



## Full wwPDB EM Validation Report ⓘ

Oct 5, 2024 – 10:53 PM EDT

PDB ID : 6DRC  
EMDB ID : EMD-7994  
Title : High IP3 Ca<sup>2+</sup> human type 3 1,4,5-inositol trisphosphate receptor  
Authors : Hite, R.K.; Paknejad, N.  
Deposited on : 2018-06-11  
Resolution : 3.92 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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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

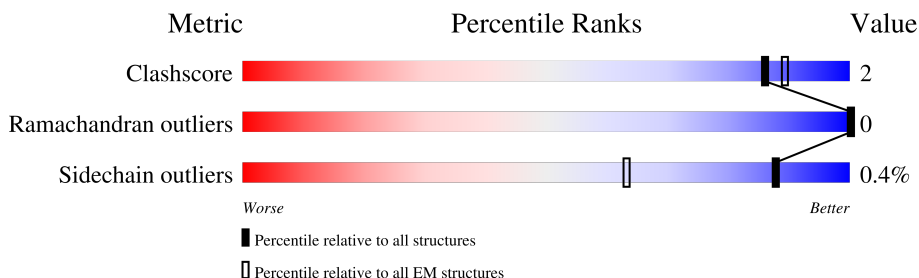
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.92 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>44%</div> <div>76% 5% 18%</div> </div>
1	B	2671	<div> <div>45%</div> <div>77% 5% 18%</div> </div>
1	C	2671	<div> <div>44%</div> <div>77% 5% 18%</div> </div>
1	D	2671	<div> <div>45%</div> <div>77% 5% 18%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 138896 atoms, of which 69420 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.

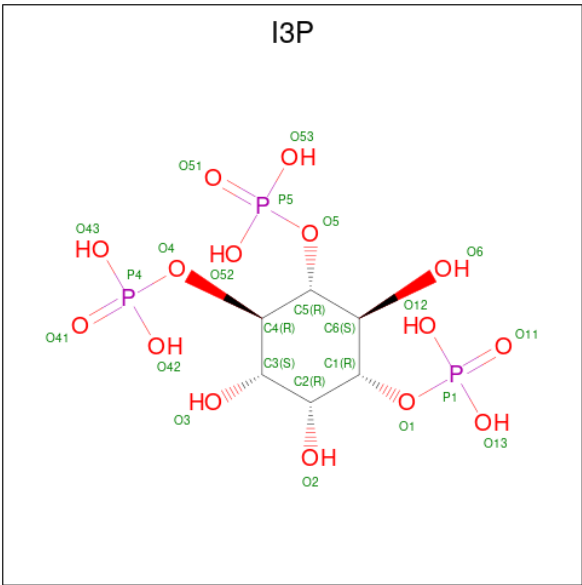
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2186	Total	C	H	N	O	S	0	0
			34688	11057	17346	2984	3195	106		
1	B	2186	Total	C	H	N	O	S	0	0
			34688	11057	17346	2984	3195	106		
1	C	2186	Total	C	H	N	O	S	0	0
			34688	11057	17346	2984	3195	106		
1	D	2186	Total	C	H	N	O	S	0	0
			34688	11057	17346	2984	3195	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 D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>15</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

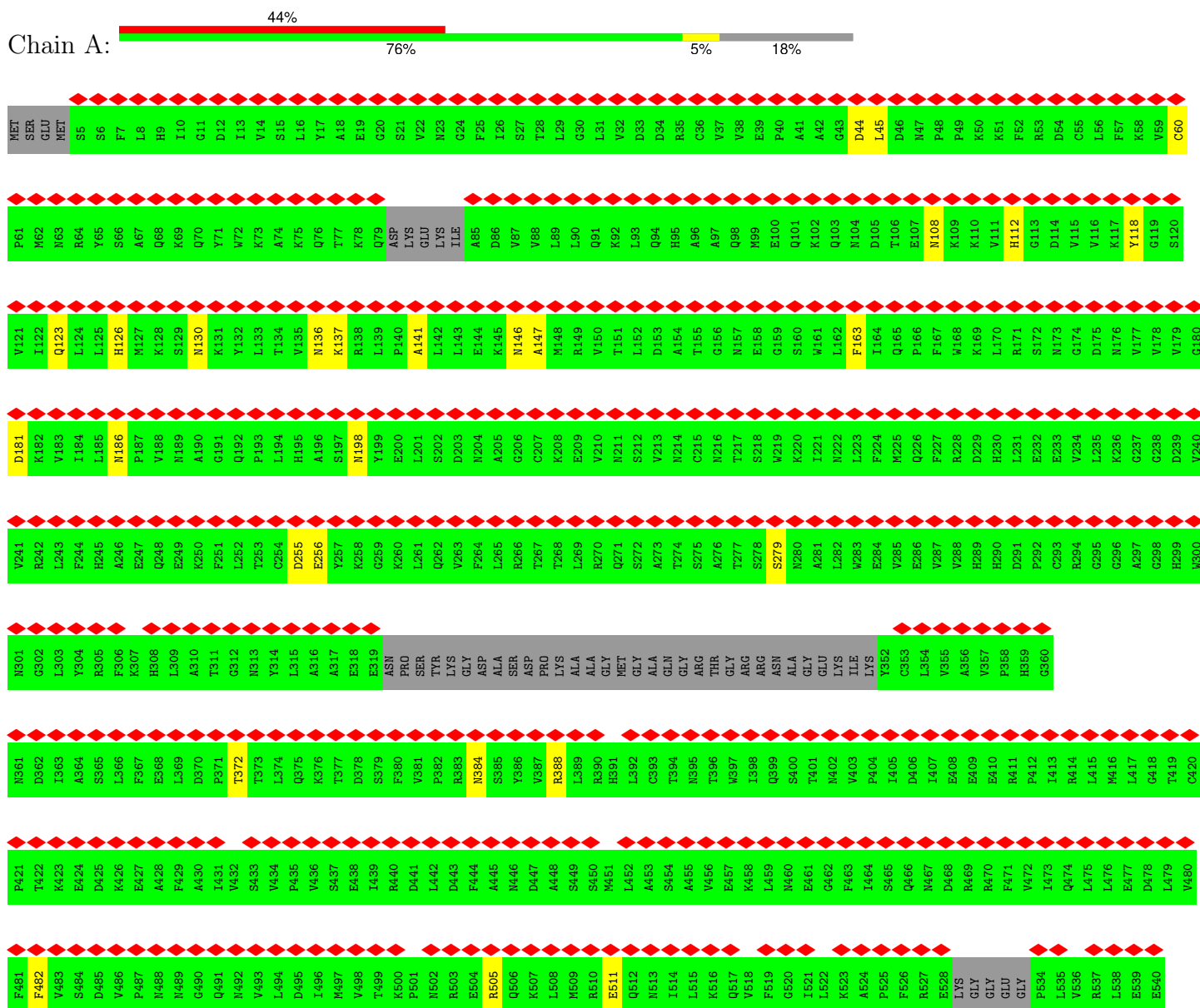
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

### 3 Residue-property plots

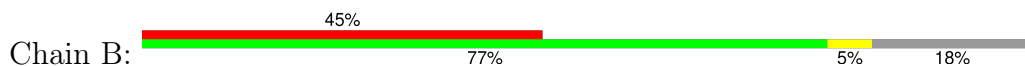
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



A1340	S1279	Q1211	L1225	L1226	H1293	D1294	R1295	H1296	V1297	E1298	Y1299	L1300	D1301	F1302	L1303	M1363	Y1364	H1365	I1366	K1367	L1368	V1369	D1370	L1371	L1372	A1373	A1374	C1375	A1376	E1377	G1378	K1379	M1380	V1381	Y1382	T1383	E1384	I1385	K1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	D1395	V1396	V1397	S1398	V1399					
GLU	ARG	THR	ASP	GLU	GLY	PHE	HIS	PRO	PRO	GLY	GLU	LYS	SER	S1166	E1167	N1168	Y1169	Q1170	I1171	V1172	K1173	G1174	I1175	L1176	E1177	R1178	L1179	M1180	K1181	M1182	C1183	G1184	V1185	G1186	E1187	Q1188	M1189	R1190	K1191	Q1192	Q1193	Q1194	R1195	K1198	N1199	A1202	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210			
F1079	R1085	M1089	H1090	K1093	Q1094	V1095	Q1096	L1097	L1098	I1099	S1100	A1101	Q1102	D1103	V1104	E1105	N1106	Y1107	K1108	V1109	I1110	K1111	S1112	E1113	L1114	D1115	R1116	V1121	E1122	K1123	S1124	E1125	L1126	W1127	V1128	D1129	K1130	LYS	GLY	GLY	GLY	GLY	GLU	VAL	ALA	GLY	ALA	LYS	LYS								
ASP	SER	GLY	ALA	ASP	GLY	THR	ALA	PRO	THR	ALA	N1022	M1023	N1024	L1025	D1026	I1027	I1028	G1029	E1030	E1033	A1034	M1035	F1036	G1037	V1038	G1039	LYS	THR	SER	S1043	M1044	L1045	E1046	V1047	D1048	D1049	E1050	G1051	R1052	M1054	R1057	H1061	M1064	Y1067	A1068	S1072											
SER	VAL	PHE	ALA	PRO	SER	LEU	ALA	GLY	SER	ALA	GLU	GLU	PRO	LEU	ASP	ARG	SER	PHE	GLU	ASN	D961	V964	M965	L972	E973	Q976	L979	L983	D984	I987	L990	L991	S992	V993	F994	K995	K996	F997	V999	E1000	V1001	F1002	P1003	M1004	GLN												
H868	N869	L870	L871	Y872	F873	G874	F875	S879	E880	R883	R886	T887	G890	C894	VAL	GLN	PRO	PRO	ALA	MET	LEU	GLN	D824	D825	K826	K827	N828	A831	N832	T833	M834	E835	E838	D839	N842	N843	V844	V845	S846	E847	A848	V849	P850	F851	A852	N853	E854	E855	K856	N857	T860	F861					
E792	K798	R801	L802	M803	T804	E805	I806	P807	T808	A809	I810	K813	D814	Y815	D816	S817	N818	L819	N820	A821	S822	R823	D824	D825	K826	K827	N828	A831	N832	T833	M834	E835	E838	D839	N842	N843	V844	V845	S846	E847	A848	V849	P850	F851	A852	N853	E854	E855	K856	N857	T860	F861					
L726	S727	Y728	Y729	R730	L733	K734	L735	F736	A737	R738	L741	D742	R743	A747	I748	D749	E750	I751	S752	Q753	Q754	L755	G756	V757	D758	L759	I760	F761	L762	C763	M764	A765	D766	E767	M768	L769	F770	F771	D772	L773	R774	A775	S776	F777	C778	H779	H783	V784	V785	V786	D787	R788	D789	F790	Q791		
I666	R667	T668	E669	R671	P672	V673	K674	GLU	MET	ALA	GLN	SER	HIS	TVR	LEU	SER	ILE	TVR	GLU	SER	E690	E691	V692	M693	L694	T695	M696	T697	D698	K699	N700	N701	E702	H703	H704	E705	K706	S640	N641	H642	I643	A644	E650	L651	I652	C653	K654	C655	V656	L657	D658	P659	K660	S662	D663	I664	L665
M601	N602	R603	L606	E607	K608	H609	I610	T611	K612	T613	E614	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	I643	A644	E650	L651	I652	C653	K654	C655	V656	L657	D658	P659	K660	S662	D663	I664	L665	

