



## Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 07:56 PM EDT

PDB ID : 6DR2  
EMDB ID : EMD-7988  
Title : Ca<sup>2+</sup>-bound human type 3 1,4,5-inositol trisphosphate receptor  
Authors : Hite, R.K.; Paknejad, N.  
Deposited on : 2018-06-11  
Resolution : 4.33 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](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) : 2.39

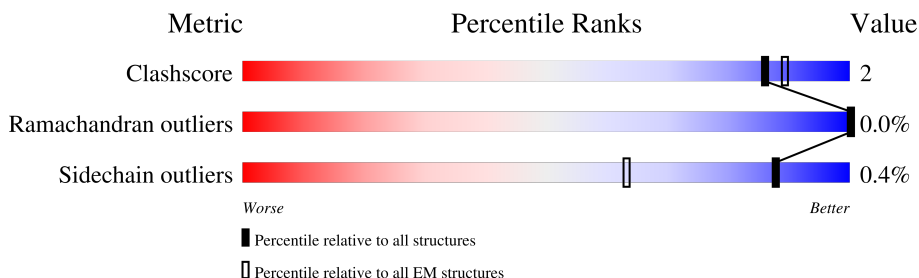
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.33 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	2671	<div> <div>38%</div> <div>77%</div> <div>5%</div> <div>18%</div> </div>
1	B	2671	<div> <div>39%</div> <div>77%</div> <div>5%</div> <div>18%</div> </div>
1	C	2671	<div> <div>39%</div> <div>76%</div> <div>5%</div> <div>18%</div> </div>
1	D	2671	<div> <div>39%</div> <div>77%</div> <div>5%</div> <div>18%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 139084 atoms, of which 69544 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 Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		
1	B	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		
1	C	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		
1	D	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

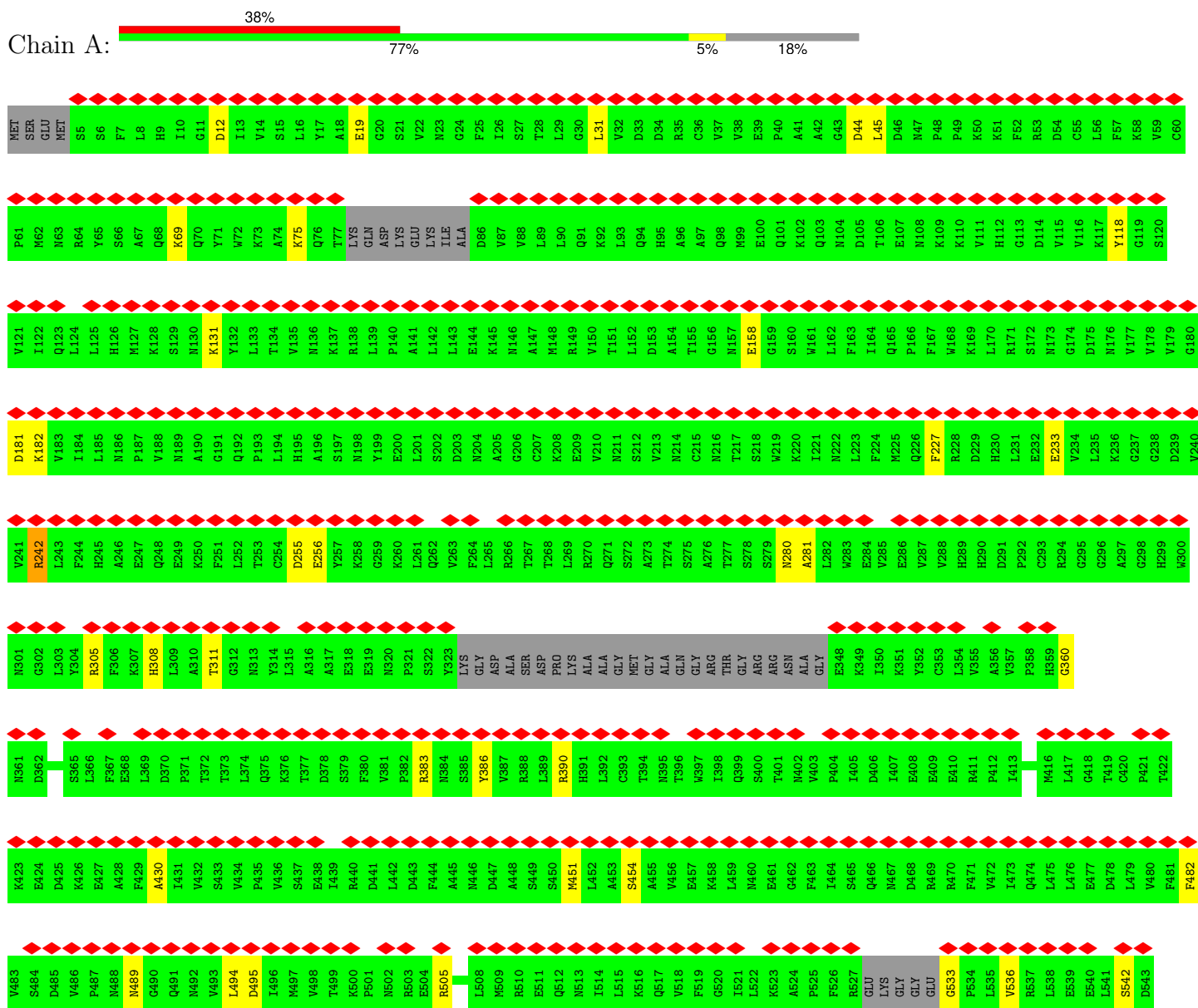
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	

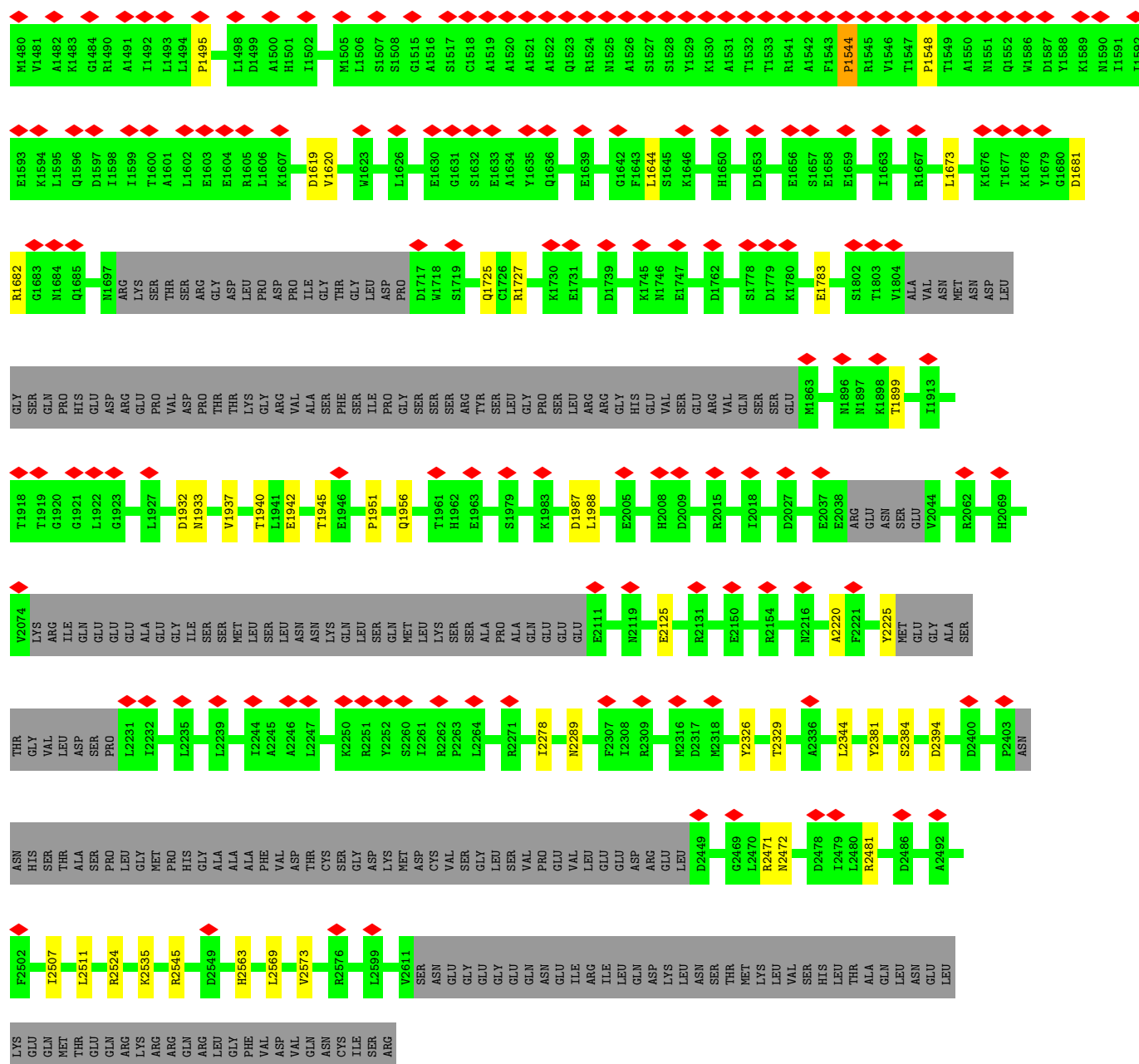
### 3 Residue-property plots

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.

