



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:11 AM UTC

PDB ID : 6R83 / pdb_00006r83
EMDB ID : EMD-4750
Title : CryoEM structure and molecular model of squid hemocyanin (Todarodes pacificus , TpH)
Authors : Tanaka, Y.; Kato, S.; Stabrin, M.; Raunser, S.; Matsui, T.; Gatsogiannis, C.
Deposited on : 2019-03-31
Resolution : 5.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

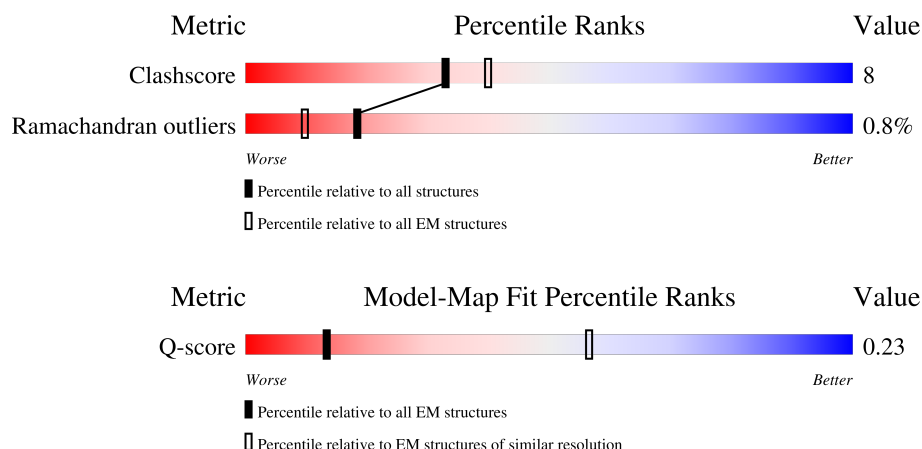
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.10 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.



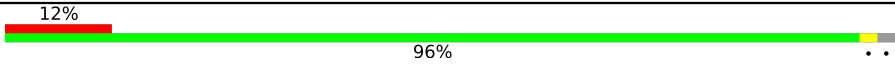
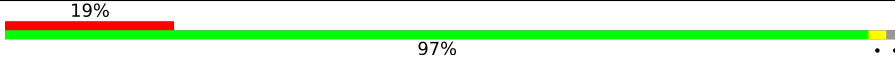
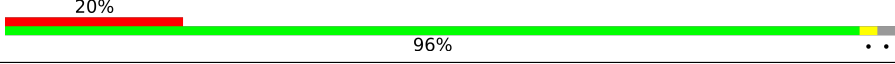
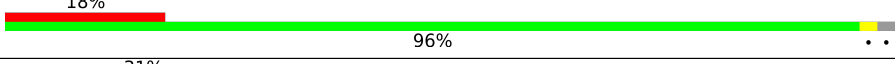
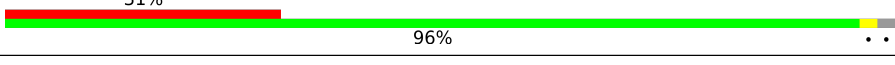
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	844 (4.60 - 5.60)

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	10a	3314	23% 96% ..
1	1a	3314	18% 96% ..
1	2a	3314	18% 96% ..
1	3a	3314	9% 96% ..
1	4a	3314	9% 96% ..

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Mol	Chain	Length	Quality of chain
1	5a	3314	
1	6a	3314	
1	7a	3314	
1	8a	3314	
1	9a	3314	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 161300 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.

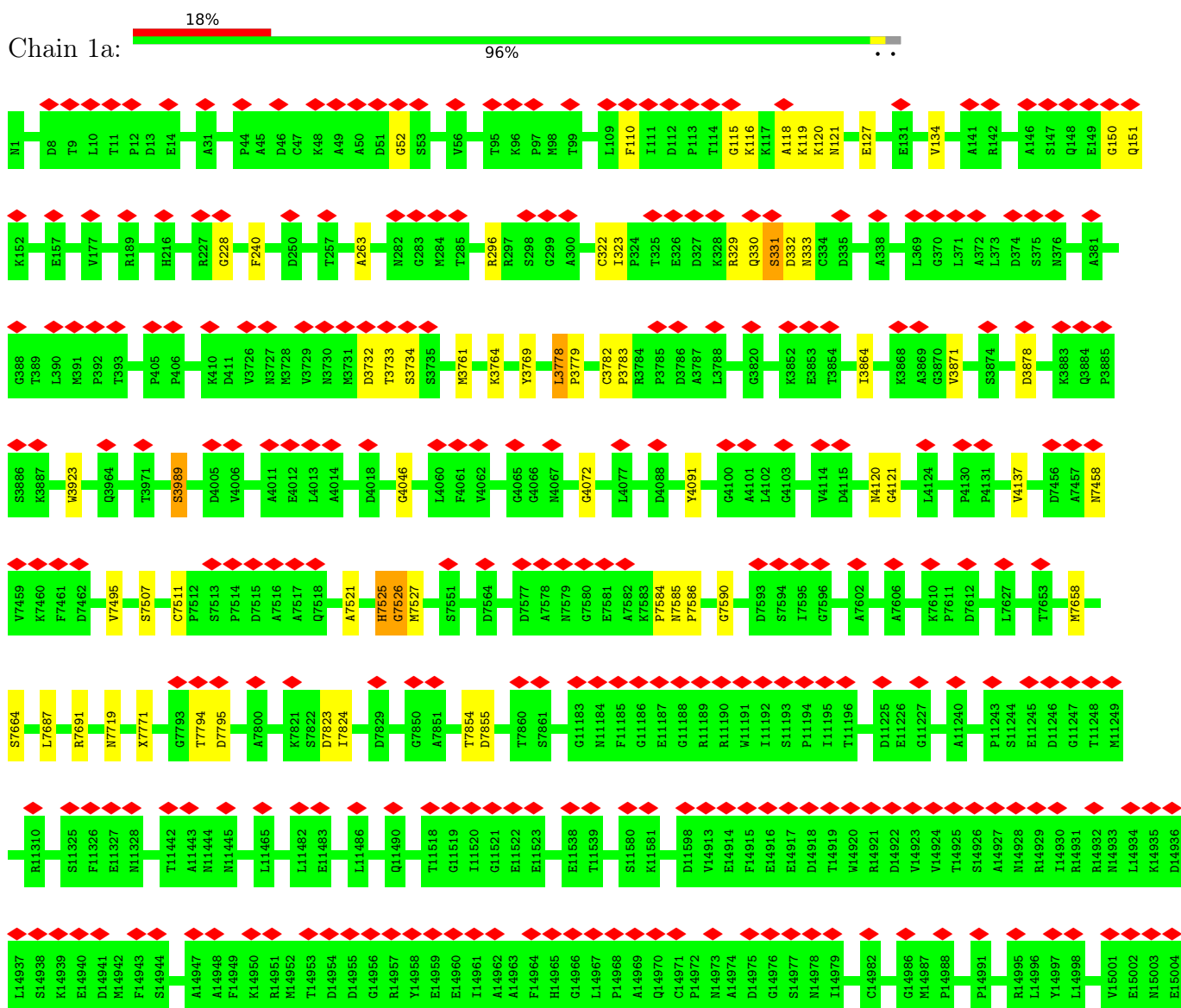
- Molecule 1 is a protein called Hemocyanin subunit 1.

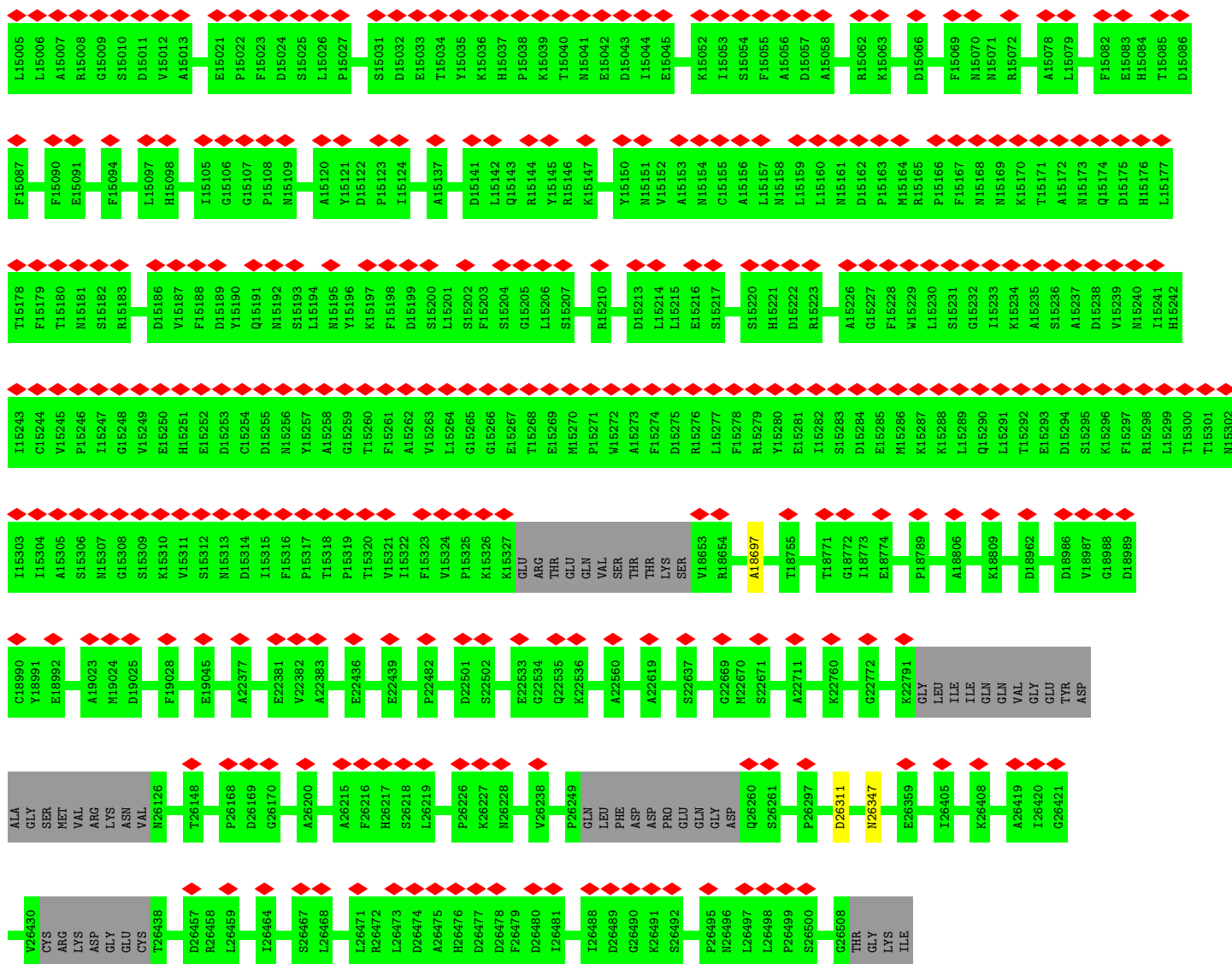
Mol	Chain	Residues	Atoms				AltConf	Trace
1	1a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	2a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	3a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	4a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	5a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	6a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	7a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	8a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	9a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	10a	3262	Total 16130	C 9606	N 3262	O 3262	0	0

3 Residue-property plots [i](#)

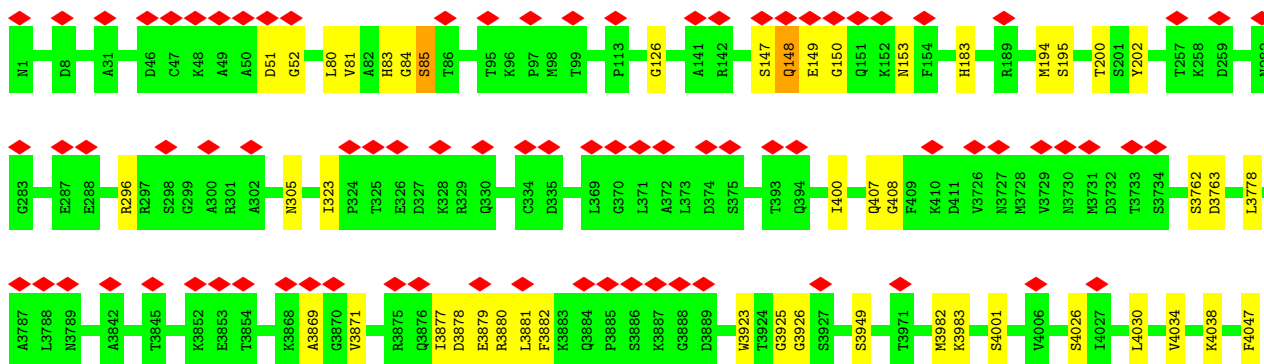
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Hemocyanin subunit 1

