



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 08:29 PM UTC

PDB ID : 6LK8 / pdb_00006lk8
EMDB ID : EMD-0909
Title : Structure of Xenopus laevis Cytoplasmic Ring subunit.
Authors : Shi, Y.; Huang, G.; Yan, C.; Zhang, Y.
Deposited on : 2019-12-18
Resolution : 5.50 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:

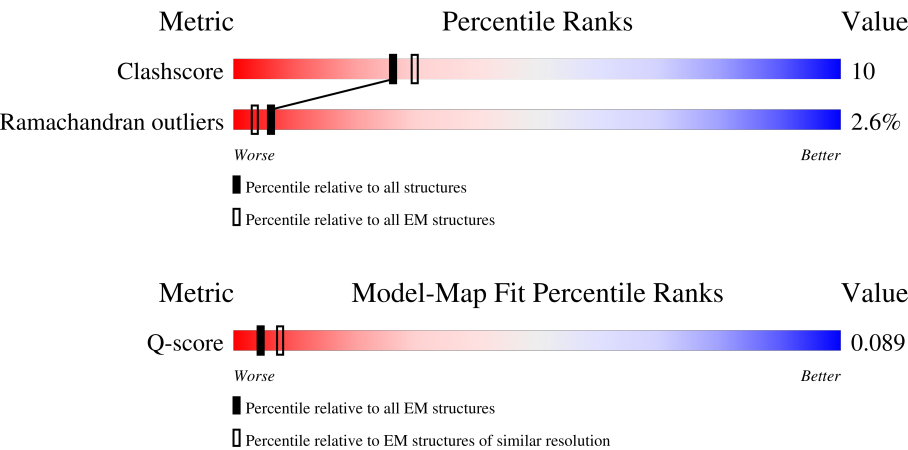
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.50 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	-
Q-score	-	25397	520 (5.00 - 6.00)

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	A	2011	27% 62% 8% 30%
1	a	2011	30% 56% 7% 37%
2	B	653	23% 68% 12% 19%
2	b	653	22% 64% 14% 21%
3	C	375	66% 10% 23%

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Mol	Chain	Length	Quality of chain
3	c	375	
4	D	322	
4	d	322	
5	E	1435	
5	e	1435	
6	F	326	
6	f	326	
7	G	923	
7	g	923	
8	H	320	
8	h	320	
9	I	916	
9	i	916	
10	J	1140	
10	j	1140	
11	S	2905	
11	T	2905	
11	U	2905	
11	V	2905	
12	K	69	
13	L	80	
14	M	73	
15	N	31	
16	O	35	
17	P	26	

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Mol	Chain	Length	Quality of chain
18	Q	391	58% 91% 8%
18	R	391	87% 72% 18% 10%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 72207 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	1409	Total	C	N	O	0	0
			6934	4116	1409	1409		
1	a	1272	Total	C	N	O	0	0
			6306	3762	1272	1272		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	532	Total	C	N	O	0	0
			2639	1575	532	532		
2	b	519	Total	C	N	O	0	0
			2574	1536	519	519		

- Molecule 3 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	289	Total	C	N	O	0	0
			1156	578	289	289		
3	c	292	Total	C	N	O	0	0
			1168	584	292	292		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	307	Total	C	N	O	0	0
			1519	905	307	307		
4	d	293	Total	C	N	O	0	0
			1450	864	293	293		

- Molecule 5 is a protein called outer Nup160.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	1030	Total	C	N	O	0	0
			5107	3047	1030	1030		
5	e	1109	Total	C	N	O	0	0
			5497	3279	1109	1109		

- Molecule 6 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	289	Total	C	N	O	0	0
			1423	845	289	289		
6	f	291	Total	C	N	O	0	0
			1433	851	291	291		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	618	Total	C	N	O	0	0
			3064	1828	618	618		
7	g	607	Total	C	N	O	0	0
			3010	1796	607	607		

- Molecule 8 is a protein called GATOR complex protein SEC13.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	291	Total	C	N	O	0	0
			1419	837	291	291		
8	h	287	Total	C	N	O	0	0
			1413	839	287	287		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	738	Total	C	N	O	0	0
			3668	2192	738	738		
9	i	727	Total	C	N	O	0	0
			3613	2159	727	727		

- Molecule 10 is a protein called outer Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	1026	Total	C	N	O	0	0
			5085	3033	1026	1026		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	1027	Total	C	N	O	0	0
			5090	3036	1027	1027		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	S	169	Total	C	N	O	0	0
			840	502	169	169		
11	T	169	Total	C	N	O	0	0
			840	502	169	169		
11	U	173	Total	C	N	O	0	0
			859	513	173	173		
11	V	169	Total	C	N	O	0	0
			840	502	169	169		

- Molecule 12 is a protein called Nup214 complex Coiled-coil region 1, helix 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	K	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 13 is a protein called Nup214 complex coiled coil region 1, helix 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	L	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 14 is a protein called Nup214 complex coiled coil region 1, helix 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	73	Total	C	N	O	0	0
			365	219	73	73		

- Molecule 15 is a protein called Nup214 complex Coiled coil region 2, helix 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	N	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 16 is a protein called Nup214 complex Coiled coil region 2, helix 2.

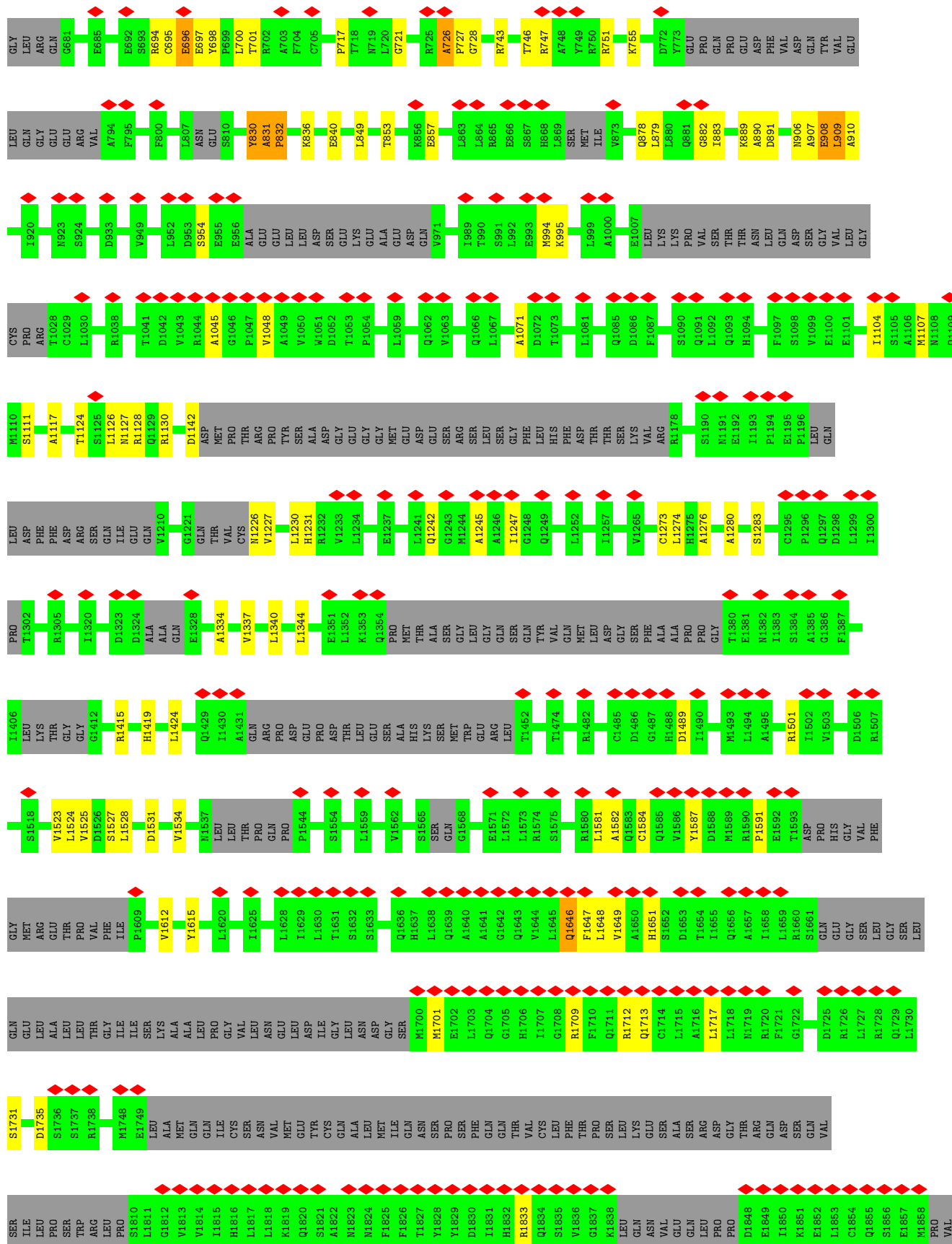
Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	35	Total	C	N	O	0	0
			175	105	35	35		

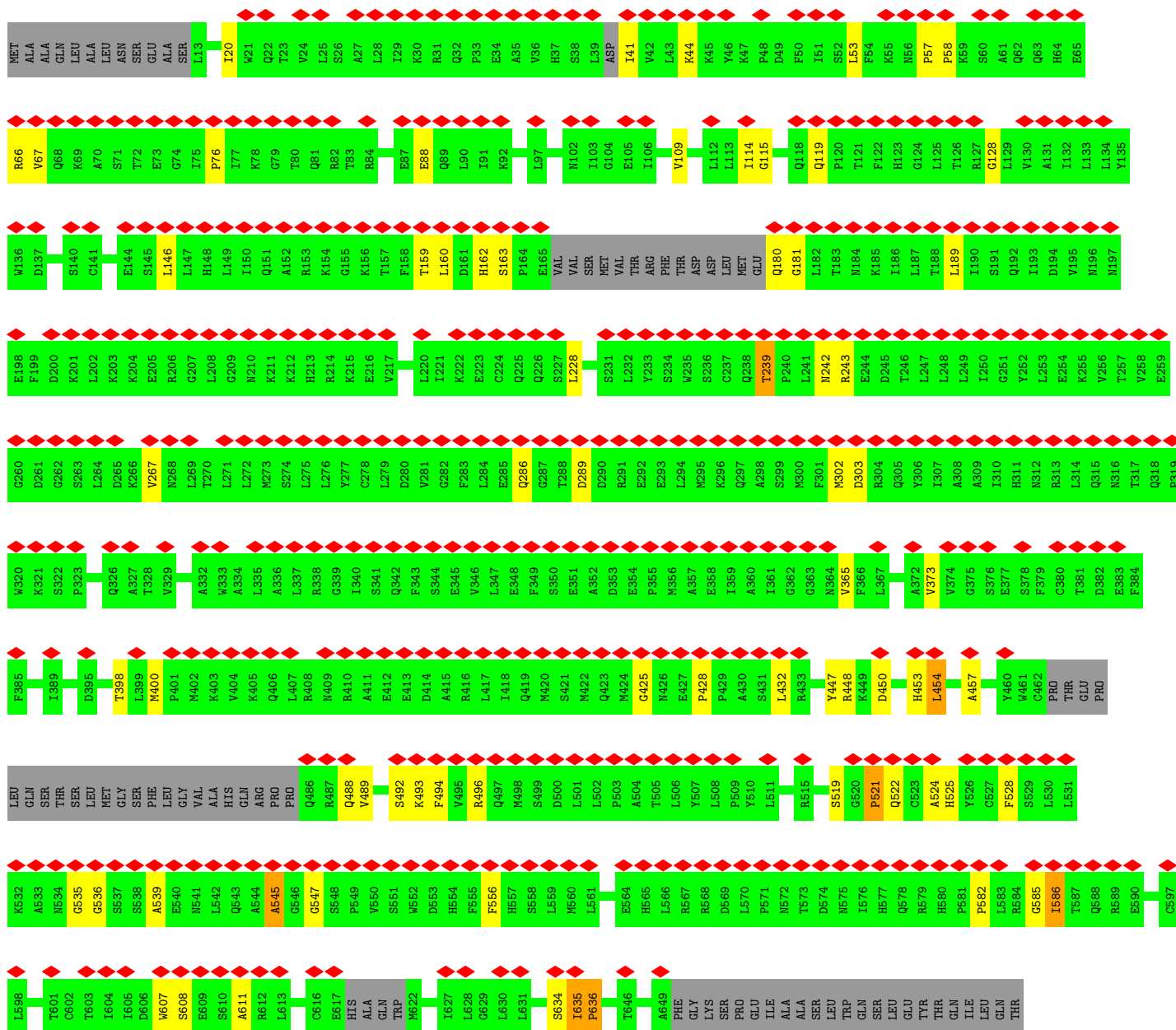
- Molecule 17 is a protein called Nup214 complex Coiled coil region 2, helix 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	P	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 18 is a protein called bridge domain.

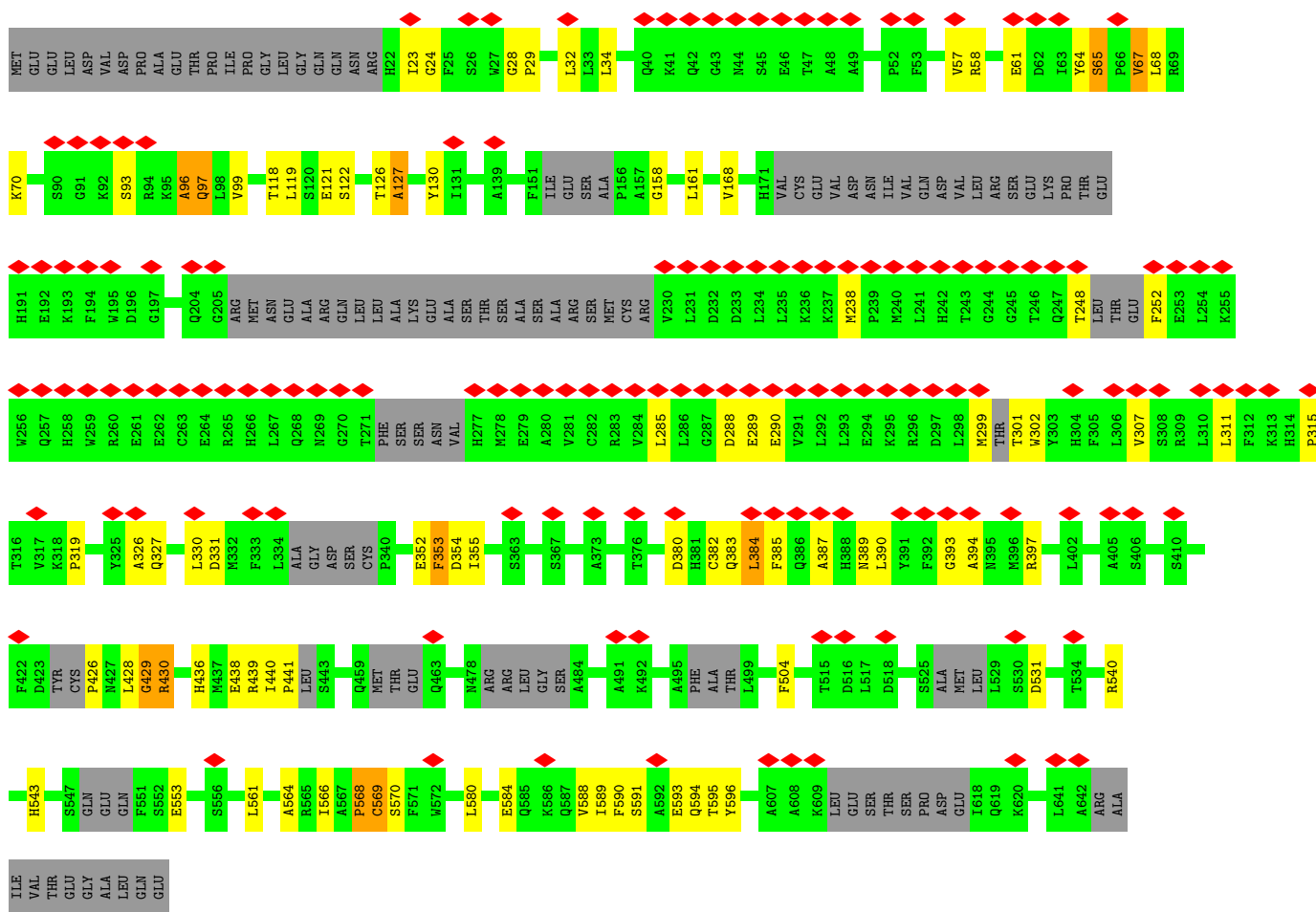
Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	387	Total	C	N	O	0	0
			1935	1161	387	387		
18	R	351	Total	C	N	O	0	0
			1755	1053	351	351		



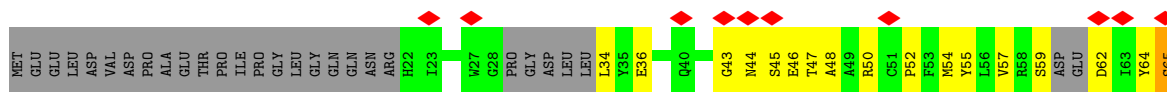


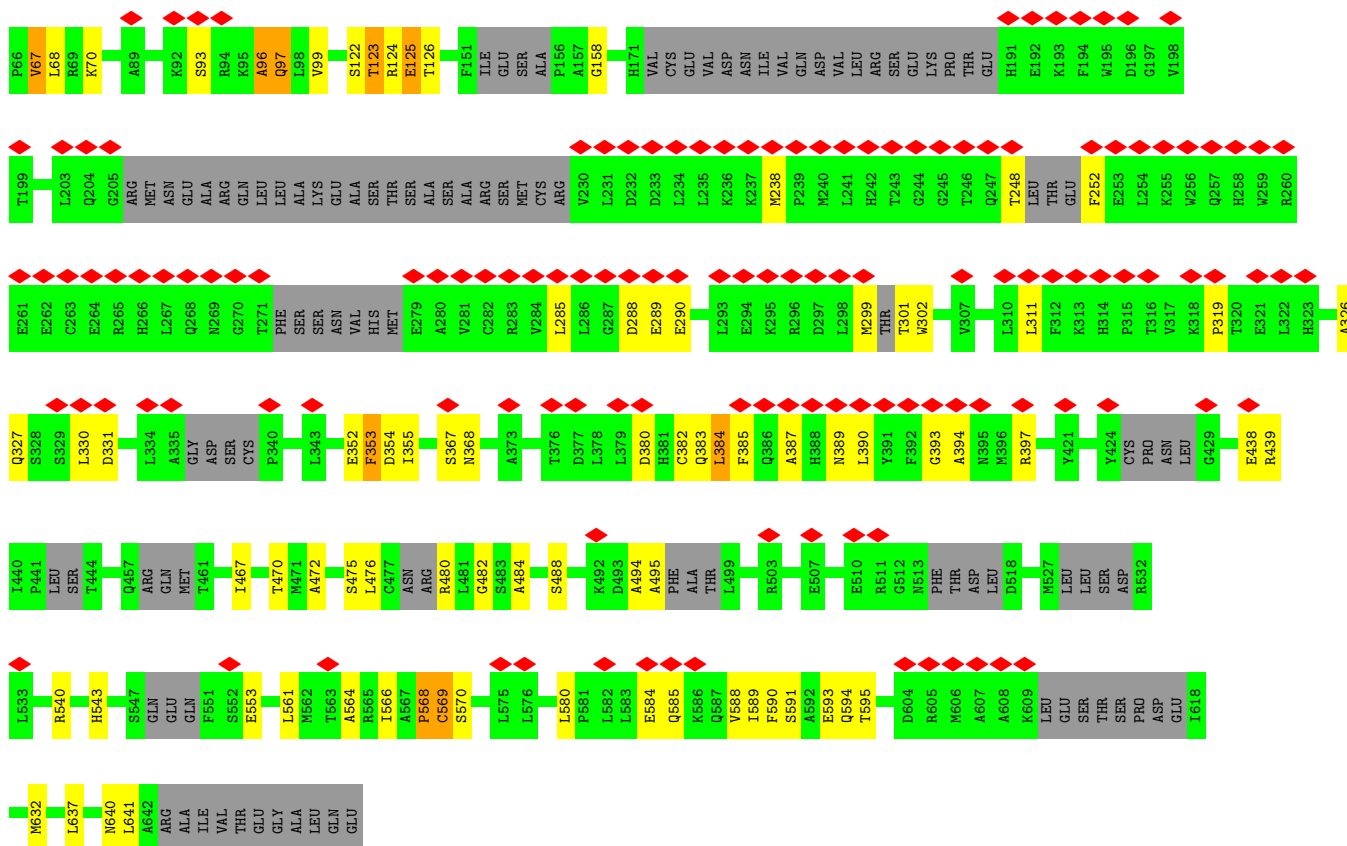


- Molecule 2: Nuclear pore complex protein Nup85

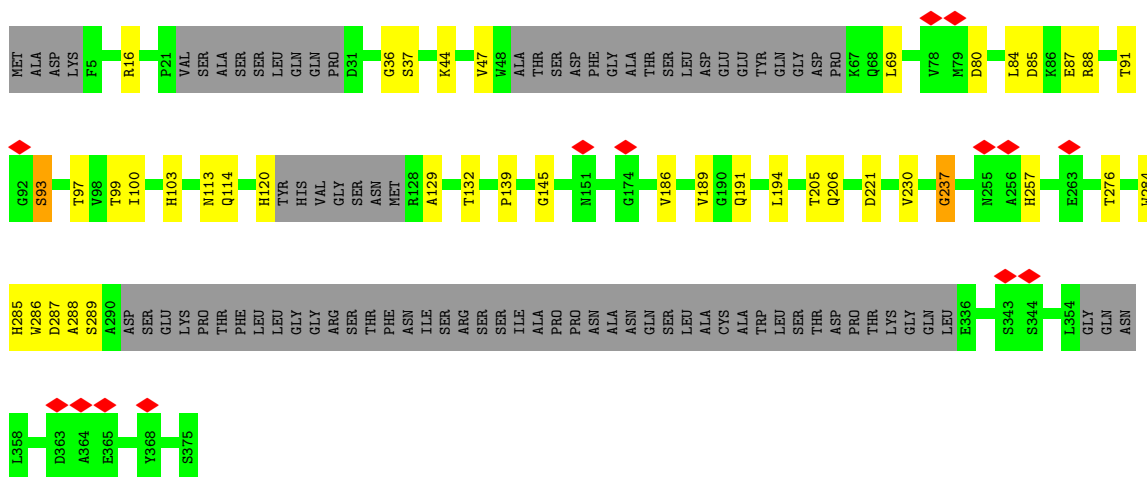


- Molecule 2: Nuclear pore complex protein Nup85

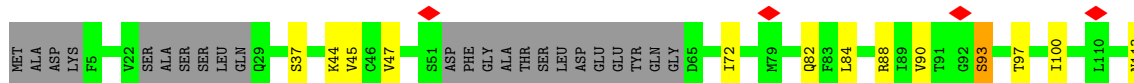


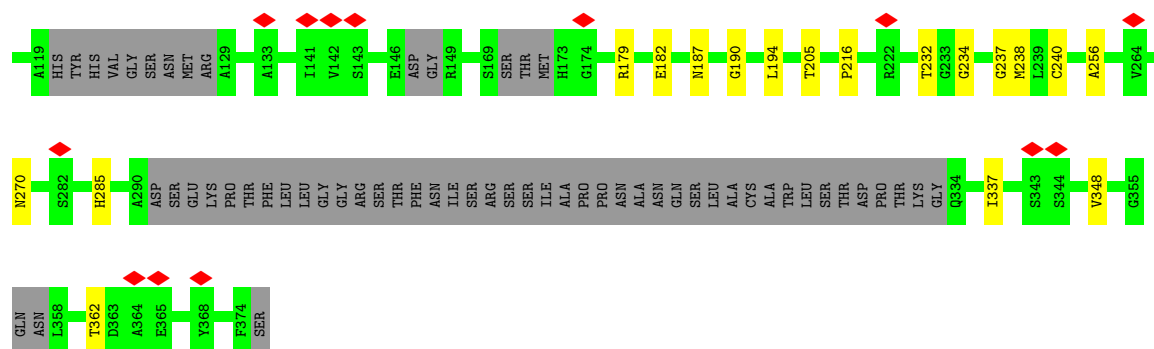


- Molecule 3: MGC154553 protein

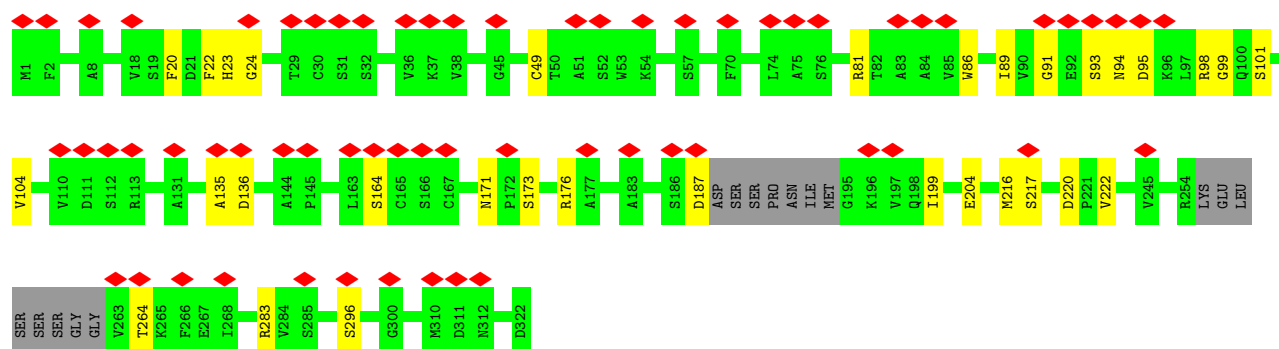
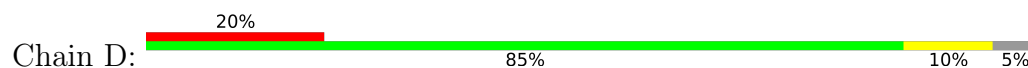


- Molecule 3: MGC154553 protein

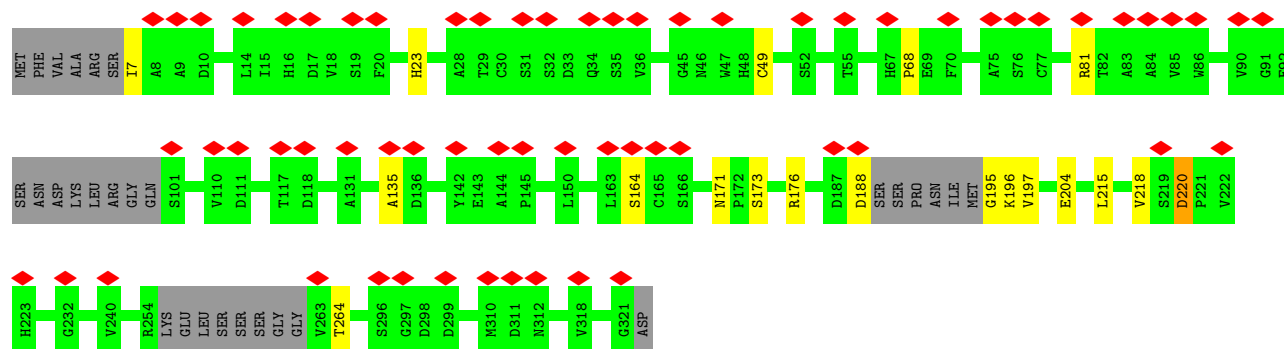
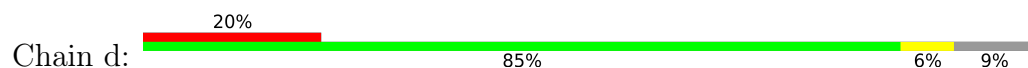




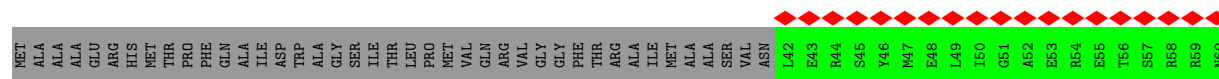
• Molecule 4: Nucleoporin SEH1-A



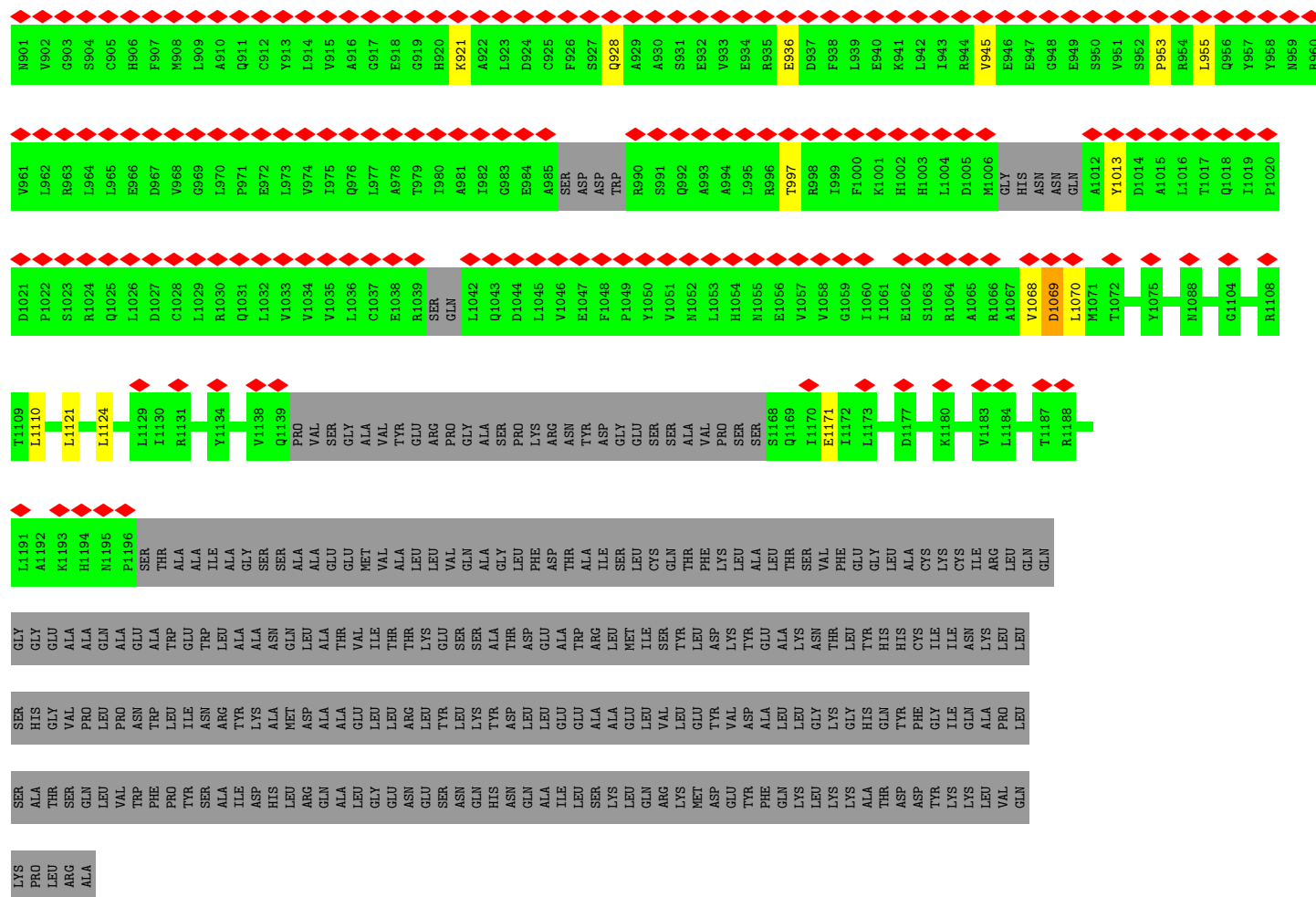
• Molecule 4: Nucleoporin SEH1-A



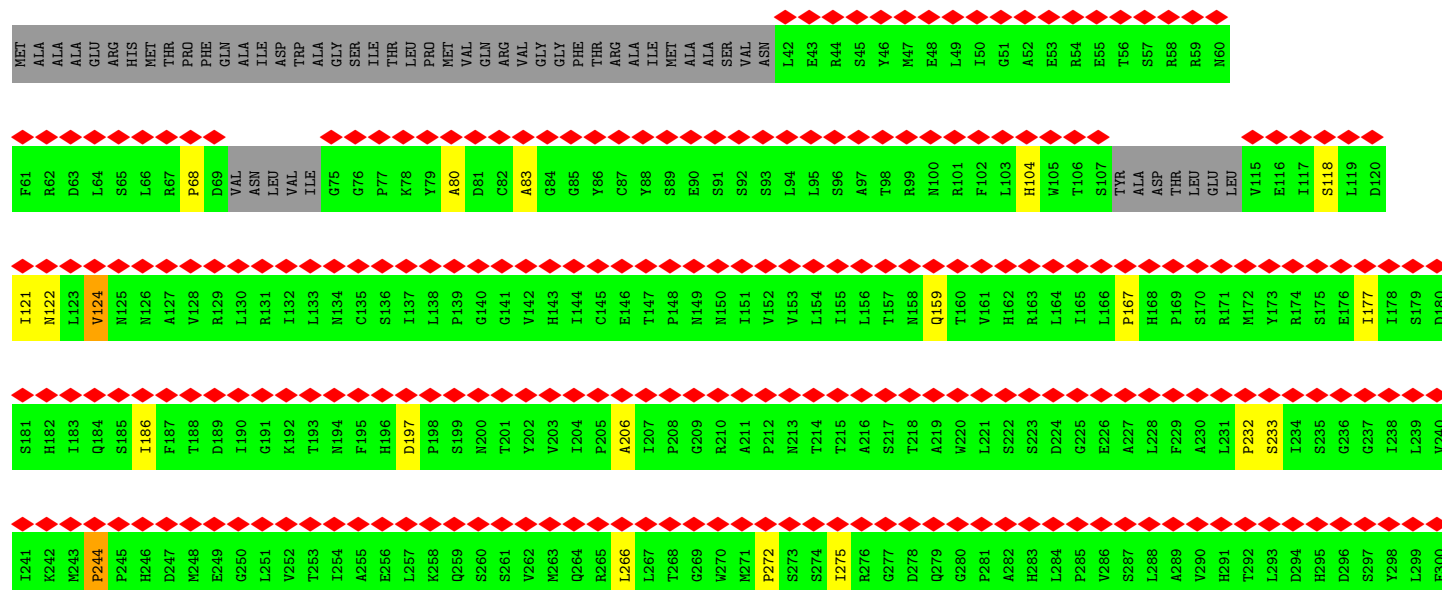
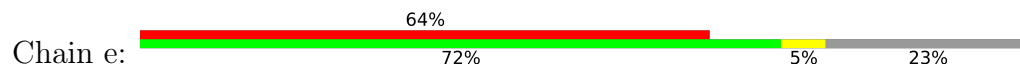
• Molecule 5: outer Nup160



