66	0
8	H	2235	0	2100	9	0
8	h	2259	0	2141	17	0
9	I	3626	0	1617	19	0
9	i	3347	0	1497	2	0
10	J	5029	0	1569	5	0
11	K	3460	0	1508	4	0
11	L	3372	0	1473	0	0
11	M	3246	0	1416	9	0
11	N	3480	0	1521	7	0
11	O	3391	0	1485	7	0
12	P	2945	0	1314	12	0
12	S	432	0	433	5	0
12	p	2267	0	1004	25	0
12	s	432	0	433	1	0
13	W	2636	0	2655	33	0
14	X	794	0	155	0	0
15	Y	1676	0	722	2	0
16	j	5094	0	2310	2	0
All	All	116163	0	76243	664	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 3.

All (664) 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)
1:a:1627:GLN:O	1:a:1631:THR:CB	1.87	1.22
12:p:614:ALA:HA	12:p:629:LEU:CB	1.70	1.21
5:e:968:VAL:HA	6:f:275:LYS:HA	1.33	1.10
12:p:618:GLU:HA	12:p:626:ALA:HB1	1.33	1.09
12:p:227:MET:CB	12:p:461:TYR:HA	1.83	1.09
12:p:618:GLU:HA	12:p:626:ALA:CB	1.87	1.04
5:E:1016:LEU:HD21	5:E:1025:GLN:HA	1.43	1.01
2:B:71:LEU:HD13	2:B:108:VAL:HG12	1.45	0.98
5:E:1136:TRP:HZ3	7:G:1673:SER:CB	1.78	0.97
5:E:1136:TRP:CZ3	7:G:1673:SER:CB	2.49	0.95
12:p:234:VAL:CB	12:p:254:ALA:HB1	1.97	0.94
2:B:71:LEU:CD1	2:B:108:VAL:HG12	1.96	0.93
5:e:910:ALA:HB2	5:e:925:CYS:HB2	1.48	0.93
12:p:193:ASN:CB	12:p:553:TYR:CB	2.48	0.92
12:p:650:VAL:CB	12:p:664:LEU:CB	2.48	0.91
5:E:1016:LEU:CD2	5:E:1025:GLN:HG2	2.03	0.89
7:G:1045:VAL:CG1	7:G:1047:LEU:HD12	2.05	0.87
5:E:1016:LEU:HD11	5:E:1028:CYS:HB2	1.56	0.87
7:G:1045:VAL:HG12	7:G:1047:LEU:HD12	1.55	0.85
2:B:71:LEU:HD12	2:B:108:VAL:HG11	1.57	0.84
12:p:617:ALA:HB3	12:p:629:LEU:CB	2.05	0.84
7:g:1071:ARG:HB3	8:h:266:HIS:HB2	1.57	0.84
5:E:1046:VAL:HG13	5:E:1085:TYR:HB2	1.59	0.84
2:B:71:LEU:CD1	2:B:108:VAL:CG1	2.55	0.84
5:E:1016:LEU:HD21	5:E:1025:GLN:CA	2.08	0.82
5:E:1016:LEU:CD1	5:E:1028:CYS:HB2	2.07	0.82
1:a:1628:LEU:O	1:a:1632:SER:N	2.12	0.82
2:B:71:LEU:HD12	2:B:108:VAL:CG1	2.09	0.81
12:p:614:ALA:HB2	12:p:629:LEU:O	1.80	0.81
5:E:1016:LEU:HD21	5:E:1025:GLN:CB	2.12	0.80
12:p:702:GLU:CB	12:p:708:ILE:N	2.45	0.80
5:e:797:LEU:HD11	5:e:879:MET:HE1	1.62	0.79
5:E:1016:LEU:HD21	5:E:1025:GLN:HG2	1.65	0.78
4:D:166:SER:HB2	4:D:187:ASP:HB2	1.66	0.77
1:A:444:GLY:HA2	1:A:516:GLY:HA3	1.66	0.75
2:b:558:LEU:HD11	2:b:575:LEU:HD22	1.68	0.75
1:A:327:ALA:HB1	1:A:360:ALA:HA	1.69	0.75
7:g:1571:TRP:HB3	7:g:1611:ILE:HG12	1.67	0.75
7:g:1071:ARG:HD2	8:h:279:SER:HB3	1.69	0.74
5:E:1042:LEU:HD22	5:E:1078:LEU:HD11	1.69	0.74
13:W:1141:LEU:HD23	13:W:1144:LYS:HD2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:p:224:LEU:HA	12:p:460:PRO:O	1.88	0.73
5:E:1016:LEU:HD12	5:E:1028:CYS:CB	2.19	0.73
5:E:1016:LEU:HD21	5:E:1025:GLN:CG	2.18	0.73
13:W:1366:PRO:HG3	5:e:990:ARG:HB3	1.70	0.73
9:I:428:GLN:O	9:I:432:VAL:N	2.22	0.73
15:Y:263:TYR:HA	15:Y:281:GLY:HA3	1.71	0.72
7:g:1257:VAL:HG13	7:g:1320:GLU:HB2	1.71	0.72
7:G:1045:VAL:CG1	7:G:1047:LEU:CD1	2.66	0.72
5:E:1016:LEU:HD23	5:E:1025:GLN:HG2	1.69	0.72
7:g:1484:LEU:HD22	7:g:1489:LEU:HD12	1.71	0.72
2:b:239:PRO:HG2	2:b:256:TRP:HA	1.72	0.72
2:b:527:MET:HG2	2:b:534:THR:HA	1.72	0.71
4:D:116:VAL:HA	4:D:134:SER:HB3	1.72	0.71
7:G:1071:ARG:HB3	8:H:266:HIS:HB2	1.72	0.70
2:b:343:LEU:HA	2:b:346:ILE:HD12	1.74	0.70
2:b:577:LEU:O	2:b:581:PRO:HD2	1.93	0.69
13:W:1188:GLN:O	13:W:1192:PRO:HD2	1.93	0.69
12:p:680:VAL:O	12:p:683:GLU:HA	1.93	0.69
5:E:1019:ILE:HG21	5:E:1024:ARG:HD2	1.75	0.69
13:W:1079:TRP:HB2	13:W:1091:ALA:HB1	1.75	0.69
5:e:1191:LEU:HD23	5:e:1202:ALA:HB2	1.73	0.69
5:e:1128:ARG:HH21	5:e:1179:GLU:HG2	1.59	0.68
9:I:187:VAL:O	9:I:191:GLN:N	2.23	0.68
13:W:1059:PRO:HG3	1:a:3:ALA:HB1	1.77	0.67
5:E:1016:LEU:CD1	5:E:1028:CYS:CB	2.73	0.67
2:B:595:THR:HB	2:B:637:LEU:HD22	1.77	0.67
3:c:262:TRP:HE1	3:c:279:GLU:HB3	1.59	0.67
6:f:166:SER:HB2	6:f:185:GLU:HB3	1.76	0.67
5:E:866:TRP:O	5:E:868:SER:N	2.27	0.66
5:e:968:VAL:CA	6:f:275:LYS:HA	2.19	0.66
5:E:962:LEU:HD13	5:E:995:LEU:HD13	1.77	0.66
7:g:1255:ARG:HD2	7:g:1257:VAL:HB	1.76	0.66
1:A:1066:GLN:HA	1:A:1069:ALA:HB3	1.76	0.66
5:e:965:LEU:HA	5:e:968:VAL:HB	1.78	0.66
12:p:614:ALA:CB	12:p:629:LEU:O	2.43	0.66
5:e:773:MET:HE1	5:e:890:TYR:HA	1.77	0.65
1:a:1013:SER:HA	1:a:1072:ASP:HA	1.79	0.65
4:D:41:LYS:HE3	4:D:45:VAL:HA	1.79	0.65
5:e:1224:ILE:HG12	5:e:1237:VAL:HG11	1.79	0.65
2:B:599:MET:HE3	2:B:637:LEU:HD12	1.80	0.64
2:b:54:MET:HE1	4:d:27:MET:HE1	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:140:VAL:O	12:S:144:VAL:HG23	1.98	0.64
4:d:166:SER:HB2	4:d:187:ASP:HB2	1.78	0.64
7:g:1552:SER:HA	7:g:1556:GLY:HA3	1.79	0.64
2:B:38:LEU:HG	2:B:40:GLN:H	1.63	0.64
13:W:1191:ASP:HB2	13:W:1192:PRO:HD3	1.79	0.64
2:b:25:PHE:HB2	2:b:32:LEU:HD11	1.80	0.63
5:e:1322:ASN:HA	5:e:1325:LYS:HE2	1.79	0.63
6:f:233:ILE:HG23	6:f:243:PRO:HB3	1.80	0.63
13:W:1092:ALA:HB2	13:W:1125:SER:HB3	1.80	0.63
7:G:1292:VAL:CG1	9:I:372:TRP:CB	2.76	0.63
11:M:723:GLU:HA	11:M:726:ALA:HB3	1.80	0.63
13:W:1059:PRO:HG3	1:a:3:ALA:CB	2.29	0.63
1:A:1641:ALA:HB1	1:A:1682:ALA:HA	1.80	0.63
5:e:1302:HIS:HB3	5:e:1324:TYR:CE1	2.34	0.62
4:d:207:ARG:HH22	5:e:1280:THR:HG21	1.64	0.62
9:I:459:SER:O	9:I:461:ILE:N	2.32	0.62
5:E:1378:TRP:CD1	7:G:1064:LEU:HD21	2.35	0.62
5:e:1192:ALA:HA	5:e:1199:ALA:HB2	1.82	0.62
7:g:1071:ARG:HH11	8:h:279:SER:HB3	1.64	0.62
5:E:973:LEU:HD21	6:F:18:TYR:H	1.65	0.62
2:B:25:PHE:HE2	4:D:285:SER:HB3	1.65	0.61
7:G:1282:HIS:C	7:G:1284:LEU:H	2.08	0.61
8:H:235:GLN:HA	8:H:263:VAL:HG13	1.80	0.61
2:b:287:GLY:HA2	2:b:312:PHE:HB3	1.83	0.61
1:a:1230:LEU:HD22	1:a:1261:LEU:HD23	1.83	0.61
5:E:1016:LEU:CD2	5:E:1025:GLN:HA	2.26	0.61
2:B:330:LEU:HD22	2:B:348:LEU:HD11	1.83	0.61
8:h:235:GLN:HA	8:h:263:VAL:HG13	1.83	0.61
1:a:1627:GLN:O	1:a:1631:THR:N	2.32	0.60
6:f:279:GLN:HG2	6:f:295:THR:HG22	1.83	0.60
9:I:233:GLU:HA	9:I:247:LYS:HA	1.83	0.60
15:Y:263:TYR:HA	15:Y:281:GLY:CA	2.31	0.60
5:E:1296:ALA:HB3	5:E:1300:LEU:HB2	1.84	0.60
5:e:968:VAL:HA	6:f:275:LYS:CA	2.22	0.60
1:a:1265:VAL:CG1	1:a:1269:LYS:HE3	2.32	0.60
6:f:232:TRP:HD1	6:f:249:ALA:HB2	1.65	0.60
8:H:82:LYS:HG2	8:H:100:THR:HG22	1.83	0.60
11:O:188:CYS:O	11:O:192:GLU:N	2.34	0.60
4:D:320:LYS:HE3	4:D:326:VAL:HA	1.83	0.59
5:E:1357:LEU:HD22	5:E:1417:LYS:HD3	1.84	0.59
2:b:155:ALA:HB1	2:b:159:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:PHE:HB2	2:B:32:LEU:HD11	1.84	0.59
5:e:1192:ALA:HA	5:e:1199:ALA:CB	2.32	0.59
3:C:178:LEU:HD13	3:C:184:LEU:HD11	1.84	0.59
8:H:267:VAL:HB	8:H:276:LEU:HD11	1.83	0.59
1:a:1217:LYS:HD3	1:a:1221:GLY:H	1.68	0.59
7:G:1071:ARG:HD2	8:H:279:SER:HB3	1.83	0.59
13:W:1065:ALA:HB1	13:W:1075:MET:HE2	1.85	0.59
5:e:766:GLN:HG3	5:e:897:TRP:HB2	1.86	0.58
2:b:25:PHE:HE2	4:d:285:SER:HB3	1.69	0.58
12:p:614:ALA:CB	12:p:629:LEU:C	2.76	0.58
13:W:1152:LEU:O	13:W:1155:GLN:HG3	2.04	0.58
1:A:520:GLY:O	1:A:523:CYS:N	2.37	0.58
4:D:13:ASP:HB3	4:D:32:SER:HB3	1.86	0.58
7:G:1181:LEU:HD11	7:G:1192:VAL:HG11	1.86	0.58
7:G:1257:VAL:HG13	7:G:1320:GLU:HB2	1.86	0.57
5:e:933:VAL:HG21	5:e:954:ARG:HB3	1.87	0.57
11:K:41:GLU:O	11:K:45:ALA:HB2	2.04	0.57
1:a:1054:PRO:C	1:a:1056:LEU:H	2.10	0.57
7:g:1167:GLY:H	7:g:1462:ALA:HB1	1.69	0.57
13:W:1159:THR:HG22	13:W:1164:HIS:HA	1.85	0.57
2:B:148:GLU:HB2	2:B:152:ILE:HD12	1.86	0.57
7:g:1124:HIS:HD2	8:h:7:THR:HB	1.69	0.57
2:B:596:TYR:HE1	5:E:1122:ALA:HB2	1.68	0.57
4:D:228:ALA:HB3	4:D:237:ILE:HB	1.86	0.57
5:e:961:VAL:HB	5:e:977:LEU:HD21	1.86	0.57
3:C:233:GLY:HA3	3:C:261:MET:HE2	1.87	0.57
7:G:1291:MET:HG2	7:G:1294:SER:HB3	1.86	0.56
2:b:148:GLU:HB2	2:b:152:ILE:HD12	1.85	0.56
5:E:1131:ARG:HG3	5:E:1133:GLU:HG2	1.87	0.56
5:e:957:TYR:O	5:e:961:VAL:HG23	2.05	0.56
7:g:1691:GLN:HB2	7:g:1692:PRO:HD3	1.87	0.56
9:I:456:ILE:O	9:I:459:SER:C	2.48	0.56
1:a:1040:GLY:O	1:a:1042:ASP:N	2.35	0.56
5:e:795:GLN:O	5:e:799:VAL:HG23	2.05	0.56
5:e:797:LEU:HD11	5:e:879:MET:CE	2.33	0.56
7:g:1257:VAL:CG1	7:g:1320:GLU:HB2	2.36	0.56
12:p:618:GLU:HA	12:p:626:ALA:HB2	1.80	0.56
5:E:973:LEU:HD21	6:F:18:TYR:N	2.20	0.56
1:a:1627:GLN:O	1:a:1631:THR:CA	2.53	0.56
1:A:1206:GLN:HE22	2:B:461:THR:HG23	1.70	0.56
1:A:1866:SER:O	1:A:1870:LYS:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:1533:LEU:HD23	7:g:1537:LEU:HD12	1.86	0.56
