



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:52 AM UTC

PDB ID : 6WHR / pdb_00006whr
EMDB ID : EMD-21673
Title : GluN1b-GluN2B NMDA receptor in non-active 2 conformation at 4 angstrom resolution
Authors : Chou, T.; Tajima, N.; Furukawa, H.
Deposited on : 2020-04-08
Resolution : 3.99 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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

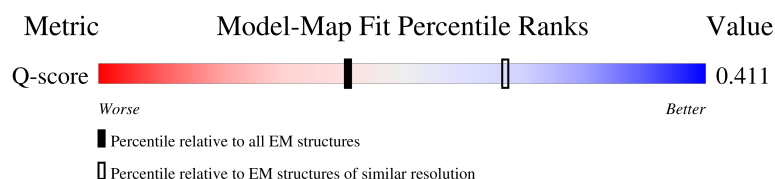
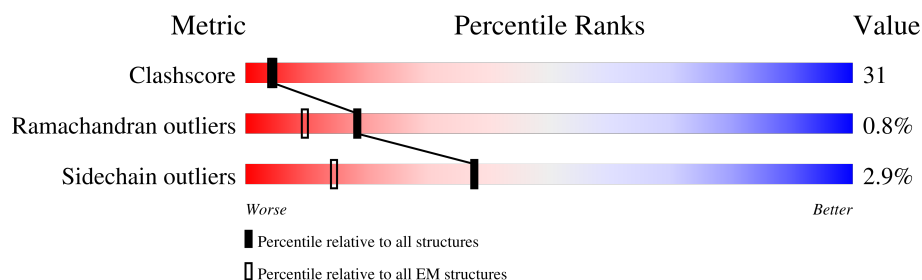
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7463 (3.49 - 4.49)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	959	
1	C	959	
2	B	883	
2	D	883	

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Mol	Chain	Length	Quality of chain
3	E	2	 50%50%
3	F	2	 50%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23370 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	799	Total	C	N	O	S	0	0
			5870	3757	980	1101	32		
1	C	799	Total	C	N	O	S	0	0
			5870	3757	980	1101	32		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	260	ASP	ASN	conflict	UNP P35439
A	371	GLN	ASN	conflict	UNP P35439
A	492	GLN	ASN	conflict	UNP P35439
A	512	GLN	ASN	conflict	UNP P35439
A	615	GLN	GLU	conflict	UNP P35439
A	616	SER	GLU	conflict	UNP P35439
A	618	SER	GLU	conflict	UNP P35439
A	619	THR	GLU	conflict	UNP P35439
A	792	GLN	ASN	conflict	UNP P35439
A	831	CYS	PHE	conflict	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	260	ASP	ASN	conflict	UNP P35439
C	371	GLN	ASN	conflict	UNP P35439
C	492	GLN	ASN	conflict	UNP P35439
C	512	GLN	ASN	conflict	UNP P35439
C	615	GLN	GLU	conflict	UNP P35439
C	616	SER	GLU	conflict	UNP P35439
C	618	SER	GLU	conflict	UNP P35439
C	619	THR	GLU	conflict	UNP P35439
C	792	GLN	ASN	conflict	UNP P35439
C	831	CYS	PHE	conflict	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	784	Total	C	N	O	S	0	0
			5717	3679	927	1078	33		
2	D	784	Total	C	N	O	S	0	0
			5717	3679	927	1078	33		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	expression tag	UNP Q00960
B	-29	GLY	-	expression tag	UNP Q00960
B	-28	THR	-	expression tag	UNP Q00960
B	-27	MET	-	expression tag	UNP Q00960
B	-26	ARG	-	expression tag	UNP Q00960
B	-25	LEU	-	expression tag	UNP Q00960
B	-24	PHE	-	expression tag	UNP Q00960
B	-23	LEU	-	expression tag	UNP Q00960
B	-22	LEU	-	expression tag	UNP Q00960
B	-21	ALA	-	expression tag	UNP Q00960
B	-20	VAL	-	expression tag	UNP Q00960
B	-19	LEU	-	expression tag	UNP Q00960
B	-18	PHE	-	expression tag	UNP Q00960
B	-17	LEU	-	expression tag	UNP Q00960
B	-16	PHE	-	expression tag	UNP Q00960
B	-15	SER	-	expression tag	UNP Q00960
B	-14	PHE	-	expression tag	UNP Q00960
B	-13	ALA	-	expression tag	UNP Q00960
B	-12	ARG	-	expression tag	UNP Q00960
B	-11	ALA	-	expression tag	UNP Q00960
B	-10	THR	-	expression tag	UNP Q00960
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960
B	26	GLY	-	expression tag	UNP Q00960
B	348	ASP	ASN	conflict	UNP Q00960
B	557	CYS	ASP	conflict	UNP Q00960
B	588	SER	CYS	conflict	UNP Q00960
B	838	SER	CYS	conflict	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-30	MET	-	expression tag	UNP Q00960
D	-29	GLY	-	expression tag	UNP Q00960
D	-28	THR	-	expression tag	UNP Q00960
D	-27	MET	-	expression tag	UNP Q00960
D	-26	ARG	-	expression tag	UNP Q00960
D	-25	LEU	-	expression tag	UNP Q00960
D	-24	PHE	-	expression tag	UNP Q00960
D	-23	LEU	-	expression tag	UNP Q00960
D	-22	LEU	-	expression tag	UNP Q00960
D	-21	ALA	-	expression tag	UNP Q00960
D	-20	VAL	-	expression tag	UNP Q00960
D	-19	LEU	-	expression tag	UNP Q00960
D	-18	PHE	-	expression tag	UNP Q00960
D	-17	LEU	-	expression tag	UNP Q00960
D	-16	PHE	-	expression tag	UNP Q00960

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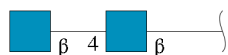
Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP Q00960
D	-14	PHE	-	expression tag	UNP Q00960
D	-13	ALA	-	expression tag	UNP Q00960
D	-12	ARG	-	expression tag	UNP Q00960
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960

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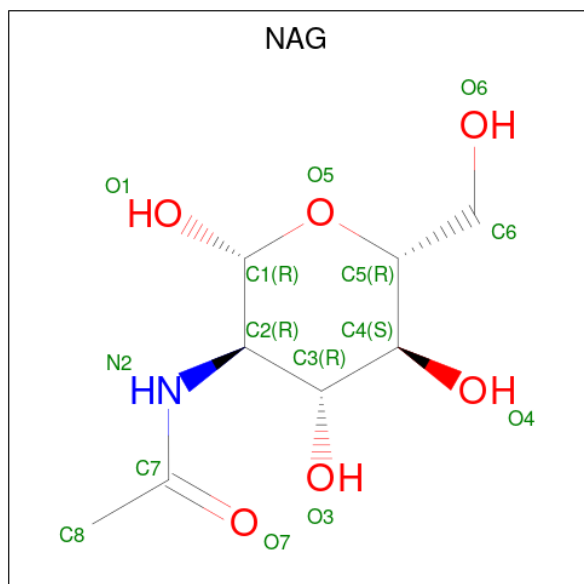
Chain	Residue	Modelled	Actual	Comment	Reference
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	588	SER	CYS	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