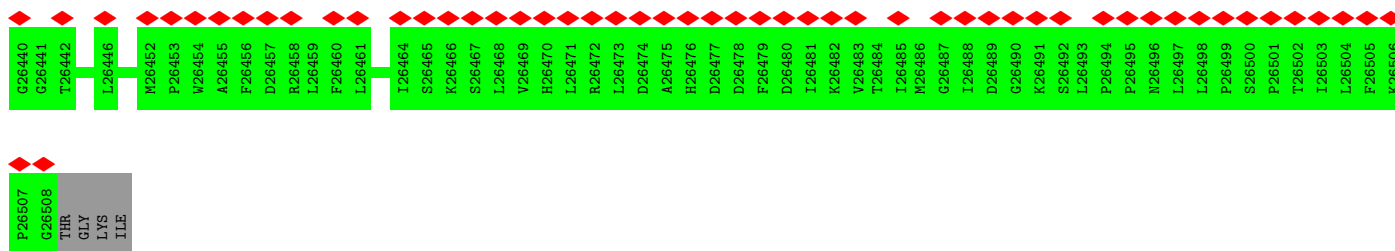




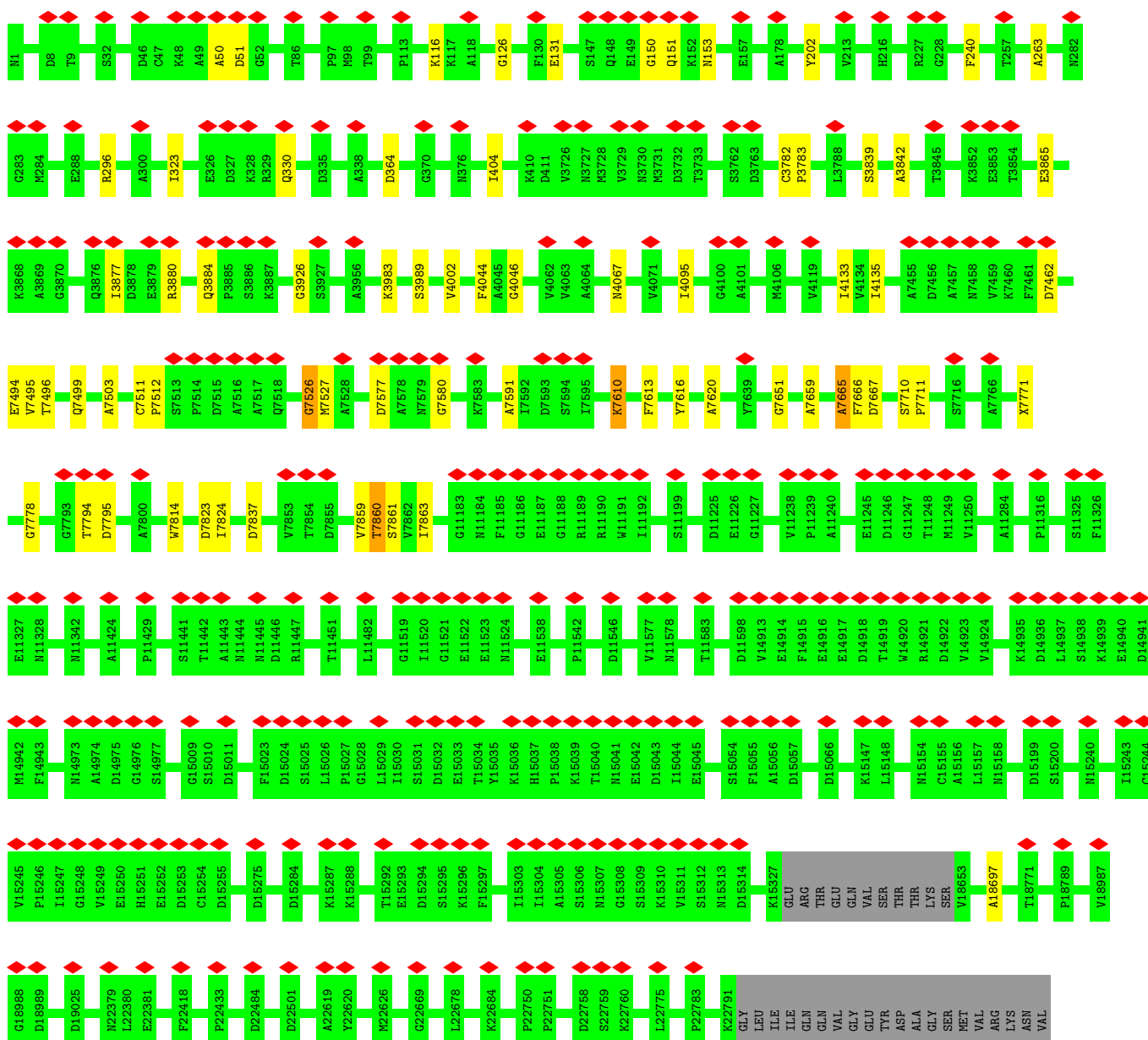
• Molecule 1: Hemocyanin subunit 1

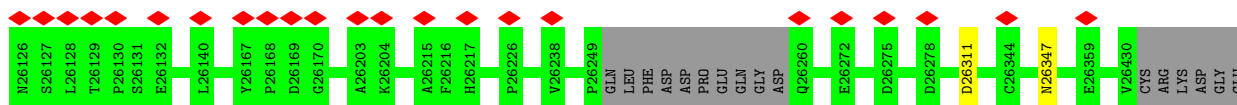


E26359	E26360	N26361	N26362	N26363	N26364	K26367	A26368	Q26369	Q26370	F26373	Y26374	R26375	Q26376	I26377	A26379	L26380	L26381	E26382	F26383	E26384	P26387	D26388	P26389	F26390	H26391	G26392	M26393	T26394	L26395	P26396	Q26397	L26398	E26399	V26400	H26401	L26402	F26403	K26404	L26405	Q26406	E26407	K26408	D26409	R26410	V26411	F26412	A26413	F26414	F26415	L26416	A26419	L26420	V26426	N26427	F26428	N26429	V26430	CYS	ARG	LYS	ASP	GLY	GLU	CYS	F26438	F26439
LEU	ILE	ILE	GLN	GLN	VAL	GLY	GLU	TYR	ASP	ALA	GLY	SER	MET	VAL	ARG	LYS	ASN	VAL	N26126	S26127	L26128	T26129	E26132	T26148	D26149	Q26166	Y26167	D26168	D26169	G26170	K26199	A26200	K26201	K26204	T26214	A26215	F26216	H26217	S26218	L26219	P26220	V26223	T26224	E26225	E26226	P26227	K26227	N26228	D26237	V26238	P26249															
GLN	LEU	PHE	ASP	ASP	PRO	GLU	GLN	GLY	ASP	Q26260	F26263	Y26264	R26265	Q26266	I26267	A26270	L26271	E26272	Q26273	R26274	D26275	F26276	C26277	E26280	I26281	Q26282	F26283	E26284	P26297	D26311	A26326	Q26329	A26330	K26333	Y26334	R26335	Q26336	L26337	Y26339	N26340	S26341	E26342	N26343	N26347	K26350	K26351	P26352	T26438	F26439																	
P15319	T15320	V15321	K15327	GLU	ARG	THR	GLU	VAL	SER	THR	THR	LYS	SER	V18653	R18654	A18697	K18708	I18742	T18755	T18771	G18772	I18773	E18774	P18789	E18790	R18795	E18796	V18797	A18806	A18895	E18958	D18986	V18987	G18988	D18989	C18990	Y18991	E18992	S19002	A19023	M19024	F19028																								
K19035	T19036	K19037	G19043	T19044	E19045	A22377	E22381	V22382	A22383	S22395	L22396	E22397	E22415	E22533	G22534	Q22535	E22551	A22560	S22637	G22669	M22670	S22671	A22677	K22684	A22685	D22686	A22711	D22712	G22717	V22718	T22741	D22742	K22745	R22746	R22747	N22748	D22768	S22769	A22790	K22791	GLY																									
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A15156	L15157	N15158	L15159	L15160	M15161	D15162	F15167	N15168	M15169	K15170	T15171	A15172	M15173	Q15174	D15175	L15176	L15177	T15178	F15179	T15180	M15181	S15182	R15183	D15186	V15187	F15188	D15189	M15192	S15193	L15194	N15195	D15199	S15204	G15205	F15228	W15229	L15230	S15231	G15232	L15233	K15234	A15235	S15236	A15237	D15238	C15244	V15245	P15246	G15248	V15249	E15250															
V15001	E15002	M15003	E15004	L15005	L15006	A15007	R15008	G15009	S15010	D15011	V15012	A15013	V15014	D15024	D15032	E15033	V15034	L15035	K15036	H15037	P15038	K15039	T15040	M15041	E15042	D15043	I15044	E15045	N15046	G15051	K15052	I15053	S15054	F15055	A15056	D15057	A15058	V15059	T15060	V15061	R15062	K15063	D15066	P15108	M15109	H15110	H15111	S15112	Y15121	A15153	M15154	C15155														
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V4062	V4063	A4064	G4065	G4066	O4072	S4073	T4084	Y4091	L4099	G4100	A4101	L4102	G4103	T4111	O4121	T4122	A4123	P4126	T4127	V4137	T4140	A7455	D7456	A7457	N7458	V7459	F7461	S7477	A7487	A7491	T7508	Q7509	W7510	C7511	P7512	S7513	F7514	D7515	A7516	A7517	G7526	M7527																								