5:E:862:LEU:O	5:E:866:TRP:N	2.33	0.56
5:e:1196:PRO:O	5:e:1199:ALA:HB3	2.05	0.55
1:A:259:GLU:O	1:A:262:GLY:N	2.33	0.55
1:A:1299:LEU:HD23	1:A:1305:ARG:HB2	1.88	0.55
5:E:1016:LEU:CD2	5:E:1025:GLN:CG	2.77	0.55
5:E:1378:TRP:HD1	7:G:1064:LEU:HD21	1.69	0.55
11:M:415:ASP:O	11:M:419:LEU:CB	2.54	0.55
7:g:1611:ILE:HB	7:g:1614:TRP:HB2	1.88	0.55
5:E:1358:GLY:HA2	5:E:1369:PRO:HB3	1.89	0.55
5:E:1388:ARG:HH12	7:G:1051:VAL:HG11	1.71	0.55
2:b:442:LEU:HD11	2:b:467:ILE:HD12	1.88	0.55
5:E:1291:LEU:O	5:E:1295:GLU:HG3	2.06	0.55
5:e:879:MET:HG2	5:e:884:TYR:HE1	1.72	0.55
5:e:1070:LEU:HD13	5:e:1103:LEU:HA	1.89	0.55
2:B:633:LEU:O	2:B:637:LEU:HG	2.06	0.55
4:D:215:LEU:HD21	4:D:250:MET:HE2	1.89	0.55
11:N:36:TYR:O	11:N:39:ALA:C	2.50	0.55
13:W:1316:LYS:HB3	13:W:1319:HIS:HB3	1.87	0.55
16:j:905:GLN:O	16:j:908:GLN:N	2.38	0.55
4:D:253:LEU:HD12	4:D:265:LYS:HB3	1.89	0.55
11:M:376:PHE:HA	11:M:381:GLY:HA3	1.89	0.55
5:e:800:LEU:HD23	5:e:961:VAL:HG22	1.89	0.55
5:e:872:PHE:CZ	5:e:874:PHE:HB3	2.42	0.55
4:d:140:ARG:HG2	4:d:158:GLU:HG2	1.89	0.55
5:e:879:MET:HG2	5:e:884:TYR:CE1	2.42	0.55
6:f:188:GLY:HA2	6:f:211:LEU:HB2	1.88	0.55
12:S:134:LEU:HA	12:S:137:TRP:HD1	1.71	0.55
7:g:1612:GLN:C	7:g:1614:TRP:H	2.13	0.55
5:e:1259:ALA:HA	5:e:1262:TRP:CD1	2.42	0.54
1:A:153:ARG:O	1:A:154:LYS:C	2.51	0.54
5:E:1016:LEU:HD12	5:E:1028:CYS:HB3	1.87	0.54
2:b:581:PRO:O	2:b:585:GLN:HG2	2.08	0.54
2:B:634:ARG:NE	5:E:1125:ASN:HB3	2.22	0.54
6:f:71:HIS:HE1	6:f:99:ALA:HB2	1.72	0.54
12:P:180:ASN:CB	7:g:1467:HIS:HA	2.38	0.54
5:E:1241:LEU:HG	5:E:1287:MET:HE2	1.90	0.54
6:f:227:VAL:HG22	6:f:257:PHE:HB2	1.90	0.54
11:O:727:TYR:O	11:O:731:ALA:CB	2.56	0.54
5:e:1306:ILE:HG21	5:e:1335:LEU:HD13	1.89	0.54
8:h:82:LYS:HG2	8:h:100:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:1612:GLN:C	7:g:1614:TRP:N	2.63	0.54
2:B:626:ASP:O	2:B:630:VAL:HG23	2.08	0.54
1:a:104:GLY:O	1:a:108:ALA:N	2.41	0.54
6:f:270:THR:HG23	6:f:302:LEU:HD22	1.90	0.54
13:W:1061:LEU:HD13	13:W:1078:LEU:HA	1.90	0.53
6:f:46:ILE:HG13	6:f:93:LEU:HD21	1.89	0.53
1:a:1224:VAL:HG12	1:a:1268:ASN:HB3	1.90	0.53
7:g:1554:ARG:HB2	8:h:68:PRO:HB3	1.91	0.53
3:C:178:LEU:HA	3:C:222:ARG:HD3	1.90	0.53
7:G:1139:SER:O	7:G:1143:PRO:HD2	2.08	0.53
5:e:868:SER:HA	5:e:900:VAL:HB	1.89	0.53
5:e:1422:THR:HG23	7:g:1060:ILE:H	1.73	0.53
2:B:542:PHE:CD1	2:B:554:ALA:HB1	2.44	0.53
11:O:26:SER:O	11:O:29:GLY:N	2.41	0.53
8:h:267:VAL:HB	8:h:276:LEU:HD11	1.90	0.53
5:e:878:LEU:HD12	5:e:887:LEU:HD13	1.91	0.53
5:e:1195:ASN:HB3	5:e:1198:THR:OG1	2.09	0.53
5:E:996:ARG:HD2	5:E:1019:ILE:HA	1.90	0.53
2:B:239:PRO:HG2	2:B:256:TRP:HA	1.91	0.53
5:e:1054:HIS:HE1	5:e:1086:ARG:HG3	1.74	0.53
9:I:459:SER:C	9:I:461:ILE:H	2.17	0.52
6:f:192:PHE:HD2	6:f:202:LEU:HB3	1.73	0.52
7:G:1323:ARG:HG2	7:G:1342:ILE:HG23	1.91	0.52
7:g:1608:CYS:HB2	7:g:1614:TRP:CD1	2.44	0.52
5:e:894:LEU:HD11	5:e:905:CYS:SG	2.50	0.52
7:G:1292:VAL:HG11	9:I:372:TRP:CB	2.40	0.52
13:W:1076:ASP:HA	13:W:1079:TRP:CD1	2.45	0.52
5:e:884:TYR:CE2	5:e:915:VAL:HG11	2.44	0.52
7:g:1083:ASN:HA	7:g:1123:VAL:HG13	1.91	0.52
1:A:1321:LEU:C	1:A:1321:LEU:HD12	2.35	0.52
3:C:10:VAL:O	3:C:365:GLU:HB3	2.10	0.52
12:P:180:ASN:HA	7:g:1467:HIS:HA	1.91	0.52
6:f:18:TYR:HD2	6:f:316:TYR:HA	1.74	0.52
12:p:614:ALA:HB1	12:p:630:TYR:HA	1.91	0.52
8:H:184:SER:HB3	8:H:194:TRP:HE1	1.75	0.52
1:a:1234:LEU:HD23	1:a:1257:ILE:HG23	1.92	0.52
12:p:630:TYR:CB	12:p:638:LYS:CB	2.88	0.52
3:C:208:PHE:HD1	3:C:248:LYS:HA	1.75	0.51
5:E:1419:LYS:HA	5:E:1422:THR:HG22	1.91	0.51
9:I:609:ARG:O	9:I:611:ARG:N	2.43	0.51
4:d:87:GLU:HB3	4:d:106:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:876:GLU:O	5:e:880:ARG:HG3	2.10	0.51
5:e:1309:LEU:HB3	5:e:1314:VAL:HG11	1.92	0.51
4:d:228:ALA:HB3	4:d:237:ILE:HB	1.90	0.51
7:g:1171:ILE:HG21	7:g:1207:GLY:HA2	1.91	0.51
7:g:1254:GLU:HG3	7:g:1275:LEU:HD11	1.92	0.51
13:W:1233:SER:O	13:W:1237:ARG:HG3	2.11	0.51
3:c:146:GLU:HA	3:c:171:THR:HG23	1.92	0.51
5:e:823:PHE:HB2	5:e:874:PHE:HD2	1.75	0.51
7:g:1318:GLN:HB3	7:g:1321:ARG:HB2	1.93	0.51
7:g:1323:ARG:HG2	7:g:1342:ILE:HG23	1.92	0.51
10:J:847:ALA:O	10:J:851:CYS:HA	2.10	0.51
5:E:1234:LEU:H	5:E:1300:LEU:HD21	1.76	0.50
2:b:611:GLU:HB3	5:e:1294:TYR:HE1	1.75	0.50
5:E:1019:ILE:HG22	5:E:1021:ASP:H	1.76	0.50
7:G:1071:ARG:CB	8:H:266:HIS:HB2	2.41	0.50
11:N:632:PHE:C	11:N:634:ASN:H	2.18	0.50
2:B:631:GLU:HG2	5:E:1129:LEU:HG	1.93	0.50
4:D:197:VAL:HB	4:D:215:LEU:HB2	1.94	0.50
7:G:1292:VAL:HG12	9:I:372:TRP:CB	2.42	0.50
3:C:187:ASN:HD21	3:C:191:GLN:HB2	1.77	0.50
5:E:1103:LEU:HD12	5:E:1107:VAL:HG13	1.94	0.50
5:e:1419:LYS:O	5:e:1422:THR:HB	2.12	0.50
9:I:723:MET:O	9:I:727:LEU:CB	2.60	0.50
1:a:1055:HIS:C	1:a:1057:ALA:H	2.20	0.50
5:E:1016:LEU:HD11	5:E:1025:GLN:HA	1.94	0.49
11:N:70:PHE:O	11:N:75:ASN:N	2.34	0.49
13:W:1155:GLN:O	13:W:1156:GLU:C	2.54	0.49
1:a:320:TRP:C	1:a:322:SER:H	2.20	0.49
2:b:571:PHE:O	2:b:575:LEU:HG	2.12	0.49
13:W:1111:ARG:HG2	13:W:1177:SER:HA	1.94	0.49
13:W:1075:MET:SD	13:W:1098:LEU:HB2	2.52	0.49
2:b:287:GLY:CA	2:b:312:PHE:HB3	2.42	0.49
1:a:1102:SER:O	1:a:1105:SER:N	2.43	0.49
5:e:1065:ALA:C	5:e:1067:ALA:H	2.21	0.49
1:A:1247:ILE:HD13	5:E:1264:ALA:HB2	1.95	0.49
2:B:591:SER:O	2:B:595:THR:HG23	2.12	0.49
2:B:646:VAL:HG13	5:E:1040:SER:O	2.12	0.49
1:a:493:LYS:O	1:a:497:GLN:N	2.27	0.49
5:e:1367:GLN:HB2	5:e:1376:LEU:HD21	1.94	0.49
10:J:153:UNK:O	10:J:166:UNK:N	2.45	0.49
5:e:1422:THR:HG23	7:g:1060:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ALA:HB1	2:B:225:ARG:HG3	1.95	0.49
9:I:157:HIS:C	9:I:160:SER:H	2.21	0.49
1:a:1628:LEU:O	1:a:1629:ILE:C	2.55	0.49
8:h:264:VAL:HA	8:h:280:GLY:HA2	1.94	0.49
1:A:1631:THR:C	1:A:1633:SER:H	2.19	0.49
12:P:659:SER:C	12:P:661:ARG:H	2.20	0.49
9:I:584:VAL:O	9:I:587:LEU:N	2.45	0.49
5:E:927:SER:HB3	5:E:954:ARG:HG2	1.95	0.48
1:A:1141:LEU:O	1:A:1143:ASP:N	2.42	0.48
11:O:19:ALA:O	11:O:23:ARG:N	2.44	0.48
3:c:17:THR:HG22	3:c:35:THR:HG22	1.95	0.48
4:d:320:LYS:HE3	4:d:326:VAL:HA	1.95	0.48
5:E:1296:ALA:C	5:E:1298:ASN:H	2.22	0.48
7:G:1282:HIS:C	7:G:1284:LEU:N	2.68	0.48
5:e:939:LEU:HD12	5:e:957:TYR:HB3	1.94	0.48
7:g:1376:GLU:HA	7:g:1379:PHE:CE1	2.48	0.48
2:b:415:TRP:HZ3	2:b:437:MET:HE1	1.79	0.48
2:B:595:THR:HB	2:B:637:LEU:HD13	1.95	0.48
2:b:124:ARG:HA	2:b:127:ALA:HB2	1.94	0.48
5:e:1350:LEU:HD22	5:e:1410:LYS:HD3	1.96	0.48
9:i:663:ILE:HA	9:i:705:LYS:O	2.14	0.48
1:A:1318:VAL:O	1:A:1321:LEU:HG	2.13	0.48
5:E:824:PHE:HA	5:E:828:ALA:HB3	1.94	0.48
11:M:70:PHE:O	11:M:75:ASN:N	2.46	0.48
1:a:112:LEU:O	1:a:116:GLU:N	2.42	0.48
5:e:968:VAL:HG22	6:f:275:LYS:HA	1.96	0.48
6:f:227:VAL:HG13	6:f:257:PHE:HD2	1.78	0.48
13:W:1130:THR:O	13:W:1131:LEU:C	2.56	0.48
1:a:1230:LEU:HD22	1:a:1261:LEU:CD2	2.44	0.48
2:b:330:LEU:HD22	2:b:348:LEU:HD11	1.96	0.48
6:f:211:LEU:HD11	6:f:226:ALA:HB1	1.96	0.48
7:G:1206:TRP:CH2	7:G:1426:LEU:HB3	2.49	0.48
1:a:1630:LEU:C	1:a:1640:ALA:HA	2.39	0.48
4:d:302:VAL:HB	4:d:319:LEU:HD12	1.95	0.48
5:E:920:HIS:O	5:E:923:LEU:HB3	2.14	0.48
11:M:128:SER:O	11:M:132:TYR:CB	2.62	0.48
12:P:187:ARG:CB	7:g:1431:GLN:HB2	2.44	0.48
5:e:1333:LEU:HD13	5:e:1348:LEU:HD23	1.95	0.48
12:p:702:GLU:CB	12:p:708:ILE:CA	2.92	0.48
7:G:1566:LEU:HD13	7:G:1598:PHE:HA	1.96	0.47
3:c:353:VAL:HB	3:c:358:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:59:ARG:O	5:E:61:PHE:N	2.47	0.47
5:E:1291:LEU:HD22	5:E:1323:ARG:HH21	1.79	0.47
5:e:773:MET:CE	5:e:890:TYR:HA	2.43	0.47
5:E:1093:GLY:HA3	5:E:1127:LEU:HD21	1.96	0.47
7:G:1257:VAL:CG1	7:G:1320:GLU:HB2	2.44	0.47
1:a:1871:TYR:HA	1:a:1874:ALA:HB3	1.96	0.47
3:c:97:THR:HG23	3:c:117:GLU:HA	1.97	0.47
6:f:172:ALA:HB3	6:f:182:MET:HE2	1.94	0.47
2:B:25:PHE:CE2	4:D:285:SER:HB3	2.48	0.47
2:B:148:GLU:HG3	2:B:149:ILE:N	2.29	0.47
5:e:823:PHE:CD2	5:e:874:PHE:HB2	2.50	0.47
6:f:282:ILE:HG21	6:f:324:THR:HG21	1.97	0.47
1:A:1557:ALA:HA	12:S:124:MET:HG3	1.96	0.47
1:A:1631:THR:C	1:A:1633:SER:N	2.71	0.47
1:A:1631:THR:O	1:A:1633:SER:N	2.48	0.47
7:G:1072:VAL:HG21	7:G:1081:VAL:HB	1.96	0.47
5:e:1302:HIS:HB3	5:e:1324:TYR:HE1	1.76	0.47
