



## wwPDB EM Validation Summary Report ⓘ

Dec 26, 2024 – 07:47 AM EST

PDB ID : 6F9E  
EMDB ID : EMD-4200  
Title : Model of the Rift Valley fever virus glycoprotein hexamer type 3  
Authors : Halldorsson, S.; Bowden, T.A.; Huiskonen, J.T.  
Deposited on : 2017-12-14  
Resolution : 13.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

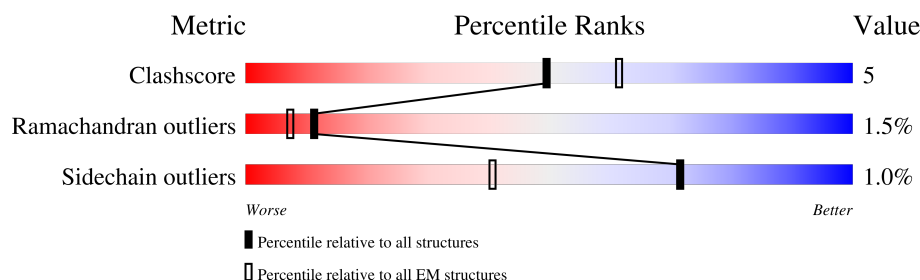
# 1 Overall quality at a glance

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  $\geq 3$ , 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>43%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>
1	C	316	<div> <div>46%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>
1	E	316	<div> <div>46%</div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div>
1	G	316	<div> <div>43%</div> <div>78%</div> <div>17%</div> <div>5%</div> </div>
1	I	316	<div> <div>41%</div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
1	K	316	<div> <div>41%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>
2	B	431	<div> <div>100%</div> <div>85%</div> <div>15%</div> </div>
2	D	431	<div> <div>100%</div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	431	<div><div></div><div>100%</div><div>84%</div><div>16%</div></div>
2	H	431	<div><div></div><div>100%</div><div>83%</div><div>16%</div></div>
2	J	431	<div><div></div><div>100%</div><div>84%</div><div>15%</div></div>
2	L	431	<div><div></div><div>100%</div><div>84%</div><div>16%</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:

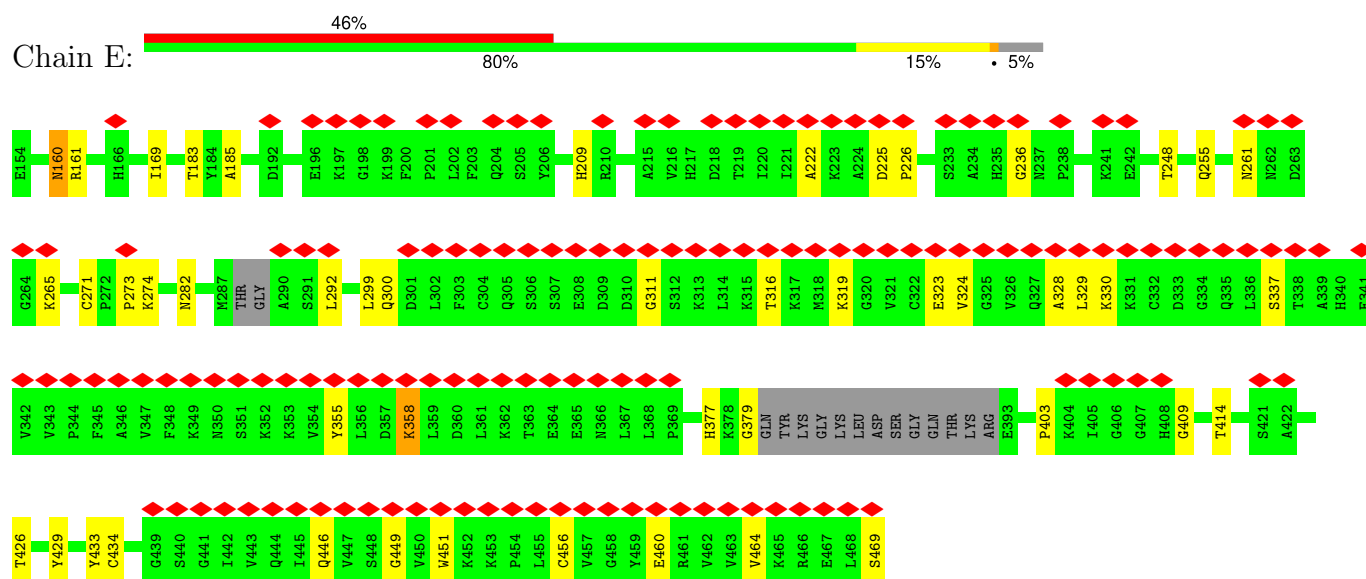
Chain	Residue	Modelled	Actual	Comment	Reference
B	688	ASP	-	expression tag	UNP A2T072
B	689	PRO	-	expression tag	UNP A2T072

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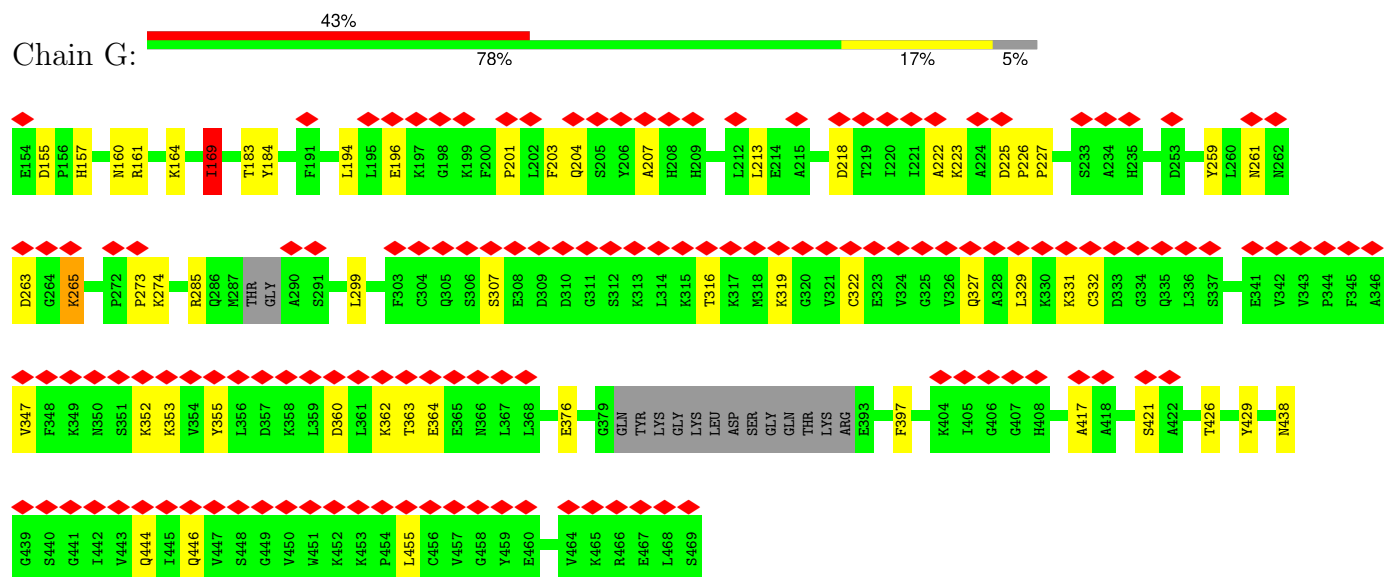
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Chain	Residue	Modelled	Actual	Comment	Reference
B	690	GLY	-	expression tag	UNP A2T072
D	688	ASP	-	expression tag	UNP A2T072
D	689	PRO	-	expression tag	UNP A2T072
D	690	GLY	-	expression tag	UNP A2T072
F	688	ASP	-	expression tag	UNP A2T072
F	689	PRO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