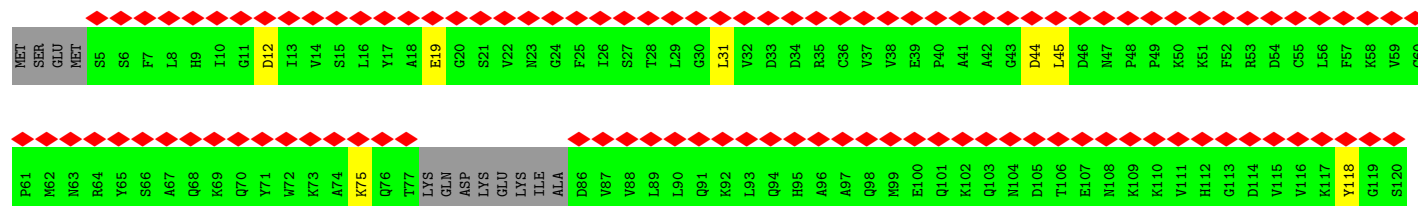
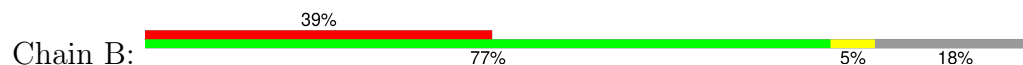
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



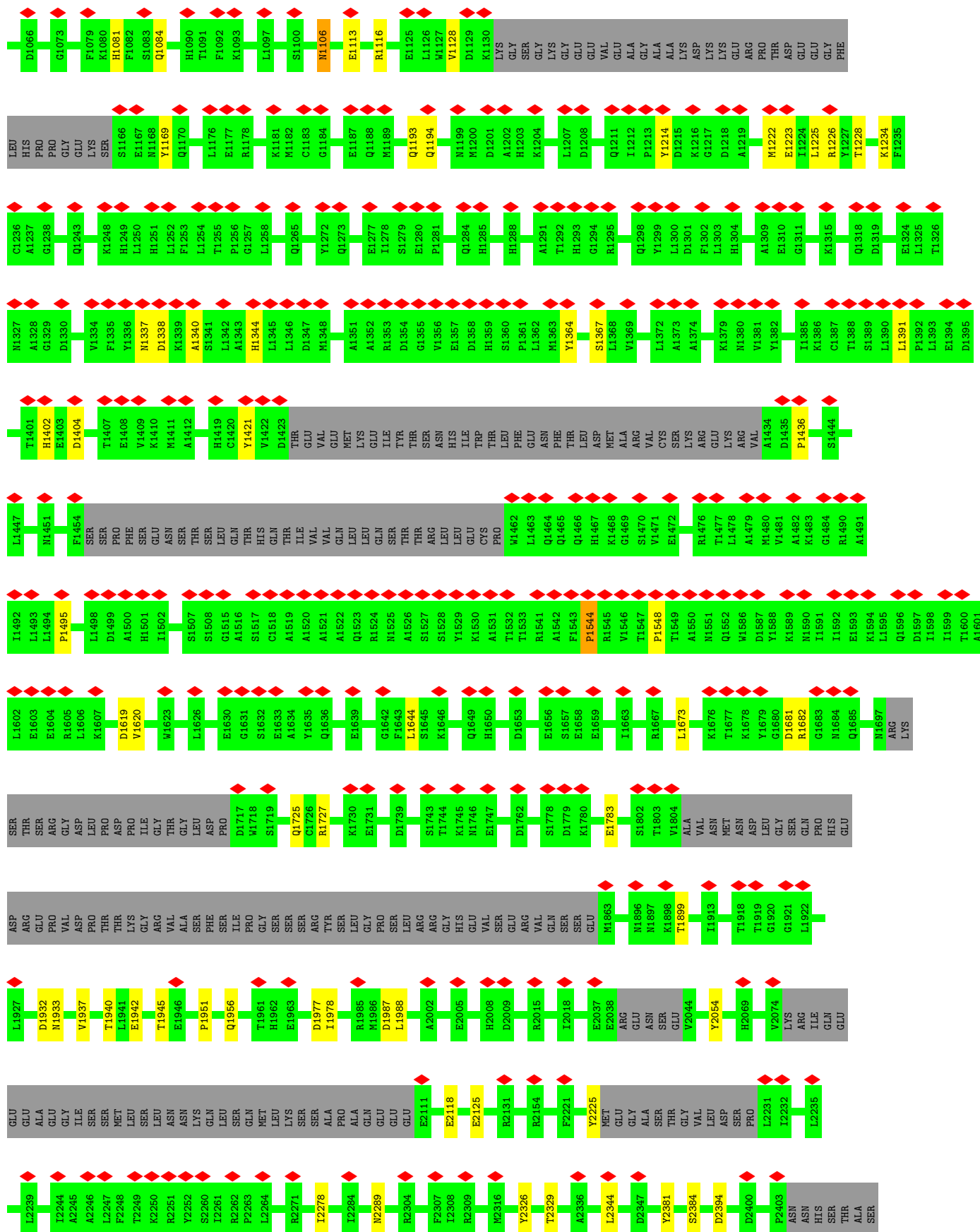




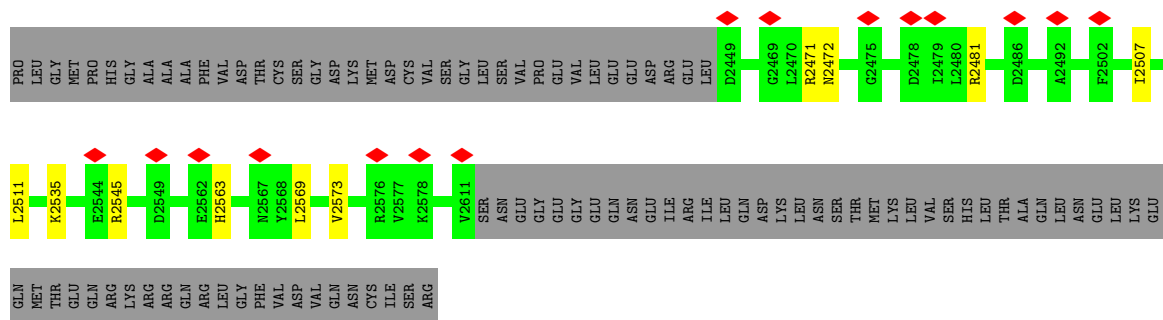
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



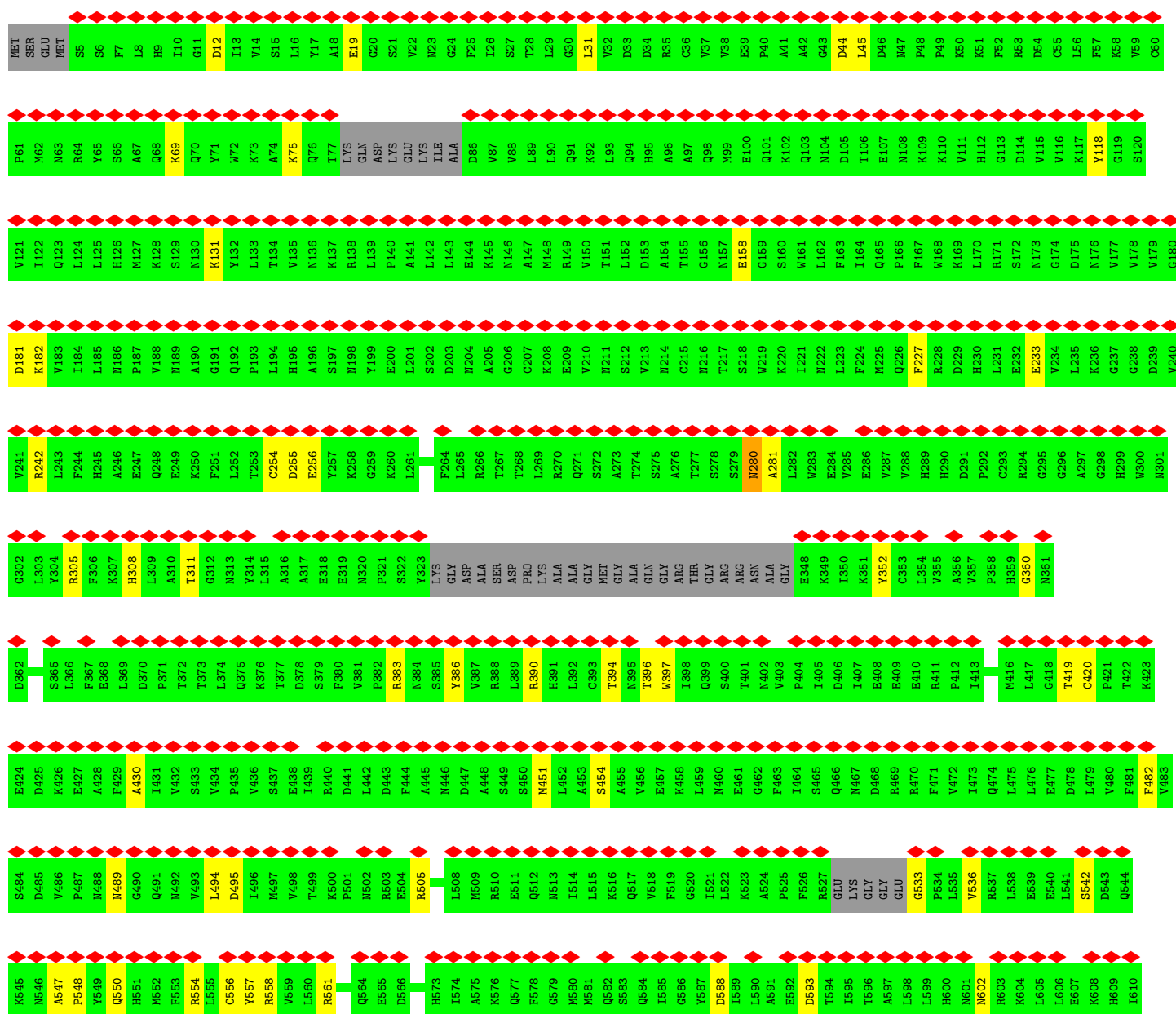
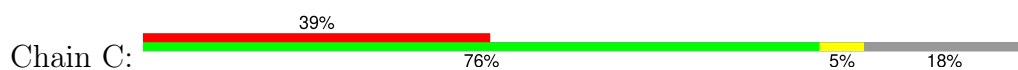
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ARG	ARG	SER	ILE	GLN	GLY	VAL	HIS	GLY	GLY	HIS	MET	MET	THR	THR	VAL	LEU	SER	ASP	ARG	GLN	LYS	GLY	ALA	ASP	GLY	THR	ALA	PRO	ALA	PHE	LEU	SER	ASP	ALA	GLY	ALA	SER	THR	THR	ALA	ALA	GLU	PRO	ASP	GLU	ASN	GLU	D961	N965	E966	T967	E973	Q976	N980	L983				
G756	V757	D758	L759	L762	C763	D766	E767	M768	L769	F770	F771	D772	L773	R774	A775	S776	F777	C778	H779	L780	M781	L782	H783	V784	H785	E792	L793	V797	R801	L802	P807	T808	A809	K813	D814	Y815	N818	L819	N820	A821	S822	D825	K826	K827	N828	A831	N832	T833											
D839	H843	V844	V845	S846	E847	A848	V849	P850	F851	A852	N853	E854	E855	K856	N857	K858	L859	T860	F861	H868	I871	Y872	F873	G874	S879	R883	R886	T887	G890	I891	I892	D893	C894	VAL	GLN	GLY	PRO	ALA	MET	LEU	GLN	ALA	TYR	GLU	ASP	PRO	GLY	LYS	VAL										
H609	T610	T611	K612	V615	E616	T617	F618	V619	S620	E621	V622	N625	R626	E627	P628	R629	F630	L631	D632	F633	L634	S635	L637	C638	V639	S640	N641	H642	Q649	E650	L651	C655	V656	L657	D658	P659	K660	N661	S662	D663	I664	L665	L666	R667	T668	E669	L670	R671	P672	V673	K674	GLU	MET	ALA					
D543	Q544	K545	N546	A547	P548	Y549	Q550	H551	M552	F553	R554	L555	C556	Y557	R558	V559	L560	R561	Q564	E565	D566	H573	L574	A575	K576	Q577	F578	G579	M580	Q582	S583	Q584	L585	G586	Y587	D588	I589	L590	A591	E592	D593	T594	L595	T596	A597	L598	L599	H600	N601	N602	R603	K604	L605	L606	E607	K608			
F482	V483	S484	D485	V486	P487	N488	N489	G490	Q491	N492	L494	D495	L496	V497	V498	T499	K500	F501	N502	R503	E504	R505	Q506	M509	R510	E511	Q512	N513	I514	L515	K516	Q517	V518	F519	G520	I521	L522	K523	A524	P525	F526	R527	GLU	LYS	GLY	GLY	G533	P534	L535	V536	R537	L538	E539	E540	L541	S542			
T422	K423	E424	D425	K426	E427	A428	F429	A430	I431	V432	S433	V434	P435	V436	S437	E438	I439	R440	D441	L442	D443	F444	A445	N446	D447	A448	S449	S450	M451	L452	A453	S454	A455	V456	E457	K458	L459	M460	E461	G462	F463	I464	S465	Q466	M467	D468	R469	R470	F471	V472	I473	Q474	L475	L476	A477	D478	L479	V480	F481
N361	D362	I363	A364	S365	L366	F367	E368	L369	D370	P371	T372	T373	L374	Q375	K376	T377	D378	S379	F380	V381	P382	R383	N384	S385	Y386	V387	R388	L389	R390	H391	L392	C393	N395	T396	W397	I398	Q399	S400	T401	N402	V403	P404	I405	D406	I407	E408	E409	E410	R411	P412	I413	M416	L417	G418	T419	C420	P421		
N301	G302	L303	Y304	R305	F306	K307	H308	L309	A310	T311	G312	N313	Y314	L315	A316	A317	E318	E319	N320	P321	S322	Y323	LYS	GLY	ASP	ALA	SER	PRO	LYS	ALA	ALA	GLY	MET	GLY	GLN	GLY	THR	ARG	ARG	ASN	ALA	GLY	E348	K349	I350	K351	Y352	C353	L354	V355	A356	V357	P358	H359	G360				
V241	R242	L243	F244	H245	A246	E247	Q248	E249	K250	F251	T252	T253	C254	D255	E256	Y257	K258	G259	K260	L261	Q262	V263	F264	L265	R266	T267	T268	L269	R270	Q271	L272	A273	T274	S275	A276	T277	S278	S279	N280	A281	L282	W283	E284	V285	E286	V287	V288	H289	H290	D291	P292	C293	R294	G295	K296	A297	G298	H299	W300
D181	K182	V183	I184	L185	N186	P187	V188	S189	A190	G191	Q192	P193	L194	H195	A196	S197	N198	Y199	E200	L201	S202	D203	N204	A205	G206	C207	K208	E209	L210	N211	L212	S213	V214	C215	N216	T217	S218	W219	K220	I221	N222	L223	F224	M225	Q226	F227	R228	D229	H230	L231	E232	E233	V234	L235	K236	G237	G238	D239	V240
V121	I122	Q123	L124	L125	H126	M127	K128	S129	M130	K131	Y132	L133	T134	V135	N136	K137	R138	L139	P140	A141	L142	L143	E144	A145	N146	A147	M148	R149	V150	T151	L152	D153	A154	T155	G156	N157	E158	G159	S160	V161	L162	F163	I164	Q165	P166	F167	W168	K169	L170	R171	S172	N173	G174	D175	N176	V177	V178	V179	G180



