



Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 07:44 AM EST

PDB ID : 6F9D
EMDB ID : EMD-4199
Title : Model of the Rift Valley fever virus glycoprotein hexamer type 2
Authors : Halldorsson, S.; Bowden, T.A.; Huiskonen, J.T.
Deposited on : 2017-12-14
Resolution : 13.30 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

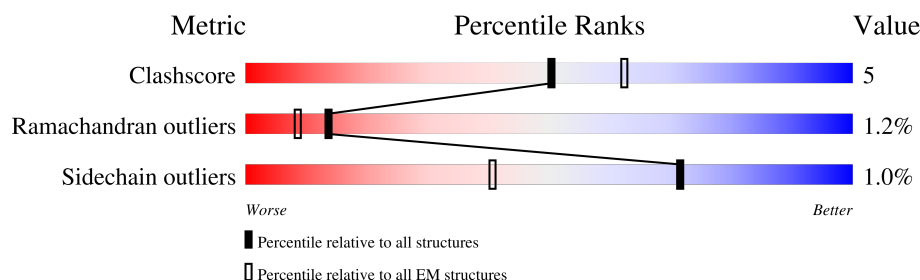
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	316	<div> <div>57%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	C	316	<div> <div>56%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
1	E	316	<div> <div>53%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>5%</div> </div> </div>
1	G	316	<div> <div>54%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	I	316	<div> <div>51%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
1	K	316	<div> <div>52%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>5%</div> </div> </div>
2	B	431	<div> <div>100%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> </div>
2	D	431	<div> <div>100%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	431	<div><div></div><div>100%</div><div>81%18%</div></div>
2	H	431	<div><div></div><div>100%</div><div>87%13%</div></div>
2	J	431	<div><div></div><div>100%</div><div>84%16%</div></div>
2	L	431	<div><div></div><div>100%</div><div>85%14%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33048 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 Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	C	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	E	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	G	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	I	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		
1	K	301	Total	C	N	O	S	0	0
			2284	1437	400	441	6		

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	D	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	F	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	H	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	J	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		
2	L	431	Total	C	N	O	S	0	0
			3224	2006	561	652	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	688	ASP	-	expression tag	UNP A2T072
B	689	PRO	-	expression tag	UNP A2T072

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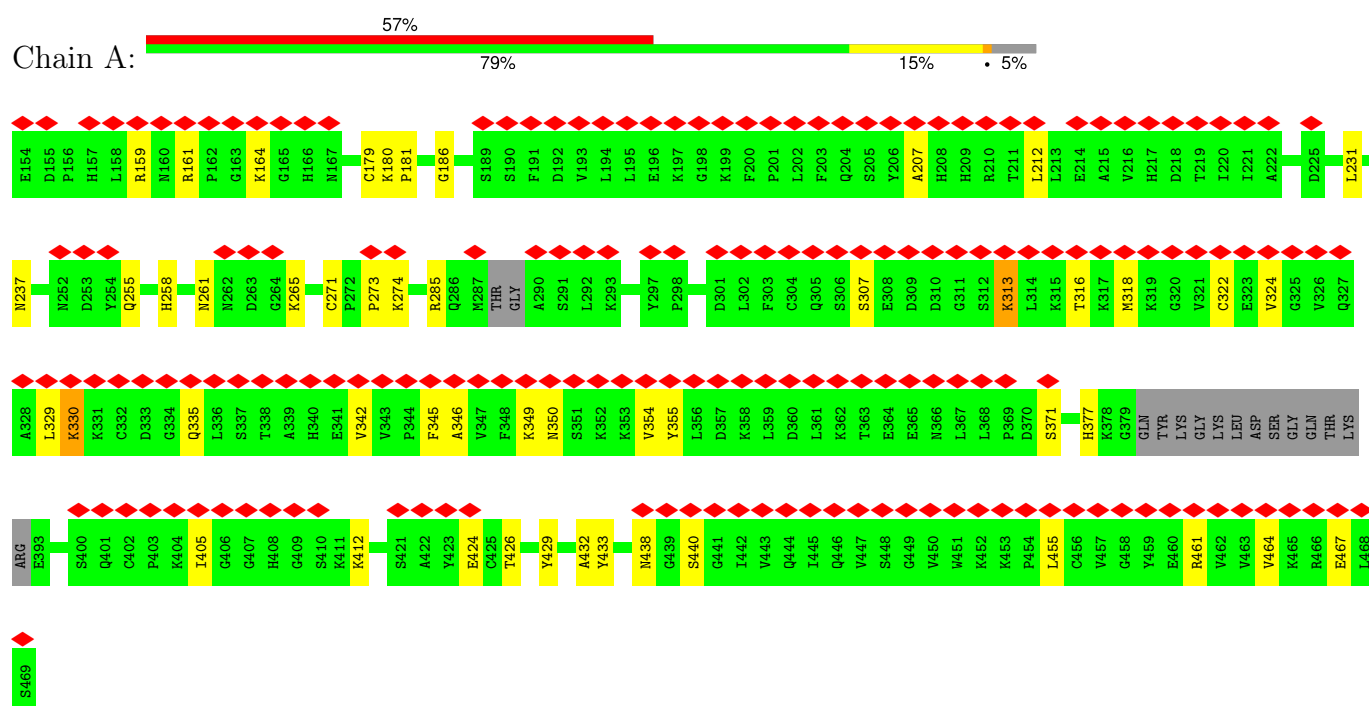
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Chain	Residue	Modelled	Actual	Comment	Reference
B	690	GLY	-	expression tag	UNP A2T072
D	688	ASP	-	expression tag	UNP A2T072
D	689	PRO	-	expression tag	UNP A2T072
D	690	GLY	-	expression tag	UNP A2T072
F	688	ASP	-	expression tag	UNP A2T072
F	689	PRO	-	expression tag	UNP A2T072
F	690	GLY	-	expression tag	UNP A2T072
H	688	ASP	-	expression tag	UNP A2T072
H	689	PRO	-	expression tag	UNP A2T072
H	690	GLY	-	expression tag	UNP A2T072
J	688	ASP	-	expression tag	UNP A2T072
J	689	PRO	-	expression tag	UNP A2T072
J	690	GLY	-	expression tag	UNP A2T072
L	688	ASP	-	expression tag	UNP A2T072
L	689	PRO	-	expression tag	UNP A2T072
L	690	GLY	-	expression tag	UNP A2T072

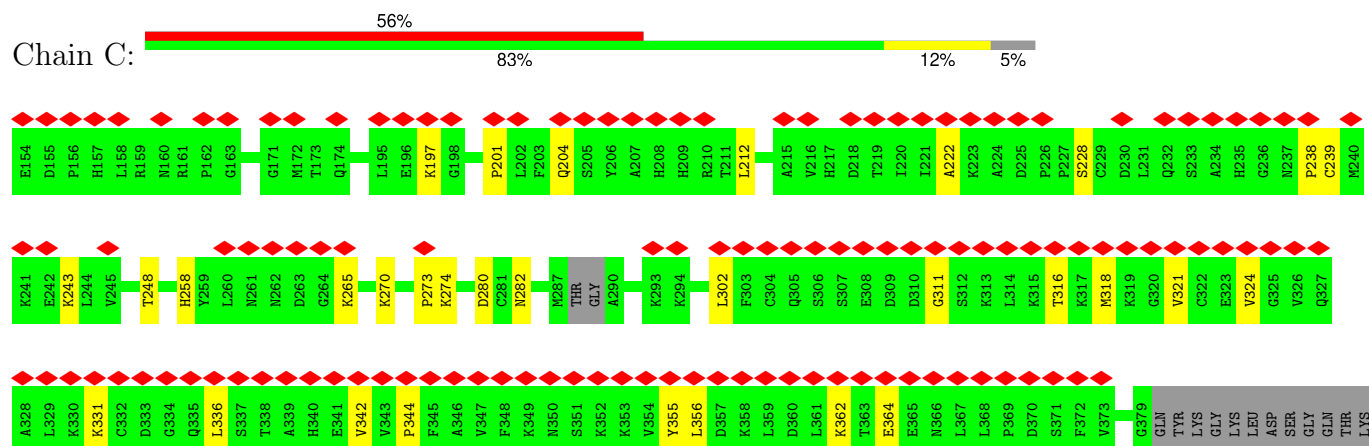
3 Residue-property plots

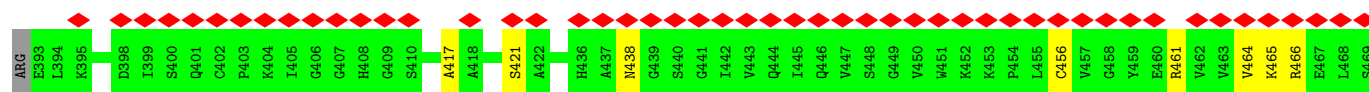
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Glycoprotein

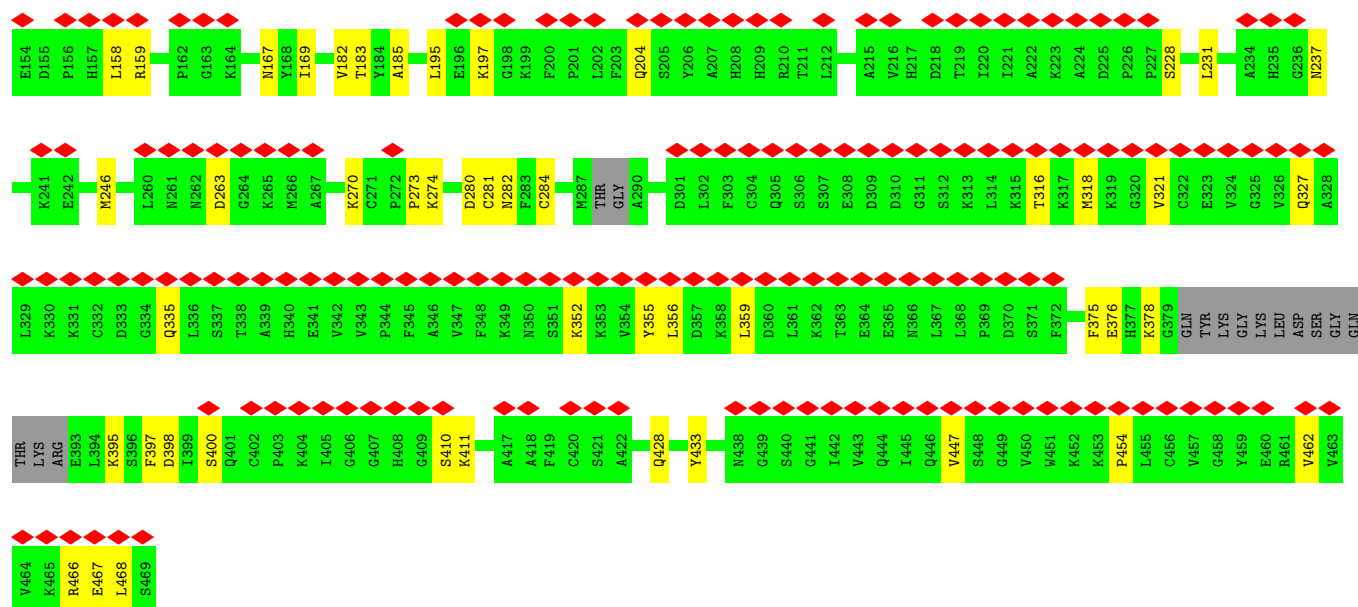
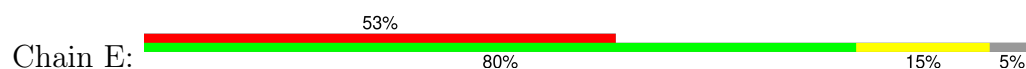


• Molecule 1: Glycoprotein

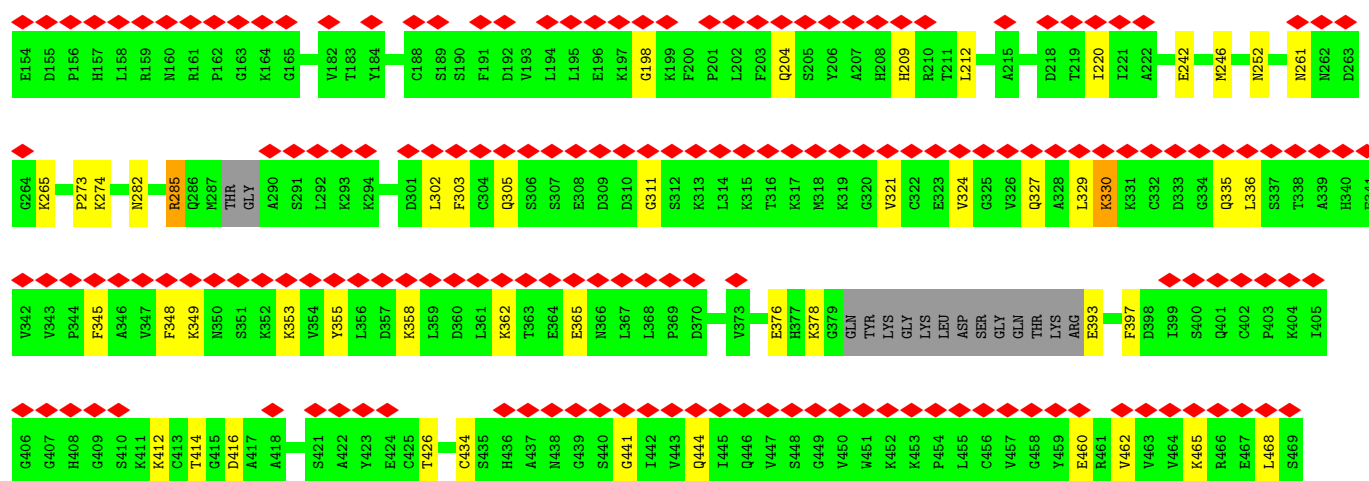
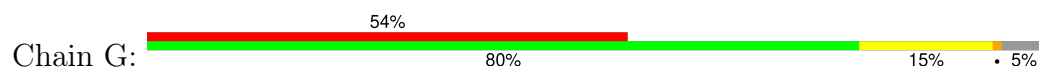




