Full wwPDB EM Validation Report (i)

Feb 5, 2026 – 10:48 pm GMT

PDB ID	:	9U0N / pdb_00009u0n
EMDB ID	:	EMD-56497
Title	:	Wild type human T cell receptor in detergent
Deposited on	:	2026-01-27
Resolution	:	3.33 Å(reported)
Based on initial model	:	9U0K

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev129
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)

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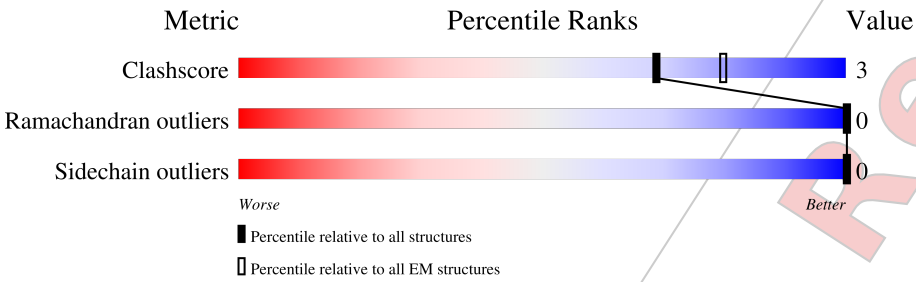
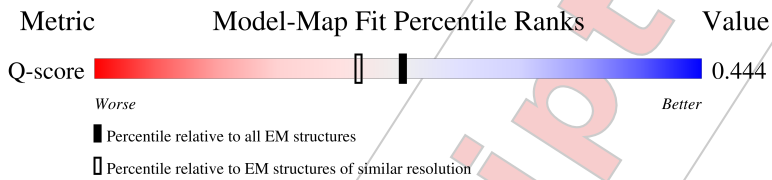
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14484 (2.83 - 3.83)

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 <=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	251	9% 89% 8% •
2	B	318	6% 81% 8% 11%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

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Mol	Chain	Length	Quality of chain
3	C	145	6% 69% 10% 21%
4	D	135	71% 9% 20%
5	E	158	6% 72% 6% 22%
5	e	158	9% 72% 6% 22%
6	Z	110	28% 69%
6	z	110	23% 74%

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2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8527 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 GPabWT T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	243	1898	1183	327	379	9	0	0

- Molecule 2 is a protein called GPabWT T cell receptor beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	284	2247	1431	379	428	9	0	0

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	114	899	578	149	165	7	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	123	LYS	-	expression tag	UNP P09693
C	124	LEU	-	expression tag	UNP P09693
C	125	GLY	-	expression tag	UNP P09693
C	126	SER	-	expression tag	UNP P09693
C	127	GLY	-	expression tag	UNP P09693
C	128	ALA	-	expression tag	UNP P09693
C	129	THR	-	expression tag	UNP P09693
C	130	ASN	-	expression tag	UNP P09693
C	131	PHE	-	expression tag	UNP P09693
C	132	SER	-	expression tag	UNP P09693
C	133	LEU	-	expression tag	UNP P09693
C	134	LEU	-	expression tag	UNP P09693
C	135	LYS	-	expression tag	UNP P09693
C	136	GLN	-	expression tag	UNP P09693
C	137	ALA	-	expression tag	UNP P09693

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Chain	Residue	Modelled	Actual	Comment	Reference
C	138	GLY	-	expression tag	UNP P09693
C	139	ASP	-	expression tag	UNP P09693
C	140	VAL	-	expression tag	UNP P09693
C	141	GLU	-	expression tag	UNP P09693
C	142	GLU	-	expression tag	UNP P09693
C	143	ASN	-	expression tag	UNP P09693
C	144	PRO	-	expression tag	UNP P09693
C	145	GLY	-	expression tag	UNP P09693