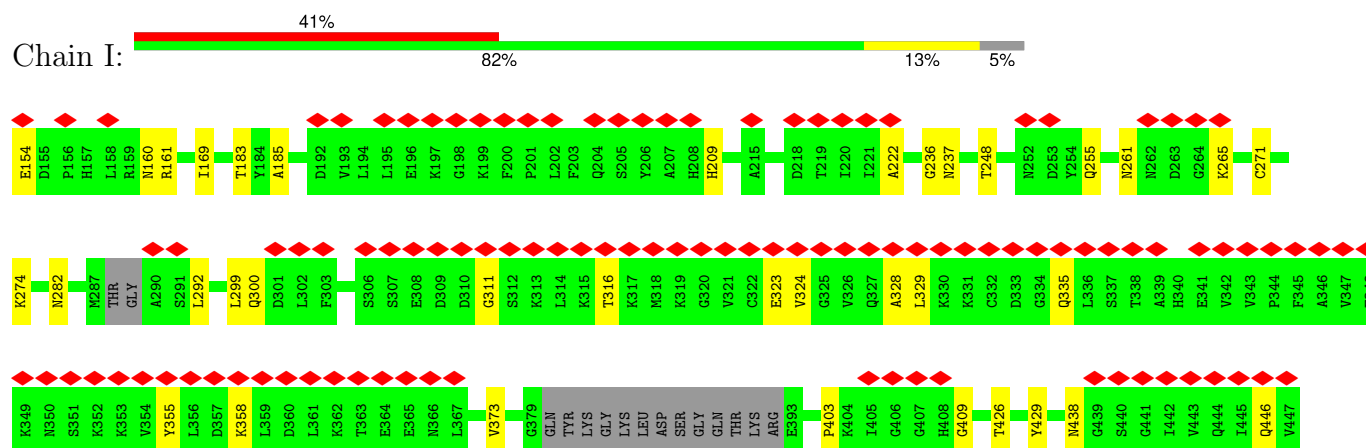


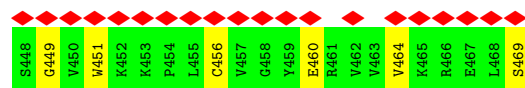


• Molecule 1: Glycoprotein

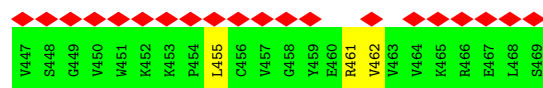
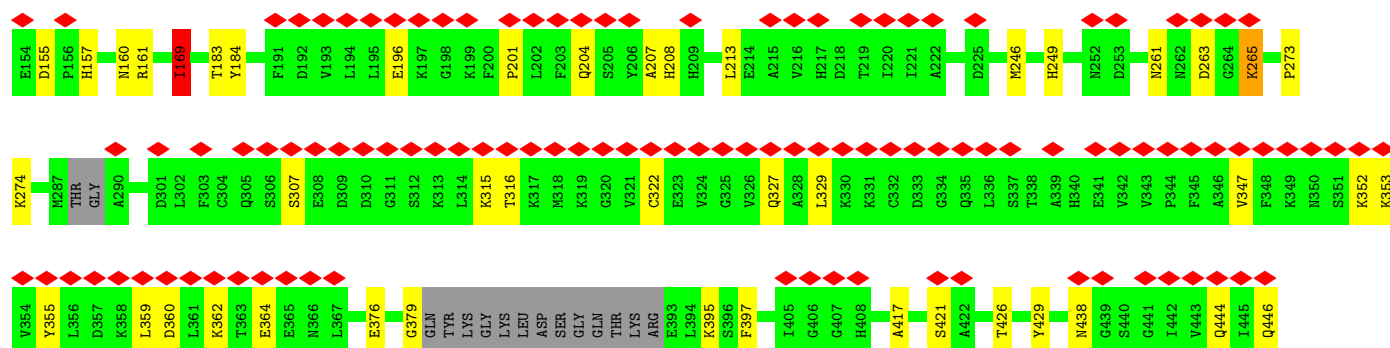
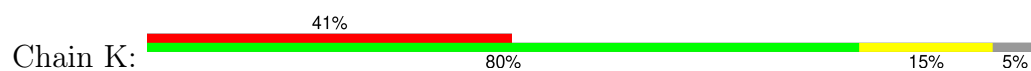


• Molecule 1: Glycoprotein

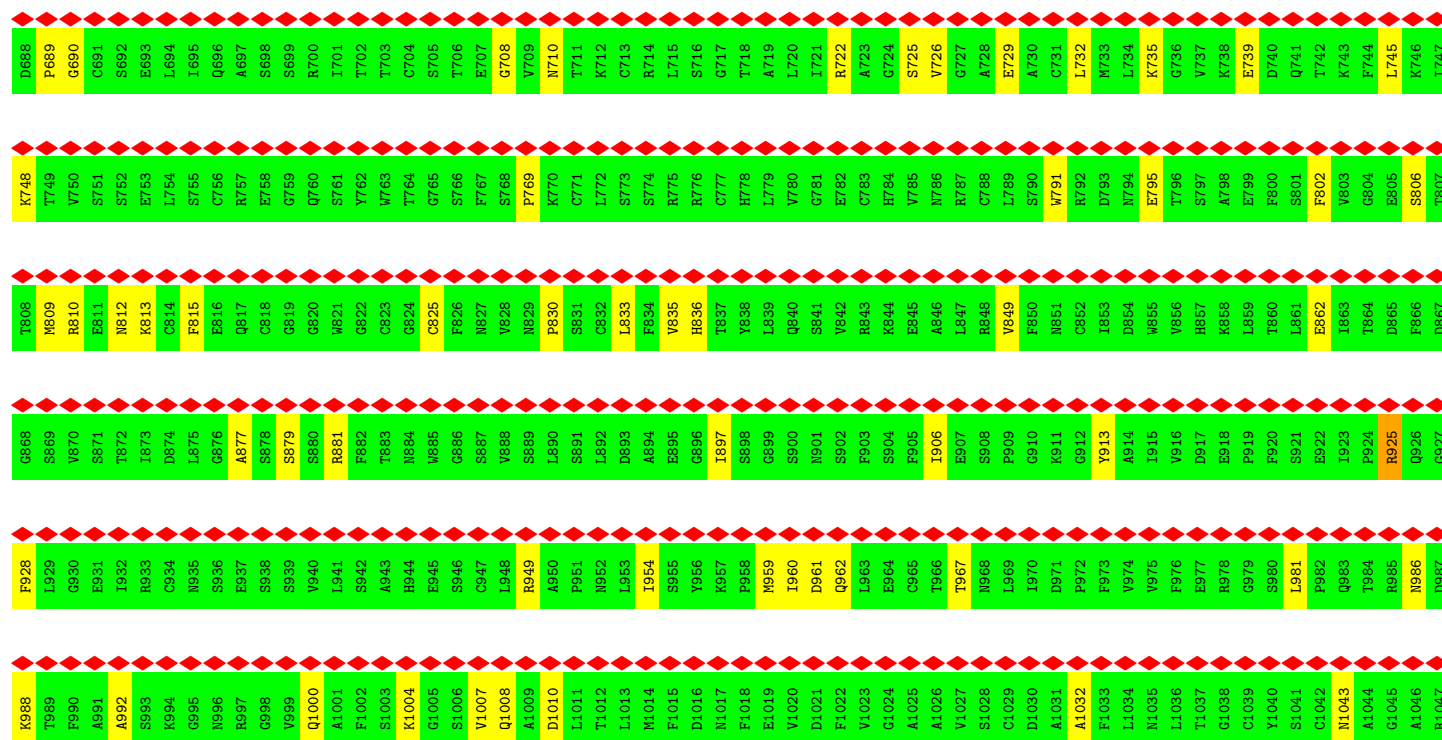
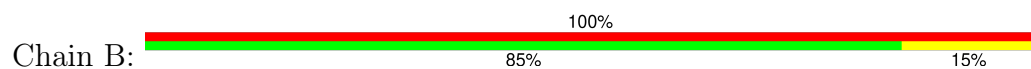