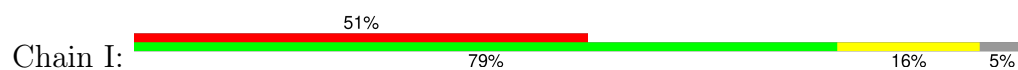
• Molecule 1: Glycoprotein

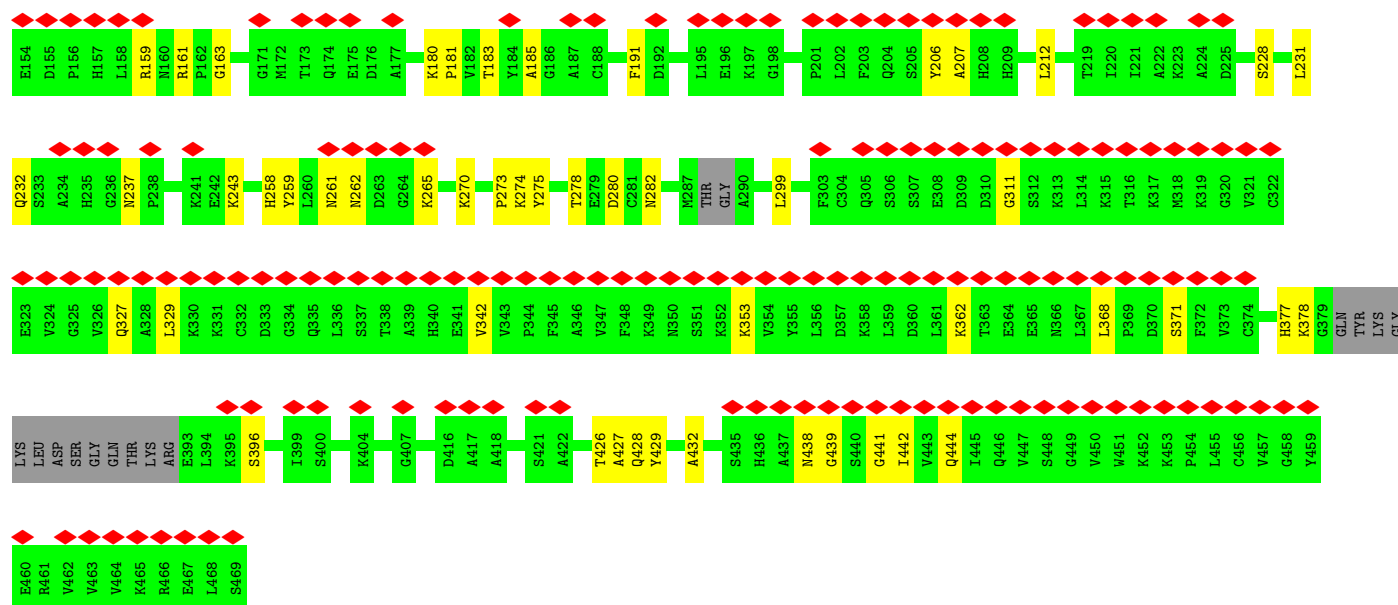


• Molecule 1: Glycoprotein

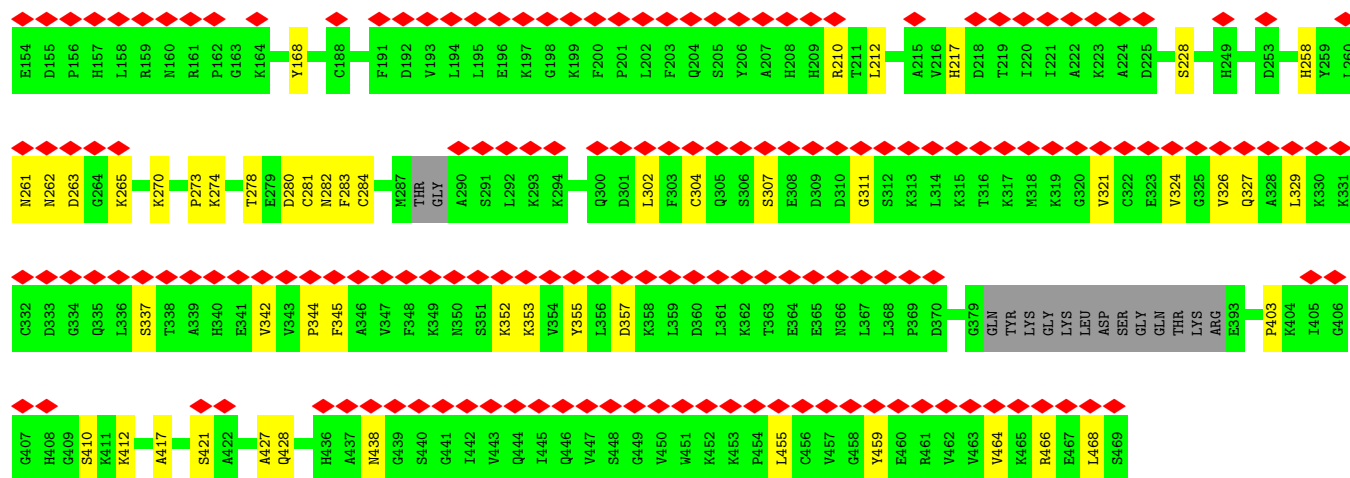
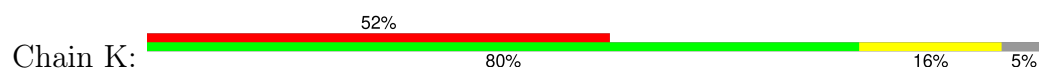


• Molecule 1: Glycoprotein

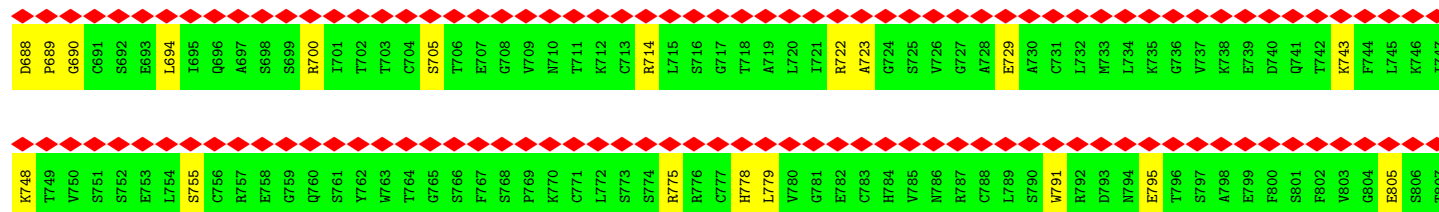
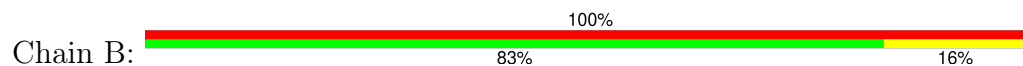