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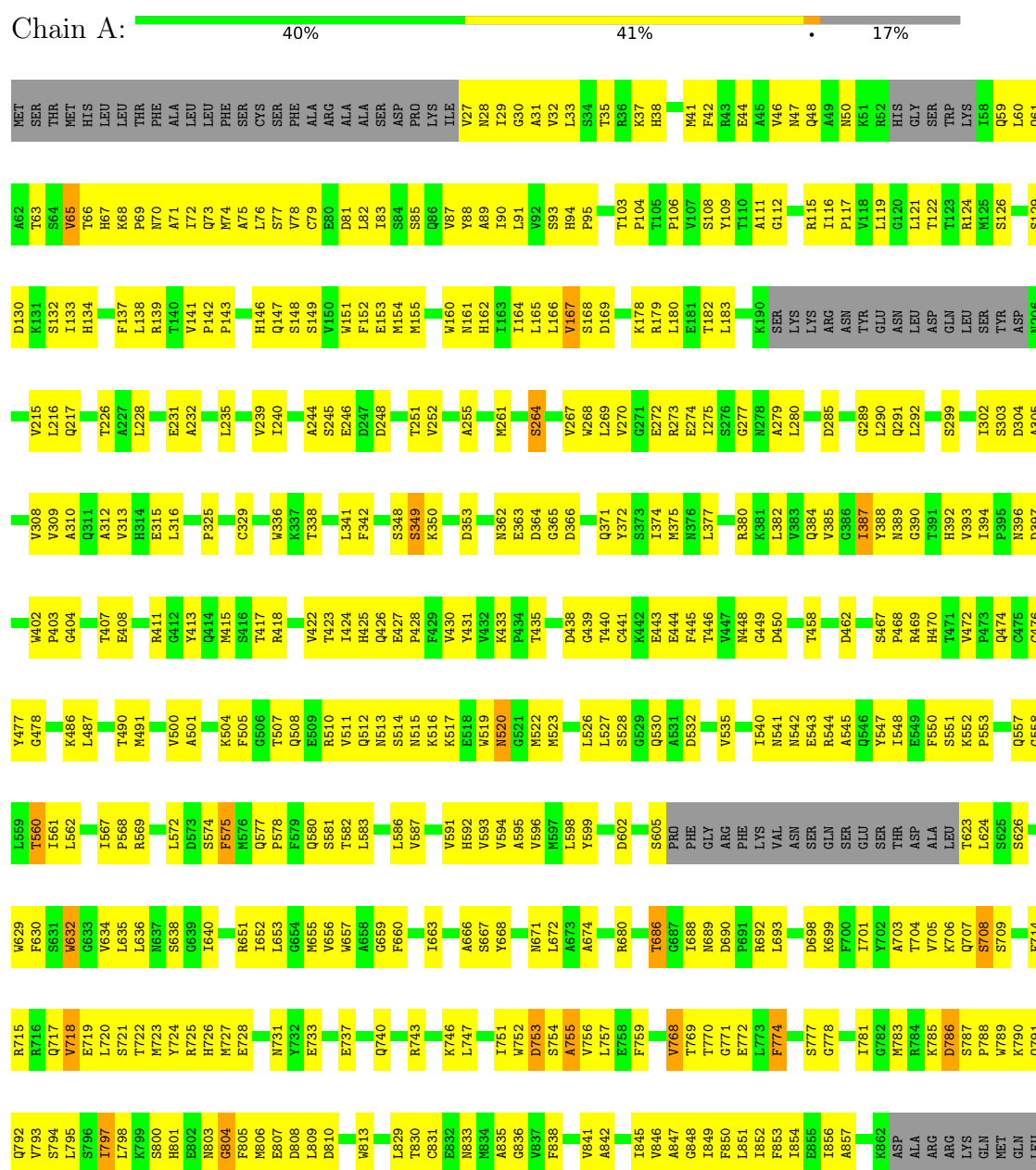
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0

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: Glutamate receptor ionotropic, NMDA 1



ASN	GLN	LYS	ASP	THR	VAL	LEU	PRO	ARG	ARG	ALA	ILE	GLU	ARG	GLU	GLU	GLY	GLN	LEU	GLN	LEU	LEU	CYS	SER	ARG	ARG	HIS	ARG	GLU	SER
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- Molecule 1: Glutamate receptor ionotropic, NMDA 1

Chain C: 40% 41% 1% 17%

GLN	PHE	V793	F714	L624	P553	P473	N396	A305	ASP	D130	A62
LYS	ALA	S794	R715	S625	Q57	Q474	D397	V308	N206	R131	T63
ASP	ALA	L795	R716	S626	Q577	Q475	Q308	V309	N207	S132	S64
THR	VAL	S796	Q717	S627	Q578	Q476	Q402	V310	N208	I133	P65
VAL	ASN	I797	W718	W629	L559	Q477	Q403	A310	N209	H134	H13
LEU	VAL	L798	E719	F630	T560	Q478	Q404	Q311	N210	L135	H67
PRO	TRP	R799	L720	S631	L561			A312	N211	S136	K68
ARG	ARG	S800	S721	W632	L562	K486	T407	V312	N212	F137	P69
ARG	LYS	H801	T722	G633	L563	L487	E408	H314	A227	L138	PHE
ALA	ASN	E902	M723	V634	L564			E315	N228	R139	ALA
ILE	LEU	N803	R724	L635	L565	T490	R411	L316	N229	T140	LEU
GLU	GLN	G804	W725	L636	L566	M491	G412		N230	V141	Q73
ARG	ASP	F805	H726	W637	L567		V413	P325	N231	P142	M74
GLU	ARG	M806	M727	S638	L568		Q414		A232	M143	LEU
GLU	LYS	E807	E728	G639	L569	A501	M415		N233	W146	LEU
GLY	SER	D808		I640	S574		S416		N234	A75	SER
GLN	GLY	L809	N731	P575	S575	K504	T417	W336	N235	H146	PHE
LEU	ARG	D810	W732	R651	W576	F505	R418	K337	N236	Q79	ALA
GLN	ALA		E733	L652	Q577	G506		T338	N237	E80	ARG
LEU	GLU	W813		L653	Q578	T507	V422		N238	D81	ALA
LEU	GLU		E737	G654	P579	Q508	T423	L341	N239	W150	ALA
CYS	PRO	L829	ASP	M655	Q580	L509	I424	F342	N240	M151	L82
SER	ASP	T830	THR	G656	Q581	R510	H425	D248	N241	F152	I83
ARG	PRO	W831	Q740	W657	S581	R511	Q426	M154	N242	M154	ASP
HIS	LYS	C831		W657	T582	V511		S348	N243	S85	PRO
ARG	LYS	E832	K746	A658	L583	Q512	E427	S349	N244	Q86	LYS
LEU	LYS	N833	L747	F660		N513	P428	W350	N245	V87	ILE
GLU	ALA	M834		G660	L586	S514	F429	F351	N246	W160	V27
ALA	THR	A835	I751	P661	L587	N515	V430	A352	N247	N161	N28
THR	PHE	G836	W752	M662	V587	K516	Y431	D353	N248	H162	I29
ARG	ARG	W837	D753	I663	V591	K517	W432	S264	N249	L91	G30
ILE	ILE	F855	A755	A666	H592	S518	K433	N362	N250	I164	A31
THR	THR	V841	W756	S667	V594	N520	T435	E363	N251	L165	S93
SER	SER	A842	L757	V668	A595	G521		D364	N252	L166	L33
THR	THR		E758		V596	M522	D438	G365	N253	V167	S34
LEU	LEU	I845	F759	R680	V597	M523	C439	D366	N254	S168	T35
ALA	ALA	V846			L598		T440		N255	D169	R36
SER	SER	A847	W768	T686	L599	L526	Q371	E272	N256	P104	K37
SER	THR	G848	T769	G687	V599	L527	Y372	E273	N257	T105	H38
PHE	PHE	I849	T770	I688	D602	L528	K442	E274	N258	P106	
LYS	LYS	F850	G771	N689		S528	E443	I374	N259	L180	M41
ARG	ARG	L851	E772	D690	S605	G528	E444	M375	N260	S108	F42
ARG	ARG		L773	P691		Q530	F445	K376	N261	Y109	R43
ARG	ARG	S852	W774	R692	PHO	A531	T446	L377	N262	T110	E44
SER	SER	I854		G693	GLY	D532	V447		N278	L183	A45
SER	SER	E855	S777	R694	GLY	B331	N448	R380	N281	G112	V46
LYS	LYS	I856	G778		PHE	V535	C449	K381	R281	K190	M47
ASP	ASP	A857					D450	L382	Y282		Q48
THR	THR		T781	D698	LYS	L540		V383	N285	LYS	Q49
SER	SER	K862	G782	K699	VAL	N541	T456	Q384		L116	
THR	THR	ASP	M783	F700	ASN	N542	C457	V385		P117	M50
GLY	GLY	ALA	W784	T701	SER	E543	T458	G386		ARG	K51
GLY	GLY	ARG	K785	A702	GLN	L544		L387		ASN	R52
GLY	GLY	ARG	D786	R703	SER	A545	D462	Y388		TYR	G120
ARG	ARG				GLU					GLU	H13
LYS	ARG	LYS	S787	V705	SER	L547		N389		ASN	GLY
GLN	GLN	THR	P788	V706	THR	L548	S467	G390		LEU	SER
ALA	ALA	MET	W789	Q707	ALA	E549	R469	T391		ASP	TRP
LEU	LEU	THR	K790	S708	ALA	F550	H470	V393		GLN	LYS
GLN	GLN	LEU	Q791	S709	LEU	S551	T471	Q393		LEU	Q59
ALA	ALA	ASP								SER	L60
										THR	L61

- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain B:



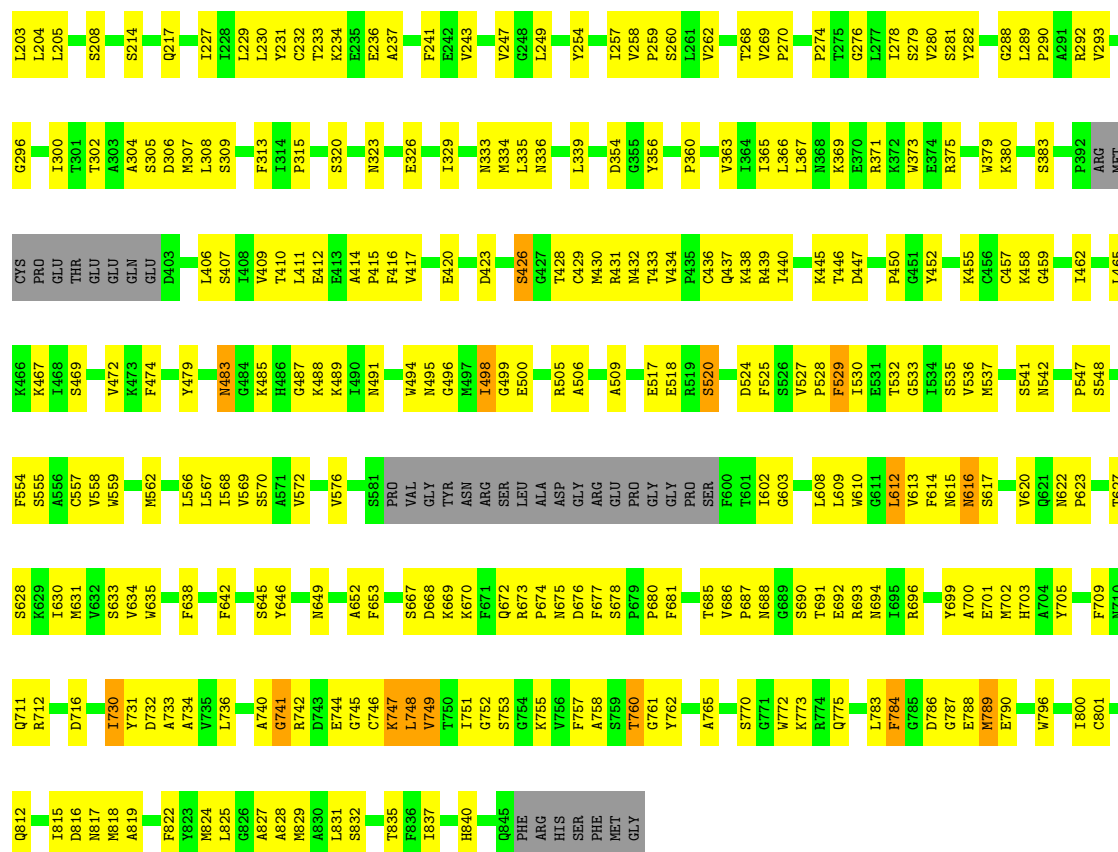
MET	LYS	I115	L203	R292	ARG	D463	S541	S617	E701	E788
GLY	SER	S116	L204	V293	MEI	I464	N542	V618	M702	M789
THR	PRO	T119	L205	G296	CYS	K467	P547	P619	H703	E790
MET	PRO	L120	S208	G296	PRO	K467	S548	V620	A704	L796
ARG	I35	I123	S214	I300	THR	S469	L551	T627	F705	M796
PHE	G36	I124	T201	T302	GLU	V472	F554	S628	F709	I800
LEU	I37	G125	T302	A304	GLN	K473	F554	K629	H710	C801
LEU	V39	I126	A304	S305	D403	F474	C557	L630	R711	Q812
ALA	I40	G129	T227	D306	D403	Y479	W558	M631	R712	L813
VAL	L41	S130	I228	M307	L406	M483	W559	V634	D716	D814
LEU	T44	S131	L229	L308	S407	G484	M562	W635	I730	I815
PHE	S45	M134	L230	F313	I408	K485	L566	F638	Y731	D816
LEU	S45	M134	Y231	F313	T410	H486	I568	I641	D732	M817
SER	D46	E47	T233	P315	T410	K488	V569	F642	A733	M818
PHE	E47	D138	K234	P315	E412	K489	S570	S645	L736	A819
ALA	V48	E139	E235	S320	E413	K490	V572	I646	A740	F822
ARG	A49	S140	E236	N323	A414	N491	V576	I655	G741	M823
ALA	I50	Q145	A237	E326	F416	W494	V576	I656	R742	M824
THR	V64	F146	F241	N323	F416	N495	V576	I656	R742	L825
GLY	V65	G147	V243	E326	V417	N495	V576	I656	R742	G826
TRP	P66	Q152	V243	E326	V417	N495	V576	I656	R742	A827
SER	R67	Q153	V243	E326	V417	N495	V576	I656	R742	A828
HIS	L70	A154	V243	E326	V417	N495	V576	I656	R742	M829
PRO	V71	S155	V243	E326	V417	N495	V576	I656	R742	A830
GLN	D77	V156	V243	E326	V417	N495	V576	I656	R742	L831
PHE	P78	M157	V243	E326	V417	N495	V576	I656	R742	S832
GLY	K79	L158	V243	E326	V417	N495	V576	I656	R742	L833
GLY	S80	F169	V243	E326	V417	N495	V576	I656	R742	T834
SER	I81	S170	V243	E326	V417	N495	V576	I656	R742	T835
GLY	I82	I171	V243	E326	V417	N495	V576	I656	R742	F836
GLY	T83	V172	V243	E326	V417	N495	V576	I656	R742	T837
SER	R84	T173	V243	E326	V417	N495	V576	I656	R742	H840
GLY	I85	T174	V243	E326	V417	N495	V576	I656	R742	Q845
SER	L88	Y175	V243	E326	V417	N495	V576	I656	R742	PHE
GLY	R92	P177	V243	E326	V417	N495	V576	I656	R742	ARG
ALA	K93	G178	V243	E326	V417	N495	V576	I656	R742	HIS
TRP	I94	Y179	V243	E326	V417	N495	V576	I656	R742	ALA
SER	Q95	Q180	V243	E326	V417	N495	V576	I656	R742	TRP
HIS	V97	D181	V243	E326	V417	N495	V576	I656	R742	SER
GLN	V98	F182	V243	E326	V417	N495	V576	I656	R742	GLY
GLU	F99	V183	V243	E326	V417	N495	V576	I656	R742	GLY
PHE	V99	N184	V243	E326	V417	N495	V576	I656	R742	GLY
GLU	F99	N184	V243	E326	V417	N495	V576	I656	R742	GLY
LYS	D101	R187	V243	E326	V417	N495	V576	I656	R742	GLY
ALA	D102	I190	V243	E326	V417	N495	V576	I656	R742	GLY
LEU	I108	S193	V243	E326	V417	N495	V576	I656	R742	GLY
VAL	A109	L199	V243	E326	V417	N495	V576	I656	R742	GLY
PRO	Q110	E200	V243	E326	V417	N495	V576	I656	R742	GLY
ARG	I111	L199	V243	E326	V417	N495	V576	I656	R742	GLY
GLY	L112	E201	V243	E326	V417	N495	V576	I656	R742	GLY
ARG	D113	F114	V243	E326	V417	N495	V576	I656	R742	GLY
SER	E201	V202	V243	E326	V417	N495	V576	I656	R742	GLY
GLN	F114	V202	V243	E326	V417	N495	V576	I656	R742	GLY

- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:



MET	LYS	S116	E701	E788
GLY	SER	T119	M702	M789
THR	PRO	L120	H703	E790
MET	PRO	I123	A704	L796
ARG	S34	I124	F705	M796
LEU	I35	G125	F709	I800
PHE	G36	I126	R710	C801
LEU	I37	G127	H711	Q812
LEU	A38	H127	R712	L813
ALA	V39	I128	R712	I814
VAL	I40	G129	D716	I815
LEU	L41	S130	I730	D816
PHE	T44	S131	Y731	M817
LEU	S45	M132	D732	M818
PHE	S45	M132	A733	A819
SER	D46	M134	L736	F822
PHE	E47	D138	A740	Y823
ALA	V48	E139	R742	M824
ARG	A49	S140	R742	L825
ALA	I50	Q145	R742	G826
THR	V64	F146	R742	A827
GLY	V65	G147	R742	A828
TRP	P66	Q152	R742	M829
SER	R67	Q153	R742	A830
HIS	L70	A154	R742	L831
PRO	V71	S155	R742	S832
GLN	D77	V156	R742	L833
PHE	P78	M157	R742	T834
GLY	K79	L158	R742	T835
GLY	S80	F169	R742	F836
SER	I81	S170	R742	T837
GLY	I82	I171	R742	H840
GLY	T83	V172	R742	Q845
SER	R84	T173	R742	PHE
GLY	I85	T174	R742	ARG
SER	L88	Y175	R742	HIS
GLY	R92	P177	R742	ALA
ALA	K93	G178	R742	TRP
TRP	I94	Y179	R742	SER
SER	Q95	Q180	R742	PHE
HIS	V97	D181	R742	MET
GLN	V98	F182	R742	GLY
GLU	F99	V183	R742	
GLU	N184	N184	R742	
LYS	D101	R187	R742	
ALA	D102	I190	R742	
LEU	I108	S193	R742	
VAL	A109	L199	R742	
PRO	Q110	E200	R742	
ARG	I111	L199	R742	
GLY	L112	E201	R742	
ARG	D113	F114	R742	
SER	E201	V202	R742	
GLN	F114	V202	R742	



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	134688	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 ($e^-/\text{\AA}^2$)	64.5	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	18.999	Depositor
Minimum map value	-8.082	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.684	Depositor
Recommended contour level	2.3	Depositor
Map size ($\text{\AA}$)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.74	1/5996 (0.0%)	0.73	0/8192
1	C	0.74	1/5996 (0.0%)	0.73	0/8192
2	B	0.68	2/5835 (0.0%)	0.70	3/7968 (0.0%)
2	D	0.68	2/5835 (0.0%)	0.70	3/7968 (0.0%)
All	All	0.71	6/23662 (0.0%)	0.72	6/32320 (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	2
1	C	0	2
2	B	0	2
2	D	0	2
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	755	ALA	CA-C	-8.24	1.41	1.52
1	C	755	ALA	CA-C	-8.21	1.41	1.52
2	D	520	SER	CA-C	-6.65	1.43	1.52
2	B	520	SER	CA-C	-6.61	1.44	1.52
2	B	789	MET	CA-C	-5.32	1.40	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	747	LYS	CA-C-N	-6.33	114.05	121.64
2	D	747	LYS	C-N-CA	-6.33	114.05	121.64
2	B	747	LYS	CA-C-N	-6.29	114.09	121.64
2	B	747	LYS	C-N-CA	-6.29	114.09	121.64
2	D	529	PHE	CB-CA-C	-5.26	103.02	111.39

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	426	GLN	Peptide
1	A	774	PHE	Peptide
2	B	429	CYS	Peptide
2	B	748	LEU	Peptide
1	C	426	GLN	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	5870	0	5528	412	0
1	C	5870	0	5528	407	0
2	B	5717	0	5359	319	0
2	D	5717	0	5359	302	0
3	E	28	0	25	1	0
3	F	28	0	25	1	0
4	A	28	0	26	0	0
4	B	42	0	39	1	0
4	C	28	0	26	0	0
4	D	42	0	39	1	0
All	All	23370	0	21954	1400	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 31.

The worst 5 of 1400 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:C:149:SER:HB2	1:C:179:ARG:HH21	1.33	0.93
1:A:149:SER:HB2	1:A:179:ARG:HH21	1.32	0.93
1:A:511:VAL:HG13	1:A:512:GLN:HG3	1.52	0.92
1:C:511:VAL:HG13	1:C:512:GLN:HG3	1.52	0.91
1:A:574:SER:HB2	1:A:577:GLN:HE21	1.36	0.91

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	791/959 (82%)	603 (76%)	182 (23%)	6 (1%)	16	52
1	C	791/959 (82%)	604 (76%)	181 (23%)	6 (1%)	16	52
2	B	778/883 (88%)	620 (80%)	151 (19%)	7 (1%)	14	48
2	D	778/883 (88%)	620 (80%)	151 (19%)	7 (1%)	14	48
All	All	3138/3684 (85%)	2447 (78%)	665 (21%)	26 (1%)	18	52

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	749	VAL
2	D	749	VAL
1	A	581	SER
2	B	431	ARG
1	C	581	SER

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	587/826 (71%)	565 (96%)	22 (4%)	30	52
1	C	587/826 (71%)	565 (96%)	22 (4%)	30	52
2	B	571/762 (75%)	559 (98%)	12 (2%)	47	65
2	D	571/762 (75%)	559 (98%)	12 (2%)	47	65
All	All	2316/3176 (73%)	2248 (97%)	68 (3%)	38	58

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	140	SER
2	D	426	SER
2	D	730	ILE
2	B	146	PHE
2	B	140	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	577	GLN
2	D	159	ASN
2	D	840	HIS
2	D	486	HIS
1	C	740	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 ⓘ

4 monosaccharides are modelled in this entry.

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	NAG	E	1	2,3	14,14,15	0.89	1 (7%)	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
3	NAG	F	1	2,3	14,14,15	0.90	1 (7%)	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.59	0	17,19,21	1.35	2 (11%)

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	NAG	E	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	6/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-3.25	1.38	1.43
3	E	1	NAG	O5-C1	-3.22	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C2-N2-C7	4.51	128.95	122.90
3	E	2	NAG	C2-N2-C7	4.51	128.94	122.90
3	E	2	NAG	C1-C2-N2	2.34	114.12	110.43
3	F	2	NAG	C1-C2-N2	2.34	114.11	110.43

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

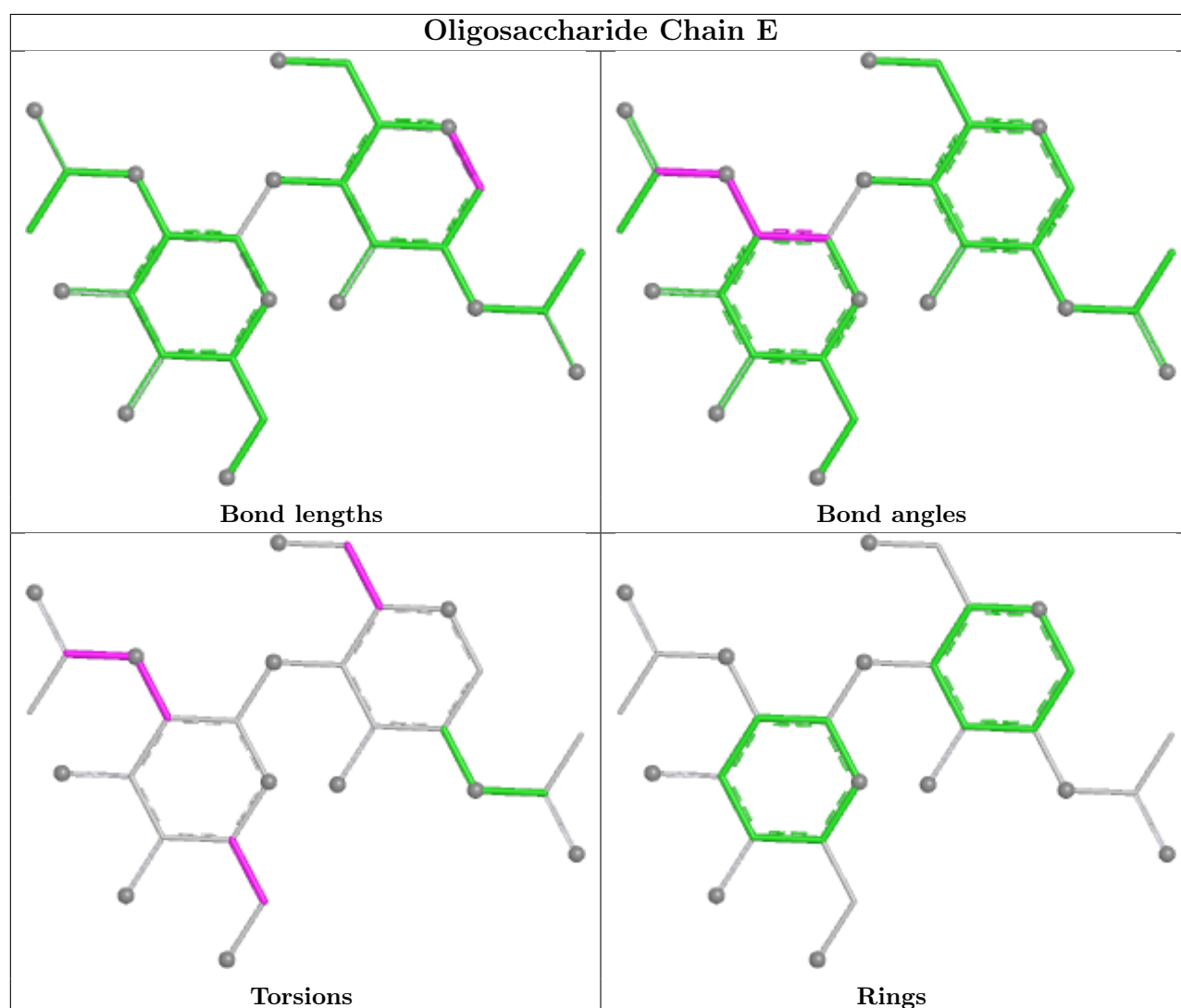
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