- Molecule 4 is a protein called T-cell surface glycoprotein CD3 delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	108	840	534	140	160	6	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	112	GLY	-	expression tag	UNP P04234
D	113	THR	-	expression tag	UNP P04234
D	114	GLY	-	expression tag	UNP P04234
D	115	SER	-	expression tag	UNP P04234
D	116	GLY	-	expression tag	UNP P04234
D	117	GLN	-	expression tag	UNP P04234
D	118	CYS	-	expression tag	UNP P04234
D	119	THR	-	expression tag	UNP P04234
D	120	ASN	-	expression tag	UNP P04234
D	121	TYR	-	expression tag	UNP P04234
D	122	ALA	-	expression tag	UNP P04234
D	123	LEU	-	expression tag	UNP P04234
D	124	LEU	-	expression tag	UNP P04234
D	125	LYS	-	expression tag	UNP P04234
D	126	LEU	-	expression tag	UNP P04234
D	127	ALA	-	expression tag	UNP P04234
D	128	GLY	-	expression tag	UNP P04234
D	129	ASP	-	expression tag	UNP P04234
D	130	VAL	-	expression tag	UNP P04234
D	131	GLU	-	expression tag	UNP P04234
D	132	SER	-	expression tag	UNP P04234
D	133	ASN	-	expression tag	UNP P04234
D	134	PRO	-	expression tag	UNP P04234
D	135	GLY	-	expression tag	UNP P04234

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- Molecule 5 is a protein called T-cell surface glycoprotein CD3 epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	123	978	619	157	194	8	0	0
5	e	124	987	625	159	195	8	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	137	GLY	-	expression tag	UNP P07766
E	138	PRO	-	expression tag	UNP P07766
E	139	GLY	-	expression tag	UNP P07766
E	140	SER	-	expression tag	UNP P07766
E	141	GLY	-	expression tag	UNP P07766
E	142	GLU	-	expression tag	UNP P07766
E	143	GLY	-	expression tag	UNP P07766
E	144	ARG	-	expression tag	UNP P07766
E	145	GLY	-	expression tag	UNP P07766
E	146	SER	-	expression tag	UNP P07766
E	147	LEU	-	expression tag	UNP P07766
E	148	LEU	-	expression tag	UNP P07766
E	149	THR	-	expression tag	UNP P07766
E	150	CYS	-	expression tag	UNP P07766
E	151	GLY	-	expression tag	UNP P07766
E	152	ASP	-	expression tag	UNP P07766
E	153	VAL	-	expression tag	UNP P07766
E	154	GLU	-	expression tag	UNP P07766
E	155	GLU	-	expression tag	UNP P07766
E	156	ASN	-	expression tag	UNP P07766
E	157	PRO	-	expression tag	UNP P07766
E	158	GLY	-	expression tag	UNP P07766
e	137	GLY	-	expression tag	UNP P07766
e	138	PRO	-	expression tag	UNP P07766
e	139	GLY	-	expression tag	UNP P07766
e	140	SER	-	expression tag	UNP P07766
e	141	GLY	-	expression tag	UNP P07766
e	142	GLU	-	expression tag	UNP P07766
e	143	GLY	-	expression tag	UNP P07766
e	144	ARG	-	expression tag	UNP P07766
e	145	GLY	-	expression tag	UNP P07766
e	146	SER	-	expression tag	UNP P07766
e	147	LEU	-	expression tag	UNP P07766
e	148	LEU	-	expression tag	UNP P07766

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Chain	Residue	Modelled	Actual	Comment	Reference
e	149	THR	-	expression tag	UNP P07766
e	150	CYS	-	expression tag	UNP P07766
e	151	GLY	-	expression tag	UNP P07766
e	152	ASP	-	expression tag	UNP P07766
e	153	VAL	-	expression tag	UNP P07766
e	154	GLU	-	expression tag	UNP P07766
e	155	GLU	-	expression tag	UNP P07766
e	156	ASN	-	expression tag	UNP P07766
e	157	PRO	-	expression tag	UNP P07766
e	158	GLY	-	expression tag	UNP P07766

- Molecule 6 is a protein called T-cell surface glycoprotein CD3 zeta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Z	34	275	191	40	43	1	0	0
			Total	C	N	O	S		
6	z	29	235	163	34	37	1	0	0