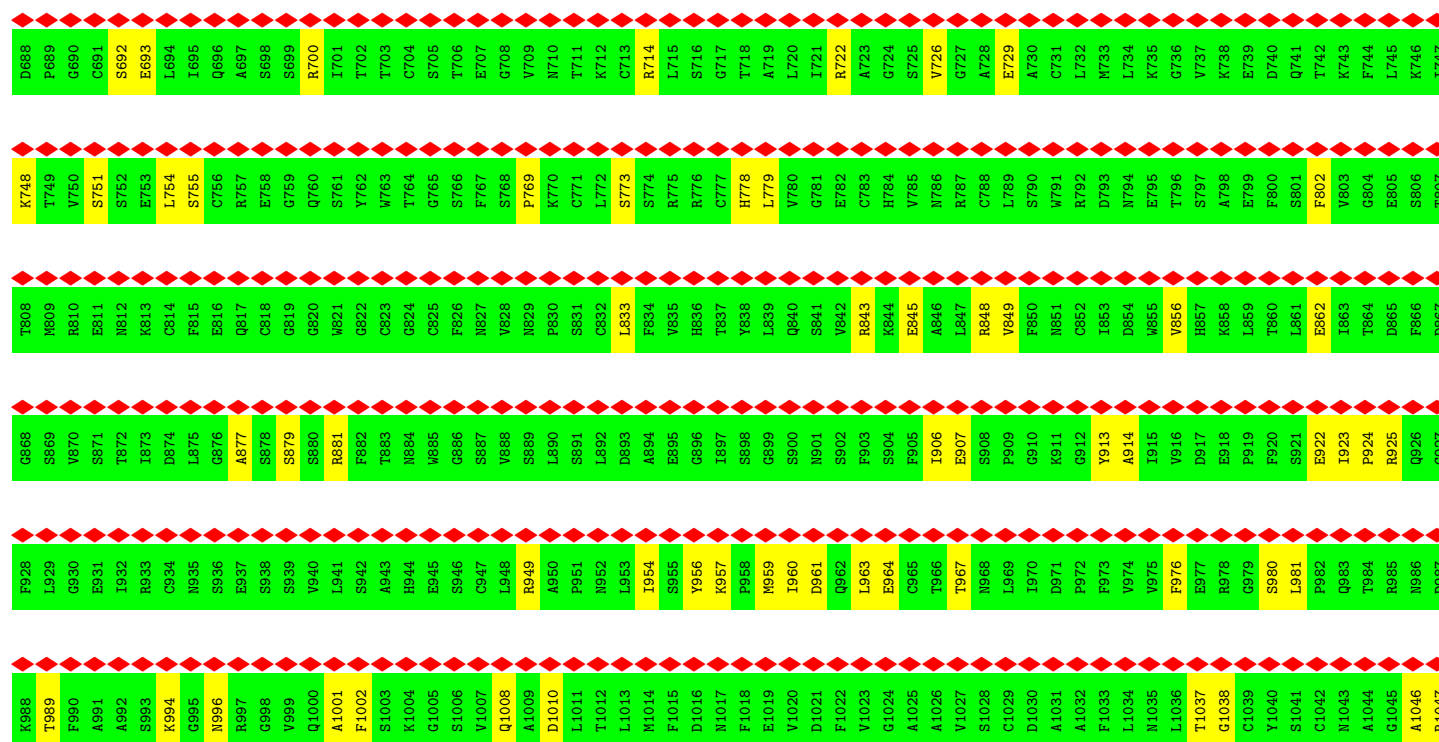


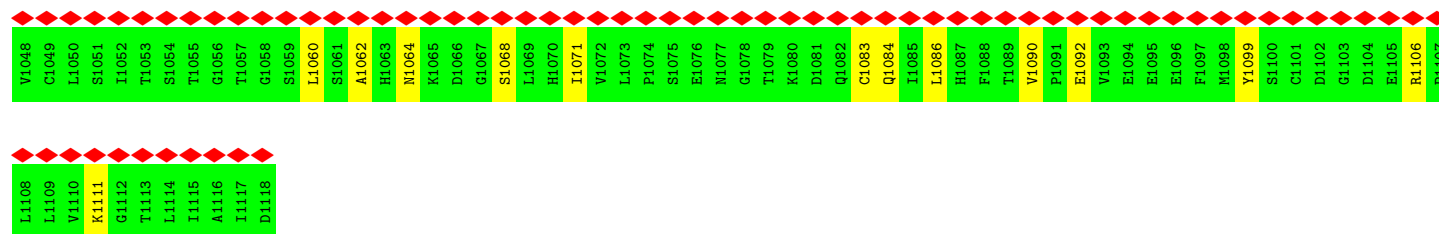
• Molecule 1: Glycoprotein



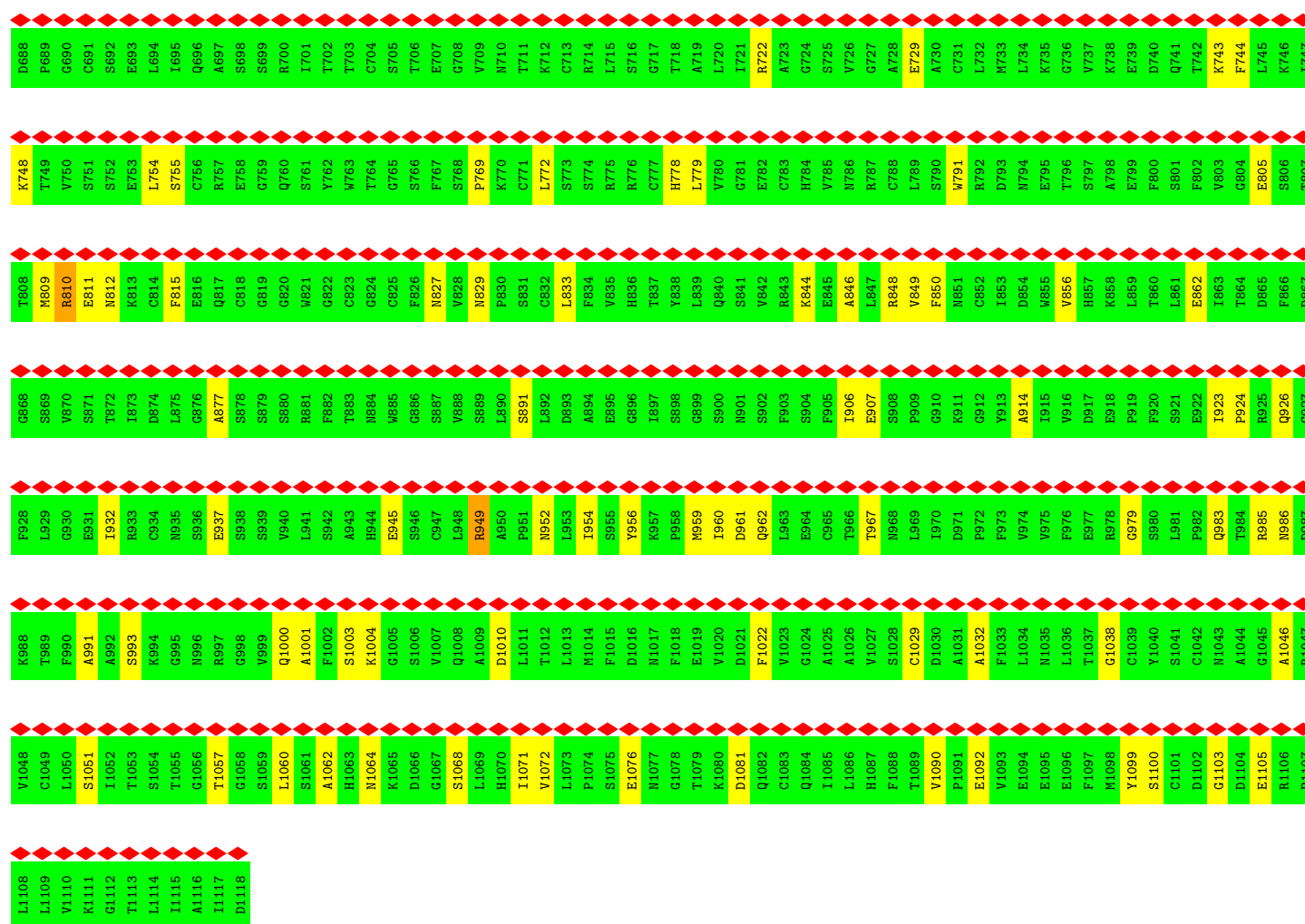
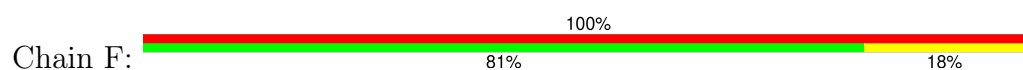
• Molecule 2: Glycoprotein



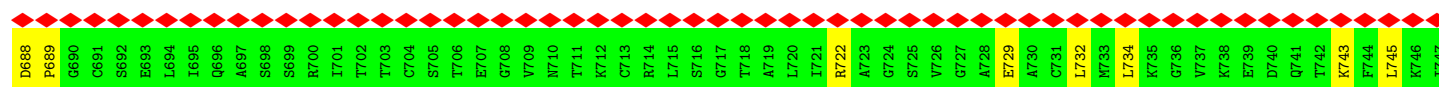
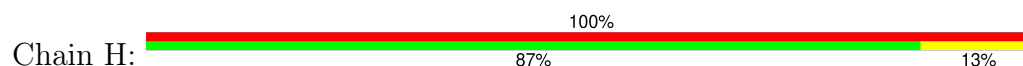




• Molecule 2: Glycoprotein

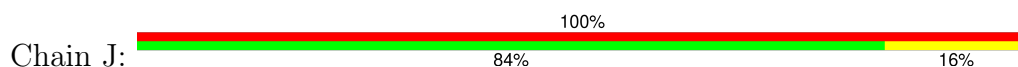


• Molecule 2: Glycoprotein

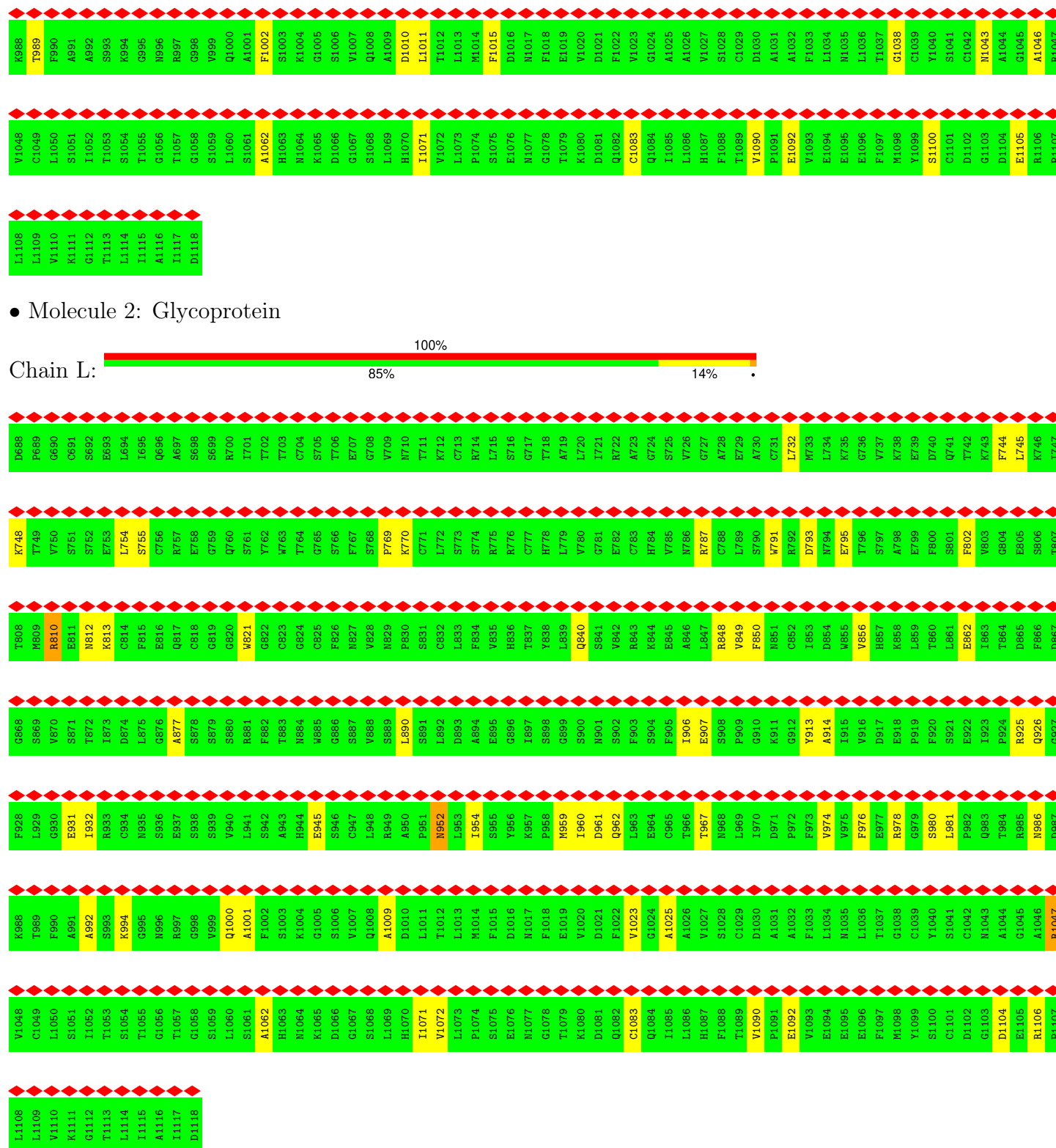


K748	T808	G868	F928	K988	V1048	L1108
T749	M809	S869	L929	T989	C1049	L1109
V750	R810	V870	G930	F990	L1050	V1110
S751	E811	S871	E931	A991	S1051	K1111
S752	N812	T872	R932	A992	T1052	G1112
E753	K813	I873	R933	S993	T1053	T1113
L754	C814	D874	C934	K994	S1054	L1114
S755	F815	L875	N935	G995	T1055	I1115
C756	E816	G876	S936	N996	G1056	A1116
R757	Q817	A877	E937	R997	T1057	I1117
E758	C818	S878	S938	G998	G1058	D1118
G759	G819	S879	S939	V999	S1059	
Q760	G820	S880	V940	Q1000	L1060	
S761	W821	R881	L941	A1001	S1061	
Y762	G822	F882	S942	F1002	A1062	
W763	C823	T883	A943	S1003	H1063	
T764	G824	N884	H944	K1004	N1064	
G765	C825	W885	E945	G1005	K1065	
S766	F826	G886	S946	S1006	D1066	
F767	N827	S887	C947	T1007	G1067	
S768	V828	S888	L948	Q1008	S1068	
P769	N829	S889	R949	A1009	L1069	
K770	P830	L890	A950	D1010	H1070	
C771	S831	S891	P951	L1011	T1071	
L772	C832	L892	N952	T1012	V1072	
S773	F833	D893	L953	L1013	L1073	
R775	V835	A894	I954	M1014	P1074	
R776	H836	E895	S955	F1015	S1075	
C777	T837	G896	Y956	D1016	E1076	
H778	Y838	I897	K957	N1017	T1077	
L779	L839	S898	P958	F1018	G1078	
V780	Q840	G899	N959	E1019	T1079	
G781	S841	S900	I960	V1020	K1080	
E782	V842	N901	D961	D1021	L1081	
C783	R843	S902	Q962	F1022	Q1082	
H784	K844	F903	L963	V1023	Q1083	
V785	E845	S904	E964	G1024	Q1084	
N786	A846	F905	C965	A1025	T1085	
R787	L847	I906	T966	A1026	L1086	
C788	R848	E907	T967	V1027	H1087	
L789	N849	S908	N968	S1028	F1088	
S790	F850	P909	L969	C1029	T1089	
W791	N851	G910	I970	D1030	V1090	
R792	C852	K911	D971	A1031	C1091	
D793	I853	G912	F972	A1032	E1092	
N794	D854	Y913	F973	F1033	V1093	
E795	W855	A914	V974	L1034	E1094	
T796	V856	I915	V975	M1035	E1095	
S797	V857	V916	F976	L1036	E1096	
A798	K858	D917	E977	T1037	F1097	
E799	L859	E918	R978	G1038	M1098	
F800	T860	P919	G979	C1039	Y1099	
S801	L861	F920	S980	Y1040	S1100	
F802	E862	S921	L981	C1041	C1101	
V803	T863	E922	P982	C1042	D1102	
G804	I864	I923	Q983	M1043	G1103	
E805	D865	P924	T984	A1044	D1104	
S806	F866	R925	N985	G1045	R1105	
T807	D867	Q926	D987	A1046	L1106	
		G927		R1047	P1107	

• Molecule 2: Glycoprotein



D688	K748	T808	G868	F928	V1048	L1108
P689	T749	M809	S869	P689	C1049	L1109
G690	V750	R810	V870	G690	L1050	V1110
C691	S751	E811	S871	C691	S1051	K1111
S692	S752	N812	T872	S692	T1052	G1112
E693	E753	K813	I873	E693	T1053	T1113
L694	L754	C814	D874	L694	S1054	L1114
I695	S755	F815	L875	I695	T1055	I1115
Q696	C756	E816	G876	Q696	G1056	A1116
A697	R757	Q817	A877	A697	T1057	I1117
S698	E758	C818	S878	S698	G1058	D1118
S699	G759	G819	S879	S699	S1059	
R700	Q760	G820	S880	R700	L1060	
I701	S761	W821	R881	I701	S1061	
T702	Y762	G822	F882	T702	A1062	
T703	W763	C823	T883	T703	H1063	
C704	T764	G824	N884	C704	N1064	
S705	G765	C825	W885	S705	K1065	
T706	S766	F826	G886	T706	D1066	
E707	F767	N827	S887	E707	G1067	
G708	S768	V828	S888	G708	S1068	
V709	P769	N829	S889	V709	L1069	
W710	K770	P830	L890	W710	H1070	
T711	C771	S831	S891	T711	T1071	
K712	L772	C832	L892	K712	V1072	
C713	S773	L833	D893	C713	L1073	
R714	S774	F834	A894	R714	P1074	
L715	R775	V835	E895	L715	S1075	
S716	R776	H836	G896	S716	E1076	
G717	C777	T837	I897	G717	T1077	
T718	H778	Y838	S898	T718	G1078	
A719	L779	L839	G899	A719	T1079	
L720	V780	Q840	S900	L720	K1080	
T721	G781	S841	N901	T721	L1081	
R722	E782	V842	S902	R722	Q1082	
A723	C783	R843	F903	A723	Q1083	
G724	H784	E844	S904	G724	Q1084	
S725	V785	E845	F905	S725	T1085	
V726	N786	A846	I906	V726	L1086	
G727	R787	L847	E907	G727	H1087	
A728	C788	R848	S908	A728	F1088	
E729	L789	N849	P909	E729	T1089	
A730	S790	F850	G910	A730	V1090	
C731	W791	N851	K911	C731	C1091	
L732	R792	C852	G912	L732	E1092	
M733	D793	I853	Y913	M733	V1093	
L734	N794	D854	A914	L734	E1094	
K735	E795	W855	I915	K735	E1095	
G736	T796	V856	V916	G736	E1096	
V737	S797	V857	D917	V737	F1097	
K738	A798	K858	E918	K738	M1098	
E739	E799	L859	P919	E739	Y1099	
D740	F800	T860	F920	D740	S1100	
Q741	S801	L861	S921	Q741	C1101	
T742	F802	E862	E922	T742	D1102	
K743	V803	T863	I923	K743	G1103	
F744	G804	D864	P924	F744	D1104	
L745	E805	D865	R925	L745	R1105	
K746	S806	F866	Q926	K746	L1106	
I747	T807	D867	G927	I747	P1107	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2995	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	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	0.101	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.7, 2.7, 2.7	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/2333	0.41	0/3136
1	C	0.24	0/2333	0.40	0/3136
1	E	0.24	0/2333	0.42	0/3136
1	G	0.24	0/2333	0.41	0/3136
1	I	0.24	0/2333	0.41	0/3136
1	K	0.24	0/2333	0.40	0/3136
2	B	0.24	0/3284	0.41	0/4431
2	D	0.24	0/3284	0.42	0/4431
2	F	0.24	0/3284	0.42	0/4431
2	H	0.24	0/3284	0.42	0/4431
2	J	0.24	0/3284	0.43	0/4431
2	L	0.24	0/3284	0.43	0/4431
All	All	0.24	0/33702	0.42	0/45402

There are no bond length outliers.