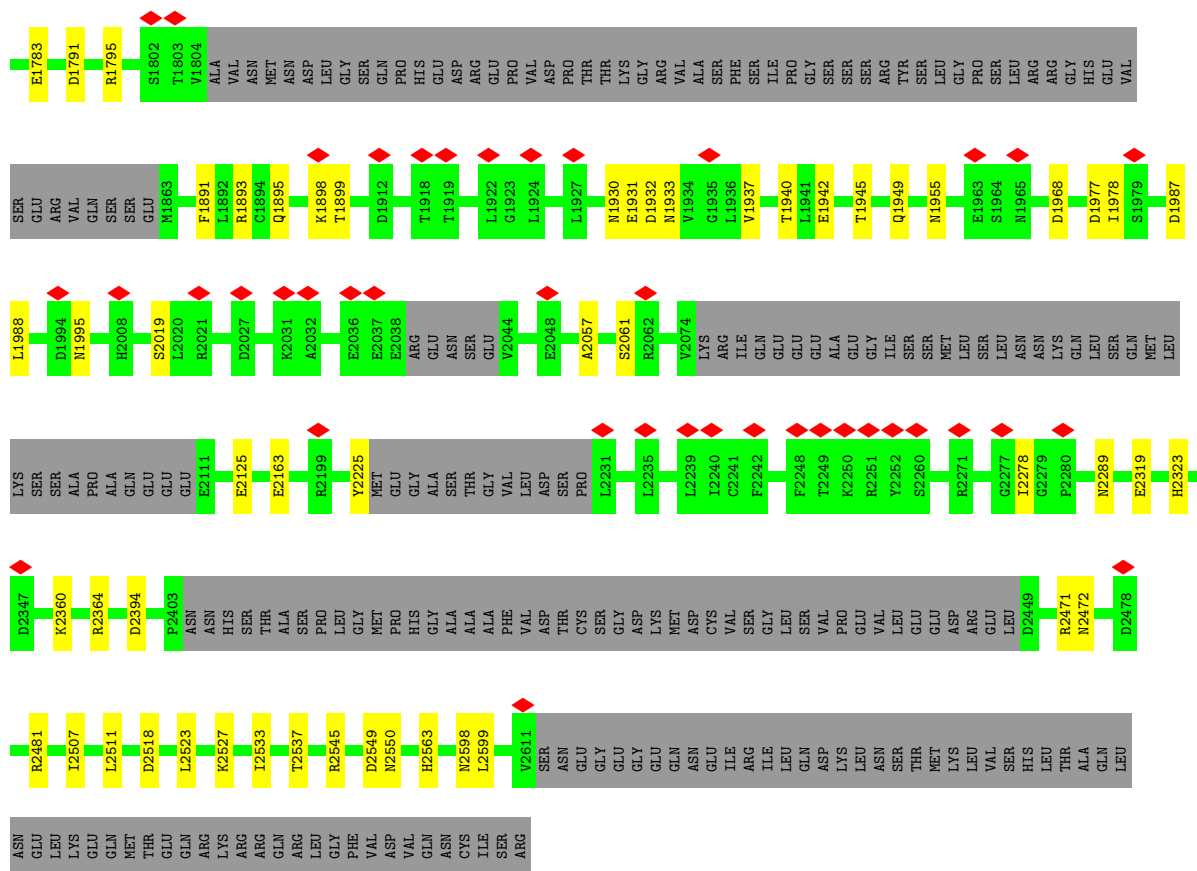
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



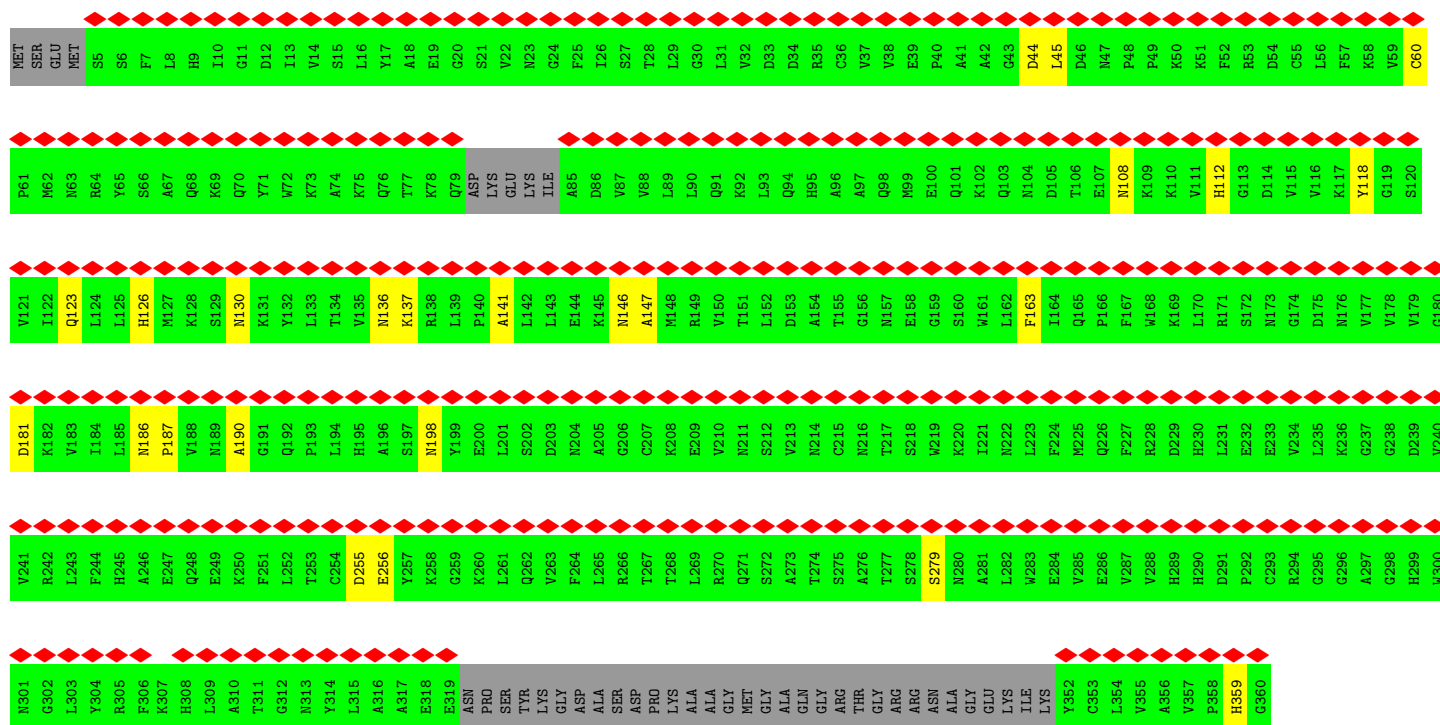
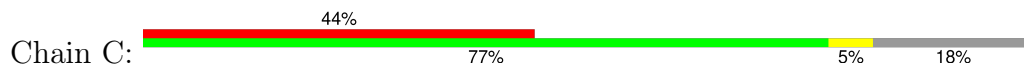
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V725	L726	S727	Y728	Y729	R730	L733	K734	L735	F736	A737	L741	D742	R743	A747	I748	D749	E750	I751	S752	Q753	Q754	L755	G756	V757	D758	L759	T760	F761	L762	C763	M764	A765	D766	E767	M768	L769	F770	F771	D772	L773	R774	A775	S776	F777	C778	H779	H785	V786	D787	R788	D789	P790	Q791	E792						
L665	I666	R667	T668	E669	L670	R671	P672	V673	Q674	GLU	MET	ALA	GLN	SER	HIS	GLU	TYR	LEU	ILE	GLU	TYR	SER	E690	E691	V692	W693	L694	T695	W696	T697	D698	K699	N700	N701	E702	H703	H704	E705	K706	S707	V708	N709	H710	Q711	L711	A712	Q713	E714	A715	R716	A717	G718	N719	A720	H721	D722	E723	N724		
N601	N602	R603	K604	L605	L606	E607	K608	H609	I610	T611	K612	T613	E614	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	H643	A644	E650	L651	I652	C653	K654	C655	V656	L657	D658	P659	K660	N661	S662	D663	I664		
F481	F482	V483	S484	K485	V486	E487	P487	N488	M489	Q490	Q491	N492	V493	L494	D495	I496	M497	V498	T499	K500	P501	N502	R503	E504	Q505	K506	K507	L508	M509	R510	E511	Q512	N513	I514	L515	K516	Q517	V518	F519	G520	I521	L522	K523	A524	P525	F526	R527	E528	LYS	GLY	GLY	GLY	P534	L535	V536	R537	L538	E539	E540	
P421	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	N460	E461	G462	F463	I464	S465	Q466	R467	D468	R469	R470	F471	V472	Q474	L475	L476	E477	D478	L479	V480		
N361	D362	I363	A364	S365	L366	F367	E368	L369	D370	F371	T372	L373	L374	Q375	K376	T377	D378	S379	F380	V381	P382	R383	N384	S385	Y386	V387	R388	L389	R390	H391	L392	C393	T394	N395	T396	W397	I398	Q399	S400	T401	N402	V403	P404	I405	D406	I407	E408	E409	E410	R411	P412	I413	R414	L415	M416	L417	T419	C420		
N301	G302	L303	Y304	R305	F306	K307	H308	L309	A310	T311	G312	N313	Y314	L315	A316	A317	E318	E319	ASN	PRO	SER	TYR	GLY	ASP	ALA	SER	ASP	PRO	LYS	ALA	GLY	MET	GLY	ALA	GLN	GLY	THR	ARG	ARG	ASN	ALA	GLY	GLY	LYS	ILE	LYS	Y352	C353	L354	V355	A356	V357	P358	H359	G360					
V241	R242	L243	F244	H245	A246	E247	Q248	E249	K250	F251	L252	T253	C254	D255	E256	Y257	K258	G259	K260	L261	Q262	V263	F264	L265	R266	T267	L268	L269	R270	Q271	S272	A273	T274	S275	A276	T277	S278	S279	N280	A281	L282	W283	E284	V285	E286	V287	V288	H289	L290	D291	P292	C293	R294	G295	G296	A297	G298	H299	W300	
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V121	I122	Q123	L124	L125	H126	M127	K128	S129	N130	K131	Y132	L133	T134	K135	N136	K137	R138	L139	P140	A141	L142	L143	E144	K145	N146	V147	M148	L149	V150	T151	L152	D153	A154	T155	G156	M157	G158	E159	Q160	W161	L162	F163	T164	Q165	E166	F167	W168	K169	L170	R171	S172	M173	D174	V175	V176	K177	Y178	V179	G180	
P61	M62	M63	M64	Y65	S66	A67	L68	Q68	R69	Q70	Y71	W72	K73	A74	K75	Q76	K77	K78	Q79	ASP	LYS	GLU	LYS	ILE	A85	D86	H87	V88	L89	L90	Q91	K92	L93	Q94	H95	A96	A97	Q98	M99	E100	Q101	K102	Q103	M104	D105	T106	E107	M108	K109	K110	V111	H112	G113	D114	V115	V116	K117	Y118	G119	S120
MET	SER	GLU	MET	S5	S6	F7	L8	H9	I10	G11	D12	I13	V14	S15	L16	Y17	A18	E19	G20	S21	V22	N23	G24	F25	I26	S27	T28	L29	G30	L31	V32	D33	D34	R35	C36	V37	V38	E39	P40	A41	A42	O43	D44	L45	D46	N47	P48	P49	K50	K51	F52	R53	D54	C55	L56	F57	K58	V59	C60	