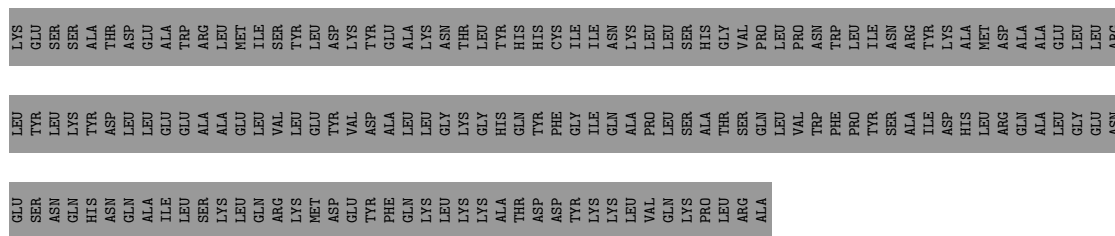
A841	S842	Q843	LEU	GLN	GLU	PRO	LEU	N849	W850	C729	GLU	S851	D852	L853	L854	K855	R856	L857	T858	N859	Y860	L861	L862	Q863	L864	L865	W866	P867	R868	Y869	P870	N871	F872	Q873	F874	A875	E876	C877	L878	M879	R880	F881	C882	Q883	Y884	T885	Q886	L887	Q888	E889	Y890	R891	R892	L893	L894	L895	P896	C898	Q899	V900
L781	A782	C783	A784	V785	P786	V787	D788	ILE	LEU	LEU	GLU	SER	ASN	LEU	GLN	HIS	LEU	SER	VAL	N859	Y860	L861	L862	Q863	L864	L865	W866	P867	R868	Y869	P870	N871	F872	Q873	F874	A875	E876	C877	L878	M879	R880	F881	C882	Q883	Y884	T885	Q886	L887	Q888	E889	Y890	R891	R892	L893	L894	L895	P896	C898	Q899	V900
I661	Q662	N663	K664	L665	Q666	D667	T668	R669	N670	P671	L672	R673	A674	L675	G676	F677	L678	L679	Q680	N681	H682	D683	E684	E685	THR	ASN	ALA	ASP	M690	E691	Q692	P693	Q694	P695	N696	T697	R698	L699	W700	L701	S702	THR	LEU	TYR	GLY	SER	ILE	T709	A710	S711	S712	V713	V714	D715	Q716	A717	C718	K720		
I721	S722	A723	T724	R725	F726	L727	T728	C729	R730	D731	L732	L733	T734	L735	Q736	H737	L738	L739	L740	R741	L742	G743	D744	M745	A746	L747	I748	G749	A750	G751	Q752	L753	L754	H755	S756	Q757	W758	E759	L760	I761	P762	R763	A764	T765	Q766	L767	L768	L769	S770	V771	V772	M773	T774	R775	W776	G777	S778	Q779	C780	
L781	A782	C783	A784	V785	P786	V787	D788	ILE	LEU	LEU	GLU	SER	ASN	LEU	GLN	HIS	LEU	SER	VAL	N859	Y860	L861	L862	Q863	L864	L865	W866	P867	R868	Y869	P870	N871	F872	Q873	F874	A875	E876	C877	L878	M879	R880	F881	C882	Q883	Y884	T885	Q886	L887	Q888	E889	Y890	R891	R892	L893	L894	L895	P896	C898	Q899	V900
I121	N122	L123	V124	N125	N126	THR	A127	ILE	V128	R129	L130	R131	I132	L133	N134	C135	S136	I137	L138	P139	G140	G141	V142	H143	I144	C145	E146	T147	P148	N149	N150	I151	V152	V153	L154	I155	L156	T157	N158	Q159	T160	V161	H162	R163	L164	I165	L166	P167	H168	P169	S170	R171	M172	Y173	ARG	SER	GLU	ILE	L119	D120
SER	HIS	ILE	GLN	SER	ILE	PHE	THR	ASP	GLY	LYS	THR	ASN	PHE	HIS	D197	P198	S199	N200	T201	Y202	V203	I204	P205	A206	I207	P208	G209	R210	A211	P212	N213	T214	T215	A216	S217	T218	A219	W220	L221	S222	S223	D224	G225	E226	A227	L228	F229	A230	L231	P232	S233	I234	S235	G236	G237	L238	I239	V240		
I241	K242	M243	P244	H245	H246	D247	M248	E249	G250	L251	V252	T253	I254	A255	E256	L257	K258	Q259	S260	V262	M263	Q264	R265	L266	L267	T268	G269	P270	A271	P272	M271	P272	S273	S274	I275	R276	G277	D278	Q279	G280	P281	A282	H283	L284	P285	V286	S287	L288	A289	V290	H291	T292	L293	D294	H295	D296	S297	Y298	L299	F300
A301	L302	C303	Q304	D305	H306	K307	L308	R309	M310	W311	S312	Y313	K314	D315	Q316	M317	C318	L319	M320	V321	A322	D323	M324	L325	E326	Y327	V328	P329	V330	S331	K332	D333	I334	R335	Q336	T337	A338	G339	T340	G341	H342	K343	L344	R345	L346	A347	F348	S349	E350	T351	L352	G353	I354	L355	Y356	L357	G358	V359	Y360	
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I721	S722	A723	T724	R725	F726	L727	T728	C729	R730	D731	L732	L733	T734	L735	Q736	H737	L738	L739	L740	R741	L742	G743	D744	M745	A746	L747	I748	G749	A750	G751	Q752	L753	L754	H755	S756	Q757	W758	E759	L760	I761	P762	R763	A764	T765	Q766	L767	L768	L769	S770	V771	V772	M773	T774	R775	W776	G777	S778	Q779	C780	



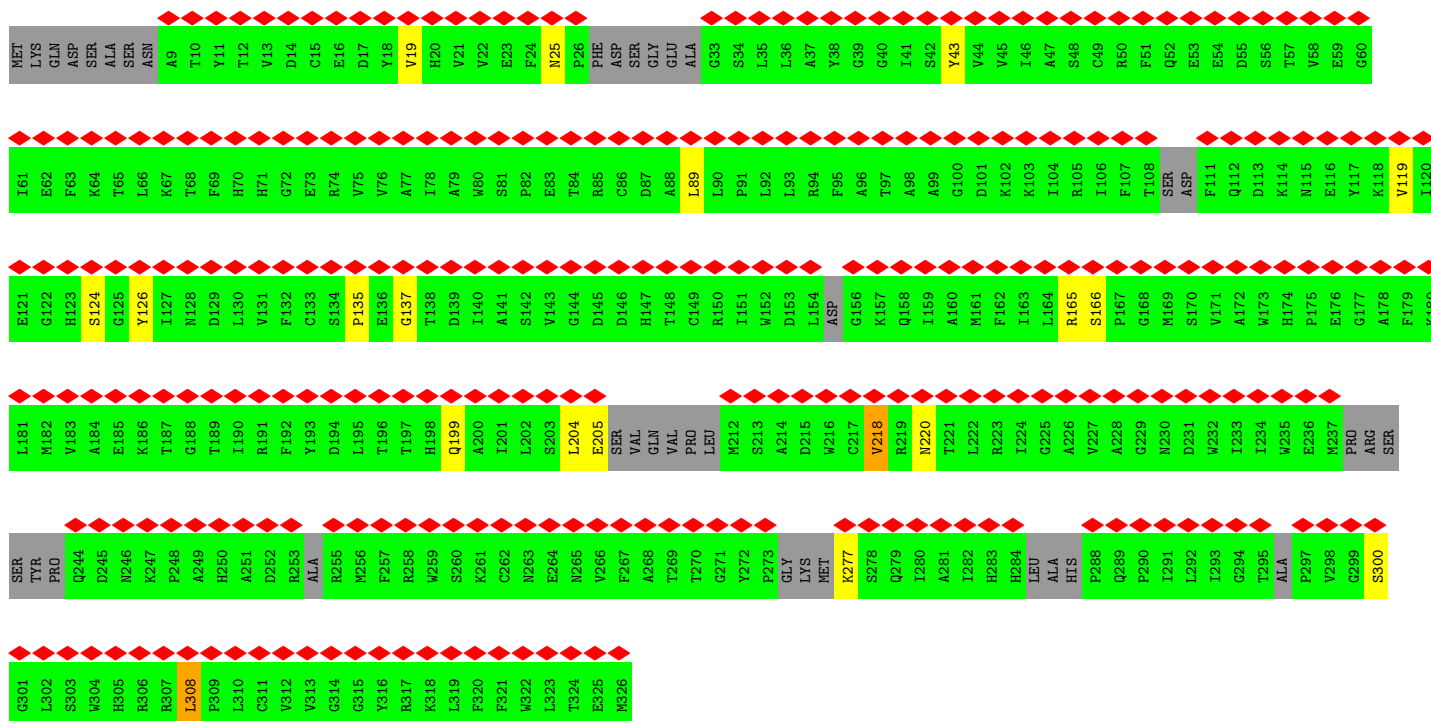
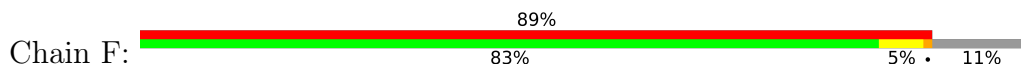
• Molecule 5: outer Nup160



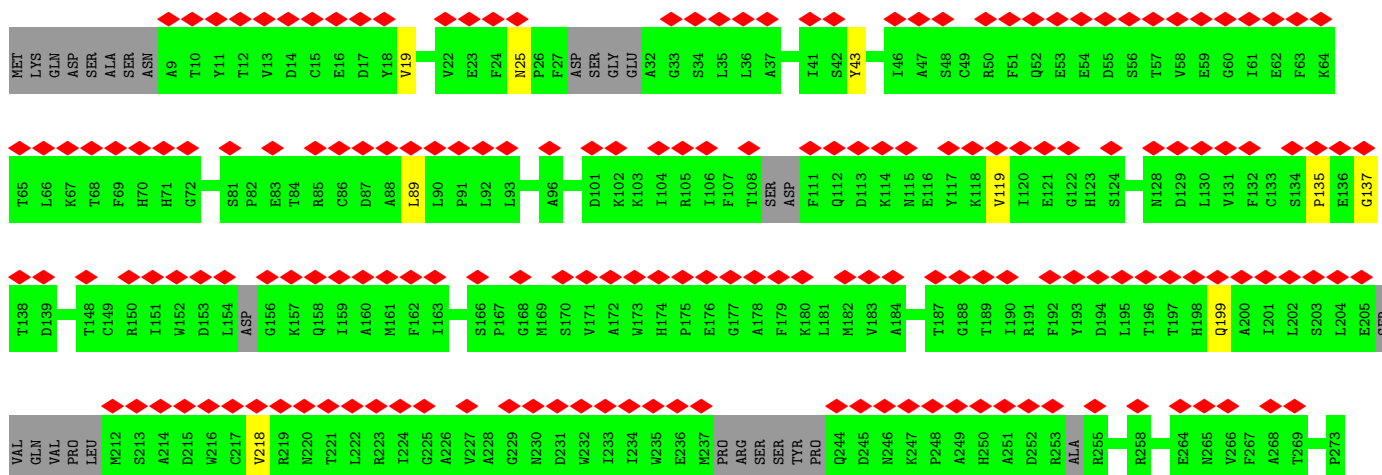
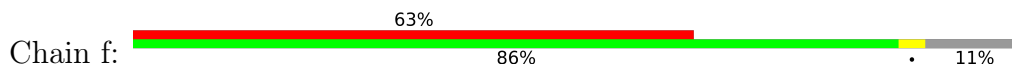


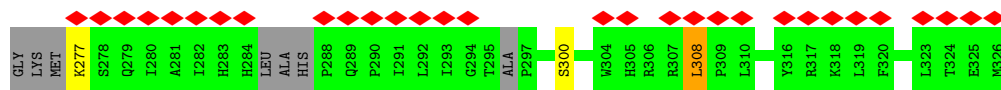


- Molecule 6: MGC83926 protein

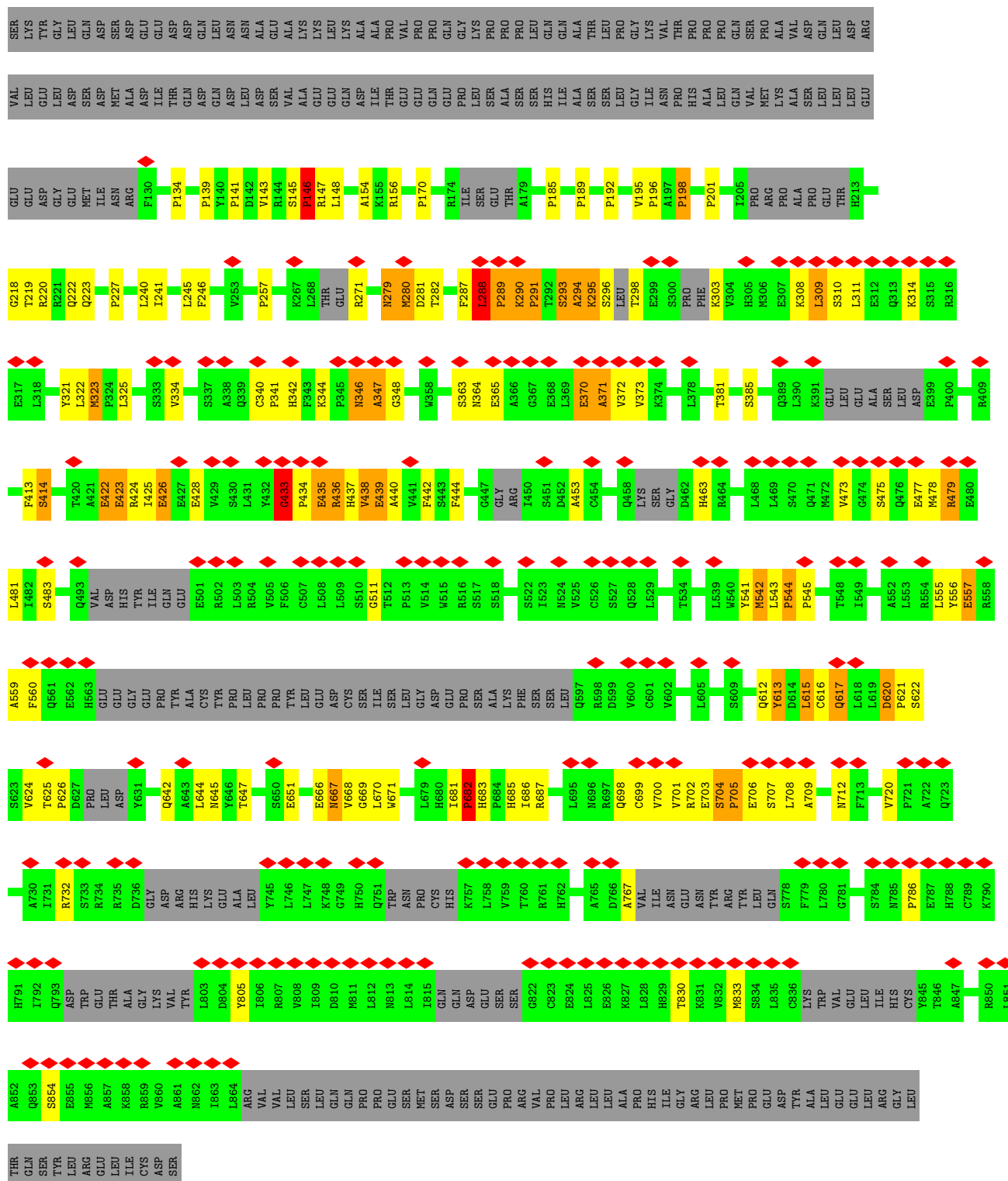


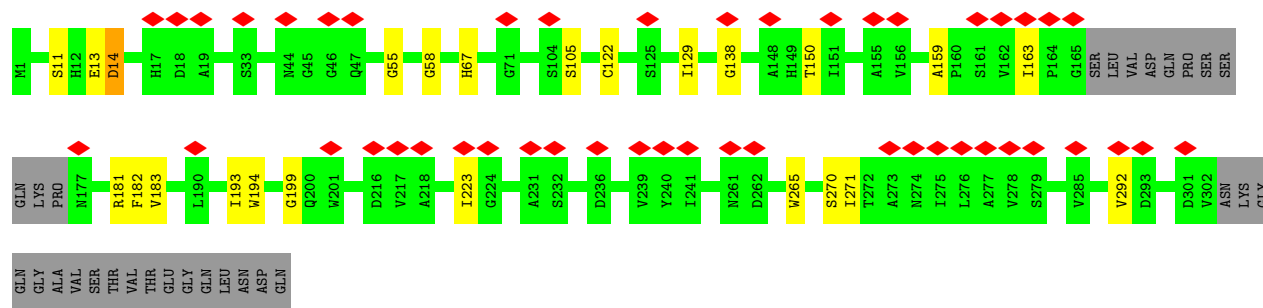
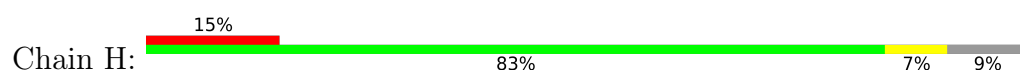
- Molecule 6: MGC83926 protein



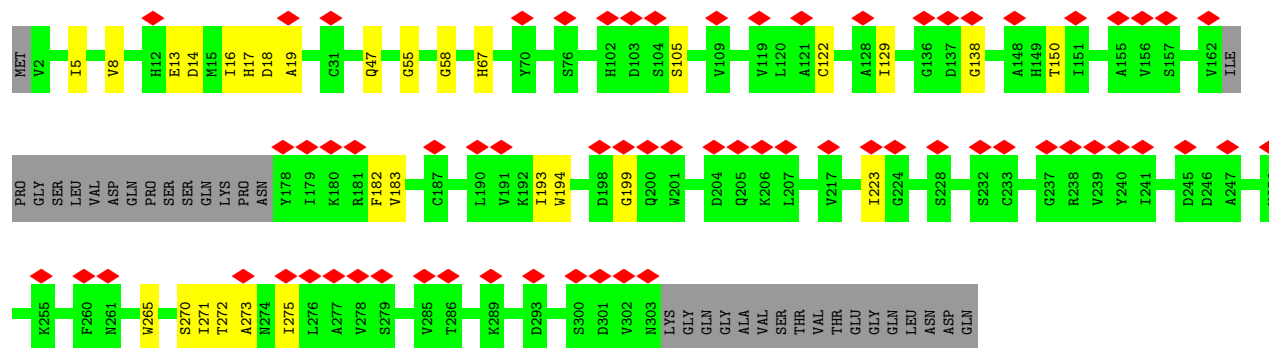
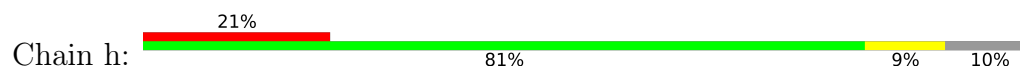


• Molecule 7: Nuclear pore complex protein Nup96

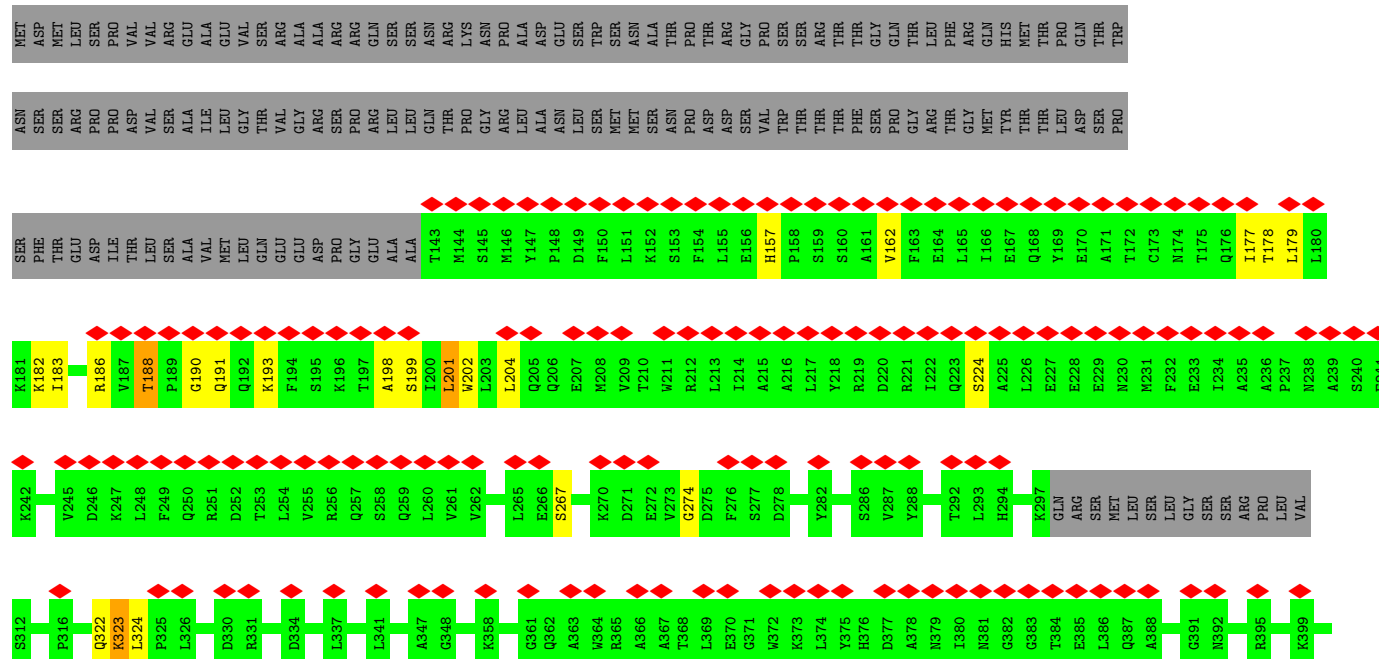
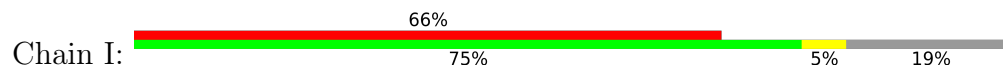