There are no bond angle outliers.

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	2284	0	2205	26	0
1	C	2284	0	2205	19	0
1	E	2284	0	2205	27	0
1	G	2284	0	2205	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2284	0	2205	26	0
1	K	2284	0	2205	26	0
2	B	3224	0	3071	38	0
2	D	3224	0	3071	35	0
2	F	3224	0	3071	43	0
2	H	3224	0	3071	28	0
2	J	3224	0	3071	36	0
2	L	3224	0	3071	34	0
All	All	33048	0	31656	348	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 5.

All (348) 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:K:212:LEU:HB2	1:K:302:LEU:HD11	1.77	0.66
2:D:748:LYS:HB3	2:D:862:GLU:HB3	1.79	0.65
2:B:1062:ALA:HB3	2:B:1071:ILE:HB	1.79	0.64
2:F:805:GLU:OE2	2:F:810:ARG:NH2	2.30	0.64
2:H:1062:ALA:HB3	2:H:1071:ILE:HB	1.78	0.64
2:F:791:TRP:HE1	2:F:812:ASN:HB3	1.62	0.63
2:L:748:LYS:HB3	2:L:862:GLU:HB3	1.81	0.63
2:D:729:GLU:HG2	2:D:748:LYS:HA	1.81	0.62
2:B:805:GLU:OE2	2:B:810:ARG:NH2	2.32	0.62
2:J:729:GLU:HG2	2:J:748:LYS:HA	1.81	0.62
2:L:1104:ASP:OD2	2:L:1106:ARG:NH1	2.33	0.62
1:E:321:VAL:HG22	1:E:466:ARG:HG2	1.82	0.61
1:E:316:THR:HG23	1:E:355:TYR:HB2	1.82	0.61
2:L:1062:ALA:HB3	2:L:1071:ILE:HB	1.83	0.61
1:E:197:LYS:HA	1:E:204:GLN:HE22	1.66	0.60
2:F:748:LYS:HB3	2:F:862:GLU:HB3	1.83	0.60
2:H:732:LEU:HB3	2:H:745:LEU:HB3	1.82	0.60
1:I:261:ASN:HD21	1:I:265:LYS:HB2	1.65	0.60
2:J:732:LEU:HB3	2:J:745:LEU:HB3	1.85	0.59
1:E:359:LEU:H	2:F:772:LEU:HG	1.68	0.58
1:G:376:GLU:HB2	1:G:397:PHE:HB2	1.85	0.58
1:K:403:PRO:HG2	1:K:412:LYS:HD3	1.86	0.58
1:C:212:LEU:HD13	1:C:302:LEU:HD11	1.86	0.58
1:E:375:PHE:HB2	1:E:433:TYR:HB3	1.84	0.58
1:E:280:ASP:OD2	1:E:282:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:HE22	2:L:821:TRP:HB2	1.70	0.57
1:C:197:LYS:HA	1:C:204:GLN:HE22	1.69	0.57
2:D:849:VAL:HG22	2:D:906:ILE:HG12	1.87	0.57
1:C:316:THR:HG23	1:C:355:TYR:HB2	1.86	0.57
2:D:906:ILE:HB	2:D:914:ALA:HB3	1.87	0.57
2:F:849:VAL:HG22	2:F:906:ILE:HG12	1.87	0.57
2:H:966:THR:HG1	2:J:879:SER:HG	1.51	0.57
1:G:336:LEU:HD11	1:G:465:LYS:HB3	1.86	0.56
2:F:1032:ALA:HB3	2:F:1051:SER:HB3	1.87	0.56
1:E:158:LEU:HD12	1:E:159:ARG:HG3	1.86	0.56
2:L:974:VAL:O	2:L:978:ARG:HB2	2.05	0.56
2:B:1064:ASN:HD21	2:B:1068:SER:H	1.51	0.56
2:F:1060:LEU:HD21	2:F:1099:TYR:HB2	1.88	0.56
1:I:262:ASN:OD1	1:I:327:GLN:NE2	2.40	0.55
2:J:849:VAL:HG22	2:J:906:ILE:HG12	1.88	0.55
2:L:732:LEU:HB3	2:L:745:LEU:HB3	1.88	0.55
1:C:212:LEU:HD23	1:C:258:HIS:HD2	1.71	0.55
1:G:198:GLY:H	1:G:204:GLN:HE22	1.54	0.55
2:J:891:SER:HB3	2:J:1010:ASP:HB2	1.88	0.55
2:F:959:MET:HB2	2:F:962:GLN:HB2	1.87	0.55
1:I:371:SER:HA	1:I:441:GLY:HA2	1.88	0.54
2:J:922:GLU:HG2	2:J:923:ILE:HG12	1.88	0.54
2:B:848:ARG:NH2	2:B:907:GLU:OE1	2.39	0.54
2:D:769:PRO:HG3	2:D:967:THR:HG23	1.89	0.54
2:J:748:LYS:HB3	2:J:862:GLU:HB3	1.88	0.54
1:K:321:VAL:HG22	1:K:466:ARG:HG2	1.88	0.54
2:H:849:VAL:HG22	2:H:906:ILE:HG12	1.89	0.54
2:H:906:ILE:HB	2:H:914:ALA:HB3	1.90	0.54
1:E:263:ASP:OD1	1:E:352:LYS:NZ	2.41	0.54
1:I:212:LEU:HD23	1:I:258:HIS:HD2	1.72	0.54
1:K:280:ASP:OD2	1:K:282:ASN:ND2	2.41	0.54
2:D:913:TYR:HB2	2:D:981:LEU:HD12	1.89	0.53
2:B:890:LEU:HD11	2:B:1009:ALA:HB1	1.89	0.53
2:J:711:THR:HB	2:J:741:GLN:HE22	1.73	0.53
2:J:989:THR:HB	2:J:1002:PHE:HB2	1.91	0.53
1:C:201:PRO:HG2	2:D:802:PHE:HB3	1.89	0.53
1:K:261:ASN:HD21	1:K:265:LYS:HB2	1.72	0.53
2:J:879:SER:OG	2:J:881:ARG:NH1	2.41	0.53
2:J:1062:ALA:HB3	2:J:1071:ILE:HB	1.89	0.53
1:A:342:VAL:HG22	1:A:461:ARG:HG2	1.91	0.53
2:H:773:SER:HB2	2:H:833:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:983:GLN:OE1	2:F:985:ARG:NH2	2.42	0.53
1:A:426:THR:HB	1:A:429:TYR:HB2	1.89	0.52
2:B:690:GLY:H	2:B:1085:ILE:HG12	1.74	0.52
1:E:376:GLU:OE1	1:E:395:LYS:NZ	2.37	0.52
1:E:467:GLU:OE1	2:H:1017:ASN:ND2	2.42	0.52
2:F:906:ILE:HB	2:F:914:ALA:HB3	1.92	0.52
1:A:330:LYS:NZ	1:A:467:GLU:OE2	2.42	0.52
2:H:876:GLY:H	2:H:879:SER:HB3	1.74	0.52
1:K:357:ASP:OD2	2:L:770:LYS:NZ	2.40	0.52
2:F:1064:ASN:HD21	2:F:1068:SER:H	1.57	0.52
2:D:773:SER:HB2	2:D:833:LEU:HD11	1.90	0.52
1:C:228:SER:HB2	1:C:270:LYS:HB2	1.92	0.52
2:F:926:GLN:NE2	2:F:952:ASN:O	2.43	0.52
2:H:734:LEU:HB3	2:H:743:LYS:HB2	1.92	0.52
2:J:693:GLU:OE2	2:J:722:ARG:NH2	2.43	0.52
2:B:791:TRP:HE1	2:B:812:ASN:HB3	1.75	0.52
1:C:243:LYS:NZ	1:C:282:ASN:OD1	2.41	0.52
2:D:1064:ASN:HD21	2:D:1068:SER:H	1.58	0.52
1:E:231:LEU:HD23	1:E:237:ASN:HD21	1.74	0.52
1:I:362:LYS:HD2	1:I:444:GLN:HB2	1.92	0.52
2:L:754:LEU:HB2	2:L:1001:ALA:HB3	1.92	0.52
2:B:722:ARG:NH2	2:B:1008:GLN:OE1	2.43	0.52
2:F:1090:VAL:HG22	2:F:1092:GLU:H	1.74	0.52
2:F:1062:ALA:HB3	2:F:1071:ILE:HB	1.92	0.51
2:J:954:ILE:HA	2:J:967:THR:HG22	1.91	0.51
1:G:412:LYS:HD2	1:G:426:THR:HG21	1.91	0.51
1:C:342:VAL:HG22	1:C:461:ARG:HG2	1.93	0.51
2:J:806:SER:O	2:J:810:ARG:NH1	2.44	0.51
2:F:744:PHE:HZ	2:F:1072:VAL:HG13	1.76	0.51
1:A:161:ARG:NH1	1:A:207:ALA:O	2.43	0.51
2:D:879:SER:OG	2:D:881:ARG:NH1	2.41	0.51
2:H:879:SER:OG	2:H:881:ARG:NH1	2.44	0.51
1:K:337:SER:HB2	1:K:468:LEU:HD22	1.93	0.51
1:E:183:THR:HG23	1:E:185:ALA:H	1.76	0.51
1:I:426:THR:HB	1:I:429:TYR:HB2	1.91	0.51
1:A:237:ASN:HD22	1:K:428:GLN:HG3	1.76	0.51
2:D:722:ARG:NH1	2:D:1010:ASP:OD1	2.43	0.51
1:G:345:PHE:HA	1:G:355:TYR:HA	1.93	0.50
1:K:263:ASP:OD1	1:K:352:LYS:NZ	2.40	0.50
1:E:428:GLN:NE2	1:G:282:ASN:O	2.44	0.50
1:I:161:ARG:NH1	1:I:207:ALA:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:721:ILE:HD13	2:J:730:ALA:HB1	1.94	0.50
2:B:795:GLU:O	2:B:812:ASN:ND2	2.44	0.50
1:I:342:VAL:HB	2:J:803:VAL:HG13	1.93	0.50
2:F:815:PHE:HB2	2:F:833:LEU:HB3	1.91	0.50
2:J:1090:VAL:HG22	2:J:1092:GLU:H	1.76	0.50
1:A:349:LYS:NZ	1:A:350:ASN:OD1	2.41	0.50
2:B:775:ARG:HH22	2:B:824:GLY:HA3	1.77	0.50
2:D:1038:GLY:HA3	2:D:1046:ALA:HA	1.92	0.50
2:L:926:GLN:NE2	2:L:952:ASN:O	2.44	0.50
2:L:1090:VAL:HG22	2:L:1092:GLU:H	1.76	0.50
2:F:1057:THR:HA	2:F:1076:GLU:HA	1.94	0.50
2:D:1062:ALA:HB3	2:D:1071:ILE:HB	1.94	0.50
1:I:428:GLN:NE2	1:K:284:CYS:O	2.45	0.50
2:B:1090:VAL:HG22	2:B:1092:GLU:H	1.77	0.49
1:I:280:ASP:OD2	1:I:282:ASN:ND2	2.45	0.49
2:J:700:ARG:HG3	2:J:701:ILE:HG23	1.94	0.49
1:A:377:HIS:NE2	1:A:432:ALA:O	2.46	0.49
2:B:875:LEU:HD21	2:B:888:VAL:HG23	1.93	0.49
1:I:206:TYR:HA	1:I:439:GLY:HA2	1.95	0.49
1:K:278:THR:OG1	1:K:280:ASP:OD1	2.30	0.49
2:L:1062:ALA:N	2:L:1071:ILE:O	2.45	0.49
2:D:726:VAL:HG22	2:D:751:SER:HA	1.95	0.49
2:D:923:ILE:HD12	2:D:924:PRO:HD2	1.95	0.49
1:I:273:PRO:HA	1:I:274:LYS:HA	1.54	0.49
2:J:1038:GLY:HA3	2:J:1046:ALA:HA	1.95	0.49
2:D:1060:LEU:HD21	2:D:1099:TYR:HB2	1.93	0.49
1:I:327:GLN:HE21	1:I:353:LYS:HB3	1.78	0.49
2:L:769:PRO:HG3	2:L:967:THR:HG23	1.94	0.49
1:A:212:LEU:HD23	1:A:258:HIS:HD2	1.78	0.48
1:E:228:SER:HB2	1:E:270:LYS:HB2	1.95	0.48
2:F:923:ILE:HD12	2:F:924:PRO:HD2	1.96	0.48
1:K:307:SER:HB3	1:K:455:LEU:HD23	1.95	0.48
1:G:378:LYS:O	1:G:393:GLU:N	2.45	0.48
2:D:843:ARG:HG3	2:D:845:GLU:H	1.79	0.48
2:B:729:GLU:HG2	2:B:748:LYS:HA	1.95	0.48
2:D:954:ILE:HA	2:D:967:THR:HG22	1.94	0.48
2:D:957:LYS:HD3	2:D:964:GLU:HB2	1.96	0.48
2:D:1046:ALA:N	2:D:1086:LEU:O	2.46	0.48
2:H:722:ARG:NH2	2:H:1008:GLN:OE1	2.46	0.48
2:F:846:ALA:HB3	2:F:937:GLU:HG3	1.94	0.48
2:B:1064:ASN:ND2	2:B:1068:SER:OG	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:OD2	1:C:282:ASN:ND2	2.47	0.47
1:G:273:PRO:HA	1:G:274:LYS:HA	1.55	0.47
2:H:791:TRP:HE1	2:H:812:ASN:HB3	1.79	0.47
1:I:243:LYS:NZ	1:I:282:ASN:OD1	2.38	0.47
1:K:342:VAL:HG11	2:L:802:PHE:HB2	1.96	0.47
1:G:355:TYR:HE1	1:G:460:GLU:HG3	1.79	0.47
2:B:694:LEU:HD22	2:B:1070:HIS:HB3	1.96	0.47
1:C:344:PRO:HG2	1:C:356:LEU:HB2	1.97	0.47
1:C:417:ALA:O	1:C:421:SER:HB3	2.13	0.47
2:F:811:GLU:OE2	2:F:956:TYR:OH	2.27	0.47
2:H:848:ARG:NH2	2:H:907:GLU:OE1	2.40	0.47
2:L:906:ILE:HB	2:L:914:ALA:HB3	1.95	0.47
1:K:210:ARG:O	1:K:304:CYS:N	2.48	0.47
1:A:255:GLN:NE2	1:A:271:CYS:O	2.42	0.47
1:G:362:LYS:HB3	1:G:444:GLN:HB2	1.97	0.47
2:H:811:GLU:OE2	2:H:956:TYR:OH	2.29	0.47
1:K:212:LEU:HD23	1:K:258:HIS:HD2	1.80	0.47
1:A:307:SER:HB3	1:A:455:LEU:HD23	1.96	0.47
2:D:959:MET:O	2:D:961:ASP:N	2.47	0.47
2:L:959:MET:O	2:L:961:ASP:N	2.48	0.47
2:D:989:THR:HB	2:D:1002:PHE:HB2	1.97	0.47
2:B:906:ILE:HB	2:B:914:ALA:HB3	1.96	0.47
1:K:273:PRO:HA	1:K:274:LYS:HA	1.46	0.47
1:G:220:ILE:O	1:G:349:LYS:NZ	2.46	0.47
1:A:261:ASN:HD21	1:A:265:LYS:HB2	1.80	0.46
2:D:1037:THR:O	2:D:1047:ARG:N	2.48	0.46
1:K:168:TYR:O	1:K:217:HIS:NE2	2.41	0.46
1:A:345:PHE:HA	1:A:355:TYR:HA	1.97	0.46