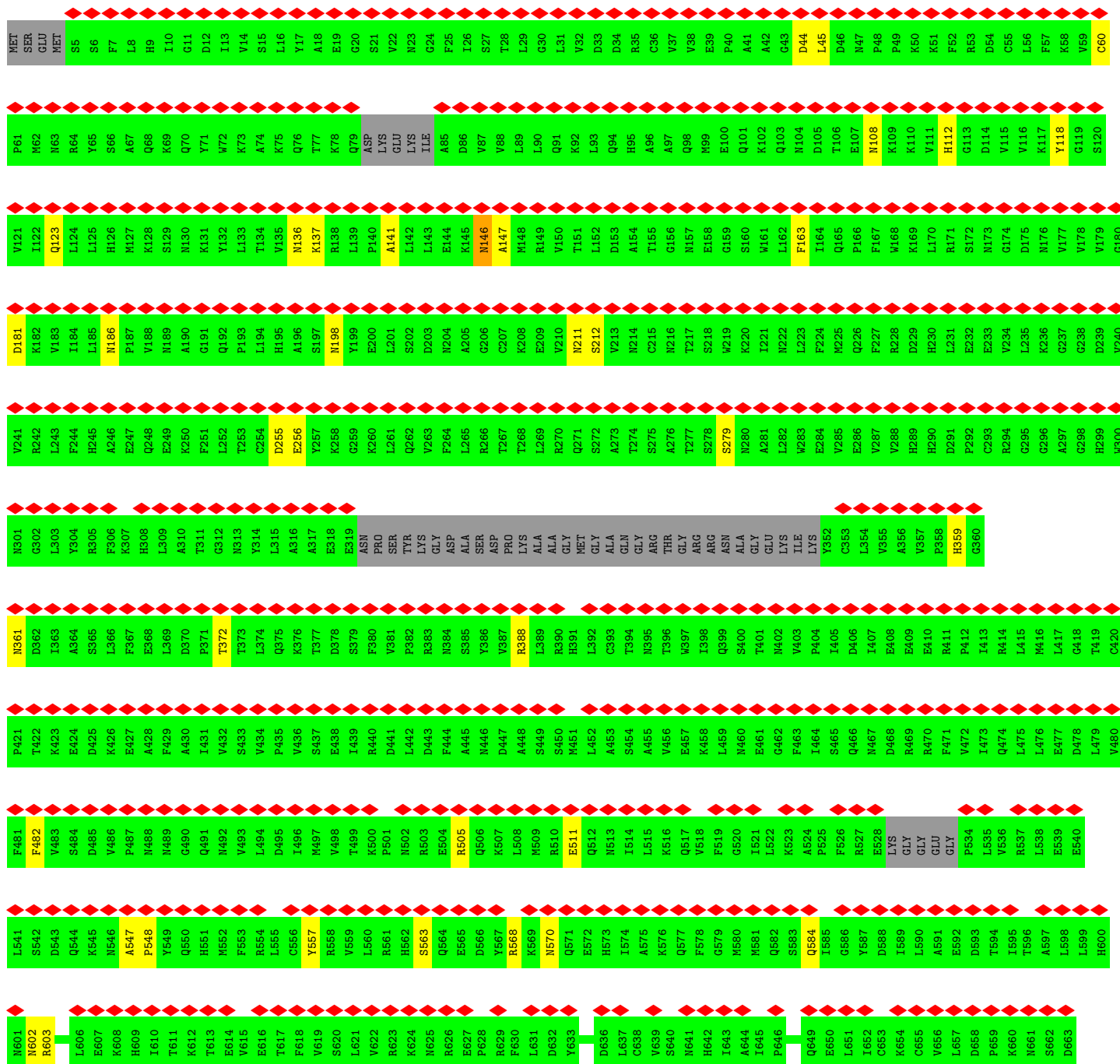
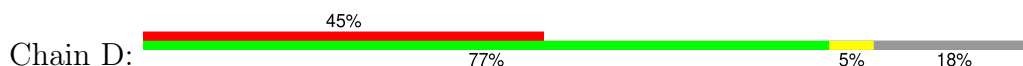
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







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







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131437	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	30.948	Depositor
Minimum map value	-23.778	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.817	Depositor
Recommended contour level	3	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: ZN, I3P, CA