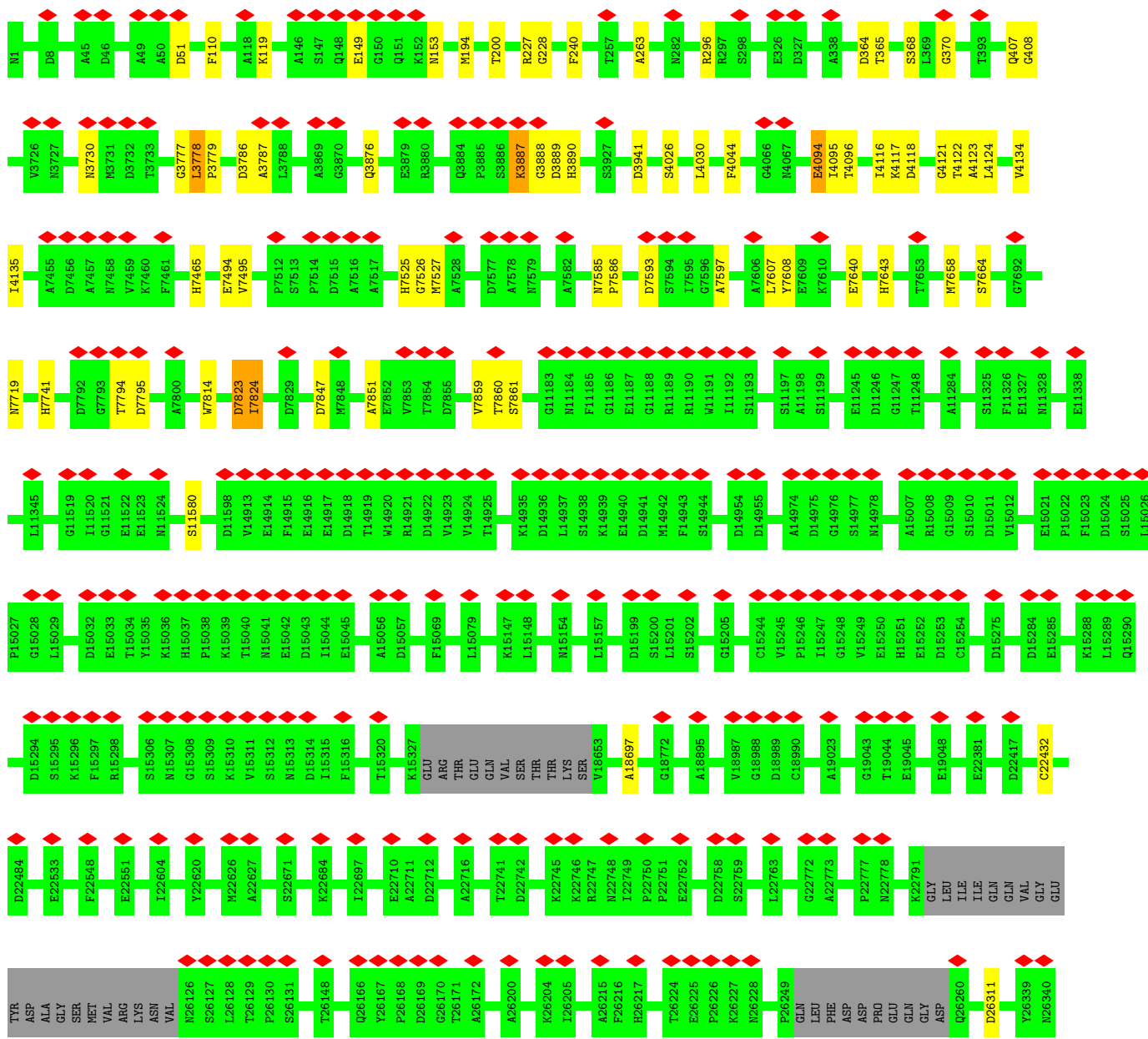


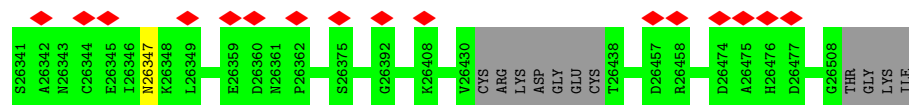
• Molecule 1: Hemocyanin subunit 1



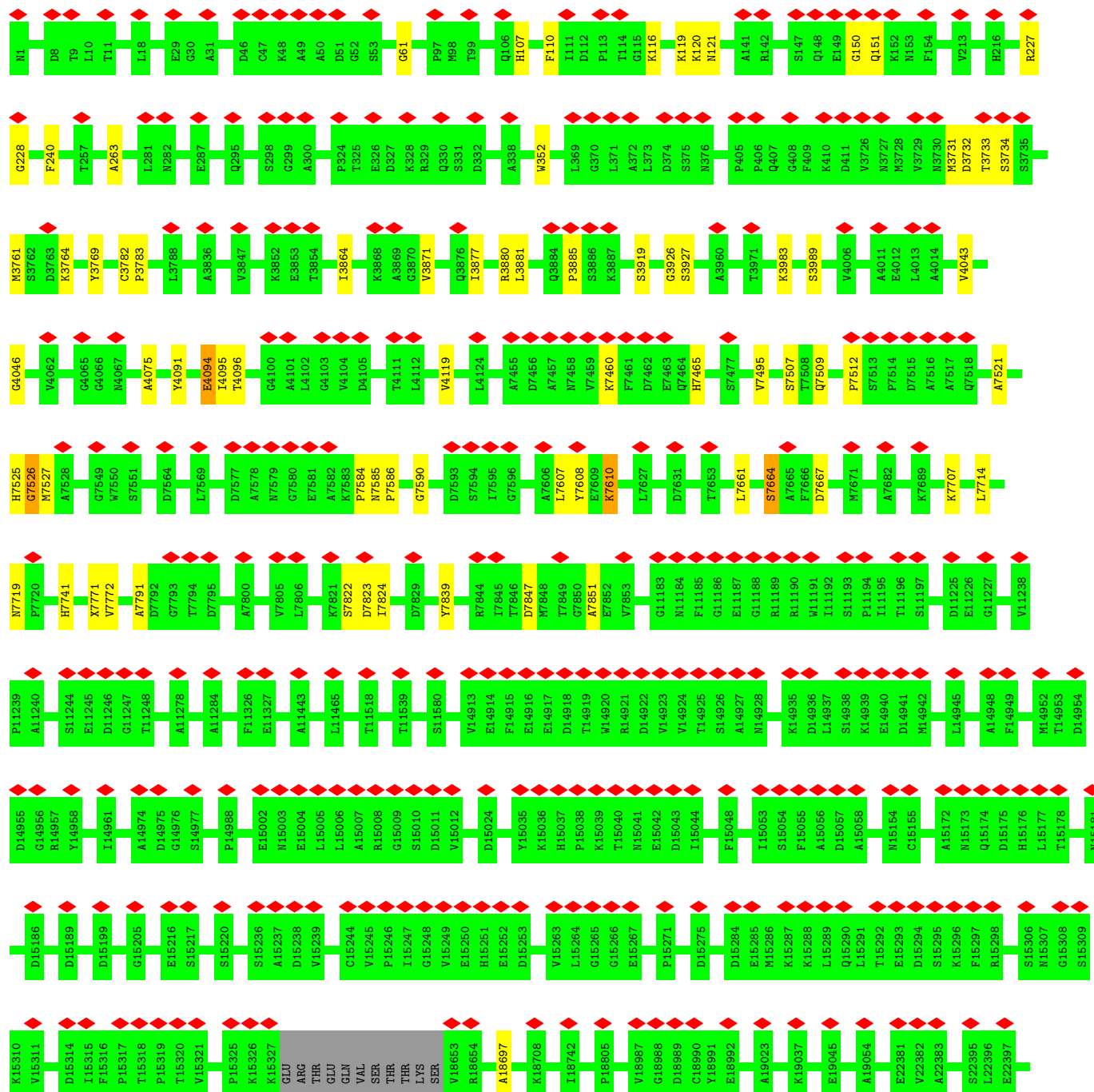


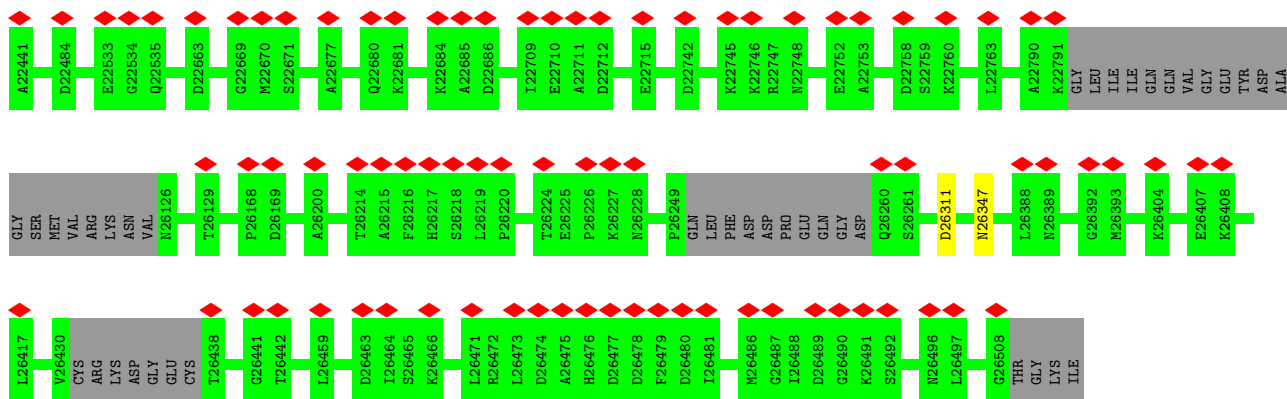
• Molecule 1: Hemocyanin subunit 1



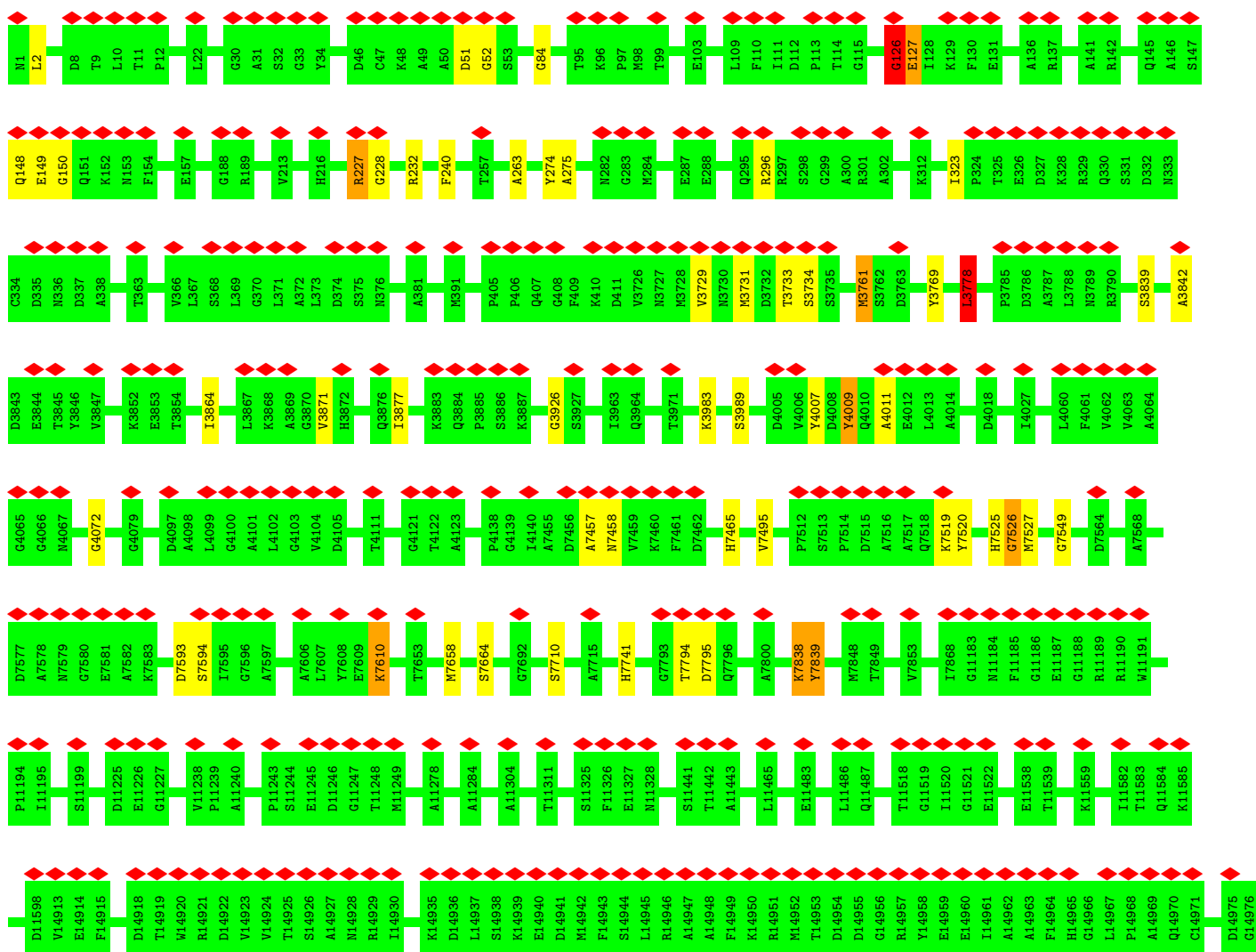


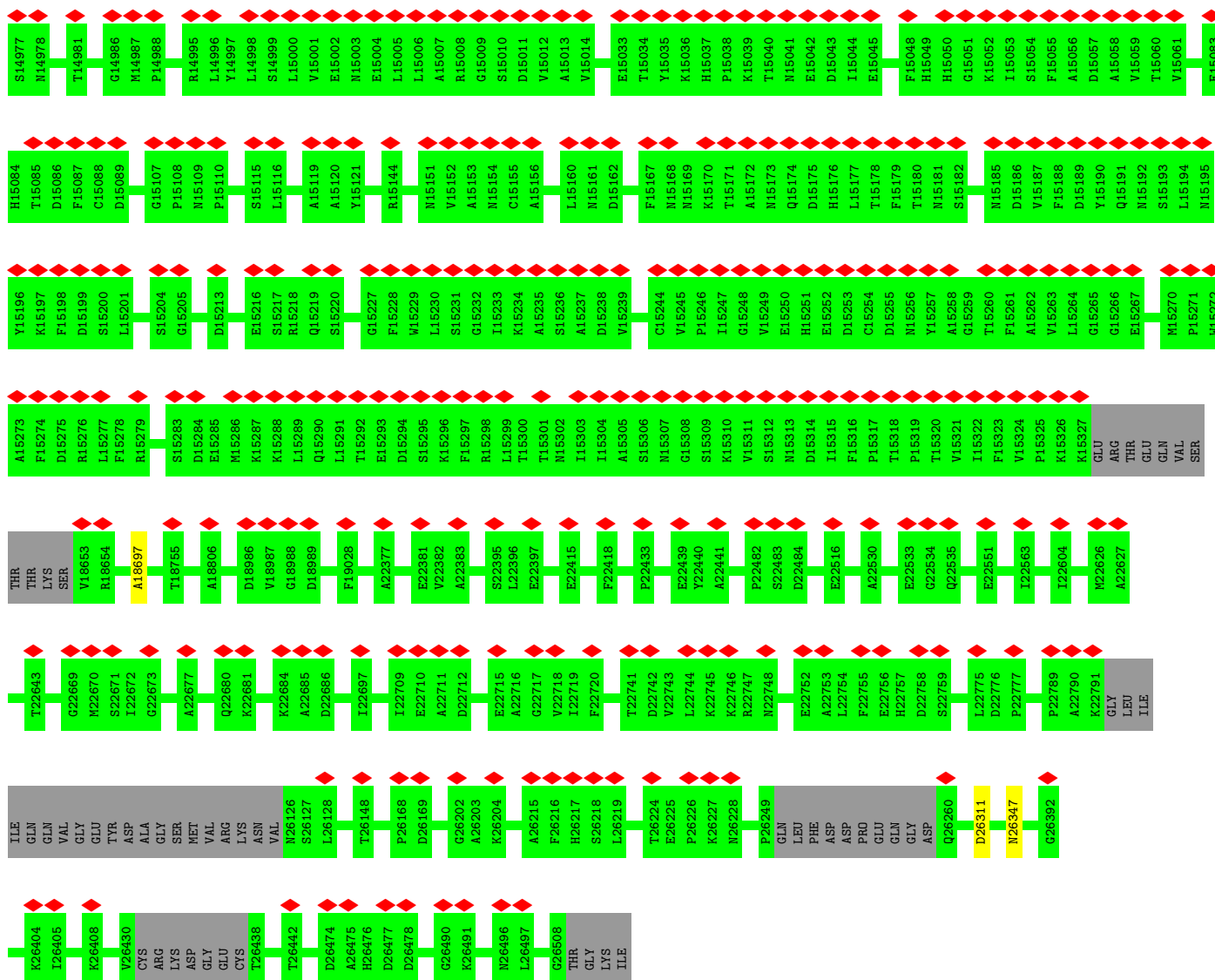
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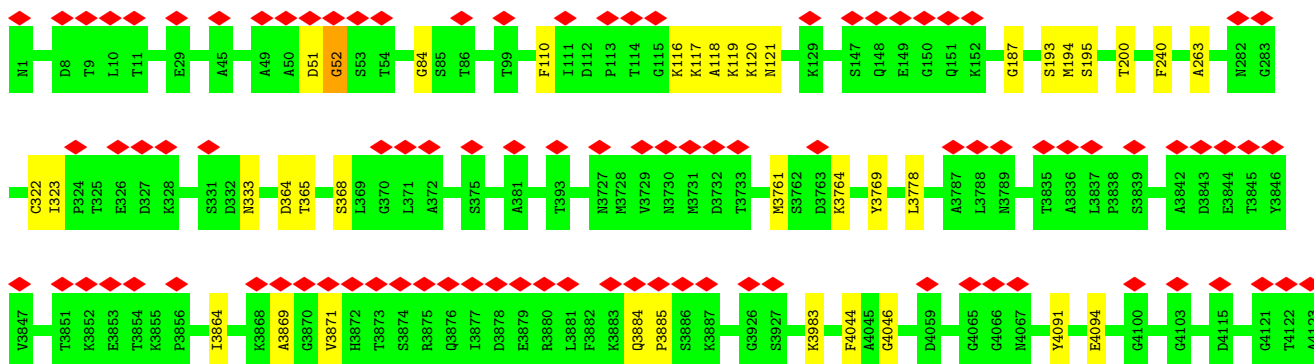


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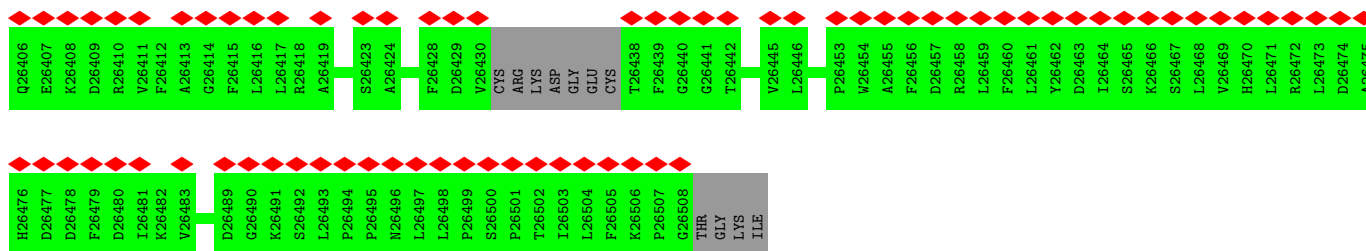




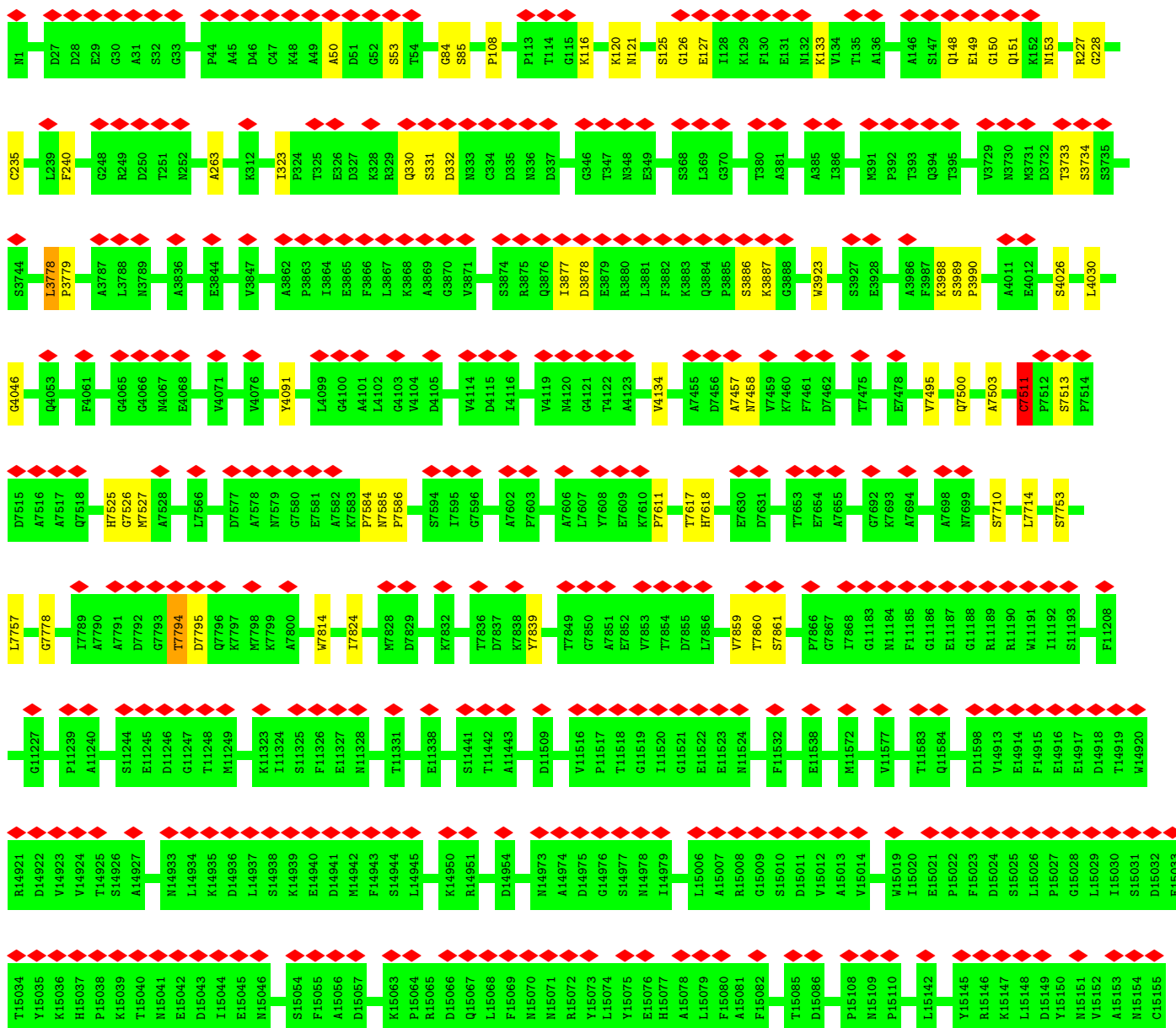
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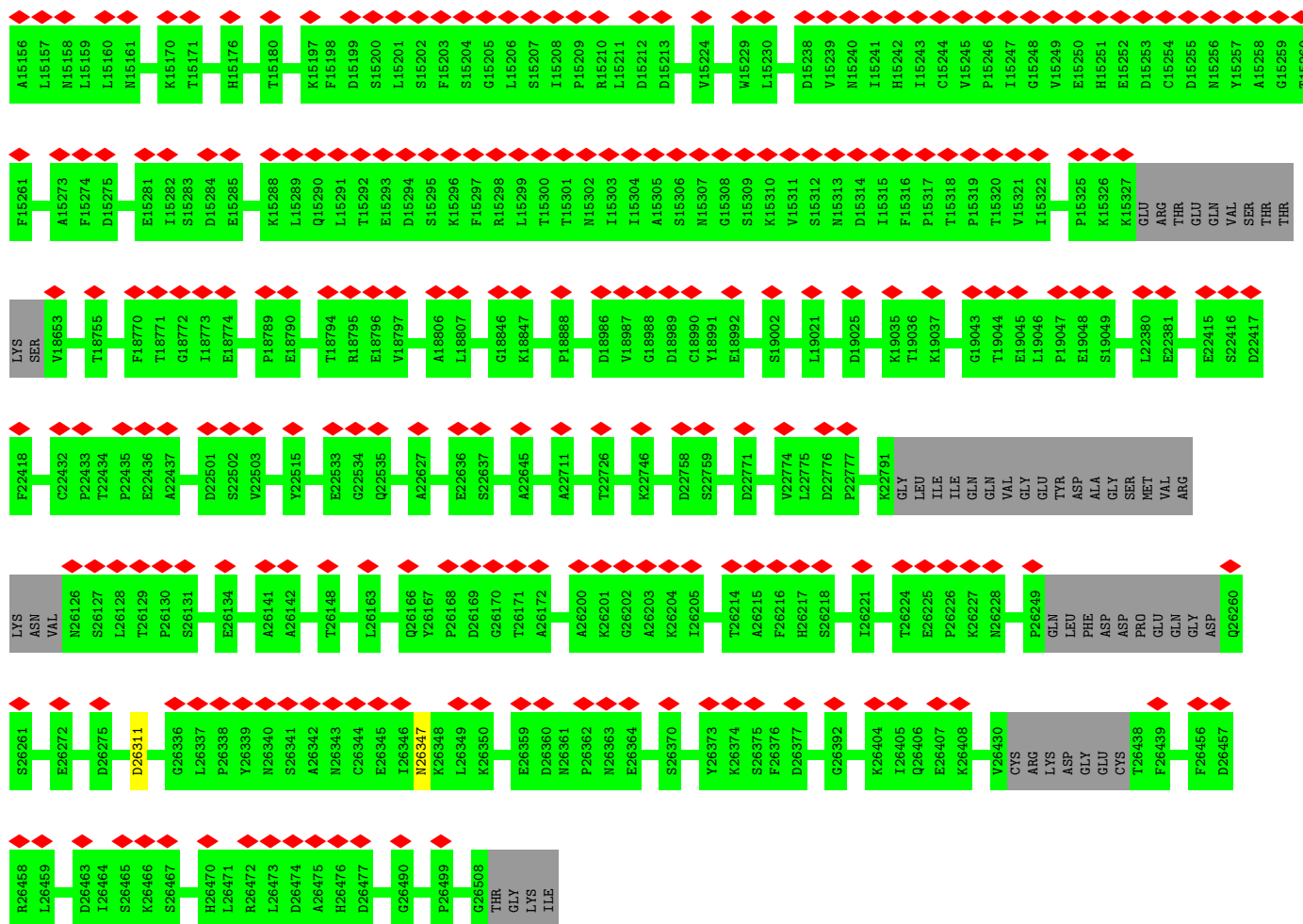