2:J:975:VAL:HA	2:J:978:ARG:HG2	1.97	0.46
1:K:417:ALA:O	1:K:421:SER:HB2	2.15	0.46
2:L:1023:VAL:HG22	2:L:1025:ALA:H	1.80	0.46
1:E:316:THR:OG1	1:E:327:GLN:OE1	2.32	0.46
1:I:278:THR:OG1	1:I:280:ASP:OD1	2.32	0.46
1:A:324:VAL:HG23	1:A:464:VAL:HG22	1.96	0.46
2:B:1023:VAL:HG22	2:B:1025:ALA:H	1.80	0.46
1:K:344:PRO:HA	1:K:459:TYR:HA	1.97	0.46
2:B:723:ALA:HB2	2:B:1011:LEU:HG	1.97	0.46
2:B:743:LYS:NZ	2:B:1021:ASP:O	2.45	0.46
2:J:695:ILE:HD13	2:J:721:ILE:HB	1.97	0.46
2:B:849:VAL:HG22	2:B:906:ILE:HG12	1.97	0.46
2:F:754:LEU:HB2	2:F:1001:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:HIS:HD2	1:G:303:PHE:HB2	1.79	0.46
1:I:428:GLN:HE22	1:K:283:PHE:HB3	1.80	0.46
2:D:722:ARG:NH2	2:D:1008:GLN:OE1	2.49	0.46
2:B:885:TRP:HH2	2:B:1013:LEU:HD22	1.81	0.46
1:E:316:THR:HG22	1:E:318:MET:H	1.81	0.46
2:F:959:MET:O	2:F:961:ASP:N	2.48	0.46
2:J:769:PRO:HG3	2:J:967:THR:HG23	1.98	0.46
1:G:246:MET:HA	1:G:462:VAL:HA	1.98	0.46
2:B:850:PHE:HE1	2:B:907:GLU:HB2	1.82	0.45
1:C:248:THR:OG1	1:C:280:ASP:O	2.32	0.45
1:E:335:GLN:HG3	1:E:468:LEU:HB3	1.98	0.45
1:K:228:SER:HB2	1:K:270:LYS:HB3	1.97	0.45
2:L:848:ARG:NH2	2:L:907:GLU:OE1	2.38	0.45
2:L:850:PHE:HE1	2:L:907:GLU:HB2	1.81	0.45
1:E:376:GLU:HB2	1:E:397:PHE:HB2	1.99	0.45
2:J:959:MET:O	2:J:961:ASP:N	2.48	0.45
1:A:405:ILE:HA	1:A:424:GLU:HB2	1.98	0.45
1:A:412:LYS:HD2	1:A:426:THR:HG21	1.98	0.45
2:B:843:ARG:NH2	2:B:971:ASP:OD2	2.49	0.45
1:G:330:LYS:HB2	2:J:714:ARG:HH21	1.82	0.45
1:A:231:LEU:O	1:K:428:GLN:NE2	2.50	0.45
1:C:222:ALA:HB3	1:C:265:LYS:HG2	1.98	0.45
1:C:324:VAL:HG23	1:C:464:VAL:HG22	1.98	0.45
2:J:817:GLN:HE22	2:J:958:PRO:HB2	1.81	0.45
2:F:979:GLY:HA2	2:F:983:GLN:HE22	1.82	0.45
1:K:262:ASN:OD1	1:K:327:GLN:NE2	2.49	0.45
1:A:313:LYS:H	1:A:313:LYS:HD2	1.80	0.45
2:L:793:ASP:OD1	2:L:813:LYS:NZ	2.50	0.45
2:F:891:SER:HB3	2:F:1010:ASP:HB2	1.99	0.45
1:G:311:GLY:HA3	1:G:348:PHE:HD2	1.81	0.45
2:H:959:MET:O	2:H:961:ASP:N	2.50	0.45
1:E:273:PRO:HA	1:E:274:LYS:HA	1.53	0.45
1:E:398:ASP:OD2	1:E:400:SER:OG	2.27	0.45
1:K:345:PHE:HA	1:K:355:TYR:HA	1.99	0.45
2:D:1090:VAL:HG22	2:D:1092:GLU:H	1.81	0.45
1:I:183:THR:HG23	1:I:185:ALA:H	1.82	0.45
1:E:468:LEU:HD12	2:F:844:LYS:HG2	1.98	0.45
2:H:850:PHE:HE1	2:H:907:GLU:HB2	1.81	0.44
2:L:954:ILE:HA	2:L:967:THR:HG22	1.98	0.44
2:L:959:MET:HB2	2:L:962:GLN:HB2	1.98	0.44
1:G:242:GLU:OE2	1:G:353:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:377:HIS:H	1:I:432:ALA:HA	1.82	0.44
1:I:163:GLY:H	1:I:396:SER:HB3	1.82	0.44
2:F:810:ARG:NH1	2:F:945:GLU:OE1	2.47	0.44
2:F:991:ALA:HB3	2:F:1000:GLN:HE21	1.81	0.44
2:H:809:MET:HB2	2:H:839:LEU:HB2	1.98	0.44
2:L:1047:ARG:H	2:L:1047:ARG:HD2	1.82	0.44
2:J:1100:SER:HB3	2:J:1105:GLU:HG3	1.98	0.44
1:A:346:ALA:N	1:A:354:VAL:O	2.50	0.44
2:B:876:GLY:H	2:B:879:SER:HB3	1.83	0.44
1:G:261:ASN:HD21	1:G:265:LYS:HB2	1.83	0.44
1:E:410:SER:OG	1:E:411:LYS:N	2.49	0.44
2:J:913:TYR:HB2	2:J:981:LEU:HD12	2.00	0.44
1:K:327:GLN:HE22	1:K:353:LYS:HB3	1.82	0.44
2:L:913:TYR:HB2	2:L:981:LEU:HD12	2.00	0.44
2:B:813:LYS:HB2	2:B:835:VAL:HB	1.99	0.43
2:B:865:ASP:OD2	2:B:869:SER:OG	2.36	0.43
2:B:973:PHE:HA	2:B:976:PHE:HB3	1.99	0.43
2:H:1062:ALA:HA	2:H:1099:TYR:HA	2.00	0.43
2:L:992:ALA:O	2:L:1000:GLN:NE2	2.51	0.43
2:B:959:MET:O	2:B:961:ASP:N	2.51	0.43
2:J:723:ALA:HB2	2:J:1011:LEU:HG	2.00	0.43
2:L:849:VAL:HG22	2:L:906:ILE:HG12	1.99	0.43
1:A:316:THR:HG22	1:A:318:MET:H	1.83	0.43
2:F:810:ARG:H	2:F:810:ARG:HD3	1.82	0.43
2:L:787:ARG:NH2	2:L:795:GLU:OE2	2.44	0.43
2:F:827:ASN:HD21	2:F:829:ASN:HD22	1.65	0.43
1:G:252:ASN:HD21	1:G:285:ARG:HH11	1.67	0.43
1:G:365:GLU:HG2	1:G:441:GLY:HA3	2.00	0.43
1:A:377:HIS:CE1	1:A:433:TYR:HB2	2.53	0.43
2:D:778:HIS:ND1	2:D:779:LEU:HG	2.34	0.43
1:E:158:LEU:HD13	1:E:195:LEU:HD22	2.01	0.43
2:F:778:HIS:ND1	2:F:779:LEU:HG	2.33	0.43
1:G:209:HIS:CE1	1:G:305:GLN:HB3	2.54	0.43
2:H:729:GLU:HA	2:H:748:LYS:HA	2.01	0.43
2:F:729:GLU:OE2	2:F:748:LYS:NZ	2.40	0.43
2:H:976:PHE:O	2:H:980:SER:OG	2.32	0.43
2:D:692:SER:OG	2:D:693:GLU:OE1	2.30	0.43
2:J:711:THR:HG21	2:J:737:VAL:HG22	2.00	0.43
2:L:770:LYS:HG3	2:L:840:GLN:HE22	1.83	0.43
1:A:273:PRO:HA	1:A:274:LYS:HA	1.48	0.42
2:D:754:LEU:HB2	2:D:1001:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1100:SER:HB3	2:F:1105:GLU:HG2	2.00	0.42
1:G:327:GLN:NE2	1:G:353:LYS:O	2.52	0.42
1:I:259:TYR:HB3	1:I:299:LEU:HB2	2.01	0.42
1:C:321:VAL:HG22	1:C:466:ARG:HG2	2.00	0.42
1:I:228:SER:HB2	1:I:270:LYS:HB2	2.00	0.42
2:D:848:ARG:NH2	2:D:907:GLU:OE1	2.36	0.42
2:F:932:ILE:HG12	2:F:949:ARG:HB2	2.01	0.42
2:J:959:MET:HB2	2:J:962:GLN:HB2	2.01	0.42
1:K:324:VAL:HG23	1:K:464:VAL:HG22	2.01	0.42
2:B:755:SER:O	2:B:856:VAL:N	2.52	0.42
2:H:762:TYR:HB2	2:H:933:ARG:HB2	2.02	0.42
2:H:778:HIS:ND1	2:H:779:LEU:HG	2.34	0.42
2:J:717:GLY:H	2:J:1015:PHE:HB2	1.84	0.42
1:G:335:GLN:HB3	1:G:468:LEU:HB2	2.00	0.42
1:I:231:LEU:HD23	1:I:237:ASN:HD21	1.84	0.42
2:J:929:LEU:HD11	2:J:972:PRO:HB3	1.99	0.42
1:A:180:LYS:HA	1:A:181:PRO:HA	1.87	0.42
2:H:817:GLN:HE22	2:H:958:PRO:HB2	1.84	0.42
2:B:743:LYS:HE3	2:B:1022:PHE:HB2	2.02	0.42
2:B:1054:SER:OG	2:B:1055:THR:N	2.53	0.42
1:C:336:LEU:HD13	1:C:465:LYS:HB3	2.01	0.42
1:E:167:ASN:HD22	1:E:182:VAL:HG21	1.84	0.42
2:J:725:SER:OG	2:J:1043:ASN:ND2	2.51	0.42
1:E:246:MET:HG2	1:E:462:VAL:HG12	2.01	0.42
2:F:1081:ASP:OD1	2:F:1081:ASP:N	2.53	0.42
2:H:773:SER:HB3	2:H:963:LEU:HB2	2.01	0.42
2:F:954:ILE:HA	2:F:967:THR:HG22	2.02	0.42
2:B:688:ASP:HB2	2:B:689:PRO:HD3	2.01	0.42
2:D:1071:ILE:HG12	2:D:1084:GLN:HE21	1.85	0.42
2:J:926:GLN:NE2	2:J:952:ASN:O	2.52	0.42
1:C:316:THR:HG22	1:C:318:MET:H	1.85	0.41
1:C:362:LYS:NZ	1:C:364:GLU:OE2	2.52	0.41
1:I:368:LEU:HD13	1:I:442:ILE:HD12	2.02	0.41
2:D:755:SER:N	2:D:856:VAL:O	2.52	0.41
2:L:744:PHE:HZ	2:L:1072:VAL:HG23	1.85	0.41
2:H:865:ASP:OD2	2:H:869:SER:OG	2.39	0.41
1:C:273:PRO:HA	1:C:274:LYS:HA	1.50	0.41
2:F:848:ARG:NH2	2:F:907:GLU:OE1	2.42	0.41
2:F:1003:SER:OG	2:F:1004:LYS:N	2.53	0.41
2:F:1038:GLY:HA3	2:F:1046:ALA:HA	2.02	0.41
2:B:913:TYR:HB2	2:B:981:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:GLN:HE22	1:I:275:TYR:HE2	1.68	0.41
2:L:931:GLU:HG3	2:L:932:ILE:HG13	2.01	0.41
2:H:688:ASP:HB2	2:H:689:PRO:HD3	2.02	0.41
2:B:755:SER:N	2:B:856:VAL:O	2.54	0.41
2:B:971:ASP:HB3	2:B:974:VAL:HG23	2.03	0.41
2:D:956:TYR:HD1	2:D:963:LEU:HD21	1.85	0.41
2:F:993:SER:HB2	2:F:1000:GLN:HB3	2.01	0.41
2:L:755:SER:O	2:L:856:VAL:N	2.44	0.41
2:L:791:TRP:HE1	2:L:812:ASN:HB3	1.86	0.41
1:E:169:ILE:HD12	1:E:169:ILE:HA	1.95	0.41
1:A:371:SER:OG	1:A:440:SER:OG	2.31	0.41
2:B:778:HIS:ND1	2:B:779:LEU:HG	2.35	0.41
2:D:755:SER:O	2:D:856:VAL:N	2.53	0.41
1:E:356:LEU:HD21	1:E:447:VAL:HG23	2.03	0.41
2:F:755:SER:O	2:F:856:VAL:N	2.44	0.41
1:G:212:LEU:HD22	1:G:302:LEU:HD11	2.03	0.41
1:G:321:VAL:HG11	1:G:324:VAL:HB	2.03	0.41
1:G:414:THR:O	1:G:434:CYS:N	2.43	0.41
1:I:180:LYS:HA	1:I:181:PRO:HA	1.92	0.41
2:B:705:SER:HB2	2:B:714:ARG:HH12	1.86	0.40
2:D:907:GLU:HG3	2:D:913:TYR:CE1	2.56	0.40
2:H:1090:VAL:HG22	2:H:1092:GLU:H	1.86	0.40
1:I:159:ARG:HG2	1:I:191:PHE:HE2	1.86	0.40
2:J:843:ARG:HG3	2:J:845:GLU:HG2	2.03	0.40
2:F:769:PRO:HG3	2:F:967:THR:HG23	2.02	0.40
2:F:743:LYS:HD3	2:F:1022:PHE:HD1	1.85	0.40
2:L:890:LEU:HD11	2:L:1009:ALA:HB1	2.02	0.40
2:L:976:PHE:O	2:L:980:SER:OG	2.35	0.40
1:A:159:ARG:NH2	1:A:186:GLY:O	2.54	0.40
2:B:857:HIS:CD2	2:B:895:GLU:HB2	2.56	0.40
2:D:976:PHE:O	2:D:980:SER:OG	2.31	0.40
2:F:850:PHE:HE1	2:F:907:GLU:HB2	1.86	0.40
1:G:358:LYS:HD2	2:H:770:LYS:HD2	2.03	0.40
2:J:810:ARG:HD2	2:J:836:HIS:CE1	2.56	0.40
2:L:810:ARG:NH1	2:L:945:GLU:OE1	2.47	0.40
1:A:316:THR:HG23	1:A:355:TYR:HB2	2.04	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	A	295/316 (93%)	254 (86%)	37 (12%)	4 (1%)	9	41
1	C	295/316 (93%)	250 (85%)	41 (14%)	4 (1%)	9	41
1	E	295/316 (93%)	260 (88%)	32 (11%)	3 (1%)	13	49
1	G	295/316 (93%)	254 (86%)	39 (13%)	2 (1%)	19	57
1	I	295/316 (93%)	256 (87%)	36 (12%)	3 (1%)	13	49
1	K	295/316 (93%)	261 (88%)	28 (10%)	6 (2%)	6	32
2	B	429/431 (100%)	380 (89%)	44 (10%)	5 (1%)	11	44
2	D	429/431 (100%)	378 (88%)	47 (11%)	4 (1%)	14	52
2	F	429/431 (100%)	380 (89%)	43 (10%)	6 (1%)	9	41
2	H	429/431 (100%)	382 (89%)	42 (10%)	5 (1%)	11	44
2	J	429/431 (100%)	376 (88%)	48 (11%)	5 (1%)	11	44
2	L	429/431 (100%)	382 (89%)	43 (10%)	4 (1%)	14	52
All	All	4344/4482 (97%)	3813 (88%)	480 (11%)	51 (1%)	14	44