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	37	GLY	-	expression tag	UNP P20963
Z	38	GLY	-	expression tag	UNP P20963
Z	39	SER	-	expression tag	UNP P20963
Z	40	GLY	-	expression tag	UNP P20963
Z	41	GLY	-	expression tag	UNP P20963
Z	42	SER	-	expression tag	UNP P20963
Z	43	LEU	-	expression tag	UNP P20963
Z	44	PRO	-	expression tag	UNP P20963
Z	45	GLU	-	expression tag	UNP P20963
Z	46	THR	-	expression tag	UNP P20963
Z	47	GLY	-	expression tag	UNP P20963
Z	48	GLY	-	expression tag	UNP P20963
Z	49	GLY	-	expression tag	UNP P20963
Z	50	SER	-	expression tag	UNP P20963
Z	51	GLY	-	expression tag	UNP P20963
Z	52	GLY	-	expression tag	UNP P20963
Z	53	SER	-	expression tag	UNP P20963
Z	54	GLY	-	expression tag	UNP P20963
Z	55	GLY	-	expression tag	UNP P20963
Z	56	SER	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	57	GLY	-	expression tag	UNP P20963
Z	58	GLY	-	expression tag	UNP P20963
Z	59	SER	-	expression tag	UNP P20963
Z	60	GLY	-	expression tag	UNP P20963
Z	61	GLY	-	expression tag	UNP P20963
Z	62	SER	-	expression tag	UNP P20963
Z	63	ARG	-	expression tag	UNP P20963
Z	64	GLY	-	expression tag	UNP P20963
Z	65	VAL	-	expression tag	UNP P20963
Z	66	PRO	-	expression tag	UNP P20963
Z	67	HIS	-	expression tag	UNP P20963
Z	68	ILE	-	expression tag	UNP P20963
Z	69	VAL	-	expression tag	UNP P20963
Z	70	MET	-	expression tag	UNP P20963
Z	71	VAL	-	expression tag	UNP P20963
Z	72	ASP	-	expression tag	UNP P20963
Z	73	ALA	-	expression tag	UNP P20963
Z	74	TYR	-	expression tag	UNP P20963
Z	75	LYS	-	expression tag	UNP P20963
Z	76	ARG	-	expression tag	UNP P20963
Z	77	TYR	-	expression tag	UNP P20963
Z	78	LYS	-	expression tag	UNP P20963
Z	79	GLY	-	expression tag	UNP P20963
Z	80	GLY	-	expression tag	UNP P20963
Z	81	TRP	-	expression tag	UNP P20963
Z	82	SER	-	expression tag	UNP P20963
Z	83	HIS	-	expression tag	UNP P20963
Z	84	PRO	-	expression tag	UNP P20963
Z	85	GLN	-	expression tag	UNP P20963
Z	86	PHE	-	expression tag	UNP P20963
Z	87	GLU	-	expression tag	UNP P20963
Z	88	LYS	-	expression tag	UNP P20963
Z	89	GLY	-	expression tag	UNP P20963
Z	90	GLY	-	expression tag	UNP P20963
Z	91	GLY	-	expression tag	UNP P20963
Z	92	SER	-	expression tag	UNP P20963
Z	93	GLY	-	expression tag	UNP P20963
Z	94	GLY	-	expression tag	UNP P20963
Z	95	GLY	-	expression tag	UNP P20963
Z	96	SER	-	expression tag	UNP P20963
Z	97	GLY	-	expression tag	UNP P20963
Z	98	GLY	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	99	SER	-	expression tag	UNP P20963
Z	100	ALA	-	expression tag	UNP P20963
Z	101	TRP	-	expression tag	UNP P20963
Z	102	SER	-	expression tag	UNP P20963
Z	103	HIS	-	expression tag	UNP P20963
Z	104	PRO	-	expression tag	UNP P20963
Z	105	GLN	-	expression tag	UNP P20963
Z	106	PHE	-	expression tag	UNP P20963
Z	107	GLU	-	expression tag	UNP P20963
Z	108	LYS	-	expression tag	UNP P20963
Z	109	ALA	-	expression tag	UNP P20963
Z	110	ALA	-	expression tag	UNP P20963
z	37	GLY	-	expression tag	UNP P20963
z	38	GLY	-	expression tag	UNP P20963
z	39	SER	-	expression tag	UNP P20963
z	40	GLY	-	expression tag	UNP P20963
z	41	GLY	-	expression tag	UNP P20963
z	42	SER	-	expression tag	UNP P20963
z	43	LEU	-	expression tag	UNP P20963
z	44	PRO	-	expression tag	UNP P20963
z	45	GLU	-	expression tag	UNP P20963
z	46	THR	-	expression tag	UNP P20963
z	47	GLY	-	expression tag	UNP P20963
z	48	GLY	-	expression tag	UNP P20963
z	49	GLY	-	expression tag	UNP P20963
z	50	SER	-	expression tag	UNP P20963
z	51	GLY	-	expression tag	UNP P20963
z	52	GLY	-	expression tag	UNP P20963
z	53	SER	-	expression tag	UNP P20963
z	54	GLY	-	expression tag	UNP P20963
z	55	GLY	-	expression tag	UNP P20963
z	56	SER	-	expression tag	UNP P20963
z	57	GLY	-	expression tag	UNP P20963
z	58	GLY	-	expression tag	UNP P20963
z	59	SER	-	expression tag	UNP P20963
z	60	GLY	-	expression tag	UNP P20963
z	61	GLY	-	expression tag	UNP P20963
z	62	SER	-	expression tag	UNP P20963
z	63	ARG	-	expression tag	UNP P20963
z	64	GLY	-	expression tag	UNP P20963
z	65	VAL	-	expression tag	UNP P20963
z	66	PRO	-	expression tag	UNP P20963