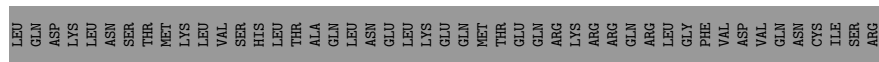


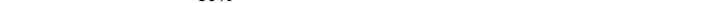


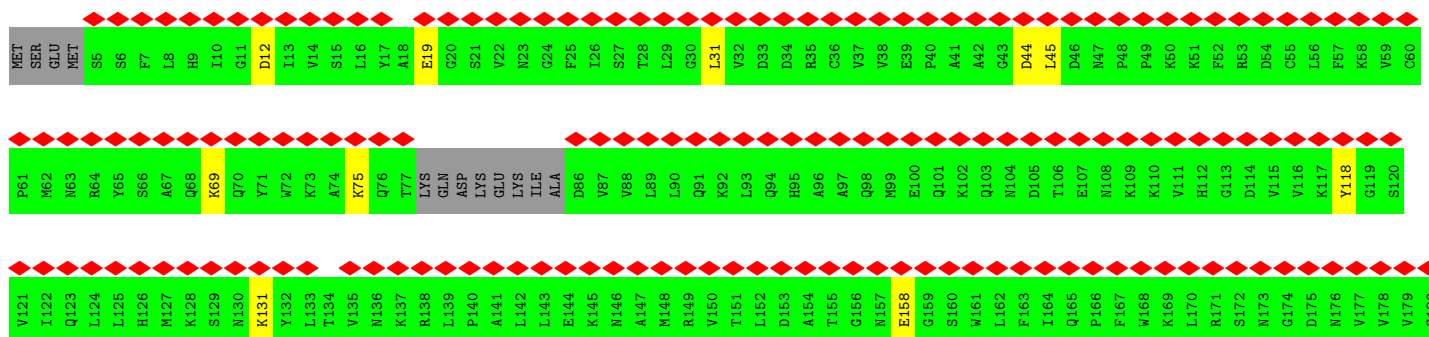
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



A1479	M1480	V1481	A1482	K1483	G1484	R1490	A1491	I1492	L1493	L1494	P1495	L1498	D1499	A1500	H1501	I1502	S1507	S1508	G1515	A1516	S1517	C1518	A1519	A1520	A1521	A1522	Q1523	R1524	N1525	A1526	S1527	S1528	Y1529	K1530	A1531	T1532	T1533	R1541	F1543	P1544	R1545	V1546	T1547	P1548	T1549	A1550	N1551	Q1552	V1586	D1587	Y1588	K1589	N1590	I1591	I1592	E1593
ARG	VAL	D1435	P1436	S1444	L1447	N1451	F1454	SER	SER	PRO	PHE	SER	GLU	ASN	SER	THR	SER	LEU	G1515	GLN	THR	HIS	GLN	THR	ILE	VAL	VAL	GLN	LEU	GLN	SER	THR	ARG	LEU	LEU	GLU	CYS	PRO	V1462	L1463	Q1464	Q1465	Q1466	H1467	K1468	G1469	S1470	V1471	E1472	R1476	T1477	L1478				
T1388	S1389	L1390	L1391	P1392	L1393	E1394	D1395	T1401	H1402	E1403	D1404	T1407	E1408	M1411	A1412	N1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	VAL	GLN	GLU	MET	LYS	GLU	ILE	THR	ASN	HIS	ILE	THR	THR	PHE	ASP	MET	ALA	ARG	VAL	CYS	SER	LYS	ARG	GLU	LYS							
K1315	Q1318	D1319	E1324	L1325	T1326	N1327	A1328	G1329	D1330	V1334	F1335	Y1336	N1337	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	K1350	A1351	A1352	R1353	D1354	G1355	V1356	E1357	D1358	H1359	S1360	F1361	L1362	M1363	Y1364	S1367	L1368	V1369	L1372	A1373	A1374	K1379	N1380	V1381	Y1382	I1385	K1386	C1387					
R1226	Y1227	T1228	K1234	F1235	C1236	A1237	G1238	Q1243	A1244	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	A1261	Q1265	Y1272	Q1273	E1277	I1278	S1279	E1280	F1281	Q1284	H1285	H1288	A1291	T1292	H1293	G1294	R1295	Y1299	L1300	D1301	F1302	L1303	H1304	A1309	E1310	G1311										
THR	ASP	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	GLU	LYS	S1166	E1167	M1168	Y1169	Q1170	L1176	E1177	R1178	K1181	M1182	C1183	G1184	E1187	Q1188	M1189	Q1193	Q1194	N1199	M1200	D1201	K1204	V1205	M1206	L1207	D1208	Q1211	I1212	P1213	D1215	K1216	G1217	D1218	A1219	M1222	E1223	I1224	L1225								
D1049	E1050	G1051	G1052	H1061	D1066	G1073	F1079	K1080	H1081	F1082	S1083	Q1084	H1090	T1091	F1092	K1093	L1097	S1100	N1106	E1113	R1116	E1125	L1126	W1127	V1128	D1129	K1130	LYS	GLY	SER	GLY	LYS	GLY	GLU	VAL	GLU	VAL	ALA	ALA	ALA	LYS	ASP	LYS	GLU	ARG	PRO										
Q976	N960	L983	D984	Y985	R986	I987	L990	K996	E997	E1000	V1001	F1002	P1003	M1004	GLN	ASP	SER	GLY	ALA	ASP	THR	GLY	THR	ALA	ALA	ALA	PHE	ASP	SER	THR	ALA	M1022	M1023	M1024	L1025	D1026	R1027	E1030	F1036	G1037	V1038	G1039	LYS	THR	SER	S1043	M1044	L1045	E1046	V1047	D1048					
T833	E838	D839	N843	S846	E847	A848	P850	F851	A852	N853	E854	E855	K856	K858	L859	T860	F861	V864	S865	H868	N869	L870	I871	Y872	F873	G874	F875	Y876	S879	R883	R886	T887	G890	I891	I892	D893	C894	VAL	GLN	GLY	PRO	PRO	ALA	ALA	MET	LEU	GLN	ALA	TYR							
Q753	Q754	L755	D758	L759	L762	C763	D766	E767	M768	L769	A852	N853	E854	E855	K856	N857	R774	A775	S776	F777	C778	H779	L780	L782	H783	Y784	H785	E792	L793	V797	R801	L802	P807	T808	A809	K813	D814	Y815	N818	L819	N820	A821	S822	D825	K826	K827	N828	A831	N832							
HIS	GLU	TYR	LEU	SER	ILE	GLU	TYR	SER	GLU	E690	E691	V692	W696	T697	D698	K699	N700	N701	E702	H703	H704	E705	R709	A712	Q713	E714	A715	R716	A717	G718	N719	A720	H721	D722	E723	N724	V725	L726	S727	Y728	Y729	R730	L733	A737	L741	D742	A747	I748	D749	E750	I751	S752				
T611	K612	V615	E616	T617	F618	V619	S620	L621	V622	R623	K624	N625	R626	E627	P628	R629	F630	L631	D632	Y633	L634	S635	D636	L637	C638	V639	S640	N641	H642	Q649	E650	L651	C655	V656	L657	D658	P659	K660	D663	I664	L665	I666	R667	T668	E669	L670	R671	P672	V673	K674	GLU	MET	ALA	GLN	SER	