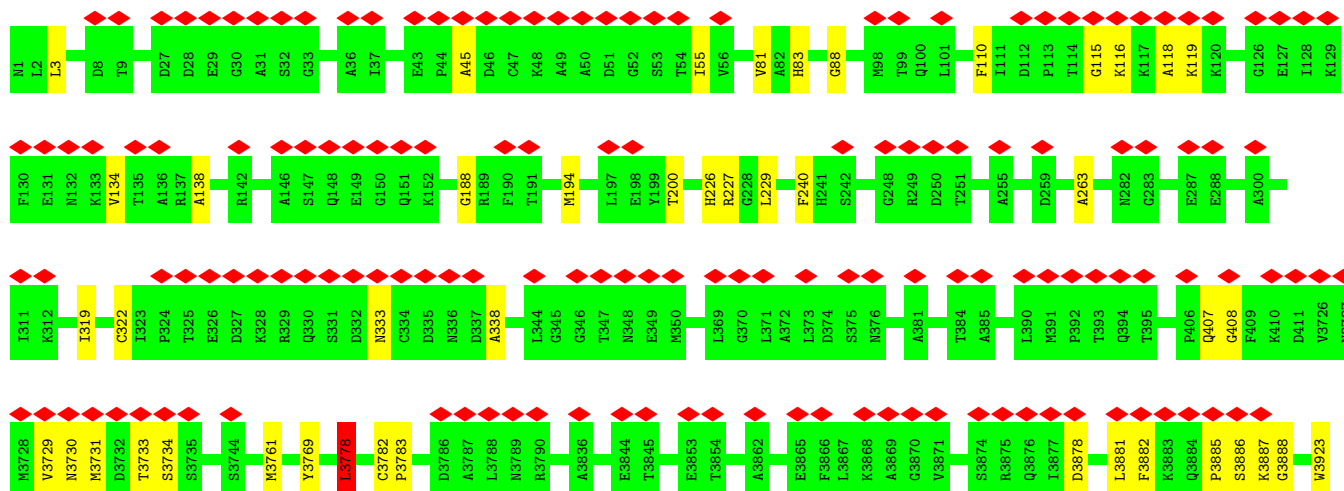


• Molecule 1: Hemocyanin subunit 1





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S15296	K15296	F15297	R15298	T15300	T15301	M15302	I15303	I15304	A15305	S15306	M15307	G15308	S15309	K15310	V15311	S15312	M15313	D15314	I15315	F15316	T15317	T15318	P15319	T15320	V15321	I15322	F15323	V15324	P15325	K15326	K15327	GLU	ARG	THR	GLU	GLN	VAL	THR	THR	LYS	SER	V18653	K18708	T18755	E18764	P18769	G18772	I18773	E18774	E18790									
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L7783	I7789	D7792	T7793	T7794	D7795	Q7796	A7800	G7801	F7805	L7806	W7814	D7823	I7824	T7825	D7829	T7836	V7841	I7845	M7848	E7852	V7853	T7854	D7855	L7856	T7860	S7861	G11183	N11184	F11185	G11186	E11187	G11188	R11189	W11190	W11191	D14922	V14923	T14924	T14925	S14926	A14927	N14928	R14929	I14930	R14931	R14932													
T4111	L4112	R4113	V4114	D4115	V4119	N4120	G4121	T4122	A4123	L4124	P4125	L4013	A4014	L4020	I4133	I4140	A7455	D7456	A7457	N7458	O7459	K7460	F7461	D7462	E7463	M7474	T7475	E7478	E7494	V7495	C7511	S7512	P7513	P7514	D7515	A7516	A7517	Q7518	K7519	G7526	M7527	A7528	R7547	S7551	T7560	D7564													
S3927	L4112	T3971	K3983	S3989	P3990	L3991	Y4009	Q4010	A4011	E4012	L4013	A4014	L4020	I4027	C4046	L4049	D4059	L4060	F4061	V4062	V4063	A4064	C4065	G4066	H4067	E4068	F4069	F4070	V4071	G4072	S4073	V4076	L4077	Y4091	E4094	D4097	L4099	G4100	A4101	L4102	G4103	V4104	D4105	M4106															

W26212	T26213	T26214	A26215	H26216	H26217	S26218	L26219	P26220	T26221	L26222	V26223	P26226	K26227	R26245	D26246	P26247	R26248	P26249	GLN	LEU	PHE	ASP	ASP	PRO	GLU	GLN	GLY	ASP	Q26260	S26261	F26262	F26263	F26264	R26265	Q26266	I26267	A26268	F26269	L26270	E26272	Q26273	R26274	D26275	F26276	C26277	D26278	F26279	Q26282	F26283	E26284	M26285	G26286	H26287	P26297		
IIE	IIE	GLN	VAL	GLY	GLU	TYR	ASP	ALA	GLY	SER	MET	VAL	ARG	LYS	ASN	VAL	R26126	S26127	L26128	T26129	E26132	T26133	L26136	L26140	T26148	D26149	A26150	Q26166	Y26167	F26168	D26169	G26170	R26180	V26181	T26182	H26185	D26196	K26199	A26200	K26201	G26202	A26203	K26204	T26205	G26206	Y26209	W26210	D26211								
V22646	D22663	H22668	G22669	W22670	S22671	L22672	G22673	A22677	L22678	K22684	A22685	D22686	I22687	A22711	D22712	E22715	A22716	G22717	V22718	D22739	I22740	T22741	D22742	K22745	K22746	R22747	N22748	I22749	P22750	E22756	H22757	D22758	S22759	K22760	L22763	G22772	A22773	P22777	P22783	P22789	A22790	K22791	GLY	LEU												
T15301	N15302	I15303	I15304	A15305	N15306	N15307	G15308	S15309	K15310	V15311	S15312	N15313	D15314	I15315	F15316	P15317	T15318	P15319	T15320	V15321	I15322	F15323	V15324	P15325	K15326	K15327	GLU	ARG	THR	GLU	GLN	VAL	SER	THR	LYS	SER	V18653	A18697	H18709	T18755	P18769	F18770	T18771	G18772	I18773	E18774	P18789	E18790	R18795	E18796	E18803					
A15235	S15236	A15237	D15238	V15239	T15243	C15244	V15245	P15246	I15247	G15248	V15249	E15250	H15251	E15252	D15253	C15254	D15255	N15256	Y15257	A15258	G15259	T15260	F15261	A15262	V15263	E15267	T15268	E15269	M15270	P15271	V15272	A15273	D15274	D15275	R15276	L15277	F15278	I15282	S15283	D15284	E15285	M15286	K15287	K15288	L15289	Q15290	L15291	T15292	E15293	D15294	S15295	K15296	F15297	L15298	T15299	T15300
A15172	H15176	L15177	T15178	T15179	T15180	N15181	S15182	R15183	P15184	N15185	D15186	V15187	F15188	D15189	Y15190	Q15191	N15192	S15193	Y15196	K15197	F15198	D15199	S15200	L15201	S15202	F15203	S15204	G15205	L15206	S15207	H15208	P15209	R15210	L15211	D15212	D15213	L15214	L15215	E15216	S15217	R15218	Q15219	H15221	D15222	R15223	V15224	F15225	A15226	G15227	F15228	W15229	L15230	S15231	G15232	I15233	K15234
I15044	E15045	I15053	S15054	F15055	A15056	D15057	A15058	V15059	K15063	P15064	R15065	D15066	Q15067	N15070	N15071	R15072	Y15073	E15083	H15084	T15085	D15086	F15087	C15088	G15107	P15108	N15109	P15110	H15111	R15144	Y15145	R15146	K15147	L15148	D15149	Y15150	N15151	V15152	A15153	N15154	C15155	A15156	L15157	N15158	L15159	L15160	N15161	D15162	P15163	N15168	N15169	K15170	T15171				
R14946	F14949	T14953	D14954	D14955	G14956	R14957	A14969	Q14970	C14971	P14972	N14973	A14974	D14975	G14976	S14977	N14978	I14979	H14980	M14987	A15007	R15008	G15009	S15010	D15011	V15012	A15013	V15014	D15018	W15019	I15020	E15021	P15022	F15023	D15024	S15025	L15026	P15027	G15028	N15029	I15030	S15031	D15032	E15033	T15034	S15035	K14938	E14939	H15037	P15038	K15039	T15040	N15041	E15042	D15043		
T11442	A11443	N11444	D11445	D11446	R11447	E11483	G11519	I11520	G11521	E11522	E11523	N11524	E11538	T11539	M11572	V11577	T11583	Q11584	K11585	T11194	I11195	T11196	S11197	D11225	E11226	F14915	E14916	E14917	D14918	T14919	W14920	R14921	D14922	V14923	V14924	T14925	S14926	L15026	P15027	N14928	L15029	I14933	L14934	F14935	D14936	L14937	S14938	E14940	D14941	M14942	F14943	S14944	L14945			
M7848	T7849	G7850	A7851	E7852	V7853	T7854	D7855	E7856	K7857	T7860	S7861	G11183	N11184	F11185	G11186	E11187	G11188	R11189	R11190	T7653	E7654	A7655	V7656	A7694	S7710	P7711	H7741	S7753	L7767	A7791	D7792	G7793	T7794	D7795	Q7796	K7797	H7798	K7799	A7800	D7823	L7824	D7829	T7836	D7837	K7838	Y7839										

P26453	W26454	A26455	F26456	D26457	R26458	L26459	F26460	L26461	Y26462	D26463	L26464	S26465	K26466	S26467	L26468	V26469	H26470	L26471	R26472	L26473	D26474	A26475	H26476	D26477	D26478	F26479	D26480	I26481	K26482	V26483	T26484	I26485	N26486	G26487	I26488	D26489	G26490	K26491																				
N26389	F26390	H26391	G26392	M26393	T26394	I26395	P26396	Q26397	L26398	E26399	V26400	H26401	L26402	K26403	K26404	I26405	Q26406	E26407	K26408	D26409	R26410	V26411	F26412	A26413	G26414	F26415	L26416	L26417	R26418	A26419	I26420	G26421	Q26422	S26423	A26424	D26425	V26426	N26427	F26428	D26429	V26430	CYS	ARG	LYS	ASP	GLY	GLU	CYS	T26438	F26439	G26440	G26441	T26442	F26443	C26444	V26445	L26446	G26447
S26303	D26311	R26323	A26326	Q26329	A26330	K26333	Y26334	R26335	G26336	L26337	P26338	Y26339	N26340	S26341	A26342	N26343	C26344	E26345	I26346	N26347	K26348	L26349	K26350	K26351	P26352	S26357	S26358	E26359	P26362	N26363	E26364	V26365	A26368	Y26373	K26374	S26375	F26376	D26377	Y26378	Q26379	Q26380	L26381	N26382	Y26383	E26384	Y26385	D26386	N26387	L26388									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196315	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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	513.0, 513.0, 513.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.14, 1.14, 1.14	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	10a	0.45	0/6115	1.09	28/8514 (0.3%)
1	1a	0.44	0/6115	1.08	20/8514 (0.2%)
1	2a	0.43	0/6115	1.04	16/8514 (0.2%)
1	3a	0.45	0/6115	1.06	23/8514 (0.3%)
1	4a	0.44	0/6115	1.04	17/8514 (0.2%)
1	5a	0.44	0/6115	1.05	24/8514 (0.3%)
1	6a	0.44	0/6115	1.08	24/8514 (0.3%)
1	7a	0.46	0/6115	1.08	17/8514 (0.2%)
1	8a	0.46	0/6115	1.05	16/8514 (0.2%)
1	9a	0.46	0/6115	1.09	13/8514 (0.2%)
All	All	0.44	0/61150	1.07	198/85140 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	10a	0	5
1	1a	0	5
1	2a	0	5
1	3a	0	3
1	4a	0	7
1	5a	0	3
1	6a	0	4
1	7a	0	7
1	8a	0	3
1	9a	0	5
All	All	0	47

There are no bond length outliers.