7:g:1302:SER:HB2	7:g:1329:SER:HA	1.96	0.47
7:g:1614:TRP:O	7:g:1615:GLU:C	2.54	0.47
12:p:617:ALA:CB	12:p:629:LEU:CB	2.86	0.47
1:a:1420:LEU:O	1:a:1424:LEU:N	2.44	0.47
7:g:1347:GLN:HE21	7:g:1347:GLN:HB2	1.53	0.47
5:E:906:HIS:O	5:E:925:CYS:HB3	2.15	0.47
11:O:377:ALA:HB3	11:O:381:GLY:H	1.80	0.47
12:P:459:GLN:HA	12:P:463:TYR:H	1.79	0.47
5:e:796:HIS:ND1	5:e:964:LEU:HD11	2.30	0.47
5:e:882:CYS:HA	5:e:884:TYR:CE2	2.49	0.47
11:O:645:LEU:O	11:O:649:ALA:HB2	2.14	0.47
12:P:180:ASN:CA	7:g:1467:HIS:HA	2.45	0.47
3:c:10:VAL:HG22	3:c:11:SER:H	1.79	0.47
1:a:1682:ALA:O	1:a:1684:LEU:N	2.47	0.47
3:C:138:SER:HA	3:C:139:PRO:HA	1.69	0.46
7:G:1376:GLU:HA	7:G:1379:PHE:CE1	2.50	0.46
5:e:872:PHE:HB3	5:e:901:ASN:OD1	2.15	0.46
7:g:1634:ILE:HG22	7:g:1639:SER:HA	1.97	0.46
1:a:1265:VAL:HG12	1:a:1269:LYS:HE3	1.97	0.46
2:b:542:PHE:CD1	2:b:554:ALA:HB1	2.50	0.46
7:g:1084:GLY:H	7:g:1123:VAL:HA	1.80	0.46
5:E:968:VAL:HG11	6:F:316:TYR:CB	2.46	0.46
11:M:246:LYS:O	11:M:248:ASP:N	2.44	0.46
12:S:113:ALA:O	12:S:116:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:ARG:HG2	2:B:434:LYS:HE3	1.98	0.46
12:P:560:ASP:O	12:P:563:GLY:N	2.49	0.46
5:E:299:LEU:O	5:E:311:TRP:N	2.37	0.46
5:E:1004:LEU:HD21	5:E:1032:LEU:HA	1.97	0.46
13:W:1078:LEU:HD23	13:W:1094:VAL:HG11	1.98	0.46
1:a:301:PHE:C	1:a:303:ASP:H	2.22	0.46
1:a:651:GLY:O	1:a:657:ALA:HB2	2.16	0.46
11:N:312:ILE:O	11:N:316:ALA:N	2.45	0.46
1:a:1771:SER:O	1:a:1772:PRO:C	2.57	0.46
2:b:262:GLU:HG3	2:b:265:ARG:HH12	1.81	0.46
7:g:1139:SER:O	7:g:1143:PRO:HD2	2.15	0.46
12:p:459:GLN:HA	12:p:463:TYR:H	1.79	0.46
1:A:1130:ARG:O	1:A:1131:SER:C	2.57	0.46
8:H:230:ILE:HG13	8:H:242:TRP:HB2	1.98	0.46
3:c:178:LEU:HD12	3:c:222:ARG:HD3	1.96	0.46
5:e:1259:ALA:O	5:e:1263:LEU:HG	2.15	0.46
7:G:1045:VAL:HG13	7:G:1047:LEU:HD11	1.97	0.46
2:b:38:LEU:HG	2:b:40:GLN:H	1.81	0.46
5:e:1096:MET:HB2	5:e:1123:CYS:HB2	1.97	0.46
8:h:190:LEU:HD22	8:h:208:GLU:HG2	1.98	0.46
2:b:579:ALA:HA	2:b:582:LEU:HD12	1.98	0.46
3:c:154:ARG:HB2	3:c:161:LEU:HD11	1.98	0.46
7:g:1290:GLN:HE21	7:g:1290:GLN:HB2	1.61	0.45
5:E:1030:ARG:HD2	5:E:1060:ILE:HG21	1.98	0.45
5:e:968:VAL:HG13	6:f:274:GLY:O	2.16	0.45
7:g:1592:TYR:CE1	7:g:1624:TYR:HE1	2.34	0.45
2:B:131:ILE:HA	2:B:134:ILE:HD12	1.98	0.45
5:E:1000:PHE:CD2	5:E:1012:ALA:HB1	2.52	0.45
1:a:1211:ILE:O	1:a:1215:GLU:HG2	2.16	0.45
1:a:1630:LEU:CB	1:a:1639:GLN:O	2.65	0.45
5:e:930:ALA:HA	5:e:933:VAL:HG23	1.97	0.45
12:p:614:ALA:HB1	12:p:629:LEU:C	2.41	0.45
1:a:1217:LYS:O	1:a:1218:ASN:C	2.60	0.45
7:g:1627:VAL:O	7:g:1628:ILE:C	2.59	0.45
2:B:519:LEU:HA	3:C:214:ARG:HH22	1.81	0.45
3:C:154:ARG:HB2	3:C:161:LEU:HD11	1.99	0.45
4:D:27:MET:HG3	4:D:39:TRP:HB2	1.98	0.45
7:G:1045:VAL:HG13	7:G:1047:LEU:CD1	2.46	0.45
7:G:1417:ARG:HB2	7:G:1422:HIS:CE1	2.51	0.45
3:c:126:ASN:O	3:c:127:MET:HB2	2.15	0.45
5:e:58:ARG:O	5:e:59:ARG:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:1224:ILE:CG1	5:e:1237:VAL:HG11	2.45	0.45
6:f:232:TRP:CD1	6:f:249:ALA:HB2	2.50	0.45
1:A:320:TRP:C	1:A:322:SER:H	2.23	0.45
3:C:260:GLU:HG2	3:C:279:GLU:HB2	1.99	0.45
6:F:140:ILE:N	6:F:152:TRP:O	2.46	0.45
13:W:1158:LEU:HD13	13:W:1193:PHE:HB3	1.99	0.45
2:b:25:PHE:CE2	4:d:285:SER:HB3	2.50	0.45
7:g:1594:TYR:O	7:g:1595:LEU:C	2.59	0.45
7:G:1139:SER:O	7:G:1140:TYR:C	2.60	0.45
9:I:345:ILE:O	9:I:348:GLY:N	2.50	0.45
1:a:1573:LEU:O	1:a:1576:GLY:N	2.43	0.45
3:c:187:ASN:HD21	3:c:191:GLN:HB2	1.82	0.45
5:e:778:SER:O	5:e:818:THR:HG21	2.16	0.45
5:e:1195:ASN:HD22	5:e:1198:THR:HG23	1.81	0.45
4:D:140:ARG:HG2	4:D:158:GLU:HG2	1.98	0.45
12:s:118:ARG:HH21	12:s:119:LYS:HG2	1.82	0.45
7:g:1171:ILE:HD12	7:g:1171:ILE:HA	1.83	0.45
2:B:580:LEU:HB3	2:B:581:PRO:HD3	1.99	0.45
3:C:191:GLN:HG2	3:C:209:SER:HB3	1.99	0.45
1:a:1775:GLN:C	1:a:1777:THR:H	2.25	0.45
2:b:290:GLU:O	2:b:293:LEU:N	2.42	0.45
5:e:904:SER:O	5:e:908:MET:HG2	2.17	0.45
1:A:1318:VAL:HA	1:A:1321:LEU:CD2	2.47	0.44
2:B:144:TRP:HH2	2:B:374:HIS:HB3	1.81	0.44
2:B:579:ALA:HA	2:B:582:LEU:HD12	2.00	0.44
12:P:444:GLN:O	12:P:449:TYR:N	2.48	0.44
5:e:901:ASN:HD22	5:e:901:ASN:HA	1.52	0.44
7:g:1422:HIS:HB2	7:g:1437:LEU:HD13	1.99	0.44
5:E:1084:ILE:O	5:E:1085:TYR:C	2.60	0.44
13:W:1151:GLN:HG2	13:W:1152:LEU:N	2.32	0.44
2:b:334:LEU:HB3	2:b:338:SER:HB2	1.98	0.44
4:d:237:ILE:HD13	4:d:249:THR:HG22	1.99	0.44
1:A:1234:LEU:HA	1:A:1234:LEU:HD13	1.74	0.44
8:H:84:ILE:HG12	8:H:98:GLU:HG3	1.98	0.44
11:K:302:GLN:HA	11:K:306:VAL:HA	1.99	0.44
7:g:1257:VAL:HG12	7:g:1258:GLU:HG3	1.99	0.44
12:p:373:ARG:HA	12:p:398:CYS:CB	2.47	0.44
3:c:149:ARG:HD3	3:c:151:ASN:HD21	1.82	0.44
5:e:993:ALA:HB2	5:e:1020:PRO:HG2	1.98	0.44
5:e:1109:THR:HG23	5:e:1112:GLY:H	1.83	0.44
7:g:1132:GLN:O	7:g:1133:LYS:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:VAL:HG13	2:B:433:LEU:HD11	1.98	0.44
3:C:12:HIS:HB3	3:C:37:SER:HB2	1.99	0.44
3:c:223:HIS:HB2	3:c:229:VAL:HB	1.99	0.44
7:G:1372:LEU:HD22	7:G:1424:LEU:HB3	1.99	0.44
11:O:727:TYR:O	11:O:731:ALA:HB3	2.18	0.44
12:P:373:ARG:HA	12:P:398:CYS:CB	2.47	0.44
1:a:100:LEU:C	1:a:102:ASN:N	2.75	0.44
1:a:1515:LEU:O	1:a:1520:TYR:N	2.51	0.44
2:B:558:LEU:HD21	2:B:578:ASP:HB2	2.00	0.44
1:a:1283:SER:O	1:a:1286:GLN:HG2	2.18	0.44
5:e:823:PHE:HB2	5:e:874:PHE:CD2	2.52	0.44
7:g:1072:VAL:HG22	7:g:1081:VAL:HB	1.99	0.44
7:G:1426:LEU:HD13	7:G:1426:LEU:HA	1.90	0.44
9:I:269:ALA:HB1	9:I:347:ALA:HB1	2.00	0.44
10:J:612:UNK:C	10:J:614:UNK:H	2.30	0.44
9:i:805:LYS:O	9:i:809:TYR:CB	2.65	0.44
3:c:19:TRP:CE3	3:c:33:PHE:HB3	2.53	0.44
6:f:25:ASN:HB2	6:f:35:LEU:HB2	1.98	0.44
12:p:574:LEU:O	12:p:575:VAL:C	2.60	0.44
5:E:982:ILE:HG12	5:E:996:ARG:HH22	1.83	0.44
5:E:1259:ALA:HA	5:E:1262:TRP:NE1	2.33	0.44
13:W:1065:ALA:HB1	13:W:1075:MET:HG2	2.00	0.44
7:g:1122:LYS:HA	7:g:1122:LYS:HD3	1.80	0.44
1:A:853:THR:O	1:A:857:GLU:N	2.49	0.43
7:G:1072:VAL:HG11	7:G:1081:VAL:O	2.18	0.43
7:g:1152:SER:HB3	7:g:1165:ASN:HD21	1.82	0.43
5:E:1357:LEU:HD21	5:E:1414:TYR:HD2	1.82	0.43
7:G:1350:TRP:HB2	7:G:1375:TYR:OH	2.18	0.43
5:E:1187:THR:HB	5:E:1214:LEU:HD11	2.00	0.43
5:E:1301:TYR:HB3	5:E:1302:HIS:H	1.66	0.43
12:P:248:SER:O	12:P:251:MET:N	2.39	0.43
2:b:22:HIS:CE1	4:d:298:ASP:HA	2.53	0.43
5:e:1376:LEU:H	5:e:1376:LEU:HD23	1.83	0.43
1:A:1241:LEU:HD13	1:A:1253:LEU:HD13	2.00	0.43
2:B:35:TYR:CE2	2:B:37:THR:HG22	2.53	0.43
5:E:1046:VAL:CG1	5:E:1085:TYR:HB2	2.40	0.43
7:G:1446:ASP:HA	7:G:1447:PRO:HD3	1.91	0.43
7:G:1484:LEU:HD22	7:G:1489:LEU:HD12	2.00	0.43
13:W:1092:ALA:CB	13:W:1125:SER:HB3	2.47	0.43
3:C:263:GLU:HB2	3:C:277:CYS:SG	2.59	0.43
5:E:975:ILE:HD11	5:E:1003:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1048:PHE:HA	5:E:1049:PRO:HD3	1.86	0.43
9:I:456:ILE:O	9:I:459:SER:O	2.37	0.43
2:b:437:MET:O	2:b:440:ILE:HG12	2.19	0.43
7:g:1206:TRP:CH2	7:g:1426:LEU:HB3	2.53	0.43
1:A:1234:LEU:HD12	1:A:1257:ILE:HG23	2.00	0.43
2:B:33:LEU:HD11	2:B:54:MET:HG2	2.00	0.43
13:W:1101:MET:HE2	13:W:1101:MET:HB3	1.83	0.43
3:c:199:LYS:HG2	3:c:201:GLY:H	1.82	0.43
7:g:1071:ARG:HB2	8:h:279:SER:OG	2.19	0.43
1:A:742:LEU:O	1:A:745:ARG:N	2.52	0.43
4:D:135:ALA:HB3	4:D:138:VAL:HB	2.01	0.43
5:E:996:ARG:NH1	5:E:1018:GLN:HB3	2.34	0.43
2:b:555:ALA:HB2	2:b:582:LEU:HD13	2.01	0.43
6:f:71:HIS:CE1	6:f:99:ALA:HB2	2.51	0.43
7:g:1607:HIS:O	7:g:1611:ILE:HG13	2.18	0.43
5:E:978:ALA:O	5:E:982:ILE:HG13	2.18	0.43
6:F:105:ARG:HA	6:F:118:LYS:O	2.18	0.43
9:I:525:TRP:O	9:I:530:LYS:N	2.42	0.43
1:A:483:ARG:O	1:A:484:PRO:C	2.62	0.43
2:B:437:MET:O	2:B:440:ILE:HG12	2.19	0.43
4:D:60:VAL:HG22	4:D:78:SER:OG	2.19	0.43
4:D:302:VAL:HB	4:D:319:LEU:HD12	2.00	0.43
5:E:962:LEU:HG	5:E:977:LEU:HD23	2.01	0.43
7:G:1193:LYS:HE3	7:G:1193:LYS:HB2	1.83	0.43
1:a:1054:PRO:C	1:a:1056:LEU:N	2.77	0.43
5:e:867:PRO:HG2	5:e:894:LEU:HB2	2.01	0.43
6:f:54:GLU:HG3	6:f:308:LEU:HD11	2.01	0.43
12:S:145:LEU:HD23	12:S:145:LEU:HA	1.89	0.43
2:b:259:TRP:CH2	2:b:285:LEU:O	2.72	0.43
7:g:1675:MET:HE2	7:g:1675:MET:HB3	1.85	0.43
16:j:924:GLU:HA	16:j:929:GLU:H	1.82	0.43
3:C:223:HIS:NE2	3:C:271:PRO:HB2	2.34	0.42
1:a:1049:ALA:HB2	1:a:1054:PRO:C	2.43	0.42