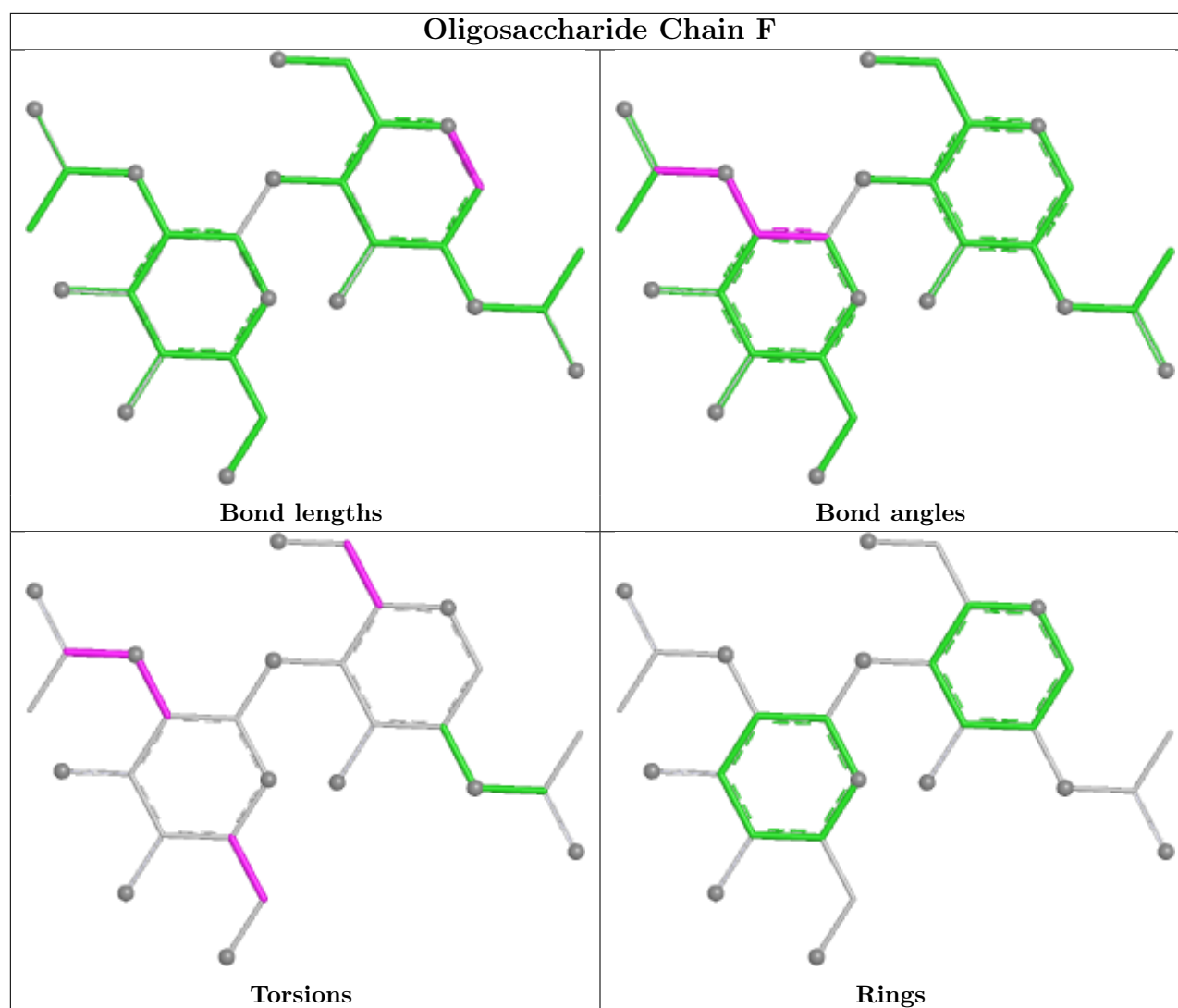
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	E	2	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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	$\# Z > 2$
4	NAG	B	904	2	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	A	1002	1	14,14,15	0.39	0	17,19,21	0.38	0
4	NAG	C	1002	1	14,14,15	0.39	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	905	2	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	A	1001	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	D	903	2	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	D	904	2	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	B	905	2	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	B	903	2	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	C	1001	1	14,14,15	0.34	0	17,19,21	0.51	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
4	NAG	B	904	2	-	3/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	D	905	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	D	903	2	-	2/6/23/26	0/1/1/1
4	NAG	D	904	2	-	3/6/23/26	0/1/1/1
4	NAG	B	905	2	-	1/6/23/26	0/1/1/1
4	NAG	B	903	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	O5-C5-C6-O6
4	C	1002	NAG	O5-C5-C6-O6
4	B	904	NAG	C4-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6
4	B	903	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	905	NAG	1	0
4	B	905	NAG	1	0

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.

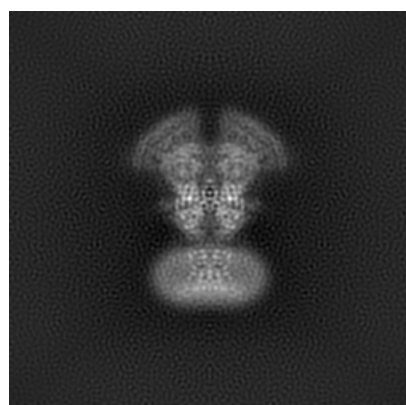
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21673. These allow visual inspection of the internal detail of the map and identification of artifacts.