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9a	3778	LEU	CA-C-N	-16.02	99.81	119.84
1	9a	3778	LEU	C-N-CA	-16.02	99.81	119.84
1	7a	7511	CYS	CA-C-N	-12.82	103.81	119.84
1	7a	7511	CYS	C-N-CA	-12.82	103.81	119.84
1	1a	3778	LEU	CA-C-N	-12.28	104.49	119.84
1	1a	3778	LEU	C-N-CA	-12.28	104.49	119.84
1	2a	7526	GLY	N-CA-C	10.60	127.10	114.48
1	9a	7526	GLY	N-CA-C	10.43	126.89	114.48
1	3a	7526	GLY	N-CA-C	9.96	126.33	114.48
1	6a	3778	LEU	CA-C-N	-9.86	109.92	120.47
1	6a	3778	LEU	C-N-CA	-9.86	109.92	120.47
1	1a	7511	CYS	CA-C-N	-9.40	107.56	120.25
1	1a	7511	CYS	C-N-CA	-9.40	107.56	120.25
1	6a	7526	GLY	N-CA-C	9.25	125.48	114.48
1	1a	3989	SER	CA-C-N	-9.21	109.43	119.19
1	1a	3989	SER	C-N-CA	-9.21	109.43	119.19
1	6a	7610	LYS	CA-C-N	-8.95	110.65	120.14
1	6a	7610	LYS	C-N-CA	-8.95	110.65	120.14
1	9a	3983	LYS	CA-C-N	-8.53	110.57	120.89
1	9a	3983	LYS	C-N-CA	-8.53	110.57	120.89
1	7a	7526	GLY	N-CA-C	8.44	126.45	114.64
1	1a	3764	LYS	N-CA-C	8.43	121.15	109.18
1	10a	7526	GLY	N-CA-C	8.42	127.94	115.64
1	1a	7526	GLY	N-CA-C	8.19	124.22	114.48
1	9a	7610	LYS	CA-C-N	-8.16	111.33	119.90
1	9a	7610	LYS	C-N-CA	-8.16	111.33	119.90
1	2a	85	SER	N-CA-C	7.89	119.03	108.38
1	10a	3778	LEU	CA-C-N	-7.78	111.63	121.04
1	10a	3778	LEU	C-N-CA	-7.78	111.63	121.04
1	6a	7710	SER	CA-C-N	-7.67	110.25	119.84
1	6a	7710	SER	C-N-CA	-7.67	110.25	119.84
1	1a	7458	ASN	N-CA-C	7.60	119.20	111.07
1	5a	7610	LYS	CA-C-N	-7.55	112.21	119.76
1	5a	7610	LYS	C-N-CA	-7.55	112.21	119.76
1	10a	7823	ASP	CA-C-N	7.46	135.12	121.70
1	10a	7823	ASP	C-N-CA	7.46	135.12	121.70
1	8a	3778	LEU	CA-C-N	-7.42	112.06	121.04
1	8a	3778	LEU	C-N-CA	-7.42	112.06	121.04
1	5a	116	LYS	CB-CA-C	-7.36	108.07	116.54
1	4a	3778	LEU	CA-C-N	-7.35	112.14	121.04
1	4a	3778	LEU	C-N-CA	-7.35	112.14	121.04
1	8a	7511	CYS	CA-C-N	-7.30	110.71	119.84
1	8a	7511	CYS	C-N-CA	-7.30	110.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1a	228	GLY	N-CA-C	7.25	125.06	114.10
1	6a	3731	MET	N-CA-C	7.18	119.66	108.96
1	8a	323	ILE	CA-C-N	7.16	127.19	119.89
1	8a	323	ILE	C-N-CA	7.16	127.19	119.89
1	4a	7823	ASP	CA-C-N	7.15	134.58	121.70
1	4a	7823	ASP	C-N-CA	7.15	134.58	121.70
1	5a	3732	ASP	N-CA-C	7.05	119.04	111.36
1	6a	7525	HIS	N-CA-C	-7.01	99.16	108.34
1	7a	117	LYS	N-CA-C	6.96	117.68	108.07
1	2a	7585	ASN	CA-C-N	-6.88	113.60	120.21
1	2a	7585	ASN	C-N-CA	-6.88	113.60	120.21
1	8a	3989	SER	CA-C-N	-6.82	111.32	119.84
1	8a	3989	SER	C-N-CA	-6.82	111.32	119.84
1	5a	228	GLY	N-CA-C	6.78	124.13	114.64
1	5a	3731	MET	N-CA-C	6.73	118.62	111.28
1	2a	3983	LYS	CA-C-N	-6.72	112.76	120.89
1	2a	3983	LYS	C-N-CA	-6.72	112.76	120.89
1	6a	126	GLY	CA-C-N	6.72	133.79	121.70
1	6a	126	GLY	C-N-CA	6.72	133.79	121.70
1	5a	3764	LYS	N-CA-C	6.64	119.97	109.81
1	5a	7714	LEU	N-CA-C	6.60	119.07	111.02
1	7a	4137	VAL	CA-C-N	6.52	126.28	119.76
1	7a	4137	VAL	C-N-CA	6.52	126.28	119.76
1	10a	404	ILE	CA-C-N	6.51	124.35	119.66
1	10a	404	ILE	C-N-CA	6.51	124.35	119.66
1	3a	3989	SER	CA-C-N	-6.44	111.80	119.84
1	3a	3989	SER	C-N-CA	-6.44	111.80	119.84
1	1a	4072	GLY	N-CA-C	6.43	119.94	111.52
1	8a	7710	SER	CA-C-N	-6.42	111.81	119.84
1	8a	7710	SER	C-N-CA	-6.42	111.81	119.84
1	7a	3983	LYS	CA-C-N	-6.42	113.07	119.56
1	7a	3983	LYS	C-N-CA	-6.42	113.07	119.56
1	6a	3989	SER	CA-C-N	-6.32	111.94	119.84
1	6a	3989	SER	C-N-CA	-6.32	111.94	119.84
1	1a	7525	HIS	N-CA-C	-6.30	100.07	108.19
1	3a	323	ILE	CA-C-N	6.22	126.24	119.90
1	3a	323	ILE	C-N-CA	6.22	126.24	119.90
1	1a	296	ARG	N-CA-C	-6.21	105.74	113.38
1	5a	3983	LYS	CA-C-N	-6.16	113.88	120.47
1	5a	3983	LYS	C-N-CA	-6.16	113.88	120.47
1	2a	83	HIS	N-CA-C	6.12	121.03	113.50
1	9a	7581	GLU	N-CA-C	6.09	117.65	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10a	3884	GLN	CA-C-N	-6.06	112.26	119.84
1	10a	3884	GLN	C-N-CA	-6.06	112.26	119.84
1	10a	7710	SER	CA-C-N	-6.06	112.26	119.84
1	10a	7710	SER	C-N-CA	-6.06	112.26	119.84
1	2a	323	ILE	CA-C-N	6.05	126.06	119.89
1	2a	323	ILE	C-N-CA	6.05	126.06	119.89
1	4a	7719	ASN	CA-C-N	6.05	126.57	120.04
1	4a	7719	ASN	C-N-CA	6.05	126.57	120.04
1	4a	3779	PRO	N-CA-C	-6.03	106.17	114.98
1	3a	3983	LYS	CA-C-N	-6.01	112.32	119.84
1	3a	3983	LYS	C-N-CA	-6.01	112.32	119.84
1	7a	323	ILE	CA-C-N	6.01	126.03	119.90
1	7a	323	ILE	C-N-CA	6.01	126.03	119.90
1	4a	296	ARG	N-CA-C	-6.00	105.79	113.23
1	10a	116	LYS	CB-CA-C	-6.00	109.07	117.23
1	10a	388	GLY	N-CA-C	-6.00	107.56	114.69
1	7a	7865	GLU	CA-C-N	5.95	125.91	119.78
1	7a	7865	GLU	C-N-CA	5.95	125.91	119.78
1	5a	7667	ASP	CA-C-N	5.94	125.62	119.56
1	5a	7667	ASP	C-N-CA	5.94	125.62	119.56
1	3a	51	ASP	N-CA-C	5.92	118.21	111.11
1	7a	7667	ASP	CA-C-N	5.91	125.58	119.56
1	7a	7667	ASP	C-N-CA	5.91	125.58	119.56
1	5a	7719	ASN	CA-C-N	5.90	126.42	120.04
1	5a	7719	ASN	C-N-CA	5.90	126.42	120.04
1	10a	3779	PRO	N-CA-C	-5.85	106.43	114.98
1	3a	7837	ASP	N-CA-C	5.82	118.21	108.73
1	5a	4094	GLU	N-CA-C	5.82	119.56	112.23
1	10a	7857	LYS	N-CA-C	5.77	118.17	109.41
1	8a	125	SER	N-CA-C	5.75	117.98	108.49
1	3a	7610	LYS	CA-C-N	-5.74	112.02	120.46
1	3a	7610	LYS	C-N-CA	-5.74	112.02	120.46
1	4a	4094	GLU	N-CA-C	5.72	118.45	111.82
1	2a	7855	ASP	N-CA-C	5.71	115.65	108.45
1	8a	7794	THR	N-CA-C	5.71	118.36	111.40
1	6a	323	ILE	CA-C-N	5.69	125.62	119.76
1	6a	323	ILE	C-N-CA	5.69	125.62	119.76
1	6a	7838	LYS	CA-C-N	5.68	131.92	121.70
1	6a	7838	LYS	C-N-CA	5.68	131.92	121.70
1	3a	3865	GLU	N-CA-C	5.68	117.14	111.07
1	4a	7495	VAL	N-CA-C	5.63	118.94	111.17
1	6a	4072	GLY	N-CA-C	5.62	119.20	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2a	4137	VAL	CA-C-N	5.62	125.38	119.76
1	2a	4137	VAL	C-N-CA	5.62	125.38	119.76
1	10a	3871	VAL	N-CA-C	5.58	116.98	110.62
1	5a	7707	LYS	CA-C-N	5.58	125.50	119.76
1	5a	7707	LYS	C-N-CA	5.58	125.50	119.76
1	6a	296	ARG	N-CA-C	-5.57	106.53	113.38
1	5a	7460	LYS	N-CA-C	5.56	115.62	108.34
1	5a	107	HIS	CA-C-N	5.54	125.21	119.56
1	5a	107	HIS	C-N-CA	5.54	125.21	119.56
1	9a	229	LEU	CA-C-N	5.52	125.45	119.76
1	9a	229	LEU	C-N-CA	5.52	125.45	119.76
1	6a	3983	LYS	CA-C-N	-5.52	114.07	119.64
1	6a	3983	LYS	C-N-CA	-5.52	114.07	119.64
1	1a	7719	ASN	CA-C-N	5.49	125.19	119.64
1	1a	7719	ASN	C-N-CA	5.49	125.19	119.64
1	8a	3779	PRO	N-CA-C	-5.49	106.97	114.98
1	8a	133	LYS	N-CA-C	5.48	117.51	109.24
1	4a	3730	ASN	N-CA-C	5.46	117.67	111.11
1	10a	7458	ASN	CA-C-N	5.46	131.52	121.70
1	10a	7458	ASN	C-N-CA	5.46	131.52	121.70
1	5a	3989	SER	CA-C-N	-5.44	113.04	119.84
1	5a	3989	SER	C-N-CA	-5.44	113.04	119.84
1	10a	3730	ASN	N-CA-C	5.41	116.90	110.19
1	2a	296	ARG	N-CA-C	-5.41	106.85	113.50
1	3a	296	ARG	N-CA-C	-5.40	106.86	113.50
1	3a	4002	VAL	CA-C-N	5.39	126.58	119.84
1	3a	4002	VAL	C-N-CA	5.39	126.58	119.84
1	10a	114	THR	CB-CA-C	-5.39	110.35	116.54
1	3a	7710	SER	CA-C-N	-5.38	113.12	119.84
1	3a	7710	SER	C-N-CA	-5.38	113.12	119.84
1	3a	404	ILE	CA-C-N	5.36	123.57	119.66
1	3a	404	ILE	C-N-CA	5.36	123.57	119.66
1	6a	7549	GLY	N-CA-C	5.33	121.27	113.48
1	6a	232	ARG	CA-C-N	5.32	125.58	119.83
1	6a	232	ARG	C-N-CA	5.32	125.58	119.83
1	7a	3764	LYS	N-CA-C	5.32	116.36	108.86
1	4a	3777	GLY	N-CA-C	5.31	119.05	110.87
1	7a	7664	SER	N-CA-C	5.27	117.44	111.11
1	8a	50	ALA	CB-CA-C	-5.27	110.48	116.54
1	8a	7525	HIS	N-CA-C	-5.27	101.81	108.45
1	10a	3879	GLU	N-CA-C	5.27	116.29	108.86
1	4a	3887	LYS	CA-C-N	5.26	131.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4a	3887	LYS	C-N-CA	5.26	131.16	121.70
1	3a	131	GLU	CB-CA-C	-5.25	110.50	116.54
1	3a	50	ALA	CB-CA-C	-5.22	110.13	117.23
1	10a	7505	HIS	N-CA-C	-5.22	106.50	112.92
1	1a	3779	PRO	N-CA-C	-5.20	101.75	112.47
1	3a	7613	PHE	CB-CA-C	-5.19	110.57	116.54
1	5a	7525	HIS	N-CA-C	-5.18	101.59	108.74
1	2a	4072	GLY	N-CA-C	5.18	118.04	110.63
1	4a	3941	ASP	CA-C-N	5.16	124.83	119.56
1	4a	3941	ASP	C-N-CA	5.16	124.83	119.56
1	9a	3989	SER	CA-C-N	-5.15	113.40	119.84
1	9a	3989	SER	C-N-CA	-5.15	113.40	119.84
1	4a	3876	GLN	N-CA-C	5.13	117.54	111.33
1	7a	7823	ASP	N-CA-C	5.13	116.95	111.36
1	5a	7526	GLY	N-CA-C	5.12	125.31	113.18
1	2a	7586	PRO	CA-C-O	-5.10	115.12	122.31
1	10a	99	THR	N-CA-C	-5.09	107.72	114.04
1	10a	4002	VAL	CA-C-N	5.08	126.19	119.84
1	10a	4002	VAL	C-N-CA	5.08	126.19	119.84
1	3a	3880	ARG	CB-CA-C	-5.06	110.35	117.23
1	10a	296	ARG	N-CA-C	-5.04	107.12	113.28
1	1a	4137	VAL	CA-C-N	5.04	125.19	119.90
1	1a	4137	VAL	C-N-CA	5.04	125.19	119.90
1	2a	3949	SER	N-CA-C	-5.02	105.81	111.28
1	1a	323	ILE	CA-C-N	5.02	125.01	119.89
1	1a	323	ILE	C-N-CA	5.02	125.01	119.89
1	10a	3941	ASP	CA-C-N	5.02	125.04	119.32
1	10a	3941	ASP	C-N-CA	5.02	125.04	119.32
1	9a	3882	PHE	N-CA-C	5.02	117.40	111.33

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	10a	18697	ALA	Peptide
1	10a	26311	ASP	Mainchain
1	10a	26347	ASN	Peptide
1	10a	3778	LEU	Peptide
1	10a	7610	LYS	Peptide
1	1a	127	GLU	Peptide
1	1a	18697	ALA	Peptide
1	1a	26311	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	1a	26347	ASN	Peptide
1	1a	3778	LEU	Peptide
1	2a	18697	ALA	Peptide
1	2a	22381	GLU	Peptide
1	2a	26311	ASP	Mainchain
1	2a	26347	ASN	Peptide
1	2a	3778	LEU	Peptide
1	3a	18697	ALA	Peptide
1	3a	26311	ASP	Mainchain
1	3a	26347	ASN	Peptide
1	4a	11580	SER	Peptide
1	4a	18697	ALA	Peptide
1	4a	22432	CYS	Peptide
1	4a	26311	ASP	Mainchain
1	4a	26347	ASN	Peptide
1	4a	3778	LEU	Peptide
1	4a	7494	GLU	Peptide
1	5a	18697	ALA	Peptide
1	5a	26311	ASP	Mainchain
1	5a	26347	ASN	Peptide
1	6a	18697	ALA	Peptide
1	6a	26311	ASP	Mainchain
1	6a	26347	ASN	Peptide
1	6a	3778	LEU	Peptide
1	7a	11581	LYS	Peptide
1	7a	18697	ALA	Peptide
1	7a	22714	GLN	Peptide
1	7a	22773	ALA	Peptide
1	7a	26311	ASP	Mainchain
1	7a	26347	ASN	Peptide
1	7a	3778	LEU	Peptide
1	8a	26311	ASP	Mainchain
1	8a	26347	ASN	Peptide
1	8a	3778	LEU	Peptide
1	9a	26311	ASP	Mainchain
1	9a	26347	ASN	Peptide
1	9a	3778	LEU	Peptide
1	9a	3881	LEU	Peptide
1	9a	7511	CYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10a	16130	0	2801	41	0
1	1a	16130	0	2801	26	0
1	2a	16130	0	2800	36	0
1	3a	16130	0	2801	27	0
1	4a	16130	0	2801	47	0
1	5a	16130	0	2801	27	0
1	6a	16130	0	2800	25	0
1	7a	16130	0	2801	45	0
1	8a	16130	0	2801	25	0
1	9a	16130	0	2801	33	0
All	All	161300	0	28008	332	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 8.