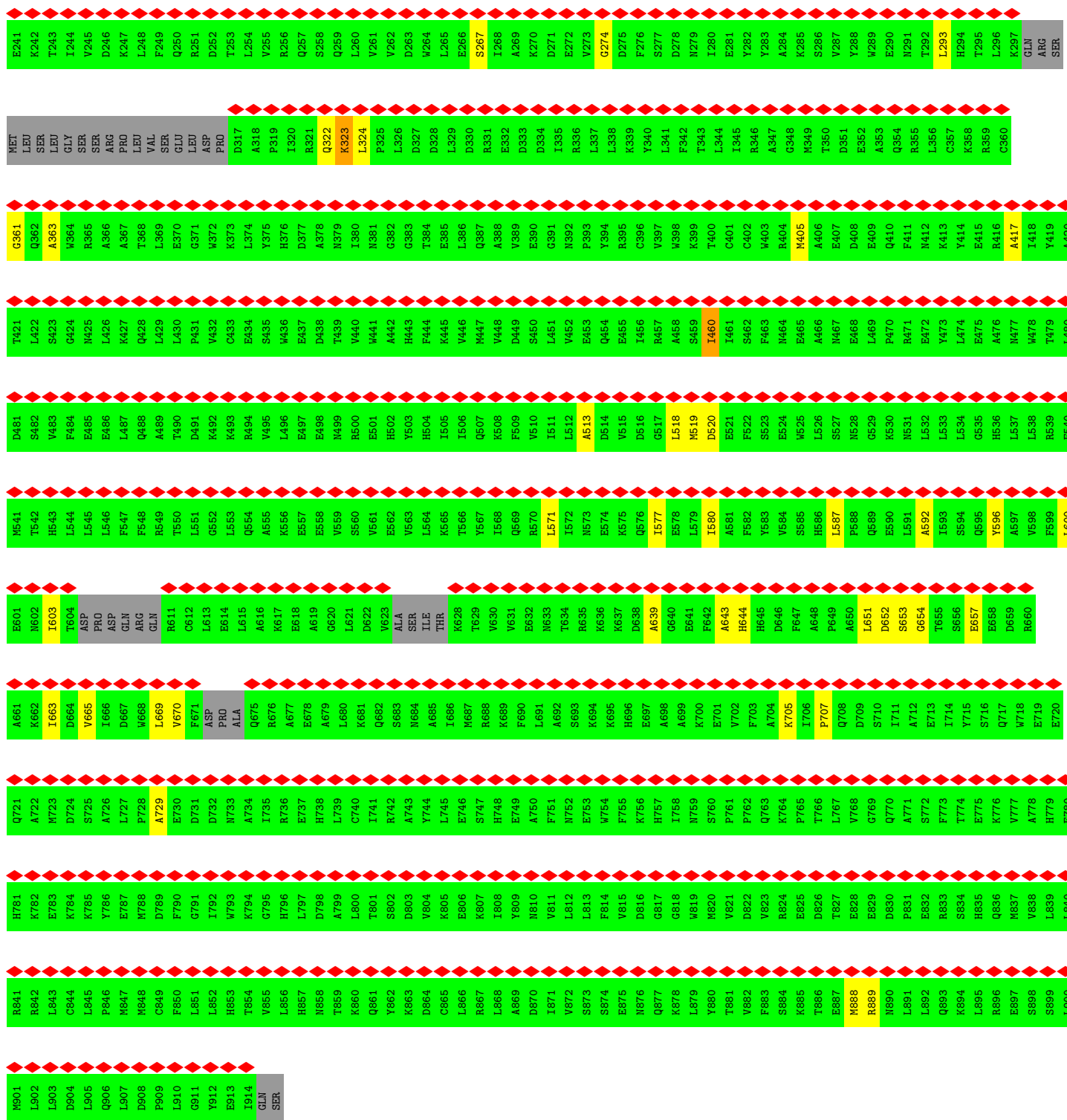


• Molecule 8: GATOR complex protein SEC13

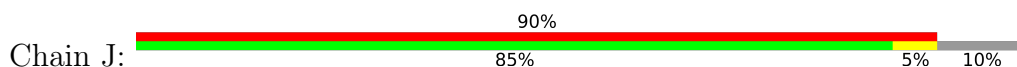


• Molecule 9: Nuclear pore complex protein



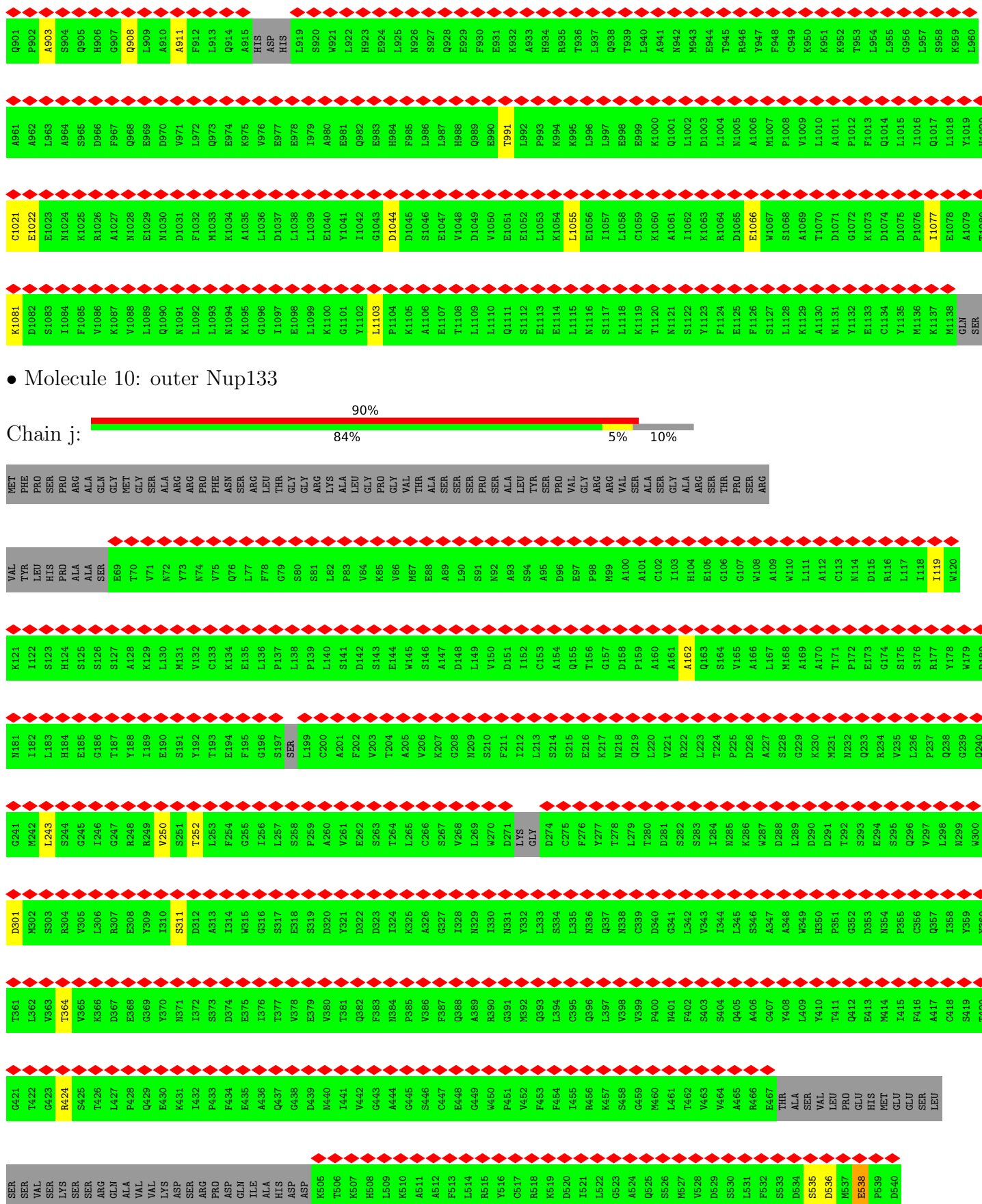


• Molecule 10: outer Nup133



MET	PHE	PRO	SER	PRO	ARG	ALA	GLN	GLY	MET	SER	GLY	LEU	GLY	THR	GLY	ARG	LYS	ALA	LEU	PRO	GLY	GLY	VAL	THR	SER	SER	SER	PRO	SER	ALA	LEU	TYR	SER	PRD	VAL	GLY	ARG	ARG	VAL	SER	ALA	GLY	ALA	ARG	THR	PRO	SER	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	TYR	LEU	HIS	PRO	ALA	ALA	SER	E69	T70	V71	N72	Y73	N74	V75	Q76	L77	F78	G79	S80	S81	L82	P83	V84	K85	V86	M87	E88	A89	L90	S91	N92	A93	S94	A95	D96	E97	P98	M99	A100	A101	C102	I103	H104	E105	G106	G107	H108	A109	W110	L111	A112	C113	N114	D115	R116	L117	I118	I119	W120
K121	I122	S123	H124	S125	S126	S127	A128	K129	V130	M131	V132	C133	K134	E135	L136	P137	L138	P139	L140	S141	D142	S143	E144	W145	S146	A147	D148	L149	V150	D151	I152	C153	A154	Q155	T156	G157	D158	P159	A160	A161	A162	Q163	S164	V165	A166	L167	M168	A169	A170	T171	P172	E173	G174	S175	S176	R177	W178	W179	P180
N181	I182	L183	H184	E185	G186	T187	Y188	L189	E190	S191	Y192	T193	E194	F195	G196	S197	SER	L199	C200	A201	F202	V203	T204	A205	V206	K207	G208	N209	S210	F211	I212	L213	S214	S215	E216	K217	N218	Q219	L220	V221	R222	L223	T224	P225	K226	A227	S228	G229	K230	M231	Q232	Q233	R234	V235	L236	P237	Q238	G239	Q240
G241	M242	L243	S244	G245	I246	G247	R248	R249	V250	S251	T252	L253	F254	G255	I256	L257	S258	P259	A260	V261	E262	S263	T264	L265	C266	S267	V268	L269	W270	D271	LVS	GLY	D274	C275	F276	Y277	T278	L279	T280	D281	S282	S283	I284	N285	K286	W287	D288	L289	D290	D291	T292	S293	E294	S295	Q296	V297	L298	N299	W300
D301	M302	S303	R304	V305	L306	R307	E308	Y309	I310	S311	D312	A313	I314	W315	G316	S317	E318	S319	D320	Y321	D322	S323	I324	K325	A326	G327	I328	N329	I330	N331	Y332	L333	S334	L335	N336	Q337	N338	C339	D340	G341	L342	V343	I344	N345	S346	A347	A348	W349	H350	F351	G352	D353	N354	P355	C356	Q357	L358	Y359	Y360
T361	L362	V363	T364	V365	K366	D367	E368	G369	Y370	N371	S372	S373	D374	E375	I376	T377	V378	E379	V380	T381	Q382	F383	N384	P385	V386	F387	Q388	A389	R390	G391	K392	Q393	L394	C395	Q396	L397	V398	V399	P400	M401	F402	S403	S404	Q405	A406	C407	Y408	L409	Y410	T411	Q412	E413	M414	I415	F416	A417	C418	S419	T420
G421	T422	G423	R424	S425	T426	L427	P428	Q429	E430	K431	L432	P433	F434	E435	A436	Q437	C438	D439	N440	I441	V442	G443	A444	G445	S446	C447	E448	G449	W450	P451	V452	F453	F454	I455	R456	K457	S458	G459	M460	L461	T462	V463	V464	A465	R466	E467	THR	ALA	SER	VAL	LEU	PRO	GLU	HIS	MET	GLU	SER	LEU	
SER	SER	VAL	LYS	SER	ARG	GLN	ALA	VAL	VAL	LYS	ASP	SER	ARG	PRO	ASP	GLN	ILE	HIS	ASP	ASP	K505	T506	K507	H508	L509	K510	A511	A512	F513	L514	R515	Y516	C517	R518	K519	D520	L521	L522	G523	A524	Q525	S526	M527	V528	D529	S530	L531	F532	S533	D534	S535	D536	M537	E538	P539	D540			
D541	E542	L543	D544	L545	A546	V547	N548	Q549	L550	S551	V552	D553	L554	L555	L556	D557	Y558	P559	A560	S561	D562	P563	R564	W565	A566	E567	S568	V569	P570	E571	E572	A573	A574	G575	F576	S577	N578	L579	S580	L581	L582	L583	L584	H585	Q586	L587	E588	D589	K590	M591	K592	A593	H594	S595	F596	F597	V598	D599	F600
L601	H602	Q603	V604	G605	L606	F607	S608	R609	L610	SER	T612	C613	D614	T615	K616	G617	M618	L619	V620	A621	T622	Q623	L624	L625	L626	S627	E628	H629	A630	E631	K632	L633	S634	A635	A636	L637	V638	L639	K640	N641	H642	H643	A644	K645	L646	P647	V648	L649	V650	N651	S652	A653	L654	Q655	L656	A657	L658	D659	K660
R661	H662	C663	T664	V665	P666	Q667	H668	L669	T670	A671	A672	D673	V674	V675	F676	R677	E678	V679	S680	Q681	H682	Q683	L684	L685	F686	E687	C688	L689	V690	D691	E692	E693	E694	A695	D696	L697	E698	S699	T700	S701	T702	D703	S704	W705	E706	W707	A708	N709	T710	V711	V712	N713	T714	L715	Q716	L717	L718	K719	D720
M721	L722	H723	V724	A725	C726	Q727	Y728	R729	Q730	S731	K732	M733	S734	L735	Y736	K737	H738	E739	G740	S741	T742	Q743	E744	F745	E746	H747	V748	F749	L750	T751	A752	S753	S754	G755	T756	A757	G758	L759	R760	S761	V762	V763	T764	R765	Q766	H767	G768	I769	L770	L771	K772	Y773	L774	P775	Q776	A777	D778	S779	G780
L781	R782	T783	L784	L785	L786	E787	Q788	L789	A790	A791	L792	L793	H794	Y795	L796	L797	D798	E799	W800	V801	M802	Q803	D804	K805	S806	I807	D808	K809	L810	A811	N812	E813	E814	R815	Y816	N817	L818	L819	E820	M821	S822	H823	P824	Q825	K826	R827	S828	Y829	L830	L831	S832	R833	K834	L835	R836	L837	L838	Q839	S840
W842	A843	S844	N845	L846	A847	E848	R849	Y850	C851	D852	F853	D854	I855	L856	W857	Q858	I859	C860	E861	M862	T863	D864	N865	Q866	S867	R868	L869	Q870	R871	Y872	M873	T874	L875	F876	A877	E878	Q879	N880	F881	S882	D883	P884	L885	R886	R887	W888	Y889	E891	K892	C893	K894	R895	C896	K897	L898	L899	S900		



K1081	C1021	A961	Q901	A841	L781	M721	R661	D541
D1082	E1022	A962	P902	W842	R782	L722	M662	E542
S1083	E1023	A963	ALA	A843	T783	H723	C663	L543
I1084	N1024	A964	SER	S844	I784	V724	T664	D544
F1085	K1025	S965	H906	N845	L785	A725	V665	L545
V1086	R1026	D966	G907	L846	I786	C726	P666	A546
K1087	A1027	F967	Q908	A847	E787	Q727	Q667	V547
V1088	N1028	Q968	L909	E848	Q788	Y728	N668	N548
L1089	E1029	E969	A910	K849	L789	R729	L669	Q549
Q1090	N1030	D970	A911	Y850	A790	Q730	T670	I550
N1091	D1031	V971	F912	C851	A791	S731	A671	S551
L1092	F1032	L972	L913	D852	L792	K732	A672	V552
L1093	M1033	Q973	Q914	F853	L793	N733	D673	D553
N1094	K1034	E974	A915	D854	N794	S734	V674	L554
K1095	A1035	K975	H916	I855	Y795	L735	Y675	I555
G1096	L1036	V976	D917	L856	L796	Y736	F676	D556
I1097	D1037	E977	H918	V857	L797	K737	R677	D557
E1098	L1038	E978	L919	Q858	D798	N738	E678	Y558
L1099	L1039	I979	S920	I859	D799	E739	V679	P559
K1100	E1040	A980	W921	C860	Y800	S740	S680	A560
G1101	Y1041	E981	L922	E861	R801	G741	Q681	S561
Y1102	I1042	Q982	H923	H862	T802	I742	M682	D562
L1103	G1043	E983	E924	T863	Q803	Q743	E683	R563
P1104	D1044	H984	L925	D864	L804	E744	I684	R564
K1105	D1045	F985	N926	N865	K805	F745	I685	W565
A1106	S1046	L986	S927	Q866	S806	E746	F686	A566
E1107	E1047	L987	Q928	S867	I807	H747	E687	E567
T1108	V1048	H988	E929	R868	D808	V748	C688	S568
L1109	D1049	Q989	E930	L869	K809	F749	L689	V569
L1110	V1050	E990	F931	Q870	L810	W750	V690	P570
Q1111	E1051	T991	K932	R871	A811	T751	D691	E571
S1112	E1052	L992	A933	W872	N812	A752	K692	E572
E1113	L1053	P993	H934	M873	E813	S753	E693	A573
E1114	K1054	K994	R935	T874	E814	S754	E694	A574
L1115	L1055	K995	T936	L875	R815	G755	A695	G575
M1116	E1056	L996	L937	F876	Y816	T756	D696	F576
S1117	I1057	L997	Q938	A877	N817	L697	I697	S577
L1118	L1058	E998	T939	E878	I818	G758	E698	N578
K1119	C1059	E999	L940	Q879	L819	I759	S699	T579
T1120	K1060	K1000	L941	N880	E820	R760	T700	S580
M1121	A1061	Q1001	N942	F881	M821	S761	N641	L581
S1122	I1062	L1002	M943	S882	E822	V762	I702	I582
Y1123	K1063	D1003	E944	D883	Y823	D703	H643	L583
F1124	L1064	L1004	T945	F884	A824	T764	S704	L584
E1125	D1065	N1005	R946	L885	Q825	R765	V705	H585
F1126	E1066	A1006	Y947	F886	K826	Q766	E706	Q586
S1127	W1067	M1007	F948	R887	R827	H767	P647	Q586
L1128	S1068	P1008	C949	W888	S828	G768	V648	L587
K1129	A1069	V1009	K950	Y889	E829	I769	L649	E588
A1130	T1070	L1010	K951	L890	L830	I770	V650	D589
M1131	D1071	A1011	K952	E891	L831	L771	N651	K590
Y1132	G1072	P1012	T953	K892	S832	K772	S652	M591
E1133	K1073	F1013	L954	G893	P833	V773	N713	K592
C1134	D1074	Q1014	L955	K894	L834	I774	I654	A593
Y1135	D1075	L1015	G956	R895	L835	P775	Q655	H594
M1136	P1076	I1016	L957	G896	I836	Q776	T716	S595
K1137	I1077	Q1017	L957	K897	L837	I717	A657	F597
M1138	E1078	L1018	S958	L898	Q838	D778	L658	V598
Q1139	T1080	Y1019	L960	L899	Q839	S779	D659	D599
SER		W1020		Q900	Y840	C780	K720	F600

• Molecule 11: Nup358 complex, clamps



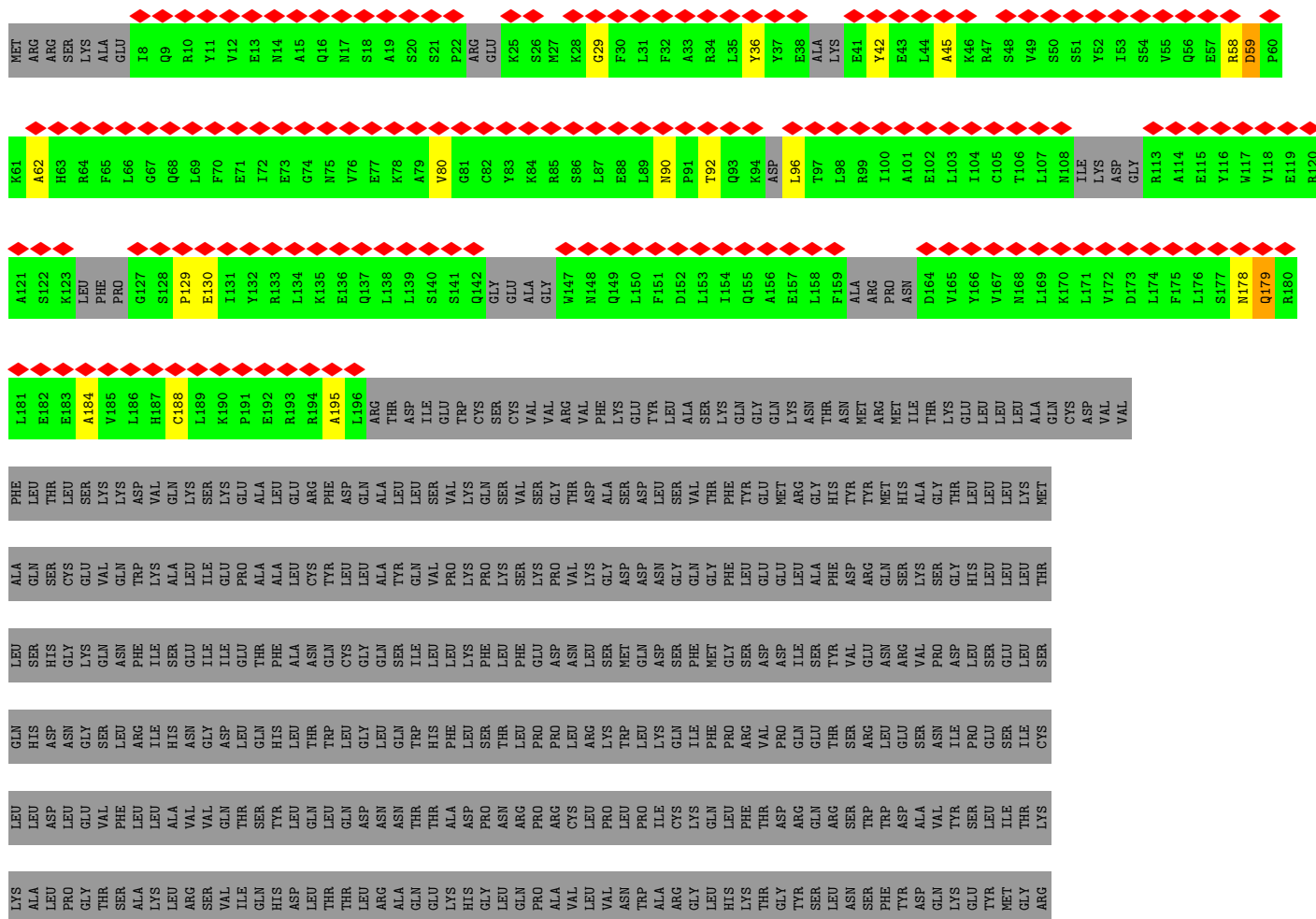
MET	ARG	ARG	SER	LYS	ALA	GLU	I8	Q9	R10	Y11	N14	A15	Q16	N17	S18	A19	S20	S21	P22	ARG	GLU	K25	S26	M27	K28	C29	F30	L31	F32	A33	R34	L35	Y36	Y37	E38	ALA	LYS	E41	Y42	E43	L44	A45	K46	R47	S48	V49	S50	S51	Y52	I53	S54	V55	Q56	E57	R58	D59	P60	K61
A62	H63	R64	F65	L66	G67	Q68	L69	F70	E71	I72	E73	G74	N75	V76	E77	K78	A79	V80	G81	C82	Y83	K84	R85	S86	L87	E88	L89	N90	P91	T92	Q93	K94	ASP	L96	T97	L98	R99	I100	A101	E102	L103	S104	C105	T106	L107	N108	I109	L110	R113	A114	E115	Y116	W117	V118	E119	R120	A121	





[illegible]

- Molecule 11: Nup358 complex, clamps





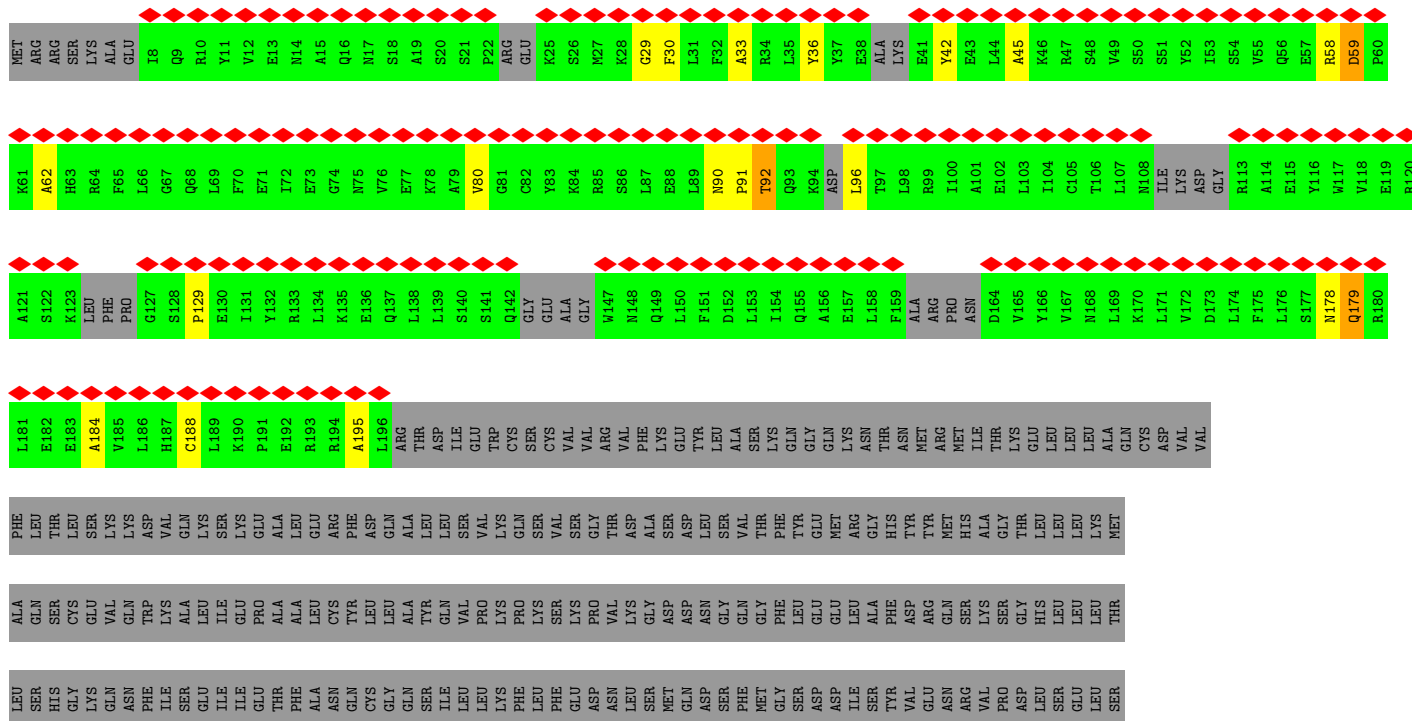






[illegible]

- Molecule 11: Nup358 complex, clamps

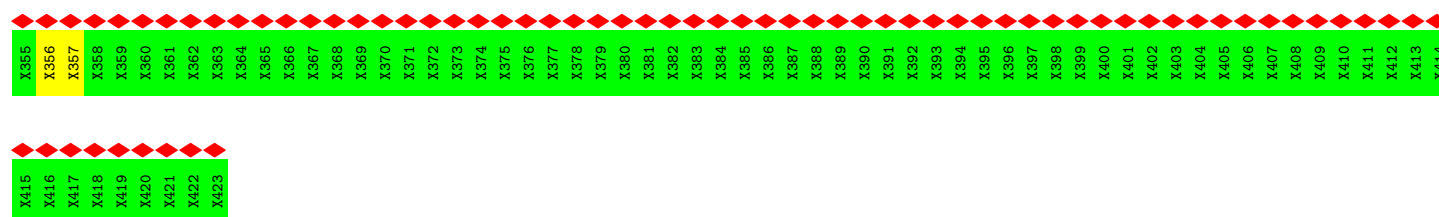




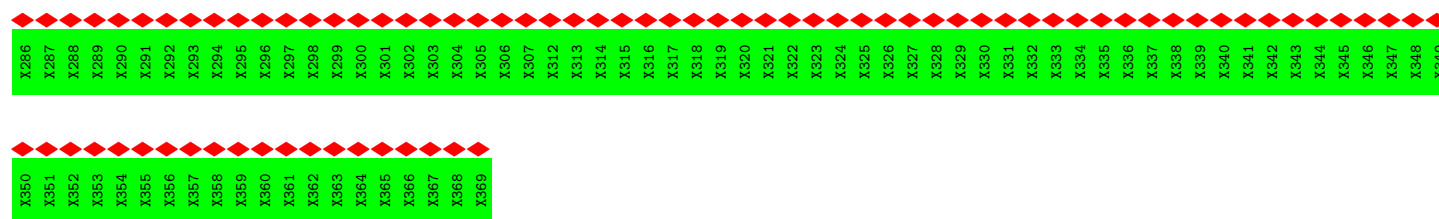


[illegible]

- Molecule 12: Nup214 complex Coiled-coil region 1, helix 1



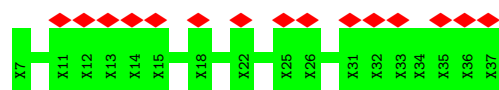
- Molecule 13: Nup214 complex coiled coil region 1, helix 2



- Molecule 14: Nup214 complex coiled coil region 1, helix 3



- Molecule 15: Nup214 complex Coiled coil region 2, helix 1

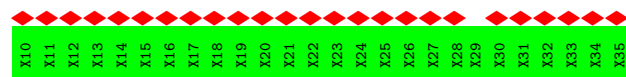


- Molecule 16: Nup214 complex Coiled coil region 2, helix 2

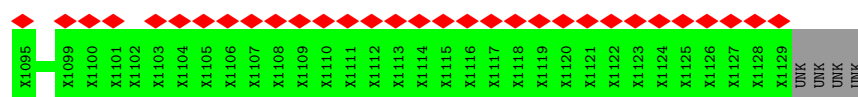
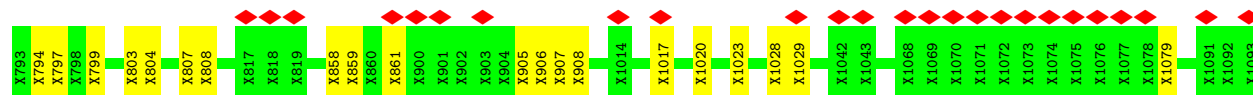
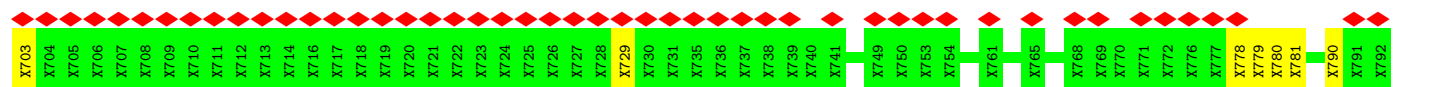
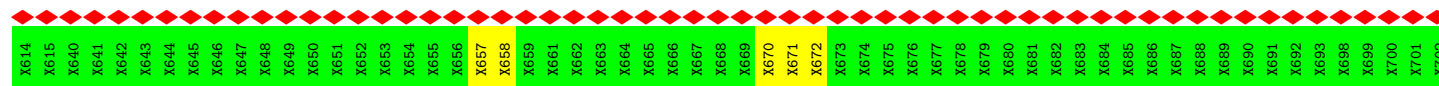
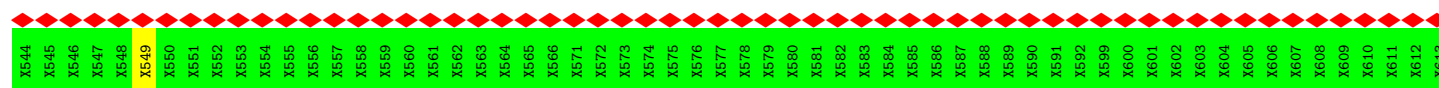
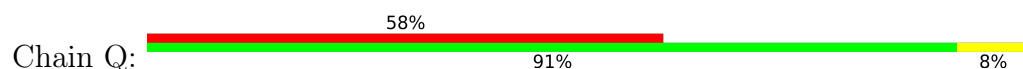




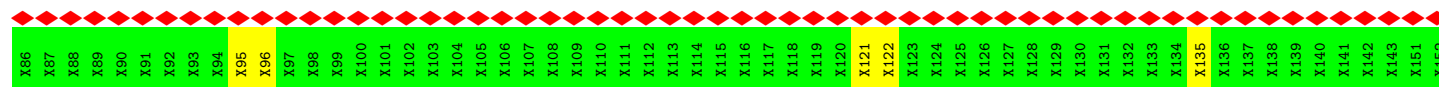
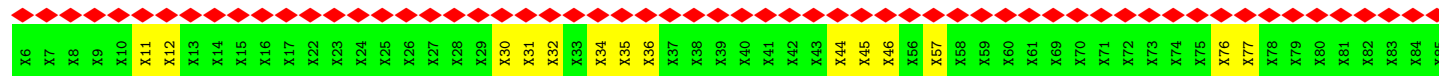
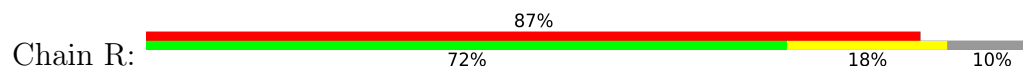
- Molecule 17: Nup214 complex Coiled coil region 2, helix 3



- Molecule 18: bridge domain



- Molecule 18: bridge domain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	616547	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	568.832, 568.832, 568.832	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.222, 2.222, 2.222	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	0.73	2/6901 (0.0%)	1.41	44/9542 (0.5%)
1	a	0.84	1/6275 (0.0%)	1.63	63/8703 (0.7%)
2	B	0.52	0/2623	1.10	11/3634 (0.3%)
2	b	0.50	0/2555	1.08	9/3534 (0.3%)
3	C	0.69	1/1150 (0.1%)	1.13	4/1427 (0.3%)
3	c	0.61	0/1160	1.03	5/1436 (0.3%)
4	D	1.07	0/1516	1.54	10/2108 (0.5%)
4	d	1.10	0/1446	1.58	9/2009 (0.4%)
5	E	0.95	0/5091	1.73	47/7076 (0.7%)
5	e	0.95	0/5486	1.73	48/7634 (0.6%)
6	F	1.02	0/1413	1.50	6/1949 (0.3%)
6	f	1.02	0/1423	1.50	6/1963 (0.3%)
7	G	0.65	2/3046 (0.1%)	1.33	39/4220 (0.9%)
7	g	0.63	6/2986 (0.2%)	1.32	43/4127 (1.0%)
8	H	1.06	0/1417	1.54	11/1959 (0.6%)
8	h	1.06	0/1411	1.55	12/1959 (0.6%)
9	I	0.90	0/3662	1.70	26/5104 (0.5%)
9	i	0.91	0/3607	1.72	30/5027 (0.6%)
10	J	0.98	2/5079 (0.0%)	1.68	41/7074 (0.6%)
10	j	0.98	2/5084 (0.0%)	1.70	47/7081 (0.7%)
11	S	0.67	0/832	1.51	10/1149 (0.9%)
11	T	0.67	0/832	1.51	10/1149 (0.9%)
11	U	0.68	0/853	1.52	12/1181 (1.0%)
11	V	0.67	0/832	1.50	8/1149 (0.7%)
All	All	0.86	16/66680 (0.0%)	1.55	551/92194 (0.6%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	289	SER	CA-C	-7.89	1.42	1.52
7	g	625	THR	C-N	6.93	1.41	1.34
10	J	1077	ILE	CA-CB	-6.77	1.46	1.54
10	j	1077	ILE	CA-CB	-6.64	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	543	LEU	C-N	6.54	1.41	1.33
7	G	620	ASP	C-N	6.49	1.42	1.34
7	g	720	VAL	C-N	6.29	1.41	1.33
7	G	720	VAL	C-N	6.26	1.41	1.33
1	A	1534	VAL	CA-C	-6.11	1.45	1.52
1	a	115	GLY	CA-C	-5.81	1.47	1.52
7	g	340	CYS	C-N	5.71	1.41	1.33
7	g	544	PRO	C-N	5.71	1.41	1.33
7	g	620	ASP	C-N	5.65	1.41	1.34
10	j	119	ILE	CA-C	-5.34	1.46	1.52
10	J	119	ILE	CA-C	-5.30	1.46	1.52
1	A	1523	VAL	CA-C	-5.28	1.46	1.52