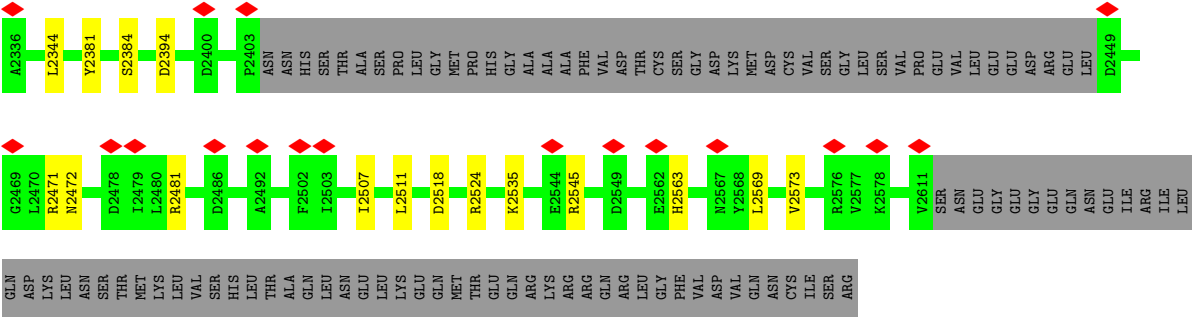


- Chain D: 









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	33807	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 ( $e^-/\text{\AA}^2$ )	61	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.663	Depositor
Minimum map value	-5.040	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.407	Depositor
Recommended contour level	1.91	Depositor
Map size (Å)	417.79202, 417.79202, 417.79202	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	0.28	0/17689	0.52	5/23903 (0.0%)
1	B	0.28	0/17689	0.52	5/23903 (0.0%)
1	C	0.28	0/17689	0.52	4/23903 (0.0%)
1	D	0.28	0/17689	0.52	5/23903 (0.0%)
All	All	0.28	0/70756	0.52	19/95612 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1544	PRO	N-CA-CB	5.67	110.10	103.30
1	A	1544	PRO	N-CA-CB	5.65	110.08	103.30
1	D	1544	PRO	N-CA-CB	5.65	110.08	103.30
1	C	1544	PRO	N-CA-CB	5.64	110.07	103.30
1	B	1495	PRO	N-CA-CB	5.61	110.03	103.30
1	A	1495	PRO	N-CA-CB	5.59	110.00	103.30
1	D	1548	PRO	N-CA-CB	5.57	109.99	103.30
1	C	1495	PRO	N-CA-CB	5.57	109.99	103.30
1	C	1548	PRO	N-CA-CB	5.57	109.98	103.30
1	D	1495	PRO	N-CA-CB	5.56	109.97	103.30
1	A	1548	PRO	N-CA-CB	5.54	109.95	103.30
1	B	1548	PRO	N-CA-CB	5.54	109.94	103.30
1	B	1436	PRO	N-CA-CB	5.45	109.84	103.30
1	D	1436	PRO	N-CA-CB	5.44	109.83	103.30
1	A	1436	PRO	N-CA-CB	5.43	109.82	103.30
1	C	1436	PRO	N-CA-CB	5.41	109.79	103.30
1	B	242	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	242	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	242	ARG	NE-CZ-NH1	5.02	122.81	120.30