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1083	CYS
1	C	239	CYS
2	D	1083	CYS
1	E	281	CYS
1	E	284	CYS
1	A	179	CYS
2	B	824	GLY
2	B	877	ALA
2	B	986	ASN
1	C	456	CYS
2	F	1029	CYS
2	J	877	ALA

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Mol	Chain	Res	Type
1	K	281	CYS
2	L	1083	CYS
1	A	164	LYS
1	A	329	LEU
2	B	960	ILE
2	D	922	GLU
2	F	877	ALA
2	F	986	ASN
2	H	824	GLY
2	H	960	ILE
1	I	329	LEU
1	I	427	ALA
2	J	809	MET
1	K	329	LEU
1	K	410	SER
1	K	427	ALA
2	D	877	ALA
2	D	960	ILE
2	F	809	MET
2	F	960	ILE
1	G	329	LEU
1	G	416	ASP
2	H	877	ALA
2	H	891	SER
1	I	311	GLY
2	J	960	ILE
2	L	877	ALA
2	L	960	ILE
2	L	986	ASN
2	F	1103	GLY
2	J	986	ASN
2	J	1083	CYS
1	K	311	GLY
1	A	322	CYS
1	K	326	VAL
1	C	238	PRO
1	C	311	GLY
1	E	454	PRO
2	H	896	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/271 (89%)	237 (98%)	4 (2%)	56	72
1	C	241/271 (89%)	239 (99%)	2 (1%)	79	85
1	E	241/271 (89%)	240 (100%)	1 (0%)	89	91
1	G	241/271 (89%)	239 (99%)	2 (1%)	79	85
1	I	241/271 (89%)	239 (99%)	2 (1%)	79	85
1	K	241/271 (89%)	240 (100%)	1 (0%)	89	91
2	B	347/371 (94%)	344 (99%)	3 (1%)	75	83
2	D	347/371 (94%)	339 (98%)	8 (2%)	45	64
2	F	347/371 (94%)	344 (99%)	3 (1%)	75	83
2	H	347/371 (94%)	345 (99%)	2 (1%)	84	88
2	J	347/371 (94%)	346 (100%)	1 (0%)	91	92
2	L	347/371 (94%)	342 (99%)	5 (1%)	62	75
All	All	3528/3852 (92%)	3494 (99%)	34 (1%)	71	82

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ARG
1	A	313	LYS
1	A	330	LYS
1	A	438	ASN
2	B	700	ARG
2	B	810	ARG
2	B	949	ARG
1	C	331	LYS
1	C	438	ASN
2	D	700	ARG
2	D	714	ARG
2	D	925	ARG
2	D	949	ARG
2	D	994	LYS

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Mol	Chain	Res	Type
2	D	996	ASN
2	D	1106	ARG
2	D	1111	LYS
1	E	378	LYS
2	F	722	ARG
2	F	810	ARG
2	F	949	ARG
1	G	285	ARG
1	G	330	LYS
2	H	786	ASN
2	H	810	ARG
1	I	378	LYS
1	I	438	ASN
2	J	925	ARG
1	K	438	ASN
2	L	810	ARG
2	L	925	ARG
2	L	952	ASN
2	L	994	LYS
2	L	1047	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	335	GLN
1	A	431	ASN
2	B	1064	ASN
1	C	166	HIS
1	C	204	GLN
1	C	438	ASN
2	D	1000	GLN
2	D	1084	GLN
1	E	160	ASN
1	E	166	HIS
2	F	829	ASN
2	F	901	ASN
2	F	1000	GLN
1	G	157	HIS
1	G	204	GLN
1	G	252	ASN
2	H	784	HIS

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Mol	Chain	Res	Type
2	H	786	ASN
2	H	944	HIS
2	H	1043	ASN
1	I	166	HIS
1	I	232	GLN
1	I	327	GLN
1	I	436	HIS
1	I	438	ASN
2	J	741	GLN
2	J	817	GLN
2	J	1000	GLN
2	J	1043	ASN
2	J	1063	HIS
2	J	1084	GLN
1	K	166	HIS
1	K	258	HIS
1	K	327	GLN
1	K	428	GLN
1	K	438	ASN
2	L	952	ASN

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](#)

There are no chain breaks in this entry.

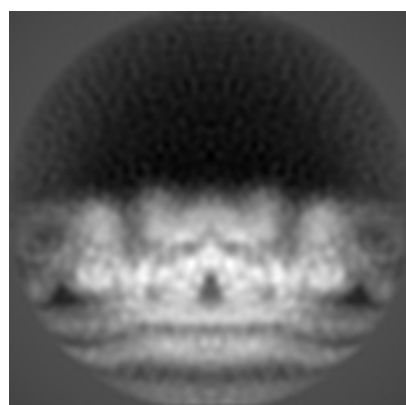
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4199. These allow visual inspection of the internal detail of the map and identification of artifacts.

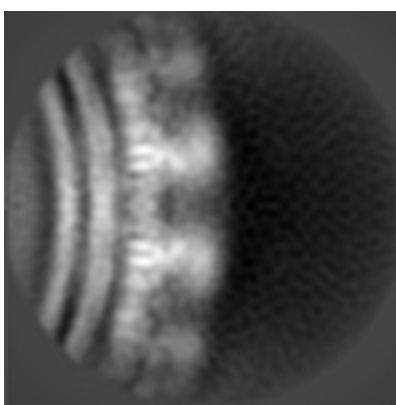
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

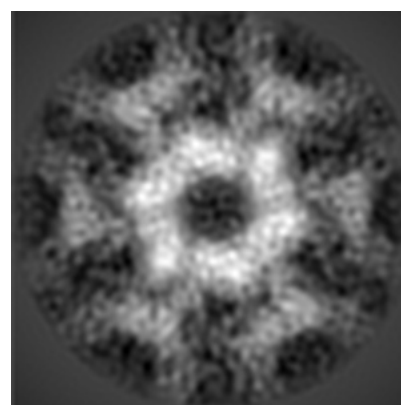
6.1.1 Primary map



X



Y

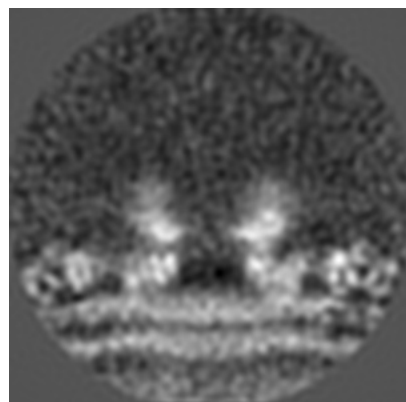


Z

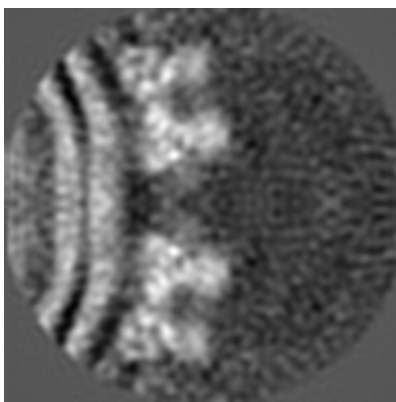
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

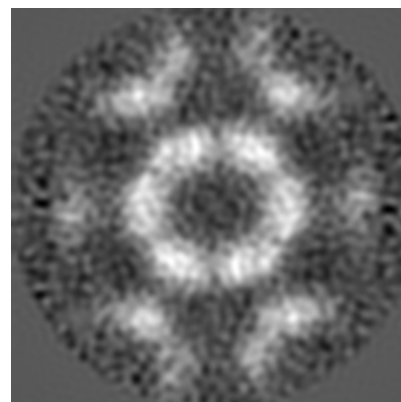
6.2.1 Primary map



X Index: 64



Y Index: 64

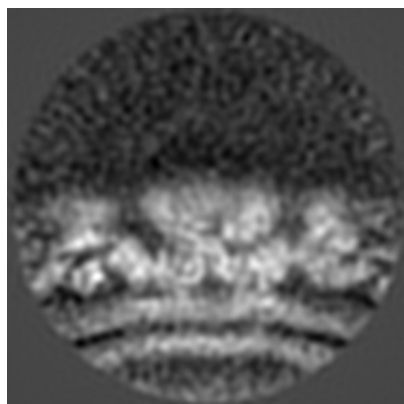


Z Index: 64

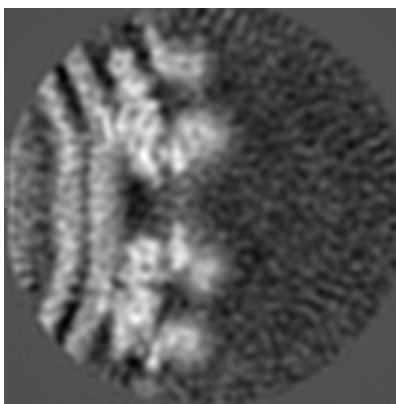
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

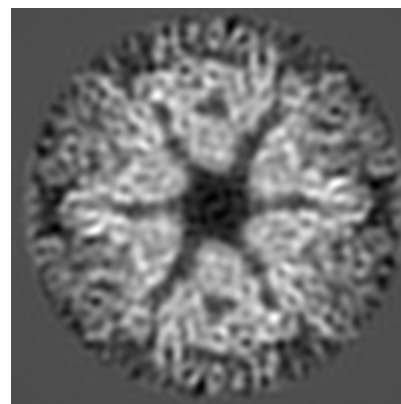
6.3.1 Primary map



X Index: 83



Y Index: 58

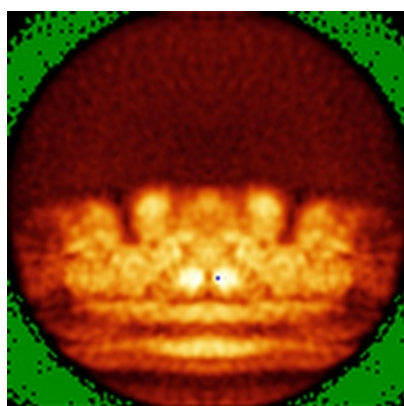


Z Index: 42

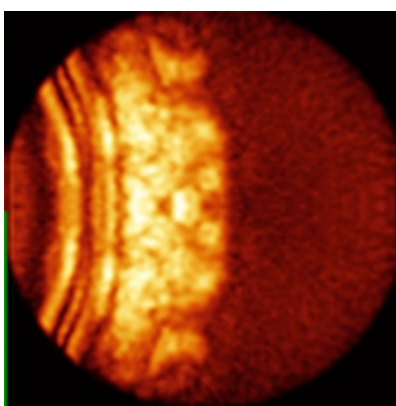
The images above show the largest variance slices of the map in three orthogonal directions.