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	0.27	0/17647	0.50	4/23845 (0.0%)
1	B	0.27	0/17647	0.50	4/23845 (0.0%)
1	C	0.27	0/17647	0.50	4/23845 (0.0%)
1	D	0.27	0/17647	0.50	4/23845 (0.0%)
All	All	0.27	0/70588	0.50	16/95380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1548	PRO	N-CA-CB	5.73	110.17	103.30
1	D	1548	PRO	N-CA-CB	5.67	110.10	103.30
1	C	1548	PRO	N-CA-CB	5.67	110.10	103.30
1	D	1495	PRO	N-CA-CB	5.67	110.10	103.30
1	B	1548	PRO	N-CA-CB	5.65	110.08	103.30
1	A	1544	PRO	N-CA-CB	5.62	110.05	103.30
1	B	1495	PRO	N-CA-CB	5.62	110.05	103.30
1	C	1544	PRO	N-CA-CB	5.62	110.04	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1495	PRO	N-CA-CB	5.62	110.04	103.30
1	A	1436	PRO	N-CA-CB	5.61	110.04	103.30
1	B	1436	PRO	N-CA-CB	5.61	110.04	103.30
1	A	1495	PRO	N-CA-CB	5.61	110.03	103.30
1	B	1544	PRO	N-CA-CB	5.60	110.02	103.30
1	D	1436	PRO	N-CA-CB	5.60	110.02	103.30
1	C	1436	PRO	N-CA-CB	5.58	110.00	103.30
1	D	1544	PRO	N-CA-CB	5.55	109.97	103.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASN	Peptide
1	B	146	ASN	Peptide
1	C	146	ASN	Peptide
1	D	146	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17342	17346	17176	75	0
1	B	17342	17346	17176	72	0
1	C	17342	17346	17176	71	0
1	D	17342	17346	17176	73	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	24	9	9	1	0
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
All	All	69476	69420	68740	278	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 (278) 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:147:ALA:HB1	1:B:1533:THR:CB	2.13	0.78
1:A:1725:GLN:NE2	1:A:1760:LEU:O	2.18	0.76
1:D:1725:GLN:NE2	1:D:1760:LEU:O	2.18	0.76
1:C:1725:GLN:NE2	1:C:1760:LEU:O	2.18	0.76
1:B:1725:GLN:NE2	1:B:1760:LEU:O	2.18	0.75
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.21	0.74
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.21	0.74
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.21	0.73
1:A:2524:ARG:NE	1:D:2518:ASP:OD2	2.17	0.73
1:A:482:PHE:O	1:A:505:ARG:NH1	2.22	0.73
1:C:482:PHE:O	1:C:505:ARG:NH1	2.22	0.73
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.21	0.73
1:B:482:PHE:O	1:B:505:ARG:NH1	2.22	0.72
1:C:1942:GLU:O	1:C:1945:THR:OG1	2.08	0.72
1:B:1942:GLU:O	1:B:1945:THR:OG1	2.08	0.71
1:D:482:PHE:O	1:D:505:ARG:NH1	2.22	0.71
1:D:1942:GLU:O	1:D:1945:THR:OG1	2.08	0.70
1:A:1942:GLU:O	1:A:1945:THR:OG1	2.08	0.70
1:B:1942:GLU:OE2	1:B:1995:ASN:ND2	2.25	0.70
1:C:1942:GLU:OE2	1:C:1995:ASN:ND2	2.25	0.70
1:D:1942:GLU:OE2	1:D:1995:ASN:ND2	2.25	0.69
1:A:1942:GLU:OE2	1:A:1995:ASN:ND2	2.25	0.69
1:D:557:TYR:OH	1:D:584:GLN:OE1	2.11	0.68
1:A:557:TYR:OH	1:A:584:GLN:OE1	2.11	0.68
1:B:1945:THR:O	1:B:1949:GLN:N	2.27	0.68
1:C:1945:THR:O	1:C:1949:GLN:N	2.27	0.68
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.27	0.67
1:D:1945:THR:O	1:D:1949:GLN:N	2.27	0.67
1:A:1945:THR:O	1:A:1949:GLN:N	2.27	0.67
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.27	0.67
1:C:557:TYR:OH	1:C:584:GLN:OE1	2.11	0.67
1:B:557:TYR:OH	1:B:584:GLN:OE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2518:ASP:OD2	1:C:2524:ARG:NE	2.22	0.66
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.27	0.66
1:D:2394:ASP:OD1	1:D:2481:ARG:NH2	2.27	0.66
1:D:563:SER:O	1:D:570:ASN:ND2	2.29	0.66
1:B:563:SER:O	1:B:570:ASN:ND2	2.29	0.66
1:C:563:SER:O	1:C:570:ASN:ND2	2.29	0.66
1:D:60:CYS:N	1:D:123:GLN:O	2.29	0.66
1:A:563:SER:O	1:A:570:ASN:ND2	2.29	0.65
1:B:60:CYS:N	1:B:123:GLN:O	2.29	0.65
1:A:60:CYS:N	1:A:123:GLN:O	2.29	0.65
1:D:1783:GLU:OE2	1:D:1899:THR:OG1	2.15	0.65
1:C:60:CYS:N	1:C:123:GLN:O	2.29	0.65
1:B:1783:GLU:OE2	1:B:1899:THR:OG1	2.15	0.64
1:A:1783:GLU:OE2	1:A:1899:THR:OG1	2.15	0.64
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.16	0.63
1:B:1391:LEU:O	1:B:1421:TYR:OH	2.16	0.63
1:C:1783:GLU:OE2	1:C:1899:THR:OG1	2.15	0.63
1:C:1391:LEU:O	1:C:1421:TYR:OH	2.16	0.62
1:D:1391:LEU:O	1:D:1421:TYR:OH	2.16	0.62
1:B:886:ARG:NE	1:B:1049:ASP:OD1	2.33	0.61
1:D:886:ARG:NE	1:D:1049:ASP:OD1	2.33	0.61
1:A:886:ARG:NE	1:A:1049:ASP:OD1	2.33	0.61
1:B:2523:LEU:O	1:B:2527:LYS:N	2.34	0.61
1:C:886:ARG:NE	1:C:1049:ASP:OD1	2.33	0.61
1:A:163:PHE:N	1:A:186:ASN:O	2.35	0.60
1:B:163:PHE:N	1:B:186:ASN:O	2.35	0.60
1:C:163:PHE:N	1:C:186:ASN:O	2.35	0.60
1:D:2523:LEU:O	1:D:2527:LYS:N	2.34	0.60
1:B:2533:ILE:O	1:B:2537:THR:N	2.35	0.59
1:C:2523:LEU:O	1:C:2527:LYS:N	2.34	0.59
1:A:2533:ILE:O	1:A:2537:THR:N	2.35	0.59
1:B:118:TYR:OH	1:B:181:ASP:OD2	2.15	0.58
1:C:2533:ILE:O	1:C:2537:THR:N	2.35	0.58
1:D:118:TYR:OH	1:D:181:ASP:OD2	2.15	0.58
1:D:163:PHE:N	1:D:186:ASN:O	2.35	0.58
1:D:2533:ILE:O	1:D:2537:THR:N	2.35	0.58
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.22	0.58
1:D:1679:TYR:O	1:D:1684:ASN:ND2	2.37	0.58
1:C:1679:TYR:O	1:C:1684:ASN:ND2	2.37	0.58
1:D:1968:ASP:OD1	1:D:2019:SER:OG	2.17	0.58
1:A:2523:LEU:O	1:A:2527:LYS:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1679:TYR:O	1:B:1684:ASN:ND2	2.37	0.58
1:A:1679:TYR:O	1:A:1684:ASN:ND2	2.37	0.57
1:C:118:TYR:OH	1:C:181:ASP:OD2	2.15	0.57
1:A:118:TYR:OH	1:A:181:ASP:OD2	2.15	0.56
1:B:1113:GLU:OE1	1:B:1116:ARG:NH2	2.39	0.56
1:A:1113:GLU:OE1	1:A:1116:ARG:NH2	2.39	0.56
1:A:2163:GLU:O	1:B:2545:ARG:NH1	2.37	0.56
1:D:1280:GLU:OE2	1:D:1284:GLN:NE2	2.39	0.56
1:B:838:GLU:O	1:B:842:ASN:ND2	2.39	0.56
1:A:838:GLU:O	1:A:842:ASN:ND2	2.39	0.55
1:D:1113:GLU:OE1	1:D:1116:ARG:NH2	2.39	0.55
1:A:1891:PHE:O	1:A:1895:GLN:NE2	2.39	0.55
1:C:1280:GLU:OE2	1:C:1284:GLN:NE2	2.39	0.55
1:D:1891:PHE:O	1:D:1895:GLN:NE2	2.39	0.55
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.22	0.55
1:B:1280:GLU:OE2	1:B:1284:GLN:NE2	2.39	0.55
1:D:838:GLU:O	1:D:842:ASN:ND2	2.39	0.55
1:A:1280:GLU:OE2	1:A:1284:GLN:NE2	2.39	0.55
1:B:1891:PHE:O	1:B:1895:GLN:NE2	2.39	0.55
1:C:1113:GLU:OE1	1:C:1116:ARG:NH2	2.39	0.55
1:C:1891:PHE:O	1:C:1895:GLN:NE2	2.39	0.55
1:C:838:GLU:O	1:C:842:ASN:ND2	2.39	0.55
1:A:1533:THR:CB	1:D:211:ASN:HB2	2.37	0.54
1:C:141:ALA:N	1:C:147:ALA:O	2.41	0.54
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.22	0.54
1:D:972:LEU:O	1:D:976:GLN:N	2.41	0.54
1:A:972:LEU:O	1:A:976:GLN:N	2.41	0.54
1:B:2507:ILE:O	1:B:2511:LEU:N	2.41	0.53
1:B:141:ALA:N	1:B:147:ALA:O	2.41	0.53
1:C:972:LEU:O	1:C:976:GLN:N	2.41	0.53
1:D:141:ALA:N	1:D:147:ALA:O	2.41	0.53
1:B:972:LEU:O	1:B:976:GLN:N	2.41	0.53
1:A:1214:TYR:OH	1:A:1222:MET:SD	2.67	0.53
1:A:372:THR:OG1	1:A:388:ARG:NH1	2.43	0.52
1:A:2507:ILE:O	1:A:2511:LEU:N	2.41	0.52
1:D:279:SER:OG	1:D:511:GLU:OE2	2.26	0.52
1:B:1214:TYR:OH	1:B:1222:MET:SD	2.67	0.52
1:B:372:THR:OG1	1:B:388:ARG:NH1	2.43	0.52
1:A:141:ALA:N	1:A:147:ALA:O	2.41	0.52
1:D:279:SER:N	1:D:511:GLU:OE2	2.43	0.52
1:D:1214:TYR:OH	1:D:1222:MET:SD	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2057:ALA:O	1:A:2061:SER:N	2.42	0.52
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.22	0.51
1:D:2057:ALA:O	1:D:2061:SER:N	2.42	0.51
1:A:279:SER:N	1:A:511:GLU:OE2	2.43	0.51
1:B:2125:GLU:OE1	1:B:2563:HIS:NE2	2.44	0.51
1:B:2057:ALA:O	1:B:2061:SER:N	2.42	0.51
1:B:1046:GLU:OE2	1:B:1052:GLY:N	2.44	0.51
1:D:1893:ARG:NH1	1:D:1955:ASN:OD1	2.44	0.51
1:A:1893:ARG:NH1	1:A:1955:ASN:OD1	2.44	0.51
1:C:372:THR:OG1	1:C:388:ARG:NH1	2.43	0.51
1:D:372:THR:OG1	1:D:388:ARG:NH1	2.43	0.51
1:D:1340:ALA:O	1:D:1344:HIS:ND1	2.43	0.51
1:A:2125:GLU:OE1	1:A:2563:HIS:NE2	2.44	0.51
1:C:1046:GLU:OE2	1:C:1052:GLY:N	2.44	0.51
1:C:1340:ALA:O	1:C:1344:HIS:ND1	2.43	0.51
1:B:1893:ARG:NH1	1:B:1955:ASN:OD1	2.44	0.50
1:C:147:ALA:HB1	1:D:1533:THR:CB	2.41	0.50
1:C:1214:TYR:OH	1:C:1222:MET:SD	2.67	0.50
1:D:1046:GLU:OE2	1:D:1052:GLY:N	2.44	0.50
1:A:1046:GLU:OE2	1:A:1052:GLY:N	2.44	0.50
1:C:279:SER:OG	1:C:511:GLU:OE2	2.26	0.50
1:C:2225:TYR:OH	1:C:2278:ILE:HG21	2.12	0.50
1:D:2225:TYR:OH	1:D:2278:ILE:HG21	2.12	0.50
1:D:2507:ILE:O	1:D:2511:LEU:N	2.41	0.50
1:C:279:SER:N	1:C:511:GLU:OE2	2.43	0.50
1:B:2225:TYR:OH	1:B:2278:ILE:HG21	2.12	0.50
1:C:2057:ALA:O	1:C:2061:SER:N	2.43	0.49
1:C:2507:ILE:O	1:C:2511:LEU:N	2.41	0.49
1:B:279:SER:N	1:B:511:GLU:OE2	2.43	0.49
1:B:1968:ASP:OD1	1:B:2019:SER:OG	2.17	0.49
1:A:1543:PHE:O	1:D:146:ASN:ND2	2.46	0.49
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.46	0.49
1:A:2225:TYR:OH	1:A:2278:ILE:HG21	2.12	0.49
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.17	0.49
1:B:1523:GLN:O	1:B:1527:SER:N	2.45	0.49
1:C:1893:ARG:NH1	1:C:1955:ASN:OD1	2.44	0.49
1:C:2125:GLU:OE1	1:C:2563:HIS:NE2	2.44	0.49
1:D:2125:GLU:OE1	1:D:2563:HIS:NE2	2.44	0.49
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.46	0.48
1:B:1340:ALA:O	1:B:1344:HIS:ND1	2.43	0.48
1:D:730:ARG:NH2	1:D:772:ASP:OD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:LYS:O	1:B:1127:TRP:NE1	2.46	0.48
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.46	0.48
1:C:1523:GLN:O	1:C:1527:SER:N	2.45	0.48
1:C:1968:ASP:OD1	1:C:2019:SER:OG	2.17	0.48
1:C:1123:LYS:O	1:C:1127:TRP:NE1	2.46	0.48
1:D:1523:GLN:O	1:D:1527:SER:N	2.45	0.48
1:A:1340:ALA:O	1:A:1344:HIS:ND1	2.43	0.48
1:B:730:ARG:NH2	1:B:772:ASP:OD2	2.47	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.46	0.48
1:C:730:ARG:NH2	1:C:772:ASP:OD2	2.47	0.47
1:D:359:HIS:ND1	1:D:361:ASN:OD1	2.47	0.47
1:A:568:ARG:NH2	3:A:3002:I3P:O3	2.47	0.47
1:C:568:ARG:NH2	3:C:3002:I3P:O3	2.47	0.47
1:A:1123:LYS:O	1:A:1127:TRP:NE1	2.46	0.47
1:A:1523:GLN:O	1:A:1527:SER:N	2.45	0.47
1:D:568:ARG:NH2	3:D:3002:I3P:O3	2.47	0.47
1:A:730:ARG:NH2	1:A:772:ASP:OD2	2.46	0.47
1:D:1123:LYS:O	1:D:1127:TRP:NE1	2.46	0.47
1:C:1930:ASN:N	1:C:1933:ASN:OD1	2.48	0.47
1:B:147:ALA:HB1	1:C:1533:THR:CB	2.44	0.47
1:B:568:ARG:NH2	3:B:3002:I3P:O3	2.47	0.47
1:A:1930:ASN:N	1:A:1933:ASN:OD1	2.48	0.46
1:A:1987:ASP:OD1	1:A:1988:LEU:N	2.49	0.46
1:D:1987:ASP:OD1	1:D:1988:LEU:N	2.49	0.46
1:B:1752:GLU:O	1:B:1756:LEU:N	2.47	0.46
1:A:1791:ASP:O	1:A:1795:ARG:N	2.49	0.46
1:B:1930:ASN:N	1:B:1933:ASN:OD1	2.48	0.46
1:C:1987:ASP:OD1	1:C:1988:LEU:N	2.49	0.46
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.49	0.45
1:B:1791:ASP:O	1:B:1795:ARG:N	2.49	0.45
1:C:1977:ASP:OD1	1:C:1978:ILE:N	2.49	0.45
1:B:2163:GLU:O	1:C:2545:ARG:NH1	2.49	0.45
1:B:1977:ASP:OD1	1:B:1978:ILE:N	2.49	0.45
1:A:1337:ASN:OD1	1:A:1338:ASP:N	2.50	0.45
1:C:1288:HIS:O	1:C:1292:THR:OG1	2.28	0.45
1:C:1791:ASP:O	1:C:1795:ARG:N	2.49	0.45
1:A:1752:GLU:O	1:A:1756:LEU:N	2.47	0.45
1:B:1337:ASN:OD1	1:B:1338:ASP:N	2.50	0.45
1:D:1930:ASN:N	1:D:1933:ASN:OD1	2.48	0.45
1:A:255:ASP:OD1	1:A:256:GLU:N	2.50	0.44
1:D:2319:GLU:O	1:D:2323:HIS:ND1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:HIS:O	1:A:130:ASN:N	2.48	0.44
1:A:1977:ASP:OD2	1:A:2031:LYS:NZ	2.33	0.44
1:B:126:HIS:O	1:B:130:ASN:N	2.48	0.44
1:A:1977:ASP:OD1	1:A:1978:ILE:N	2.49	0.44
1:C:1752:GLU:O	1:C:1756:LEU:N	2.47	0.44
1:D:1791:ASP:O	1:D:1795:ARG:N	2.49	0.44
1:C:384:ASN:OD1	1:C:1898:LYS:NZ	2.45	0.44
1:A:2319:GLU:O	1:A:2323:HIS:ND1	2.47	0.44
1:D:1337:ASN:OD1	1:D:1338:ASP:N	2.50	0.44
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.51	0.44
1:B:359:HIS:ND1	1:B:361:ASN:OD1	2.47	0.44
1:C:547:ALA:HB3	1:C:548:PRO:HD3	2.00	0.44
1:C:2319:GLU:O	1:C:2323:HIS:ND1	2.47	0.44
1:C:2598:ASN:OD1	1:C:2599:LEU:N	2.51	0.44
1:D:1752:GLU:O	1:D:1756:LEU:N	2.47	0.44
1:A:547:ALA:HB3	1:A:548:PRO:HD3	2.00	0.43
1:A:719:ASN:ND2	1:A:722:ASP:OD2	2.51	0.43
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.51	0.43
1:C:1337:ASN:OD1	1:C:1338:ASP:N	2.50	0.43
1:C:2549:ASP:OD1	1:C:2550:ASN:N	2.51	0.43
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.51	0.43
1:A:1257:GLY:H	1:A:1299:TYR:HH	1.65	0.43
1:A:44:ASP:OD1	1:A:45:LEU:N	2.52	0.43
1:D:2549:ASP:OD1	1:D:2550:ASN:N	2.51	0.43
1:B:44:ASP:OD1	1:B:45:LEU:N	2.52	0.43
1:B:547:ALA:HB3	1:B:548:PRO:HD3	2.00	0.43
1:B:862:GLU:O	1:B:865:SER:OG	2.24	0.43
1:A:1048:ASP:OD1	1:A:1049:ASP:N	2.52	0.43
1:D:547:ALA:HB3	1:D:548:PRO:HD3	2.00	0.43
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.52	0.43
1:C:719:ASN:ND2	1:C:722:ASP:OD2	2.51	0.43
1:D:255:ASP:OD1	1:D:256:GLU:N	2.50	0.43
1:D:1647:LEU:O	1:D:1651:THR:OG1	2.28	0.43
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.52	0.43
1:D:1977:ASP:OD1	1:D:1978:ILE:N	2.49	0.43
1:B:255:ASP:OD1	1:B:256:GLU:N	2.50	0.43
1:B:719:ASN:ND2	1:B:722:ASP:OD2	2.51	0.42
1:C:44:ASP:OD1	1:C:45:LEU:N	2.52	0.42
1:A:1225:LEU:O	1:A:1228:THR:OG1	2.35	0.42
1:B:2549:ASP:OD1	1:B:2550:ASN:N	2.51	0.42
1:D:2598:ASN:OD1	1:D:2599:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:OD1	1:D:45:LEU:N	2.52	0.42
1:D:719:ASN:ND2	1:D:722:ASP:OD2	2.51	0.42
1:B:2319:GLU:O	1:B:2323:HIS:ND1	2.47	0.42
1:A:2549:ASP:OD1	1:A:2550:ASN:N	2.51	0.42
1:B:384:ASN:OD1	1:B:1898:LYS:NZ	2.45	0.42
1:B:1619:ASP:O	1:B:1623:TRP:N	2.51	0.42
1:A:1930:ASN:OD1	1:A:1931:GLU:N	2.51	0.42
1:A:1533:THR:HA	1:D:212:SER:N	2.34	0.42
1:C:359:HIS:ND1	1:C:361:ASN:OD1	2.47	0.42
1:D:2148:THR:OG1	1:D:2151:THR:OG1	2.36	0.42
1:B:2360:LYS:O	1:B:2364:ARG:N	2.47	0.42
1:C:1257:GLY:H	1:C:1299:TYR:HH	1.68	0.42
1:A:384:ASN:OD1	1:A:1898:LYS:NZ	2.45	0.41
1:A:1533:THR:HA	1:D:212:SER:H	1.85	0.41
1:D:602:ASN:OD1	1:D:603:ARG:N	2.54	0.41
1:B:602:ASN:OD1	1:B:603:ARG:N	2.54	0.41
1:C:255:ASP:OD1	1:C:256:GLU:N	2.50	0.41
1:D:108:ASN:O	1:D:112:HIS:N	2.53	0.41
1:D:1930:ASN:OD1	1:D:1931:GLU:N	2.51	0.41
1:B:136:ASN:OD1	1:B:137:LYS:N	2.54	0.41
1:D:1257:GLY:H	1:D:1299:TYR:HH	1.68	0.41
1:D:1619:ASP:O	1:D:1623:TRP:N	2.51	0.41
1:A:602:ASN:OD1	1:A:603:ARG:N	2.54	0.41
1:A:1647:LEU:O	1:A:1651:THR:OG1	2.28	0.41
1:B:279:SER:OG	1:B:511:GLU:OE2	2.26	0.41
1:C:136:ASN:OD1	1:C:137:LYS:N	2.54	0.41
1:C:2360:LYS:O	1:C:2364:ARG:N	2.47	0.41
1:A:2360:LYS:O	1:A:2364:ARG:N	2.47	0.41
1:A:2545:ARG:NH1	1:D:2163:GLU:O	2.54	0.41
1:C:108:ASN:O	1:C:112:HIS:N	2.53	0.41
1:A:1619:ASP:O	1:A:1623:TRP:N	2.51	0.41
1:B:1257:GLY:H	1:B:1299:TYR:HH	1.67	0.40
1:A:108:ASN:O	1:A:112:HIS:N	2.53	0.40
1:B:108:ASN:O	1:B:112:HIS:N	2.53	0.40
1:C:126:HIS:O	1:C:130:ASN:N	2.48	0.40
1:D:136:ASN:OD1	1:D:137:LYS:N	2.54	0.40
1:C:602:ASN:OD1	1:C:603:ARG:N	2.54	0.40
1:B:1930:ASN:OD1	1:B:1931:GLU:N	2.51	0.40
1:A:136:ASN:OD1	1:A:137:LYS:N	2.54	0.40
1:C:187:PRO:HG2	1:C:190:ALA:HB3	2.04	0.40
1:C:2367:ARG:NE	1:D:2352:GLU:OE2	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	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
1	B	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
1	C	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
1	D	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
All	All	8568/10684 (80%)	8144 (95%)	424 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
1	B	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
1	C	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
1	D	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
All	All	7512/9540 (79%)	7484 (100%)	28 (0%)	88	91