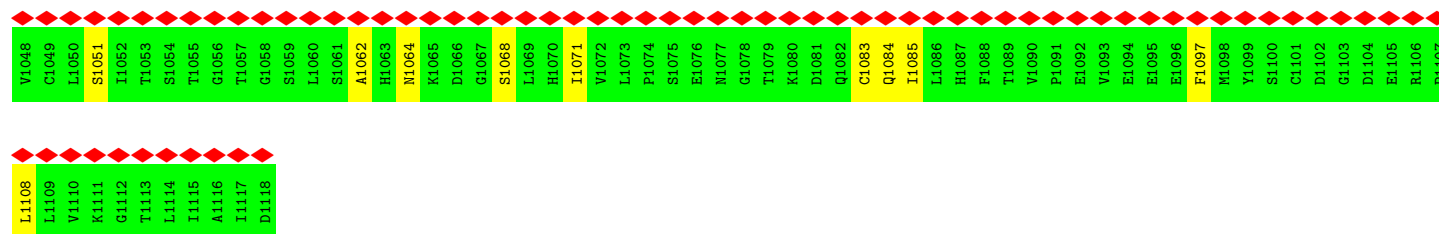
• Molecule 1: Glycoprotein



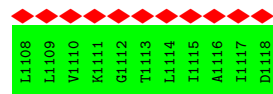
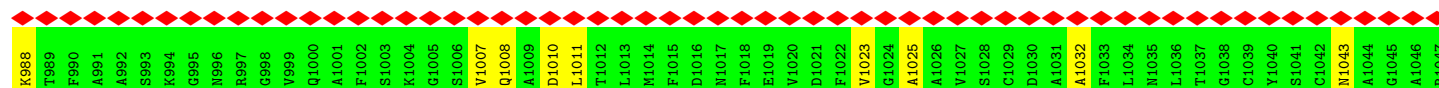
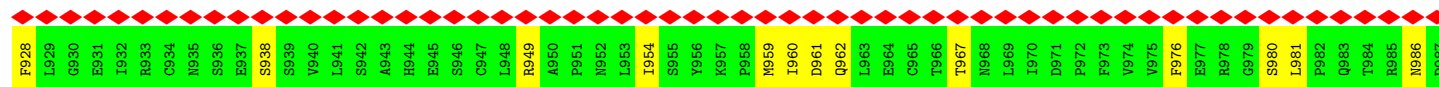
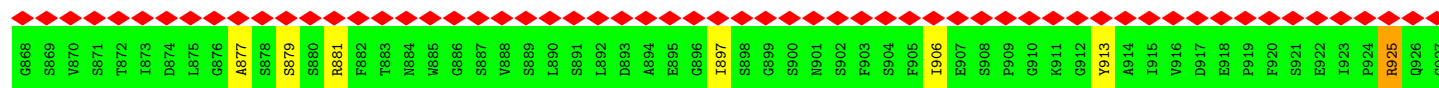
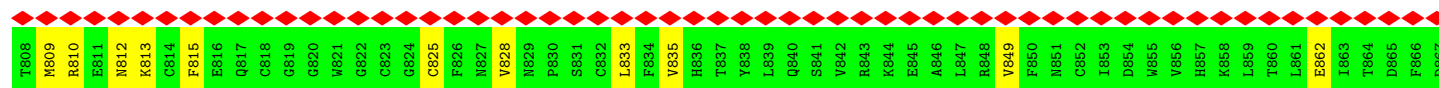
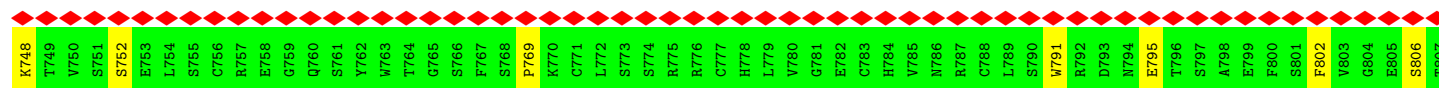
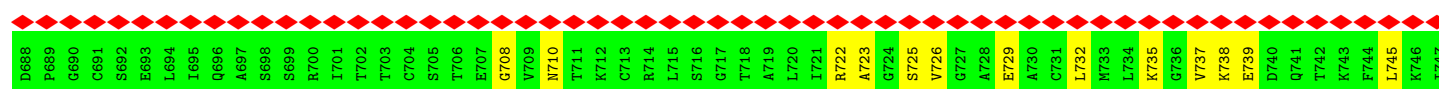
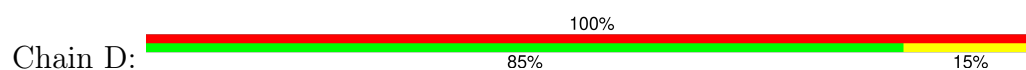
• Molecule 2: Glycoprotein



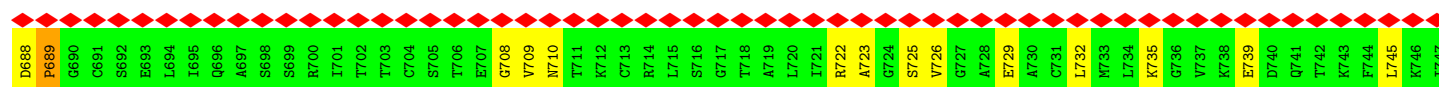
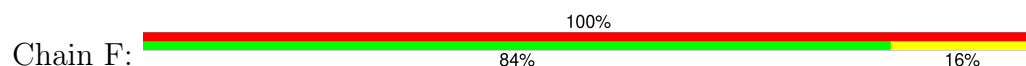




• Molecule 2: Glycoprotein

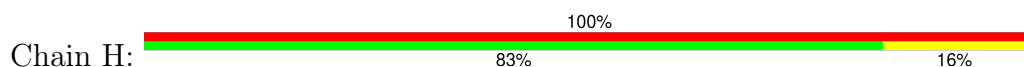


• Molecule 2: Glycoprotein



K748	T808	G868	F928	K988	V1048	L1108
T749	M809	S869	L929	T989	C1049	L1109
V750	R810	S870	G930	F990	L1050	V1110
S751	E811	S871	E931	A991	S1051	K1111
S752	N812	T872	I932	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	V1007	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	L833	D893	L953	L1013	L1073	
S774	F834	A894	I954	M1014	P1074	
R775	V835	E895	S955	F1015	S1075	
R776	H836	G896	Y956	D1016	E1076	
C777	T837	I897	K957	M1017	M1077	
H778	Y838	S898	P958	F1018	G1078	
L779	L839	G899	N959	E1019	T1079	
W780	Q840	S900	I960	V1020	K1080	
G781	S841	N901	D961	D1021	D1081	
E782	V842	S902	Q962	F1022	Q1082	
C783	R843	F903	L963	V1023	C1083	
H784	K844	S904	E964	G1024	Q1084	
V785	E845	F905	C965	A1025	I1085	
N786	A846	I906	T966	A1026	L1086	
R787	L847	E907	T967	V1027	H1087	
C788	R848	S908	N968	S1028	F1088	
L789	V849	P909	L969	C1029	T1089	
S790	F850	G910	I970	D1030	V1090	
W791	N851	K911	D971	A1031	P1091	
R792	C852	G912	P972	A1032	E1092	
D793	I853	Y913	F973	F1033	V1093	
N794	D854	A914	V974	L1034	E1094	
E795	W855	I915	V975	M1035	E1095	
T796	V856	V916	F976	L1036	E1096	
S797	H857	D917	E977	T1037	F1097	
A798	K858	E918	R978	G1038	M1098	
E799	L859	P919	G979	C1039	Y1099	
F800	T860	F920	S980	Y1040	S1100	
S801	L861	S921	L981	C1041	G1101	
F802	E862	E922	P982	C1042	D1102	
V803	I863	I923	Q983	M1043	G1103	
G804	T864	P924	T984	A1044	D1104	
E805	D865	R925	N985	G1045	E1105	
S806	F866	Q926	N986	A1046	R1106	
T807	D867	G927	D987	R1047	P1107	

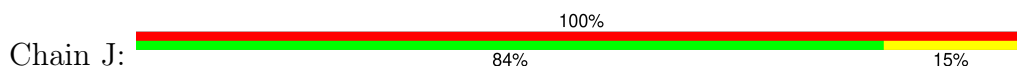
• Molecule 2: Glycoprotein



D688	K748	T808	G868	F928	V1048	L1108
P689	T749	M809	S869	L929	C1049	L1109
G690	V750	R810	S870	G930	L1050	V1110
C691	S751	E811	S871	E931	S1051	K1111
S692	S752	N812	T872	I932	T1052	G1112
F693	E753	K813	I873	R933	T1053	T1113
L694	L754	C814	D874	C934	S1054	L1114
T695	S755	F815	L875	N935	T1055	I1115
G696	C756	E816	G876	S936	G1056	A1116
A697	R757	Q817	A877	E937	T1057	I1117
S698	E758	C818	S878	S938	G1058	D1118
S699	G759	G819	S879	S939	S1059	
R700	Q760	G820	S880	V940	L1060	
I701	S761	W821	R881	L941	S1061	
T702	Y762	G822	F882	S942	A1062	
T703	W763	C823	T883	A943	H1063	
C704	T764	G824	N884	H944	N1064	
S705	G765	W885	E945	G1005	K1065	
T706	S766	G886	S946	S1006	D1066	
E707	F767	S887	C947	V1007	G1067	
G708	S768	S888	L948	Q1008	S1068	
V709	P769	N829	R949	A1009	L1069	
N710	K770	P830	A950	D1010	H1070	
T711	C771	S831	P951	L1011	T1071	
K712	L772	C832	N952	T1012	V1072	
C713	S773	L833	D893	L1013	L1073	
R714	S774	F834	A894	M1014	P1074	
L715	R775	V835	E895	F1015	S1075	
S716	R776	H836	G896	D1016	E1076	
G717	C777	T837	I897	M1017	M1077	
T718	H778	Y838	S898	F1018	G1078	
A719	L779	L839	G899	E1019	T1079	
L720	W780	Q840	S900	V1020	K1080	
I721	G781	S841	N901	D1021	D1081	
R722	E782	V842	S902	F1022	Q1082	
A723	C783	R843	F903	V1023	C1083	
G724	H784	K844	S904	G1024	Q1084	
S725	V785	E845	F905	A1025	I1085	
V726	N786	A846	I906	A1026	L1086	
G727	R787	L847	E907	V1027	H1087	
A728	C788	R848	S908	S1028	F1088	
E729	L789	V849	P909	C1029	T1089	
A730	S790	F850	G910	D1030	V1090	
C731	W791	N851	K911	A1031	P1091	
L732	R792	C852	G912	A1032	E1092	
M733	D793	I853	Y913	F1033	V1093	
L734	N794	D854	A914	L1034	E1094	
K735	E795	W855	I915	M1035	E1095	
G736	T796	V856	V916	L1036	E1096	
V737	S797	H857	D917	T1037	F1097	
K738	A798	K858	E918	G1038	M1098	
E739	E799	L859	P919	C1039	Y1099	
D740	F800	T860	F920	Y1040	S1100	
Q741	S801	L861	S921	C1041	G1101	
T742	F802	E862	E922	C1042	D1102	
K743	V803	I863	I923	M1043	G1103	
F744	G804	T864	P924	A1044	D1104	
L745	E805	D865	R925	G1045	E1105	
K746	S806	F866	Q926	A1046	R1106	
I747	T807	D867	G927	R1047	P1107	