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Chain	Residue	Modelled	Actual	Comment	Reference
z	67	HIS	-	expression tag	UNP P20963
z	68	ILE	-	expression tag	UNP P20963
z	69	VAL	-	expression tag	UNP P20963
z	70	MET	-	expression tag	UNP P20963
z	71	VAL	-	expression tag	UNP P20963
z	72	ASP	-	expression tag	UNP P20963
z	73	ALA	-	expression tag	UNP P20963
z	74	TYR	-	expression tag	UNP P20963
z	75	LYS	-	expression tag	UNP P20963
z	76	ARG	-	expression tag	UNP P20963
z	77	TYR	-	expression tag	UNP P20963
z	78	LYS	-	expression tag	UNP P20963
z	79	GLY	-	expression tag	UNP P20963
z	80	GLY	-	expression tag	UNP P20963
z	81	TRP	-	expression tag	UNP P20963
z	82	SER	-	expression tag	UNP P20963
z	83	HIS	-	expression tag	UNP P20963
z	84	PRO	-	expression tag	UNP P20963
z	85	GLN	-	expression tag	UNP P20963
z	86	PHE	-	expression tag	UNP P20963
z	87	GLU	-	expression tag	UNP P20963
z	88	LYS	-	expression tag	UNP P20963
z	89	GLY	-	expression tag	UNP P20963
z	90	GLY	-	expression tag	UNP P20963
z	91	GLY	-	expression tag	UNP P20963
z	92	SER	-	expression tag	UNP P20963
z	93	GLY	-	expression tag	UNP P20963
z	94	GLY	-	expression tag	UNP P20963
z	95	GLY	-	expression tag	UNP P20963
z	96	SER	-	expression tag	UNP P20963
z	97	GLY	-	expression tag	UNP P20963
z	98	GLY	-	expression tag	UNP P20963
z	99	SER	-	expression tag	UNP P20963
z	100	ALA	-	expression tag	UNP P20963
z	101	TRP	-	expression tag	UNP P20963
z	102	SER	-	expression tag	UNP P20963
z	103	HIS	-	expression tag	UNP P20963
z	104	PRO	-	expression tag	UNP P20963
z	105	GLN	-	expression tag	UNP P20963
z	106	PHE	-	expression tag	UNP P20963
z	107	GLU	-	expression tag	UNP P20963
z	108	LYS	-	expression tag	UNP P20963