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17382	17386	17215	68	0
1	B	17382	17386	17215	68	0
1	C	17382	17386	17215	72	0
1	D	17382	17386	17215	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	69540	69544	68860	275	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 2.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2524:ARG:NE	1:D:2518:ASP:OD2	2.13	0.82
1:A:561:ARG:NH1	1:A:593:ASP:O	2.21	0.74
1:C:561:ARG:NH1	1:C:593:ASP:O	2.21	0.73
1:B:561:ARG:NH1	1:B:593:ASP:O	2.21	0.73
1:D:561:ARG:NH1	1:D:593:ASP:O	2.21	0.73
1:A:1783:GLU:OE2	1:A:1899:THR:OG1	2.09	0.71
1:D:1783:GLU:OE2	1:D:1899:THR:OG1	2.09	0.70
1:B:1783:GLU:OE2	1:B:1899:THR:OG1	2.09	0.70
1:C:1783:GLU:OE2	1:C:1899:THR:OG1	2.09	0.69
1:A:1942:GLU:O	1:A:1945:THR:OG1	2.12	0.68
1:D:1942:GLU:O	1:D:1945:THR:OG1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1942:GLU:O	1:C:1945:THR:OG1	2.12	0.67
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.13	0.67
1:C:1391:LEU:O	1:C:1421:TYR:OH	2.13	0.66
1:D:1391:LEU:O	1:D:1421:TYR:OH	2.13	0.66
1:A:550:GLN:OE1	1:A:554:ARG:NE	2.29	0.66
1:C:550:GLN:OE1	1:C:554:ARG:NE	2.29	0.66
1:D:550:GLN:OE1	1:D:554:ARG:NE	2.29	0.65
1:B:550:GLN:OE1	1:B:554:ARG:NE	2.29	0.65
1:B:1391:LEU:O	1:B:1421:TYR:OH	2.13	0.65
1:A:815:TYR:OH	1:A:984:ASP:OD2	2.15	0.65
1:D:815:TYR:OH	1:D:984:ASP:OD2	2.15	0.65
1:C:352:TYR:O	1:C:419:THR:OG1	2.13	0.64
1:A:31:LEU:O	1:A:131:LYS:NZ	2.25	0.64
1:B:1942:GLU:O	1:B:1945:THR:OG1	2.12	0.64
1:D:886:ARG:NE	1:D:1049:ASP:OD1	2.31	0.64
1:B:815:TYR:OH	1:B:984:ASP:OD2	2.15	0.64
1:A:886:ARG:NE	1:A:1049:ASP:OD1	2.31	0.63
1:C:815:TYR:OH	1:C:984:ASP:OD2	2.15	0.63
1:A:305:ARG:NH1	1:A:360:GLY:O	2.32	0.63
1:B:886:ARG:NE	1:B:1049:ASP:OD1	2.31	0.63
1:C:886:ARG:NE	1:C:1049:ASP:OD1	2.31	0.62
1:D:305:ARG:NH1	1:D:360:GLY:O	2.32	0.62
1:C:305:ARG:NH1	1:C:360:GLY:O	2.32	0.62
1:A:1951:PRO:O	1:A:1956:GLN:NE2	2.33	0.62
1:C:1951:PRO:O	1:C:1956:GLN:NE2	2.33	0.61
1:D:1951:PRO:O	1:D:1956:GLN:NE2	2.33	0.61
1:B:12:ASP:OD1	1:B:227:PHE:N	2.34	0.61
1:B:305:ARG:NH1	1:B:360:GLY:O	2.32	0.61
1:C:12:ASP:OD1	1:C:227:PHE:N	2.34	0.61
1:B:31:LEU:O	1:B:131:LYS:NZ	2.25	0.61
1:D:12:ASP:OD1	1:D:227:PHE:N	2.34	0.61
1:B:1951:PRO:O	1:B:1956:GLN:NE2	2.33	0.61
1:C:31:LEU:O	1:C:131:LYS:NZ	2.25	0.61
1:A:12:ASP:OD1	1:A:227:PHE:N	2.34	0.60
1:D:1194:GLN:NE2	1:D:1234:LYS:O	2.34	0.60
1:D:233:GLU:OE1	1:D:383:ARG:NH2	2.36	0.59
1:B:1194:GLN:NE2	1:B:1234:LYS:O	2.34	0.59
1:A:1194:GLN:NE2	1:A:1234:LYS:O	2.34	0.59
1:C:1194:GLN:NE2	1:C:1234:LYS:O	2.34	0.59
1:C:233:GLU:OE1	1:C:383:ARG:NH2	2.36	0.58
1:B:1106:ASN:OD1	1:B:1193:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:O	1:D:131:LYS:NZ	2.25	0.58
1:D:1106:ASN:OD1	1:D:1193:GLN:NE2	2.37	0.58
1:A:1106:ASN:OD1	1:A:1193:GLN:NE2	2.37	0.58
1:B:1113:GLU:OE1	1:B:1116:ARG:NH2	2.37	0.58
1:A:233:GLU:OE1	1:A:383:ARG:NH2	2.36	0.58
1:D:1113:GLU:OE1	1:D:1116:ARG:NH2	2.37	0.57
1:C:1113:GLU:OE1	1:C:1116:ARG:NH2	2.37	0.57
1:B:233:GLU:OE1	1:B:383:ARG:NH2	2.36	0.57
1:D:2381:TYR:O	1:D:2384:SER:OG	2.21	0.57
1:C:1106:ASN:OD1	1:C:1193:GLN:NE2	2.37	0.57
1:A:482:PHE:O	1:A:505:ARG:NH1	2.38	0.57
1:A:1113:GLU:OE1	1:A:1116:ARG:NH2	2.37	0.57
1:B:482:PHE:O	1:B:505:ARG:NH1	2.38	0.56
1:C:482:PHE:O	1:C:505:ARG:NH1	2.38	0.56
1:D:482:PHE:O	1:D:505:ARG:NH1	2.38	0.56
1:A:2381:TYR:O	1:A:2384:SER:OG	2.21	0.56
1:B:2225:TYR:OH	1:B:2278:ILE:HG21	2.06	0.55
1:C:2381:TYR:O	1:C:2384:SER:OG	2.21	0.55
1:B:2381:TYR:O	1:B:2384:SER:OG	2.21	0.55
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.40	0.55
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.40	0.55
1:A:2225:TYR:OH	1:A:2278:ILE:HG21	2.06	0.55
1:D:2394:ASP:OD1	1:D:2481:ARG:NH2	2.40	0.55
1:C:2225:TYR:OH	1:C:2278:ILE:HG21	2.07	0.55
1:D:2225:TYR:OH	1:D:2278:ILE:HG21	2.06	0.55
1:B:494:LEU:O	1:B:558:ARG:NE	2.40	0.54
1:C:494:LEU:O	1:C:558:ARG:NE	2.40	0.54
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.40	0.54
1:A:774:ARG:HE	1:A:859:LEU:HD13	1.73	0.54
1:A:494:LEU:O	1:A:558:ARG:NE	2.40	0.54
1:D:774:ARG:HE	1:D:859:LEU:HD13	1.73	0.54
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.23	0.54
1:D:494:LEU:O	1:D:558:ARG:NE	2.40	0.54
1:C:774:ARG:HE	1:C:859:LEU:HD13	1.73	0.53
1:B:352:TYR:O	1:B:419:THR:OG1	2.13	0.53
1:D:19:GLU:OE1	1:D:182:LYS:NZ	2.37	0.53
1:D:352:TYR:O	1:D:419:THR:OG1	2.13	0.53
1:A:1046:GLU:OE2	1:A:1052:GLY:N	2.42	0.53
1:B:774:ARG:HE	1:B:859:LEU:HD13	1.73	0.53
1:D:1046:GLU:OE2	1:D:1052:GLY:N	2.42	0.53
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ARG:NH2	1:B:697:THR:O	2.42	0.53
1:B:1214:TYR:OH	1:B:1222:MET:SD	2.66	0.53
1:C:626:ARG:NH2	1:C:697:THR:O	2.42	0.53
1:C:1046:GLU:OE2	1:C:1052:GLY:N	2.42	0.53
1:A:1214:TYR:OH	1:A:1222:MET:SD	2.66	0.52
1:B:1046:GLU:OE2	1:B:1052:GLY:N	2.42	0.52
1:A:118:TYR:OH	1:A:181:ASP:OD2	2.28	0.52
1:C:822:SER:O	1:C:826:LYS:NZ	2.43	0.52
1:D:822:SER:O	1:D:826:LYS:NZ	2.43	0.52
1:C:118:TYR:OH	1:C:181:ASP:OD2	2.28	0.52
1:D:2125:GLU:OE1	1:D:2563:HIS:NE2	2.43	0.52
1:A:626:ARG:NH2	1:A:697:THR:O	2.42	0.52
1:B:822:SER:O	1:B:826:LYS:NZ	2.43	0.52
1:D:495:ASP:OD1	1:D:558:ARG:NH2	2.43	0.52
1:A:822:SER:O	1:A:826:LYS:NZ	2.43	0.52
1:B:118:TYR:OH	1:B:181:ASP:OD2	2.28	0.52
1:A:19:GLU:OE1	1:A:182:LYS:NZ	2.37	0.52
1:D:626:ARG:NH2	1:D:697:THR:O	2.42	0.52
1:C:495:ASP:OD1	1:C:558:ARG:NH2	2.43	0.51
1:C:2125:GLU:OE1	1:C:2563:HIS:NE2	2.43	0.51
1:D:118:TYR:OH	1:D:181:ASP:OD2	2.28	0.51
1:A:495:ASP:OD1	1:A:558:ARG:NH2	2.43	0.51
1:C:1214:TYR:OH	1:C:1222:MET:SD	2.66	0.51
1:B:495:ASP:OD1	1:B:558:ARG:NH2	2.43	0.51
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.23	0.50
1:B:19:GLU:OE1	1:B:182:LYS:NZ	2.37	0.50
1:D:1214:TYR:OH	1:D:1222:MET:SD	2.66	0.50
1:D:547:ALA:HB3	1:D:548:PRO:HD3	1.94	0.50
1:B:2125:GLU:OE1	1:B:2563:HIS:NE2	2.43	0.50
1:A:547:ALA:HB3	1:A:548:PRO:HD3	1.94	0.49
1:A:1619:ASP:OD1	1:A:1620:VAL:N	2.46	0.49
1:B:1225:LEU:O	1:B:1228:THR:OG1	2.27	0.49
1:B:547:ALA:HB3	1:B:548:PRO:HD3	1.94	0.49
1:B:1619:ASP:OD1	1:B:1620:VAL:N	2.46	0.49
1:D:242:ARG:NE	1:D:281:ALA:O	2.45	0.49
1:A:2125:GLU:OE1	1:A:2563:HIS:NE2	2.43	0.49
1:B:386:TYR:CE1	1:B:430:ALA:HB2	2.48	0.49
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.23	0.49
1:A:242:ARG:NE	1:A:281:ALA:O	2.45	0.49
1:B:2507:ILE:O	1:B:2511:LEU:N	2.43	0.49
1:A:451:MET:O	1:A:454:SER:OG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ARG:NE	1:B:281:ALA:O	2.45	0.49
1:C:1619:ASP:OD1	1:C:1620:VAL:N	2.46	0.49
1:C:19:GLU:OE1	1:C:182:LYS:NZ	2.37	0.49
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.46	0.48
1:C:242:ARG:NE	1:C:281:ALA:O	2.45	0.48
1:D:1619:ASP:OD1	1:D:1620:VAL:N	2.46	0.48
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.46	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.46	0.48
1:A:386:TYR:CE1	1:A:430:ALA:HB2	2.48	0.48
1:C:386:TYR:CE1	1:C:430:ALA:HB2	2.48	0.48
1:C:542:SER:OG	1:C:588:ASP:OD2	2.32	0.48
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.46	0.48
1:A:542:SER:OG	1:A:588:ASP:OD2	2.32	0.48
1:B:542:SER:OG	1:B:588:ASP:OD2	2.32	0.48
1:C:547:ALA:HB3	1:C:548:PRO:HD3	1.94	0.48
1:D:75:LYS:NZ	1:D:489:ASN:O	2.47	0.47
1:D:386:TYR:CE1	1:D:430:ALA:HB2	2.48	0.47
1:C:75:LYS:NZ	1:C:489:ASN:O	2.47	0.47
1:C:1225:LEU:O	1:C:1228:THR:OG1	2.27	0.47
1:A:75:LYS:NZ	1:A:489:ASN:O	2.47	0.47
1:A:1644:LEU:HD22	1:A:1727:ARG:NH2	2.30	0.47
1:D:1644:LEU:HD22	1:D:1727:ARG:NH2	2.30	0.47
1:B:2326:TYR:O	1:B:2329:THR:OG1	2.30	0.47
1:C:1644:LEU:HD22	1:C:1727:ARG:NH2	2.30	0.47
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.48	0.47
1:D:542:SER:OG	1:D:588:ASP:OD2	2.32	0.47
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.48	0.46
1:B:1644:LEU:HD22	1:B:1727:ARG:NH2	2.30	0.46
1:A:1225:LEU:O	1:A:1228:THR:OG1	2.27	0.46
1:B:75:LYS:NZ	1:B:489:ASN:O	2.47	0.46
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.48	0.46
1:D:1081:HIS:O	1:D:1084:GLN:NE2	2.49	0.46
1:B:1081:HIS:O	1:B:1084:GLN:NE2	2.49	0.46
1:A:1081:HIS:O	1:A:1084:GLN:NE2	2.49	0.46
1:C:533:GLY:N	1:C:536:VAL:O	2.49	0.46
1:D:533:GLY:N	1:D:536:VAL:O	2.49	0.46
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.48	0.46
1:A:533:GLY:N	1:A:536:VAL:O	2.49	0.45
1:B:533:GLY:N	1:B:536:VAL:O	2.49	0.45
1:D:1225:LEU:O	1:D:1228:THR:OG1	2.27	0.45
1:C:1081:HIS:O	1:C:1084:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2507:ILE:O	1:D:2511:LEU:N	2.43	0.45
1:A:2507:ILE:O	1:A:2511:LEU:N	2.43	0.45
1:A:2535:LYS:O	1:A:2545:ARG:NH2	2.48	0.45
1:A:758:ASP:OD1	1:A:759:LEU:N	2.50	0.45
1:D:758:ASP:OD1	1:D:759:LEU:N	2.50	0.45
1:B:758:ASP:OD1	1:B:759:LEU:N	2.50	0.45
1:D:44:ASP:OD1	1:D:45:LEU:N	2.50	0.45
1:A:741:LEU:O	1:A:783:HIS:ND1	2.48	0.44
1:C:2326:TYR:O	1:C:2329:THR:OG1	2.30	0.44
1:D:2326:TYR:O	1:D:2329:THR:OG1	2.30	0.44
1:B:255:ASP:OD1	1:B:256:GLU:N	2.51	0.44
1:C:44:ASP:OD1	1:C:45:LEU:N	2.50	0.44
1:A:1337:ASN:OD1	1:A:1338:ASP:N	2.51	0.44
1:C:255:ASP:OD1	1:C:256:GLU:N	2.51	0.44
1:D:255:ASP:OD1	1:D:256:GLU:N	2.51	0.44
1:A:2220:ALA:HB2	1:D:2381:TYR:HE1	1.81	0.44
1:C:758:ASP:OD1	1:C:759:LEU:N	2.50	0.44
1:C:2518:ASP:OD2	1:D:2524:ARG:NE	2.40	0.44
1:A:255:ASP:OD1	1:A:256:GLU:N	2.51	0.43
1:B:1337:ASN:OD1	1:B:1338:ASP:N	2.51	0.43
1:C:1337:ASN:OD1	1:C:1338:ASP:N	2.51	0.43
1:D:1337:ASN:OD1	1:D:1338:ASP:N	2.51	0.43
1:B:44:ASP:OD1	1:B:45:LEU:N	2.50	0.43
1:C:741:LEU:O	1:C:783:HIS:ND1	2.48	0.43
1:B:308:HIS:HD1	1:B:311:THR:HG1	1.64	0.43
1:D:2205:GLY:O	1:D:2208:SER:OG	2.30	0.43
1:A:2220:ALA:HB2	1:D:2381:TYR:CE1	2.54	0.43
1:C:2507:ILE:O	1:C:2511:LEU:N	2.43	0.43
1:B:308:HIS:ND1	1:B:311:THR:OG1	2.47	0.43
1:B:2569:LEU:O	1:B:2573:VAL:HG23	2.19	0.43
1:A:44:ASP:OD1	1:A:45:LEU:N	2.50	0.43
1:A:2569:LEU:O	1:A:2573:VAL:HG23	2.19	0.43
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.52	0.43
1:C:2569:LEU:O	1:C:2573:VAL:HG23	2.19	0.43
1:A:308:HIS:ND1	1:A:311:THR:OG1	2.47	0.42
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.52	0.42
1:D:69:LYS:NZ	1:D:158:GLU:OE1	2.51	0.42
1:D:1930:ASN:OD1	1:D:1931:GLU:N	2.51	0.42
1:C:1968:ASP:OD1	1:C:2019:SER:OG	2.25	0.42
1:A:69:LYS:NZ	1:A:158:GLU:OE1	2.51	0.42
1:B:1681:ASP:OD1	1:B:1682:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1681:ASP:OD1	1:D:1682:ARG:N	2.53	0.42
1:A:1681:ASP:OD1	1:A:1682:ARG:N	2.53	0.42
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.53	0.42
1:D:2569:LEU:O	1:D:2573:VAL:HG23	2.19	0.42
1:D:853:ASN:O	1:D:857:ASN:ND2	2.52	0.42
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.52	0.42
1:B:741:LEU:O	1:B:783:HIS:ND1	2.48	0.42
1:B:1364:TYR:O	1:B:1367:SER:OG	2.31	0.42
1:A:1048:ASP:OD1	1:A:1049:ASP:N	2.52	0.42
1:A:2326:TYR:O	1:A:2329:THR:OG1	2.30	0.42
1:C:308:HIS:ND1	1:C:311:THR:OG1	2.47	0.42
1:C:1930:ASN:OD1	1:C:1931:GLU:N	2.51	0.42
1:C:2054:TYR:OH	1:C:2118:GLU:OE1	2.38	0.42
1:D:741:LEU:O	1:D:783:HIS:ND1	2.48	0.42
1:B:853:ASN:O	1:B:857:ASN:ND2	2.52	0.42
1:B:2326:TYR:CZ	1:B:2344:LEU:HD22	2.55	0.42
1:C:853:ASN:O	1:C:857:ASN:ND2	2.52	0.42
1:C:2326:TYR:CZ	1:C:2344:LEU:HD22	2.55	0.42
1:D:2326:TYR:CZ	1:D:2344:LEU:HD22	2.55	0.42
1:B:2535:LYS:O	1:B:2545:ARG:NH2	2.48	0.41
1:C:1223:GLU:OE1	1:C:1226:ARG:NH2	2.54	0.41
1:C:1402:HIS:NE2	1:C:1404:ASP:OD2	2.53	0.41
1:C:1128:VAL:O	1:C:1169:TYR:OH	2.38	0.41
1:D:556:CYS:SG	1:D:557:TYR:N	2.94	0.41
1:D:1128:VAL:O	1:D:1169:TYR:OH	2.38	0.41
1:A:1673:LEU:HD22	1:A:1725:GLN:HG3	2.03	0.41
1:B:1340:ALA:O	1:B:1344:HIS:ND1	2.53	0.41
1:C:69:LYS:NZ	1:C:158:GLU:OE1	2.51	0.41
1:D:1402:HIS:NE2	1:D:1404:ASP:OD2	2.53	0.41
1:D:1987:ASP:OD1	1:D:1988:LEU:N	2.54	0.41
1:D:2535:LYS:O	1:D:2545:ARG:NH2	2.48	0.41
1:A:853:ASN:O	1:A:857:ASN:ND2	2.52	0.41
1:A:1128:VAL:O	1:A:1169:TYR:OH	2.38	0.41
1:A:2326:TYR:CZ	1:A:2344:LEU:HD22	2.55	0.41
1:B:1128:VAL:O	1:B:1169:TYR:OH	2.38	0.41
1:B:1223:GLU:OE1	1:B:1226:ARG:NH2	2.54	0.41
1:B:1673:LEU:HD22	1:B:1725:GLN:HG3	2.02	0.41
1:B:2054:TYR:OH	1:B:2118:GLU:OE1	2.38	0.41
1:C:394:THR:OG1	1:C:396:THR:OG1	2.18	0.41
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.54	0.41
1:C:451:MET:O	1:C:454:SER:OG	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1977:ASP:OD1	1:D:1978:ILE:N	2.54	0.41
1:A:1987:ASP:OD1	1:A:1988:LEU:N	2.54	0.41
1:A:556:CYS:SG	1:A:557:TYR:N	2.94	0.41
1:A:1223:GLU:OE1	1:A:1226:ARG:NH2	2.54	0.41
1:D:1673:LEU:HD22	1:D:1725:GLN:HG3	2.03	0.41
1:A:1402:HIS:NE2	1:A:1404:ASP:OD2	2.53	0.41
1:B:1402:HIS:NE2	1:B:1404:ASP:OD2	2.53	0.41
1:B:1977:ASP:OD1	1:B:1978:ILE:N	2.54	0.41
1:C:1673:LEU:HD22	1:C:1725:GLN:HG3	2.03	0.41
1:B:556:CYS:SG	1:B:557:TYR:N	2.94	0.41
1:C:556:CYS:SG	1:C:557:TYR:N	2.94	0.41
1:C:1987:ASP:OD1	1:C:1988:LEU:N	2.54	0.40
1:D:1223:GLU:OE1	1:D:1226:ARG:NH2	2.53	0.40
1:A:1364:TYR:O	1:A:1367:SER:OG	2.31	0.40
1:C:397:TRP:O	1:C:420:CYS:N	2.54	0.40
1:C:254:CYS:O	1:C:280:ASN:ND2	2.46	0.40
1:C:1891:PHE:O	1:C:1895:GLN:NE2	2.55	0.40
1:D:397:TRP:O	1:D:420:CYS:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2147/2671 (80%)	2055 (96%)	91 (4%)	1 (0%)	100	100
1	B	2147/2671 (80%)	2054 (96%)	92 (4%)	1 (0%)	100	100
1	C	2147/2671 (80%)	2055 (96%)	91 (4%)	1 (0%)	100	100
1	D	2147/2671 (80%)	2053 (96%)	93 (4%)	1 (0%)	100	100
All	All	8588/10684 (80%)	8217 (96%)	367 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	1544	PRO
1	B	1544	PRO
1	C	1544	PRO
1	D	1544	PRO