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	1106	ASN
1	A	1415	ASN
1	A	1418	ASN
1	A	2289	ASN
1	A	2471	ARG
1	A	2472	ASN
1	B	198	ASN
1	B	1106	ASN
1	B	1415	ASN
1	B	1418	ASN
1	B	2289	ASN
1	B	2471	ARG
1	B	2472	ASN
1	C	198	ASN
1	C	1106	ASN
1	C	1415	ASN
1	C	1418	ASN
1	C	2289	ASN
1	C	2471	ARG
1	C	2472	ASN
1	D	198	ASN
1	D	1106	ASN
1	D	1415	ASN
1	D	1418	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. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1725	GLN
1	A	2550	ASN
1	B	1725	GLN
1	C	1725	GLN
1	C	1897	ASN
1	D	146	ASN
1	D	1725	GLN

### 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 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	I3P	A	3002	-	24,24,24	1.35	3 (12%)	39,39,39	0.84	0
3	I3P	D	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	0
3	I3P	C	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	0
3	I3P	B	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3002	I3P	P1-O1	3.31	1.65	1.59
3	A	3002	I3P	P1-O1	3.29	1.65	1.59
3	A	3002	I3P	P4-O4	3.29	1.65	1.59
3	C	3002	I3P	P4-O4	3.28	1.65	1.59
3	B	3002	I3P	P5-O5	3.26	1.65	1.59
3	A	3002	I3P	P5-O5	3.25	1.65	1.59
3	B	3002	I3P	P4-O4	3.25	1.65	1.59
3	C	3002	I3P	P1-O1	3.24	1.65	1.59
3	B	3002	I3P	P1-O1	3.24	1.65	1.59
3	D	3002	I3P	P4-O4	3.22	1.65	1.59
3	C	3002	I3P	P5-O5	3.21	1.65	1.59
3	D	3002	I3P	P5-O5	3.19	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	I3P	C5-O5-P5-O51
3	B	3002	I3P	C5-O5-P5-O51
3	C	3002	I3P	C5-O5-P5-O51
3	D	3002	I3P	C5-O5-P5-O51
3	A	3002	I3P	C5-O5-P5-O53
3	B	3002	I3P	C5-O5-P5-O53
3	C	3002	I3P	C5-O5-P5-O53
3	D	3002	I3P	C5-O5-P5-O53

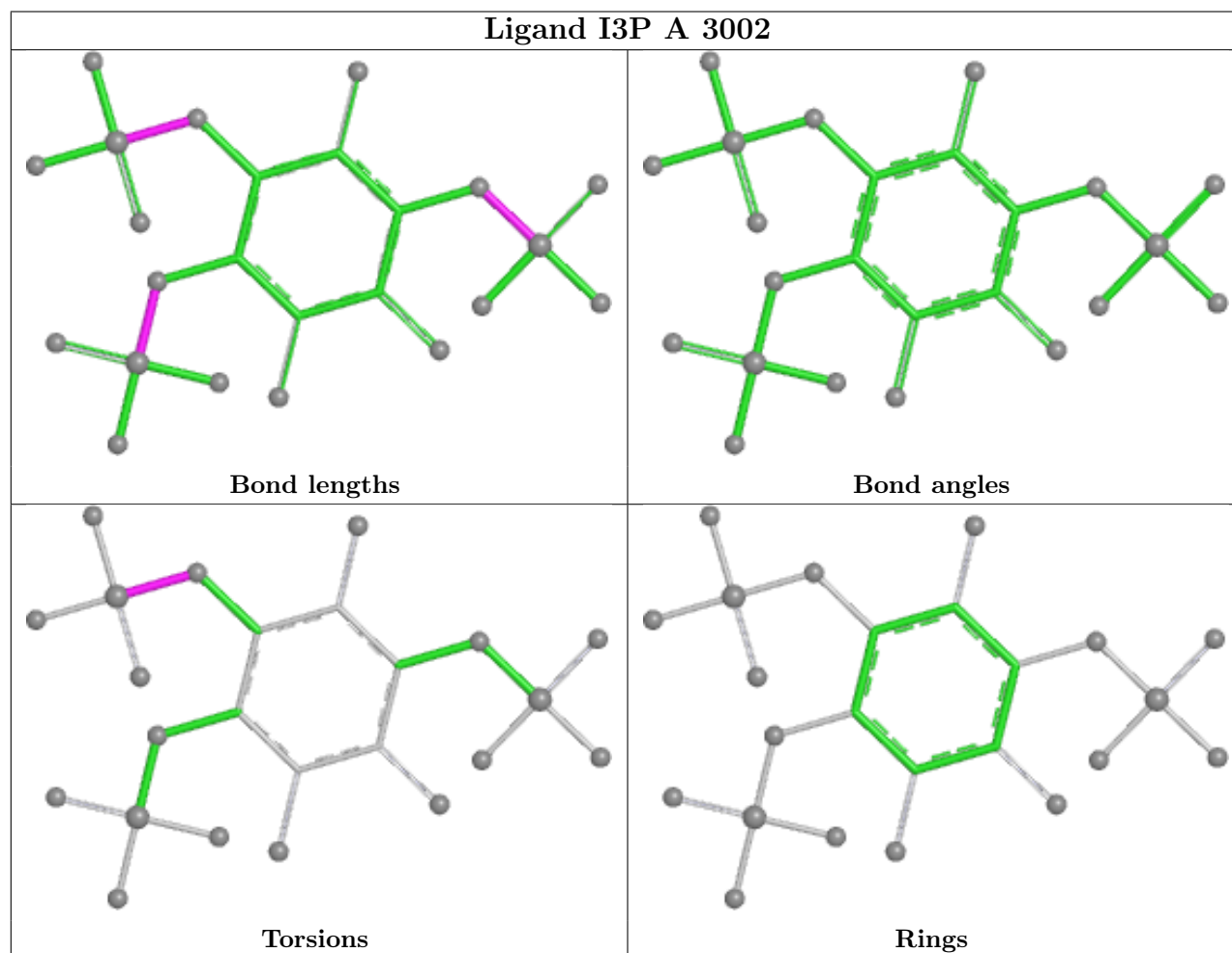
There are no ring outliers.

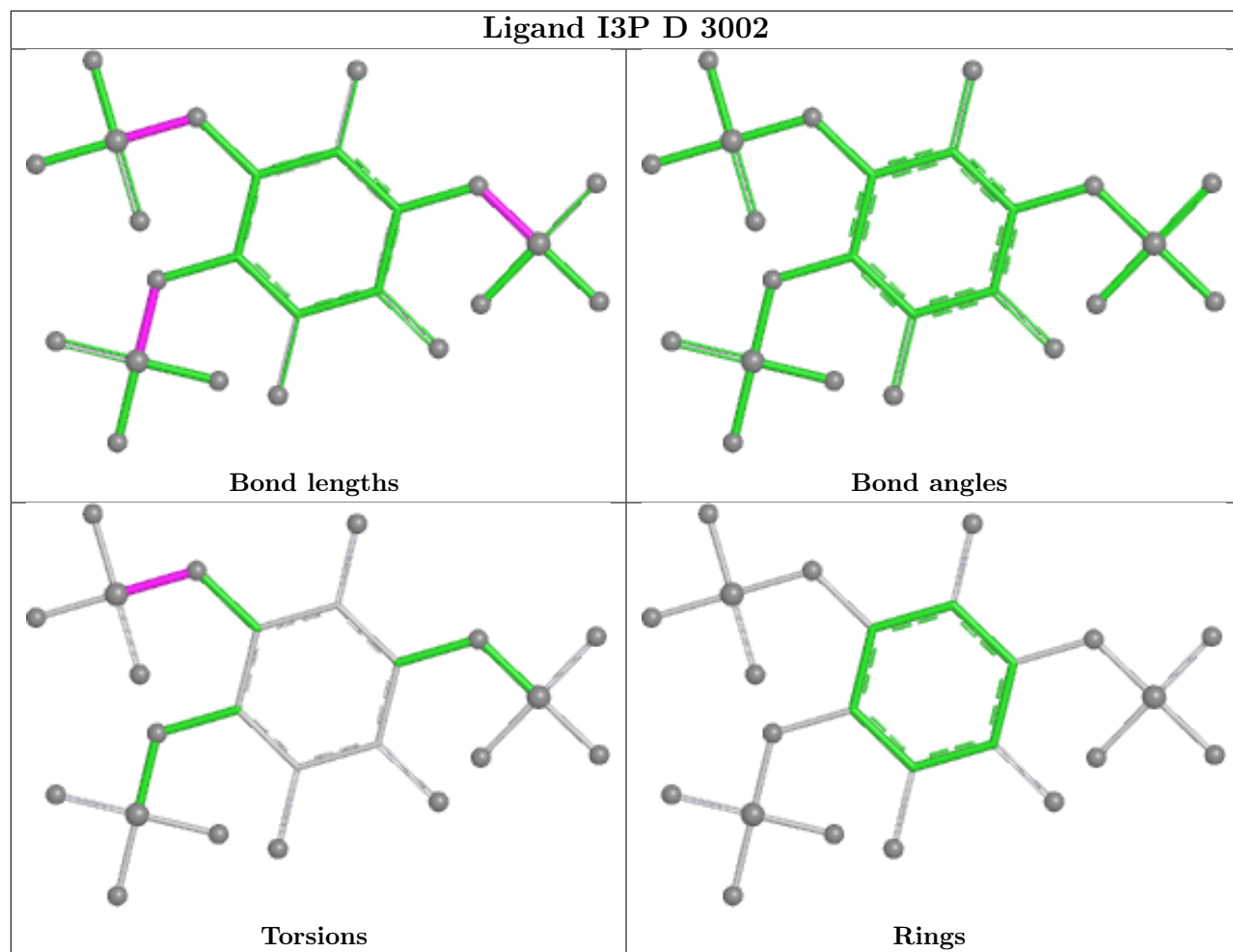
4 monomers are involved in 4 short contacts:

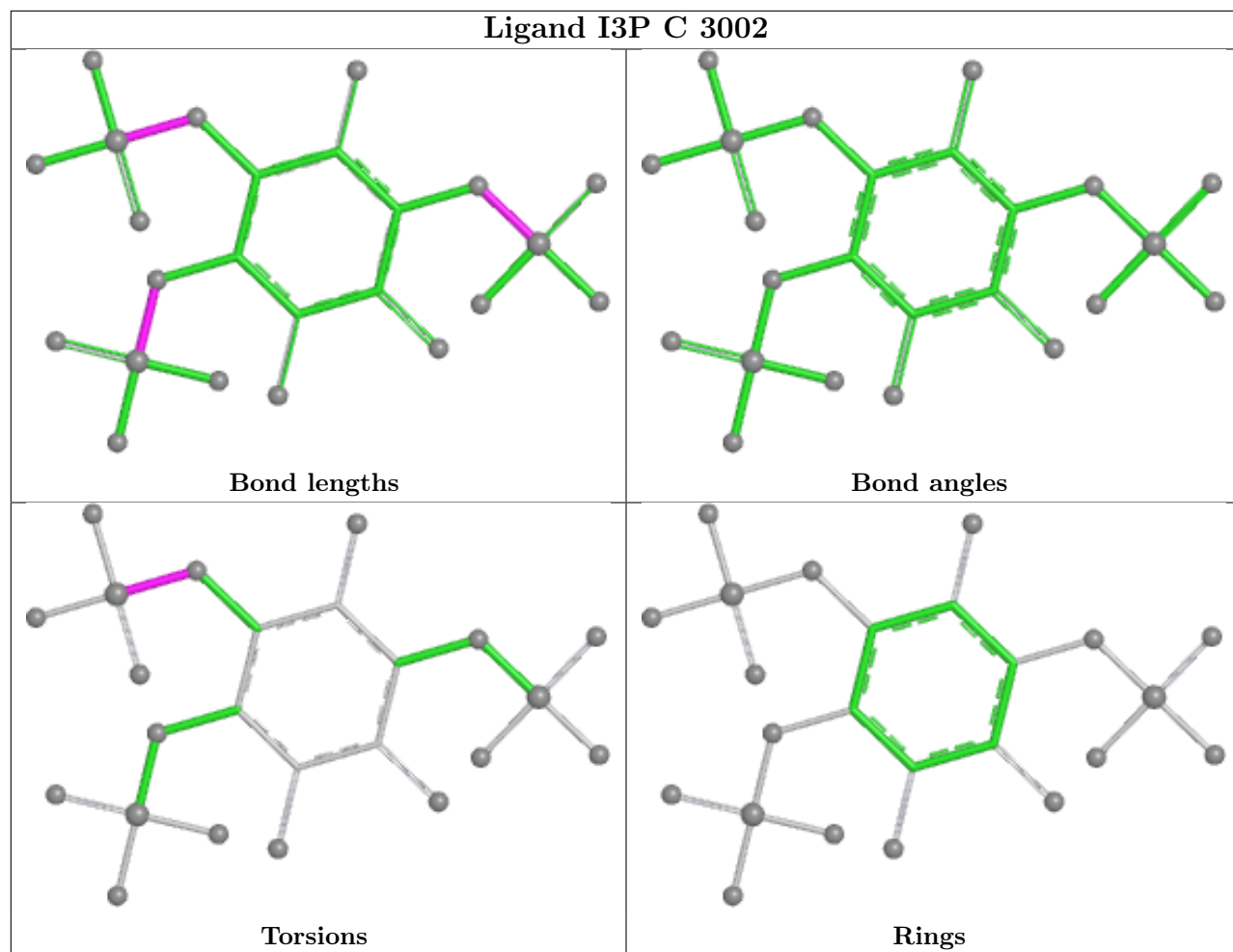
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	I3P	1	0
3	D	3002	I3P	1	0
3	C	3002	I3P	1	0
3	B	3002	I3P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

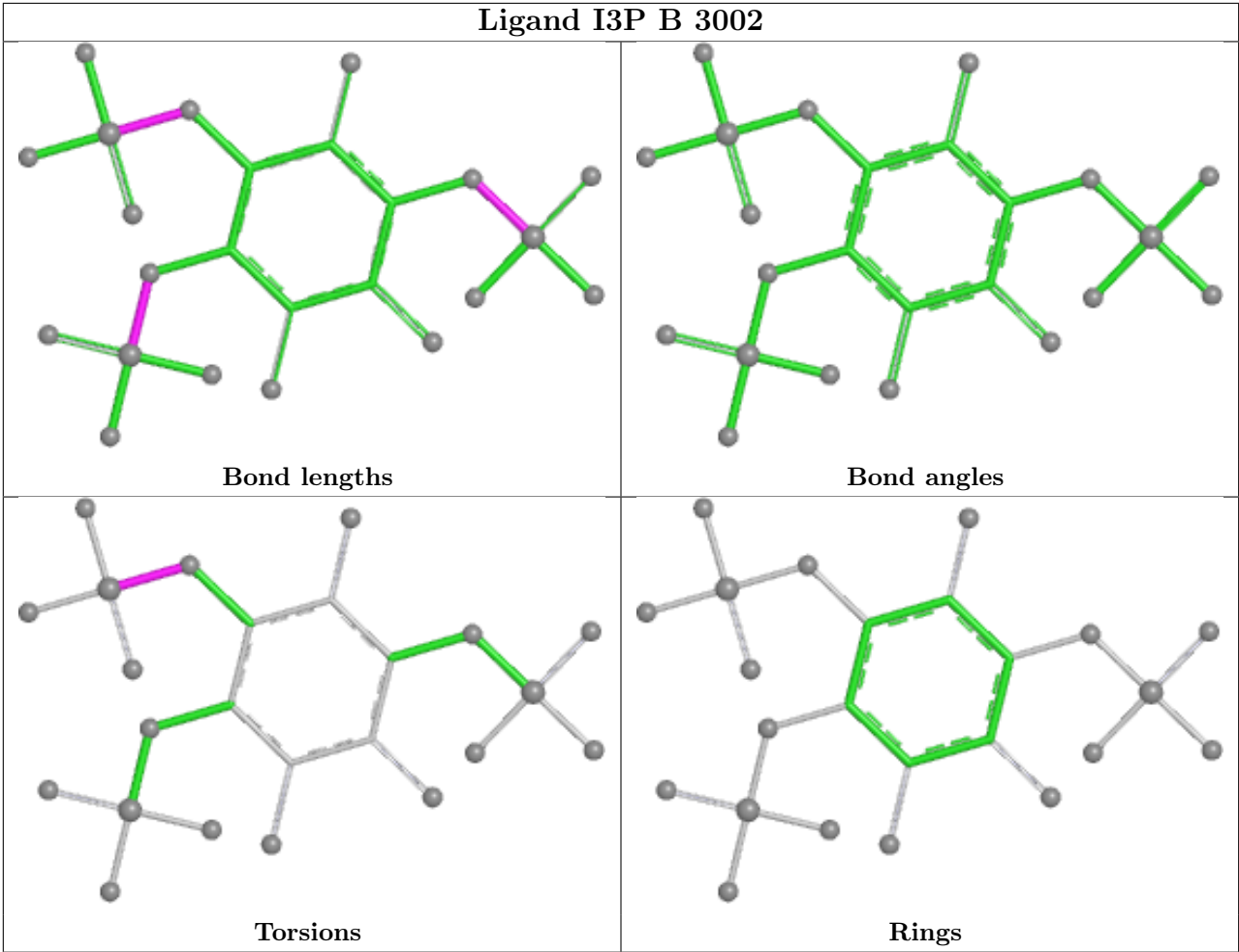
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	56.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1552:GLN	C	1586:TRP	N	56.29
1	C	1552:GLN	C	1586:TRP	N	56.29
1	D	1552:GLN	C	1586:TRP	N	56.29
1	A	1533:THR	C	1541:ARG	N	17.36
1	B	1533:THR	C	1541:ARG	N	17.36
1	C	1533:THR	C	1541:ARG	N	17.36
1	D	1533:THR	C	1541:ARG	N	17.36
1	A	1484:GLY	C	1490:ARG	N	12.73
1	B	1484:GLY	C	1490:ARG	N	12.73
1	C	1484:GLY	C	1490:ARG	N	12.73
1	D	1484:GLY	C	1490:ARG	N	12.73
1	A	1508:SER	C	1515:GLY	N	11.13
1	B	1508:SER	C	1515:GLY	N	11.13
1	C	1508:SER	C	1515:GLY	N	11.13
1	D	1508:SER	C	1515:GLY	N	11.13
1	A	2252:TYR	C	2260:SER	N	6.36
1	B	2252:TYR	C	2260:SER	N	6.36
1	C	2252:TYR	C	2260:SER	N	6.36
1	D	2252:TYR	C	2260:SER	N	6.36

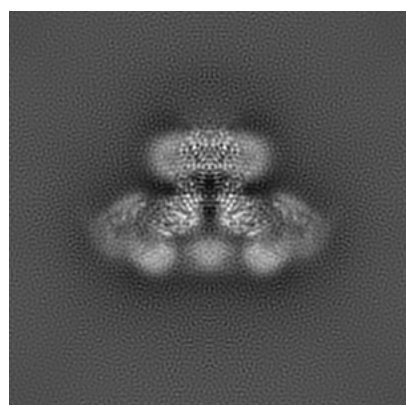
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7994. These allow visual inspection of the internal detail of the map and identification of artifacts.

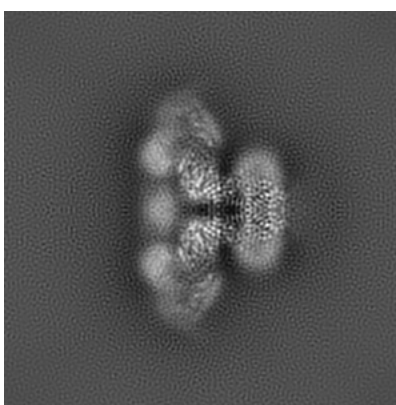
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

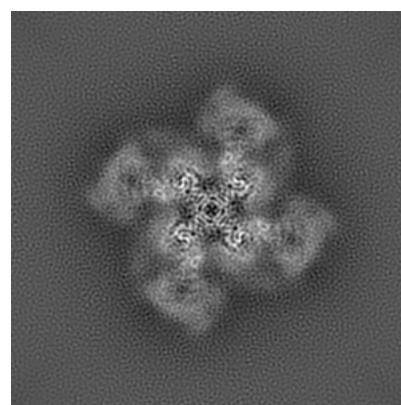
#### 6.1.1 Primary map



X



Y

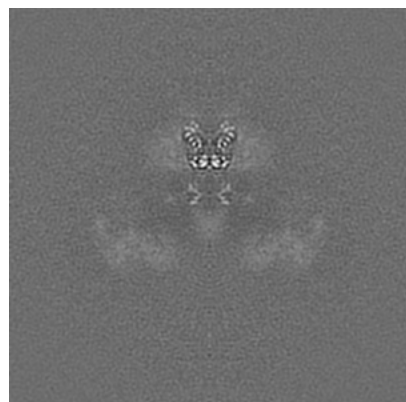


Z

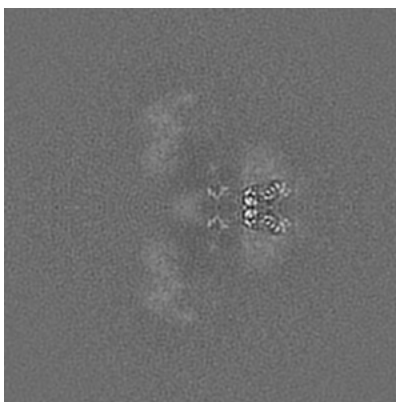
The images above show the map projected in three orthogonal directions.

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

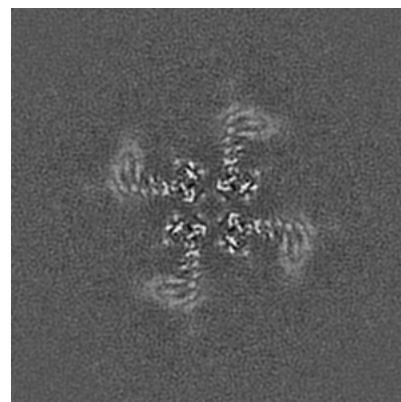
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

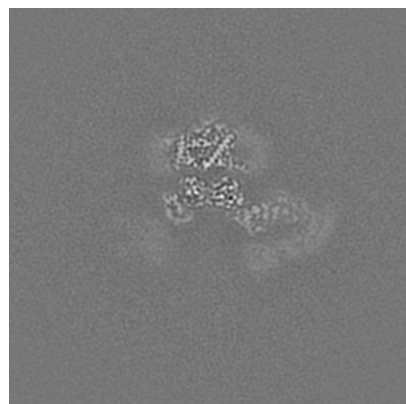


Z Index: 192

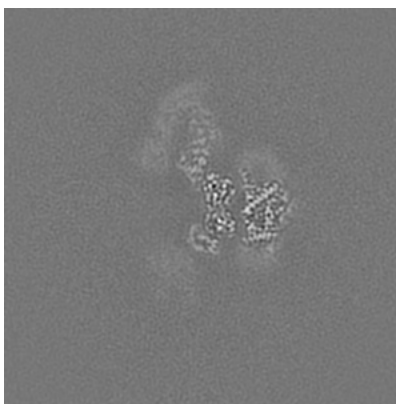
The images above show central slices of the map in three orthogonal directions.