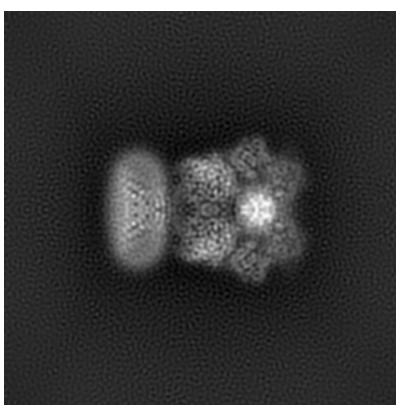
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

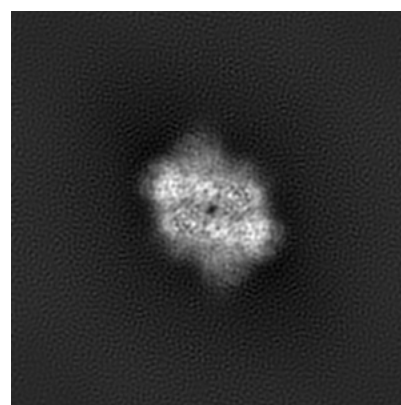
6.1.1 Primary map



X



Y

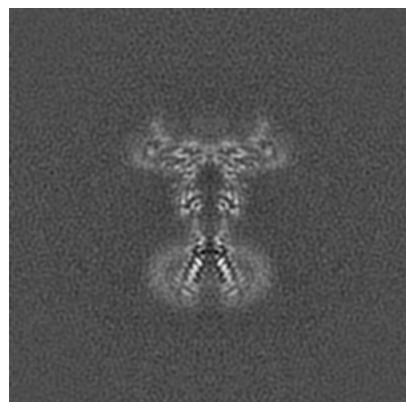


Z

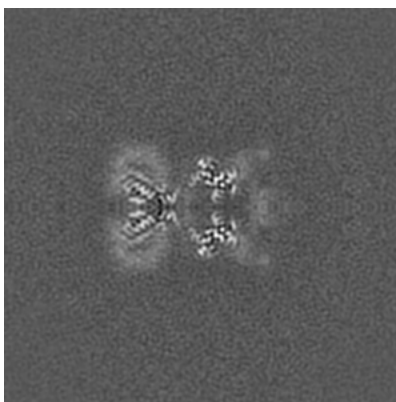
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

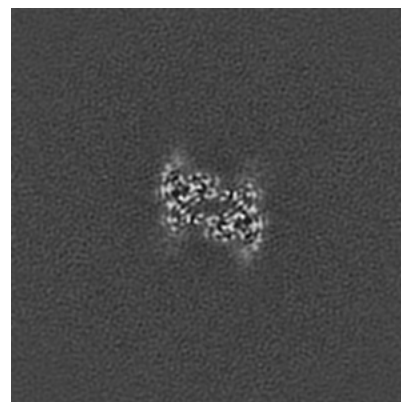
6.2.1 Primary map



X Index: 128



Y Index: 128

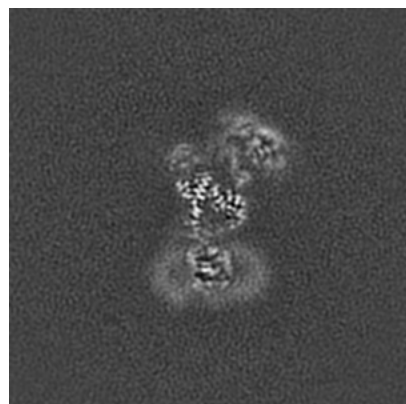


Z Index: 128

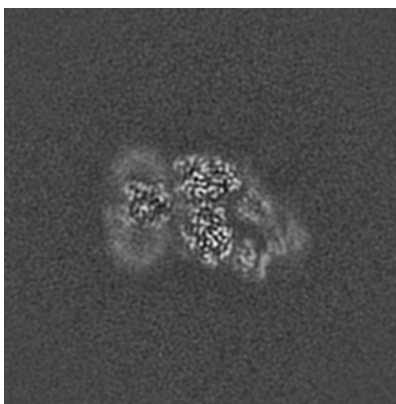
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

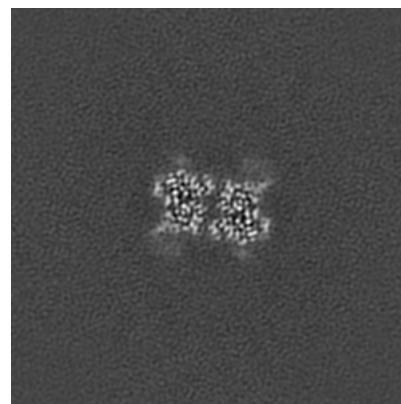
6.3.1 Primary map



X Index: 117



Y Index: 137

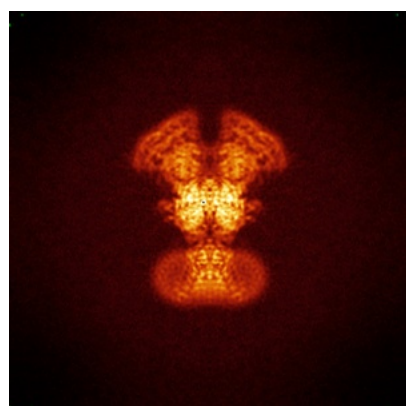


Z Index: 135

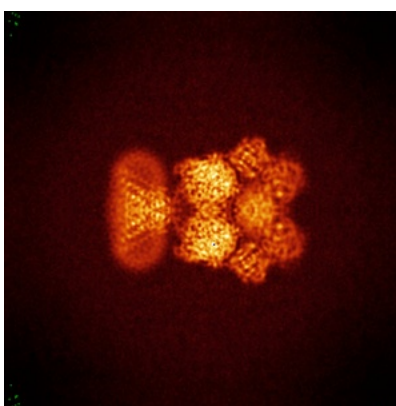
The images above show the largest variance slices of the map in three orthogonal directions.

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

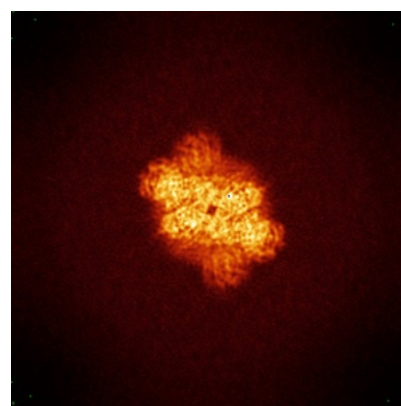
6.4.1 Primary map



X



Y



Z

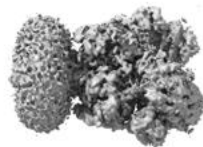
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

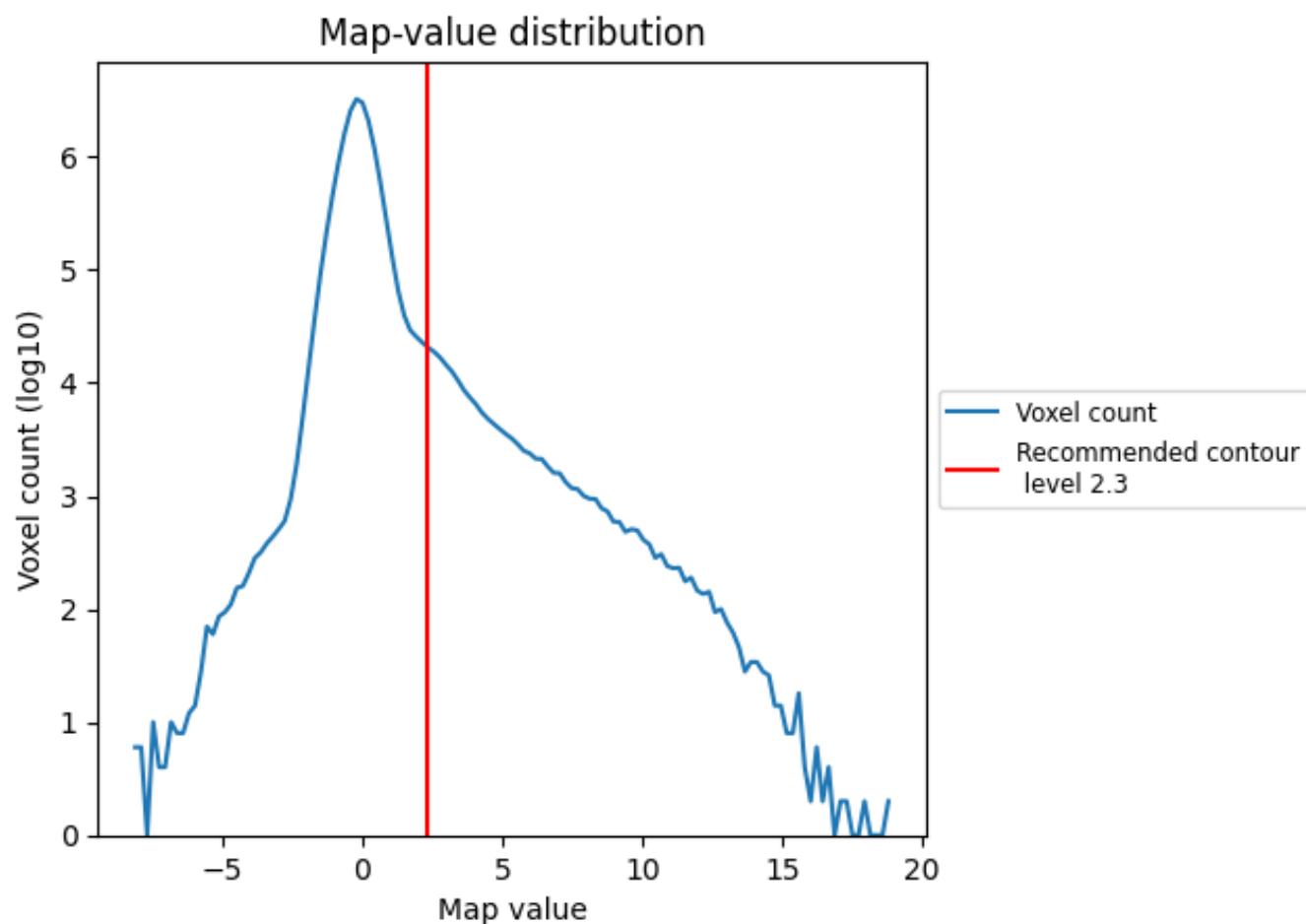
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