All (551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	1007	MET	CA-C-N	14.59	134.47	120.03
10	j	1007	MET	C-N-CA	14.59	134.47	120.03
7	G	671	TRP	N-CA-C	11.78	124.12	111.28
1	a	1573	LEU	N-CA-C	10.32	123.49	111.11
1	A	1528	LEU	N-CA-C	-10.28	99.28	112.23
5	e	635	LEU	N-CA-C	10.08	122.27	111.28
2	b	67	VAL	N-CA-C	-9.18	101.85	111.58
2	B	67	VAL	N-CA-C	-9.13	101.90	111.58
9	I	587	LEU	CA-C-N	8.98	129.01	119.05
9	I	587	LEU	C-N-CA	8.98	129.01	119.05
9	i	587	LEU	CA-C-N	8.95	128.99	119.05
9	i	587	LEU	C-N-CA	8.95	128.99	119.05
5	E	602	ALA	N-CA-C	8.92	120.61	111.07
5	e	602	ALA	N-CA-C	8.92	120.61	111.07
1	A	1531	ASP	N-CA-C	-8.91	101.48	111.82
5	E	206	ALA	CA-C-N	8.82	125.80	120.24
5	E	206	ALA	C-N-CA	8.82	125.80	120.24
1	A	1525	VAL	N-CA-C	-8.81	102.14	110.42
5	e	206	ALA	CA-C-N	8.79	125.78	120.24
5	e	206	ALA	C-N-CA	8.79	125.78	120.24
7	g	166	LYS	N-CA-C	-8.63	101.88	111.28
9	I	201	LEU	N-CA-C	-8.56	102.03	111.36
1	a	519	SER	N-CA-C	8.23	119.87	111.07
1	A	1130	ARG	N-CA-C	7.89	119.51	111.07
9	i	162	VAL	N-CA-C	7.82	117.92	110.42
7	G	620	ASP	CA-C-N	-7.79	110.94	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	620	ASP	C-N-CA	-7.79	110.94	119.19
9	I	162	VAL	N-CA-C	7.74	117.85	110.42
1	a	428	PRO	N-CA-C	7.73	120.13	110.70
4	D	171	ASN	CA-C-N	7.70	127.88	119.87
4	D	171	ASN	C-N-CA	7.70	127.88	119.87
4	d	171	ASN	CA-C-N	7.69	127.87	119.87
4	d	171	ASN	C-N-CA	7.69	127.87	119.87
7	G	220	ARG	N-CA-C	-7.64	102.95	111.28
10	j	1022	GLU	CA-C-N	7.63	130.84	120.38
10	j	1022	GLU	C-N-CA	7.63	130.84	120.38
7	G	147	ARG	N-CA-C	7.61	122.00	109.06
5	e	244	PRO	CA-C-N	7.60	127.14	119.24
5	e	244	PRO	C-N-CA	7.60	127.14	119.24
7	g	873	PRO	N-CA-CB	7.57	110.42	103.08
1	A	1534	VAL	N-CA-C	-7.56	103.49	110.82
5	E	244	PRO	CA-C-N	7.55	127.09	119.24
5	E	244	PRO	C-N-CA	7.55	127.09	119.24
10	J	1022	GLU	CA-C-N	7.54	130.71	120.38
10	J	1022	GLU	C-N-CA	7.54	130.71	120.38
5	E	865	LEU	CA-C-N	7.54	129.51	120.09
5	E	865	LEU	C-N-CA	7.54	129.51	120.09
7	G	198	PRO	N-CA-CB	7.53	111.16	103.25
7	G	196	PRO	N-CA-CB	7.50	110.31	103.33
7	g	543	LEU	CA-C-N	-7.45	112.71	120.38
7	g	543	LEU	C-N-CA	-7.45	112.71	120.38
1	a	41	ILE	CA-C-N	7.43	130.64	120.46
1	a	41	ILE	C-N-CA	7.43	130.64	120.46
1	A	41	ILE	CA-C-N	7.42	130.63	120.46
1	A	41	ILE	C-N-CA	7.42	130.63	120.46
7	G	148	LEU	N-CA-C	-7.35	103.78	112.89
1	A	701	THR	N-CA-C	7.35	119.29	111.28
5	E	859	ASN	N-CA-C	7.34	119.28	111.28
5	e	859	ASN	N-CA-C	7.29	119.22	111.28
8	h	8	VAL	N-CA-C	7.28	118.05	110.62
7	G	146	PRO	N-CA-CB	7.25	110.58	102.60
1	a	1304	HIS	N-CA-C	-7.25	103.38	111.28
2	B	429	GLY	N-CA-C	-7.22	104.02	112.83
3	C	189	VAL	N-CA-C	-7.20	105.50	111.91
7	g	161	GLY	N-CA-C	-7.18	104.11	112.73
7	G	139	PRO	N-CA-CB	7.18	110.40	103.51
9	i	181	LYS	N-CA-C	7.08	118.79	111.14
10	j	1007	MET	N-CA-C	7.07	116.27	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1333	VAL	N-CA-C	7.02	117.78	110.62
1	a	365	VAL	N-CA-C	6.99	117.75	110.62
1	A	365	VAL	N-CA-C	6.94	117.70	110.62
7	g	163	LEU	N-CA-C	-6.93	103.73	111.28
1	A	57	PRO	N-CA-C	6.87	119.08	110.70
1	a	634	SER	N-CA-C	6.87	118.77	111.28
7	G	682	PRO	CB-CA-C	6.86	122.88	111.56
9	i	200	ILE	CA-C-N	6.85	129.35	120.44
9	i	200	ILE	C-N-CA	6.85	129.35	120.44
1	a	57	PRO	N-CA-C	6.85	119.05	110.70
10	J	538	GLU	O-C-N	-6.82	113.48	121.32
7	g	170	PRO	N-CA-CB	6.80	110.39	103.25
10	J	558	TYR	CA-C-N	6.78	126.41	119.56
10	J	558	TYR	C-N-CA	6.78	126.41	119.56
10	j	558	TYR	CA-C-N	6.76	126.39	119.56
10	j	558	TYR	C-N-CA	6.76	126.39	119.56
10	j	538	GLU	O-C-N	-6.76	113.55	121.32
7	g	185	PRO	N-CA-CB	6.74	110.41	103.00
1	a	802	LEU	N-CA-C	6.72	118.40	111.14
1	a	803	MET	N-CA-C	6.71	118.39	111.14
7	g	201	PRO	N-CA-CB	6.71	110.38	103.00
7	g	544	PRO	CA-C-N	-6.69	113.09	119.85
7	g	544	PRO	C-N-CA	-6.69	113.09	119.85
7	g	340	CYS	CA-C-N	-6.66	113.12	119.85
7	g	340	CYS	C-N-CA	-6.66	113.12	119.85
1	A	1534	VAL	CB-CA-C	-6.66	103.32	112.04
9	I	729	ALA	CA-C-N	6.63	129.16	120.28
9	I	729	ALA	C-N-CA	6.63	129.16	120.28
11	U	22	PRO	CA-C-N	6.62	134.19	121.54
11	U	22	PRO	C-N-CA	6.62	134.19	121.54
11	U	38	GLU	N-CA-C	-6.61	104.07	111.28
10	j	243	LEU	CA-C-N	6.60	132.49	123.11
10	j	243	LEU	C-N-CA	6.60	132.49	123.11
1	A	1126	LEU	N-CA-C	6.59	118.46	111.28
9	i	729	ALA	CA-C-N	6.59	129.10	120.28
9	i	729	ALA	C-N-CA	6.59	129.10	120.28
10	J	243	LEU	CA-C-N	6.57	132.43	123.11
10	J	243	LEU	C-N-CA	6.57	132.43	123.11
1	a	450	ASP	CA-C-N	6.56	126.33	119.05
1	a	450	ASP	C-N-CA	6.56	126.33	119.05
7	g	681	ILE	O-C-N	6.55	124.72	120.07
7	G	134	PRO	N-CA-CB	6.54	110.52	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	720	VAL	CA-C-N	-6.54	112.77	119.83
7	g	720	VAL	C-N-CA	-6.54	112.77	119.83
7	g	146	PRO	N-CA-CB	6.53	110.52	103.33
7	G	189	PRO	N-CA-CB	6.53	110.51	103.33
7	G	227	PRO	N-CA-CB	6.53	110.51	103.33
10	j	867	SER	CA-C-N	6.53	129.56	120.29
10	j	867	SER	C-N-CA	6.53	129.56	120.29
7	g	189	PRO	N-CA-CB	6.52	110.50	103.33
9	i	417	ALA	N-CA-C	6.52	118.39	111.28
7	G	170	PRO	N-CA-CB	6.51	110.50	103.33
7	G	201	PRO	N-CA-CB	6.51	110.49	103.33
7	g	874	PRO	N-CA-CB	6.51	110.49	103.33
7	g	206	PRO	N-CA-CB	6.51	110.49	103.33
7	G	720	VAL	CA-C-N	-6.50	112.81	119.83
7	G	720	VAL	C-N-CA	-6.50	112.81	119.83
9	I	417	ALA	N-CA-C	6.50	118.37	111.28
1	a	20	ILE	CB-CA-C	-6.50	103.36	112.14
7	g	227	PRO	N-CA-CB	6.50	110.48	103.33
1	a	800	PHE	N-CA-C	-6.50	104.20	111.28
10	J	867	SER	CA-C-N	6.49	129.50	120.29
10	J	867	SER	C-N-CA	6.49	129.50	120.29
7	g	192	PRO	N-CA-CB	6.48	110.46	103.33
7	G	185	PRO	N-CA-CB	6.48	110.45	103.33
7	g	208	PRO	N-CA-CB	6.48	110.45	103.33
7	g	198	PRO	N-CA-CB	6.47	110.45	103.33
7	g	620	ASP	CA-C-N	-6.46	111.88	119.05
7	g	620	ASP	C-N-CA	-6.46	111.88	119.05
11	T	80	VAL	N-CA-CB	6.46	119.32	110.54
7	g	786	PRO	N-CA-CB	6.45	110.43	103.33
7	g	210	PRO	N-CA-CB	6.45	110.42	103.33
11	U	80	VAL	N-CA-CB	6.44	119.30	110.54
10	j	1008	PRO	N-CA-C	6.44	121.06	111.41
11	S	80	VAL	N-CA-CB	6.43	119.28	110.54
7	G	192	PRO	N-CA-CB	6.42	110.39	103.33
11	V	80	VAL	N-CA-CB	6.41	119.25	110.54
7	g	257	PRO	N-CA-CB	6.41	110.38	103.33
7	G	786	PRO	N-CA-CB	6.40	110.37	103.33
1	a	521	PRO	CA-C-N	6.38	129.12	120.44
1	a	521	PRO	C-N-CA	6.38	129.12	120.44
11	T	42	TYR	N-CA-C	6.37	118.22	111.28
7	G	257	PRO	N-CA-CB	6.36	110.33	103.33
5	E	760	LEU	CA-C-N	6.35	125.41	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	760	LEU	C-N-CA	6.35	125.41	120.33
8	h	150	THR	N-CA-C	6.35	117.87	111.07
11	S	42	TYR	N-CA-C	6.35	118.20	111.28
11	V	42	TYR	N-CA-C	6.33	118.18	111.28
5	e	828	ALA	N-CA-C	6.33	119.66	110.42
8	H	150	THR	N-CA-C	6.32	117.83	111.07
7	G	141	PRO	N-CA-CB	6.31	110.27	103.33
5	E	828	ALA	N-CA-C	6.29	119.60	110.42
7	g	150	PRO	N-CA-CB	6.29	110.25	103.33
1	a	1299	LEU	N-CA-C	6.26	120.02	112.38
5	e	782	ALA	N-CA-C	6.24	118.16	111.36
7	g	196	PRO	N-CA-CB	6.23	110.42	103.44
2	b	123	THR	N-CA-C	-6.22	101.46	110.24
5	E	782	ALA	N-CA-C	6.22	118.14	111.36
10	j	773	VAL	N-CA-C	-6.20	106.69	112.83
8	H	138	GLY	O-C-N	-6.20	115.58	121.77
5	e	760	LEU	CA-C-N	6.20	125.29	120.33
5	e	760	LEU	C-N-CA	6.20	125.29	120.33
7	g	625	THR	CA-C-N	-6.18	113.27	120.12
7	g	625	THR	C-N-CA	-6.18	113.27	120.12
1	a	373	VAL	N-CA-C	6.16	116.32	110.53
5	E	634	HIS	CA-C-N	6.14	129.12	120.28
5	E	634	HIS	C-N-CA	6.14	129.12	120.28
10	J	773	VAL	N-CA-C	-6.14	106.75	112.83
1	a	67	VAL	N-CA-C	6.13	116.30	110.42
1	A	700	LEU	O-C-N	-6.12	115.63	122.12
4	d	264	THR	N-CA-CB	6.12	119.75	110.45
4	D	264	THR	N-CA-CB	6.11	119.73	110.45
1	a	88	GLU	N-CA-C	6.09	119.55	111.75
8	h	138	GLY	O-C-N	-6.09	115.68	121.77
1	A	180	GLN	CA-C-N	6.08	126.69	120.00
1	A	180	GLN	C-N-CA	6.08	126.69	120.00
1	A	67	VAL	N-CA-C	6.08	116.26	110.42
10	j	913	LEU	N-CA-C	-6.07	104.66	111.28
9	i	195	SER	CA-C-N	6.07	129.53	120.31
9	i	195	SER	C-N-CA	6.07	129.53	120.31
1	a	180	GLN	CA-C-N	6.07	126.67	120.00
1	a	180	GLN	C-N-CA	6.07	126.67	120.00
1	a	752	ALA	N-CA-C	6.05	117.88	111.28
7	G	143	VAL	N-CA-C	6.04	116.78	110.62
9	I	177	ILE	CB-CA-C	-6.04	104.15	111.88
5	e	593	GLU	N-CA-C	6.03	117.83	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	324	LEU	CA-C-O	-6.02	111.91	120.16
6	F	199	GLN	N-CA-C	6.02	117.51	111.07
9	i	177	ILE	CB-CA-C	-6.02	104.18	111.88
9	i	324	LEU	CA-C-O	-6.02	111.92	120.16
1	A	1128	ARG	N-CA-C	6.01	118.69	108.90
1	A	88	GLU	N-CA-C	6.00	119.43	111.75
2	B	61	GLU	N-CA-C	5.99	117.81	111.28
11	U	96	LEU	N-CA-CB	-5.99	101.07	110.06
1	A	57	PRO	CA-C-O	-5.97	111.91	120.56
1	a	57	PRO	CA-C-O	-5.96	111.92	120.56
3	C	93	SER	CA-C-N	5.93	129.03	120.38
3	C	93	SER	C-N-CA	5.93	129.03	120.38
7	g	217	VAL	CA-C-N	5.93	126.52	120.00
7	g	217	VAL	C-N-CA	5.93	126.52	120.00
6	f	199	GLN	N-CA-C	5.91	117.40	111.07
5	E	483	ARG	CA-C-N	5.91	132.83	121.54
5	E	483	ARG	C-N-CA	5.91	132.83	121.54
1	A	53	LEU	CB-CA-C	-5.90	109.78	116.63
1	a	1554	SER	CA-C-N	5.89	128.50	120.54
1	a	1554	SER	C-N-CA	5.89	128.50	120.54
5	e	483	ARG	CA-C-N	5.86	132.74	121.54
5	e	483	ARG	C-N-CA	5.86	132.74	121.54
5	e	864	LEU	N-CA-C	5.86	119.08	109.76
1	a	267	VAL	CA-C-N	5.86	128.41	120.38
1	a	267	VAL	C-N-CA	5.86	128.41	120.38
5	e	601	ASP	CA-C-N	5.85	128.05	120.44
5	e	601	ASP	C-N-CA	5.85	128.05	120.44
1	a	53	LEU	CB-CA-C	-5.85	109.84	116.63
8	H	163	ILE	CA-C-N	5.85	125.55	119.82
8	H	163	ILE	C-N-CA	5.85	125.55	119.82
4	d	135	ALA	CA-C-N	5.84	129.19	120.31
4	d	135	ALA	C-N-CA	5.84	129.19	120.31
1	A	267	VAL	CA-C-N	5.83	128.36	120.38
1	A	267	VAL	C-N-CA	5.83	128.36	120.38
8	H	270	SER	CA-C-N	5.82	127.90	120.56
8	H	270	SER	C-N-CA	5.82	127.90	120.56
1	a	1300	ILE	CB-CA-C	-5.82	108.18	114.35
4	D	49	CYS	CA-C-N	5.81	128.34	120.44
4	D	49	CYS	C-N-CA	5.81	128.34	120.44
9	I	603	ILE	N-CA-C	5.80	116.54	110.62
8	h	270	SER	CA-C-N	5.80	127.87	120.56
8	h	270	SER	C-N-CA	5.80	127.87	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	601	ASP	CA-C-N	5.79	127.96	120.44
5	E	601	ASP	C-N-CA	5.79	127.96	120.44
2	b	290	GLU	N-CA-C	5.78	117.58	111.28
1	A	181	GLY	N-CA-C	-5.78	105.38	112.77
1	a	181	GLY	N-CA-C	-5.78	105.38	112.77
9	i	603	ILE	N-CA-C	5.77	116.50	110.62
1	a	795	PHE	N-CA-C	5.76	117.23	111.07
1	a	66	ARG	CA-C-N	5.76	127.81	120.56
1	a	66	ARG	C-N-CA	5.76	127.81	120.56
11	U	95	ASP	CA-C-N	5.75	128.26	120.38
11	U	95	ASP	C-N-CA	5.75	128.26	120.38
2	B	290	GLU	N-CA-C	5.75	117.55	111.28
10	J	311	SER	CA-C-N	5.74	127.98	120.28
10	J	311	SER	C-N-CA	5.74	127.98	120.28
10	j	311	SER	CA-C-N	5.74	127.97	120.28
10	j	311	SER	C-N-CA	5.74	127.97	120.28
5	E	80	ALA	CA-C-N	5.73	129.40	120.75
5	E	80	ALA	C-N-CA	5.73	129.40	120.75
9	i	157	HIS	O-C-N	-5.72	115.33	120.71
5	E	1013	TYR	N-CA-C	5.71	117.51	111.28
5	E	1069	ASP	CA-C-N	5.70	130.24	120.72
5	E	1069	ASP	C-N-CA	5.70	130.24	120.72
5	e	1069	ASP	CA-C-N	5.70	130.24	120.72
5	e	1069	ASP	C-N-CA	5.70	130.24	120.72
5	e	80	ALA	CA-C-N	5.70	129.35	120.75
5	e	80	ALA	C-N-CA	5.70	129.35	120.75
9	I	520	ASP	CA-C-N	5.69	127.91	120.28
9	I	520	ASP	C-N-CA	5.69	127.91	120.28
1	A	66	ARG	CA-C-N	5.69	127.72	120.56
1	A	66	ARG	C-N-CA	5.69	127.72	120.56
1	a	398	THR	N-CA-CB	5.68	118.31	110.07
5	e	936	GLU	CA-C-N	5.68	128.46	120.28
5	e	936	GLU	C-N-CA	5.68	128.46	120.28
1	a	398	THR	N-CA-C	5.67	117.26	111.14
2	B	384	LEU	N-CA-C	5.66	117.53	111.36
1	A	15	GLY	O-C-N	5.65	123.11	121.07
2	b	384	LEU	N-CA-C	5.65	117.52	111.36
9	i	520	ASP	CA-C-N	5.65	127.85	120.28
9	i	520	ASP	C-N-CA	5.65	127.85	120.28
1	A	398	THR	N-CA-CB	5.64	118.25	110.07
5	e	1013	TYR	N-CA-C	5.64	117.43	111.28
1	a	146	LEU	CA-C-N	5.64	128.15	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	146	LEU	C-N-CA	5.64	128.15	120.54
9	I	157	HIS	O-C-N	-5.63	115.42	120.71
5	E	233	SER	O-C-N	-5.63	116.97	123.33
5	E	754	LEU	N-CA-C	5.62	117.49	111.36
1	A	398	THR	N-CA-C	5.61	117.20	111.14
8	H	67	HIS	CA-C-N	5.61	125.32	119.82
8	H	67	HIS	C-N-CA	5.61	125.32	119.82
10	j	1081	LYS	CA-C-N	5.61	128.59	120.79
10	j	1081	LYS	C-N-CA	5.61	128.59	120.79
5	E	936	GLU	CA-C-N	5.61	128.35	120.28
5	E	936	GLU	C-N-CA	5.61	128.35	120.28
8	h	138	GLY	CA-C-O	-5.60	113.51	121.52
9	i	322	GLN	CA-C-N	5.60	132.23	121.54
9	i	322	GLN	C-N-CA	5.60	132.23	121.54
10	j	790	ALA	N-CA-C	5.60	117.06	111.07
1	A	67	VAL	N-CA-CB	-5.59	104.01	110.55
8	H	138	GLY	CA-C-O	-5.59	113.52	121.52
3	c	93	SER	CA-C-N	5.59	128.04	120.38
3	c	93	SER	C-N-CA	5.59	128.04	120.38
5	e	754	LEU	N-CA-C	5.58	117.45	111.36
1	A	365	VAL	CB-CA-C	-5.58	104.60	112.14
9	I	322	GLN	CA-C-N	5.58	132.20	121.54
9	I	322	GLN	C-N-CA	5.58	132.20	121.54
4	d	49	CYS	CA-C-N	5.58	128.21	120.29
4	d	49	CYS	C-N-CA	5.58	128.21	120.29
7	G	544	PRO	CA-C-N	-5.57	112.87	119.84
7	G	544	PRO	C-N-CA	-5.57	112.87	119.84
8	h	67	HIS	CA-C-N	5.57	125.28	119.82
8	h	67	HIS	C-N-CA	5.57	125.28	119.82
11	T	96	LEU	N-CA-CB	-5.57	101.04	110.50
1	a	365	VAL	CB-CA-C	-5.57	104.62	112.14
11	V	96	LEU	N-CA-CB	-5.56	101.05	110.50
11	S	96	LEU	N-CA-CB	-5.55	101.06	110.50
2	B	158	GLY	O-C-N	5.55	123.07	121.07
9	i	267	SER	CB-CA-C	-5.55	101.58	110.79
1	a	432	LEU	N-CA-C	5.55	117.77	111.11
5	e	233	SER	O-C-N	-5.54	117.07	123.33
10	j	832	SER	CA-C-O	-5.54	112.58	120.16
2	B	568	PRO	N-CA-C	-5.53	105.84	113.53
9	I	267	SER	CB-CA-C	-5.53	101.60	110.79
10	J	790	ALA	N-CA-C	5.53	116.99	111.07
6	f	137	GLY	N-CA-C	-5.53	103.04	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	991	THR	N-CA-CB	5.53	118.49	110.47
10	j	605	GLY	O-C-N	-5.53	115.51	122.70
10	J	694	GLU	N-CA-C	5.52	118.01	111.33
10	j	991	THR	N-CA-CB	5.52	118.48	110.47
6	F	137	GLY	N-CA-C	-5.52	103.05	110.56
10	J	1021	CYS	CA-C-N	5.52	127.67	120.28
10	J	1021	CYS	C-N-CA	5.52	127.67	120.28
5	E	593	GLU	N-CA-C	5.51	117.70	109.59
1	a	489	VAL	N-CA-C	-5.51	99.88	108.81
5	E	955	LEU	CA-C-N	5.51	128.22	120.28
5	E	955	LEU	C-N-CA	5.51	128.22	120.28
1	a	189	LEU	N-CA-C	5.51	117.37	111.36
10	j	603	GLN	N-CA-C	5.51	117.09	111.14
2	b	568	PRO	N-CA-C	-5.51	105.87	113.53
1	A	954	SER	N-CA-C	5.51	118.80	111.75
10	j	693	GLU	CA-C-O	-5.50	115.03	120.70
11	T	29	GLY	CA-C-N	5.50	127.65	120.28
11	T	29	GLY	C-N-CA	5.50	127.65	120.28
11	V	59	ASP	N-CA-C	5.49	121.95	109.81
1	a	67	VAL	N-CA-CB	-5.49	104.13	110.55
11	T	59	ASP	N-CA-C	5.49	121.94	109.81
11	V	29	GLY	CA-C-N	5.49	127.63	120.28
11	V	29	GLY	C-N-CA	5.49	127.63	120.28
11	S	29	GLY	CA-C-N	5.49	127.63	120.28
11	S	29	GLY	C-N-CA	5.49	127.63	120.28
5	e	955	LEU	CA-C-N	5.49	128.18	120.28
5	e	955	LEU	C-N-CA	5.49	128.18	120.28
10	J	603	GLN	N-CA-C	5.48	117.06	111.14
10	J	605	GLY	O-C-N	-5.48	115.58	122.70
10	J	832	SER	CA-C-O	-5.47	112.66	120.16
11	S	59	ASP	N-CA-C	5.47	121.90	109.81
10	J	1081	LYS	CA-C-N	5.47	128.39	120.79
10	J	1081	LYS	C-N-CA	5.47	128.39	120.79
10	J	424	ARG	N-CA-C	5.45	117.22	111.28
10	j	694	GLU	N-CA-C	5.44	117.92	111.33
10	j	364	THR	N-CA-CB	5.44	119.11	110.57
7	g	300	SER	CA-C-N	-5.43	113.05	119.84
7	g	300	SER	C-N-CA	-5.43	113.05	119.84
7	G	323	MET	CA-C-N	-5.43	113.05	119.84
7	G	323	MET	C-N-CA	-5.43	113.05	119.84
1	A	908	GLU	CB-CA-C	-5.42	110.34	116.63
1	a	425	GLY	O-C-N	-5.42	118.48	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	109	VAL	N-CA-C	5.41	116.19	110.72
1	a	228	LEU	N-CA-C	5.41	117.18	111.28
10	j	424	ARG	N-CA-C	5.41	117.18	111.28
7	g	619	LEU	N-CA-C	-5.41	105.38	111.28
10	j	1021	CYS	CA-C-N	5.41	127.52	120.28
10	j	1021	CYS	C-N-CA	5.41	127.52	120.28
11	U	164	ASP	CA-C-O	5.40	126.54	120.92
9	i	323	LYS	N-CA-C	5.40	122.31	110.80
1	a	888	LYS	N-CA-C	-5.40	105.39	111.28
9	i	157	HIS	CA-C-N	5.40	125.48	119.32
9	i	157	HIS	C-N-CA	5.40	125.48	119.32
1	A	1071	ALA	CA-C-N	5.40	127.78	120.38
1	A	1071	ALA	C-N-CA	5.40	127.78	120.38
9	I	157	HIS	CA-C-N	5.40	125.47	119.32
9	I	157	HIS	C-N-CA	5.40	125.47	119.32
10	J	364	THR	N-CA-CB	5.40	119.05	110.57
10	J	693	GLU	CA-C-O	-5.39	115.15	120.70
10	J	1044	ASP	CA-C-N	5.39	127.76	120.38
10	J	1044	ASP	C-N-CA	5.39	127.76	120.38
9	I	323	LYS	N-CA-C	5.38	122.25	110.80
1	A	109	VAL	N-CA-C	5.37	116.14	110.72
7	g	433	GLY	CA-C-N	-5.37	113.13	119.84
7	g	433	GLY	C-N-CA	-5.37	113.13	119.84
4	D	136	ASP	N-CA-C	-5.36	106.00	112.54
10	j	162	ALA	O-C-N	-5.36	116.44	122.12
8	H	58	GLY	CA-C-N	5.36	125.66	119.93
8	H	58	GLY	C-N-CA	5.36	125.66	119.93
1	A	114	ILE	N-CA-C	5.36	116.08	110.62
10	J	535	SER	N-CA-C	-5.35	107.30	112.97
5	e	788	ASP	CA-C-N	5.35	129.42	120.64
5	e	788	ASP	C-N-CA	5.35	129.42	120.64
1	a	492	SER	N-CA-C	5.35	117.19	111.36
10	j	1044	ASP	CA-C-N	5.34	127.70	120.38
10	j	1044	ASP	C-N-CA	5.34	127.70	120.38
7	G	681	ILE	CB-CA-C	-5.34	108.69	114.35
10	J	669	LEU	CA-C-N	5.33	131.30	121.70
10	J	669	LEU	C-N-CA	5.33	131.30	121.70
3	c	270	ASN	N-CA-C	-5.33	98.14	108.59
7	G	433	GLY	CA-C-N	-5.32	113.19	119.84
7	G	433	GLY	C-N-CA	-5.32	113.19	119.84
8	h	5	ILE	N-CA-C	5.32	116.05	110.62
10	j	669	LEU	CA-C-N	5.32	131.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	669	LEU	C-N-CA	5.32	131.28	121.70
10	J	162	ALA	O-C-N	-5.32	116.48	122.12
5	e	1144	ALA	N-CA-C	5.31	117.93	109.96
11	U	95	ASP	CA-C-O	5.31	126.10	120.10
10	j	535	SER	N-CA-C	-5.31	107.34	112.97
9	i	592	ALA	N-CA-C	5.31	119.68	112.04
5	e	121	ILE	N-CA-C	-5.30	107.58	112.83
5	E	124	VAL	O-C-N	-5.29	115.95	122.57
1	a	114	ILE	N-CA-C	5.29	116.02	110.62
2	B	311	LEU	N-CA-C	5.28	116.84	111.14
5	e	657	ILE	CA-C-N	5.28	127.61	120.38
5	e	657	ILE	C-N-CA	5.28	127.61	120.38
7	g	154	ALA	N-CA-C	5.28	117.11	111.36
1	a	1339	THR	N-CA-C	5.27	117.03	111.28
8	h	58	GLY	CA-C-N	5.27	125.57	119.93
8	h	58	GLY	C-N-CA	5.27	125.57	119.93
1	a	428	PRO	CA-C-N	5.27	125.97	120.12
1	a	428	PRO	C-N-CA	5.27	125.97	120.12
5	e	856	ARG	N-CA-C	5.27	117.10	111.36
1	a	1610	ALA	O-C-N	-5.26	115.76	120.71
6	f	277	LYS	CA-C-N	5.26	129.83	122.36
6	f	277	LYS	C-N-CA	5.26	129.83	122.36
2	b	311	LEU	N-CA-C	5.25	116.82	111.14
5	E	121	ILE	N-CA-C	-5.25	107.63	112.83
5	E	657	ILE	CA-C-N	5.25	127.57	120.38
5	E	657	ILE	C-N-CA	5.25	127.57	120.38
5	e	466	ALA	N-CA-C	5.24	121.39	109.81
1	A	994	MET	N-CA-C	5.24	116.67	111.07
5	E	599	ASP	CA-C-N	5.24	127.63	120.46
5	E	599	ASP	C-N-CA	5.24	127.63	120.46
9	i	577	ILE	N-CA-C	5.23	115.96	110.62
6	f	308	LEU	O-C-N	-5.23	115.30	121.32
6	F	277	LYS	CA-C-N	5.23	129.79	122.36
6	F	277	LYS	C-N-CA	5.23	129.79	122.36
10	j	705	VAL	CA-C-N	5.23	127.81	120.28
10	j	705	VAL	C-N-CA	5.23	127.81	120.28
1	a	488	GLN	N-CA-C	5.22	118.77	111.30
1	A	275	LEU	N-CA-C	5.22	117.05	111.36
11	S	195	ALA	CA-C-N	5.22	131.10	121.70
11	S	195	ALA	C-N-CA	5.22	131.10	121.70
11	V	195	ALA	CA-C-N	5.22	131.10	121.70
11	V	195	ALA	C-N-CA	5.22	131.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	466	ALA	N-CA-C	5.22	121.34	109.81
11	T	195	ALA	CA-C-N	5.22	131.09	121.70
11	T	195	ALA	C-N-CA	5.22	131.09	121.70
5	e	599	ASP	CA-C-N	5.21	127.60	120.46
5	e	599	ASP	C-N-CA	5.21	127.60	120.46
5	e	124	VAL	O-C-N	-5.21	116.06	122.57
9	i	188	THR	O-C-N	-5.20	115.34	121.32
9	I	592	ALA	N-CA-C	5.20	119.68	112.45
7	G	340	CYS	CA-C-N	-5.19	113.35	119.84
7	G	340	CYS	C-N-CA	-5.19	113.35	119.84
4	d	204	GLU	N-CA-C	5.19	117.36	111.02
9	I	188	THR	CA-C-N	5.19	124.81	119.05
9	I	188	THR	C-N-CA	5.19	124.81	119.05
1	a	163	SER	CA-C-N	5.19	124.64	119.24
1	a	163	SER	C-N-CA	5.19	124.64	119.24
2	b	96	ALA	N-CA-C	-5.19	105.63	111.28
9	I	519	MET	CA-C-N	5.18	127.18	120.44
9	I	519	MET	C-N-CA	5.18	127.18	120.44
2	b	385	PHE	N-CA-C	5.18	117.88	110.68
10	J	811	ALA	N-CA-C	5.18	116.93	111.28
5	E	167	PRO	CA-C-N	5.18	126.22	120.06
5	E	167	PRO	C-N-CA	5.18	126.22	120.06
7	G	344	LYS	CA-C-N	-5.18	113.37	119.84
7	G	344	LYS	C-N-CA	-5.18	113.37	119.84
10	J	705	VAL	CA-C-N	5.18	127.74	120.28
10	J	705	VAL	C-N-CA	5.18	127.74	120.28
5	e	887	LEU	CA-C-N	5.18	127.22	120.28
5	e	887	LEU	C-N-CA	5.18	127.22	120.28
7	g	704	SER	CA-C-N	-5.18	113.37	119.84
7	g	704	SER	C-N-CA	-5.18	113.37	119.84
9	I	577	ILE	N-CA-C	5.18	115.90	110.62
10	j	621	ALA	N-CA-C	5.17	116.92	111.28
10	J	250	VAL	CB-CA-C	-5.17	105.14	111.92
10	j	699	SER	CA-C-N	5.17	127.21	120.28
10	j	699	SER	C-N-CA	5.17	127.21	120.28
7	G	704	SER	CA-C-N	-5.17	113.38	119.84
7	G	704	SER	C-N-CA	-5.17	113.38	119.84
10	j	916	HIS	N-CA-C	-5.17	102.73	110.23
9	i	518	LEU	N-CA-CB	5.17	117.72	110.12
10	j	811	ALA	N-CA-C	5.17	116.91	111.28
5	E	887	LEU	CA-C-N	5.16	127.20	120.28
5	E	887	LEU	C-N-CA	5.16	127.20	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	239	THR	CA-C-N	5.16	125.46	119.47
1	a	239	THR	C-N-CA	5.16	125.46	119.47
9	i	519	MET	CA-C-N	5.16	127.15	120.44
9	i	519	MET	C-N-CA	5.16	127.15	120.44
1	A	1117	ALA	N-CA-C	5.16	116.90	111.28
2	B	385	PHE	N-CA-C	5.15	117.84	110.68
5	e	233	SER	CA-C-N	5.15	130.97	121.70
5	e	233	SER	C-N-CA	5.15	130.97	121.70
6	F	308	LEU	O-C-N	-5.15	115.40	121.32
9	i	644	HIS	CB-CA-C	-5.15	110.66	116.63
9	I	518	LEU	N-CA-CB	5.15	117.69	110.12
1	A	239	THR	CA-C-N	5.15	125.44	119.47
1	A	239	THR	C-N-CA	5.15	125.44	119.47
1	A	1489	ASP	N-CA-C	5.14	116.89	111.28
2	B	96	ALA	N-CA-C	-5.14	105.67	111.28
10	J	1055	LEU	N-CA-C	5.14	116.69	111.14
5	E	997	THR	N-CA-CB	5.14	118.25	110.28
2	b	158	GLY	O-C-N	5.14	122.92	121.07
4	d	173	SER	N-CA-CB	5.14	117.44	109.48
6	f	300	SER	CB-CA-C	-5.13	102.79	110.90
5	e	997	THR	N-CA-CB	5.13	118.24	110.28
10	j	250	VAL	CB-CA-C	-5.13	105.20	111.92
4	D	204	GLU	N-CA-C	5.12	117.27	111.02
10	j	1055	LEU	N-CA-C	5.12	116.67	111.14
4	D	173	SER	N-CA-CB	5.11	117.39	109.48
6	F	300	SER	CB-CA-C	-5.10	102.84	110.90
5	E	68	PRO	N-CA-C	5.10	122.98	112.47
5	E	233	SER	CA-C-N	5.10	130.88	121.70
5	E	233	SER	C-N-CA	5.10	130.88	121.70
5	e	68	PRO	N-CA-C	5.09	122.96	112.47
10	J	699	SER	CA-C-N	5.09	127.10	120.28
10	J	699	SER	C-N-CA	5.09	127.10	120.28
5	E	945	VAL	CA-C-N	5.08	127.09	120.28
5	E	945	VAL	C-N-CA	5.08	127.09	120.28
3	c	47	VAL	CA-C-N	5.08	131.24	121.54
3	c	47	VAL	C-N-CA	5.08	131.24	121.54
5	e	167	PRO	CA-C-N	5.08	126.10	120.06
5	e	167	PRO	C-N-CA	5.08	126.10	120.06
7	G	288	LEU	CA-C-N	-5.06	113.52	119.84
7	G	288	LEU	C-N-CA	-5.06	113.52	119.84
11	U	100	ILE	CB-CA-C	-5.06	105.50	111.97
10	J	621	ALA	N-CA-C	5.06	116.79	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	669	LEU	O-C-N	-5.05	115.66	122.43
1	a	556	PHE	CA-C-N	5.05	127.01	120.44
1	a	556	PHE	C-N-CA	5.05	127.01	120.44
10	j	243	LEU	CB-CA-C	5.05	118.08	109.80
4	D	135	ALA	CA-C-N	5.04	129.15	120.72
4	D	135	ALA	C-N-CA	5.04	129.15	120.72
1	a	1489	ASP	N-CA-C	5.04	116.77	111.28
1	A	1646	GLN	N-CA-C	5.03	121.51	110.80
11	S	130	GLU	CA-C-N	5.03	127.93	120.74
11	S	130	GLU	C-N-CA	5.03	127.93	120.74
11	T	130	GLU	CA-C-N	5.03	127.93	120.74
11	T	130	GLU	C-N-CA	5.03	127.93	120.74
1	A	1142	ASP	N-CA-CB	5.02	119.04	110.50
8	h	275	ILE	N-CA-CB	5.02	116.00	110.53
2	B	436	HIS	N-CA-C	-5.01	105.90	111.36
11	U	130	GLU	CA-C-N	5.01	127.91	120.74
11	U	130	GLU	C-N-CA	5.01	127.91	120.74
3	C	237	GLY	N-CA-C	-5.01	104.14	114.16
5	e	1042	LEU	N-CA-C	5.01	117.47	111.71
10	J	243	LEU	CB-CA-C	5.00	118.01	109.80
10	j	669	LEU	O-C-N	-5.00	115.72	122.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6934	0	3045	142	0
1	a	6306	0	2772	108	0
2	B	2639	0	1163	74	0
2	b	2574	0	1141	85	0
3	C	1156	0	304	21	0
3	c	1168	0	303	15	0
4	D	1519	0	694	32	0
4	d	1450	0	658	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	5107	0	2254	18	0
5	e	5497	0	2427	51	0
6	F	1423	0	645	12	0
6	f	1433	0	653	0	0
7	G	3064	0	1339	139	0
7	g	3010	0	1311	182	0
8	H	1419	0	647	15	0
8	h	1413	0	649	27	0
9	I	3668	0	1635	32	0
9	i	3613	0	1617	38	0
10	J	5085	0	2301	23	0
10	j	5090	0	2300	35	0
11	S	840	0	366	9	0
11	T	840	0	366	5	0
11	U	859	0	382	14	0
11	V	840	0	366	7	0
12	K	345	0	72	1	0
13	L	400	0	84	0	0
14	M	365	0	75	1	0
15	N	155	0	34	0	0
16	O	175	0	37	0	0
17	P	130	0	28	0	0
18	Q	1935	0	438	27	0
18	R	1755	0	443	58	0
All	All	72207	0	30549	1042	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 10.