2:B:415:TRP:O	2:B:419:VAL:HG23	2.19	0.42
3:c:263:GLU:HB2	3:c:277:CYS:SG	2.59	0.42
7:g:1467:HIS:H	7:g:1467:HIS:CD2	2.36	0.42
11:K:41:GLU:O	11:K:45:ALA:CB	2.67	0.42
5:e:872:PHE:CE1	5:e:874:PHE:HB3	2.54	0.42
5:e:1367:GLN:H	5:e:1376:LEU:HD11	1.84	0.42
7:G:1492:TRP:O	7:G:1496:VAL:HG23	2.19	0.42
11:M:632:PHE:C	11:M:634:ASN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1229:LEU:O	1:a:1233:VAL:HG23	2.19	0.42
5:e:797:LEU:HG	5:e:880:ARG:HG2	2.00	0.42
7:g:1071:ARG:HB3	8:h:266:HIS:CB	2.39	0.42
8:h:216:ASP:HB3	8:h:266:HIS:HA	2.01	0.42
5:E:1422:THR:HB	7:G:1060:ILE:HB	2.01	0.42
1:a:1630:LEU:O	1:a:1640:ALA:HB2	2.18	0.42
5:e:824:PHE:HD2	5:e:861:LEU:HD22	1.83	0.42
6:f:131:VAL:HG22	6:f:171:VAL:HG13	2.01	0.42
7:g:1334:TRP:HD1	7:g:1342:ILE:HD12	1.85	0.42
4:D:134:SER:HB2	4:D:135:ALA:H	1.69	0.42
5:e:1220:PHE:O	5:e:1224:ILE:HG13	2.19	0.42
5:e:1419:LYS:HB3	5:e:1419:LYS:HE2	1.80	0.42
7:g:1142:MET:HB2	7:g:1143:PRO:CD	2.50	0.42
7:G:1347:GLN:HE21	7:G:1347:GLN:HB2	1.57	0.42
13:W:1165:HIS:CE1	13:W:1167:THR:HB	2.55	0.42
2:b:638:ALA:HB1	5:e:1084:ILE:HG21	2.01	0.42
2:B:355:ILE:H	2:B:355:ILE:HG13	1.67	0.42
5:e:1194:HIS:CE1	5:e:1217:ALA:HB1	2.54	0.42
12:p:444:GLN:O	12:p:449:TYR:N	2.48	0.42
5:E:1117:VAL:HG13	5:E:1182:TYR:HE2	1.85	0.42
5:E:1378:TRP:HA	7:G:1064:LEU:HD11	2.02	0.42
10:J:850:TYR:O	10:J:852:ASP:N	2.52	0.42
12:P:622:LEU:O	12:P:626:ALA:CB	2.68	0.42
5:e:893:LEU:HD23	5:e:893:LEU:HA	1.87	0.42
5:e:1064:ARG:HA	5:e:1064:ARG:HD3	1.84	0.42
5:e:1178:LEU:HD23	5:e:1178:LEU:HA	1.77	0.42
7:g:1126:GLU:HB2	8:h:4:VAL:HA	2.01	0.42
1:A:1294:ALA:O	1:A:1295:CYS:C	2.63	0.42
5:E:109:ALA:O	5:E:136:SER:HA	2.20	0.42
7:G:1045:VAL:CG1	7:G:1047:LEU:HD11	2.46	0.42
9:I:219:ARG:O	9:I:223:GLN:CB	2.68	0.42
11:N:36:TYR:O	11:N:39:ALA:O	2.37	0.42
3:c:138:SER:HA	3:c:139:PRO:HA	1.72	0.42
4:d:207:ARG:HH12	5:e:1280:THR:HG22	1.83	0.42
5:e:867:PRO:HB2	5:e:894:LEU:HD13	2.02	0.42
7:g:1126:GLU:HA	8:h:5:ILE:HG12	2.02	0.42
7:g:1350:TRP:HB2	7:g:1375:TYR:OH	2.20	0.42
2:B:207:MET:HE2	2:B:207:MET:HB2	1.84	0.41
2:B:580:LEU:HD22	2:B:580:LEU:HA	1.70	0.41
3:C:184:LEU:HB3	3:C:192:LEU:HD11	2.02	0.41
3:C:267:HIS:HB3	3:C:270:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1142:MET:HB2	7:G:1143:PRO:CD	2.50	0.41
13:W:1140:GLU:O	13:W:1144:LYS:HG3	2.20	0.41
2:b:341:GLU:HG2	2:b:342:PRO:HD2	2.02	0.41
7:g:1320:GLU:HA	7:g:1323:ARG:HG3	2.02	0.41
2:B:556:SER:HA	2:B:559:LEU:HD23	2.02	0.41
2:B:558:LEU:HD11	2:B:575:LEU:HD22	2.01	0.41
13:W:1076:ASP:HA	13:W:1079:TRP:HD1	1.84	0.41
13:W:1168:VAL:O	13:W:1172:VAL:HG23	2.20	0.41
2:b:599:MET:O	2:b:603:GLU:HG2	2.19	0.41
5:e:1267:GLN:HE21	5:e:1267:GLN:HB3	1.72	0.41
1:a:1630:LEU:CB	1:a:1639:GLN:C	2.93	0.41
5:e:1096:MET:HE2	5:e:1096:MET:HA	2.01	0.41
5:e:1104:GLY:O	5:e:1105:ARG:C	2.62	0.41
7:g:1434:LEU:HD22	7:g:1460:LEU:HD21	2.01	0.41
1:A:585:GLY:O	1:A:586:ILE:C	2.64	0.41
13:W:1285:THR:O	13:W:1289:ILE:HG13	2.19	0.41
5:e:715:CYS:SG	5:e:820:VAL:HG12	2.61	0.41
5:e:1297:LYS:HA	5:e:1297:LYS:HD2	1.80	0.41
5:E:921:LYS:HD3	6:F:100:GLY:CA	2.50	0.41
5:E:1075:TYR:HA	5:E:1078:LEU:HB2	2.01	0.41
11:M:571:PRO:O	11:M:572:ALA:C	2.64	0.41
2:b:409:PHE:HZ	2:b:419:VAL:HG22	1.85	0.41
4:d:18:VAL:HG12	4:d:29:THR:HG22	2.01	0.41
5:e:869:ASN:HB3	5:e:872:PHE:HB2	2.02	0.41
5:e:1070:LEU:HD21	5:e:1102:ARG:HG2	2.03	0.41
7:g:1190:ALA:O	7:g:1193:LYS:HG2	2.19	0.41
2:B:240:MET:HE3	2:B:240:MET:HB2	1.97	0.41
1:a:1300:ILE:HB	1:a:1301:PRO:HD3	2.01	0.41
4:d:74:LEU:HD23	4:d:74:LEU:HA	1.85	0.41
10:J:442:UNK:N	10:J:454:UNK:O	2.53	0.41
11:K:376:PHE:HA	11:K:381:GLY:HA3	2.03	0.41
12:P:216:LEU:O	12:P:218:ASP:N	2.54	0.41
2:b:156:PRO:HG2	2:b:159:PRO:HG2	2.03	0.41
5:e:962:LEU:HG	5:e:977:LEU:HD23	2.02	0.41
2:B:85:SER:O	2:B:85:SER:OG	2.34	0.41
3:C:283:LEU:HD21	3:C:358:LEU:HD21	2.03	0.41
6:f:310:LEU:HD21	6:f:321:PHE:HD1	1.86	0.41
12:p:582:ASP:HA	12:p:586:GLY:O	2.20	0.41
1:A:1132:HIS:O	1:A:1133:THR:C	2.63	0.41
3:C:359:VAL:HG23	3:C:369:VAL:HG22	2.03	0.41
5:E:1124:LEU:HD22	5:E:1178:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1419:LYS:HE3	5:E:1419:LYS:HB3	1.83	0.41
5:E:1422:THR:O	5:E:1423:ASP:C	2.62	0.41
7:G:1489:LEU:HD23	7:G:1489:LEU:HA	1.92	0.41
9:I:502:HIS:O	9:I:506:ILE:N	2.44	0.41
11:N:654:ALA:HB2	11:N:669:ALA:HB3	2.03	0.41
2:b:453:ARG:HG2	3:c:279:GLU:OE1	2.21	0.41
7:g:1139:SER:O	7:g:1140:TYR:C	2.60	0.41
7:g:1317:ILE:HG22	7:g:1318:GLN:H	1.86	0.41
7:g:1623:ASP:O	7:g:1624:TYR:C	2.64	0.41
8:h:246:ASP:HB3	8:h:249:THR:HG23	2.02	0.41
1:A:1229:LEU:HD22	1:A:1232:ARG:HH21	1.86	0.41
2:B:450:LYS:HE2	3:C:262:TRP:CZ2	2.56	0.41
4:D:235:PHE:HB3	4:D:251:LYS:HG2	2.03	0.41
2:b:638:ALA:HB2	5:e:1084:ILE:HD13	2.03	0.41
7:g:1187:GLU:H	7:g:1187:GLU:HG3	1.74	0.41
2:B:369:TRP:O	2:B:370:TRP:C	2.63	0.40
13:W:1184:LYS:O	13:W:1185:MET:C	2.63	0.40
5:e:1224:ILE:HG22	5:e:1228:GLN:HE21	1.86	0.40
5:e:1259:ALA:O	5:e:1260:TRP:C	2.64	0.40
2:B:140:MET:HE1	2:B:368:ASN:HB3	2.03	0.40
2:B:160:LEU:HD21	2:B:322:LEU:HD11	2.04	0.40
6:F:18:TYR:O	6:F:40:GLY:HA2	2.21	0.40
7:G:1045:VAL:HA	7:G:1046:PRO:HD3	1.96	0.40
5:e:891:VAL:HG13	5:e:905:CYS:HB3	2.02	0.40
6:f:106:ILE:HD11	6:f:120:ILE:HD11	2.02	0.40
8:h:212:ASP:HB3	8:h:235:GLN:HB3	2.03	0.40
2:B:187:LYS:HE3	2:B:187:LYS:HB3	1.90	0.40
11:N:248:ASP:CB	11:N:300:MET:HA	2.50	0.40
1:a:743:ARG:O	1:a:744:TYR:C	2.64	0.40
2:b:131:ILE:HD13	2:b:131:ILE:HA	1.94	0.40
1:A:580:HIS:O	1:A:581:PRO:C	2.64	0.40
1:A:1281:LEU:HD12	1:A:1281:LEU:HA	1.94	0.40
11:M:104:ILE:C	11:M:114:ALA:HB2	2.46	0.40
13:W:1366:PRO:CG	5:e:990:ARG:HB3	2.47	0.40
1:a:1:MET:C	1:a:3:ALA:H	2.29	0.40
2:b:452:LEU:HD12	2:b:452:LEU:HA	1.85	0.40
5:e:1429:VAL:O	5:e:1430:GLN:C	2.63	0.40
1:A:674:ARG:O	1:A:676:THR:N	2.55	0.40
1:A:1125:SER:C	1:A:1127:ASN:H	2.30	0.40
2:B:433:LEU:HD12	2:B:433:LEU:HA	1.88	0.40
5:E:971:PRO:HG3	5:E:1002:HIS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:979:THR:HA	5:E:982:ILE:HD12	2.02	0.40
5:E:1263:LEU:HD22	5:E:1282:GLU:HG3	2.02	0.40
7:G:1203:GLU:HG2	7:G:1209:LEU:HD22	2.03	0.40
7:G:1298:ARG:NH1	7:G:1301:ILE:HG21	2.37	0.40
13:W:1366:PRO:HA	13:W:1370:LEU:HD23	2.02	0.40
2:b:129:LYS:HB3	2:b:129:LYS:HE2	1.79	0.40
2:b:137:LEU:HA	2:b:137:LEU:HD23	1.85	0.40
7:g:1477:HIS:HE1	7:g:1499:HIS:HB3	1.86	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	A	1759/2011 (88%)	1626 (92%)	129 (7%)	4 (0%)	43	72
1	a	1691/2011 (84%)	1552 (92%)	131 (8%)	8 (0%)	24	56
2	B	584/653 (89%)	564 (97%)	19 (3%)	1 (0%)	43	72
2	b	579/653 (89%)	562 (97%)	15 (3%)	2 (0%)	36	65
3	C	315/375 (84%)	303 (96%)	12 (4%)	0	100	100
3	c	299/375 (80%)	284 (95%)	14 (5%)	1 (0%)	36	65
4	D	310/360 (86%)	298 (96%)	12 (4%)	0	100	100
4	d	306/360 (85%)	293 (96%)	13 (4%)	0	100	100
5	E	1298/1435 (90%)	1239 (96%)	56 (4%)	3 (0%)	43	72
5	e	1227/1435 (86%)	1167 (95%)	59 (5%)	1 (0%)	48	78
6	F	324/326 (99%)	312 (96%)	12 (4%)	0	100	100
6	f	320/326 (98%)	308 (96%)	11 (3%)	1 (0%)	36	65
7	G	545/1742 (31%)	508 (93%)	35 (6%)	2 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	595/1742 (34%)	543 (91%)	50 (8%)	2 (0%)	36	65
8	H	284/320 (89%)	274 (96%)	9 (3%)	1 (0%)	30	60
8	h	284/320 (89%)	274 (96%)	8 (3%)	2 (1%)	18	50
9	I	719/916 (78%)	675 (94%)	43 (6%)	1 (0%)	48	78
9	i	657/916 (72%)	628 (96%)	29 (4%)	0	100	100
10	J	449/1140 (39%)	422 (94%)	27 (6%)	0	100	100
11	K	681/2905 (23%)	623 (92%)	57 (8%)	1 (0%)	48	78
11	L	659/2905 (23%)	614 (93%)	45 (7%)	0	100	100
11	M	638/2905 (22%)	575 (90%)	62 (10%)	1 (0%)	43	72
11	N	683/2905 (24%)	614 (90%)	68 (10%)	1 (0%)	48	78
11	O	661/2905 (23%)	613 (93%)	47 (7%)	1 (0%)	43	72
12	P	581/820 (71%)	539 (93%)	42 (7%)	0	100	100
12	S	50/820 (6%)	49 (98%)	1 (2%)	0	100	100
12	p	424/820 (52%)	401 (95%)	21 (5%)	2 (0%)	24	56
12	s	50/820 (6%)	46 (92%)	4 (8%)	0	100	100
13	W	318/1388 (23%)	305 (96%)	12 (4%)	1 (0%)	36	65
15	Y	323/728 (44%)	308 (95%)	11 (3%)	4 (1%)	10	40
16	j	1022/1140 (90%)	960 (94%)	62 (6%)	0	100	100
All	All	18635/38477 (48%)	17479 (94%)	1116 (6%)	40 (0%)	44	72