All (332) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5a:3864:ILE:N	1:5a:3871:VAL:O	2.07	0.87
1:10a:3864:ILE:N	1:10a:3871:VAL:O	2.15	0.78
1:6a:7838:LYS:HA	1:6a:7839:TYR:CB	2.15	0.76
1:2a:3881:LEU:N	1:2a:3882:PHE:HA	2.00	0.76
1:1a:118:ALA:HB1	1:1a:119:LYS:HA	1.69	0.75
1:1a:3864:ILE:N	1:1a:3871:VAL:O	2.16	0.74
1:5a:240:PHE:HA	1:5a:263:ALA:HB3	1.69	0.74
1:9a:7823:ASP:O	1:9a:7825:THR:N	2.22	0.72
1:1a:110:PHE:N	1:1a:119:LYS:O	2.23	0.70
1:4a:4094:GLU:O	1:4a:4096:THR:N	2.24	0.70
1:10a:7526:GLY:N	1:10a:7527:MET:HA	2.06	0.69
1:8a:7794:THR:N	1:8a:7795:ASP:HA	2.08	0.69
1:2a:7457:ALA:HA	1:2a:7458:ASN:C	2.19	0.68
1:6a:3864:ILE:N	1:6a:3871:VAL:O	2.26	0.67
1:2a:194:MET:HA	1:2a:200:THR:HA	1.76	0.67
1:4a:7658:MET:HA	1:4a:7664:SER:HA	1.75	0.67
1:8a:240:PHE:HA	1:8a:263:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5a:7771:UNK:HA	1:5a:7823:ASP:HA	1.77	0.67
1:3a:240:PHE:HA	1:3a:263:ALA:HB3	1.77	0.66
1:7a:7526:GLY:N	1:7a:7527:MET:HA	2.10	0.65
1:9a:110:PHE:N	1:9a:119:LYS:O	2.29	0.65
1:7a:4044:PHE:HA	1:7a:4094:GLU:HA	1.79	0.65
1:3a:7651:GLY:HA3	1:3a:7659:ALA:HB2	1.77	0.64
1:2a:7458:ASN:HA	1:2a:7459:VAL:C	2.22	0.64
1:7a:118:ALA:HB1	1:7a:119:LYS:HA	1.79	0.64
1:3a:7526:GLY:N	1:3a:7527:MET:HA	2.13	0.63
1:7a:240:PHE:HA	1:7a:263:ALA:HB3	1.81	0.63
1:9a:7526:GLY:N	1:9a:7527:MET:HA	2.13	0.63
1:1a:7526:GLY:N	1:1a:7527:MET:HA	2.12	0.62
1:5a:4094:GLU:O	1:5a:4096:THR:N	2.33	0.62
1:4a:3889:ASP:N	1:4a:3890:HIS:HA	2.15	0.61
1:7a:7503:ALA:O	1:7a:7506:GLY:N	2.20	0.61
1:9a:240:PHE:HA	1:9a:263:ALA:HB3	1.83	0.60
1:4a:240:PHE:HA	1:4a:263:ALA:HB3	1.82	0.60
1:6a:7526:GLY:N	1:6a:7527:MET:HA	2.16	0.60
1:8a:7457:ALA:HA	1:8a:7458:ASN:C	2.27	0.60
1:10a:126:GLY:HA3	1:10a:202:TYR:O	2.00	0.60
1:2a:7526:GLY:N	1:2a:7527:MET:HA	2.16	0.60
1:3a:7771:UNK:HA	1:3a:7823:ASP:O	2.01	0.59
1:1a:3761:MET:HA	1:1a:3769:TYR:CB	2.32	0.59
1:5a:7526:GLY:N	1:5a:7527:MET:HA	2.16	0.59
1:8a:330:GLN:O	1:8a:332:ASP:N	2.35	0.59
1:5a:110:PHE:N	1:5a:119:LYS:O	2.35	0.58
1:3a:4046:GLY:N	1:3a:4133:ILE:O	2.30	0.58
1:4a:3888:GLY:C	1:4a:3890:HIS:HA	2.28	0.58
1:8a:7526:GLY:N	1:8a:7527:MET:HA	2.18	0.58
1:1a:7771:UNK:HA	1:1a:7823:ASP:O	2.03	0.57
1:2a:305:ASN:N	1:2a:400:ILE:O	2.27	0.57
1:6a:240:PHE:HA	1:6a:263:ALA:HB3	1.87	0.57
1:10a:119:LYS:CB	1:10a:120:LYS:HA	2.34	0.57
1:3a:126:GLY:HA3	1:3a:202:TYR:O	2.04	0.57
1:1a:330:GLN:O	1:1a:332:ASP:N	2.31	0.57
1:4a:7465:HIS:HA	1:4a:7741:HIS:O	2.04	0.57
1:10a:7618:HIS:O	1:10a:7620:ALA:N	2.38	0.57
1:7a:7778:GLY:N	1:7a:7814:TRP:O	2.36	0.57
1:6a:148:GLN:C	1:6a:150:GLY:H	2.13	0.56
1:4a:4116:ILE:O	1:4a:4124:LEU:N	2.37	0.56
1:3a:4044:PHE:N	1:3a:4135:ILE:O	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:10a:7823:ASP:HA	1:10a:7824:ILE:CB	2.36	0.56
1:2a:80:LEU:O	1:2a:84:GLY:HA2	2.05	0.56
1:3a:7494:GLU:C	1:3a:7496:THR:H	2.13	0.56
1:4a:110:PHE:N	1:4a:119:LYS:O	2.37	0.56
1:2a:7487:ALA:O	1:2a:7491:ALA:N	2.38	0.55
1:2a:3879:GLU:C	1:2a:3881:LEU:HA	2.32	0.55
1:1a:4120:ASN:N	1:1a:4121:GLY:HA2	2.22	0.55
1:5a:7585:ASN:N	1:5a:7586:PRO:HA	2.22	0.55
1:10a:7607:LEU:CB	1:10a:7608:TYR:HA	2.36	0.55
1:4a:7823:ASP:HA	1:4a:7824:ILE:CB	2.37	0.55
1:3a:3839:SER:HA	1:3a:3842:ALA:HB3	1.88	0.55
1:4a:7526:GLY:N	1:4a:7527:MET:HA	2.20	0.55
1:8a:235:CYS:HA	1:8a:4134:VAL:O	2.07	0.55
1:10a:7794:THR:N	1:10a:7795:ASP:HA	2.22	0.55
1:5a:7791:ALA:HA	1:5a:7839:TYR:H	1.73	0.54
1:4a:7607:LEU:CB	1:4a:7608:TYR:HA	2.38	0.54
1:10a:7503:ALA:C	1:10a:7505:HIS:H	2.15	0.54
1:3a:7794:THR:N	1:3a:7795:ASP:HA	2.24	0.53
1:3a:3877:ILE:O	1:3a:3926:GLY:HA3	2.08	0.53
1:5a:61:GLY:HA3	1:5a:352:TRP:CB	2.38	0.53
1:9a:194:MET:HA	1:9a:200:THR:HA	1.90	0.53
1:1a:150:GLY:HA2	1:1a:151:GLN:C	2.33	0.53
1:4a:7847:ASP:N	1:4a:7851:ALA:O	2.36	0.53
1:8a:7585:ASN:N	1:8a:7586:PRO:HA	2.24	0.53
1:1a:7687:LEU:O	1:1a:7691:ARG:N	2.40	0.52
1:1a:7585:ASN:N	1:1a:7586:PRO:HA	2.24	0.52
1:6a:7593:ASP:N	1:6a:7594:SER:HA	2.24	0.52
1:2a:3880:ARG:N	1:2a:3881:LEU:HA	2.25	0.52
1:3a:7859:VAL:C	1:3a:7861:SER:H	2.18	0.52
1:8a:3878:ASP:HA	1:8a:3923:TRP:O	2.09	0.52
1:10a:7485:ALA:HB1	1:10a:7548:ASN:O	2.09	0.52
1:6a:3877:ILE:O	1:6a:3926:GLY:HA3	2.10	0.52
1:7a:7526:GLY:HA2	1:7a:7814:TRP:CB	2.40	0.52
1:2a:148:GLN:C	1:2a:150:GLY:H	2.18	0.51
1:7a:7465:HIS:HA	1:7a:7741:HIS:O	2.10	0.51
1:8a:120:LYS:H	1:8a:121:ASN:HA	1.75	0.51
1:10a:7593:ASP:O	1:10a:7597:ALA:N	2.44	0.51
1:3a:7591:ALA:HB3	1:3a:7666:PHE:O	2.10	0.51
1:3a:150:GLY:HA2	1:3a:151:GLN:C	2.35	0.51
1:4a:7859:VAL:O	1:4a:7861:SER:N	2.44	0.51
1:2a:126:GLY:HA3	1:2a:202:TYR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9a:115:GLY:HA2	1:9a:116:LYS:CB	2.41	0.51
1:9a:3782:CYS:HA	1:9a:3783:PRO:C	2.36	0.51
1:4a:4121:GLY:HA2	1:4a:4122:THR:C	2.36	0.50
1:6a:7593:ASP:H	1:6a:7594:SER:HA	1.76	0.50
1:5a:3880:ARG:N	1:5a:3881:LEU:HA	2.25	0.50
1:8a:108:PRO:O	1:8a:121:ASN:N	2.42	0.50
1:9a:7658:MET:HA	1:9a:7664:SER:HA	1.93	0.50
1:6a:7794:THR:H	1:6a:7795:ASP:HA	1.77	0.50
1:9a:7585:ASN:N	1:9a:7586:PRO:HA	2.26	0.50
1:10a:240:PHE:HA	1:10a:263:ALA:HB3	1.94	0.50
1:5a:120:LYS:H	1:5a:121:ASN:HA	1.78	0.49
1:7a:120:LYS:N	1:7a:121:ASN:HA	2.27	0.49
1:3a:7778:GLY:N	1:3a:7814:TRP:O	2.41	0.49
1:6a:2:LEU:H	1:6a:274:TYR:HA	1.76	0.49
1:2a:3982:MET:N	1:2a:4001:SER:O	2.27	0.49
1:10a:187:GLY:HA3	1:10a:195:SER:N	2.27	0.49
1:2a:7790:ALA:HA	1:2a:7796:GLN:O	2.12	0.49
1:8a:148:GLN:HA	1:8a:149:GLU:C	2.38	0.49
1:3a:7665:ALA:C	1:3a:7667:ASP:H	2.21	0.49
1:6a:126:GLY:HA3	1:6a:127:GLU:CB	2.43	0.49
1:7a:194:MET:HA	1:7a:200:THR:HA	1.95	0.49
1:8a:7500:GLN:O	1:8a:7503:ALA:N	2.45	0.48
1:5a:3761:MET:HA	1:5a:3769:TYR:CB	2.42	0.48
1:5a:3877:ILE:O	1:5a:3926:GLY:HA3	2.13	0.48
1:7a:3884:GLN:HA	1:7a:3885:PRO:C	2.38	0.48
1:1a:240:PHE:HA	1:1a:263:ALA:HB3	1.96	0.48
1:7a:110:PHE:N	1:7a:119:LYS:O	2.37	0.48
1:3a:7577:ASP:C	1:3a:7580:GLY:H	2.21	0.48
1:2a:7526:GLY:HA2	1:2a:7814:TRP:CB	2.44	0.48
1:9a:118:ALA:HB1	1:9a:119:LYS:HA	1.96	0.48
1:2a:4026:SER:O	1:2a:4030:LEU:N	2.35	0.47
1:5a:7465:HIS:HA	1:5a:7741:HIS:O	2.13	0.47
1:1a:7507:SER:HA	1:1a:7521:ALA:HA	1.95	0.47
1:2a:81:VAL:HA	1:2a:85:SER:H	1.79	0.47
1:7a:3761:MET:HA	1:7a:3769:TYR:CB	2.43	0.47
1:5a:7507:SER:HA	1:5a:7521:ALA:HA	1.96	0.47
1:10a:150:GLY:HA2	1:10a:152:LYS:N	2.30	0.47
1:9a:7458:ASN:HA	1:9a:7459:VAL:C	2.39	0.47
1:2a:51:ASP:HA	1:2a:52:GLY:HA3	1.70	0.47
1:2a:7513:SER:HA	1:2a:7516:ALA:H	1.80	0.47
1:9a:3733:THR:HA	1:9a:3734:SER:HA	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6a:51:ASP:HA	1:6a:52:GLY:HA2	1.58	0.47
1:10a:7791:ALA:HA	1:10a:7839:TYR:H	1.80	0.47
1:4a:194:MET:HA	1:4a:200:THR:HA	1.97	0.47
1:3a:7771:UNK:HA	1:3a:7823:ASP:HA	1.96	0.47
1:7a:3864:ILE:N	1:7a:3871:VAL:O	2.30	0.47
1:3a:7499:GLN:O	1:3a:7503:ALA:N	2.48	0.47
1:2a:7794:THR:N	1:2a:7795:ASP:HA	2.30	0.46
1:4a:4026:SER:O	1:4a:4030:LEU:N	2.48	0.46
1:8a:7617:THR:HA	1:8a:7618:HIS:HA	1.69	0.46
1:9a:3761:MET:HA	1:9a:3769:TYR:CB	2.46	0.46
1:8a:7511:CYS:O	1:8a:7513:SER:N	2.48	0.46
1:9a:4046:GLY:HA2	1:9a:4091:TYR:O	2.16	0.46
1:1a:3732:ASP:C	1:1a:3734:SER:HA	2.41	0.46
1:6a:2:LEU:O	1:6a:275:ALA:N	2.47	0.46
1:7a:187:GLY:HA3	1:7a:195:SER:CB	2.46	0.46
1:10a:234:ASN:O	1:10a:4135:ILE:HA	2.16	0.46
1:2a:147:SER:O	1:2a:149:GLU:N	2.49	0.46
1:3a:7771:UNK:N	1:3a:7863:ILE:O	2.49	0.46
1:5a:7771:UNK:HA	1:5a:7823:ASP:O	2.15	0.46
1:6a:148:GLN:O	1:6a:150:GLY:N	2.49	0.46
1:2a:7543:ASN:O	1:2a:7547:ARG:N	2.32	0.45
1:4a:7640:GLU:O	1:4a:7643:HIS:N	2.50	0.45
1:4a:3786:ASP:HA	1:4a:3787:ALA:HA	1.69	0.45
1:5a:3927:SER:HA	1:5a:4119:VAL:O	2.16	0.45
1:1a:329:ARG:C	1:1a:331:SER:H	2.24	0.45
1:6a:3839:SER:HA	1:6a:3842:ALA:HB3	1.98	0.45
1:8a:126:GLY:HA3	1:8a:127:GLU:HA	1.72	0.45
1:8a:3733:THR:HA	1:8a:3734:SER:HA	1.65	0.45
1:2a:7578:ALA:HA	1:2a:7579:ASN:HA	1.55	0.45
1:7a:7585:ASN:N	1:7a:7586:PRO:HA	2.32	0.45
1:4a:4044:PHE:N	1:4a:4135:ILE:O	2.41	0.45
1:6a:7794:THR:N	1:6a:7795:ASP:HA	2.32	0.45
1:8a:3886:SER:HA	1:8a:3887:LYS:HA	1.54	0.45
1:10a:3761:MET:HA	1:10a:3769:TYR:CB	2.46	0.45
1:2a:7687:LEU:O	1:2a:7691:ARG:N	2.50	0.45
1:4a:3887:LYS:CB	1:4a:3888:GLY:HA2	2.47	0.45
1:4a:4044:PHE:O	1:4a:4134:VAL:HA	2.17	0.45
1:4a:4094:GLU:C	1:4a:4096:THR:H	2.24	0.45
1:9a:3886:SER:HA	1:9a:3887:LYS:HA	1.42	0.45
1:7a:193:SER:C	1:7a:195:SER:H	2.25	0.45
1:7a:7771:UNK:HA	1:7a:7823:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:10a:132:ASN:HA	1:10a:133:LYS:HA	1.84	0.45
1:10a:3886:SER:HA	1:10a:3887:LYS:HA	1.47	0.44
1:4a:7526:GLY:HA2	1:4a:7814:TRP:CB	2.48	0.44
1:4a:7585:ASN:N	1:4a:7586:PRO:HA	2.32	0.44
1:9a:226:HIS:HA	1:9a:227:ARG:HA	1.55	0.44
1:10a:7654:GLU:C	1:10a:7656:VAL:H	2.26	0.44
1:6a:7658:MET:HA	1:6a:7664:SER:HA	2.00	0.44
1:7a:4046:GLY:HA2	1:7a:4091:TYR:O	2.17	0.44
1:4a:407:GLN:HA	1:4a:408:GLY:HA2	1.68	0.44
1:10a:4046:GLY:HA2	1:10a:4091:TYR:O	2.18	0.44
1:4a:7525:HIS:C	1:4a:7527:MET:HA	2.42	0.44
1:6a:3733:THR:HA	1:6a:3734:SER:HA	1.60	0.44
1:8a:4026:SER:O	1:8a:4030:LEU:N	2.40	0.44
1:2a:183:HIS:O	1:2a:195:SER:HA	2.17	0.44
1:3a:7616:TYR:O	1:3a:7620:ALA:HB3	2.18	0.44
1:4a:4117:LYS:HA	1:4a:4123:ALA:HA	2.00	0.44
1:10a:7614:GLY:HA2	1:10a:7615:LYS:HA	1.82	0.44
1:2a:7508:THR:O	1:2a:7510:TRP:N	2.51	0.43
1:8a:4046:GLY:HA2	1:8a:4091:TYR:O	2.18	0.43
1:8a:7753:SER:O	1:8a:7757:LEU:N	2.50	0.43
1:5a:7661:LEU:HA	1:5a:7664:SER:CB	2.48	0.43
1:10a:150:GLY:HA2	1:10a:151:GLN:C	2.42	0.43
1:9a:322:CYS:HA	1:9a:333:ASN:O	2.18	0.43
1:1a:7658:MET:HA	1:1a:7664:SER:HA	2.01	0.43
1:6a:7519:LYS:HA	1:6a:7520:TYR:HA	1.87	0.43
1:9a:138:ALA:O	1:9a:188:GLY:HA3	2.19	0.43
1:1a:120:LYS:N	1:1a:121:ASN:HA	2.34	0.43
1:5a:4043:VAL:O	1:5a:4094:GLU:O	2.36	0.43
1:9a:45:ALA:HB1	1:9a:55:ILE:C	2.43	0.43
1:6a:227:ARG:HA	1:6a:228:GLY:HA3	1.86	0.43
1:8a:84:GLY:HA2	1:8a:85:SER:C	2.43	0.43
1:9a:407:GLN:HA	1:9a:408:GLY:HA2	1.69	0.43
1:5a:7772:VAL:N	1:5a:7822:SER:O	2.49	0.43
1:1a:322:CYS:HA	1:1a:333:ASN:O	2.18	0.42
1:5a:7847:ASP:N	1:5a:7851:ALA:O	2.38	0.42
1:7a:7500:GLN:O	1:7a:7503:ALA:HB3	2.19	0.42
1:4a:4118:ASP:C	1:4a:4121:GLY:H	2.26	0.42
1:5a:7607:LEU:CB	1:5a:7608:TYR:HA	2.49	0.42
1:8a:149:GLU:O	1:8a:151:GLN:N	2.53	0.42
1:1a:7854:THR:HA	1:1a:7855:ASP:HA	1.80	0.42
1:5a:3919:SER:HA	1:5a:4075:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7a:7794:THR:N	1:7a:7795:ASP:HA	2.34	0.42
1:8a:7778:GLY:N	1:8a:7814:TRP:O	2.46	0.42
1:1a:3733:THR:N	1:1a:3734:SER:HA	2.33	0.42
1:3a:7771:UNK:O	1:3a:7863:ILE:N	2.52	0.42
1:5a:3782:CYS:HA	1:5a:3783:PRO:C	2.45	0.42
1:7a:322:CYS:HA	1:7a:333:ASN:O	2.20	0.42
1:9a:81:VAL:C	1:9a:83:HIS:N	2.76	0.42
1:1a:7794:THR:N	1:1a:7795:ASP:HA	2.34	0.42
1:10a:7458:ASN:HA	1:10a:7459:VAL:CB	2.49	0.42
1:1a:3878:ASP:HA	1:1a:3923:TRP:O	2.19	0.42
1:1a:7525:HIS:C	1:1a:7527:MET:HA	2.45	0.42
1:8a:7859:VAL:O	1:8a:7861:SER:N	2.53	0.42
1:2a:3881:LEU:N	1:2a:3882:PHE:CA	2.77	0.42
1:3a:7511:CYS:HA	1:3a:7512:PRO:HA	1.70	0.42
1:7a:51:ASP:HA	1:7a:52:GLY:HA2	1.66	0.42
1:9a:7614:GLY:HA2	1:9a:7615:LYS:HA	1.79	0.42
1:5a:4046:GLY:HA2	1:5a:4091:TYR:O	2.20	0.41
1:7a:7460:LYS:HA	1:7a:7461:PHE:HA	1.57	0.41
1:9a:7526:GLY:HA2	1:9a:7814:TRP:CB	2.50	0.41
1:1a:4046:GLY:HA2	1:1a:4091:TYR:O	2.19	0.41
1:3a:7577:ASP:O	1:3a:7580:GLY:N	2.52	0.41
1:5a:3733:THR:HA	1:5a:3734:SER:HA	1.67	0.41
1:6a:7457:ALA:HA	1:6a:7458:ASN:HA	1.68	0.41
1:2a:3878:ASP:HA	1:2a:3923:TRP:O	2.19	0.41
1:4a:227:ARG:HA	1:4a:228:GLY:HA2	1.92	0.41
1:6a:3729:VAL:CB	1:6a:4011:ALA:HB2	2.50	0.41
1:8a:227:ARG:HA	1:8a:228:GLY:HA2	1.85	0.41
1:10a:3732:ASP:C	1:10a:3734:SER:HA	2.44	0.41
1:2a:7823:ASP:O	1:2a:7825:THR:N	2.54	0.41
1:10a:128:ILE:N	1:10a:133:LYS:O	2.49	0.41
1:1a:3782:CYS:HA	1:1a:3783:PRO:C	2.46	0.41
1:2a:3762:SER:HA	1:2a:3763:ASP:HA	1.54	0.41
1:4a:7794:THR:N	1:4a:7795:ASP:HA	2.35	0.41
1:6a:3761:MET:HA	1:6a:3769:TYR:CB	2.49	0.41
1:4a:7593:ASP:O	1:4a:7597:ALA:N	2.48	0.41
1:2a:148:GLN:C	1:2a:150:GLY:N	2.77	0.41
1:2a:4047:PHE:O	1:2a:4091:TYR:N	2.32	0.41
1:9a:319:ILE:O	1:9a:338:ALA:N	2.51	0.41
1:9a:3:LEU:O	1:9a:88:GLY:N	2.48	0.41
1:10a:81:VAL:C	1:10a:83:HIS:N	2.77	0.41
1:10a:7753:SER:O	1:10a:7757:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1a:115:GLY:HA2	1:1a:116:LYS:CB	2.51	0.40
1:2a:3877:ILE:O	1:2a:3926:GLY:N	2.54	0.40
1:2a:4034:VAL:O	1:2a:4038:LYS:N	2.54	0.40
1:9a:3878:ASP:HA	1:9a:3923:TRP:O	2.21	0.40
1:9a:7607:LEU:CB	1:9a:7608:TYR:HA	2.51	0.40
1:10a:7484:THR:C	1:10a:7486:MET:H	2.29	0.40
1:2a:407:GLN:HA	1:2a:408:GLY:HA2	1.78	0.40
1:6a:7465:HIS:HA	1:6a:7741:HIS:O	2.21	0.40
1:2a:3869:ALA:C	1:2a:3871:VAL:H	2.28	0.40
1:10a:7465:HIS:HA	1:10a:7741:HIS:O	2.21	0.40
1:3a:3782:CYS:HA	1:3a:3783:PRO:C	2.45	0.40
1:5a:150:GLY:HA2	1:5a:151:GLN:HA	1.77	0.40
1:6a:4007:TYR:O	1:6a:4009:TYR:N	2.55	0.40
1:9a:3887:LYS:CB	1:9a:3888:GLY:HA2	2.52	0.40
1:7a:7838:LYS:HA	1:7a:7839:TYR:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	10a	1237/3314 (37%)	1157 (94%)	69 (6%)	11 (1%)	14	50
1	1a	1237/3314 (37%)	1167 (94%)	62 (5%)	8 (1%)	21	58
1	2a	1237/3314 (37%)	1176 (95%)	53 (4%)	8 (1%)	21	58
1	3a	1237/3314 (37%)	1167 (94%)	57 (5%)	13 (1%)	11	45
1	4a	1237/3314 (37%)	1185 (96%)	46 (4%)	6 (0%)	24	63
1	5a	1237/3314 (37%)	1164 (94%)	62 (5%)	11 (1%)	14	50
1	6a	1237/3314 (37%)	1169 (94%)	57 (5%)	11 (1%)	14	50
1	7a	1237/3314 (37%)	1143 (92%)	84 (7%)	10 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8a	1237/3314 (37%)	1162 (94%)	59 (5%)	16 (1%)	9	40
1	9a	1237/3314 (37%)	1151 (93%)	76 (6%)	10 (1%)	16	53
All	All	12370/33140 (37%)	11641 (94%)	625 (5%)	104 (1%)	18	53