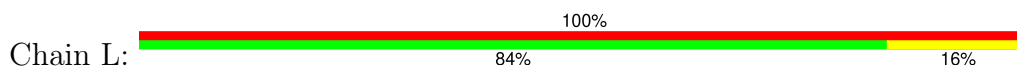
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L1109	C1049	T989
V1110	L1050	F990
K1111	S1051	A991
G1112	T1052	A992
T1113	T1053	S993
L1114	S1054	K994
I1115	T1055	G995
A1116	G1056	N996
I1117	T1057	R997
D1118	G1058	G998
	S1059	V999
	L1060	Q1000
	S1061	A1001
	A1062	F1002
	H1063	S1003
	M1064	K1004
	K1065	G1005
	D1066	S1006
	G1067	V1007
	S1068	Q1008
	L1069	A1009
	H1070	L1010
	T1071	L1011
	V1072	T1012
	L1073	L1013
	T1074	M1014
	S1075	F1015
	E1076	D1016
	M1077	N1017
	G1078	F1018
	T1079	E1019
	K1080	V1020
	D1081	D1021
	G1082	F1022
	C1083	V1023
	Q1084	G1024
	I1085	A1025
	L1086	A1026
	H1087	V1027
	F1088	S1028
	T1089	C1029
	V1090	D1030
	P1091	A1031
	E1092	A1032
	V1093	F1033
	E1094	L1034
	E1095	N1035
	E1096	L1036
	F1097	T1037
	M1098	G1038
	V1099	C1039
	S1100	V1040
	C1101	S1041
	D1102	C1042
	G1103	N1043
	D1104	A1044
	E1105	G1045
	L1106	A1046
	P1107	V1047

- Molecule 2: Glycoprotein



L1108	V1048	K988	F928	G868	T808	K748	D688
L1109	C1049	T989	L929	S869	M809	T749	P689
V1110	L1050	F990	G930	V870	R810	V750	G690
K1111	S1051	A991	E931	S871	E811	S751	C691
G1112	I1052	A992	I932	T872	M812	S752	S692
T1113	T1053	S993	R933	I873	K813	E753	E693
L1114	S1054	K994	C934	D874	C814	L894	L694
I1115	T1055	G995	N935	L875	F815	S755	I695
A1116	G1056	N996	S936	G876	E816	C756	Q696
I1117	T1057	R997	E937	A877	Q817	R757	A697
D1118	G1058	G998	S938	S878	E818	E758	S698
	S1059	V999	S939	S879	G819	G759	S699
	L1060	Q1000	V940	S880	G820	Q760	R700
	S1061	A1001	L941	R881	M821	S761	I701
	A1062	F1002	S942	T882	G822	Y762	T702
	H1063	S1003	A943	T883	C823	W763	T703
	N1064	K1004	H944	M884	G824	T764	C704
	K1065	G1005	E945	W885	C825	G765	S705
	D1066	S1006	S946	G886	F826	S766	S706
	G1067	Y1007	C947	S887	M827	F767	E707
	S1068	Q1008	L948	V888	V828	S768	G708
	L1069	A1009	R949	S889	M829	P769	Y709
	H1070	D1010	A950	L890	P830	K770	N710
	I1071	L1011	P951	S891	S831	C771	T711
	T1072	T1012	N952	L892	C832	L772	K712
	L1073	L1013	L953	D893	L833	S773	C713
	T1074	M1014	I954	A894	F834	S774	R714
	S1075	F1015	S955	E895	V835	R775	L715
	E1076	D1016	Y956	G896	H836	R776	S716
	N1077	N1017	K957	I897	T837	C777	G717
	G1078	F1018	P958	S898	V838	H778	T718
	T1079	E1019	M959	G899	L839	L779	A719
	K1080	V1020	I960	S900	Q840	V780	L720
	D1081	D1021	D961	M901	S841	G781	I721
	Q1082	F1022	Q962	S902	V842	E782	R722
	C1083	V1023	L963	F903	R843	C783	A723
	Q1084	G1024	E964	S904	K844	H784	G724
	I1085	A1025	C965	F905	E845	V785	S725
	L1086	A1026	T966	I906	A846	M786	V726
	H1087	V1027	T967	E907	L847	R787	G727
	T1088	S1028	N968	S908	R848	C788	A728
	T1089	C1029	L969	P909	V849	L789	E729
	V1090	D1030	I970	G910	F850	S790	A730
	P1091	A1031	D971	K911	M851	W791	C731
	E1092	A1032	P972	G912	C852	R792	L732
	V1093	F1033	F973	Y913	T853	D793	M733
	E1094	L1034	V974	A914	D854	L794	L734
	E1095	N1035	V975	I915	W855	E795	K735
	E1096	L1036	F976	V916	V856	T796	G736
	F1097	T1037	E977	D917	H857	S797	V737
	M1098	G1038	R978	E918	K858	A798	K738
	V1099	C1039	G979	P919	L859	E799	E739
	S1100	Y1040	S980	F920	T860	F800	D740
	C1101	S1041	L981	S921	L861	S801	Q741
	D1102	C1042	P982	E922	E862	F802	T742
	G1103	N1043	Q983	I923	T863	V803	K743
	E1104	A1044	T984	P924	K864	G804	F744
	E1105	G1045	R985	R925	D865	E805	L745
	L1106	A1046	N986	Q926	F866	S806	K746
	P1107	B1047	E987	G927	D867	T807	L747

- Molecule 2: Glycoprotein



L1108	V1048	K988	F928	G868	T808	K748	D688
L1109	C1049	T989	L929	S869	M809	T749	P689
V1110	L1050	F990	G930	V870	R810	V750	G690
K1111	S1051	A991	E931	S871	E811	S751	C691
G1112	I1052	A992	I932	T872	N812	S752	S692
T1113	T1053	S993	R933	I873	K813	E753	E693
L1114	S1054	K994	C934	D874	C814	L754	L694
I1115	T1055	G995	N935	L875	F815	S755	I695
A1116	G1056	N996	S936	G876	E816	C756	Q696
I1117	T1057	R997	E937	A877	Q817	R757	A697
D1118	G1058	G998	S938	S878	C818	E758	S698
	S1059	V999	S939	S879	G819	G759	S699
	L1060	Q1000	V940	S880	G820	Q760	R700
	S1061	A1001	L941	R881	W821	S761	I701
	A1062	F1002	S942	F882	G822	Y762	T702
	H1063	S1003	A943	T883	C823	W763	T703
	N1064	K1004	H944	N884	G824	T764	C704
	K1065	G1005	E945	W885	C825	G765	S705
	D1066	S1006	S946	G886	F826	S766	T706
	G1067	V1007	C947	S887	N827	F767	E707
	S1068	Q1008	L948	V888	W828	S768	G708
	L1069	A1009	R949	S889	N829	P769	V709
	H1070	D1010	A950	L890	P830	K770	N710
	I1071	L1011	P951	S891	S831	C771	T711
	V1072	T1012	N952	L892	C832	L772	K712
	L1073	L1013	L953	D893	L833	S773	C713
	P1074	M1014	I954	A894	F834	S774	R714
	S1075	F1015	S955	E895	W835	R775	L715
	E1076	D1016	Y956	G896	H836	R776	S716
	N1077	N1017	K957	I897	T837	C777	G717
	G1078	F1018	P958	S898	Y838	H778	T718
	T1079	E1019	N959	G899	L839	L779	A719
	K1080	V1020	I960	S900	Q840	W780	L720
	D1081	D1021	D961	N901	S841	G781	I721
	Q1082	F1022	Q962	S902	V842	E782	R722
	C1083	V1023	L963	F903	R843	C783	A723
	Q1084	G1024	E964	S904	K844	H784	G724
	I1085	A1025	C965	F905	E845	V785	S725
	L1086	A1026	T966	I906	A846	N786	V726
	H1087	V1027	T967	E907	L847	R787	G727
	F1088	S1028	N968	S908	R848	C788	A728
	T1089	C1029	L969	P909	V849	L789	E729
	V1090	D1030	I970	G910	F850	S790	A730
	P1091	A1031	D971	K911	N851	W791	C731
	E1092	A1032	P972	G912	C852	R792	L732
	V1093	F1033	F973	Y913	T853	D793	M733
	E1094	L1034	V974	A914	D854	N794	L734
	E1095	N1035	V975	I915	W855	E795	K735
	E1096	L1036	F976	V916	V856	T796	G736
	F1097	T1037	E977	D917	H857	S797	V737
	M1098	G1038	R978	E918	K858	A798	K738
	V1099	C1039	G979	P919	L859	E799	E739
	S1100	Y1040	S980	F920	T860	F800	D740
	C1101	S1041	L981	S921	L861	S801	Q741
	D1102	C1042	P982	E922	E862	F802	T742
	G1103	N1043	Q983	I923	T863	V803	K743
	D1104	A1044	T984	P924	T864	G804	F744
	E1105	G1045	R985	R925	D865	E905	L745
	R1106	A1046	N986	Q926	F866	S806	K746
	P1107	R1047	D987	G927	D867	T807	I747

## 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	0.121	Depositor
Minimum map value	-0.060	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.40	0/3136
1	C	0.24	0/2333	0.41	0/3136
1	E	0.24	0/2333	0.40	0/3136
1	G	0.24	0/2333	0.41	0/3136
1	I	0.24	0/2333	0.40	0/3136
1	K	0.24	0/2333	0.41	0/3136
2	B	0.24	0/3284	0.42	0/4431
2	D	0.24	0/3284	0.42	0/4431
2	F	0.24	0/3284	0.43	1/4431 (0.0%)
2	H	0.24	0/3284	0.42	0/4431
2	J	0.24	0/3284	0.42	0/4431
2	L	0.24	0/3284	0.42	0/4431
All	All	0.24	0/33702	0.42	1/45402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	689	PRO	C-N-CA	5.95	134.78	122.30

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	21	0
1	C	2284	0	2205	27	0
1	E	2284	0	2205	27	0
1	G	2284	0	2205	32	0
1	I	2284	0	2205	21	0
1	K	2284	0	2205	27	0
2	B	3224	0	3071	34	0
2	D	3224	0	3071	35	0
2	F	3224	0	3071	36	0
2	H	3224	0	3071	42	0
2	J	3224	0	3071	35	0
2	L	3224	0	3071	38	0
All	All	33048	0	31656	353	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.