### 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	1883/2385 (79%)	1876 (100%)	7 (0%)	89	91
1	B	1883/2385 (79%)	1876 (100%)	7 (0%)	89	91
1	C	1883/2385 (79%)	1875 (100%)	8 (0%)	89	91
1	D	1883/2385 (79%)	1876 (100%)	7 (0%)	89	91
All	All	7532/9540 (79%)	7503 (100%)	29 (0%)	88	91

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	390	ARG
1	A	602	ASN
1	A	1106	ASN
1	A	2289	ASN
1	A	2471	ARG
1	A	2472	ASN
1	B	280	ASN
1	B	390	ARG
1	B	602	ASN
1	B	1106	ASN
1	B	2289	ASN
1	B	2471	ARG
1	B	2472	ASN
1	C	280	ASN
1	C	390	ARG
1	C	602	ASN
1	C	1106	ASN

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Mol	Chain	Res	Type
1	C	1418	ASN
1	C	2289	ASN
1	C	2471	ARG
1	C	2472	ASN
1	D	280	ASN
1	D	390	ARG
1	D	602	ASN
1	D	1106	ASN
1	D	2289	ASN
1	D	2471	ARG
1	D	2472	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
1	B	5
1	C	5
1	D	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1552:GLN	C	1586:TRP	N	55.70
1	B	1552:GLN	C	1586:TRP	N	55.70
1	C	1552:GLN	C	1586:TRP	N	55.70
1	D	1552:GLN	C	1586:TRP	N	55.70
1	A	1533:THR	C	1541:ARG	N	15.48
1	B	1533:THR	C	1541:ARG	N	15.48
1	C	1533:THR	C	1541:ARG	N	15.48
1	D	1533:THR	C	1541:ARG	N	15.48
1	A	1484:GLY	C	1490:ARG	N	11.29
1	B	1484:GLY	C	1490:ARG	N	11.29
1	C	1484:GLY	C	1490:ARG	N	11.29
1	D	1484:GLY	C	1490:ARG	N	11.29
1	A	1508:SER	C	1515:GLY	N	10.86
1	B	1508:SER	C	1515:GLY	N	10.86
1	C	1508:SER	C	1515:GLY	N	10.86
1	D	1508:SER	C	1515:GLY	N	10.86
1	A	2252:TYR	C	2260:SER	N	6.44
1	B	2252:TYR	C	2260:SER	N	6.44
1	C	2252:TYR	C	2260:SER	N	6.44
1	D	2252:TYR	C	2260:SER	N	6.44

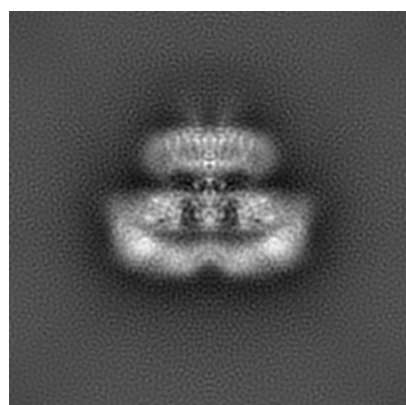
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7988. These allow visual inspection of the internal detail of the map and identification of artifacts.

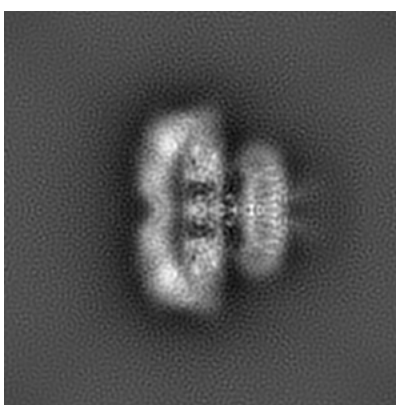
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

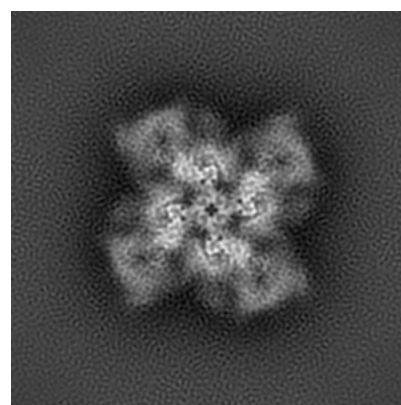
#### 6.1.1 Primary map



X



Y

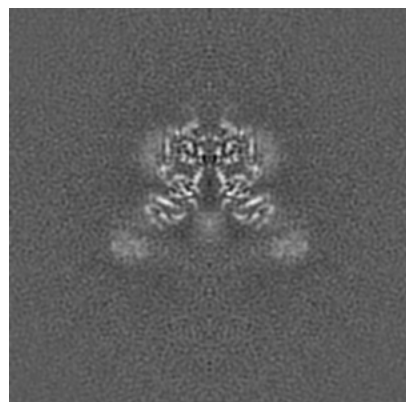


Z

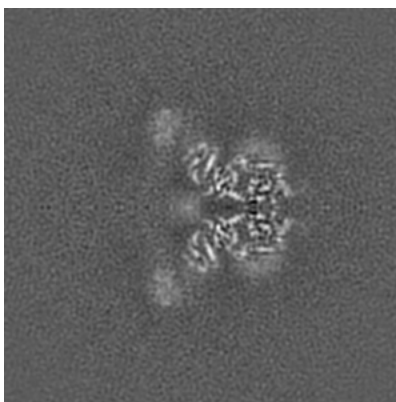
The images above show the map projected in three orthogonal directions.

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

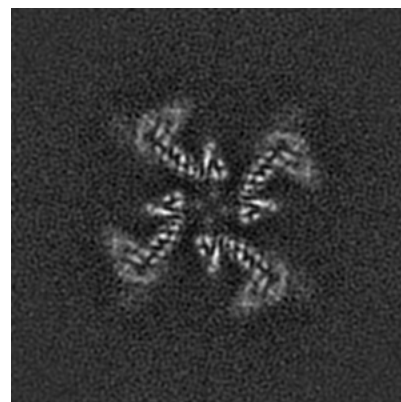
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

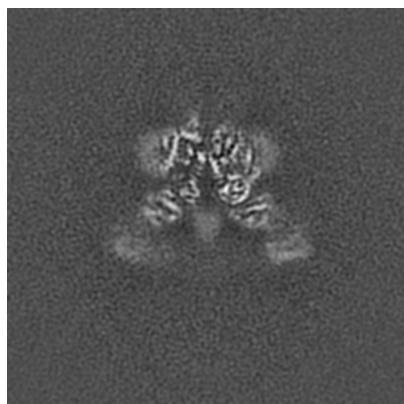


Z Index: 192

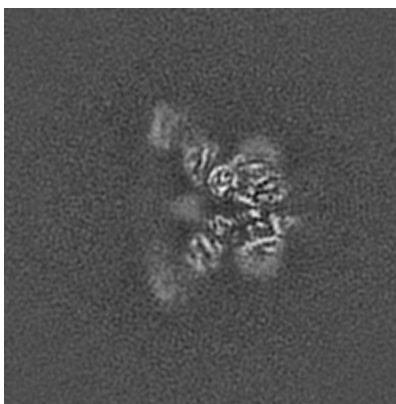
The images above show central slices of the map in three orthogonal directions.