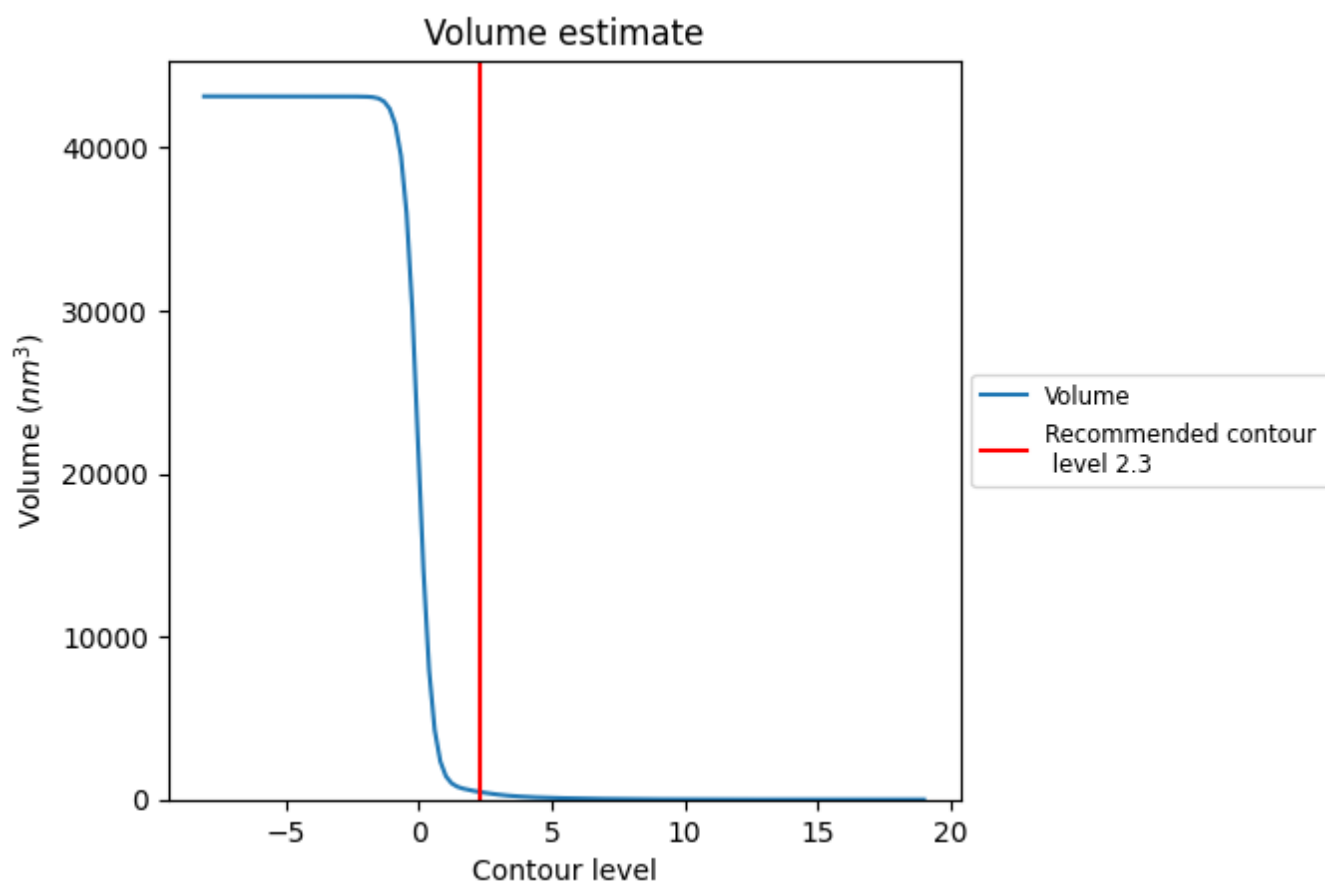
This section contains the results of statistical analysis of the map.

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.

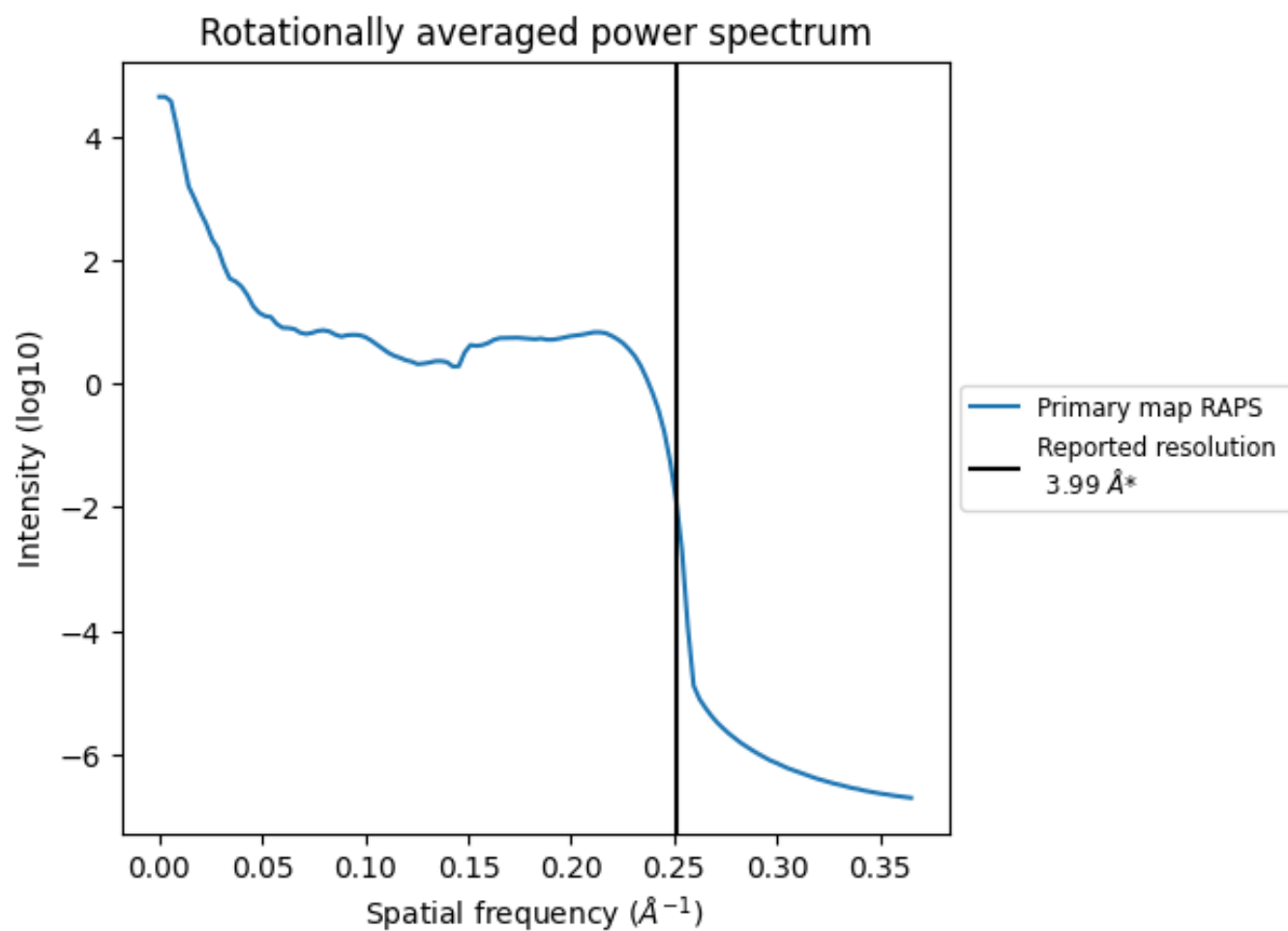
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 463 nm^3 ; this corresponds to an approximate mass of 418 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8 Fourier-Shell correlation