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	460	ILE
15	Y	271	LYS
1	a	57	PRO
1	a	58	PRO
1	a	1095	LEU
1	a	1628	LEU
1	a	1629	ILE
1	a	1772	PRO
7	g	1616	THR
1	A	153	ARG
1	A	1632	SER
5	E	1301	TYR
7	G	1463	LEU

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Mol	Chain	Res	Type
2	b	426	PRO
3	c	127	MET
12	p	202	GLN
1	a	101	TYR
8	h	139	PRO
12	p	402	ASP
1	A	127	ARG
5	E	1299	THR
11	O	27	MET
15	Y	282	PRO
15	Y	287	PRO
7	g	1068	ARG
1	A	1772	PRO
5	e	1066	ARG
2	B	52	PRO
5	E	1051	VAL
15	Y	295	TYR
1	a	502	LEU
6	f	273	PRO
8	H	139	PRO
11	N	22	PRO
13	W	1289	ILE
2	b	52	PRO
11	M	627	PRO
7	G	1503	PRO
11	K	627	PRO
8	h	5	ILE

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	A	100/1779 (6%)	98 (98%)	2 (2%)	48	64
1	a	77/1779 (4%)	73 (95%)	4 (5%)	21	47
2	B	517/580 (89%)	500 (97%)	17 (3%)	33	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	447/580 (77%)	432 (97%)	15 (3%)	32	55
3	C	288/329 (88%)	282 (98%)	6 (2%)	47	64
3	c	276/329 (84%)	267 (97%)	9 (3%)	33	55
4	D	273/310 (88%)	265 (97%)	8 (3%)	37	57
4	d	266/310 (86%)	262 (98%)	4 (2%)	57	68
5	E	382/1256 (30%)	364 (95%)	18 (5%)	23	48
5	e	545/1256 (43%)	520 (95%)	25 (5%)	24	49
6	f	266/275 (97%)	262 (98%)	4 (2%)	57	68
7	G	384/1474 (26%)	356 (93%)	28 (7%)	13	40
7	g	490/1474 (33%)	459 (94%)	31 (6%)	16	43
8	H	236/273 (86%)	230 (98%)	6 (2%)	42	61
8	h	245/273 (90%)	240 (98%)	5 (2%)	48	64
12	S	47/721 (6%)	44 (94%)	3 (6%)	16	43
12	s	47/721 (6%)	44 (94%)	3 (6%)	16	43
13	W	295/1219 (24%)	290 (98%)	5 (2%)	53	67
All	All	5181/14938 (35%)	4988 (96%)	193 (4%)	31	54