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

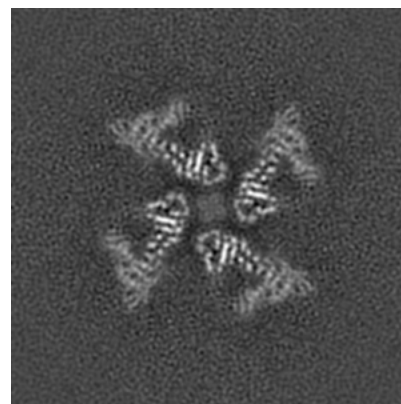
### 6.3.1 Primary map



X Index: 189



Y Index: 195

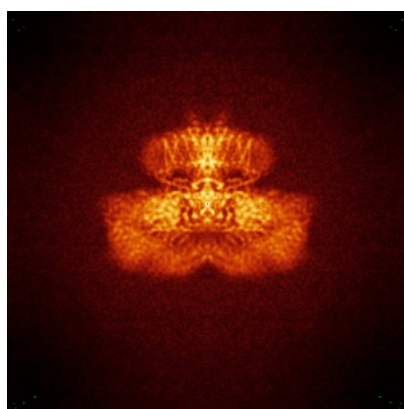


Z Index: 187

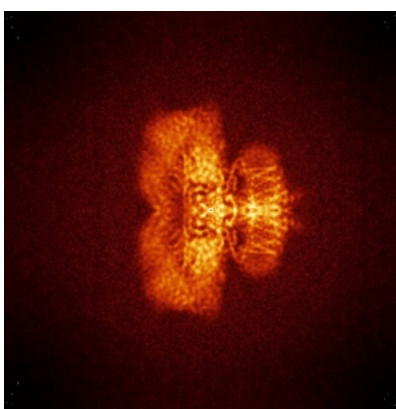
The images above show the largest variance slices of the map in three orthogonal directions.

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

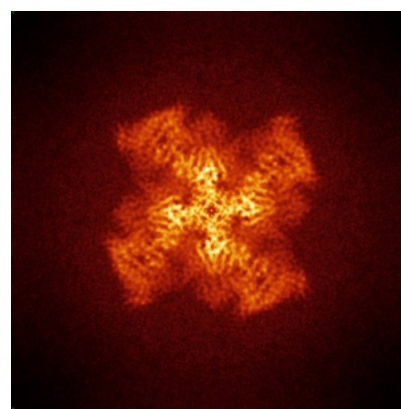
### 6.4.1 Primary map



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

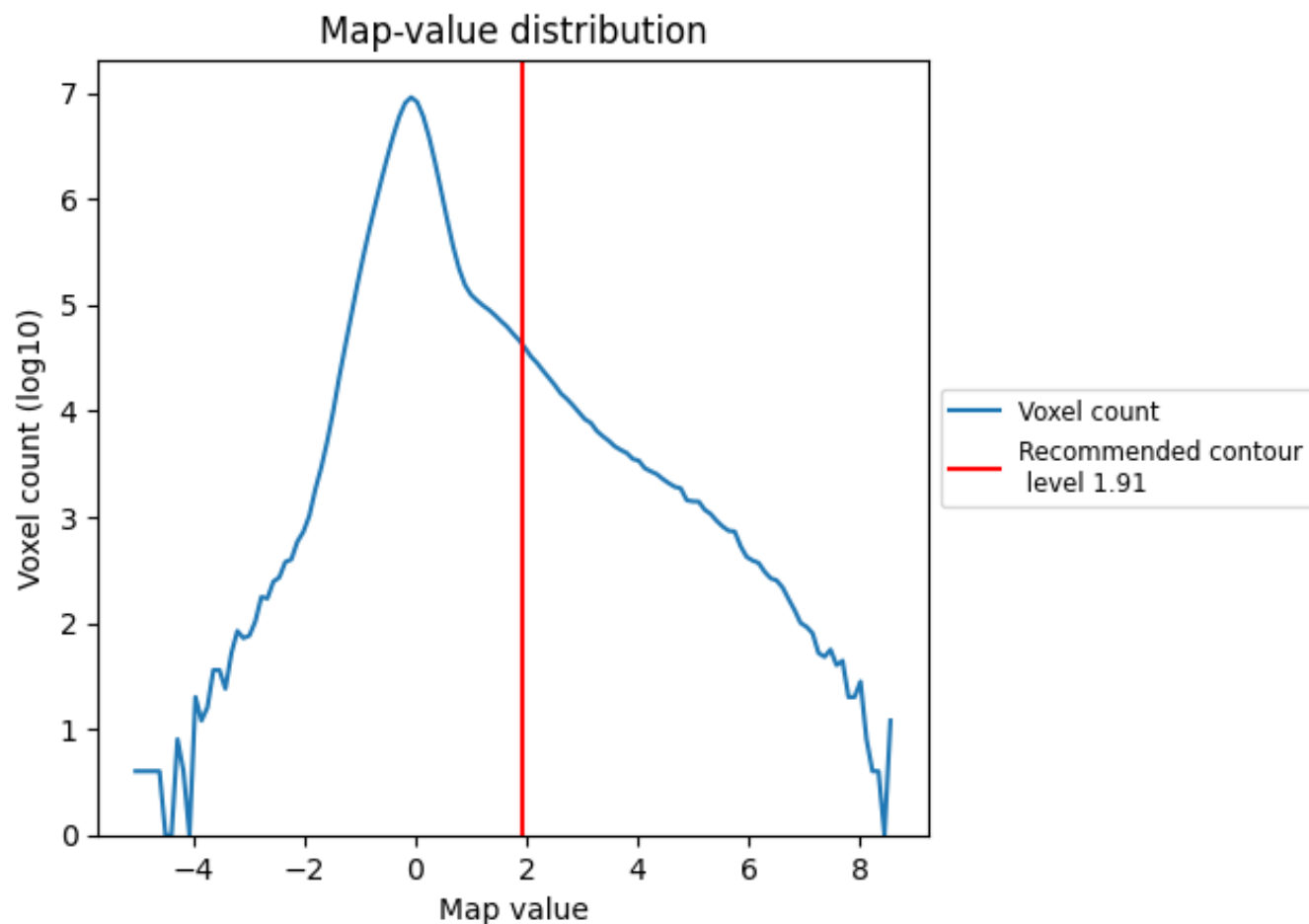
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

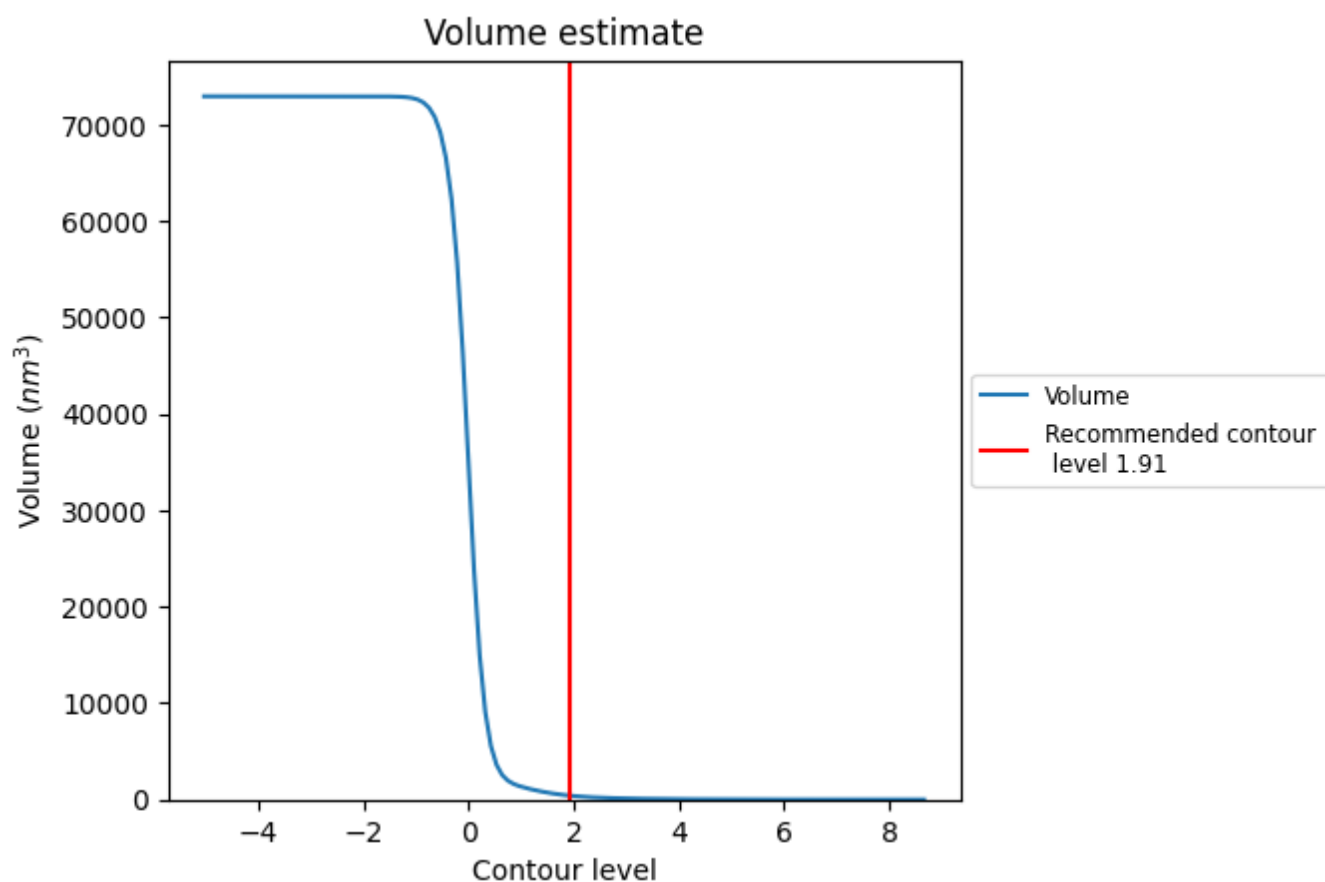
This section contains the results of statistical analysis of the map.