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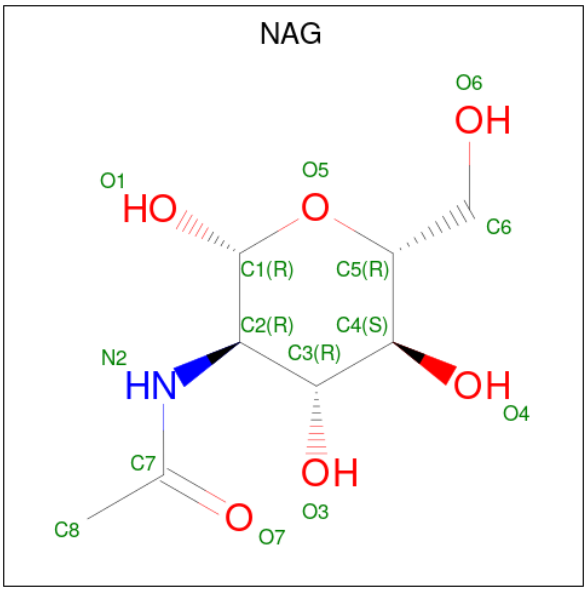
Chain	Residue	Modelled	Actual	Comment	Reference
z	109	ALA	-	expression tag	UNP P20963
z	110	ALA	-	expression tag	UNP P20963

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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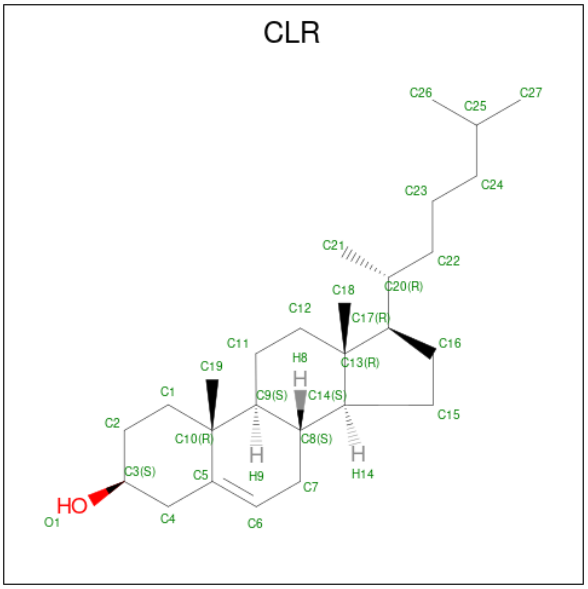
- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	C	1	28	27	1	0

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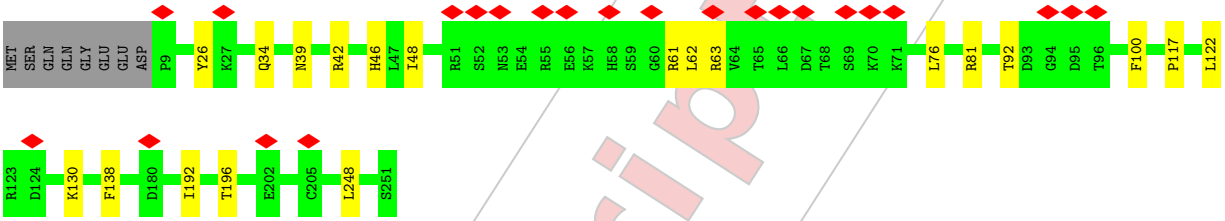
3 Residue-property plots (i)

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.