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1227	VAL
1	A	1287	LEU
2	B	40	GLN
2	B	56	LEU
2	B	118	THR
2	B	123	THR
2	B	148	GLU
2	B	187	LYS
2	B	207	MET
2	B	228	CYS
2	B	452	LEU
2	B	496	PHE
2	B	546	TYR
2	B	559	LEU
2	B	580	LEU
2	B	597	GLU
2	B	602	LEU

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Mol	Chain	Res	Type
2	B	612	SER
2	B	633	LEU
3	C	78	VAL
3	C	89	ILE
3	C	112	VAL
3	C	215	VAL
3	C	260	GLU
3	C	351	LEU
4	D	18	VAL
4	D	63	VAL
4	D	90	VAL
4	D	114	THR
4	D	148	MET
4	D	194	MET
4	D	264	THR
4	D	318	VAL
5	E	997	THR
5	E	1029	LEU
5	E	1046	VAL
5	E	1078	LEU
5	E	1085	TYR
5	E	1107	VAL
5	E	1173	LEU
5	E	1178	LEU
5	E	1213	LEU
5	E	1234	LEU
5	E	1235	THR
5	E	1250	GLN
5	E	1301	TYR
5	E	1337	LEU
5	E	1350	LEU
5	E	1370	LEU
5	E	1377	VAL
5	E	1394	ASN
7	G	1047	LEU
7	G	1058	LEU
7	G	1059	LEU
7	G	1064	LEU
7	G	1065	PHE
7	G	1071	ARG
7	G	1072	VAL
7	G	1168	VAL

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Mol	Chain	Res	Type
7	G	1181	LEU
7	G	1182	SER
7	G	1206	TRP
7	G	1209	LEU
7	G	1284	LEU
7	G	1285	SER
7	G	1287	LEU
7	G	1308	TRP
7	G	1312	GLN
7	G	1316	TYR
7	G	1333	VAL
7	G	1347	GLN
7	G	1358	LEU
7	G	1365	THR
7	G	1398	GLU
7	G	1421	VAL
7	G	1426	LEU
7	G	1487	VAL
7	G	1505	ILE
7	G	1513	LEU
8	H	42	VAL
8	H	109	VAL
8	H	162	VAL
8	H	230	ILE
8	H	257	LEU
8	H	282	ASP
12	S	128	TYR
12	S	137	TRP
12	S	144	VAL
13	W	1088	PHE
13	W	1114	TYR
13	W	1151	GLN
13	W	1154	ILE
13	W	1176	ASP
12	s	120	ARG
12	s	122	PHE
12	s	137	TRP
1	a	1234	LEU
1	a	1247	ILE
1	a	1286	GLN
1	a	1287	LEU
2	b	36	GLU

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Mol	Chain	Res	Type
2	b	56	LEU
2	b	57	VAL
2	b	67	VAL
2	b	87	GLU
2	b	123	THR
2	b	129	LYS
2	b	317	VAL
2	b	362	PHE
2	b	438	GLU
2	b	480	ARG
2	b	502	ASP
2	b	548	GLN
2	b	559	LEU
2	b	597	GLU
3	c	78	VAL
3	c	83	PHE
3	c	122	HIS
3	c	123	VAL
3	c	147	ASP
3	c	183	ILE
3	c	260	GLU
3	c	337	ILE
3	c	371	ARG
4	d	63	VAL
4	d	148	MET
4	d	159	ILE
4	d	284	VAL
5	e	799	VAL
5	e	885	THR
5	e	894	LEU
5	e	898	CYS
5	e	901	ASN
5	e	902	VAL
5	e	923	LEU
5	e	933	VAL
5	e	939	LEU
5	e	957	TYR
5	e	968	VAL
5	e	970	LEU
5	e	1026	LEU
5	e	1046	VAL
5	e	1078	LEU

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Mol	Chain	Res	Type
5	e	1079	LEU
5	e	1102	ARG
5	e	1124	LEU
5	e	1246	ILE
5	e	1260	TRP
5	e	1268	LEU
5	e	1271	VAL
5	e	1324	TYR
5	e	1377	VAL
5	e	1407	LEU
6	f	119	VAL
6	f	190	ILE
6	f	207	VAL
6	f	227	VAL
7	g	1070	PHE
7	g	1072	VAL
7	g	1081	VAL
7	g	1127	LYS
7	g	1137	LEU
7	g	1153	VAL
7	g	1200	THR
7	g	1206	TRP
7	g	1245	GLU
7	g	1257	VAL
7	g	1284	LEU
7	g	1285	SER
7	g	1287	LEU
7	g	1290	GLN
7	g	1292	VAL
7	g	1296	GLU
7	g	1317	ILE
7	g	1322	LEU
7	g	1333	VAL
7	g	1347	GLN
7	g	1365	THR
7	g	1426	LEU
7	g	1435	CYS
7	g	1443	VAL
7	g	1467	HIS
7	g	1472	ARG
7	g	1513	LEU
7	g	1520	VAL

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Mol	Chain	Res	Type
7	g	1565	LEU
7	g	1608	CYS
7	g	1679	VAL
8	h	14	ASP
8	h	42	VAL
8	h	47	GLN
8	h	109	VAL
8	h	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1206	GLN
1	A	1268	ASN
2	B	40	GLN
2	B	42	GLN
2	B	76	HIS
2	B	100	GLN
2	B	104	ASN
2	B	133	GLN
2	B	242	HIS
2	B	257	GLN
2	B	459	GLN
3	C	113	ASN
3	C	173	HIS
3	C	246	HIS
3	C	270	ASN
3	C	273	HIS
3	C	339	ASN
4	D	11	HIS
4	D	23	HIS
4	D	48	HIS
4	D	56	HIS
4	D	198	GLN
4	D	268	ASN
4	D	273	GLN
5	E	1025	GLN
5	E	1083	HIS
5	E	1228	GLN
5	E	1302	HIS
5	E	1416	GLN
7	G	1150	ASN

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Mol	Chain	Res	Type
7	G	1165	ASN
7	G	1180	ASN
7	G	1220	ASN
7	G	1290	GLN
7	G	1347	GLN
7	G	1370	GLN
7	G	1422	HIS
7	G	1431	GLN
7	G	1471	HIS
7	G	1515	ASN
8	H	261	ASN
12	S	142	GLN
12	S	146	HIS
13	W	1164	HIS
13	W	1204	HIS
13	W	1274	ASN
12	s	142	GLN
1	a	1286	GLN
2	b	22	HIS
2	b	40	GLN
2	b	42	GLN
2	b	76	HIS
2	b	83	GLN
2	b	145	ASN
2	b	171	HIS
2	b	257	GLN
2	b	314	HIS
2	b	436	HIS
2	b	548	GLN
3	c	68	GLN
3	c	114	GLN
3	c	151	ASN
3	c	173	HIS
4	d	125	HIS
4	d	152	GLN
4	d	268	ASN
4	d	269	HIS
4	d	276	ASN
4	d	280	GLN
5	e	869	ASN
5	e	883	GLN
5	e	888	GLN

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Mol	Chain	Res	Type
5	e	920	HIS
5	e	1003	HIS
5	e	1054	HIS
5	e	1073	HIS
5	e	1083	HIS
5	e	1088	ASN
5	e	1125	ASN
5	e	1195	ASN
5	e	1228	GLN
5	e	1249	GLN
5	e	1267	GLN
5	e	1307	ASN
5	e	1367	GLN
7	g	1083	ASN
7	g	1124	HIS
7	g	1150	ASN
7	g	1165	ASN
7	g	1180	ASN
7	g	1220	ASN
7	g	1290	GLN
7	g	1309	ASN
7	g	1347	GLN
7	g	1370	GLN
7	g	1467	HIS
7	g	1499	HIS
7	g	1515	ASN
7	g	1581	HIS
8	h	261	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

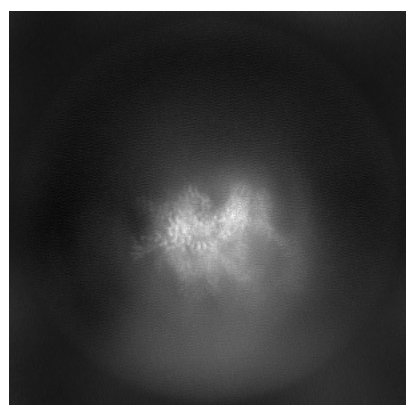
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31600. These allow visual inspection of the internal detail of the map and identification of artifacts.

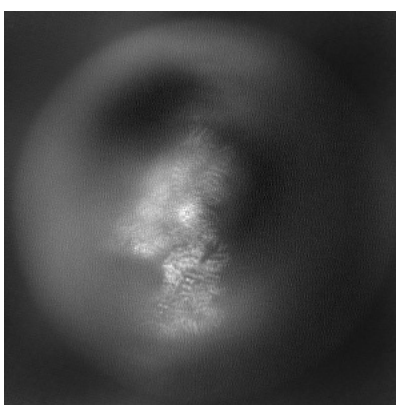
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

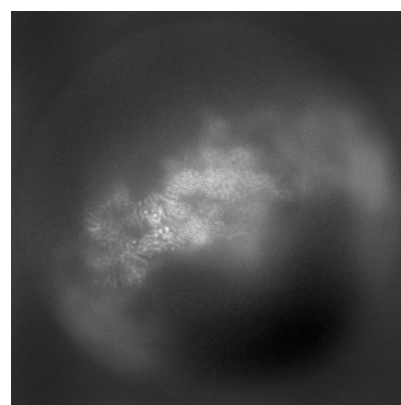
6.1.1 Primary map



X



Y

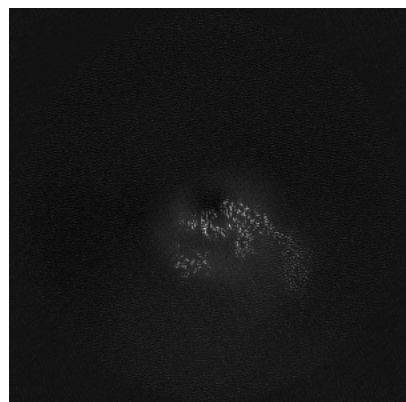


Z

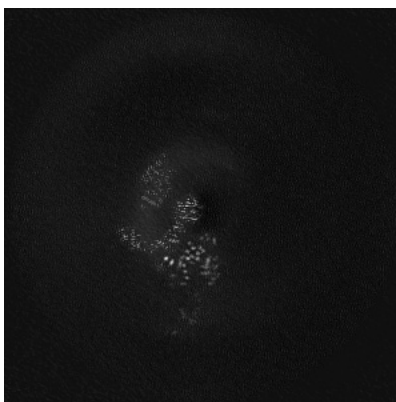
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