The worst 5 of 353 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)
2:H:926:GLN:NE2	2:H:931:GLU:OE2	2.27	0.67
2:D:959:MET:HB2	2:D:962:GLN:HB2	1.79	0.65
2:F:959:MET:HB2	2:F:962:GLN:HB2	1.79	0.64
2:D:1062:ALA:HB3	2:D:1071:ILE:HB	1.80	0.64
2:B:959:MET:HB2	2:B:962:GLN:HB2	1.79	0.64

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%)	251 (85%)	39 (13%)	5 (2%)	<b>7</b> 37

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	295/316 (93%)	253 (86%)	38 (13%)	4 (1%)	9	41
1	E	295/316 (93%)	254 (86%)	37 (12%)	4 (1%)	9	41
1	G	295/316 (93%)	250 (85%)	39 (13%)	6 (2%)	6	32
1	I	295/316 (93%)	254 (86%)	37 (12%)	4 (1%)	9	41
1	K	295/316 (93%)	252 (85%)	39 (13%)	4 (1%)	9	41
2	B	429/431 (100%)	372 (87%)	51 (12%)	6 (1%)	9	41
2	D	429/431 (100%)	370 (86%)	53 (12%)	6 (1%)	9	41
2	F	429/431 (100%)	372 (87%)	50 (12%)	7 (2%)	8	38
2	H	429/431 (100%)	374 (87%)	49 (11%)	6 (1%)	9	41
2	J	429/431 (100%)	372 (87%)	50 (12%)	7 (2%)	8	38
2	L	429/431 (100%)	372 (87%)	50 (12%)	7 (2%)	8	38
All	All	4344/4482 (97%)	3746 (86%)	532 (12%)	66 (2%)	11	40

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	CYS
2	B	825	CYS
2	D	825	CYS
1	E	456	CYS
2	F	709	VAL

### 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%)	238 (99%)	3 (1%)	67	78
1	C	241/271 (89%)	239 (99%)	2 (1%)	79	85
1	E	241/271 (89%)	237 (98%)	4 (2%)	56	72
1	G	241/271 (89%)	239 (99%)	2 (1%)	79	85
1	I	241/271 (89%)	238 (99%)	3 (1%)	67	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	241/271 (89%)	238 (99%)	3 (1%)	67	78
2	B	347/371 (94%)	344 (99%)	3 (1%)	75	83
2	D	347/371 (94%)	345 (99%)	2 (1%)	84	88
2	F	347/371 (94%)	344 (99%)	3 (1%)	75	83
2	H	347/371 (94%)	344 (99%)	3 (1%)	75	83
2	J	347/371 (94%)	343 (99%)	4 (1%)	67	78
2	L	347/371 (94%)	344 (99%)	3 (1%)	75	83
All	All	3528/3852 (92%)	3493 (99%)	35 (1%)	71	82

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	1047	ARG
1	K	160	ASN
2	L	925	ARG
1	E	358	LYS
1	E	282	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	438	ASN
2	L	1000	GLN
2	H	1000	GLN
2	L	1070	HIS
1	K	160	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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.

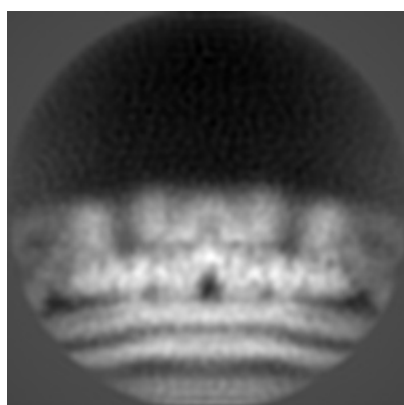
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4200. These allow visual inspection of the internal detail of the map and identification of artifacts.

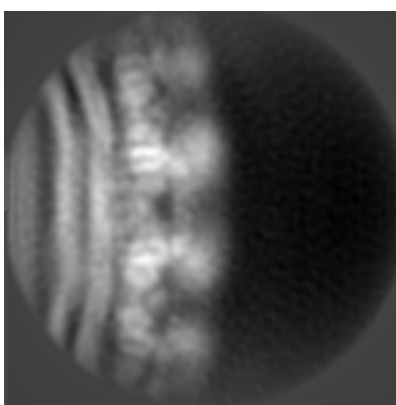
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

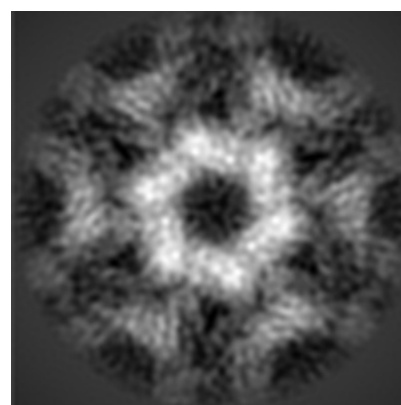
#### 6.1.1 Primary map



X



Y

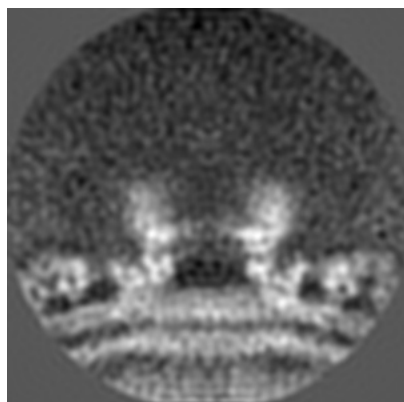


Z

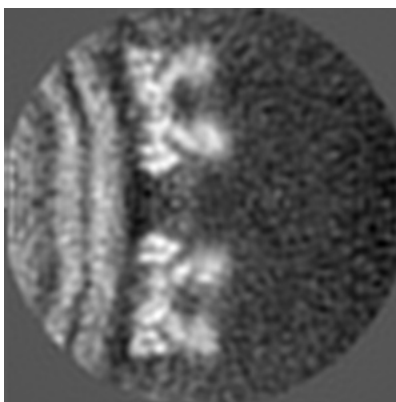
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

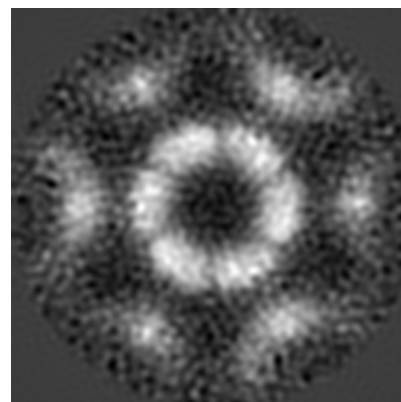
#### 6.2.1 Primary map



X Index: 64



Y Index: 64

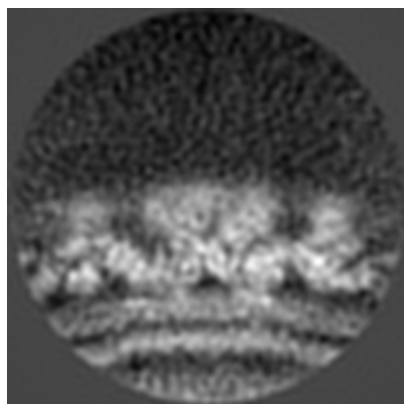


Z Index: 64

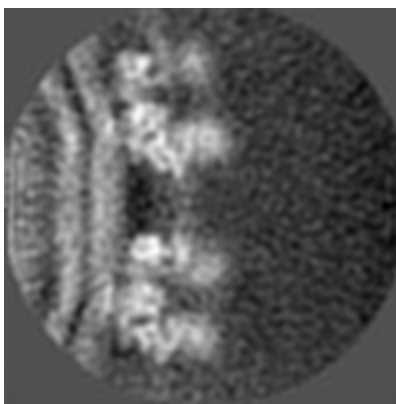
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

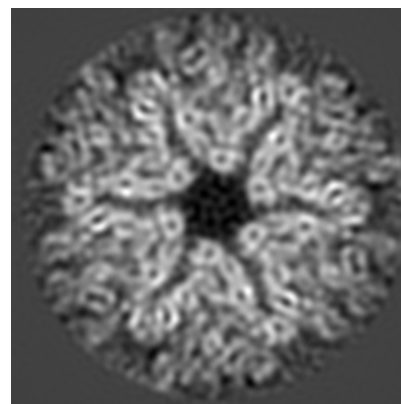
### 6.3.1 Primary map



X Index: 82



Y Index: 60

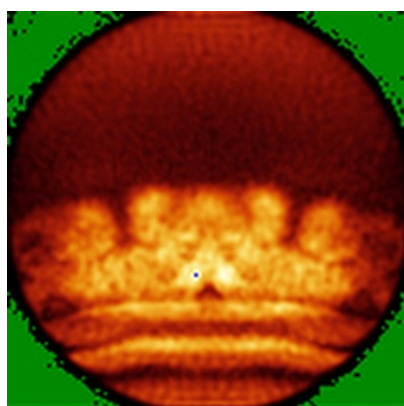


Z Index: 43

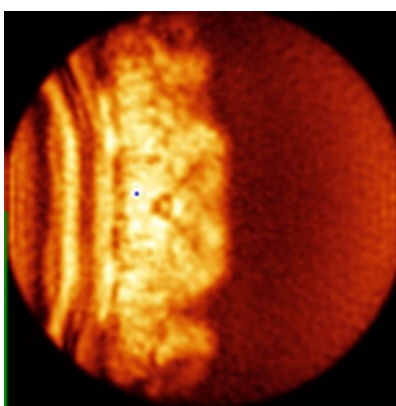
The images above show the largest variance slices of the map in three orthogonal directions.