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

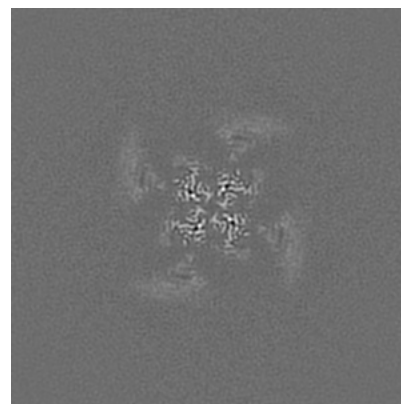
### 6.3.1 Primary map



X Index: 207



Y Index: 177

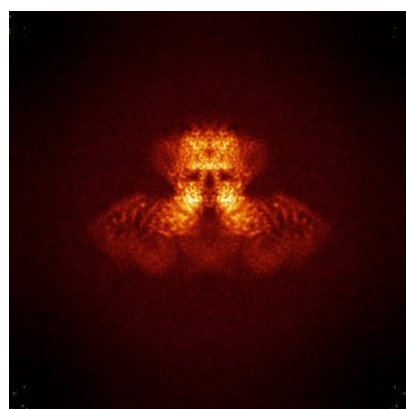


Z Index: 201

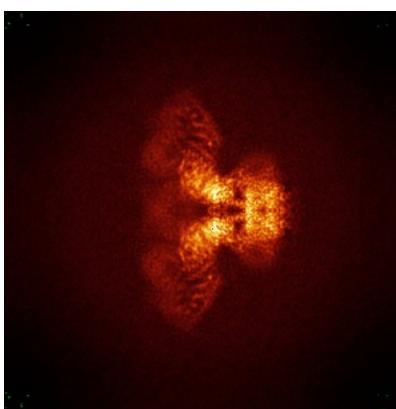
The images above show the largest variance slices of the map in three orthogonal directions.

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

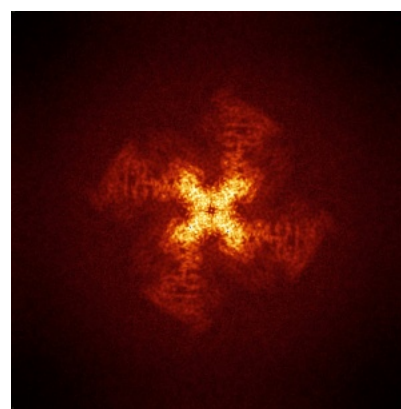
### 6.4.1 Primary map



X



Y

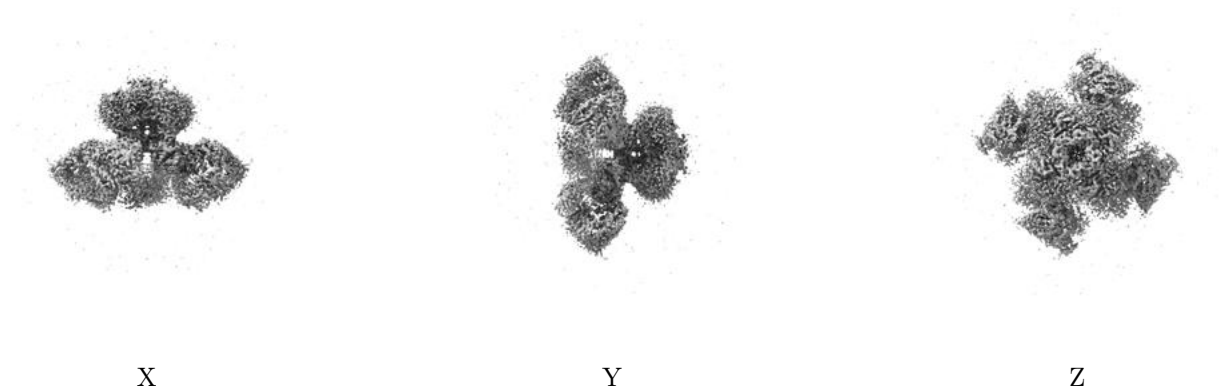


Z

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

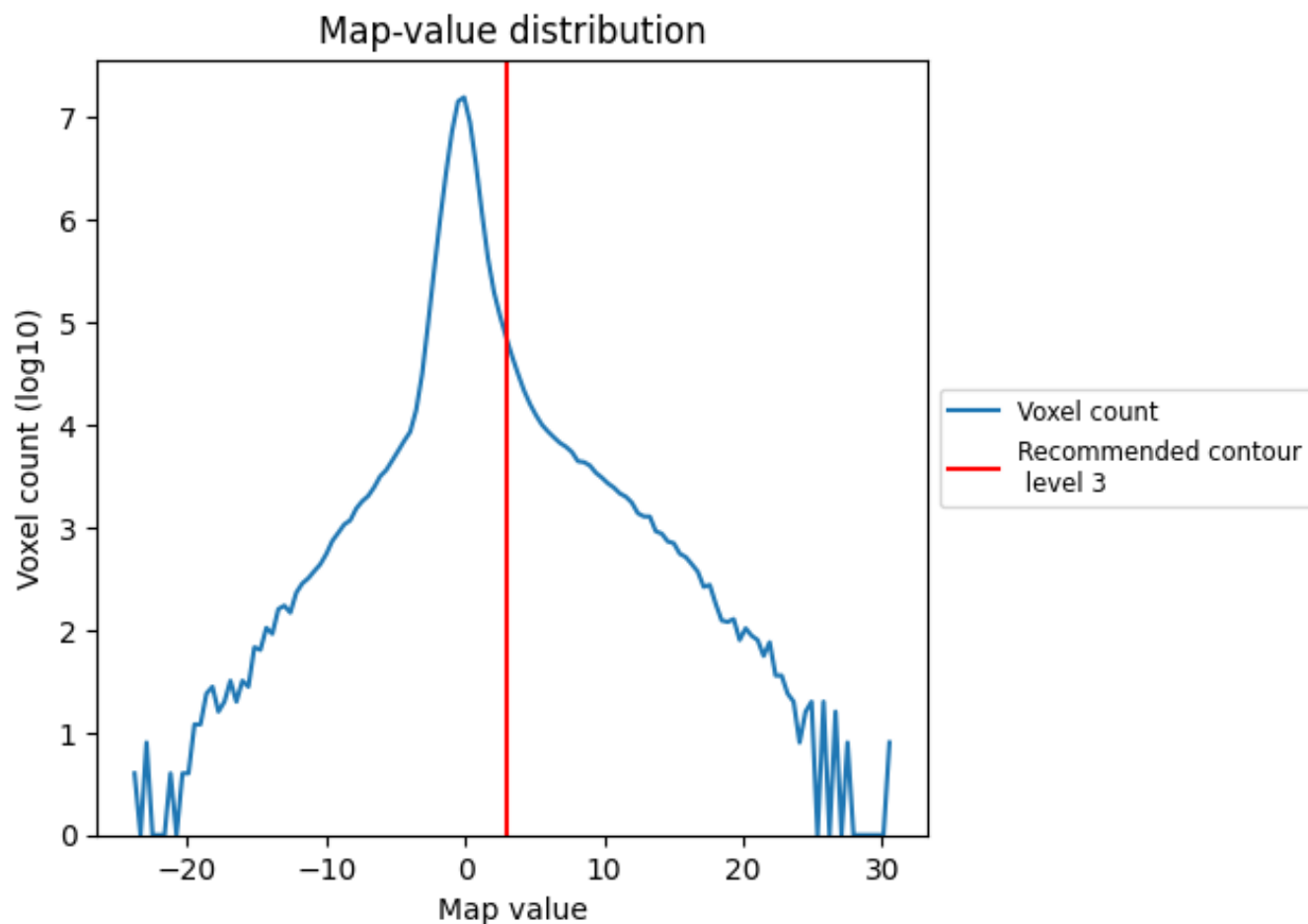
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

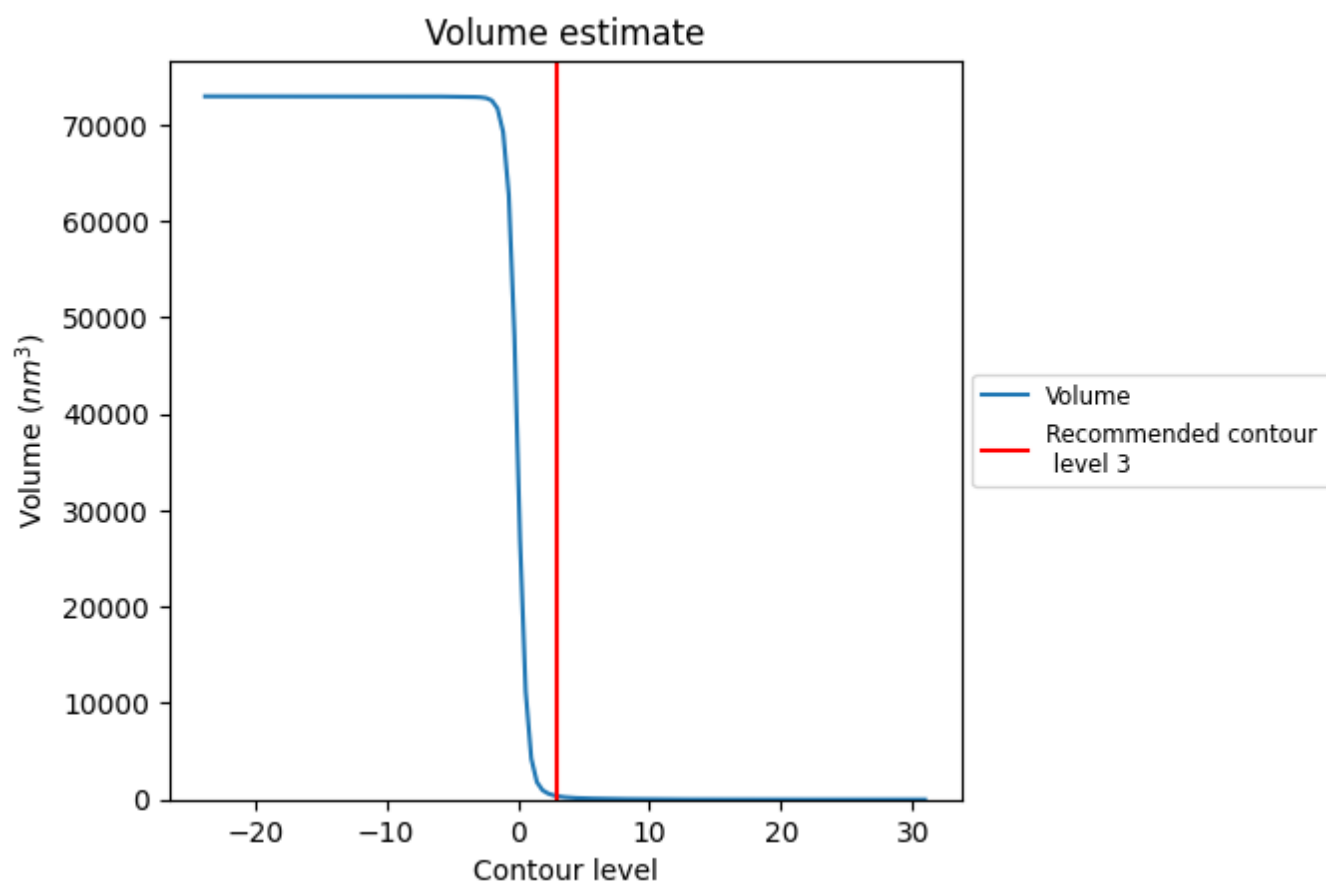
This section contains the results of statistical analysis of the map.