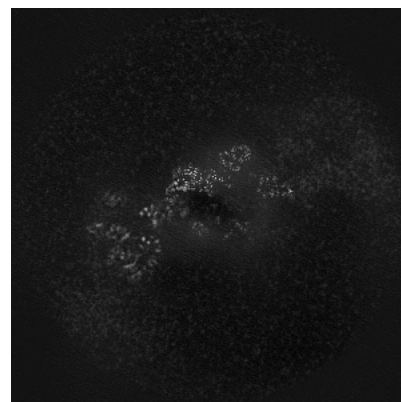
6.2.1 Primary map



X Index: 256



Y Index: 256

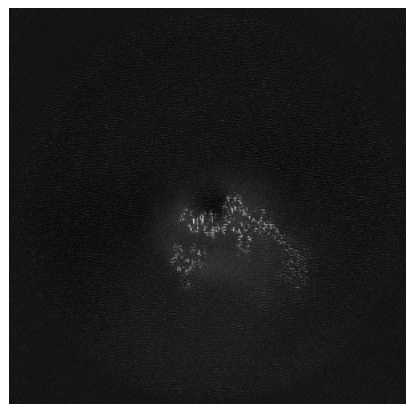


Z Index: 256

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

6.3 Largest variance slices [i](#)

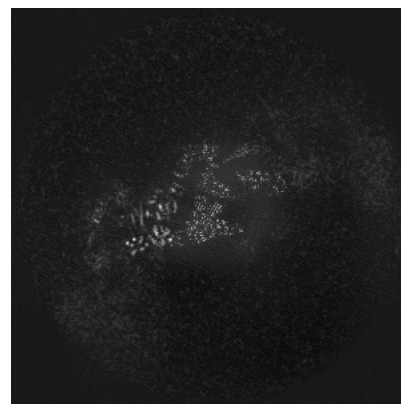
6.3.1 Primary map



X Index: 252



Y Index: 223

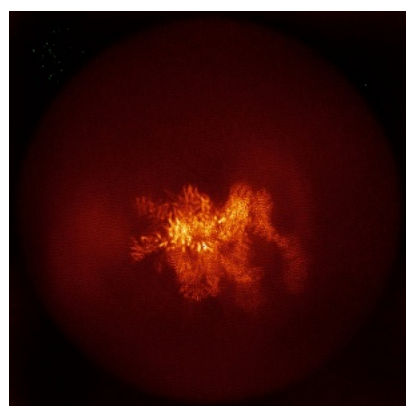


Z Index: 236

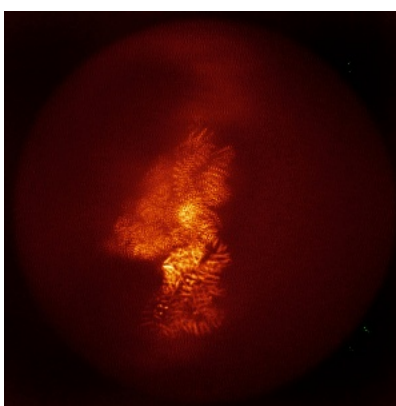
The images above show the largest variance slices of the map in three orthogonal directions.

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

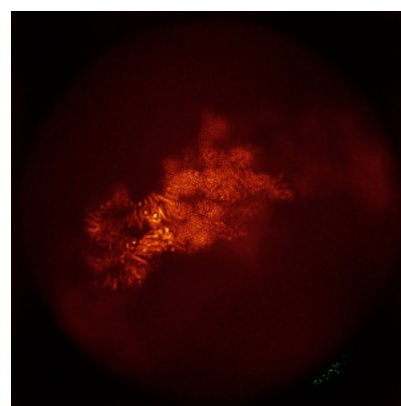
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

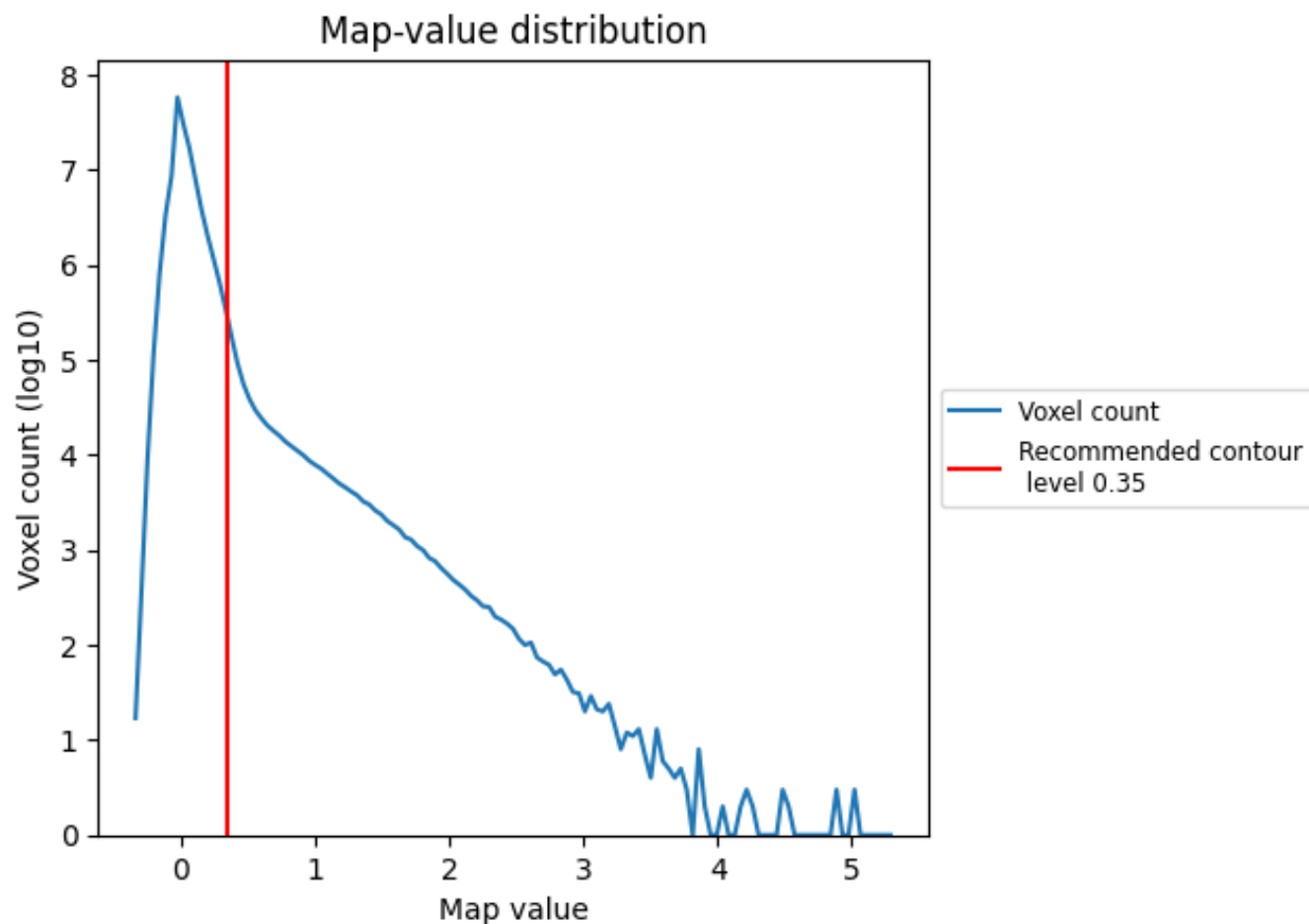
6.6 Mask visualisation

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

7 Map analysis [i](#)

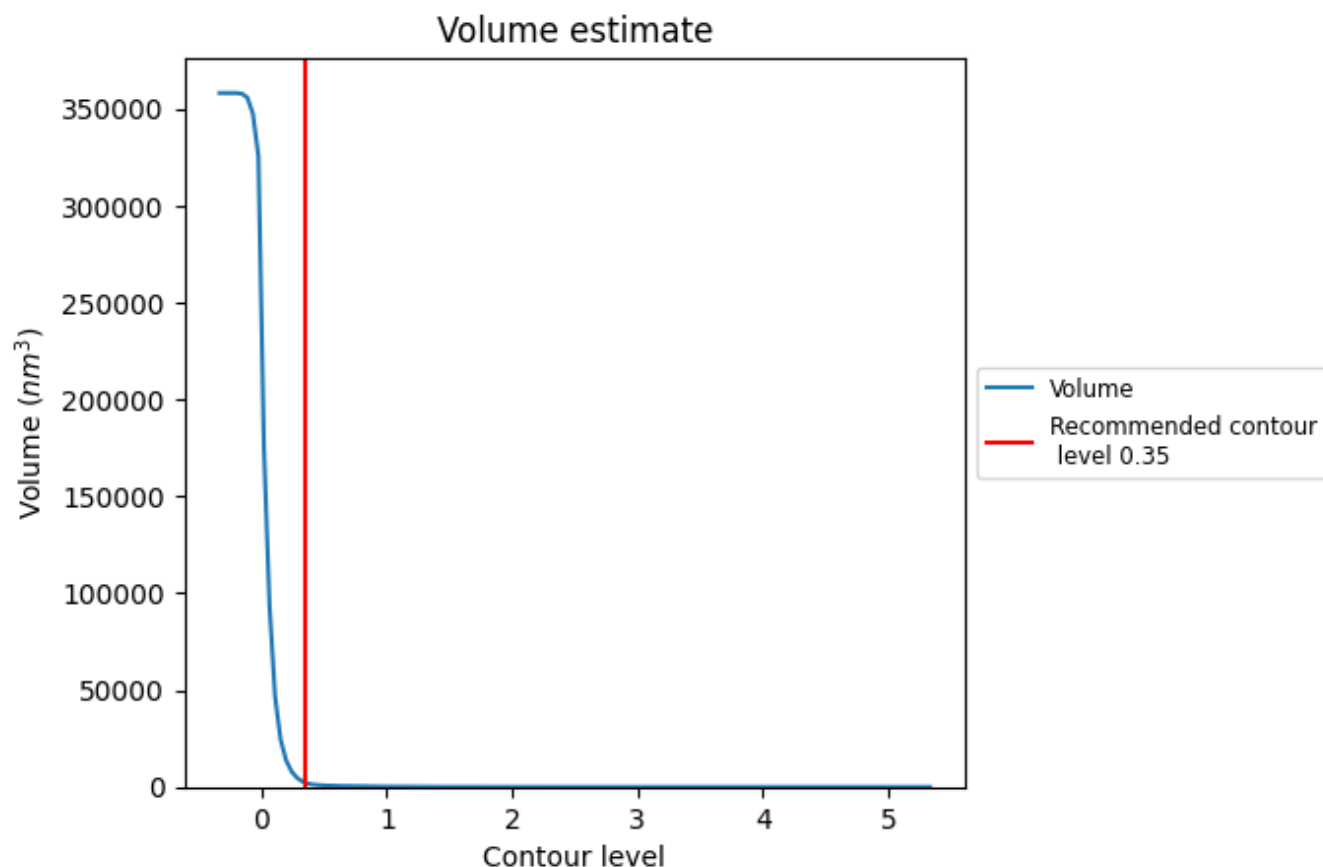
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