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

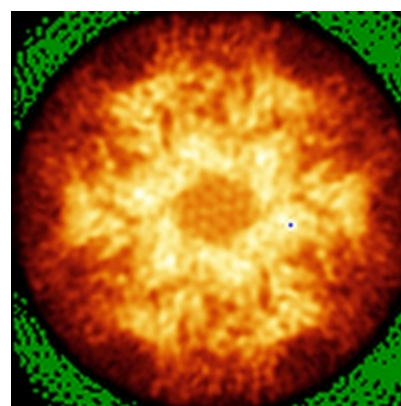
6.4.1 Primary map



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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

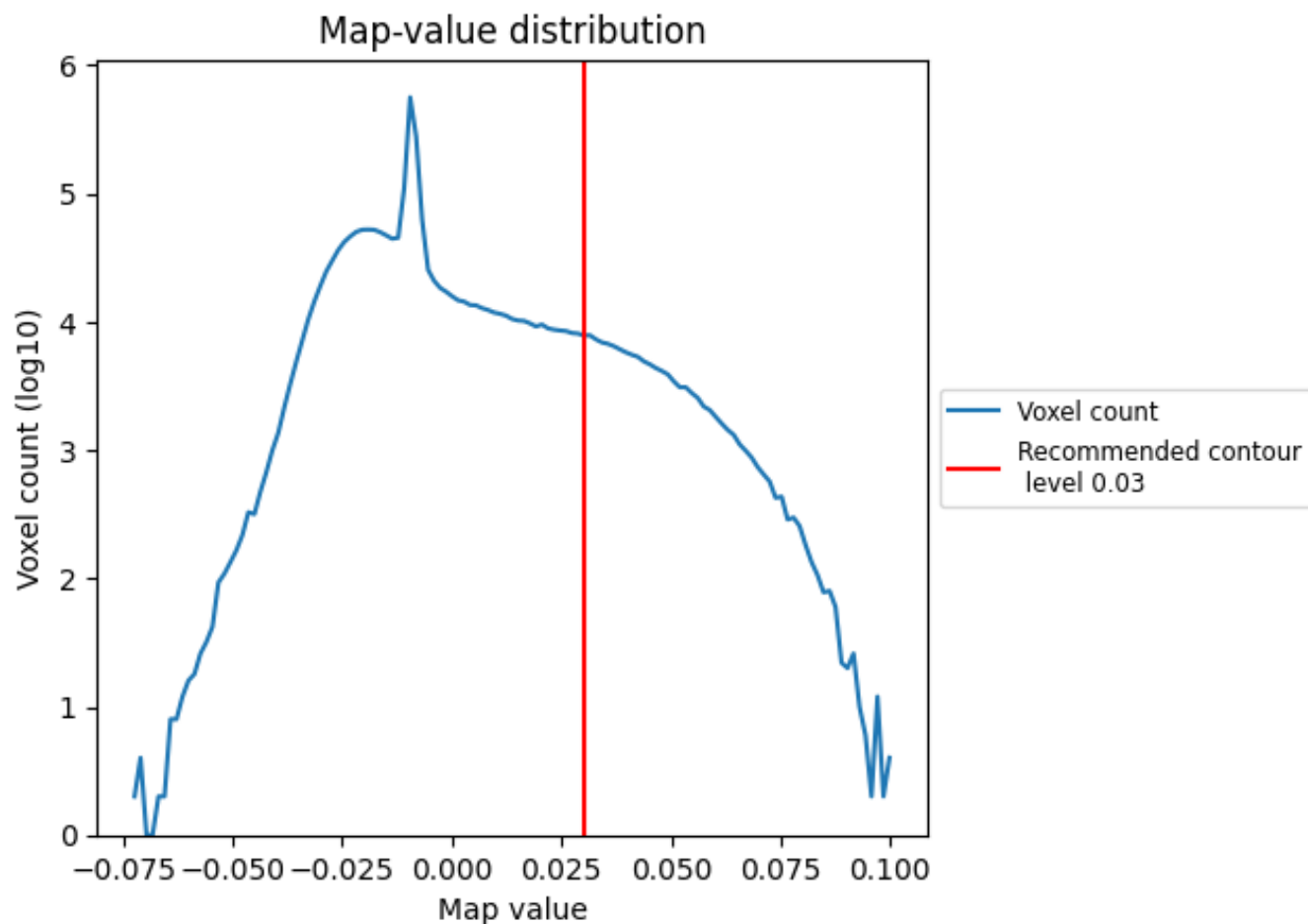
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

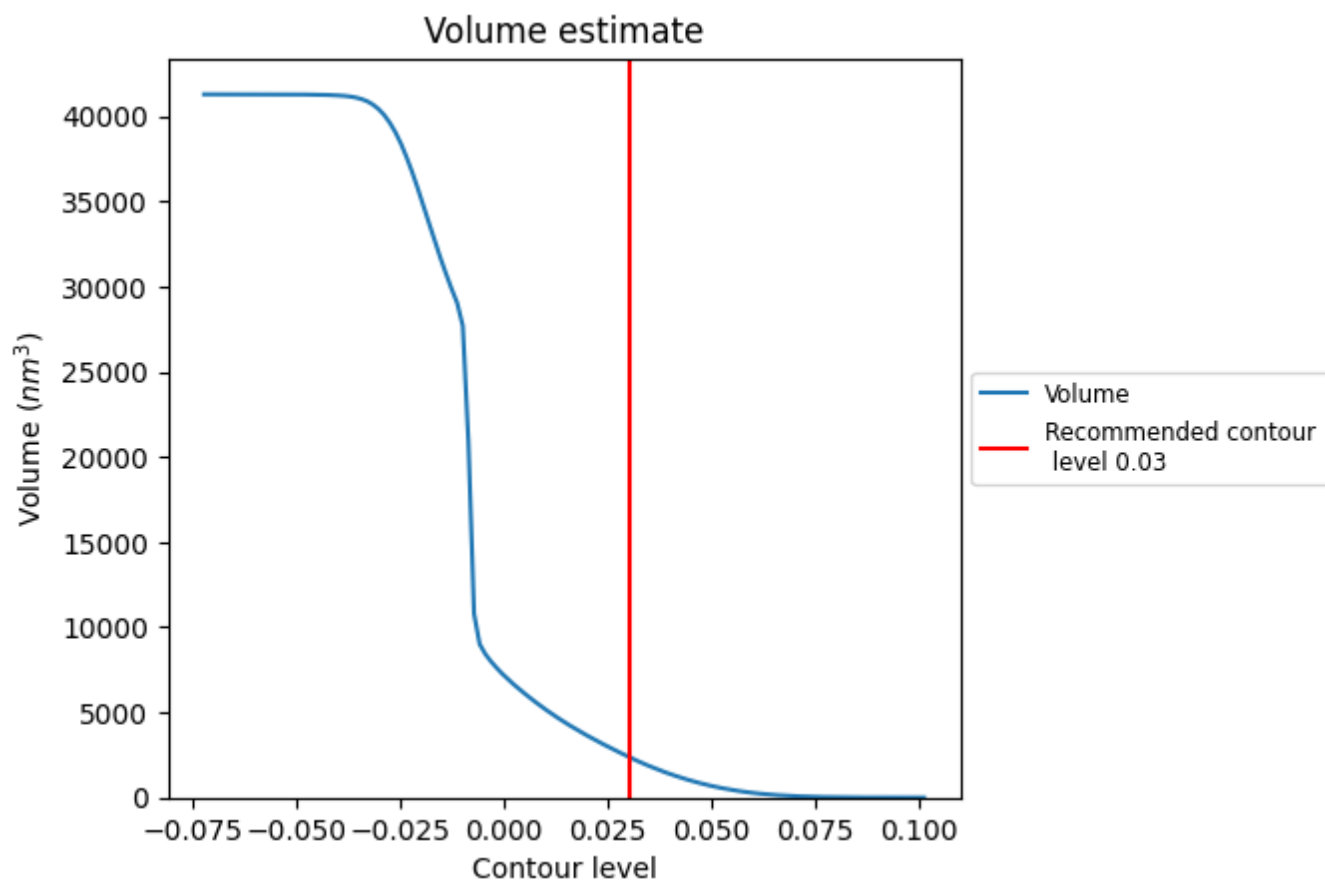
This section contains the results of statistical analysis of the map.

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.

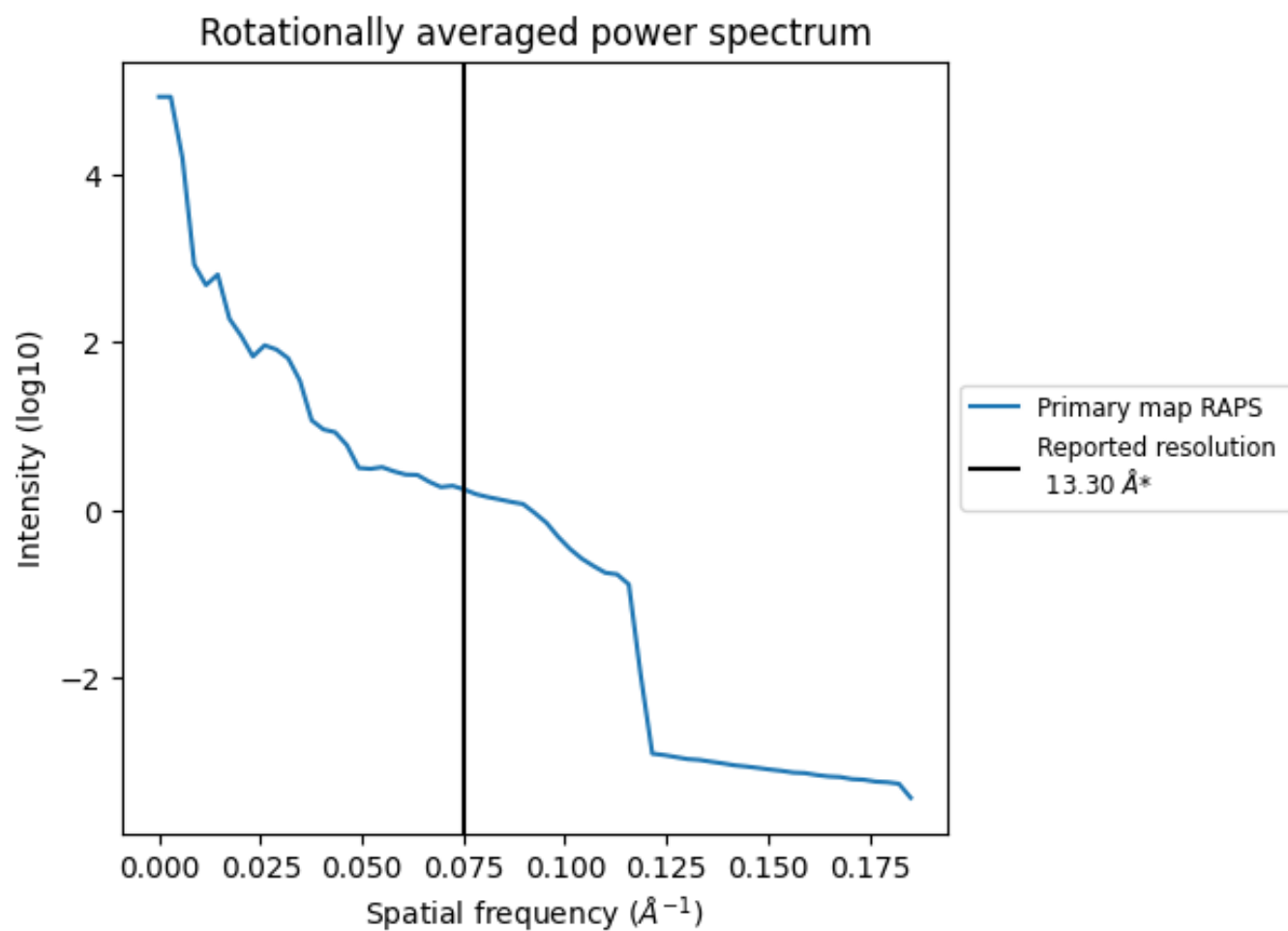
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2388 nm³; this corresponds to an approximate mass of 2157 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 ⓘ