### 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](#)

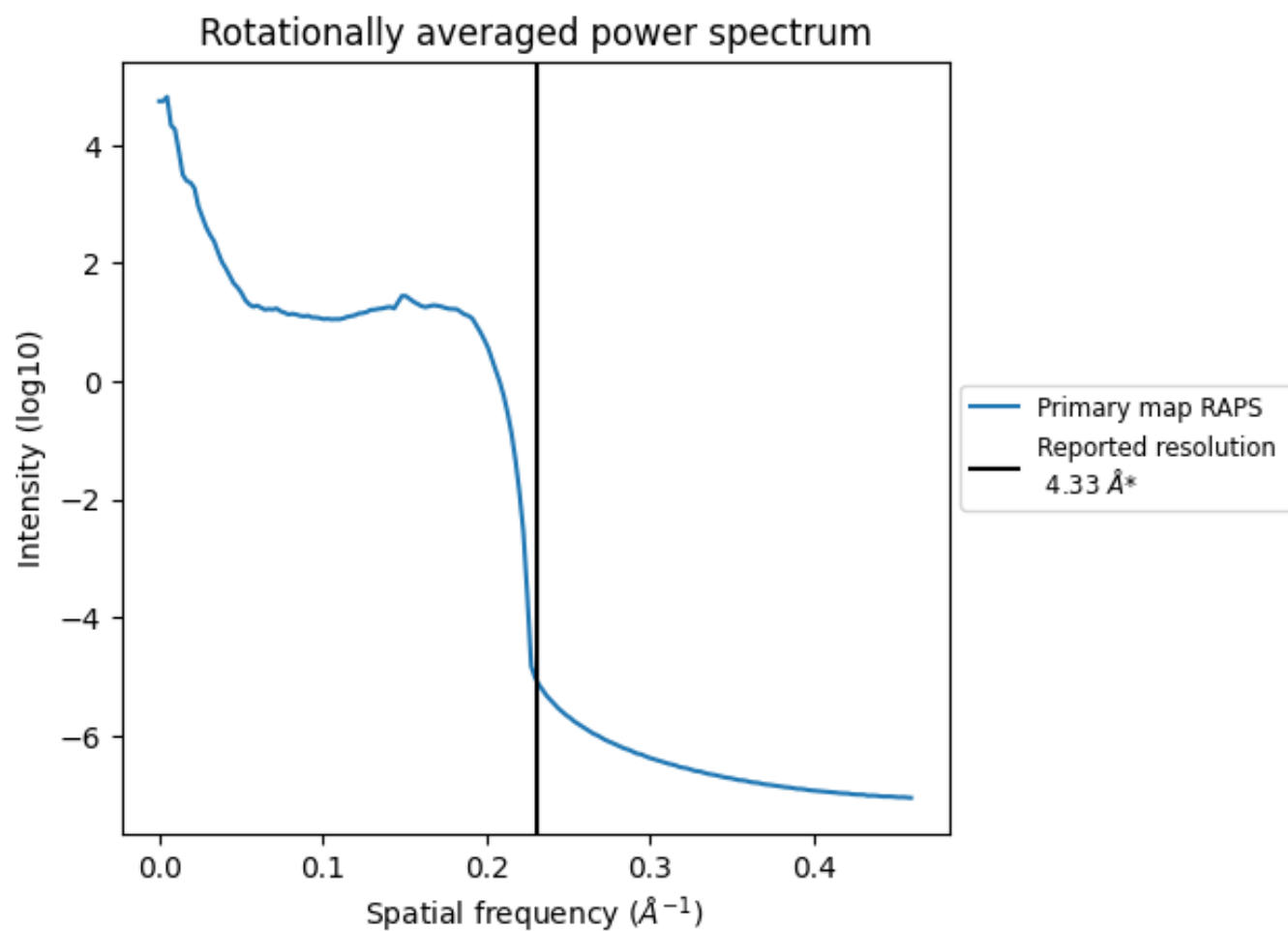


The volume at the recommended contour level is 413 nm<sup>3</sup>; this corresponds to an approximate mass of 373 kDa.

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 0.231 Å<sup>-1</sup>

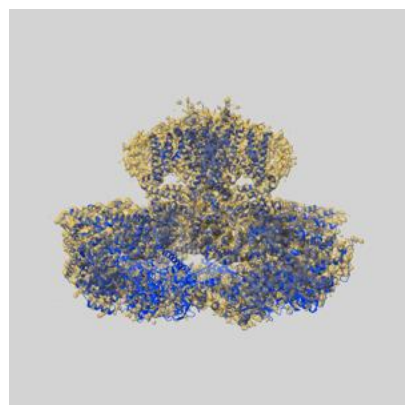
## 8 Fourier-Shell correlation ⓘ

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

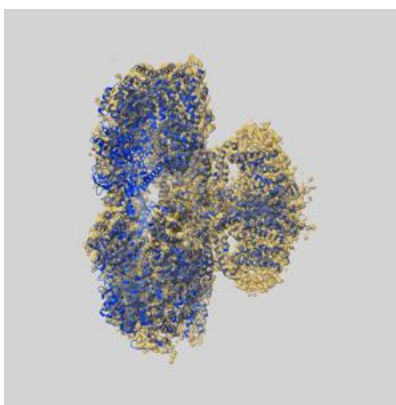
## 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-7988 and PDB model 6DR2. Per-residue inclusion information can be found in section 3 on page 4.

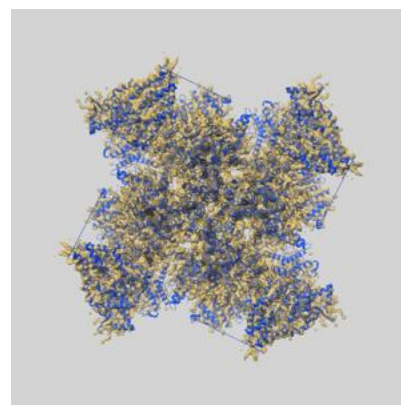
### 9.1 Map-model overlay ⓘ



X



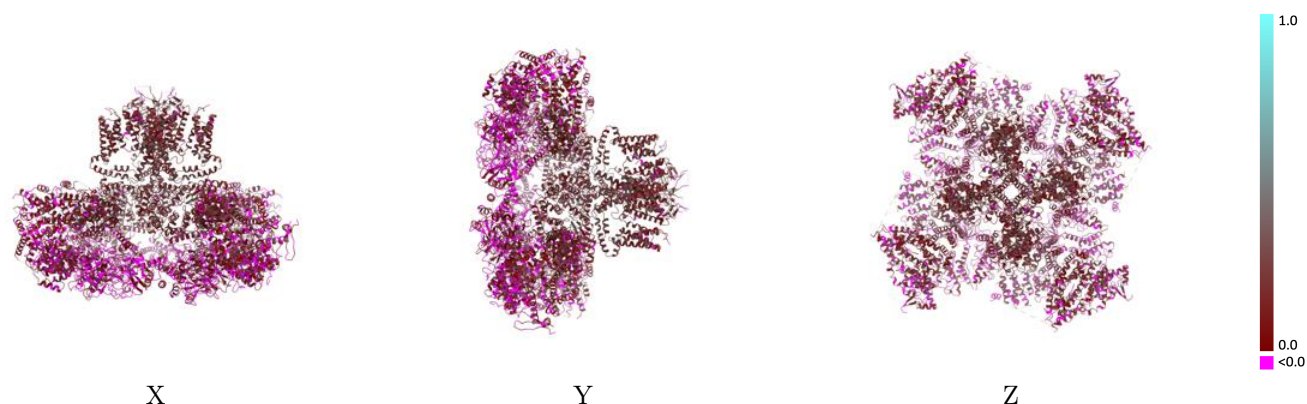
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.91 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](#)



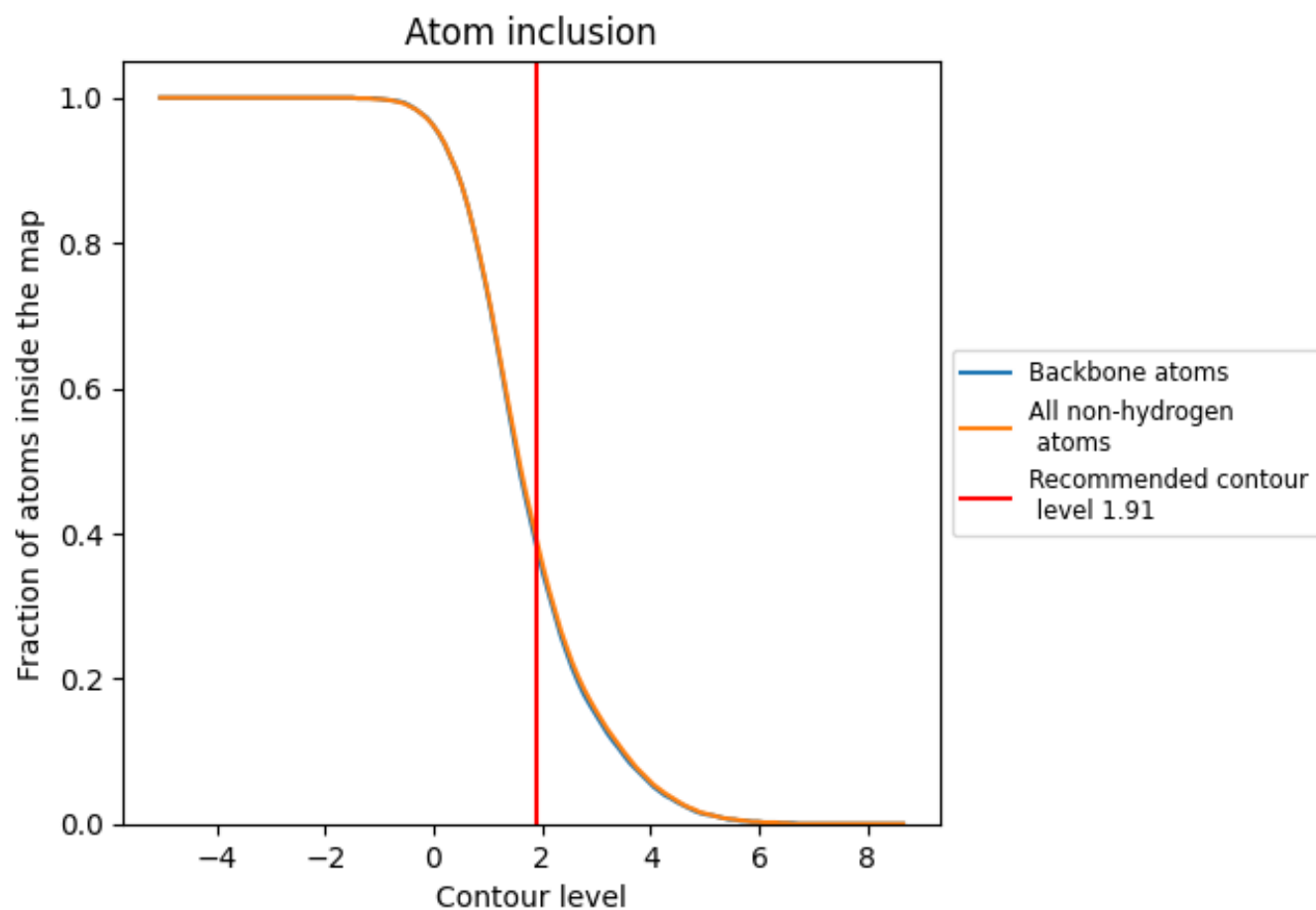
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.91).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 39% 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 (1.91) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3890	<div></div> 0.1290
A	<div></div> 0.3980	<div></div> 0.1300
B	<div></div> 0.3980	<div></div> 0.1290
C	<div></div> 0.3970	<div></div> 0.1300
D	<div></div> 0.3960	<div></div> 0.1270