All (1042) 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)
7:g:285:TYR:CB	7:g:294:ALA:HA	1.27	1.63
9:i:888:MET:CB	10:j:964:ALA:CB	1.76	1.57
2:B:23:ILE:CB	4:D:296:SER:CB	1.77	1.56
1:A:517:LEU:CB	1:A:527:CYS:CB	1.80	1.54
9:I:186:ARG:CB	9:I:191:GLN:HA	1.36	1.51
5:e:1152:SER:HA	7:g:847:ALA:CB	1.39	1.48
7:G:699:CYS:HA	7:G:703:GLU:CB	1.43	1.47
7:g:699:CYS:HA	7:g:703:GLU:CB	1.43	1.47
7:G:666:GLU:HA	7:G:670:LEU:CB	1.41	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:285:TYR:CB	7:g:294:ALA:CA	1.95	1.45
2:b:302:TRP:CB	2:b:327:GLN:HA	1.47	1.44
2:b:354:ASP:CB	2:b:355:ILE:HA	1.43	1.44
5:e:1155:ARG:N	7:g:765:ALA:HB1	1.32	1.44
7:g:704:SER:CB	7:g:732:ARG:CB	1.96	1.44
7:G:704:SER:CB	7:G:732:ARG:CB	1.96	1.44
7:G:463:HIS:CB	9:I:405:MET:CB	1.96	1.44
1:A:1424:LEU:CB	1:A:1501:ARG:CB	1.97	1.43
7:g:496:HIS:CB	9:i:293:LEU:CB	1.95	1.42
5:e:1155:ARG:CB	7:g:765:ALA:HB3	1.49	1.42
9:i:663:ILE:CB	9:i:705:LYS:CB	1.97	1.41
10:J:903:ALA:HB1	10:J:908:GLN:CB	1.50	1.41
5:e:1152:SER:CA	7:g:847:ALA:HA	1.47	1.41
2:B:354:ASP:CB	2:B:355:ILE:HA	1.43	1.41
2:B:593:GLU:HA	5:E:1121:LEU:CB	1.51	1.41
5:e:1152:SER:N	7:g:847:ALA:HA	1.31	1.41
2:B:302:TRP:CB	2:B:327:GLN:HA	1.47	1.40
9:I:663:ILE:CB	9:I:705:LYS:CB	1.97	1.40
2:B:504:PHE:CB	2:B:531:ASP:CB	1.99	1.40
7:g:660:SER:CB	8:h:273:ALA:HA	1.52	1.39
10:J:903:ALA:CB	10:J:908:GLN:CB	2.01	1.39
2:b:439:ARG:O	4:d:23:HIS:CB	1.73	1.37
7:G:296:SER:O	7:G:298:THR:CB	1.70	1.37
5:e:1152:SER:CB	7:g:847:ALA:C	1.97	1.37
4:D:91:GLY:O	4:D:99:GLY:CA	1.71	1.36
7:g:285:TYR:N	7:g:294:ALA:HB2	1.39	1.36
5:e:1152:SER:CA	7:g:847:ALA:CA	2.02	1.35
5:e:1155:ARG:CB	7:g:765:ALA:CB	2.02	1.35
5:e:1152:SER:CA	7:g:847:ALA:CB	2.07	1.32
5:e:1152:SER:CB	7:g:847:ALA:O	1.76	1.32
9:i:888:MET:CB	10:j:964:ALA:CA	2.08	1.31
5:e:1155:ARG:CA	7:g:765:ALA:HB1	1.58	1.31
5:E:928:GLN:CB	6:F:124:SER:O	1.79	1.30
7:g:288:LEU:HA	8:h:271:ILE:CB	1.59	1.30
2:B:566:ILE:O	2:B:569:CYS:CB	1.78	1.30
1:a:1295:CYS:O	1:a:1297:GLN:N	1.63	1.30
18:R:377:UNK:CB	18:R:380:UNK:CB	2.10	1.30
7:G:287:PHE:CB	7:G:291:PRO:HA	1.62	1.29
2:b:566:ILE:O	2:b:569:CYS:CB	1.78	1.29
5:e:1153:PRO:HA	7:g:765:ALA:O	1.32	1.29
2:B:29:PRO:CB	4:D:23:HIS:C	2.06	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:785:VAL:CB	5:e:889:GLU:CB	2.10	1.29
9:i:651:LEU:CB	9:i:652:ASP:HA	1.59	1.28
9:I:651:LEU:CB	9:I:652:ASP:HA	1.59	1.27
7:G:805:TYR:HA	7:G:833:MET:CB	1.63	1.27
7:g:475:SER:CB	7:g:544:PRO:CB	2.11	1.27
2:B:29:PRO:CB	4:D:24:GLY:N	1.98	1.26
5:e:1151:ALA:H	7:g:850:ARG:CB	1.46	1.26
5:e:1152:SER:CB	7:g:847:ALA:CA	2.13	1.25
1:A:694:ARG:CB	1:A:695:CYS:CB	2.15	1.23
1:a:767:TYR:CB	1:a:845:TYR:HA	1.67	1.23
9:i:888:MET:CB	10:j:964:ALA:HB2	1.46	1.23
7:G:805:TYR:CA	7:G:833:MET:CB	2.15	1.23
2:B:568:PRO:O	2:B:570:SER:N	1.72	1.22
5:e:1152:SER:CB	7:g:847:ALA:HB1	1.68	1.22
2:B:593:GLU:CA	5:E:1121:LEU:CB	2.17	1.22
1:A:908:GLU:O	1:A:910:ALA:N	1.71	1.22
11:U:154:ILE:CB	11:U:171:LEU:CB	2.18	1.22
7:G:666:GLU:CA	7:G:670:LEU:CB	2.18	1.21
2:b:568:PRO:O	2:b:570:SER:N	1.72	1.21
1:a:1290:ILE:O	1:a:1294:ALA:N	1.73	1.21
7:g:296:SER:O	8:h:18:ASP:C	1.84	1.21
1:A:747:ARG:CB	1:A:755:LYS:CB	2.18	1.20
7:g:285:TYR:CB	7:g:294:ALA:CB	2.20	1.20
7:G:294:ALA:O	7:G:303:LYS:O	1.57	1.20
9:i:888:MET:C	10:j:964:ALA:HB1	1.65	1.20
18:R:185:UNK:HA	18:R:195:UNK:O	1.39	1.19
1:a:1420:LEU:CB	1:a:1494:LEU:CB	2.22	1.18
5:e:1153:PRO:CA	7:g:765:ALA:O	1.91	1.17
5:e:1152:SER:CB	7:g:847:ALA:CB	2.24	1.16
18:Q:670:UNK:O	18:Q:672:UNK:N	1.78	1.16
7:g:345:PRO:CB	7:g:643:ALA:CA	2.24	1.16
1:A:412:GLU:CB	1:A:432:LEU:CB	2.23	1.15
9:i:651:LEU:CB	9:i:652:ASP:CA	2.23	1.15
10:j:920:SER:O	10:j:924:GLU:CB	1.93	1.14
1:a:807:LEU:O	1:a:811:PRO:CB	1.96	1.14
1:A:889:LYS:CA	1:A:890:ALA:HB3	1.77	1.13
2:B:168:VAL:CB	2:B:307:VAL:CB	2.25	1.13
7:g:345:PRO:CB	7:g:643:ALA:HA	1.78	1.13
2:b:439:ARG:O	4:d:23:HIS:CA	1.95	1.12
1:A:694:ARG:CB	1:A:695:CYS:CA	2.25	1.12
2:B:593:GLU:CB	5:E:1121:LEU:CB	2.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:346:ASN:O	7:G:348:GLY:N	1.82	1.12
9:I:651:LEU:CB	9:I:652:ASP:CA	2.23	1.12
11:U:172:VAL:HA	11:U:184:ALA:HB1	1.31	1.12
9:i:888:MET:CB	10:j:964:ALA:HA	1.76	1.12
7:G:805:TYR:CB	7:G:833:MET:CB	2.27	1.11
7:g:699:CYS:CA	7:g:703:GLU:CB	2.29	1.11
7:G:699:CYS:CA	7:G:703:GLU:CB	2.29	1.11
4:d:188:ASP:C	4:d:220:ASP:O	1.93	1.11
7:G:281:ASP:H	7:G:282:THR:CB	1.62	1.11
18:Q:794:UNK:CB	18:Q:797:UNK:H	1.63	1.11
2:b:472:ALA:HB1	2:b:488:SER:CB	1.80	1.10
2:B:299:MET:CB	2:B:301:THR:N	2.15	1.10
10:J:903:ALA:HB1	10:J:908:GLN:CA	1.81	1.10
5:e:1152:SER:HA	7:g:847:ALA:HB2	1.33	1.10
4:D:93:SER:O	4:D:95:ASP:N	1.84	1.09
2:b:299:MET:CB	2:b:301:THR:N	2.15	1.09
7:g:463:HIS:CB	9:i:405:MET:CB	2.30	1.09
7:g:345:PRO:CB	7:g:643:ALA:O	1.99	1.09
4:D:91:GLY:C	4:D:99:GLY:HA2	1.76	1.09
1:A:889:LYS:CB	1:A:890:ALA:HB3	1.83	1.09
1:a:856:LYS:O	1:a:873:VAL:CB	2.01	1.09
5:e:1152:SER:HA	7:g:847:ALA:CA	1.70	1.09
10:j:915:ALA:HB2	10:j:923:HIS:CB	1.82	1.08
1:A:889:LYS:HA	1:A:890:ALA:HB3	1.31	1.08
1:a:914:ALA:HB2	1:a:987:LEU:HA	1.29	1.08
1:A:227:SER:O	1:A:229:ALA:N	1.85	1.07
9:I:186:ARG:CB	9:I:191:GLN:CA	2.31	1.07
2:b:354:ASP:CB	2:b:355:ILE:CA	2.29	1.07
2:B:354:ASP:CB	2:B:355:ILE:CA	2.29	1.07
18:R:12:UNK:CB	18:R:45:UNK:HA	1.85	1.07
1:a:528:PHE:CB	1:a:611:ALA:HB2	1.84	1.06
7:G:287:PHE:CB	7:G:291:PRO:CA	2.33	1.06
11:U:36:TYR:CB	11:U:45:ALA:HB2	1.85	1.06
5:e:1152:SER:CA	7:g:847:ALA:HB1	1.76	1.06
2:B:302:TRP:CB	2:B:327:GLN:CA	2.34	1.05
7:G:288:LEU:HA	8:H:271:ILE:CB	1.85	1.05
10:J:903:ALA:HB3	10:J:908:GLN:CB	1.82	1.04
5:e:1155:ARG:N	7:g:765:ALA:CB	2.20	1.04
2:b:302:TRP:CB	2:b:327:GLN:CA	2.34	1.04
7:g:285:TYR:N	7:g:294:ALA:CB	2.20	1.04
1:a:1124:THR:O	1:a:1128:ARG:N	1.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:197:VAL:CB	4:d:215:LEU:O	2.05	1.03
2:b:439:ARG:O	4:d:23:HIS:HA	1.56	1.03
1:A:150:ILE:CB	1:A:234:SER:CB	2.37	1.02
1:a:635:ILE:CB	1:a:636:PRO:CB	2.36	1.02
1:A:1226:ASN:O	1:A:1231:HIS:N	1.91	1.02
1:a:635:ILE:CA	1:a:636:PRO:CB	2.32	1.02
1:A:1226:ASN:O	1:A:1230:LEU:CA	2.07	1.02
1:a:1124:THR:CB	1:a:1128:ARG:CB	2.37	1.02
1:A:1107:MET:CB	1:A:1280:ALA:HB2	1.90	1.01
8:H:159:ALA:CB	8:H:181:ARG:O	2.08	1.01
1:A:726:ALA:HB1	7:G:246:PHE:O	1.58	1.01
18:Q:790:UNK:O	18:Q:799:UNK:CB	2.08	1.01
1:a:767:TYR:CB	1:a:845:TYR:CA	2.38	1.01
7:g:663:ALA:HB1	8:h:272:THR:CB	1.91	1.01
10:J:898:LEU:CB	10:J:908:GLN:O	2.10	1.00
2:b:585:GLN:CB	2:b:632:MET:CB	2.39	1.00
1:A:1226:ASN:O	1:A:1230:LEU:CB	2.10	0.99
7:g:345:PRO:CB	7:g:643:ALA:C	2.35	0.99
1:A:694:ARG:CB	1:A:695:CYS:HA	1.90	0.99
7:g:496:HIS:O	9:i:293:LEU:HA	1.61	0.98
4:D:89:ILE:O	4:D:101:SER:HA	1.61	0.98
1:A:743:ARG:O	1:A:747:ARG:N	1.95	0.98
7:G:381:THR:O	7:G:385:SER:CB	2.12	0.98
7:g:682:PRO:CB	7:g:683:HIS:CB	2.41	0.98
7:g:381:THR:O	7:g:385:SER:CB	2.12	0.97
7:g:433:GLY:O	7:g:435:GLU:N	1.98	0.97
5:e:1153:PRO:C	7:g:765:ALA:O	2.07	0.97
9:i:889:ARG:N	10:j:964:ALA:HB1	1.80	0.97
2:b:382:CYS:O	2:b:384:LEU:N	1.97	0.97
7:g:422:GLU:O	7:g:424:ARG:N	1.98	0.97
7:G:422:GLU:O	7:G:424:ARG:N	1.98	0.96
2:b:637:LEU:CB	5:e:1079:LEU:CB	2.43	0.96
1:A:747:ARG:C	1:A:755:LYS:CB	2.37	0.96
7:G:433:GLY:O	7:G:435:GLU:N	1.97	0.96
10:J:903:ALA:CB	10:J:908:GLN:CA	2.38	0.96
5:e:1155:ARG:CA	7:g:765:ALA:CB	2.34	0.96
1:a:635:ILE:HA	1:a:636:PRO:CB	1.94	0.96
9:i:888:MET:CB	10:j:964:ALA:HB1	1.84	0.96
2:B:382:CYS:O	2:B:384:LEU:N	1.97	0.95
1:A:879:LEU:O	1:A:883:ILE:CB	2.15	0.95
7:G:685:HIS:O	7:G:687:ARG:N	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:197:VAL:CB	4:d:215:LEU:CB	2.44	0.95
9:i:653:SER:O	9:i:657:GLU:N	1.99	0.95
1:a:807:LEU:O	1:a:811:PRO:N	1.99	0.95
7:G:666:GLU:O	7:G:669:GLY:N	2.00	0.95
7:g:666:GLU:O	7:g:668:VAL:N	2.00	0.95
1:A:1227:VAL:O	1:A:1231:HIS:CB	2.13	0.94
5:E:452:ASP:O	6:F:205:GLU:CB	2.15	0.94
7:g:295:LYS:CB	8:h:19:ALA:HB3	1.96	0.94
9:i:571:LEU:CB	9:i:580:ILE:CB	2.46	0.94
1:A:520:GLY:O	1:A:524:ALA:N	2.01	0.94
7:g:296:SER:O	8:h:19:ALA:N	2.00	0.94
9:i:888:MET:C	10:j:964:ALA:CB	2.39	0.94
7:g:485:GLN:O	7:g:486:LEU:O	1.86	0.94
9:I:653:SER:O	9:I:657:GLU:N	1.99	0.94
2:b:439:ARG:C	4:d:23:HIS:HA	1.92	0.94
4:d:188:ASP:O	4:d:220:ASP:O	1.85	0.94
7:g:666:GLU:O	7:g:669:GLY:N	2.01	0.94
9:I:571:LEU:CB	9:I:580:ILE:CB	2.46	0.93
5:e:1151:ALA:N	7:g:850:ARG:CB	2.32	0.93
2:B:161:LEU:CB	2:B:315:PRO:O	2.16	0.93
4:D:91:GLY:O	4:D:99:GLY:HA2	0.77	0.93
7:g:663:ALA:CB	8:h:272:THR:CB	2.46	0.93
1:A:889:LYS:CB	1:A:890:ALA:C	2.41	0.93
1:a:1124:THR:CA	1:a:1128:ARG:CB	2.47	0.92
1:a:914:ALA:HB1	1:a:990:THR:CB	1.99	0.92
1:A:437:GLU:CB	1:A:509:PRO:CB	2.48	0.92
1:A:747:ARG:CB	1:A:755:LYS:CA	2.46	0.92
1:a:524:ALA:C	1:a:608:SER:CB	2.43	0.92
1:A:1226:ASN:O	1:A:1230:LEU:N	2.02	0.92
1:a:1124:THR:C	1:a:1128:ARG:CB	2.42	0.92
2:b:472:ALA:CB	2:b:488:SER:CB	2.48	0.92
8:H:159:ALA:HB3	8:H:181:ARG:O	1.71	0.91
2:b:45:SER:H	2:b:46:GLU:HA	1.34	0.91
1:A:518:ALA:HA	1:A:524:ALA:HA	1.52	0.91
7:g:496:HIS:O	9:i:293:LEU:CB	2.18	0.91
1:a:901:CYS:CB	1:a:944:LEU:HA	2.00	0.90
1:a:1124:THR:O	1:a:1128:ARG:CB	2.20	0.90
1:a:1431:ALA:HB1	1:a:1505:VAL:N	1.86	0.90
2:b:593:GLU:HA	5:e:1121:LEU:CB	2.02	0.90
7:g:285:TYR:CA	7:g:294:ALA:HB2	2.00	0.90
2:B:64:TYR:O	2:B:68:LEU:CB	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:423:GLU:HA	7:G:426:GLU:CB	2.02	0.90
2:b:593:GLU:CB	5:e:1121:LEU:CB	2.50	0.90
2:b:64:TYR:O	2:b:68:LEU:CB	2.19	0.90
7:g:285:TYR:H	7:g:294:ALA:HB2	1.02	0.90
7:G:287:PHE:CB	7:G:291:PRO:C	2.45	0.90
7:G:701:VAL:O	7:G:704:SER:N	2.05	0.90
2:B:238:MET:CB	2:B:285:LEU:CB	2.50	0.90
2:b:238:MET:CB	2:b:285:LEU:CB	2.50	0.89
1:A:437:GLU:CB	1:A:509:PRO:CA	2.50	0.89
7:g:423:GLU:HA	7:g:426:GLU:CB	2.02	0.89
8:H:159:ALA:HB2	8:H:181:ARG:O	1.73	0.89
1:a:1431:ALA:HA	1:a:1505:VAL:CB	2.02	0.89
2:B:439:ARG:HA	4:D:23:HIS:HA	1.52	0.89
1:a:524:ALA:HB2	1:a:607:TRP:CB	2.02	0.89
5:e:1155:ARG:H	7:g:765:ALA:HB1	1.32	0.89
7:G:219:THR:HA	7:G:271:ARG:CB	2.03	0.88
1:a:1304:HIS:O	1:a:1306:GLN:N	2.06	0.88
7:g:496:HIS:O	9:i:293:LEU:CA	2.20	0.88
1:A:889:LYS:CA	1:A:890:ALA:CB	2.51	0.88
5:E:454:GLN:H	6:F:205:GLU:CB	1.86	0.88
7:G:767:ALA:CB	7:G:854:SER:O	2.21	0.88
7:g:701:VAL:O	7:g:704:SER:N	2.05	0.88
7:g:285:TYR:CB	7:g:294:ALA:HB2	1.98	0.88
1:a:1243:GLY:O	1:a:1244:MET:C	2.13	0.88
1:a:1278:ARG:CB	1:a:1328:GLU:CB	2.51	0.88
1:A:889:LYS:HA	1:A:890:ALA:CB	2.04	0.88
2:B:29:PRO:CB	4:D:22:PHE:O	2.21	0.88
1:A:747:ARG:CB	1:A:755:LYS:HA	2.03	0.88
10:J:903:ALA:HB1	10:J:908:GLN:N	1.89	0.88
9:I:179:LEU:O	9:I:182:LYS:O	1.92	0.87
10:j:989:GLN:CB	10:j:1009:VAL:CB	2.53	0.87
2:B:161:LEU:CB	2:B:315:PRO:C	2.48	0.86
7:G:219:THR:CB	7:G:271:ARG:CB	2.53	0.86
5:e:1153:PRO:HA	7:g:765:ALA:C	1.99	0.86
1:A:1334:ALA:HB2	1:A:1415:ARG:CB	2.05	0.86
7:g:438:VAL:O	7:g:440:ALA:N	2.08	0.86
7:G:438:VAL:O	7:G:440:ALA:N	2.08	0.86
2:B:588:VAL:O	2:B:590:PHE:N	2.09	0.86
1:a:1243:GLY:O	1:a:1244:MET:O	1.91	0.86
7:G:321:TYR:O	7:G:323:MET:N	2.09	0.86
2:B:24:GLY:HA2	4:D:283:ARG:CB	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:905:UNK:O	18:Q:908:UNK:N	2.08	0.85
1:A:379:PHE:H	1:A:382:ASP:CB	1.89	0.85
2:b:588:VAL:O	2:b:590:PHE:N	2.09	0.85
7:g:660:SER:CB	8:h:273:ALA:CA	2.48	0.85
1:A:390:HIS:CB	1:A:456:LEU:HA	2.07	0.85
7:g:296:SER:C	8:h:17:HIS:O	2.19	0.85
18:R:31:UNK:HA	18:R:77:UNK:CB	2.06	0.84
7:g:389:GLN:O	7:g:409:ARG:CB	2.25	0.84
1:A:1226:ASN:CB	1:A:1230:LEU:H	1.90	0.84
5:E:451:SER:O	6:F:205:GLU:CB	2.25	0.84
2:b:44:ASN:N	2:b:45:SER:HA	1.90	0.84
11:S:36:TYR:CB	11:S:45:ALA:HB2	2.08	0.84
1:A:889:LYS:CB	1:A:890:ALA:CB	2.55	0.84
7:g:288:LEU:CA	8:h:271:ILE:CB	2.52	0.84
11:T:36:TYR:CB	11:T:45:ALA:HB2	2.08	0.83
7:G:295:LYS:CB	7:G:298:THR:N	2.41	0.83
1:a:901:CYS:CB	1:a:944:LEU:CA	2.56	0.83
7:G:707:SER:O	7:G:709:ALA:N	2.11	0.83
7:g:707:SER:O	7:g:709:ALA:N	2.11	0.83
7:G:296:SER:C	7:G:298:THR:CB	2.51	0.83
2:B:29:PRO:CB	4:D:24:GLY:CA	2.56	0.83
11:V:36:TYR:CB	11:V:45:ALA:HB2	2.08	0.82
9:I:651:LEU:CB	9:I:652:ASP:CB	2.57	0.82
9:i:651:LEU:CB	9:i:652:ASP:CB	2.57	0.82
7:g:283:ILE:CB	8:h:18:ASP:HA	2.09	0.82
7:G:666:GLU:O	7:G:668:VAL:N	2.11	0.82
7:g:543:LEU:CB	7:g:548:THR:CB	2.58	0.82
9:i:888:MET:CA	10:j:964:ALA:CB	2.58	0.82
5:e:1151:ALA:C	7:g:847:ALA:HA	2.04	0.82
1:A:695:CYS:O	1:A:697:GLU:N	2.13	0.81
2:b:593:GLU:CA	5:e:1121:LEU:CB	2.58	0.81
8:H:182:PHE:O	8:H:194:TRP:N	2.12	0.81
7:g:617:GLN:O	7:g:620:ASP:N	2.13	0.81
7:G:281:ASP:N	7:G:282:THR:CB	2.44	0.81
2:b:540:ARG:CB	2:b:553:GLU:O	2.28	0.81
18:R:381:UNK:CB	18:R:416:UNK:HA	2.11	0.81
1:a:525:HIS:N	1:a:608:SER:CB	2.44	0.81
1:A:457:ALA:HA	1:A:523:CYS:CB	2.11	0.81
7:g:296:SER:O	8:h:18:ASP:CA	2.28	0.81
7:g:406:ASN:CB	7:g:546:THR:CB	2.59	0.80
7:G:281:ASP:CB	7:G:282:THR:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:ARG:CB	2:B:553:GLU:O	2.28	0.80
5:e:1155:ARG:H	7:g:765:ALA:CB	1.89	0.80
10:J:898:LEU:CB	10:J:911:ALA:HB3	2.11	0.80
5:e:1155:ARG:H	7:g:765:ALA:CA	1.94	0.80
1:a:798:PRO:O	1:a:802:LEU:N	2.15	0.80
1:a:1302:THR:CB	1:a:1305:ARG:CB	2.60	0.80
2:b:476:LEU:N	2:b:484:ALA:CB	2.45	0.80
18:R:12:UNK:CB	18:R:44:UNK:O	2.31	0.79
1:a:528:PHE:CB	1:a:611:ALA:CB	2.60	0.79
1:A:437:GLU:CB	1:A:509:PRO:C	2.55	0.79
1:a:524:ALA:CB	1:a:607:TRP:CB	2.60	0.79
2:B:439:ARG:CA	4:D:23:HIS:HA	2.13	0.79
11:U:172:VAL:CA	11:U:184:ALA:HB1	2.10	0.79
7:G:288:LEU:O	7:G:290:LYS:HA	1.81	0.79
2:B:591:SER:O	2:B:595:THR:N	2.15	0.79
7:g:491:LYS:O	7:g:495:ASP:N	2.16	0.78
7:G:682:PRO:CB	7:G:683:HIS:HA	2.13	0.78
7:g:682:PRO:CB	7:g:683:HIS:CA	2.61	0.78
11:U:172:VAL:HA	11:U:184:ALA:CB	2.14	0.78
18:R:273:UNK:O	18:R:276:UNK:N	2.16	0.78
1:a:1285:ARG:O	1:a:1289:GLU:CB	2.32	0.78
1:A:515:ARG:O	1:A:518:ALA:HB3	1.83	0.78
5:e:1152:SER:N	7:g:847:ALA:CA	2.27	0.78
7:g:627:ASP:CB	7:g:628:PRO:HA	2.14	0.78
18:R:185:UNK:HA	18:R:195:UNK:C	2.13	0.77
1:a:914:ALA:CB	1:a:990:THR:CB	2.63	0.77
1:A:1226:ASN:CB	1:A:1230:LEU:N	2.48	0.77
2:b:389:ASN:O	2:b:393:GLY:N	2.18	0.77
2:B:543:HIS:CB	2:B:553:GLU:CB	2.63	0.77
1:A:747:ARG:CA	1:A:755:LYS:CB	2.62	0.77
7:G:219:THR:CA	7:G:271:ARG:CB	2.63	0.77
1:a:767:TYR:CB	1:a:845:TYR:CB	2.63	0.77
1:a:524:ALA:HB3	1:a:607:TRP:C	2.10	0.76
9:I:199:SER:HA	9:I:202:TRP:CB	2.14	0.76
1:a:887:SER:O	1:a:891:ASP:CB	2.33	0.76
7:G:805:TYR:CB	7:G:830:THR:O	2.33	0.76
10:j:867:SER:H	10:j:910:ALA:CB	1.99	0.76
1:A:1226:ASN:O	1:A:1230:LEU:C	2.29	0.75
18:R:184:UNK:O	18:R:196:UNK:HA	1.86	0.75
2:b:543:HIS:CB	2:b:553:GLU:CB	2.63	0.75
2:b:591:SER:O	2:b:595:THR:N	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1290:ILE:O	1:a:1294:ALA:CB	2.34	0.75
2:B:389:ASN:O	2:B:393:GLY:N	2.18	0.75
18:Q:803:UNK:O	18:Q:807:UNK:CB	2.35	0.75
7:g:345:PRO:CB	7:g:643:ALA:CB	2.64	0.75
7:g:489:TRP:CB	9:i:361:GLY:O	2.34	0.75
1:A:518:ALA:CA	1:A:524:ALA:HA	2.17	0.75
1:a:528:PHE:CB	1:a:611:ALA:N	2.50	0.75
8:h:13:GLU:N	8:h:14:ASP:HA	2.01	0.75
1:A:437:GLU:CB	1:A:509:PRO:O	2.35	0.74
18:Q:804:UNK:O	18:Q:808:UNK:CB	2.35	0.74
18:R:173:UNK:O	18:R:174:UNK:CB	2.35	0.74
1:a:901:CYS:CB	1:a:944:LEU:N	2.50	0.74
9:i:888:MET:CA	10:j:964:ALA:HB1	2.17	0.74
18:Q:905:UNK:O	18:Q:907:UNK:N	2.20	0.74
1:a:457:ALA:CB	1:a:522:GLN:CB	2.65	0.74
18:R:121:UNK:O	18:R:122:UNK:CB	2.36	0.74
9:I:198:ALA:O	9:I:202:TRP:N	2.19	0.74
9:i:639:ALA:O	9:i:643:ALA:N	2.20	0.74
1:A:1107:MET:CA	1:A:1280:ALA:HB2	2.17	0.74
1:A:1591:PRO:HA	1:A:1612:VAL:CB	2.17	0.74
10:j:867:SER:CB	10:j:910:ALA:HA	2.18	0.74
1:A:1591:PRO:HA	1:A:1612:VAL:HA	1.68	0.74
18:Q:657:UNK:O	18:Q:658:UNK:CB	2.35	0.73
18:R:184:UNK:O	18:R:197:UNK:N	2.20	0.73
4:d:188:ASP:CB	4:d:196:LYS:H	2.01	0.73
1:a:1428:LEU:N	1:a:1501:ARG:CB	2.51	0.73
9:i:663:ILE:CA	9:i:705:LYS:CB	2.66	0.73
7:G:296:SER:O	7:G:298:THR:CA	2.37	0.73
1:a:1420:LEU:C	1:a:1494:LEU:CB	2.61	0.73
1:A:390:HIS:CB	1:A:456:LEU:CA	2.66	0.72
9:I:759:ASN:CB	18:Q:549:UNK:HA	2.18	0.72
1:a:635:ILE:CB	1:a:636:PRO:O	2.37	0.72
7:G:287:PHE:O	8:H:271:ILE:N	2.15	0.72
9:I:663:ILE:CA	9:I:705:LYS:CB	2.66	0.72
1:a:457:ALA:HB1	1:a:522:GLN:CB	2.20	0.72
7:g:389:GLN:O	7:g:409:ARG:HA	1.89	0.72
7:g:345:PRO:HA	7:g:643:ALA:HB1	1.72	0.72
1:A:517:LEU:O	1:A:524:ALA:HA	1.90	0.72
18:Q:905:UNK:O	18:Q:906:UNK:C	2.37	0.72
3:c:194:LEU:O	3:c:205:THR:N	2.22	0.72
7:G:666:GLU:HA	7:G:670:LEU:CA	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:164:GLN:O	7:g:167:PHE:CB	2.38	0.71
2:b:45:SER:N	2:b:46:GLU:HA	2.00	0.71
2:b:124:ARG:O	2:b:125:GLU:C	2.32	0.71
2:b:580:LEU:O	2:b:584:GLU:N	2.23	0.71
1:A:1124:THR:O	1:A:1127:ASN:O	2.09	0.71
1:a:1431:ALA:HB1	1:a:1504:SER:C	2.15	0.71
7:G:346:ASN:O	7:G:347:ALA:C	2.33	0.71
5:e:1155:ARG:CB	7:g:765:ALA:C	2.64	0.71
7:g:475:SER:CB	7:g:544:PRO:CA	2.69	0.71
2:B:580:LEU:O	2:B:584:GLU:N	2.23	0.71
1:a:901:CYS:CB	1:a:943:LYS:C	2.64	0.71
18:R:34:UNK:HA	18:R:46:UNK:C	2.20	0.71
2:b:96:ALA:O	2:b:99:VAL:N	2.23	0.71
2:b:476:LEU:N	2:b:484:ALA:HB1	2.06	0.71
1:A:517:LEU:CA	1:A:527:CYS:CB	2.69	0.70
7:G:666:GLU:CB	7:G:670:LEU:CB	2.69	0.70
10:J:896:GLY:O	10:J:911:ALA:HB1	1.91	0.70
1:a:1428:LEU:HA	1:a:1501:ARG:CB	2.21	0.70
7:G:219:THR:O	7:G:223:GLN:N	2.23	0.70
9:i:665:VAL:O	9:i:669:LEU:N	2.23	0.70
2:B:96:ALA:O	2:B:99:VAL:N	2.23	0.70
7:G:422:GLU:O	7:G:425:ILE:N	2.24	0.70
7:g:281:ASP:CB	8:h:16:ILE:O	2.39	0.70
7:g:345:PRO:CB	7:g:643:ALA:HB1	2.21	0.70
1:A:1226:ASN:CA	1:A:1230:LEU:CB	2.69	0.70
8:H:13:GLU:O	8:H:14:ASP:O	2.10	0.70
1:a:525:HIS:HA	1:a:608:SER:CB	2.19	0.70
18:Q:1017:UNK:HA	18:Q:1079:UNK:CB	2.21	0.70
7:g:345:PRO:CA	7:g:643:ALA:HB1	2.22	0.70
7:g:422:GLU:O	7:g:425:ILE:N	2.24	0.70
7:g:663:ALA:HB3	8:h:272:THR:CB	2.21	0.70
1:A:517:LEU:C	1:A:527:CYS:CB	2.64	0.70
2:B:29:PRO:CB	4:D:22:PHE:C	2.65	0.69
2:B:568:PRO:C	2:B:570:SER:H	1.99	0.69
18:Q:794:UNK:CB	18:Q:797:UNK:N	2.47	0.69
18:R:12:UNK:CB	18:R:45:UNK:CA	2.67	0.69
7:g:287:PHE:O	7:g:288:LEU:C	2.35	0.69
1:A:408:ARG:HA	1:A:432:LEU:CB	2.22	0.69
1:a:1291:ILE:O	1:a:1295:CYS:CB	2.40	0.69
1:A:1524:LEU:HA	1:A:1527:SER:CB	2.21	0.69
7:G:617:GLN:O	7:G:620:ASP:CB	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:1155:ARG:H	7:g:765:ALA:C	2.00	0.69
7:G:280:MET:CB	8:H:265:TRP:CB	2.70	0.69
1:A:1701:MET:CB	1:A:1833:ARG:CA	2.71	0.69
18:R:95:UNK:O	18:R:96:UNK:CB	2.40	0.69
1:A:1226:ASN:C	1:A:1230:LEU:CB	2.66	0.69
7:g:146:PRO:O	7:g:150:PRO:N	2.26	0.69
1:A:747:ARG:O	1:A:755:LYS:CB	2.41	0.69
1:A:889:LYS:CB	1:A:890:ALA:CA	2.70	0.69
9:I:665:VAL:O	9:I:669:LEU:N	2.23	0.69
7:g:285:TYR:CA	7:g:294:ALA:CB	2.66	0.69
2:b:475:SER:C	2:b:484:ALA:HB2	2.18	0.68
1:A:1226:ASN:CB	1:A:1230:LEU:CB	2.70	0.68
2:B:568:PRO:C	2:B:570:SER:N	2.51	0.68
7:G:699:CYS:CB	7:G:703:GLU:CB	2.71	0.68
18:R:184:UNK:HA	18:R:302:UNK:CB	2.23	0.68
2:b:390:LEU:O	2:b:394:ALA:N	2.27	0.68
7:g:491:LYS:O	7:g:495:ASP:CB	2.40	0.68
7:g:699:CYS:CB	7:g:703:GLU:CB	2.71	0.68
5:E:451:SER:O	6:F:205:GLU:N	2.26	0.68
10:J:898:LEU:N	10:J:911:ALA:CB	2.57	0.68
11:S:88:GLU:O	7:g:825:LEU:CB	2.42	0.68
5:E:921:LYS:HA	6:F:126:TYR:CB	2.24	0.68
7:G:424:ARG:O	7:G:428:GLU:CB	2.42	0.68
5:e:1152:SER:H	7:g:850:ARG:CB	2.06	0.68
1:a:914:ALA:CA	1:a:990:THR:CB	2.72	0.68
7:G:296:SER:C	7:G:298:THR:HA	2.18	0.68
1:a:1428:LEU:CA	1:a:1501:ARG:CB	2.72	0.68
5:e:1151:ALA:HB3	7:g:846:THR:O	1.92	0.68
7:g:285:TYR:H	7:g:294:ALA:CB	1.93	0.67
18:Q:703:UNK:HA	18:Q:729:UNK:CB	2.25	0.67
4:D:93:SER:C	4:D:95:ASP:N	2.52	0.67
7:g:424:ARG:O	7:g:428:GLU:CB	2.42	0.67
7:g:266:ASP:CB	7:g:277:ASP:CB	2.72	0.67
8:H:183:VAL:HA	8:H:193:ILE:HA	1.75	0.67
18:R:35:UNK:N	18:R:45:UNK:O	2.27	0.67
2:b:54:MET:CB	4:d:7:ILE:N	2.58	0.67
2:b:568:PRO:C	2:b:570:SER:H	1.99	0.67
10:j:915:ALA:CB	10:j:923:HIS:CB	2.69	0.67
9:I:201:LEU:O	9:I:204:LEU:N	2.28	0.67
7:G:666:GLU:O	7:G:667:ASN:C	2.38	0.67
1:A:1226:ASN:N	1:A:1230:LEU:CB	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ILE:CA	4:D:296:SER:CB	2.71	0.67
18:R:31:UNK:CA	18:R:77:UNK:CB	2.72	0.67
7:g:707:SER:CB	7:g:712:ASN:CB	2.73	0.67
9:i:888:MET:CA	10:j:964:ALA:HB2	2.22	0.67
1:A:379:PHE:N	1:A:382:ASP:CB	2.58	0.66
1:A:387:ARG:CA	1:A:455:GLU:CB	2.73	0.66
1:A:387:ARG:CB	1:A:455:GLU:CB	2.73	0.66
18:R:215:UNK:HA	18:R:272:UNK:N	2.10	0.66
4:D:91:GLY:O	4:D:98:ARG:O	2.13	0.66
5:e:1155:ARG:CB	7:g:766:ASP:N	2.58	0.66
2:B:390:LEU:O	2:B:394:ALA:N	2.27	0.66
2:B:65:SER:CB	2:B:68:LEU:CB	2.74	0.66
1:A:518:ALA:HA	1:A:524:ALA:CA	2.21	0.66
7:G:707:SER:CB	7:G:712:ASN:CB	2.73	0.66
1:a:807:LEU:O	1:a:811:PRO:CA	2.44	0.66
1:a:524:ALA:CB	1:a:607:TRP:C	2.69	0.65
18:R:217:UNK:HA	18:R:269:UNK:HA	1.78	0.65
2:b:65:SER:CB	2:b:68:LEU:CB	2.74	0.65
10:J:903:ALA:CB	10:J:908:GLN:HA	2.27	0.65
2:b:439:ARG:CA	4:d:23:HIS:HA	2.27	0.65
8:h:182:PHE:O	8:h:194:TRP:N	2.29	0.65
1:A:908:GLU:O	1:A:909:LEU:C	2.34	0.65
7:G:346:ASN:C	7:G:348:GLY:N	2.48	0.65
1:A:1591:PRO:HA	1:A:1612:VAL:CA	2.27	0.65
7:G:308:LYS:O	7:G:309:LEU:C	2.40	0.65
9:I:190:GLY:O	9:I:193:LYS:N	2.30	0.65
4:d:197:VAL:CB	4:d:215:LEU:C	2.70	0.65
7:g:389:GLN:O	7:g:409:ARG:CA	2.44	0.65
1:A:1226:ASN:C	1:A:1230:LEU:H	2.05	0.64
1:a:528:PHE:CB	1:a:611:ALA:CA	2.75	0.64
7:g:666:GLU:O	7:g:667:ASN:C	2.38	0.64
10:j:912:PHE:O	10:j:915:ALA:HB3	1.97	0.64
2:b:475:SER:O	2:b:480:ARG:N	2.30	0.64
3:c:100:ILE:O	3:c:113:ASN:N	2.30	0.64
2:B:29:PRO:N	4:D:24:GLY:HA3	2.12	0.64
7:g:626:PRO:O	7:g:627:ASP:C	2.40	0.64
2:B:302:TRP:CB	2:B:327:GLN:CB	2.76	0.64
18:R:31:UNK:C	18:R:77:UNK:CB	2.76	0.64
18:R:375:UNK:N	18:R:382:UNK:CB	2.61	0.64
1:A:1111:SER:HA	1:A:1283:SER:CB	2.28	0.64
18:Q:790:UNK:C	18:Q:799:UNK:CB	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:700:VAL:O	7:G:732:ARG:HA	1.98	0.64
1:a:635:ILE:CB	1:a:636:PRO:C	2.71	0.64
7:g:296:SER:C	8:h:17:HIS:C	2.65	0.64
1:A:515:ARG:HA	1:A:518:ALA:HB3	1.80	0.64
1:A:836:LYS:O	1:A:840:GLU:CB	2.46	0.64
7:g:218:GLY:O	7:g:222:GLN:N	2.26	0.64
18:R:314:UNK:HA	18:R:326:UNK:HA	1.79	0.63
18:R:329:UNK:HA	18:R:348:UNK:HA	1.80	0.63
7:g:370:GLU:O	7:g:371:ALA:C	2.40	0.63
7:G:698:GLN:O	7:G:703:GLU:CB	2.45	0.63
1:a:807:LEU:C	1:a:811:PRO:CB	2.70	0.63
2:b:47:THR:HA	2:b:48:ALA:C	2.22	0.63
7:G:370:GLU:O	7:G:371:ALA:C	2.41	0.63
18:R:76:UNK:O	18:R:77:UNK:CB	2.46	0.63
18:R:328:UNK:N	18:R:349:UNK:O	2.32	0.63
4:d:188:ASP:O	4:d:220:ASP:C	2.41	0.63
1:A:1227:VAL:HA	1:A:1231:HIS:CB	2.28	0.63
18:R:185:UNK:CA	18:R:195:UNK:O	2.32	0.63
7:g:700:VAL:O	7:g:732:ARG:HA	1.98	0.63
1:A:908:GLU:C	1:A:910:ALA:N	2.56	0.63
7:G:644:LEU:O	7:G:645:ASN:CB	2.47	0.63
7:G:767:ALA:CB	7:G:854:SER:C	2.71	0.63
1:a:1290:ILE:O	1:a:1294:ALA:CA	2.46	0.63
10:j:865:ASN:CB	10:j:907:GLY:HA2	2.29	0.63
2:B:23:ILE:C	4:D:296:SER:CB	2.72	0.63
2:B:352:GLU:O	2:B:353:PHE:CB	2.47	0.63
2:b:302:TRP:CB	2:b:327:GLN:CB	2.76	0.63
2:b:352:GLU:O	2:b:353:PHE:CB	2.47	0.63
1:a:525:HIS:CA	1:a:608:SER:CB	2.75	0.63
2:b:590:PHE:O	2:b:594:GLN:N	2.31	0.63
7:g:698:GLN:O	7:g:703:GLU:CB	2.45	0.63
2:b:475:SER:C	2:b:484:ALA:CB	2.71	0.62
7:g:296:SER:C	8:h:18:ASP:CA	2.72	0.62