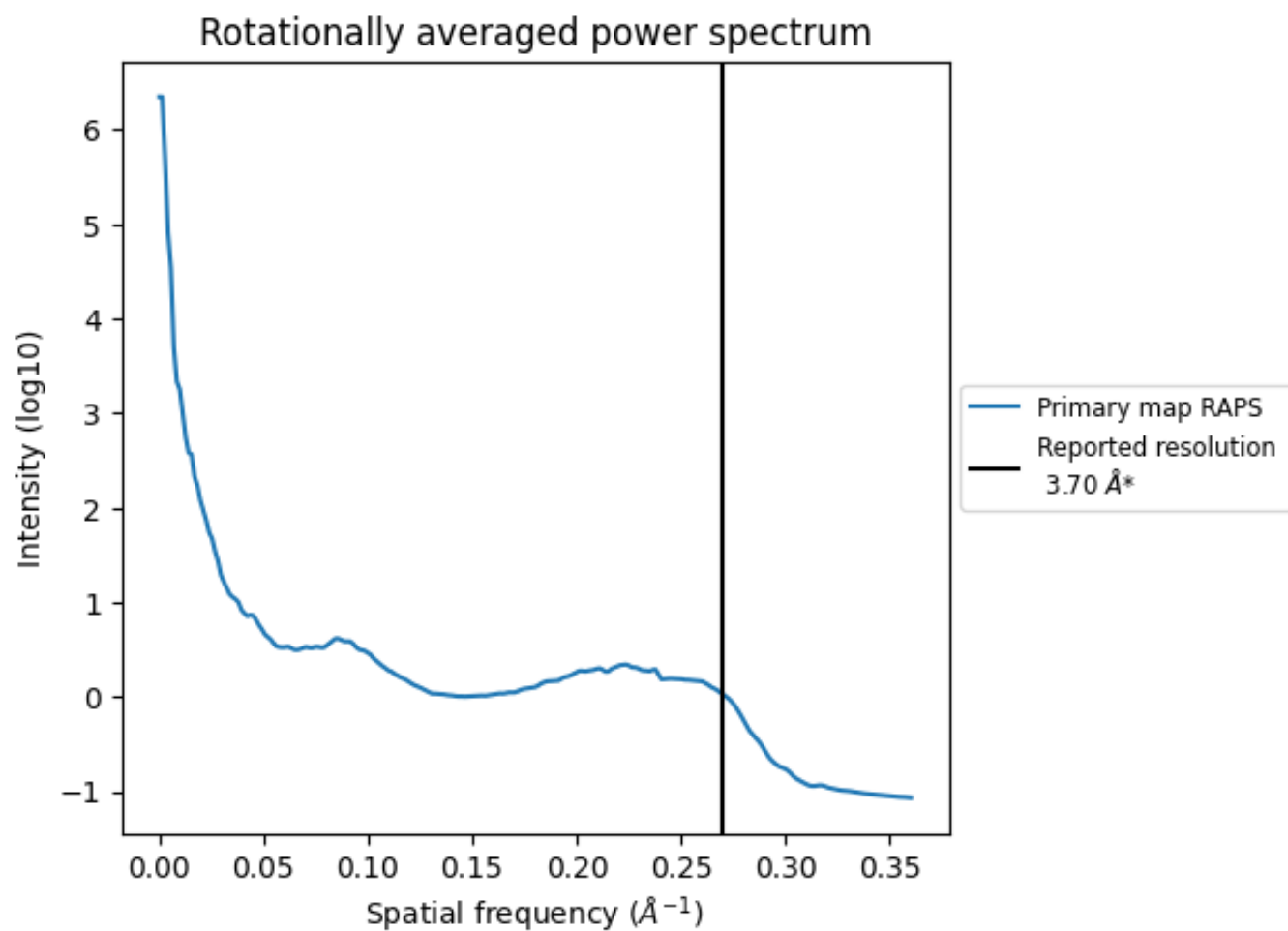
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2248 nm^3 ; this corresponds to an approximate mass of 2031 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 0.270 Å⁻¹

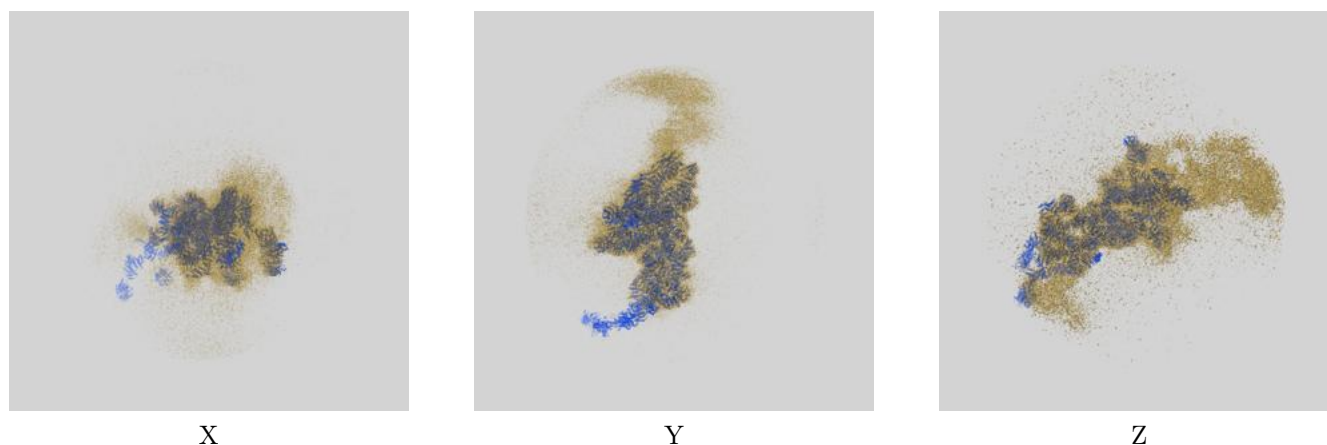
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

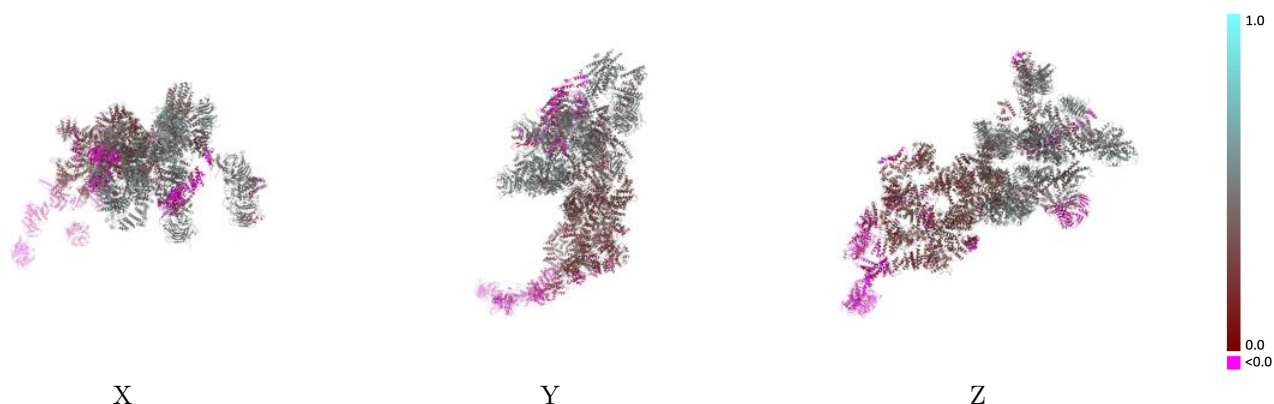
This section contains information regarding the fit between EMDB map EMD-31600 and PDB model 7FIK. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



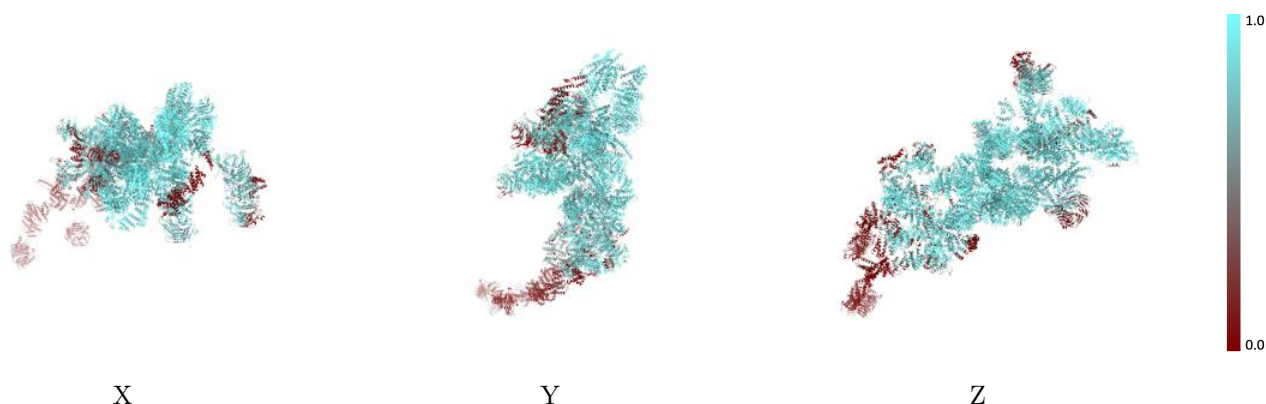
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



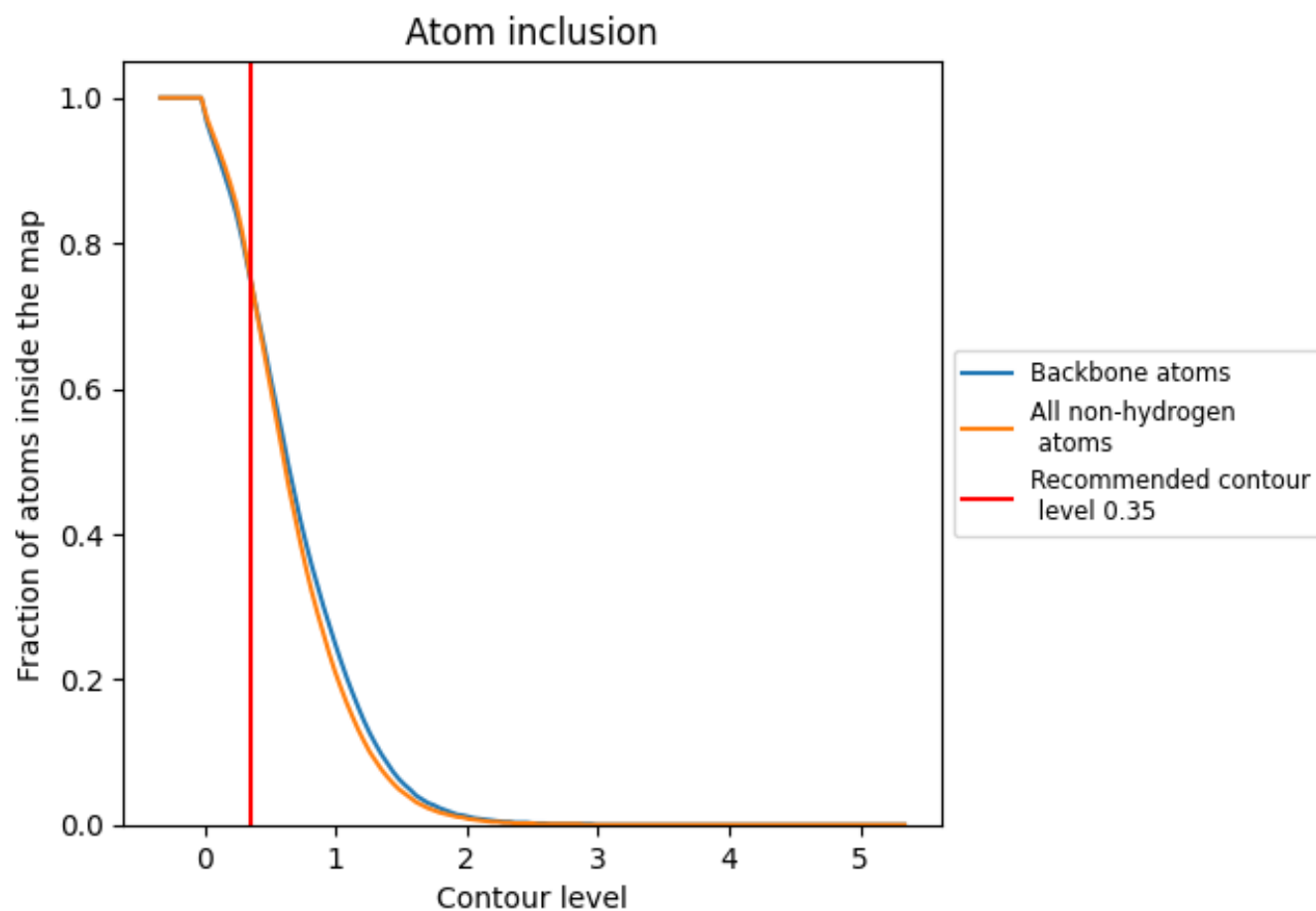
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.3460
A	 0.9580	 0.4790
B	 0.8710	 0.4340
C	 0.9490	 0.5030
D	 0.9220	 0.4710
E	 0.7110	 0.4090
F	 0.7750	 0.4700
G	 0.8890	 0.3440
H	 0.9590	 0.4710
I	 0.8330	 0.2830
J	 0.1110	 0.0820
K	 0.7490	 0.2950
L	 0.5250	 0.2780
M	 0.9400	 0.3220
N	 0.6850	 0.2870
O	 0.7840	 0.2290
P	 0.8780	 0.2830
S	 0.9190	 0.4340
W	 0.9640	 0.4950
X	 0.2370	 0.0090
Y	 0.2550	 -0.0240
a	 0.9670	 0.4830
b	 0.8760	 0.4240
c	 0.9290	 0.4670
d	 0.9660	 0.4690
e	 0.8850	 0.4500
f	 0.9850	 0.5100
g	 0.8900	 0.3330
h	 0.9510	 0.3740
i	 0.3530	 0.1570
j	 0.0000	 -0.0560
p	 0.1080	 -0.0130
s	 0.9530	 0.3980