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1a	134	VAL
1	1a	331	SER
1	1a	3989	SER
1	2a	148	GLN
1	3a	7495	VAL
1	4a	51	ASP
1	4a	7824	ILE
1	5a	4095	ILE
1	6a	127	GLU
1	6a	4009	TYR
1	7a	7511	CYS
1	8a	331	SER
1	8a	7714	LEU
1	9a	4009	TYR
1	9a	7824	ILE
1	10a	7824	ILE
1	1a	7495	VAL
1	2a	3925	GLY
1	2a	4121	GLY
1	3a	4067	ASN
1	4a	153	ASN
1	4a	4095	ILE
1	4a	7860	THR
1	5a	7590	GLY
1	6a	84	GLY
1	6a	149	GLU
1	6a	3761	MET
1	7a	84	GLY
1	7a	7580	GLY
1	8a	116	LYS
1	8a	150	GLY
1	8a	3877	ILE
1	8a	3988	LYS
1	10a	149	GLU

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Mol	Chain	Res	Type
1	10a	7459	VAL
1	2a	153	ASN
1	2a	7509	GLN
1	2a	7856	LEU
1	3a	4095	ILE
1	3a	7462	ASP
1	3a	7665	ALA
1	3a	7860	THR
1	4a	149	GLU
1	5a	227	ARG
1	5a	7509	GLN
1	6a	227	ARG
1	6a	7495	VAL
1	8a	7495	VAL
1	8a	7839	TYR
1	9a	134	VAL
1	9a	3731	MET
1	9a	7495	VAL
1	10a	333	ASN
1	10a	7860	THR
1	3a	116	LYS
1	3a	330	GLN
1	5a	3885	PRO
1	5a	7664	SER
1	6a	3778	LEU
1	6a	7839	TYR
1	7a	3869	ALA
1	7a	7495	VAL
1	8a	153	ASN
1	9a	7512	PRO
1	9a	7584	PRO
1	10a	7495	VAL
1	10a	7503	ALA
1	1a	7590	GLY
1	2a	7512	PRO
1	3a	3884	GLN
1	7a	7512	PRO
1	7a	7584	PRO
1	8a	53	SER
1	8a	7611	PRO
1	10a	3778	LEU
1	3a	153	ASN

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Mol	Chain	Res	Type
1	5a	7512	PRO
1	7a	116	LYS
1	8a	7511	CYS
1	8a	7584	PRO
1	8a	7860	THR
1	10a	7584	PRO
1	1a	7584	PRO
1	1a	7824	ILE
1	3a	7610	LYS
1	5a	7584	PRO
1	8a	3990	PRO
1	9a	7459	VAL
1	1a	52	GLY
1	2a	7824	ILE
1	6a	7610	LYS
1	7a	7824	ILE
1	8a	7824	ILE
1	3a	7711	PRO
1	5a	7495	VAL
1	5a	7610	LYS
1	6a	126	GLY
1	5a	7824	ILE
1	7a	52	GLY
1	9a	3778	LEU
1	10a	7549	GLY
1	10a	7711	PRO
1	3a	7824	ILE
1	9a	3885	PRO

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
1	3a	1
1	4a	1
1	7a	1
1	10a	1
1	8a	1
1	2a	1
1	1a	1
1	6a	1
1	5a	1
1	9a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3a	11598:ASP	C	14913:VAL	N	29.53
1	4a	11598:ASP	C	14913:VAL	N	27.35
1	7a	11598:ASP	C	14913:VAL	N	27.29
1	10a	11598:ASP	C	14913:VAL	N	25.41
1	8a	11598:ASP	C	14913:VAL	N	24.86
1	2a	11598:ASP	C	14913:VAL	N	19.86
1	1a	11598:ASP	C	14913:VAL	N	19.26
1	6a	11598:ASP	C	14913:VAL	N	17.88
1	5a	11598:ASP	C	14913:VAL	N	17.67
1	9a	11598:ASP	C	14913:VAL	N	4.91

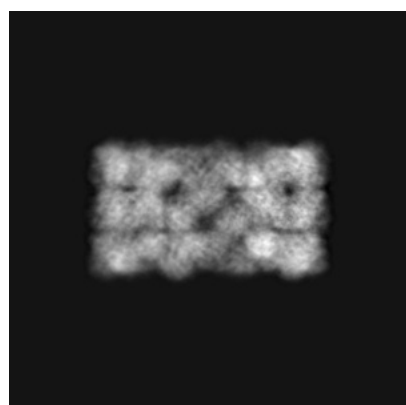
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4750. These allow visual inspection of the internal detail of the map and identification of artifacts.

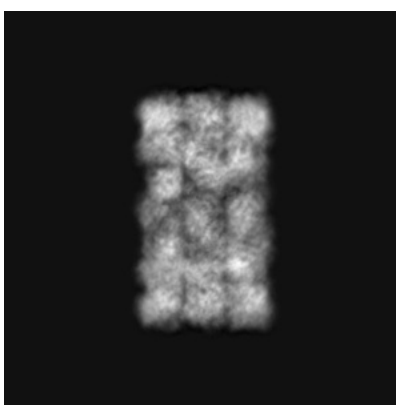
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

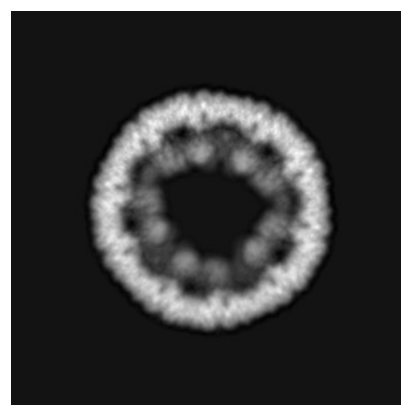
6.1.1 Primary map



X



Y

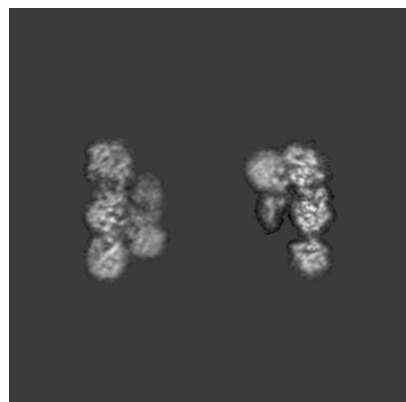


Z

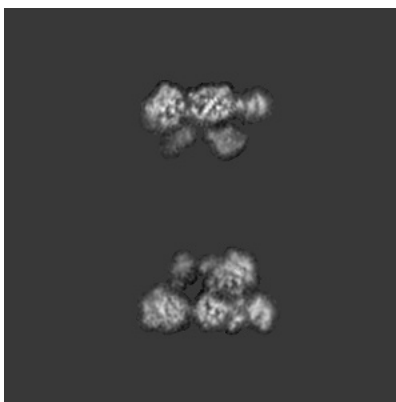
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225



Y Index: 225

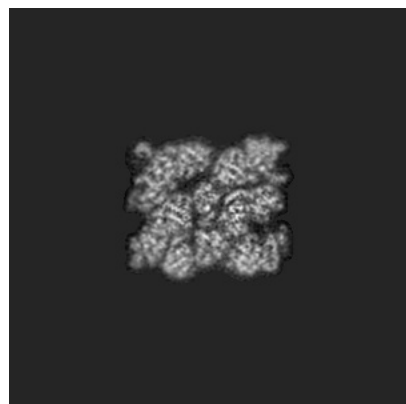


Z Index: 225

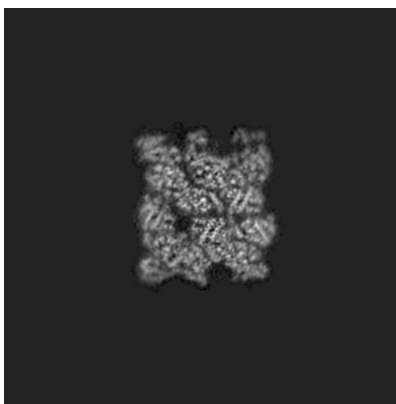
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

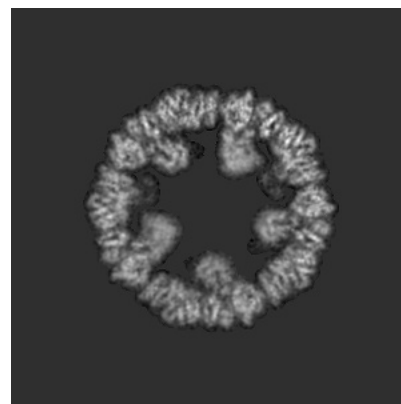
6.3.1 Primary map



X Index: 331



Y Index: 333

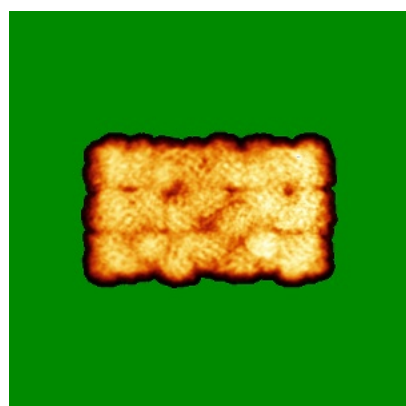


Z Index: 181

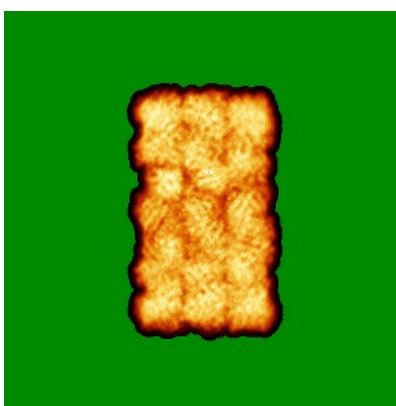
The images above show the largest variance slices of the map in three orthogonal directions.

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

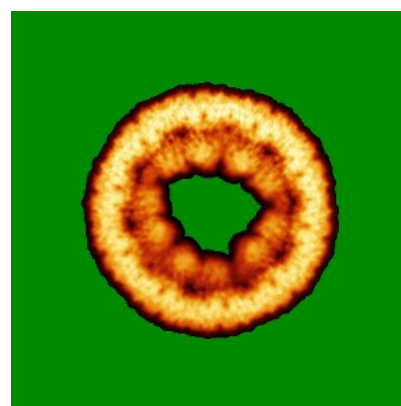
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

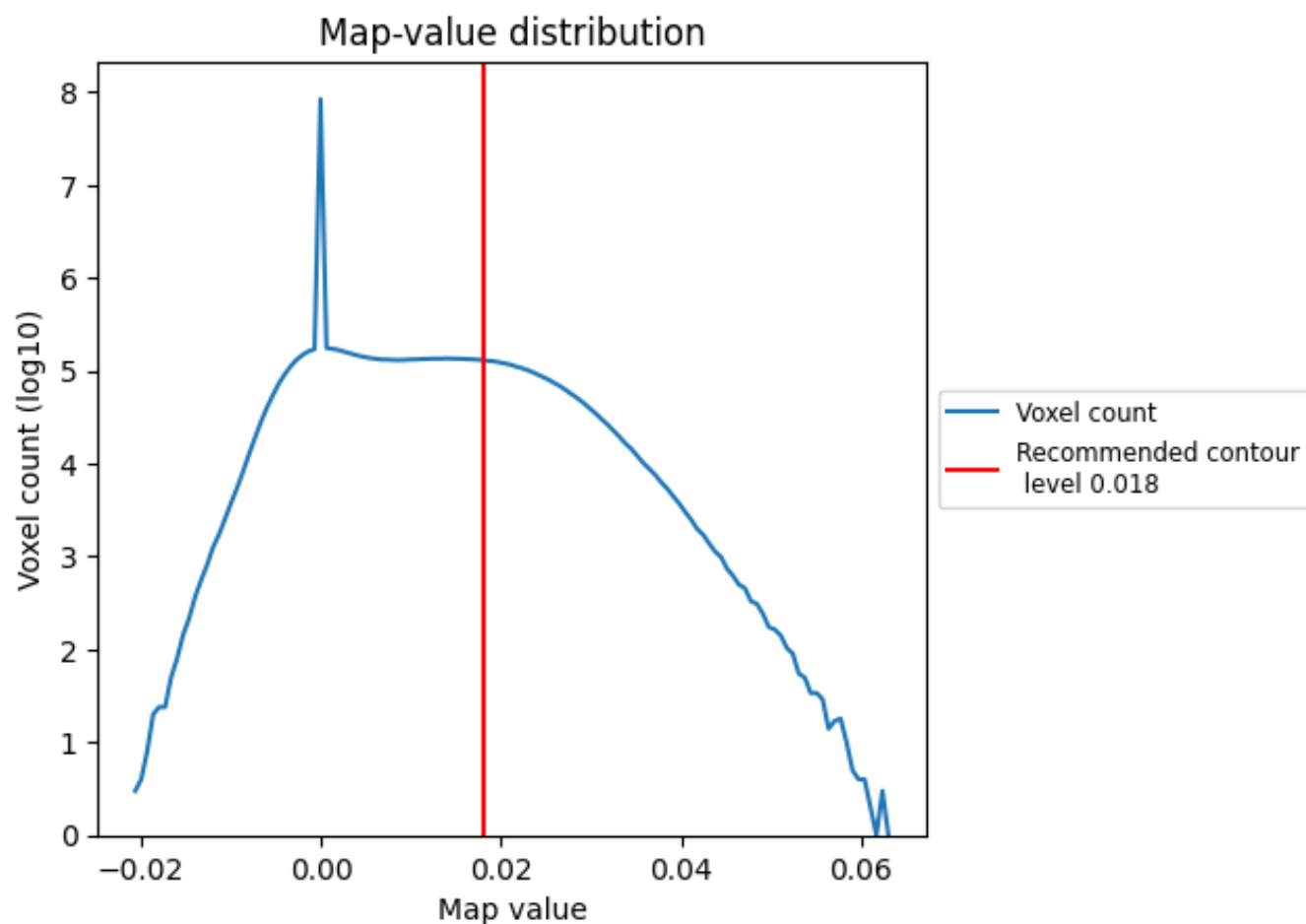
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