7:G:422:GLU:O	7:G:423:GLU:C	2.41	0.62
1:a:457:ALA:HB3	1:a:522:GLN:CB	2.29	0.62
7:g:422:GLU:O	7:g:423:GLU:C	2.41	0.62
7:g:496:HIS:C	9:i:293:LEU:CB	2.73	0.62
2:B:28:GLY:HA2	4:D:20:PHE:CB	2.29	0.62
4:d:197:VAL:CB	4:d:215:LEU:CA	2.76	0.62
18:Q:778:UNK:O	18:Q:779:UNK:C	2.47	0.62
12:K:356:UNK:O	12:K:357:UNK:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:670:UNK:C	18:Q:672:UNK:N	2.62	0.62
2:B:248:THR:CB	2:B:252:PHE:N	2.63	0.62
2:b:43:GLY:HA2	2:b:44:ASN:CB	2.29	0.62
1:a:1124:THR:O	1:a:1128:ARG:CA	2.47	0.62
2:b:248:THR:CB	2:b:252:PHE:N	2.63	0.62
7:g:161:GLY:O	7:g:164:GLN:N	2.33	0.62
9:i:670:VAL:CB	9:i:707:PRO:CB	2.78	0.61
18:Q:778:UNK:O	18:Q:781:UNK:N	2.33	0.61
2:B:29:PRO:N	4:D:24:GLY:CA	2.63	0.61
1:a:453:HIS:O	1:a:454:LEU:C	2.43	0.61
7:g:538:HIS:O	7:g:542:MET:CB	2.47	0.61
1:a:914:ALA:HA	1:a:990:THR:CB	2.31	0.61
2:b:288:ASP:N	2:b:289:GLU:HA	2.16	0.61
9:I:670:VAL:CB	9:I:707:PRO:CB	2.78	0.61
18:Q:670:UNK:O	18:Q:671:UNK:C	2.49	0.61
1:a:635:ILE:CB	1:a:636:PRO:CA	2.78	0.61
1:a:1295:CYS:C	1:a:1297:GLN:N	2.52	0.61
3:c:45:VAL:O	3:c:72:ILE:N	2.31	0.61
7:g:703:GLU:O	7:g:707:SER:CB	2.49	0.61
7:G:703:GLU:O	7:G:707:SER:CB	2.49	0.60
1:A:500:ASP:O	1:A:507:TYR:N	2.34	0.60
2:B:440:ILE:O	2:B:441:PRO:C	2.45	0.60
8:h:183:VAL:HA	8:h:193:ILE:HA	1.83	0.60
7:G:346:ASN:C	7:G:348:GLY:H	2.09	0.60
7:g:301:PRO:O	8:h:47:GLN:CB	2.49	0.60
1:A:1649:VAL:C	1:A:1651:HIS:H	2.09	0.59
2:B:288:ASP:N	2:B:289:GLU:HA	2.16	0.59
7:g:215:ARG:O	7:g:219:THR:N	2.34	0.59
10:j:867:SER:H	10:j:910:ALA:HB2	1.66	0.59
1:A:460:TYR:CB	1:A:523:CYS:CB	2.79	0.59
7:g:423:GLU:CA	7:g:426:GLU:CB	2.80	0.59
3:C:87:GLU:O	3:C:103:HIS:N	2.33	0.59
1:a:1304:HIS:O	1:a:1307:LEU:N	2.31	0.59
1:A:387:ARG:HA	1:A:455:GLU:CB	2.32	0.59
1:A:437:GLU:CB	1:A:509:PRO:HA	2.31	0.59
2:B:590:PHE:O	2:B:594:GLN:N	2.30	0.59
2:b:568:PRO:C	2:b:570:SER:N	2.51	0.59
7:g:494:VAL:O	7:g:495:ASP:C	2.44	0.59
1:A:515:ARG:HA	1:A:518:ALA:CB	2.33	0.59
11:T:58:ARG:O	11:T:62:ALA:HB3	2.03	0.59
7:g:296:SER:C	8:h:18:ASP:HA	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:452:ASP:C	6:F:205:GLU:CB	2.76	0.58
7:G:423:GLU:CA	7:G:426:GLU:CB	2.80	0.58
11:S:58:ARG:O	11:S:62:ALA:HB3	2.03	0.58
2:b:476:LEU:HA	2:b:484:ALA:HB3	1.85	0.58
1:A:889:LYS:CB	1:A:891:ASP:N	2.66	0.58
1:a:949:VAL:O	1:a:1034:LEU:CB	2.51	0.58
7:g:363:SER:C	7:g:365:GLU:H	2.12	0.58
1:A:1273:CYS:O	1:A:1276:ALA:N	2.35	0.58
2:b:438:GLU:CB	2:b:467:ILE:CB	2.82	0.58
5:e:1155:ARG:CB	7:g:765:ALA:CA	2.81	0.58
7:g:281:ASP:HA	8:h:17:HIS:HA	1.86	0.58
1:A:1731:SER:O	1:A:1735:ASP:N	2.27	0.58
7:g:485:GLN:O	7:g:486:LEU:C	2.47	0.58
7:g:682:PRO:CB	7:g:683:HIS:HA	2.32	0.58
7:G:334:VAL:HA	7:G:342:HIS:O	2.04	0.58
9:i:596:TYR:O	9:i:600:LEU:N	2.30	0.58
2:B:23:ILE:CB	4:D:296:SER:CA	2.78	0.58
7:G:245:LEU:HA	7:G:246:PHE:C	2.29	0.58
11:U:36:TYR:CB	11:U:45:ALA:CB	2.73	0.58
1:A:515:ARG:O	1:A:518:ALA:N	2.37	0.58
11:V:58:ARG:O	11:V:62:ALA:HB3	2.03	0.58
1:a:854:LEU:O	1:a:919:SER:CB	2.52	0.58
1:A:836:LYS:O	1:A:840:GLU:N	2.30	0.58
1:A:878:GLN:O	1:A:882:GLY:N	2.27	0.57
7:G:296:SER:C	7:G:298:THR:CA	2.76	0.57
1:a:1427:TYR:C	1:a:1501:ARG:CB	2.77	0.57
2:b:476:LEU:HA	2:b:480:ARG:O	2.04	0.57
3:c:348:VAL:O	3:c:362:THR:N	2.36	0.57
1:a:521:PRO:HA	1:a:607:TRP:O	2.05	0.57
3:c:285:HIS:O	3:c:337:ILE:CA	2.53	0.57
5:e:1152:SER:O	7:g:764:ALA:O	2.21	0.57
18:R:213:UNK:O	18:R:272:UNK:CB	2.52	0.57
3:C:16:ARG:N	3:C:36:GLY:O	2.36	0.57
7:g:325:LEU:C	7:g:327:ILE:H	2.13	0.57
7:G:363:SER:C	7:G:365:GLU:H	2.12	0.57
1:a:493:LYS:O	1:a:496:ARG:N	2.38	0.57
18:R:322:UNK:CB	18:R:354:UNK:O	2.53	0.57
7:g:556:TYR:O	7:g:559:ALA:HB3	2.05	0.57
18:R:135:UNK:HA	18:R:216:UNK:HA	1.87	0.57
7:G:463:HIS:CB	9:I:405:MET:CA	2.83	0.56
1:a:1431:ALA:CA	1:a:1505:VAL:CB	2.80	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:1028:UNK:O	18:Q:1029:UNK:C	2.52	0.56
18:R:210:UNK:CB	18:R:276:UNK:HA	2.35	0.56
2:b:44:ASN:N	2:b:45:SER:CA	2.67	0.56
1:A:227:SER:O	1:A:228:LEU:C	2.47	0.56
7:G:287:PHE:CB	7:G:290:LYS:O	2.53	0.56
7:G:767:ALA:HB2	7:G:854:SER:CB	2.35	0.56
7:G:805:TYR:N	7:G:833:MET:CB	2.68	0.56
1:a:1124:THR:HA	1:a:1128:ARG:CB	2.35	0.56
3:c:179:ARG:O	3:c:182:GLU:N	2.39	0.56
7:g:666:GLU:C	7:g:668:VAL:N	2.62	0.56
10:j:867:SER:CB	10:j:910:ALA:O	2.53	0.56
3:C:93:SER:N	3:C:97:THR:O	2.32	0.56
1:A:743:ARG:HA	1:A:746:THR:CB	2.36	0.56
2:b:640:ASN:C	5:e:1076:TYR:CB	2.78	0.56
7:G:666:GLU:N	7:G:670:LEU:CB	2.68	0.56
18:R:183:UNK:O	18:R:302:UNK:N	2.39	0.56
1:a:1431:ALA:CB	1:a:1505:VAL:N	2.66	0.56
2:b:475:SER:CB	2:b:484:ALA:HB2	2.36	0.56
7:G:556:TYR:O	7:G:559:ALA:HB3	2.05	0.55
18:Q:905:UNK:C	18:Q:907:UNK:N	2.68	0.55
18:R:184:UNK:O	18:R:196:UNK:C	2.53	0.55
1:a:524:ALA:O	1:a:608:SER:CB	2.53	0.55
2:b:45:SER:H	2:b:46:GLU:CA	2.14	0.55
2:B:428:LEU:O	2:B:429:GLY:C	2.49	0.55
7:G:621:PRO:O	7:G:624:VAL:N	2.39	0.55
3:c:232:THR:O	3:c:240:CYS:N	2.37	0.55
18:R:330:UNK:N	18:R:347:UNK:O	2.39	0.55
7:G:666:GLU:HA	7:G:670:LEU:N	2.21	0.55
9:I:596:TYR:O	9:I:600:LEU:N	2.30	0.55
18:R:212:UNK:N	18:R:276:UNK:O	2.40	0.55
5:E:451:SER:CB	6:F:204:LEU:HA	2.37	0.55
8:H:13:GLU:O	8:H:14:ASP:C	2.49	0.55
10:J:898:LEU:CB	10:J:908:GLN:HA	2.36	0.55
1:A:906:ASN:O	1:A:907:ALA:HB3	2.06	0.55
8:h:122:CYS:O	8:h:129:ILE:HA	2.06	0.55
10:j:566:ALA:HB2	10:j:573:ALA:HB1	1.89	0.55
7:G:682:PRO:CB	7:G:683:HIS:CA	2.84	0.55
1:A:831:ALA:H	1:A:832:PRO:CB	2.20	0.54
7:g:167:PHE:O	7:g:168:ALA:HB3	2.08	0.54
7:G:295:LYS:CB	7:G:303:LYS:HA	2.36	0.54
2:b:327:GLN:O	2:b:331:ASP:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:234:GLY:N	3:c:238:MET:O	2.37	0.54
1:A:849:LEU:O	1:A:853:THR:CB	2.55	0.54
7:G:287:PHE:O	8:H:271:ILE:CB	2.56	0.54
10:j:867:SER:N	10:j:910:ALA:CB	2.71	0.54
1:a:856:LYS:C	1:a:873:VAL:CB	2.80	0.54
7:g:627:ASP:CB	7:g:628:PRO:CA	2.85	0.54
3:C:194:LEU:O	3:C:205:THR:N	2.40	0.54
7:G:767:ALA:HB1	7:G:854:SER:O	2.05	0.54
18:Q:859:UNK:C	18:Q:861:UNK:HA	2.38	0.54
18:R:31:UNK:N	18:R:77:UNK:O	2.41	0.54
1:A:515:ARG:O	1:A:518:ALA:CB	2.54	0.54
2:B:387:ALA:HB3	2:B:390:LEU:CB	2.38	0.54
3:C:237:GLY:HA3	3:C:257:HIS:H	1.73	0.54
9:I:199:SER:O	9:I:202:TRP:CB	2.56	0.54
9:I:652:ASP:C	9:I:654:GLY:H	2.16	0.54
10:J:903:ALA:HB1	10:J:908:GLN:H	1.69	0.54
7:g:293:SER:O	7:g:294:ALA:HB2	2.07	0.54
2:B:327:GLN:O	2:B:331:ASP:CB	2.55	0.53
2:B:561:LEU:O	2:B:564:ALA:O	2.26	0.53
11:U:25:LYS:HA	9:i:460:ILE:CB	2.38	0.53
18:R:186:UNK:O	18:R:195:UNK:N	2.41	0.53
18:R:216:UNK:O	18:R:270:UNK:N	2.42	0.53
9:i:652:ASP:C	9:i:654:GLY:H	2.16	0.53
7:g:475:SER:CB	7:g:544:PRO:HA	2.38	0.53
3:C:91:THR:O	3:C:99:THR:N	2.39	0.53
10:J:566:ALA:HB2	10:J:573:ALA:HB1	1.89	0.53
9:i:653:SER:O	9:i:657:GLU:CB	2.57	0.53
7:G:282:THR:CB	8:H:265:TRP:CB	2.87	0.53
2:b:387:ALA:HB3	2:b:390:LEU:CB	2.38	0.53
1:A:908:GLU:O	1:A:910:ALA:CA	2.55	0.53
1:A:1104:ILE:HA	1:A:1276:ALA:CB	2.38	0.53
2:B:29:PRO:CB	4:D:23:HIS:O	2.54	0.53
1:a:1290:ILE:O	1:a:1294:ALA:HB3	2.07	0.53
3:c:37:SER:N	3:c:44:LYS:O	2.41	0.53
7:G:767:ALA:HB1	7:G:854:SER:C	2.34	0.52
18:Q:1017:UNK:CA	18:Q:1079:UNK:CB	2.86	0.52
1:a:808:ASN:O	1:a:812:MET:CB	2.57	0.52
1:a:948:PHE:O	1:a:981:LYS:CB	2.57	0.52
1:A:831:ALA:N	1:A:832:PRO:CB	2.72	0.52
1:A:1334:ALA:CB	1:A:1415:ARG:CB	2.83	0.52
7:G:642:GLN:HA	7:G:647:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:46:GLU:CB	2:b:50:ARG:CB	2.87	0.52
9:I:653:SER:O	9:I:657:GLU:CB	2.57	0.52
7:g:279:ASN:CB	7:g:281:ASP:N	2.72	0.52
1:A:853:THR:O	1:A:857:GLU:N	2.40	0.52
7:G:218:GLY:O	7:G:222:GLN:N	2.37	0.52
18:R:328:UNK:O	18:R:349:UNK:N	2.43	0.52
18:R:431:UNK:N	18:R:436:UNK:O	2.43	0.52
7:g:165:SER:C	7:g:168:ALA:H	2.17	0.52
10:j:865:ASN:O	10:j:910:ALA:HB2	2.09	0.52
3:C:221:ASP:O	3:C:230:VAL:CA	2.57	0.52
11:S:88:GLU:O	7:g:825:LEU:CA	2.58	0.52
2:B:34:LEU:CB	2:B:57:VAL:O	2.57	0.52
10:J:903:ALA:CB	10:J:908:GLN:N	2.65	0.52
1:a:1282:GLU:O	1:a:1286:GLN:CB	2.57	0.52
2:b:561:LEU:O	2:b:564:ALA:O	2.27	0.51
2:B:126:THR:O	2:B:127:ALA:HB3	2.09	0.51
18:R:184:UNK:O	18:R:196:UNK:CA	2.56	0.51
18:R:375:UNK:O	18:R:382:UNK:CB	2.58	0.51
2:B:439:ARG:CB	4:D:23:HIS:HA	2.41	0.51
7:g:422:GLU:C	7:g:424:ARG:N	2.69	0.51
1:A:387:ARG:O	1:A:455:GLU:CB	2.59	0.51
7:G:613:TYR:C	7:G:615:LEU:H	2.18	0.51
7:g:295:LYS:CB	8:h:19:ALA:CB	2.79	0.51
7:g:487:VAL:N	7:g:490:ASN:CB	2.73	0.51
1:A:830:TYR:O	1:A:831:ALA:HB2	2.11	0.51
1:a:539:ALA:HB1	1:a:545:ALA:HB1	1.92	0.51
3:C:100:ILE:O	3:C:113:ASN:N	2.42	0.51
7:G:439:GLU:O	7:G:442:PHE:N	2.44	0.51
1:A:227:SER:C	1:A:229:ALA:N	2.61	0.51
9:i:663:ILE:HA	9:i:705:LYS:CB	2.41	0.51
3:c:93:SER:N	3:c:97:THR:O	2.38	0.50
10:j:865:ASN:C	10:j:910:ALA:HB2	2.36	0.50
10:j:867:SER:CB	10:j:910:ALA:CA	2.88	0.50
1:A:390:HIS:CB	1:A:456:LEU:N	2.74	0.50
4:D:86:TRP:HA	4:D:104:VAL:O	2.12	0.50
9:I:663:ILE:HA	9:I:705:LYS:CB	2.41	0.50
11:V:36:TYR:CB	11:V:45:ALA:CB	2.87	0.50
18:R:31:UNK:O	18:R:32:UNK:CB	2.59	0.50
10:j:920:SER:O	10:j:924:GLU:CA	2.57	0.50
7:G:624:VAL:HA	8:H:292:VAL:CB	2.41	0.50
2:b:475:SER:CB	2:b:484:ALA:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:MET:HA	1:A:1280:ALA:HB2	1.93	0.50
11:T:178:ASN:O	11:T:179:GLN:CB	2.60	0.50
1:a:751:ARG:O	1:a:755:LYS:CB	2.59	0.50
7:G:287:PHE:C	7:G:290:LYS:O	2.54	0.50
7:G:370:GLU:O	7:G:373:VAL:N	2.45	0.50
7:g:370:GLU:O	7:g:373:VAL:N	2.45	0.50
2:b:641:LEU:N	5:e:1076:TYR:CB	2.75	0.50
7:g:439:GLU:O	7:g:442:PHE:N	2.44	0.50
7:G:767:ALA:HB2	7:G:854:SER:C	2.37	0.50
7:g:282:THR:CB	8:h:265:TRP:CB	2.90	0.50
11:S:178:ASN:O	11:S:179:GLN:CB	2.60	0.50
11:T:36:TYR:CB	11:T:45:ALA:CB	2.87	0.50
18:R:30:UNK:O	18:R:31:UNK:CB	2.59	0.50
1:A:1107:MET:CB	1:A:1276:ALA:O	2.60	0.49
18:Q:1017:UNK:CB	18:Q:1079:UNK:CB	2.90	0.49
1:A:721:GLY:HA3	1:A:728:GLY:HA3	1.94	0.49
18:Q:1020:UNK:O	18:Q:1023:UNK:CB	2.59	0.49
2:b:45:SER:N	2:b:46:GLU:CA	2.73	0.49
10:j:911:ALA:O	10:j:915:ALA:N	2.45	0.49
18:R:12:UNK:CB	18:R:46:UNK:N	2.75	0.49
1:A:500:ASP:HA	1:A:506:LEU:CB	2.42	0.49
10:J:903:ALA:HB2	10:J:908:GLN:HA	1.94	0.49
11:V:178:ASN:O	11:V:179:GLN:CB	2.59	0.49
2:b:476:LEU:CA	2:b:484:ALA:HB3	2.42	0.49
1:A:515:ARG:CA	1:A:518:ALA:HB3	2.42	0.49
1:A:517:LEU:O	1:A:523:CYS:C	2.55	0.49
2:B:380:ASP:CB	2:B:397:ARG:CB	2.91	0.49
3:C:47:VAL:O	3:C:69:LEU:N	2.45	0.49
2:B:439:ARG:O	2:B:440:ILE:C	2.52	0.49
7:G:281:ASP:CB	7:G:282:THR:CA	2.88	0.49
7:G:433:GLY:C	7:G:435:GLU:N	2.70	0.49
7:g:165:SER:O	7:g:168:ALA:N	2.46	0.49
7:g:486:LEU:O	7:g:488:ASP:N	2.45	0.49
5:E:892:ARG:CB	6:F:166:SER:CB	2.91	0.49
7:G:541:TYR:O	7:G:542:MET:C	2.56	0.49
7:G:666:GLU:C	7:G:668:VAL:N	2.71	0.48
1:a:1304:HIS:C	1:a:1306:GLN:N	2.67	0.48
2:b:326:ALA:O	2:b:330:LEU:CB	2.61	0.48
18:R:216:UNK:N	18:R:270:UNK:O	2.45	0.48
2:b:641:LEU:HA	5:e:1076:TYR:CB	2.43	0.48
3:C:276:THR:O	3:C:284:TRP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:GLY:O	4:D:98:ARG:C	2.56	0.48
7:G:240:LEU:O	7:G:241:ILE:C	2.55	0.48
7:g:511:GLY:HA2	7:g:541:TYR:O	2.14	0.48
2:b:380:ASP:CB	2:b:397:ARG:CB	2.91	0.48
1:A:1581:LEU:O	1:A:1584:CYS:N	2.45	0.48
2:B:29:PRO:CB	4:D:23:HIS:CA	2.88	0.48
3:c:237:GLY:O	3:c:256:ALA:N	2.46	0.48
7:g:621:PRO:O	7:g:625:THR:N	2.38	0.48
7:G:702:ARG:O	7:G:706:GLU:N	2.25	0.48
1:a:1295:CYS:C	1:a:1297:GLN:H	2.01	0.48
7:G:621:PRO:O	7:G:622:SER:C	2.55	0.48
8:H:122:CYS:O	8:H:129:ILE:HA	2.14	0.48
1:A:515:ARG:O	1:A:519:SER:N	2.47	0.48
2:B:326:ALA:O	2:B:330:LEU:CB	2.61	0.48
18:R:12:UNK:O	18:R:45:UNK:CB	2.61	0.48
1:a:447:TYR:O	1:a:448:ARG:C	2.54	0.48
18:R:12:UNK:O	18:R:45:UNK:HA	2.14	0.48
7:G:279:ASN:C	7:G:282:THR:CB	2.86	0.48
7:g:702:ARG:O	7:g:706:GLU:N	2.25	0.47
10:j:865:ASN:CB	10:j:907:GLY:CA	2.92	0.47
1:A:1104:ILE:HA	1:A:1276:ALA:HB1	1.95	0.47
11:U:176:LEU:HA	11:U:181:LEU:CB	2.44	0.47
18:R:190:UNK:O	18:R:191:UNK:CB	2.58	0.47
1:a:1424:LEU:CB	1:a:1497:ALA:HB3	2.44	0.47
10:j:854:ASP:O	10:j:858:GLN:CB	2.62	0.47
1:A:515:ARG:C	1:A:518:ALA:HB3	2.39	0.47
1:A:743:ARG:O	1:A:746:THR:N	2.48	0.47
8:H:13:GLU:C	8:H:14:ASP:O	2.58	0.47
1:a:1431:ALA:HB2	1:a:1501:ARG:O	2.13	0.47
1:A:908:GLU:C	1:A:910:ALA:H	2.19	0.47
7:G:541:TYR:O	7:G:543:LEU:N	2.47	0.47
10:J:898:LEU:CB	10:J:908:GLN:C	2.86	0.47
7:g:478:MET:O	7:g:479:ARG:C	2.57	0.47
10:j:867:SER:CB	10:j:913:LEU:CB	2.92	0.47
9:I:190:GLY:O	9:I:191:GLN:C	2.56	0.47
1:a:1424:LEU:CB	1:a:1497:ALA:CB	2.92	0.47
7:g:156:ARG:HA	7:g:157:THR:HA	1.65	0.47
7:G:557:GLU:C	7:G:559:ALA:H	2.22	0.47
2:b:470:THR:CB	4:d:68:PRO:O	2.63	0.47
3:c:187:ASN:O	3:c:190:GLY:N	2.47	0.47
7:g:707:SER:C	7:g:709:ALA:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:CYS:O	1:A:696:GLU:C	2.57	0.47
1:A:1587:TYR:O	1:A:1615:TYR:CB	2.63	0.47
7:G:613:TYR:C	7:G:615:LEU:N	2.73	0.47
11:S:88:GLU:O	7:g:825:LEU:HA	2.15	0.47
1:a:854:LEU:C	1:a:919:SER:CB	2.87	0.47
2:b:476:LEU:CA	2:b:484:ALA:CB	2.92	0.47
7:g:389:GLN:CB	7:g:412:ALA:HB3	2.45	0.47
7:g:557:GLU:C	7:g:559:ALA:H	2.22	0.47
3:C:84:LEU:N	3:C:88:ARG:O	2.48	0.47
7:G:707:SER:C	7:G:709:ALA:N	2.73	0.47
2:b:472:ALA:HB1	2:b:488:SER:CA	2.42	0.47
10:j:920:SER:O	10:j:924:GLU:N	2.47	0.47
1:A:1227:VAL:C	1:A:1231:HIS:CB	2.85	0.47
7:G:444:PHE:CB	7:G:453:ALA:CB	2.93	0.47
7:G:478:MET:O	7:G:479:ARG:C	2.57	0.47
1:a:1431:ALA:CB	1:a:1505:VAL:CB	2.92	0.47
1:A:242:ASN:HA	1:A:243:ARG:HA	1.55	0.46
7:G:296:SER:H	7:G:298:THR:HA	1.80	0.46
7:G:323:MET:C	7:G:325:LEU:N	2.73	0.46
9:I:652:ASP:O	9:I:654:GLY:N	2.42	0.46
18:Q:858:UNK:O	18:Q:861:UNK:HA	2.15	0.46
1:a:1331:PRO:CB	1:a:1415:ARG:CB	2.93	0.46
11:S:36:TYR:CB	11:S:45:ALA:CB	2.87	0.46
7:g:160:MET:O	7:g:163:LEU:CB	2.62	0.46
7:G:436:ARG:HA	7:G:437:HIS:HA	1.74	0.46
2:b:96:ALA:O	2:b:97:GLN:C	2.59	0.46
5:e:1155:ARG:HA	7:g:765:ALA:HB1	1.77	0.46
7:g:325:LEU:C	7:g:327:ILE:N	2.73	0.46
3:C:80:ASP:O	3:C:91:THR:CA	2.63	0.46
7:G:279:ASN:C	7:G:281:ASP:N	2.73	0.46
1:a:528:PHE:CB	1:a:611:ALA:H	2.28	0.46
18:R:267:UNK:O	18:R:268:UNK:CB	2.63	0.46
9:i:652:ASP:O	9:i:654:GLY:N	2.42	0.46
2:B:96:ALA:O	2:B:97:GLN:C	2.58	0.46
10:J:896:GLY:O	10:J:911:ALA:CB	2.63	0.46
11:U:172:VAL:CB	11:U:184:ALA:HB1	2.45	0.46
7:G:511:GLY:O	7:G:542:MET:O	2.34	0.46
7:G:685:HIS:C	7:G:687:ARG:N	2.72	0.46
10:j:915:ALA:O	10:j:916:HIS:C	2.59	0.46
1:A:520:GLY:HA3	1:A:523:CYS:CB	2.46	0.46
9:I:199:SER:CA	9:I:202:TRP:CB	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:472:ALA:CB	2:b:488:SER:CA	2.93	0.46
2:B:119:LEU:O	2:B:122:SER:CB	2.64	0.46
3:C:37:SER:N	3:C:44:LYS:O	2.33	0.46
3:C:194:LEU:N	3:C:206:GLN:O	2.49	0.46
7:G:438:VAL:C	7:G:440:ALA:N	2.73	0.46
11:T:184:ALA:O	11:T:188:CYS:N	2.49	0.46
4:d:195:GLY:C	4:d:218:VAL:CB	2.89	0.46
7:g:438:VAL:C	7:g:440:ALA:N	2.73	0.46
7:g:486:LEU:N	9:i:363:ALA:CB	2.79	0.46
1:A:515:ARG:O	1:A:518:ALA:CA	2.63	0.45
1:A:517:LEU:O	1:A:524:ALA:CA	2.62	0.45
1:a:887:SER:O	1:a:891:ASP:N	2.44	0.45
2:b:64:TYR:O	2:b:65:SER:CB	2.65	0.45
5:e:1152:SER:HA	7:g:847:ALA:HA	1.44	0.45
1:A:227:SER:C	1:A:229:ALA:H	2.19	0.45
2:B:596:TYR:CB	5:E:1124:LEU:CB	2.94	0.45
10:J:898:LEU:CB	10:J:911:ALA:CB	2.90	0.45
2:b:494:ALA:O	2:b:495:ALA:HB3	2.17	0.45
11:U:175:PHE:C	11:U:181:LEU:CB	2.90	0.45
1:a:1183:ILE:C	1:a:1185:ASP:H	2.24	0.45
7:g:444:PHE:CB	7:g:453:ALA:CB	2.93	0.45
4:D:187:ASP:O	4:D:222:VAL:N	2.48	0.45
7:G:557:GLU:C	7:G:559:ALA:N	2.73	0.45
7:g:161:GLY:O	7:g:164:GLN:CB	2.65	0.45
1:A:832:PRO:O	1:A:836:LYS:N	2.44	0.45
3:C:186:VAL:CA	3:C:191:GLN:O	2.64	0.45
11:S:184:ALA:O	11:S:188:CYS:N	2.49	0.45
1:A:1649:VAL:C	1:A:1651:HIS:N	2.73	0.45
2:B:67:VAL:O	2:B:70:LYS:N	2.50	0.45
3:C:132:THR:H	3:C:145:GLY:HA2	1.82	0.45
9:I:178:THR:O	9:I:182:LYS:N	2.46	0.45
11:V:184:ALA:O	11:V:188:CYS:N	2.49	0.45
1:a:854:LEU:CB	1:a:919:SER:CB	2.95	0.45
7:g:219:THR:O	7:g:223:GLN:N	2.47	0.45
2:b:67:VAL:O	2:b:70:LYS:N	2.50	0.45
10:j:867:SER:N	10:j:910:ALA:HB1	2.31	0.45
1:A:1242:GLN:O	1:A:1245:ALA:O	2.34	0.45
2:B:64:TYR:O	2:B:65:SER:CB	2.65	0.45
4:D:91:GLY:O	4:D:99:GLY:N	2.42	0.45
7:G:767:ALA:HB2	7:G:854:SER:O	2.12	0.45
7:g:557:GLU:C	7:g:559:ALA:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:683:HIS:HA	7:g:684:PRO:HA	1.69	0.45
1:A:1591:PRO:CA	1:A:1612:VAL:CB	2.91	0.44
11:U:25:LYS:N	9:i:460:ILE:CB	2.80	0.44
18:R:12:UNK:C	18:R:45:UNK:HA	2.47	0.44
7:g:370:GLU:O	7:g:372:VAL:N	2.51	0.44
7:G:475:SER:O	7:G:544:PRO:CB	2.64	0.44
1:a:242:ASN:HA	1:a:243:ARG:HA	1.55	0.44
7:g:433:GLY:C	7:g:435:GLU:N	2.70	0.44
7:g:296:SER:O	8:h:18:ASP:HA	2.10	0.44
7:G:154:ALA:C	7:G:156:ARG:H	2.26	0.44
7:G:701:VAL:O	7:G:705:PRO:N	2.50	0.44
1:a:1575:SER:O	1:a:1579:VAL:N	2.40	0.44
5:E:634:HIS:HA	6:F:165:ARG:HA	1.99	0.44
11:U:147:TRP:CB	11:U:178:ASN:CB	2.95	0.44
2:b:439:ARG:CB	4:d:23:HIS:HA	2.47	0.44
2:B:382:CYS:C	2:B:384:LEU:N	2.75	0.44
3:C:85:ASP:N	3:C:88:ARG:O	2.41	0.44
11:U:36:TYR:O	11:U:39:ALA:O	2.36	0.44
18:R:253:UNK:O	18:R:257:UNK:N	2.51	0.44
7:G:288:LEU:C	7:G:290:LYS:HA	2.41	0.44
1:a:748:ALA:O	1:a:755:LYS:CB	2.65	0.44
3:c:82:GLN:O	3:c:90:VAL:N	2.36	0.44
1:A:1227:VAL:CA	1:A:1231:HIS:CB	2.94	0.44
7:G:296:SER:N	7:G:298:THR:CA	2.81	0.43
5:e:787:VAL:C	5:e:789:ILE:H	2.26	0.43
7:g:701:VAL:O	7:g:705:PRO:N	2.50	0.43
7:G:370:GLU:O	7:G:372:VAL:N	2.51	0.43
9:I:182:LYS:HA	9:I:183:ILE:HA	1.47	0.43
10:J:898:LEU:N	10:J:911:ALA:HB3	2.32	0.43
2:b:122:SER:O	2:b:123:THR:C	2.56	0.43
7:g:496:HIS:CA	9:i:293:LEU:CB	2.84	0.43
1:A:1581:LEU:O	1:A:1582:ALA:C	2.61	0.43
7:G:293:SER:O	7:G:294:ALA:HB3	2.18	0.43
7:G:767:ALA:HB2	7:G:854:SER:CA	2.48	0.43
1:a:1420:LEU:CA	1:a:1494:LEU:CB	2.94	0.43
2:b:475:SER:O	2:b:480:ARG:O	2.37	0.43
14:M:386:UNK:O	14:M:390:UNK:CB	2.66	0.43
7:G:625:THR:O	7:G:626:PRO:C	2.62	0.43
2:b:34:LEU:CB	2:b:57:VAL:O	2.67	0.43
1:A:289:ASP:HA	1:A:302:MET:H	1.83	0.43
3:C:120:HIS:O	3:C:129:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:281:ASP:N	7:G:282:THR:CA	2.80	0.43
1:a:493:LYS:O	1:a:494:PHE:C	2.62	0.43
4:D:93:SER:H	4:D:98:ARG:CB	2.32	0.43
7:G:289:PRO:HA	7:G:290:LYS:HA	1.70	0.43
7:G:296:SER:CA	7:G:298:THR:CB	2.96	0.43
1:a:289:ASP:HA	1:a:302:MET:H	1.83	0.43
1:a:854:LEU:CB	1:a:916:ILE:HA	2.49	0.43
5:E:1068:VAL:C	5:E:1070:LEU:H	2.27	0.43
11:U:36:TYR:O	11:U:39:ALA:C	2.62	0.43
1:a:585:GLY:O	1:a:586:ILE:CB	2.67	0.43
1:A:520:GLY:O	1:A:524:ALA:CB	2.66	0.43
18:R:188:UNK:N	18:R:193:UNK:O	2.52	0.43
2:B:118:THR:O	2:B:121:GLU:CB	2.67	0.42
7:g:444:PHE:CB	7:g:453:ALA:HB2	2.49	0.42
1:A:585:GLY:O	1:A:586:ILE:CB	2.66	0.42
2:b:36:GLU:O	2:b:55:TYR:CB	2.68	0.42
2:B:438:GLU:O	2:B:439:ARG:C	2.63	0.42
4:D:216:MET:O	4:D:217:SER:CB	2.67	0.42
7:G:308:LYS:O	7:G:310:SER:O	2.37	0.42
1:a:1304:HIS:C	1:a:1306:GLN:H	2.27	0.42
7:G:624:VAL:O	7:G:625:THR:C	2.61	0.42
3:C:286:TRP:O	3:C:288:ALA:N	2.53	0.42
7:G:444:PHE:CB	7:G:453:ALA:HB2	2.50	0.42
7:g:413:PHE:O	7:g:414:SER:C	2.62	0.42
1:A:1647:PHE:O	1:A:1648:LEU:C	2.63	0.42
1:A:1709:ARG:CB	1:A:1717:LEU:CB	2.98	0.42
2:B:426:PRO:C	2:B:428:LEU:N	2.76	0.42
7:G:422:GLU:C	7:G:424:ARG:N	2.69	0.42
2:b:591:SER:HA	2:b:594:GLN:CB	2.50	0.42
7:g:164:GLN:O	7:g:168:ALA:N	2.52	0.42
1:A:879:LEU:O	1:A:883:ILE:N	2.52	0.42
1:A:1340:LEU:O	1:A:1344:LEU:N	2.33	0.42
18:R:11:UNK:CB	18:R:46:UNK:CB	2.97	0.42
18:R:36:UNK:CB	18:R:57:UNK:CB	2.98	0.42
2:B:591:SER:HA	2:B:594:GLN:CB	2.50	0.42
5:E:104:HIS:O	5:E:118:SER:HA	2.20	0.42
7:G:413:PHE:O	7:G:414:SER:C	2.62	0.42
18:R:321:UNK:O	18:R:322:UNK:CB	2.66	0.41
1:a:524:ALA:HB1	1:a:608:SER:N	2.35	0.41
2:b:45:SER:CB	2:b:46:GLU:HA	2.50	0.41
5:e:1068:VAL:C	5:e:1070:LEU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:363:SER:C	7:g:365:GLU:N	2.77	0.41
8:h:122:CYS:O	8:h:129:ILE:CA	2.67	0.41
3:C:285:HIS:O	3:C:287:ASP:N	2.52	0.41
18:R:214:UNK:O	18:R:272:UNK:O	2.38	0.41
3:c:84:LEU:N	3:c:88:ARG:O	2.53	0.41
5:e:104:HIS:O	5:e:118:SER:HA	2.20	0.41
7:g:285:TYR:CB	7:g:294:ALA:N	2.73	0.41
7:G:279:ASN:CB	7:G:282:THR:CB	2.99	0.41
1:A:1337:VAL:CB	1:A:1419:HIS:CB	2.99	0.41
1:A:27:ALA:HB1	1:A:32:GLN:O	2.21	0.41
7:G:296:SER:CB	7:G:298:THR:CB	2.98	0.41
1:A:605:ILE:O	1:A:612:ARG:CB	2.68	0.41
10:J:897:LYS:C	10:J:911:ALA:CB	2.93	0.41
1:A:831:ALA:CA	1:A:832:PRO:CB	2.99	0.41
3:C:100:ILE:N	3:C:114:GLN:O	2.50	0.41
5:E:655:ASP:C	5:E:657:ILE:H	2.29	0.41
6:F:218:VAL:C	6:F:220:ASN:H	2.29	0.41
9:I:759:ASN:CB	18:Q:549:UNK:CA	2.94	0.41
18:Q:778:UNK:C	18:Q:780:UNK:N	2.83	0.41
1:A:695:CYS:C	1:A:697:GLU:N	2.77	0.41
7:G:444:PHE:CB	7:G:453:ALA:HB1	2.51	0.41
1:A:1524:LEU:C	1:A:1527:SER:H	2.28	0.41
2:B:32:LEU:C	2:B:58:ARG:CB	2.94	0.41
5:E:454:GLN:N	6:F:205:GLU:CB	2.68	0.41
7:G:145:SER:HA	7:G:146:PRO:HA	1.61	0.41
7:G:617:GLN:O	7:G:620:ASP:CA	2.69	0.41
7:G:767:ALA:HB3	7:G:854:SER:O	2.13	0.41
9:I:201:LEU:O	9:I:202:TRP:C	2.63	0.41
9:I:652:ASP:C	9:I:654:GLY:N	2.79	0.41
18:R:446:UNK:O	18:R:448:UNK:N	2.53	0.41
7:g:444:PHE:CB	7:g:453:ALA:HB1	2.51	0.41
10:J:898:LEU:CB	10:J:908:GLN:CA	2.99	0.40
11:V:30:PHE:O	11:V:33:ALA:HB3	2.21	0.40
9:i:652:ASP:C	9:i:654:GLY:N	2.79	0.40
7:G:346:ASN:O	7:G:348:GLY:CA	2.64	0.40
11:S:30:PHE:O	11:S:33:ALA:HB3	2.21	0.40
11:V:91:PRO:O	11:V:92:THR:CB	2.70	0.40
2:b:59:SER:O	2:b:62:ASP:N	2.54	0.40
7:g:386:LEU:CB	7:g:608:TYR:CB	2.99	0.40
2:B:29:PRO:CB	4:D:24:GLY:HA3	2.47	0.40
10:j:920:SER:C	10:j:924:GLU:CB	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:LEU:C	2:B:430:ARG:N	2.77	0.40
1:a:886:ARG:O	1:a:887:SER:CB	2.70	0.40
3:c:93:SER:O	3:c:97:THR:N	2.54	0.40
1:A:387:ARG:C	1:A:455:GLU:CB	2.94	0.40
7:G:279:ASN:O	7:G:281:ASP:N	2.54	0.40
10:J:903:ALA:HB2	10:J:908:GLN:CA	2.40	0.40
2:b:367:SER:HA	2:b:368:ASN:C	2.47	0.40
5:e:655:ASP:C	5:e:657:ILE:H	2.29	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	1343/2011 (67%)	1264 (94%)	50 (4%)	29 (2%)	5	28
1	a	1210/2011 (60%)	1131 (94%)	53 (4%)	26 (2%)	5	29
2	B	500/653 (77%)	471 (94%)	18 (4%)	11 (2%)	5	28
2	b	481/653 (74%)	454 (94%)	15 (3%)	12 (2%)	4	25
3	C	277/375 (74%)	211 (76%)	65 (24%)	1 (0%)	30	67
3	c	276/375 (74%)	212 (77%)	63 (23%)	1 (0%)	30	67
4	D	301/322 (94%)	275 (91%)	20 (7%)	6 (2%)	6	30
4	d	285/322 (88%)	261 (92%)	20 (7%)	4 (1%)	9	39
5	E	998/1435 (70%)	900 (90%)	71 (7%)	27 (3%)	4	25
5	e	1087/1435 (76%)	967 (89%)	87 (8%)	33 (3%)	3	22
6	F	269/326 (82%)	244 (91%)	17 (6%)	8 (3%)	3	22
6	f	271/326 (83%)	245 (90%)	18 (7%)	8 (3%)	3	22
7	G	582/923 (63%)	473 (81%)	56 (10%)	53 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	559/923 (61%)	475 (85%)	39 (7%)	45 (8%)	1	9
8	H	287/320 (90%)	257 (90%)	24 (8%)	6 (2%)	5	29
8	h	283/320 (88%)	255 (90%)	24 (8%)	4 (1%)	9	39
9	I	726/916 (79%)	692 (95%)	28 (4%)	6 (1%)	16	54
9	i	715/916 (78%)	681 (95%)	27 (4%)	7 (1%)	12	48
10	J	1014/1140 (89%)	925 (91%)	69 (7%)	20 (2%)	6	30
10	j	1015/1140 (89%)	930 (92%)	67 (7%)	18 (2%)	6	33
11	S	153/2905 (5%)	146 (95%)	2 (1%)	5 (3%)	3	20
11	T	153/2905 (5%)	146 (95%)	2 (1%)	5 (3%)	3	20
11	U	161/2905 (6%)	148 (92%)	9 (6%)	4 (2%)	4	25
11	V	153/2905 (5%)	146 (95%)	2 (1%)	5 (3%)	3	20
All	All	13099/28462 (46%)	11909 (91%)	846 (6%)	344 (3%)	6	25