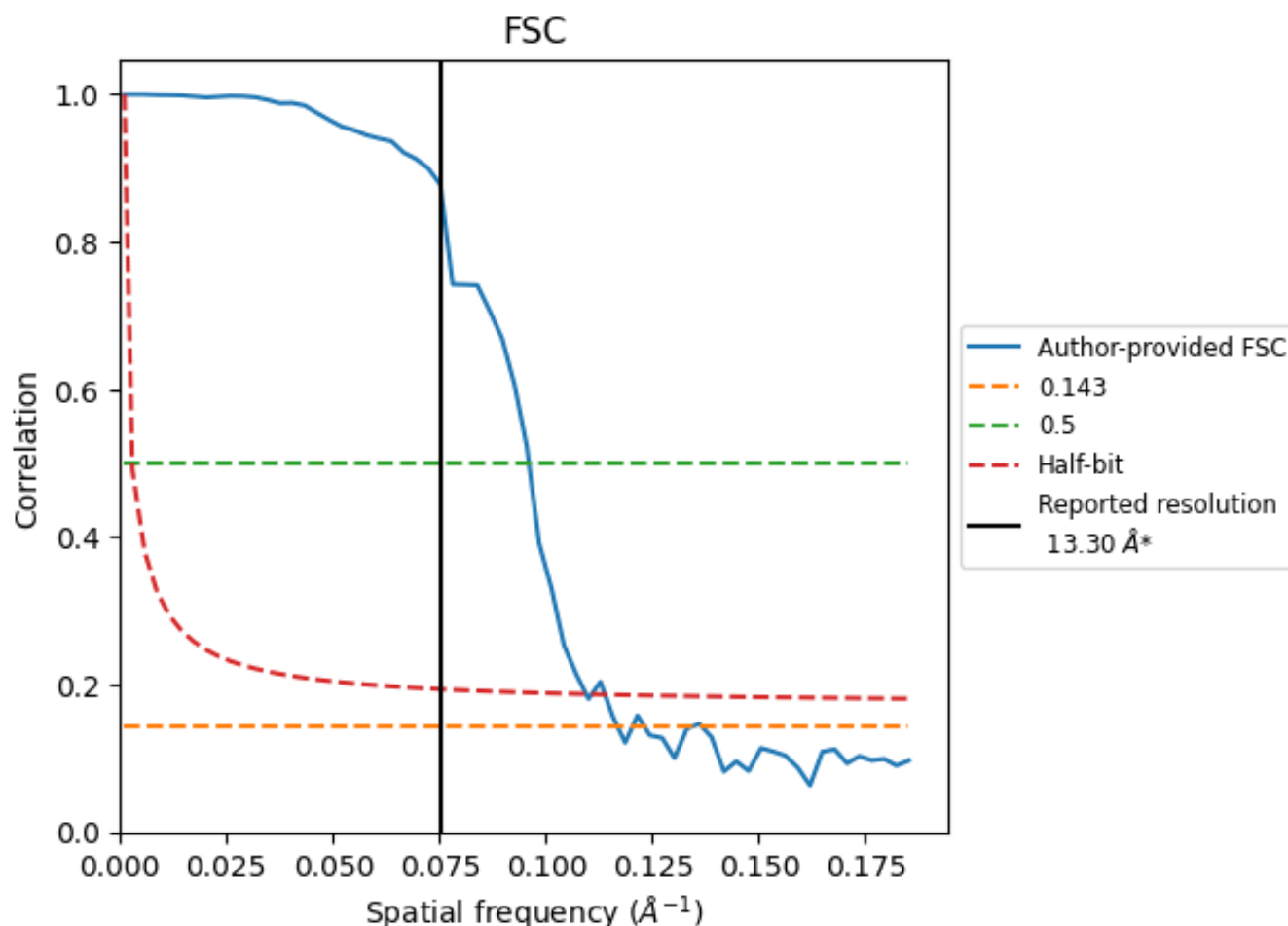


*Reported resolution corresponds to spatial frequency of 0.075 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.075 Å⁻¹

8.2 Resolution estimates [i](#)

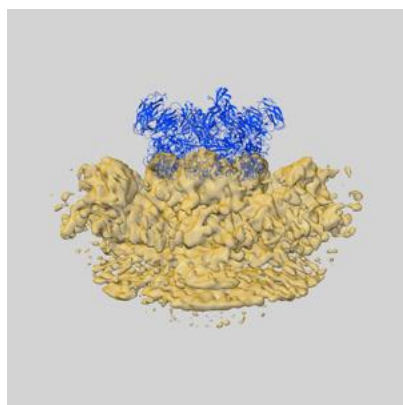
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.30	-	-
Author-provided FSC curve	8.56	10.42	9.14
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.56 differs from the reported value 13.3 by more than 10 %

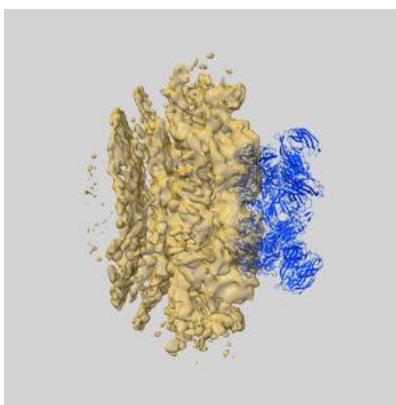
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4199 and PDB model 6F9D. Per-residue inclusion information can be found in section [3](#) on page [6](#).

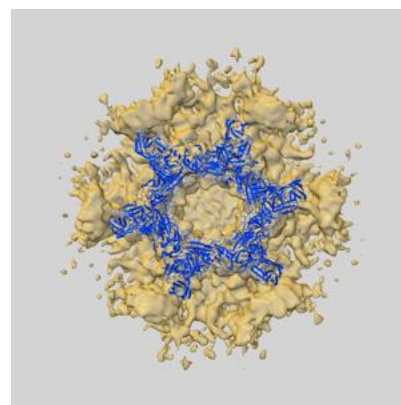
9.1 Map-model overlay [i](#)



X



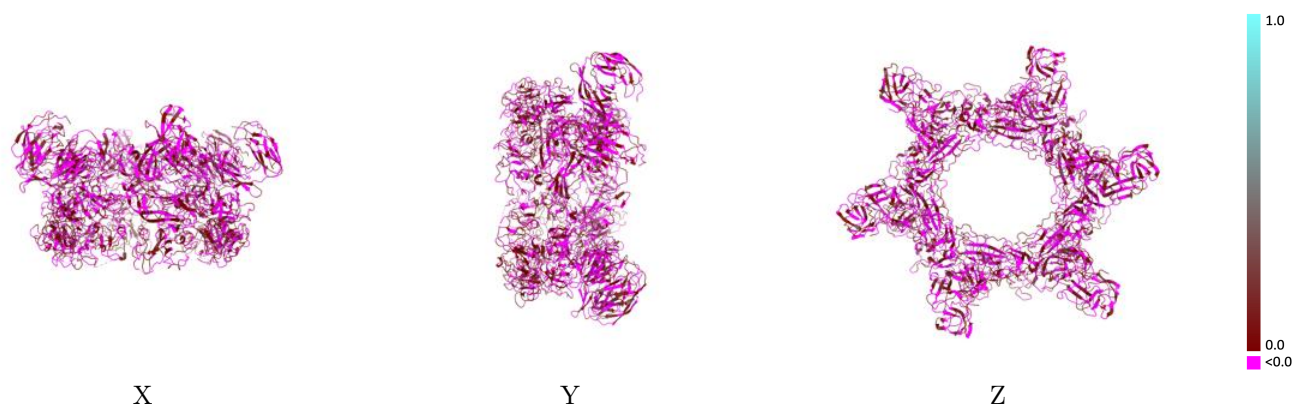
Y



Z

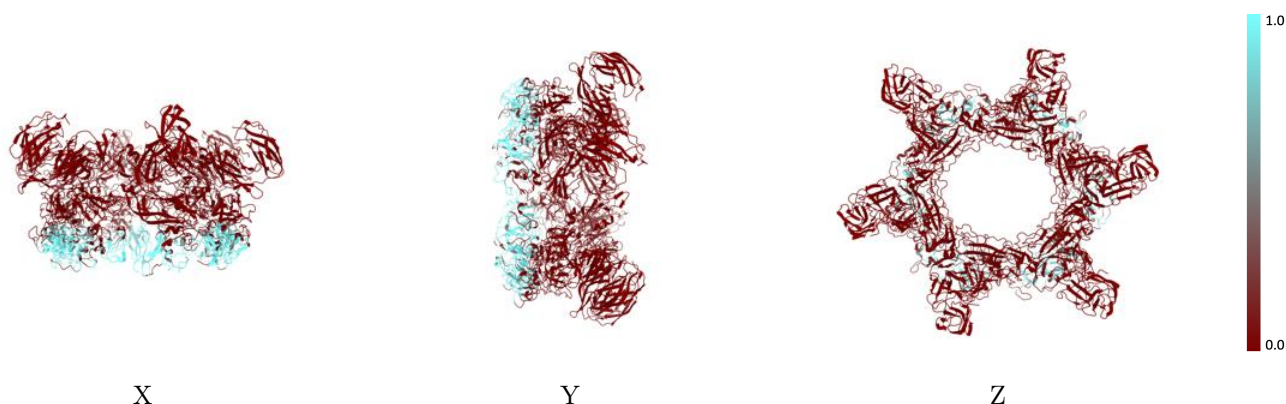
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



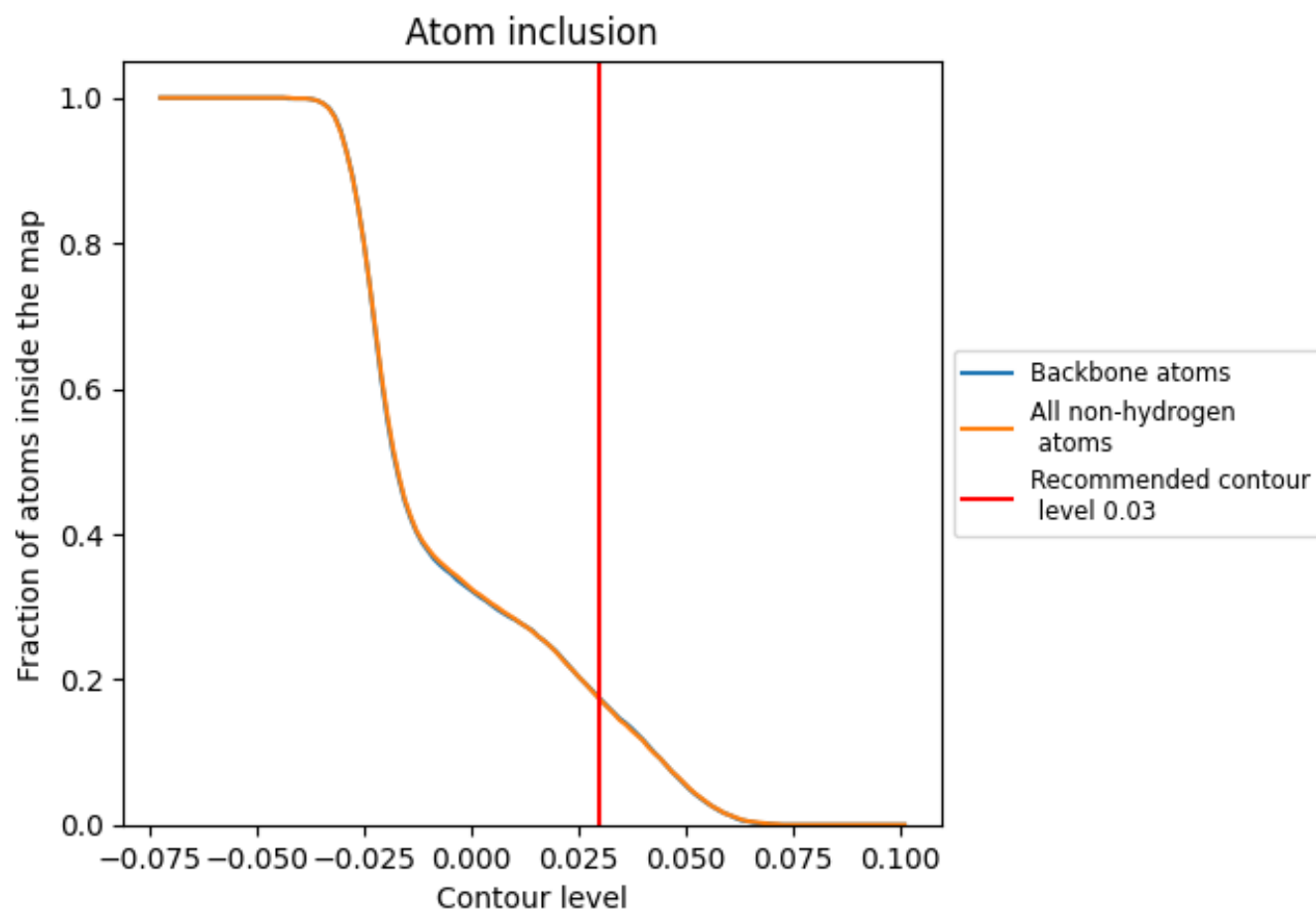
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 17% of all backbone atoms, 17% 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	 0.1730	 0.0080
A	 0.3810	 0.0150
B	 0.0000	 0.0020
C	 0.4000	 0.0300
D	 0.0000	 0.0010
E	 0.4180	 0.0220
F	 0.0000	 0.0030
G	 0.4200	 0.0260
H	 0.0000	 -0.0070
I	 0.4490	 0.0250
J	 0.0000	 -0.0040
K	 0.4260	 0.0180
L	 0.0000	 -0.0110