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

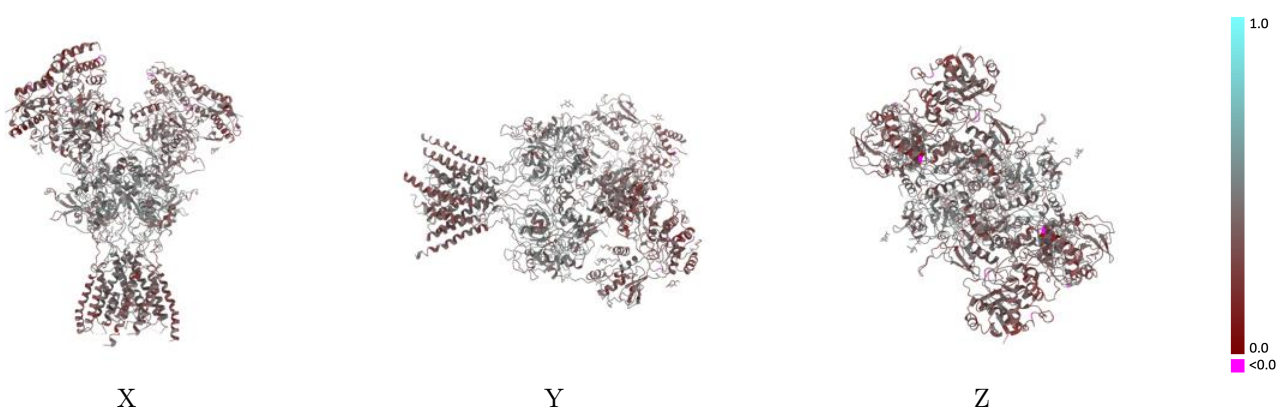
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21673 and PDB model 6WHR. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

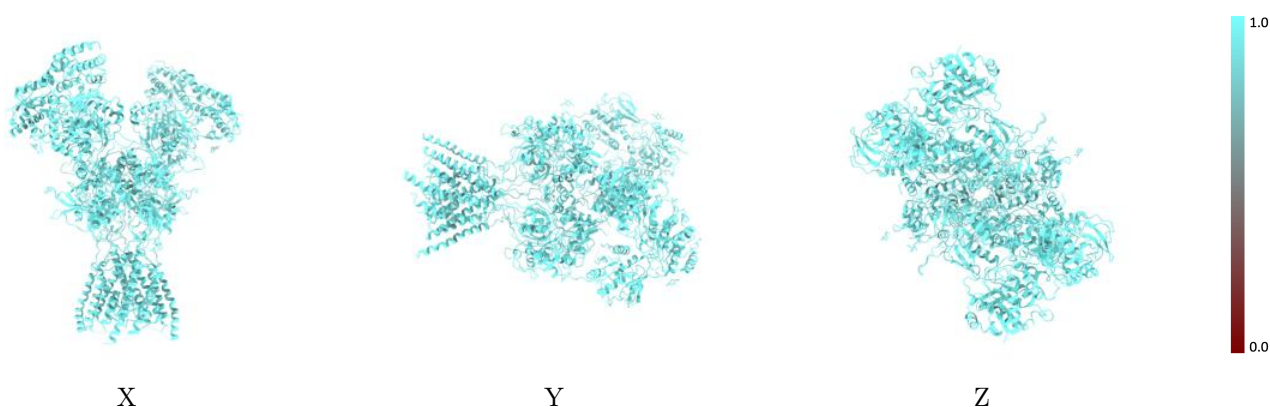
This section was not generated.

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



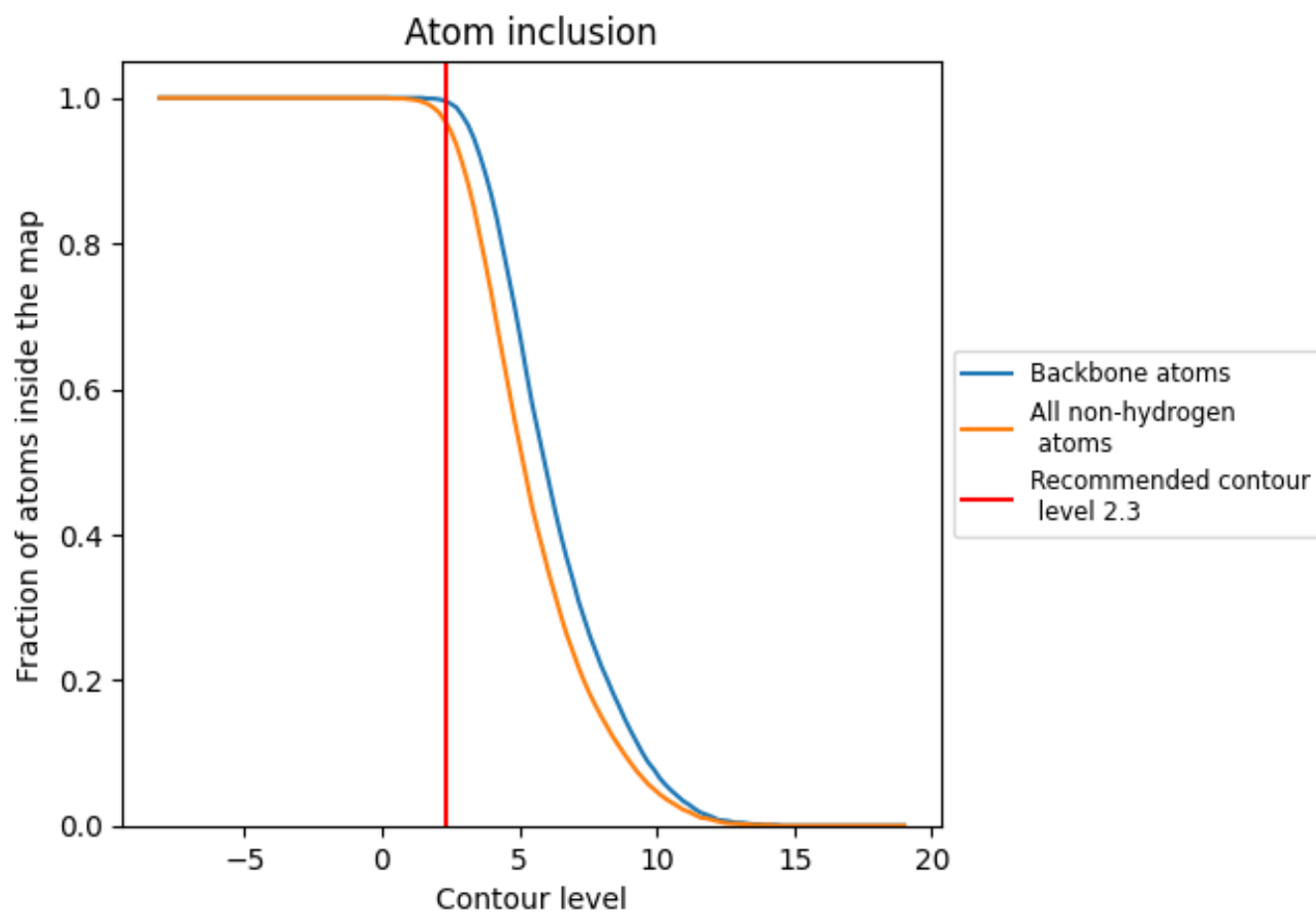
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9680	0.4110
A	0.9710	0.4130
B	0.9650	0.4100
C	0.9730	0.4130
D	0.9650	0.4100
E	1.0000	0.4630
F	0.9640	0.4700

1.0

0.0

<0.0