All (344) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	228	LEU
1	A	239	THR
1	A	586	ILE
1	A	696	GLU
1	A	698	TYR
1	A	726	ALA
1	A	727	PRO
1	A	831	ALA
1	A	832	PRO
1	A	909	LEU
1	A	1048	VAL
1	A	1247	ILE
1	A	1646	GLN
1	A	1713	GLN
2	B	383	GLN
2	B	569	CYS
2	B	589	ILE
3	C	139	PRO
4	D	94	ASN
4	D	164	SER
5	E	451	SER

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Mol	Chain	Res	Type
5	E	896	PRO
5	E	953	PRO
6	F	43	TYR
6	F	119	VAL
6	F	308	LEU
7	G	198	PRO
7	G	288	LEU
7	G	293	SER
7	G	294	ALA
7	G	295	LYS
7	G	309	LEU
7	G	322	LEU
7	G	347	ALA
7	G	422	GLU
7	G	423	GLU
7	G	426	GLU
7	G	438	VAL
7	G	473	VAL
7	G	616	CYS
7	G	667	ASN
7	G	682	PRO
7	G	686	ILE
7	G	708	LEU
8	H	14	ASP
9	I	188	THR
9	I	224	SER
9	I	323	LYS
10	J	252	THR
10	J	538	GLU
10	J	561	SER
10	J	567	GLU
10	J	574	ALA
10	J	609	ARG
10	J	666	PRO
10	J	851	CYS
10	J	1066	GLU
11	S	59	ASP
11	S	90	ASN
11	S	92	THR
11	S	179	GLN
11	T	59	ASP
11	T	90	ASN

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Mol	Chain	Res	Type
11	T	92	THR
11	T	179	GLN
11	U	23	ARG
11	U	92	THR
11	V	59	ASP
11	V	90	ASN
11	V	92	THR
11	V	179	GLN
1	a	239	THR
1	a	454	LEU
1	a	582	PRO
1	a	586	ILE
1	a	636	PRO
1	a	1244	MET
1	a	1247	ILE
1	a	1250	ARG
1	a	1296	PRO
1	a	1305	ARG
2	b	52	PRO
2	b	383	GLN
2	b	569	CYS
2	b	589	ILE
4	d	164	SER
5	e	451	SER
5	e	896	PRO
5	e	953	PRO
5	e	1141	VAL
6	f	43	TYR
6	f	119	VAL
6	f	308	LEU
7	g	282	THR
7	g	294	ALA
7	g	302	PHE
7	g	315	SER
7	g	321	TYR
7	g	323	MET
7	g	422	GLU
7	g	423	GLU
7	g	426	GLU
7	g	438	VAL
7	g	473	VAL
7	g	486	LEU

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Mol	Chain	Res	Type
7	g	487	VAL
7	g	627	ASP
7	g	667	ASN
7	g	682	PRO
7	g	684	PRO
7	g	708	LEU
9	i	188	THR
9	i	224	SER
9	i	323	LYS
10	j	252	THR
10	j	538	GLU
10	j	561	SER
10	j	567	GLU
10	j	574	ALA
10	j	609	ARG
10	j	666	PRO
10	j	1066	GLU
1	A	1274	LEU
2	B	93	SER
2	B	319	PRO
4	D	176	ARG
5	E	83	ALA
5	E	266	LEU
5	E	331	SER
6	F	19	VAL
6	F	89	LEU
6	F	218	VAL
7	G	433	GLY
7	G	434	PRO
7	G	439	GLU
7	G	479	ARG
7	G	481	LEU
7	G	483	SER
7	G	560	PHE
7	G	615	LEU
8	H	11	SER
8	H	105	SER
8	H	223	ILE
10	J	575	GLY
1	a	159	THR
1	a	535	GLY
1	a	635	ILE

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Mol	Chain	Res	Type
2	b	93	SER
2	b	319	PRO
4	d	176	ARG
4	d	220	ASP
5	e	83	ALA
5	e	186	ILE
5	e	266	LEU
5	e	331	SER
5	e	1142	SER
6	f	19	VAL
6	f	89	LEU
6	f	218	VAL
7	g	328	GLU
7	g	371	ALA
7	g	433	GLY
7	g	434	PRO
7	g	439	GLU
7	g	479	ARG
7	g	481	LEU
7	g	483	SER
7	g	560	PHE
8	h	105	SER
8	h	223	ILE
10	j	575	GLY
1	A	58	PRO
1	A	303	ASP
1	A	751	ARG
1	A	995	LYS
1	A	1712	ARG
2	B	97	GLN
5	E	122	ASN
5	E	232	PRO
5	E	329	PRO
5	E	442	PRO
5	E	483	ARG
5	E	486	SER
5	E	566	GLY
5	E	1171	GLU
7	G	289	PRO
7	G	291	PRO
7	G	311	LEU
7	G	346	ASN

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Mol	Chain	Res	Type
7	G	364	ASN
7	G	371	ALA
7	G	435	GLU
7	G	436	ARG
7	G	542	MET
7	G	651	GLU
8	H	199	GLY
9	I	460	ILE
10	J	560	ALA
10	J	571	GLU
10	J	742	ILE
10	J	751	THR
10	J	852	ASP
11	U	91	PRO
1	a	58	PRO
1	a	162	HIS
1	a	303	ASP
1	a	545	ALA
2	b	97	GLN
2	b	126	THR
5	e	122	ASN
5	e	232	PRO
5	e	329	PRO
5	e	442	PRO
5	e	483	ARG
5	e	486	SER
5	e	566	GLY
5	e	1069	ASP
5	e	1171	GLU
7	g	317	GLU
7	g	319	GLN
7	g	364	ASN
7	g	435	GLU
7	g	436	ARG
7	g	651	GLU
8	h	199	GLY
9	i	460	ILE
10	j	560	ALA
10	j	571	GLU
10	j	742	ILE
10	j	751	THR
1	A	44	LYS

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	717	PRO
1	A	830	TYR
1	A	1045	ALA
2	B	130	TYR
2	B	353	PHE
2	B	430	ARG
4	D	220	ASP
5	E	159	GLN
5	E	244	PRO
5	E	444	PRO
5	E	484	LYS
5	E	565	LYS
5	E	598	ASP
5	E	1069	ASP
5	E	1110	LEU
6	F	135	PRO
7	G	146	PRO
7	G	290	LYS
7	G	314	LYS
7	G	370	GLU
7	G	477	GLU
7	G	555	LEU
7	G	705	PRO
8	H	55	GLY
9	I	513	ALA
1	a	44	LYS
1	a	160	LEU
1	a	286	GLN
2	b	125	GLU
2	b	353	PHE
5	e	159	GLN
5	e	244	PRO
5	e	444	PRO
5	e	484	LYS
5	e	565	LYS
5	e	598	ASP
5	e	1110	LEU
5	e	1139	GLN
6	f	135	PRO
7	g	293	SER
7	g	301	PRO

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Mol	Chain	Res	Type
7	g	346	ASN
7	g	370	GLU
7	g	477	GLU
7	g	485	GLN
7	g	555	LEU
7	g	705	PRO
8	h	55	GLY
9	i	513	ALA
1	A	76	PRO
1	A	502	LEU
2	B	65	SER
2	B	127	ALA
4	D	199	ILE
5	E	124	VAL
5	E	272	PRO
5	E	784	ALA
5	E	865	LEU
7	G	341	PRO
7	G	612	GLN
7	G	613	TYR
7	G	617	GLN
10	J	570	PRO
1	a	76	PRO
1	a	547	GLY
2	b	65	SER
5	e	124	VAL
5	e	272	PRO
5	e	784	ALA
5	e	866	TRP
7	g	324	PRO
7	g	325	LEU
7	g	414	SER
10	j	301	ASP
10	j	570	PRO
4	D	81	ARG
6	F	25	ASN
7	G	279	ASN
7	G	280	MET
7	G	414	SER
7	G	557	GLU
10	J	301	ASP
10	J	536	ASP

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Mol	Chain	Res	Type
10	J	1103	LEU
4	d	81	ARG
5	e	197	ASP
6	f	25	ASN
7	g	557	GLU
10	j	536	ASP
10	j	1103	LEU
5	E	275	ILE
10	J	605	GLY
1	a	119	GLN
1	a	128	GLY
1	a	536	GLY
5	e	177	ILE
5	e	275	ILE
9	i	183	ILE
10	j	605	GLY
1	A	400	MET
1	a	400	MET
7	G	195	VAL
7	G	545	PRO
11	S	129	PRO
11	T	129	PRO
11	U	129	PRO
11	V	129	PRO
2	b	482	GLY
3	c	216	PRO
9	I	274	GLY
9	i	274	GLY

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	Q	21
18	R	18
13	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	235:UNK	C	245:UNK	N	21.64
1	Q	861:UNK	C	900:UNK	N	21.11
1	R	387:UNK	C	416:UNK	N	18.78
1	Q	1112:UNK	C	1113:UNK	N	18.48
1	R	198:UNK	C	210:UNK	N	17.94
1	Q	1076:UNK	C	1077:UNK	N	17.45
1	Q	693:UNK	C	698:UNK	N	17.08
1	R	290:UNK	C	299:UNK	N	16.87
1	R	177:UNK	C	183:UNK	N	16.41
1	Q	1056:UNK	C	1057:UNK	N	15.19
1	Q	1016:UNK	C	1017:UNK	N	14.44
1	Q	731:UNK	C	735:UNK	N	13.78
1	Q	592:UNK	C	599:UNK	N	13.32
1	L	307:UNK	C	312:UNK	N	13.26
1	Q	1029:UNK	C	1030:UNK	N	12.80
1	Q	916:UNK	C	1011:UNK	N	12.52
1	Q	1040:UNK	C	1041:UNK	N	12.26
1	Q	1093:UNK	C	1095:UNK	N	12.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	17:UNK	C	22:UNK	N	11.85
1	Q	714:UNK	C	716:UNK	N	9.51
1	Q	750:UNK	C	753:UNK	N	9.51
1	Q	566:UNK	C	571:UNK	N	9.34
1	Q	819:UNK	C	828:UNK	N	8.54
1	Q	772:UNK	C	776:UNK	N	7.99
1	R	46:UNK	C	56:UNK	N	7.67
1	Q	837:UNK	C	846:UNK	N	7.48
1	Q	615:UNK	C	640:UNK	N	6.57
1	R	61:UNK	C	69:UNK	N	5.86
1	R	143:UNK	C	151:UNK	N	4.88
1	R	217:UNK	C	219:UNK	N	4.68
1	R	282:UNK	C	284:UNK	N	4.67
1	R	449:UNK	C	451:UNK	N	4.52
1	R	428:UNK	C	430:UNK	N	4.18
1	R	354:UNK	C	356:UNK	N	4.11
1	R	343:UNK	C	345:UNK	N	3.88
1	R	367:UNK	C	369:UNK	N	3.59
1	Q	794:UNK	C	797:UNK	N	3.52
1	Q	659:UNK	C	661:UNK	N	3.49
1	R	317:UNK	C	319:UNK	N	3.37
1	R	451:UNK	C	452:UNK	N	3.13

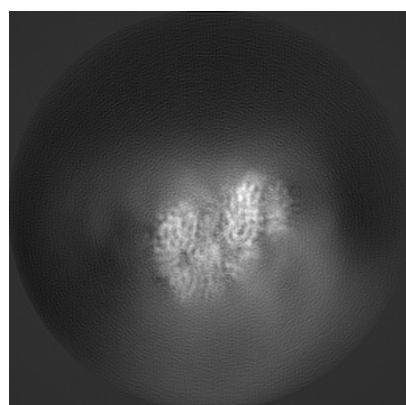
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0909. These allow visual inspection of the internal detail of the map and identification of artifacts.