### 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.

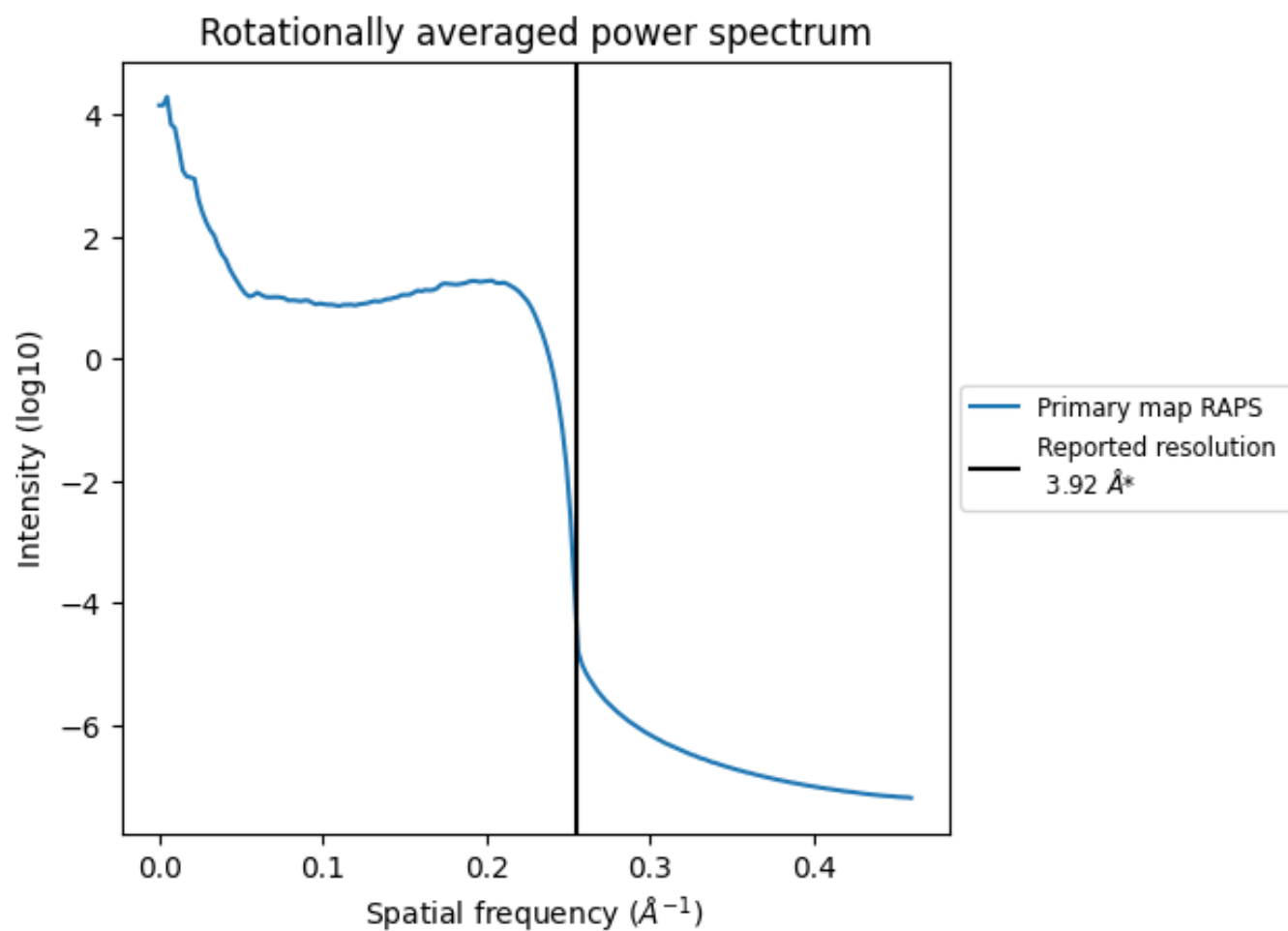
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm<sup>3</sup>; this corresponds to an approximate mass of 327 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 0.255 Å<sup>-1</sup>



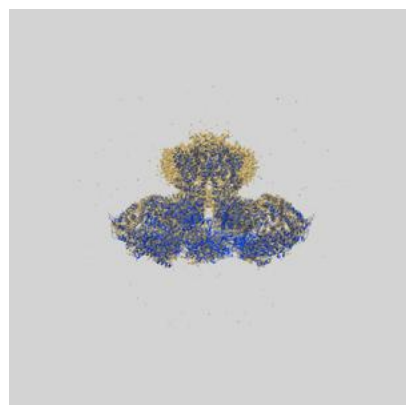
## 8 Fourier-Shell correlation

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

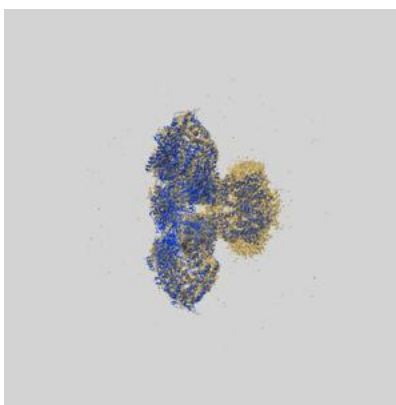
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7994 and PDB model 6DRC. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

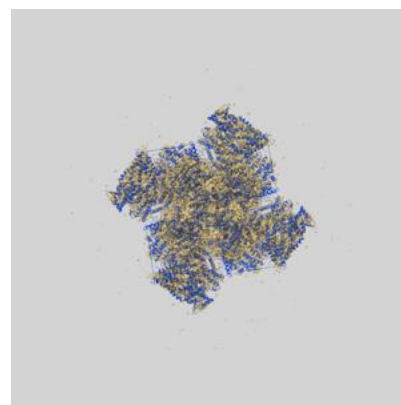
### 9.1 Map-model overlay [i](#)



X



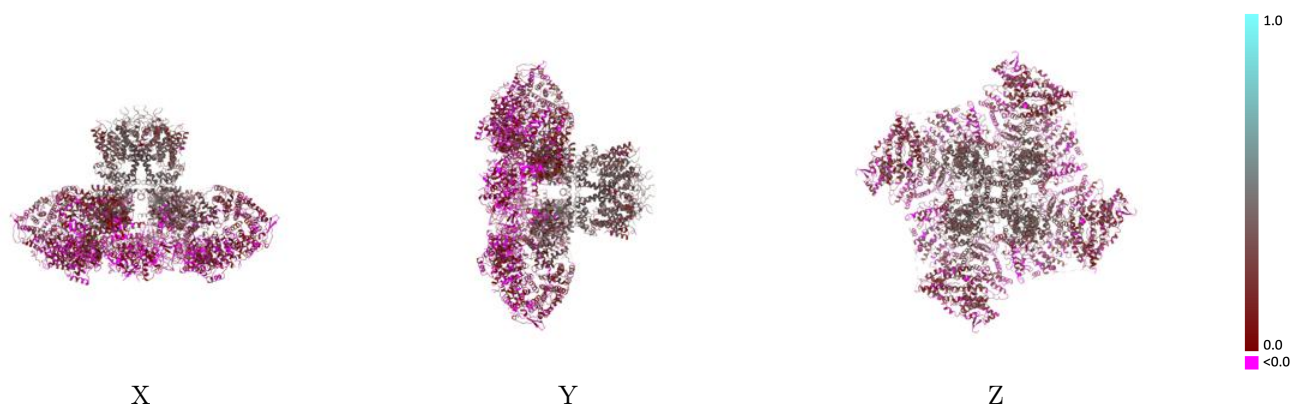
Y



Z

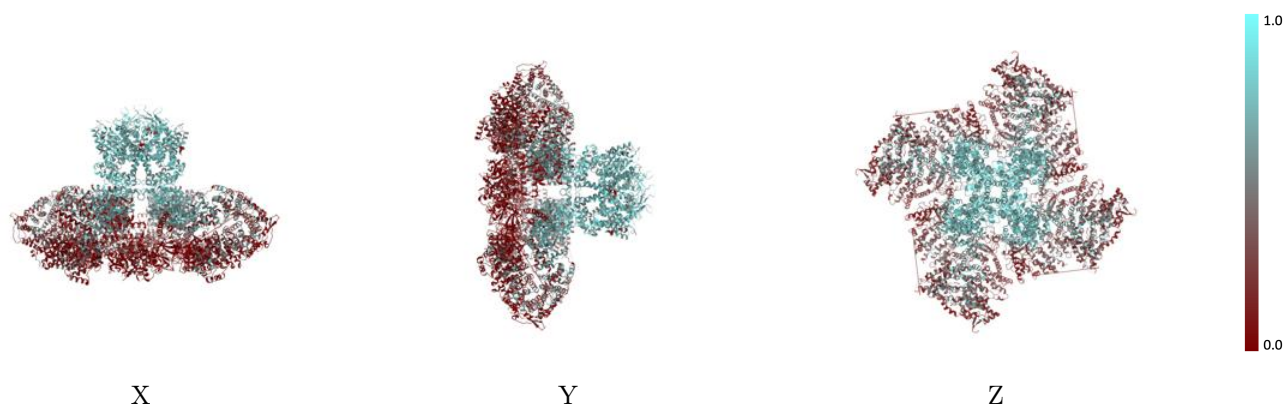
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



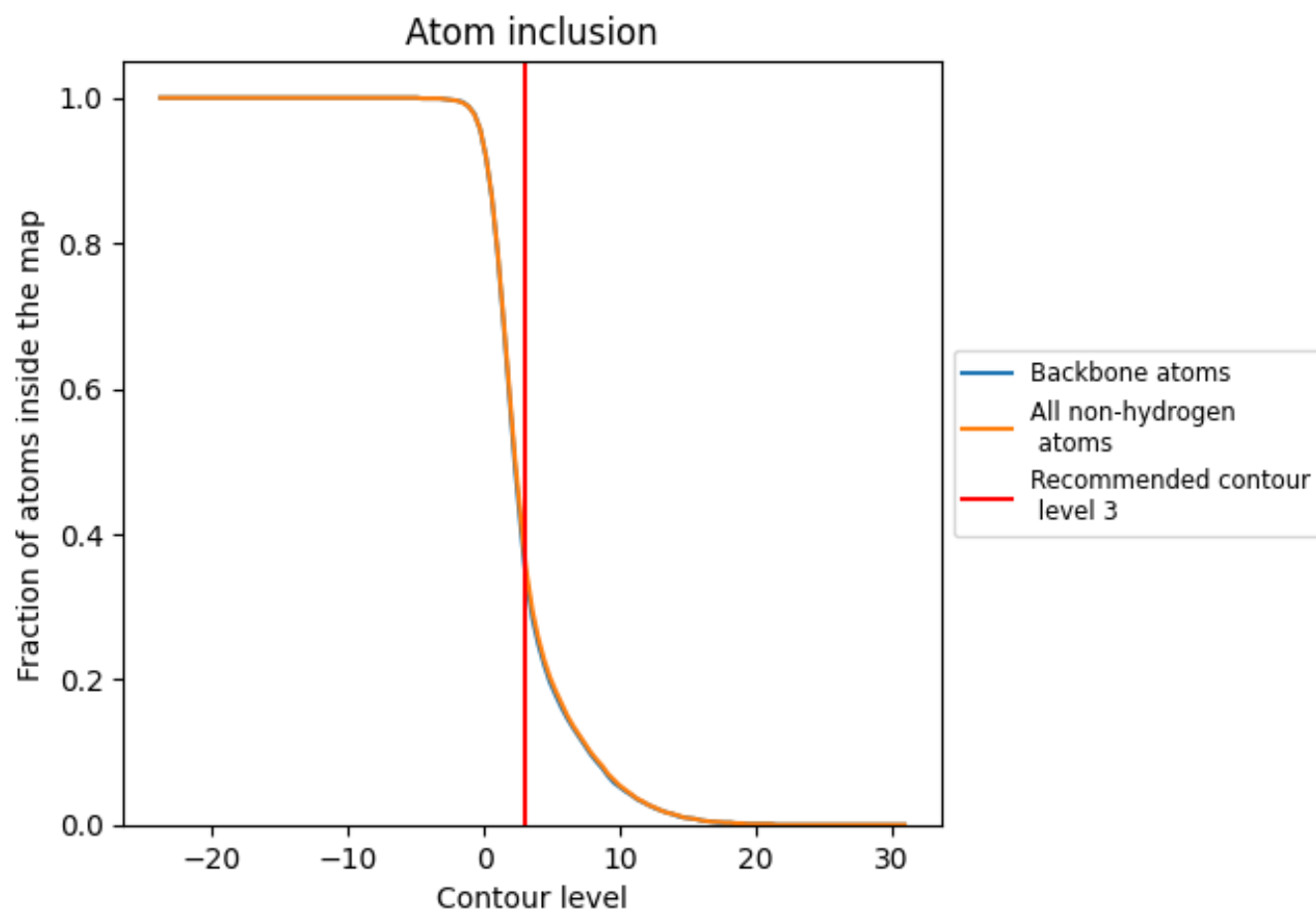
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 36% of all backbone atoms, 37% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3700	<div></div> 0.1790
A	<div></div> 0.3770	<div></div> 0.1790
B	<div></div> 0.3770	<div></div> 0.1790
C	<div></div> 0.3760	<div></div> 0.1790
D	<div></div> 0.3770	<div></div> 0.1790