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

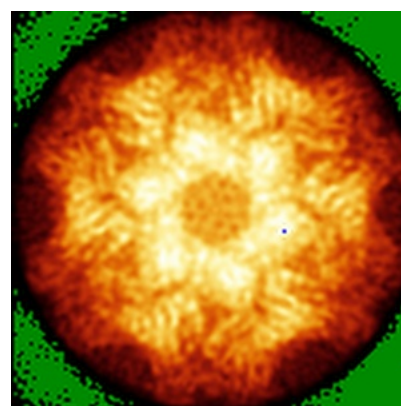
### 6.4.1 Primary map



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.

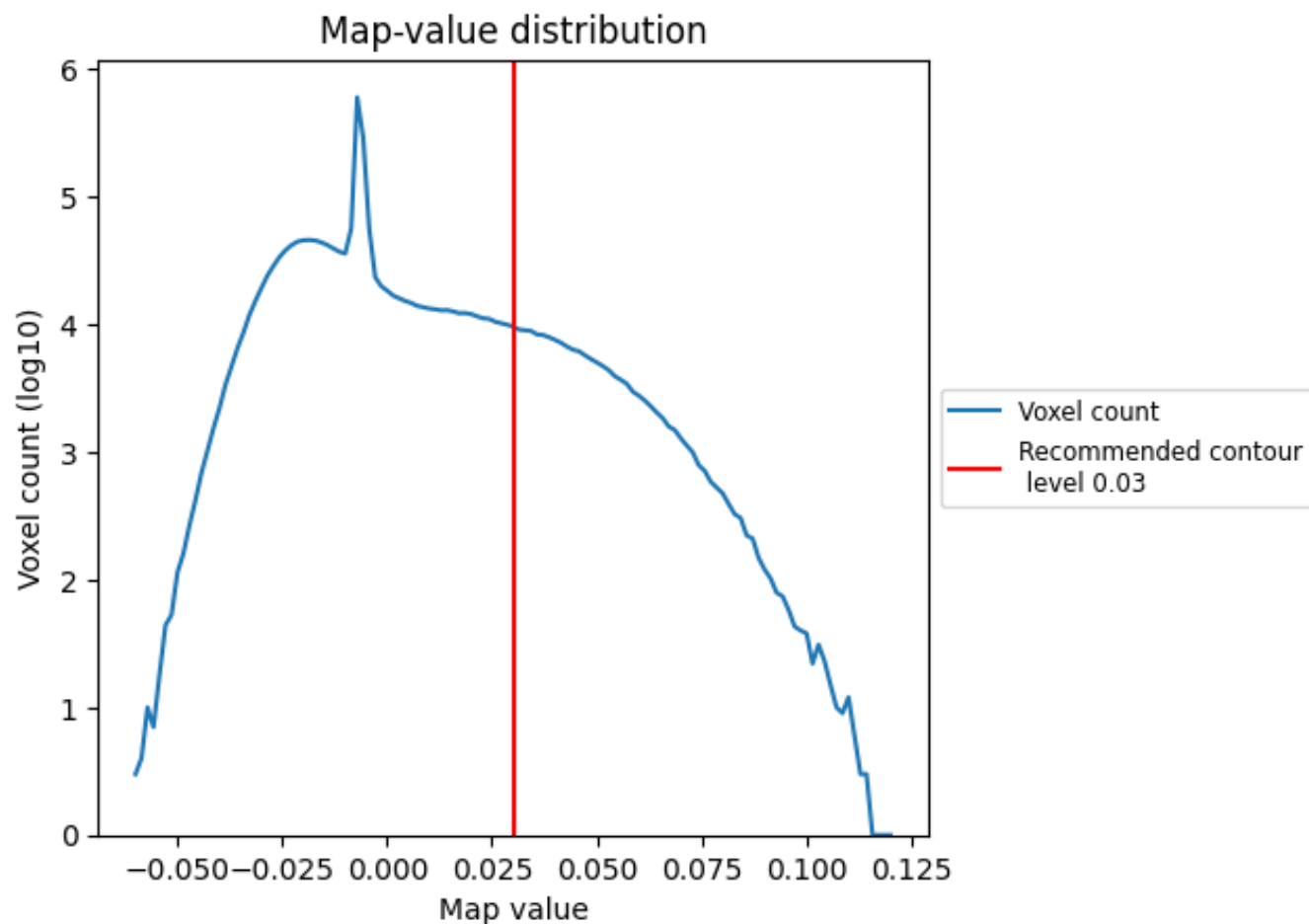
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

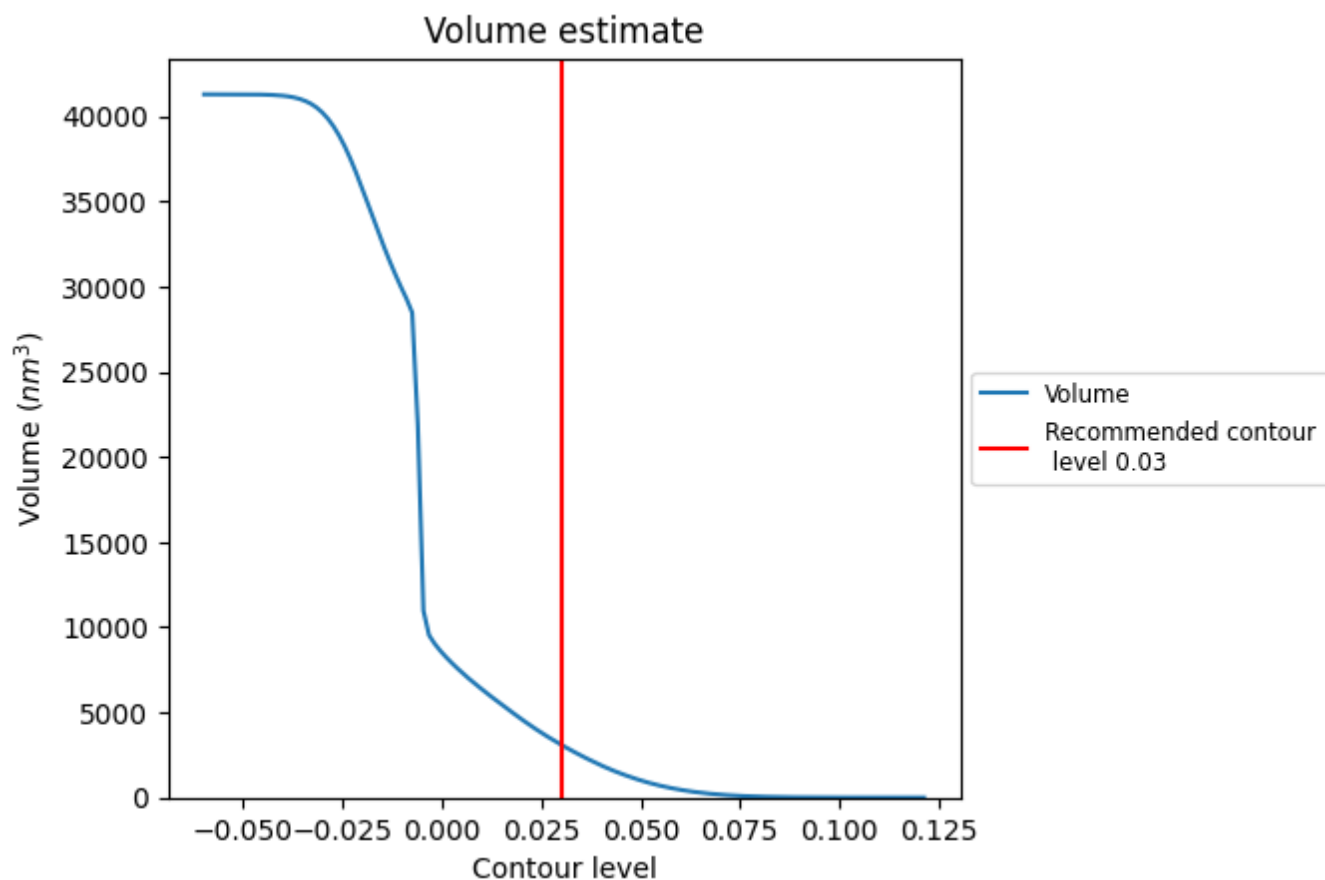
This section contains the results of statistical analysis of the map.