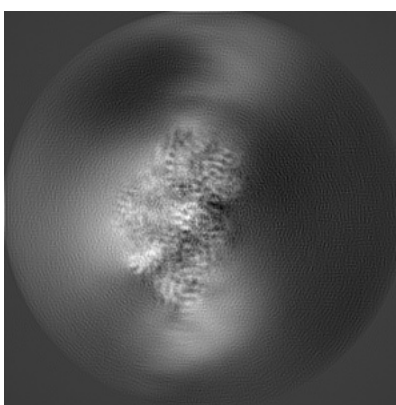
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

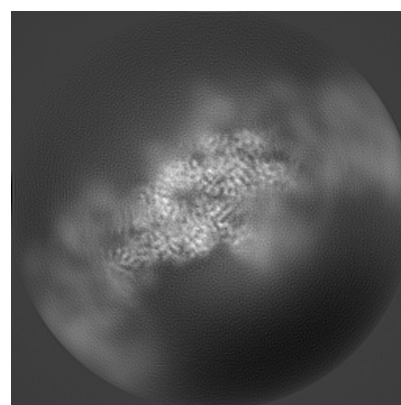
6.1.1 Primary map



X



Y

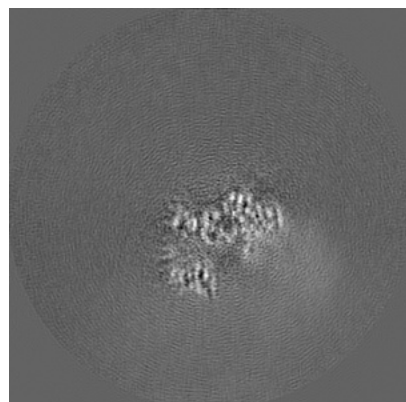


Z

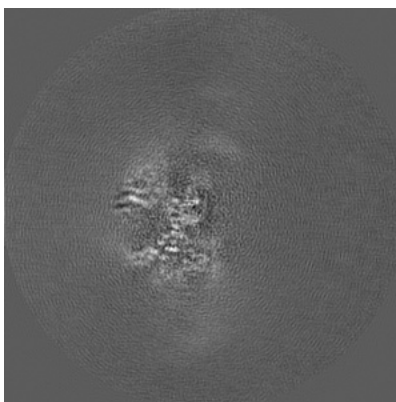
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

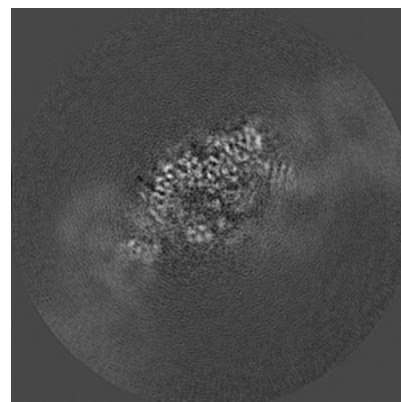
6.2.1 Primary map



X Index: 128



Y Index: 128

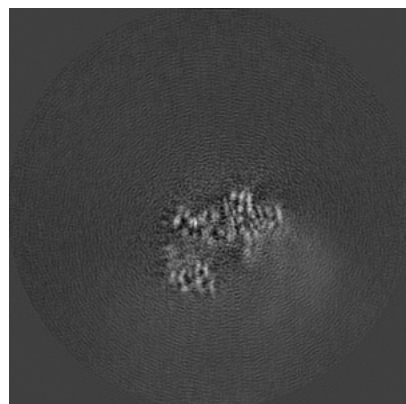


Z Index: 128

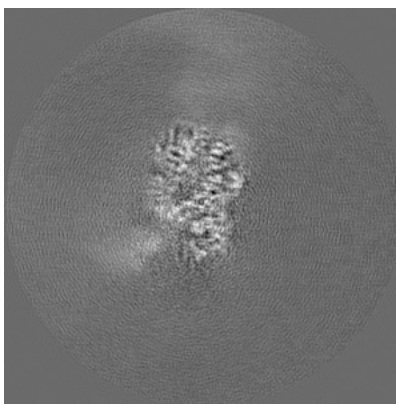
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

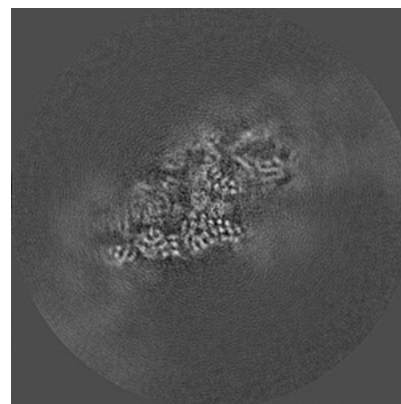
6.3.1 Primary map



X Index: 127



Y Index: 152

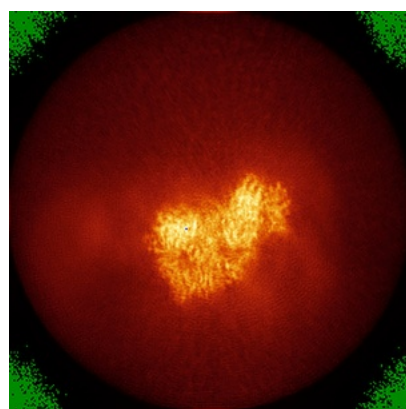


Z Index: 117

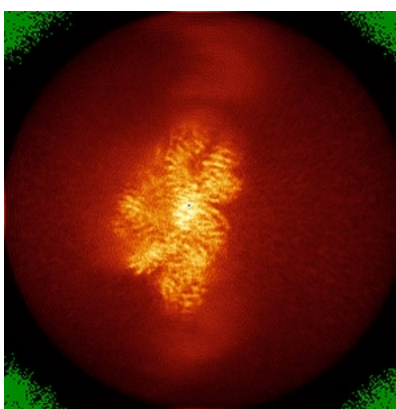
The images above show the largest variance slices of the map in three orthogonal directions.

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

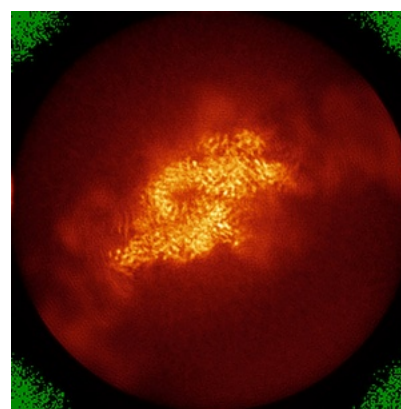
6.4.1 Primary map



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.

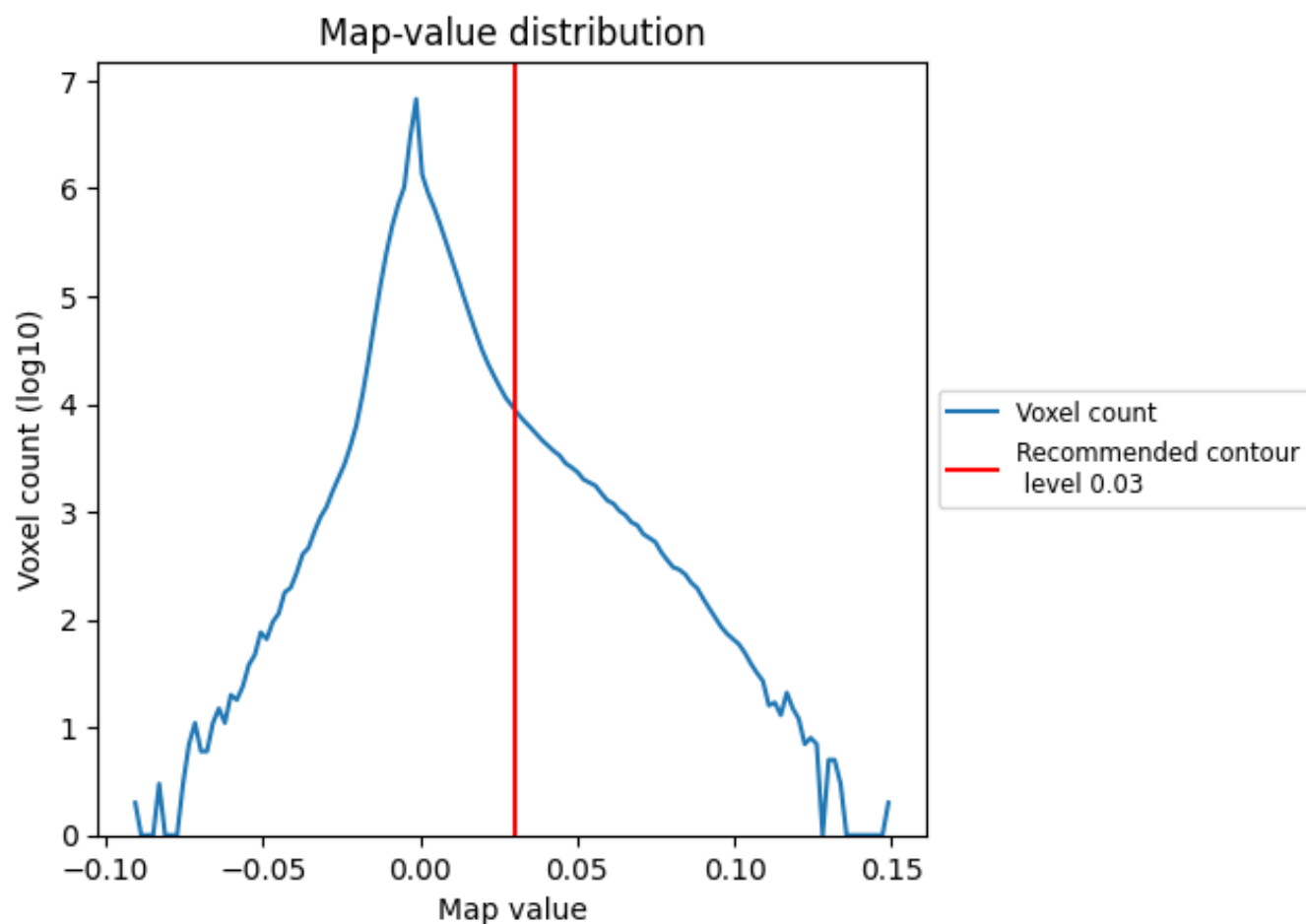
6.6 Mask visualisation

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

7 Map analysis [i](#)

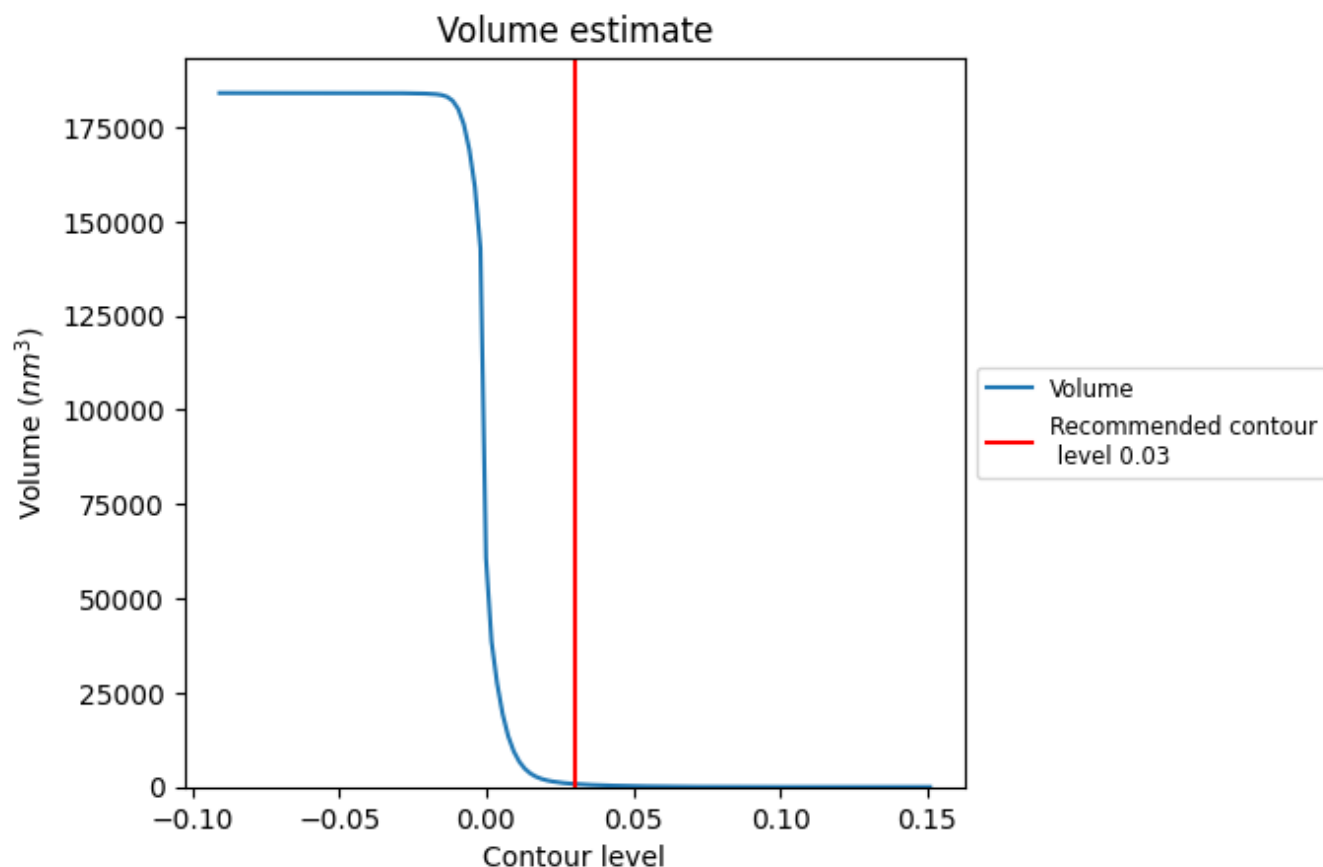
This section contains the results of statistical analysis of the map.

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.

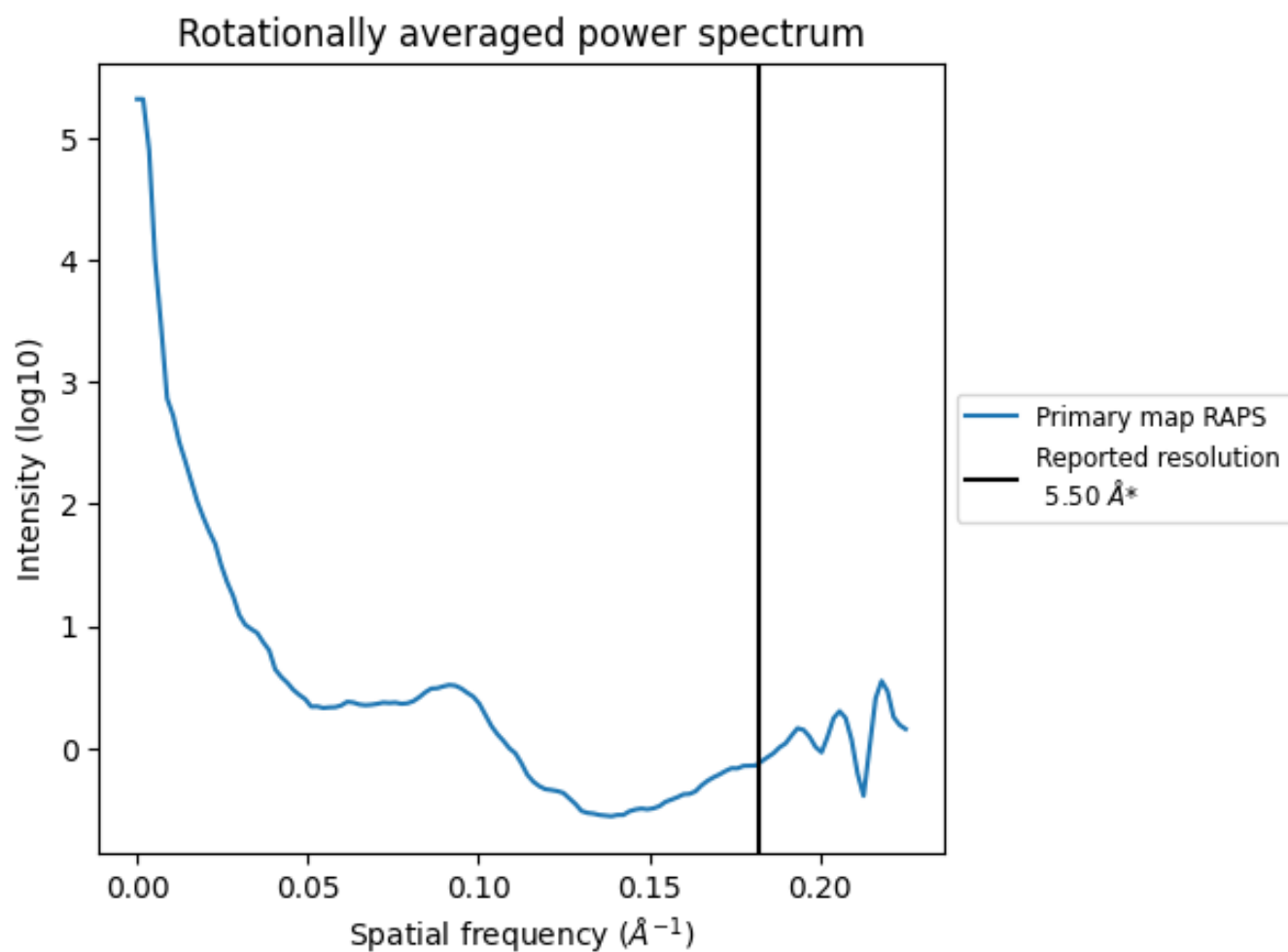
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 803 nm³; this corresponds to an approximate mass of 725 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 0.182 Å⁻¹

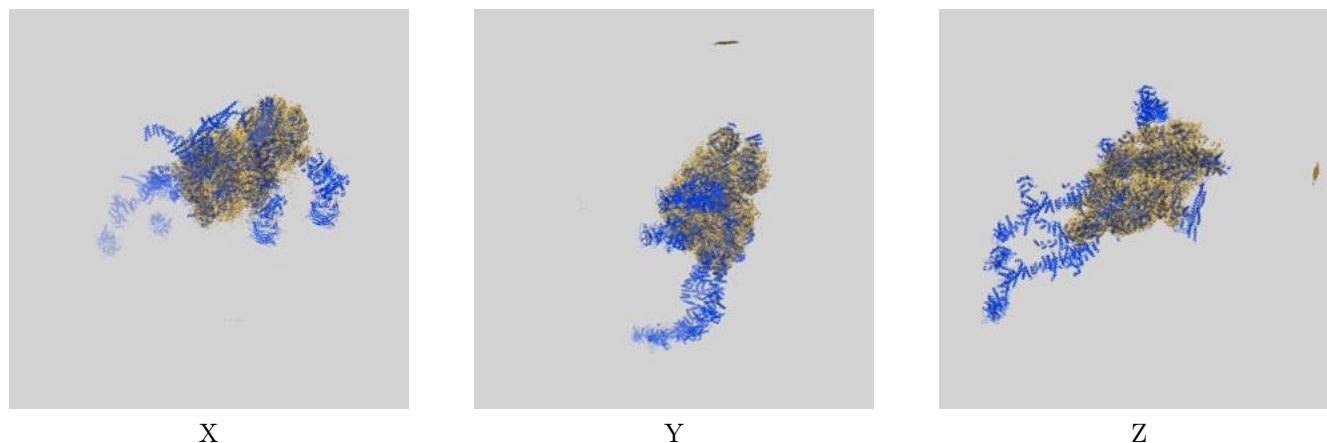
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

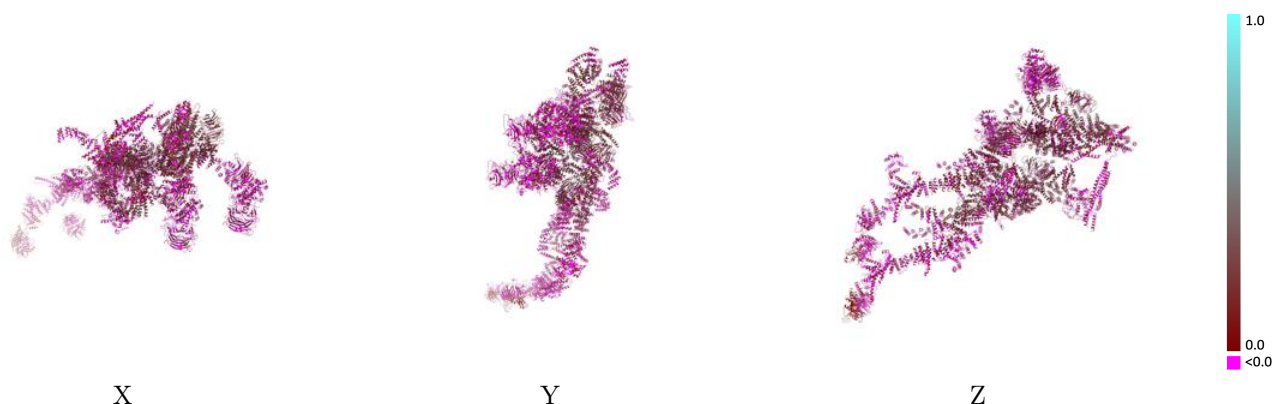
This section contains information regarding the fit between EMDB map EMD-0909 and PDB model 6LK8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



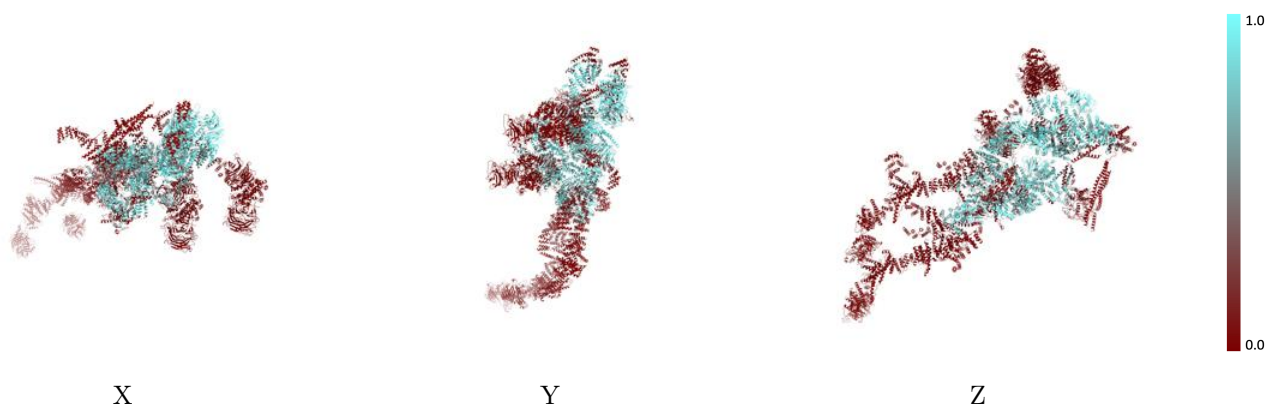
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



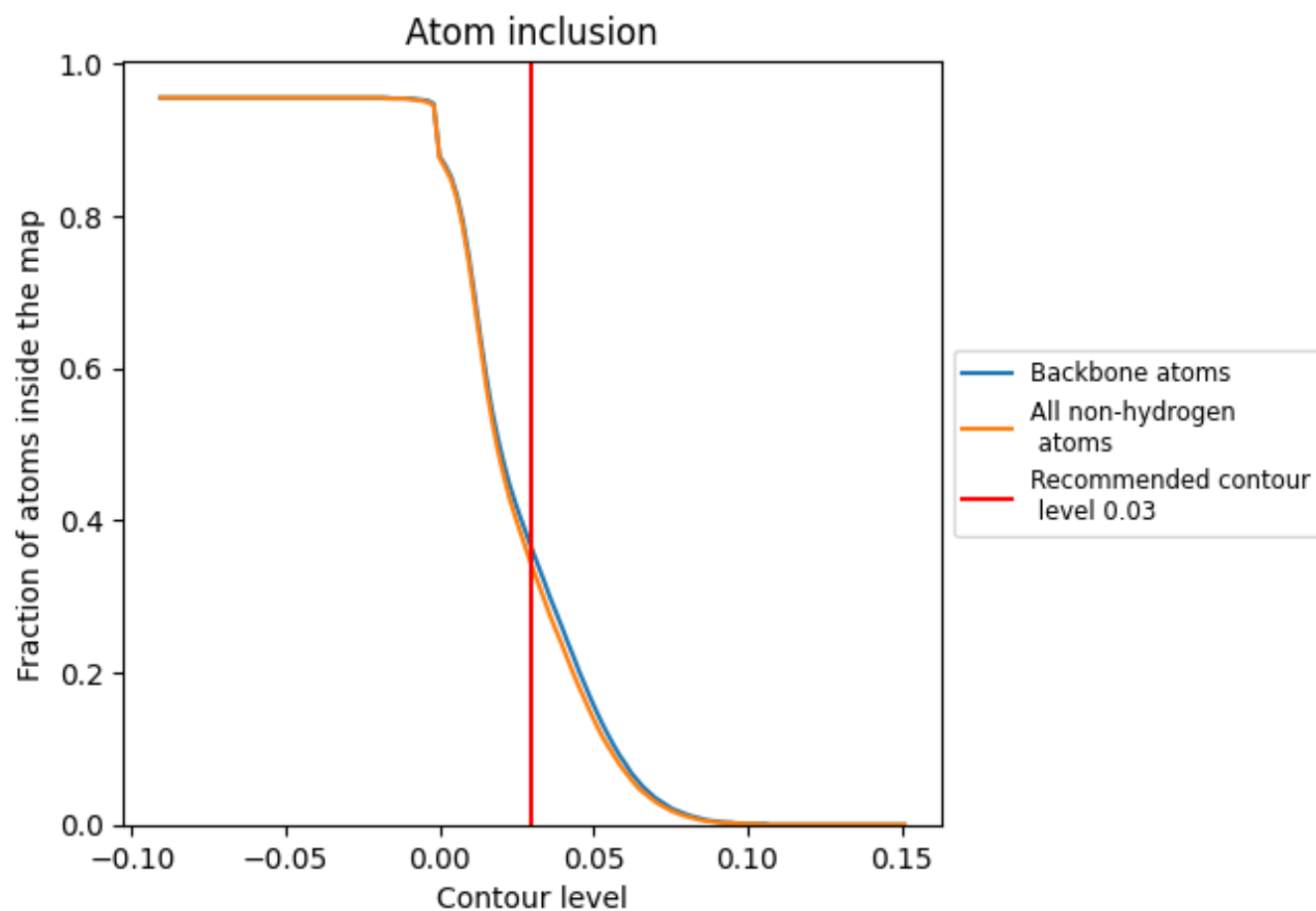
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 36% of all backbone atoms, 34% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3390	 0.0890
A	 0.6000	 0.1430
B	 0.6840	 0.1880
C	 0.8950	 0.2270
D	 0.7460	 0.1650
E	 0.0750	 0.0220
F	 0.0000	 0.0160
G	 0.6470	 0.1730
H	 0.7810	 0.1790
I	 0.1830	 0.0930
J	 0.0000	 0.0030
K	 0.0000	 0.0110
L	 0.0000	 0.0100
M	 0.0000	 0.0220
N	 0.4520	 0.1270
O	 0.0800	 0.0580
P	 0.0850	 0.0380
Q	 0.4120	 0.1510
R	 0.0550	 0.0080
S	 0.0670	 0.0560
T	 0.0500	 0.0150
U	 0.0000	 0.0300
V	 0.0000	 0.0190
a	 0.5030	 0.1030
b	 0.6740	 0.1800
c	 0.8780	 0.2470
d	 0.7290	 0.1740
e	 0.1730	 0.0260
f	 0.2990	 0.0300
g	 0.5760	 0.1550
h	 0.7090	 0.1850
i	 0.0000	 0.0190
j	 0.0000	 0.0120