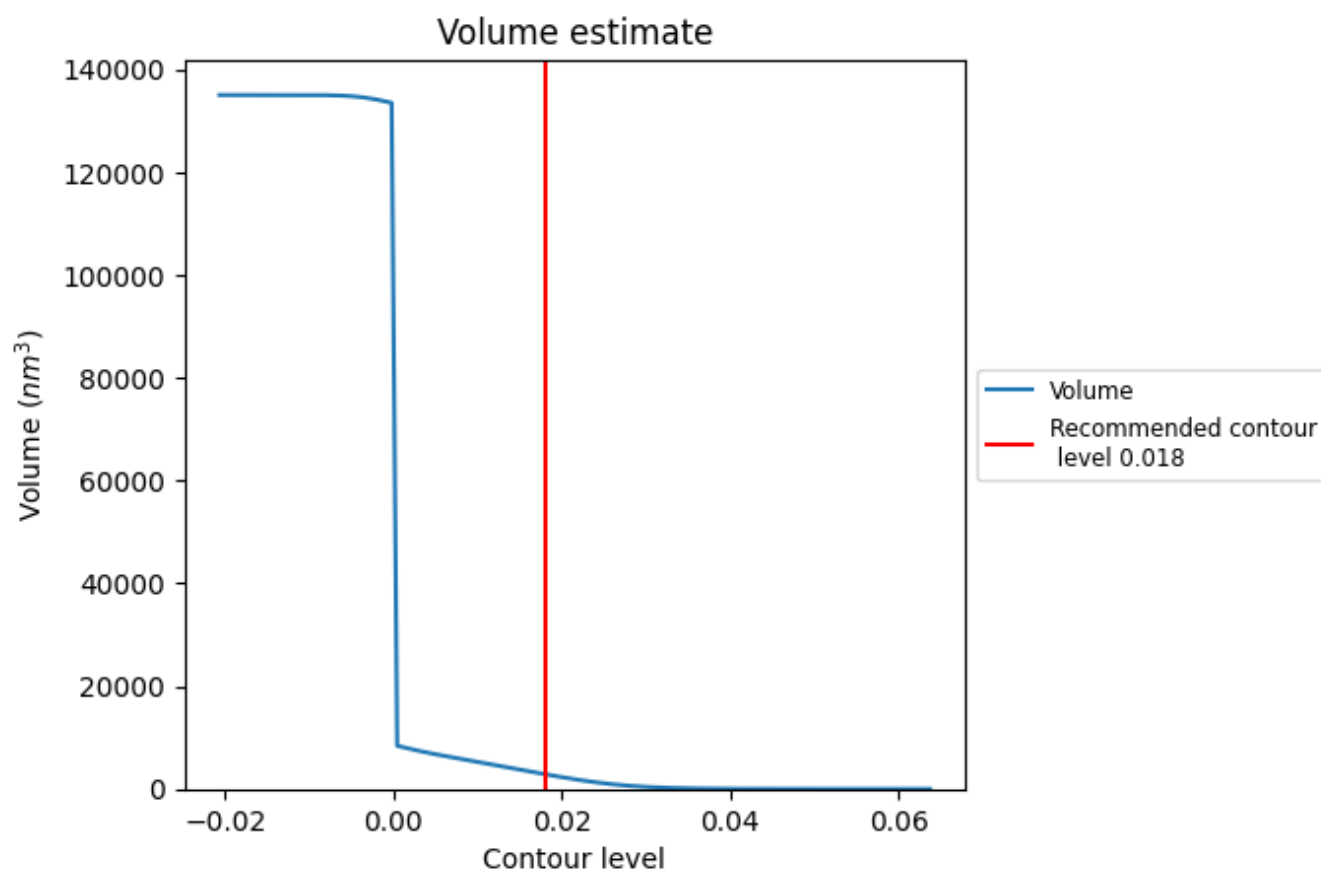
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

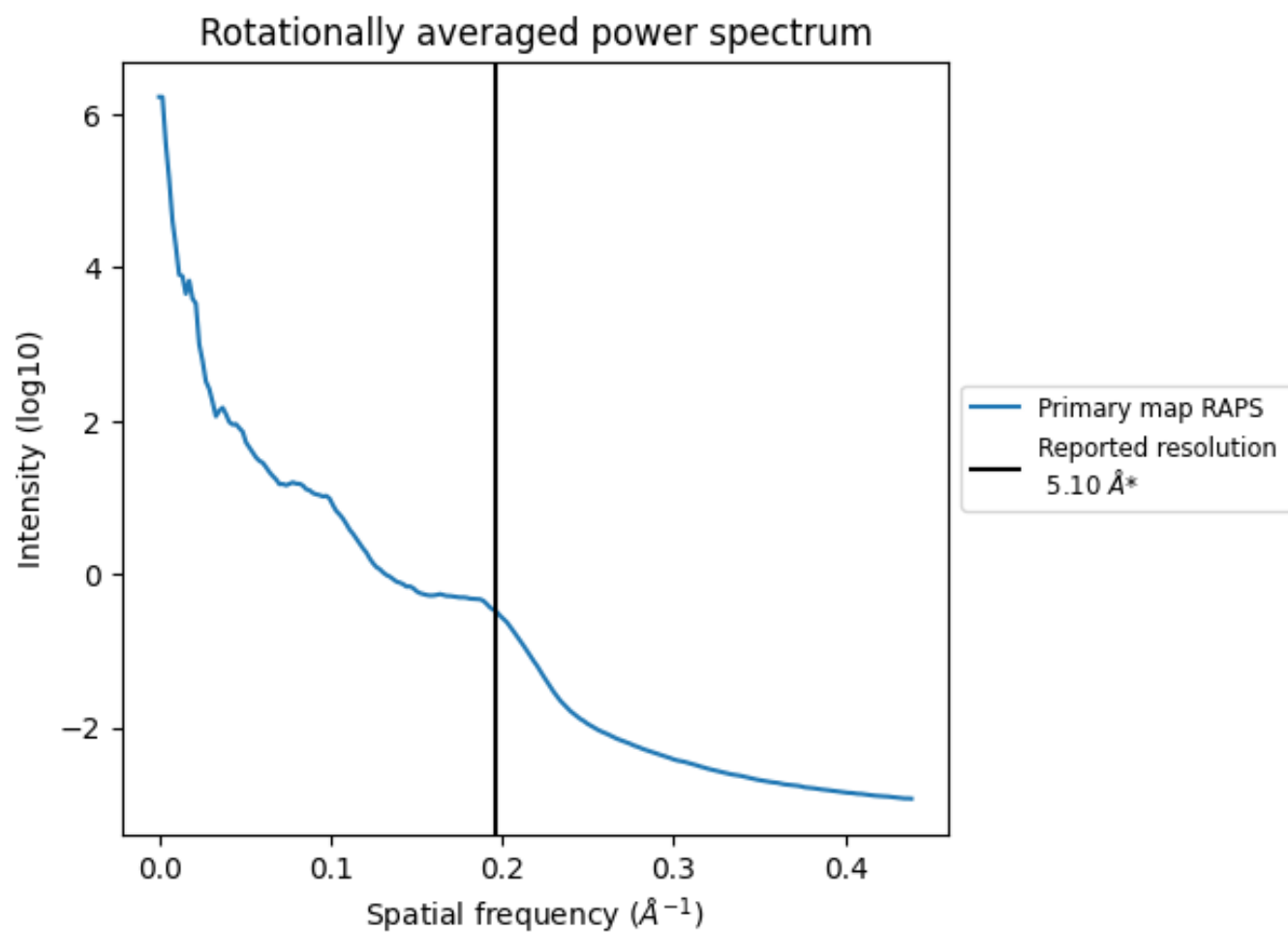
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2864 nm^3 ; this corresponds to an approximate mass of 2587 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 0.196 Å⁻¹

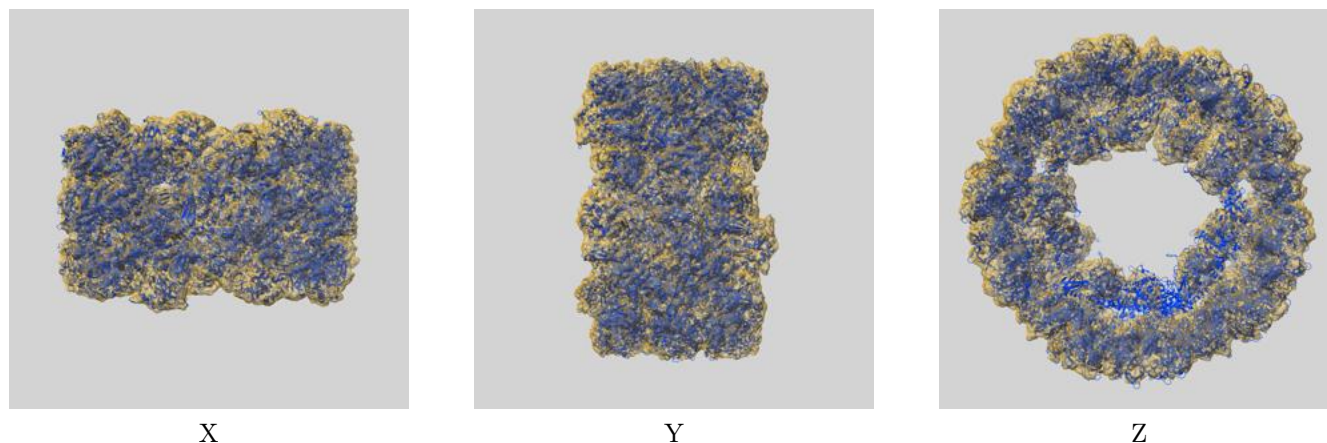
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

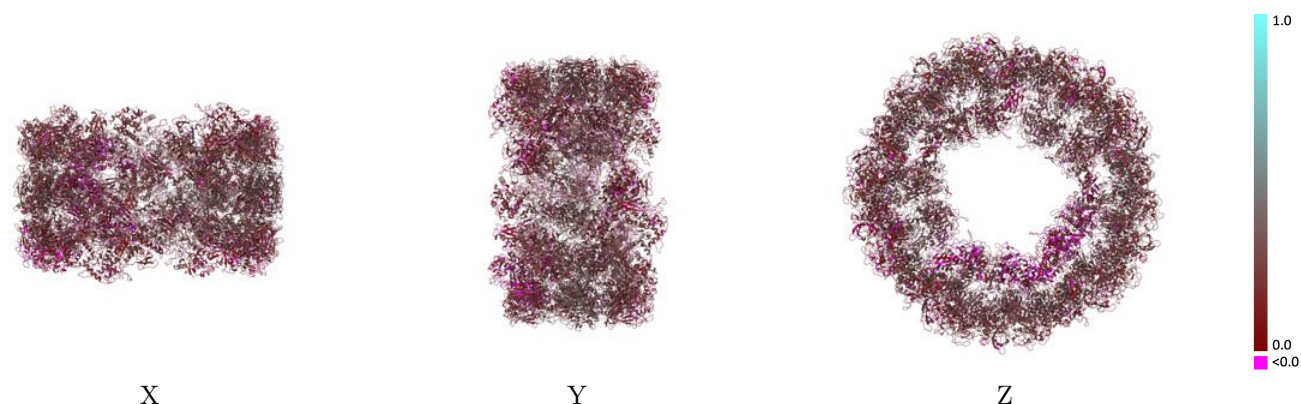
This section contains information regarding the fit between EMDB map EMD-4750 and PDB model 6R83. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



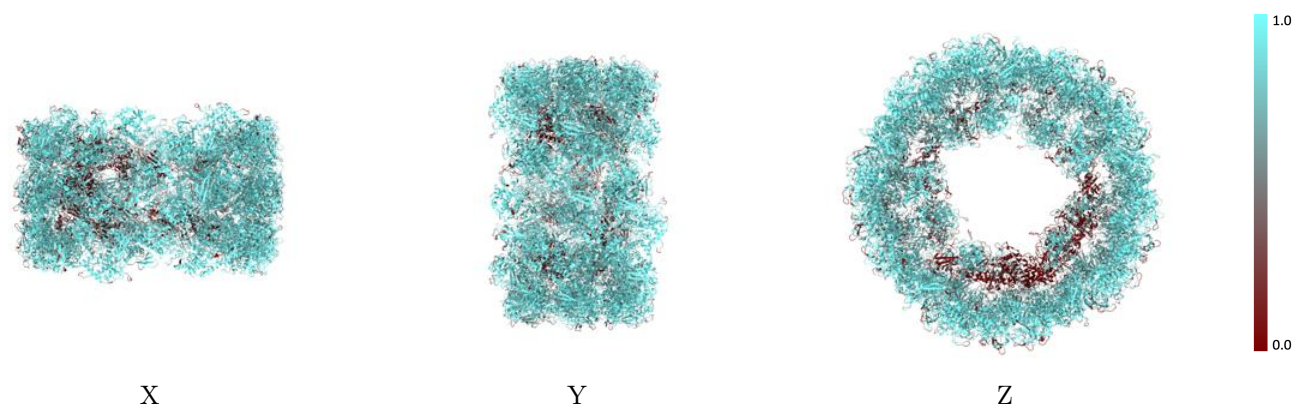
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



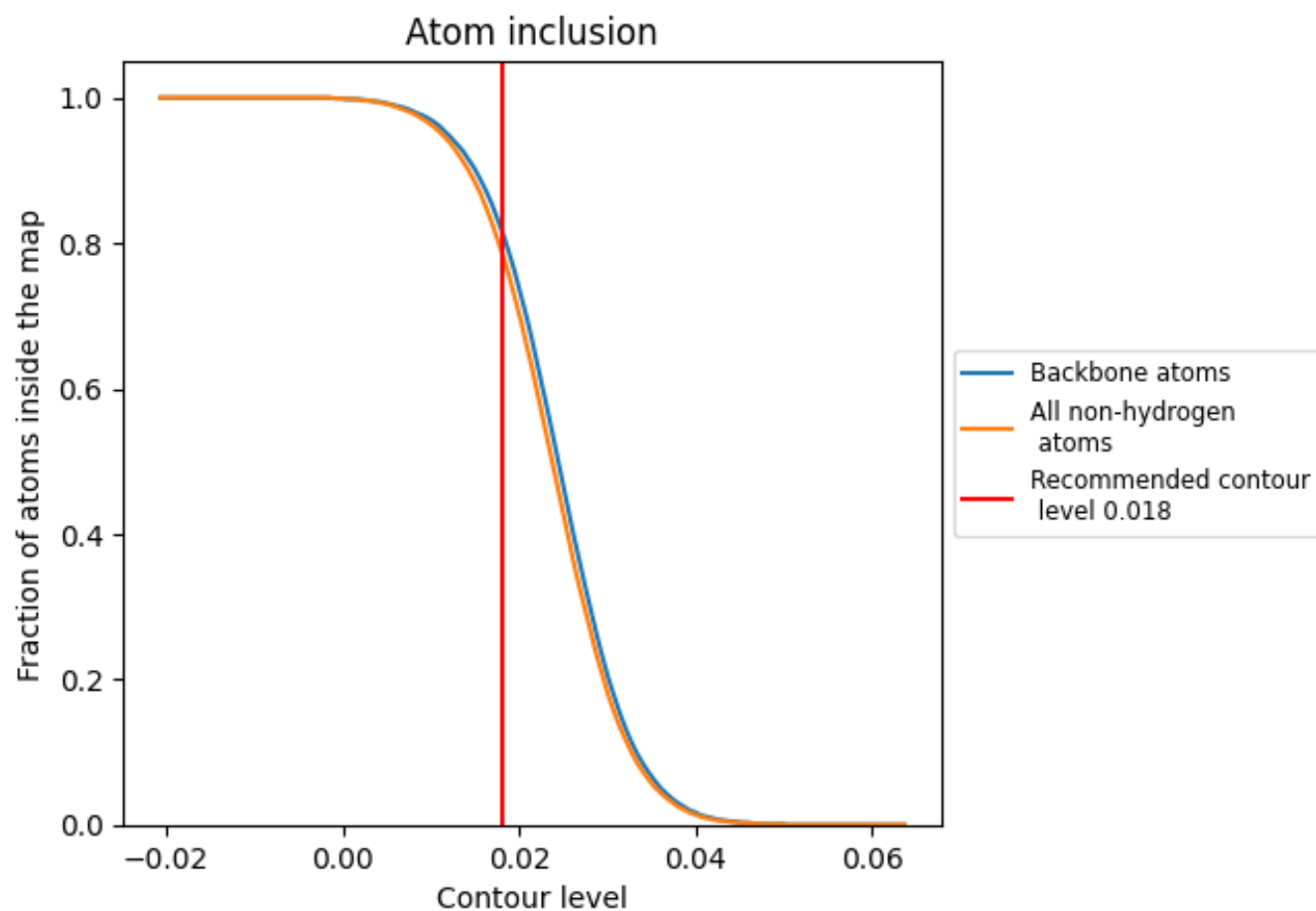
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.2300
10a	0.7430	0.2150
1a	0.7860	0.2310
2a	0.7830	0.2310
3a	0.8730	0.2430
4a	0.8780	0.2550
5a	0.8320	0.2410
6a	0.7810	0.2290
7a	0.7740	0.2260
8a	0.7840	0.2350
9a	0.6620	0.1930

1.0

0.0

<0.0