### 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.

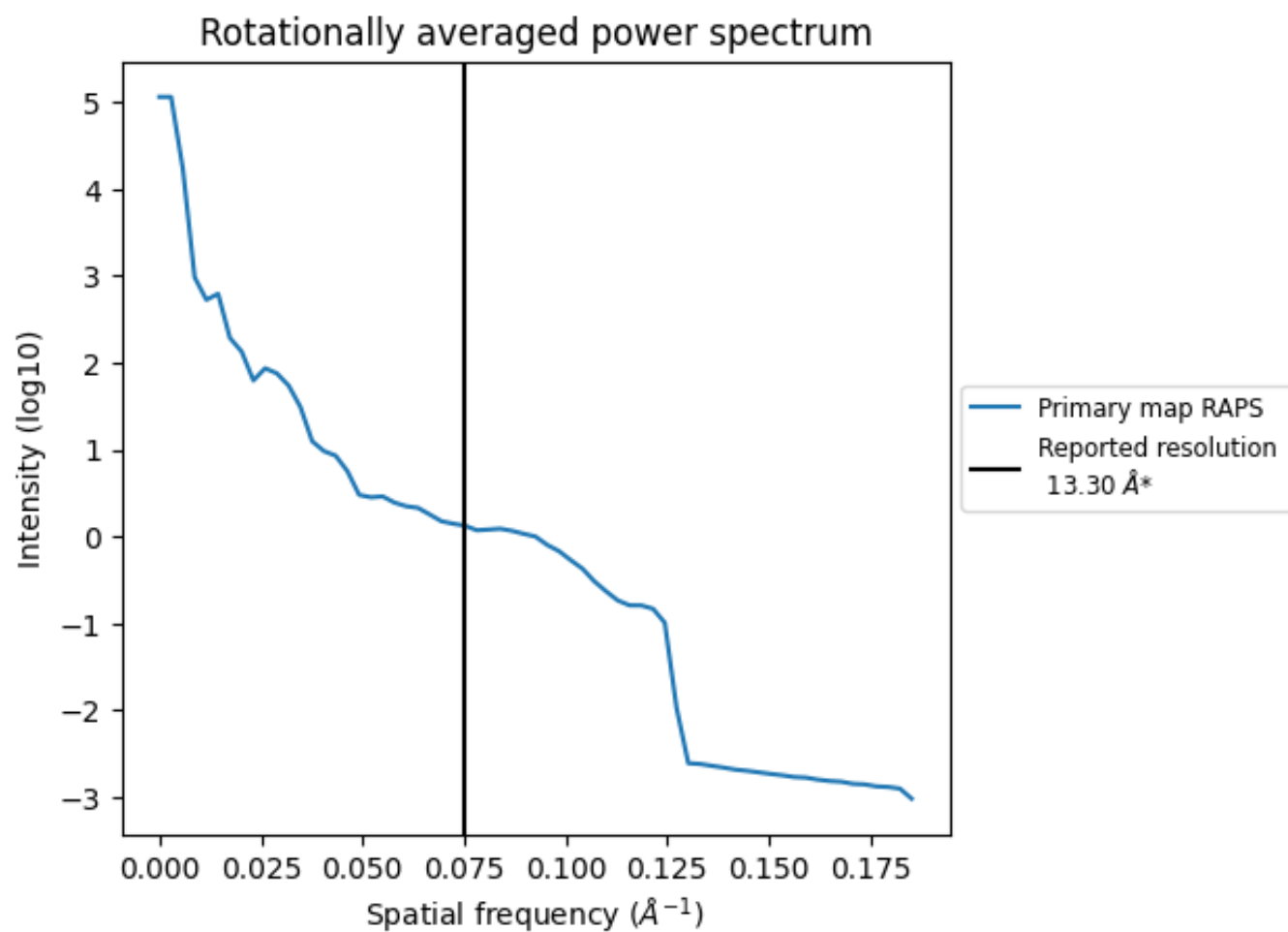
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3102 nm<sup>3</sup>; this corresponds to an approximate mass of 2802 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 ⓘ



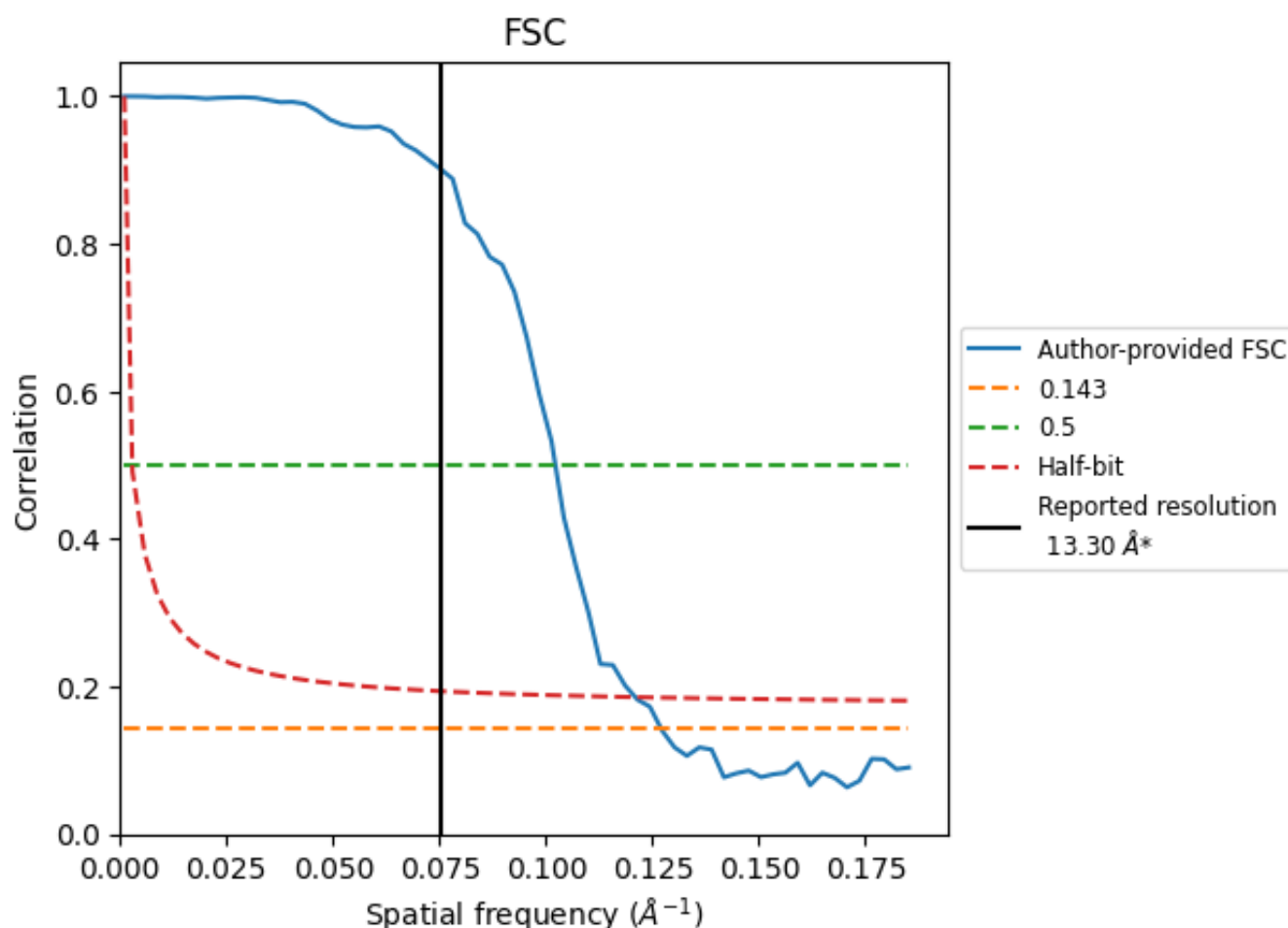
\*Reported resolution corresponds to spatial frequency of 0.075 Å<sup>-1</sup>



## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

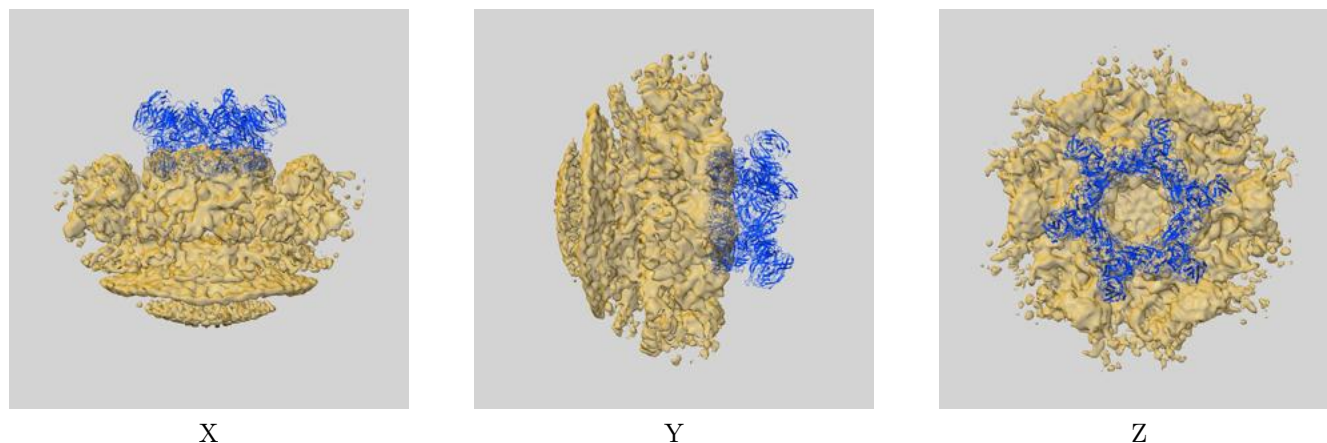
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.30	-	-
Author-provided FSC curve	7.87	9.78	8.26
Unmasked-calculated*	-	-	-

\*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 7.87 differs from the reported value 13.3 by more than 10 %

## 9 Map-model fit [i](#)

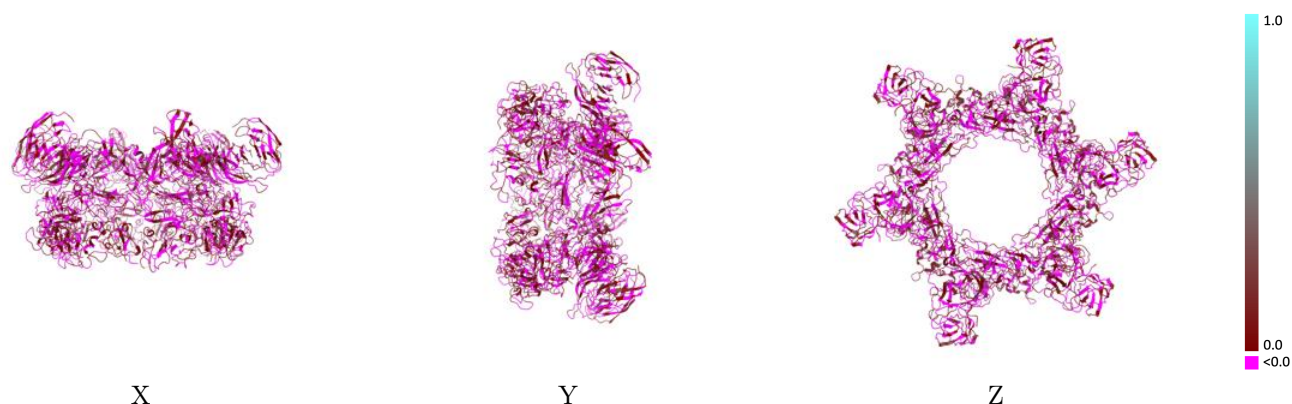
This section contains information regarding the fit between EMDB map EMD-4200 and PDB model 6F9E. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



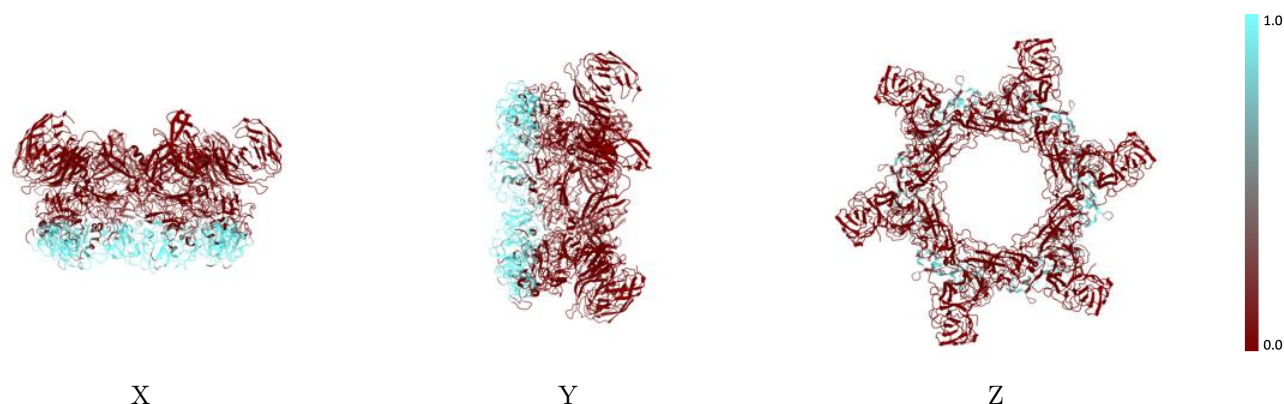
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



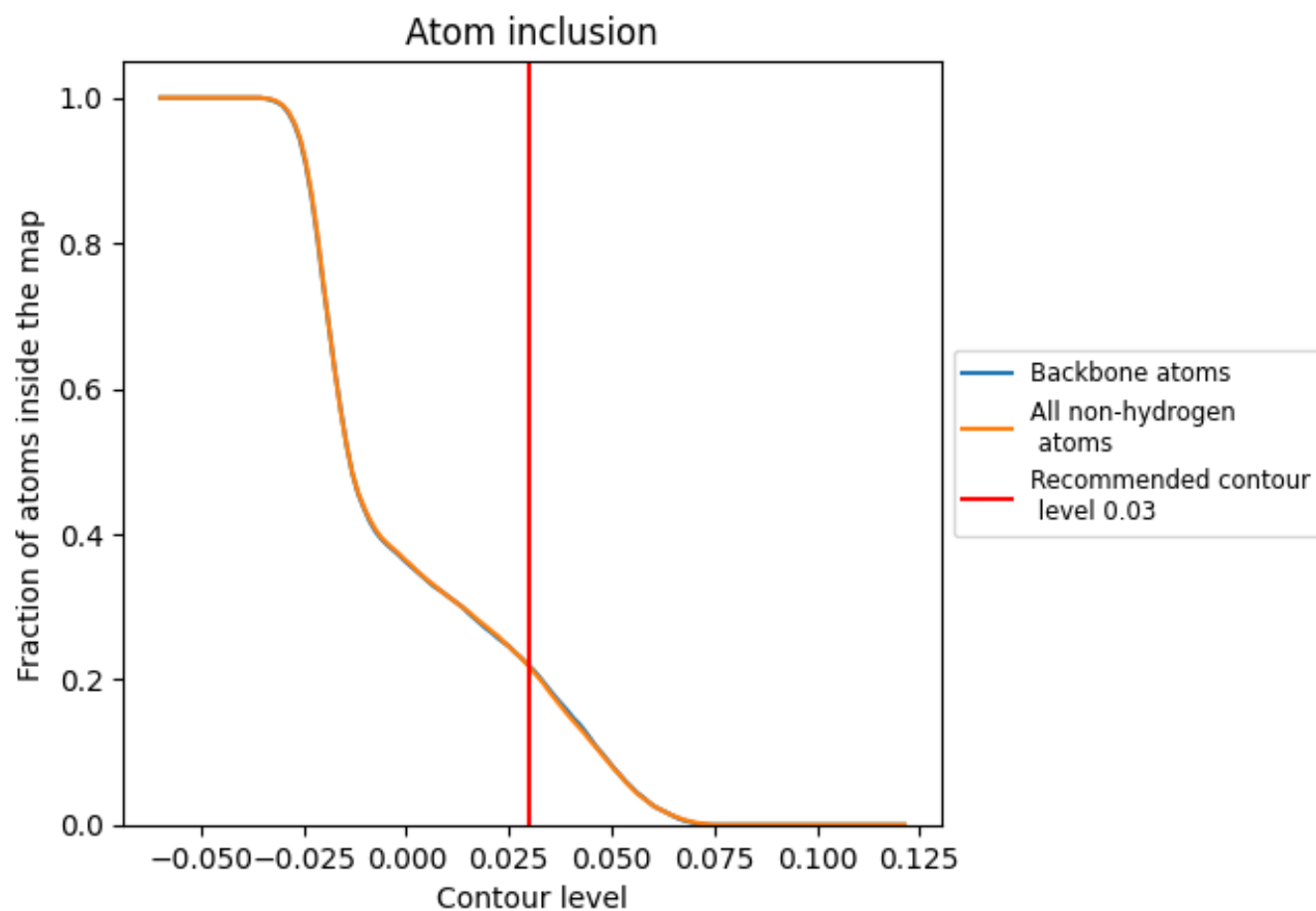
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 22% of all backbone atoms, 22% 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	 0.2170	 0.0090
A	 0.5180	 0.0220
B	 0.0010	 0.0060
C	 0.4960	 0.0190
D	 0.0000	 0.0010
E	 0.5060	 0.0260
F	 0.0000	 -0.0000
G	 0.5210	 0.0210
H	 0.0000	 -0.0040
I	 0.5380	 0.0250
J	 0.0010	 -0.0020
K	 0.5430	 0.0180
L	 0.0000	 -0.0010