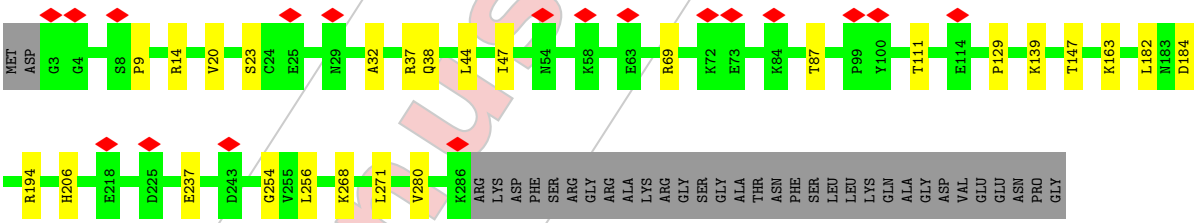
- Molecule 1: GPabWT T cell receptor alpha chain

Chain A:



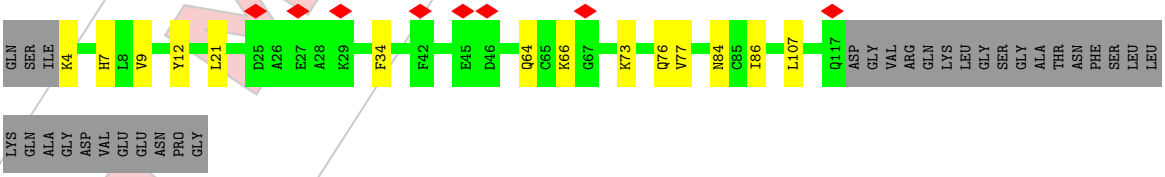
- Molecule 2: GPabWT T cell receptor beta chain

Chain B:



- Molecule 3: T-cell surface glycoprotein CD3 gamma chain

Chain C:



- Molecule 4: T-cell surface glycoprotein CD3 delta chain

Chain D:

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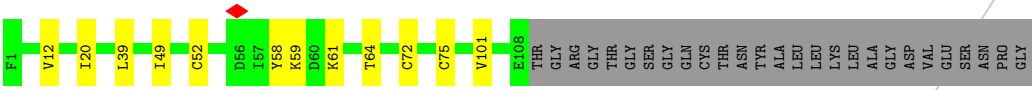
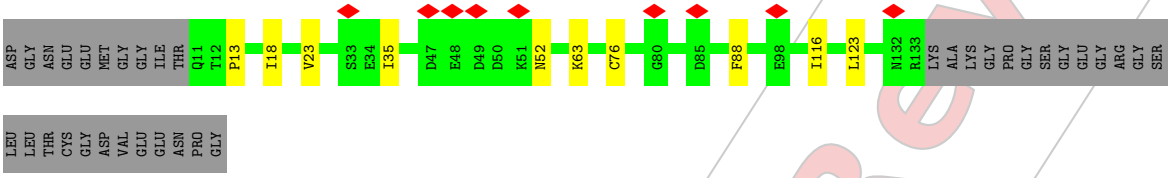
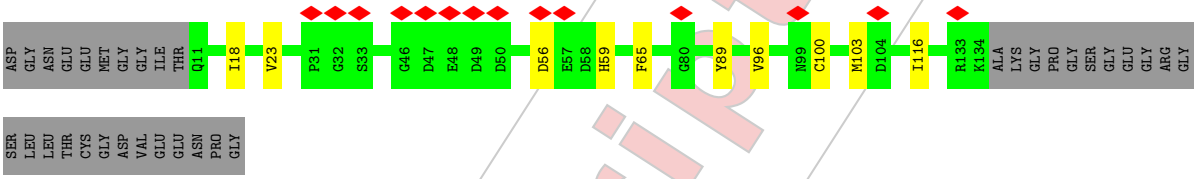


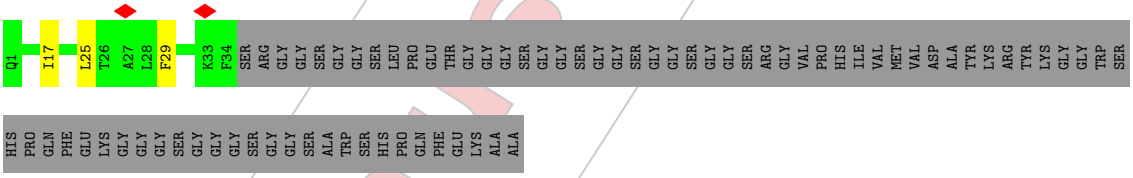
• Molecule 5: T-cell surface glycoprotein CD3 epsilon chain



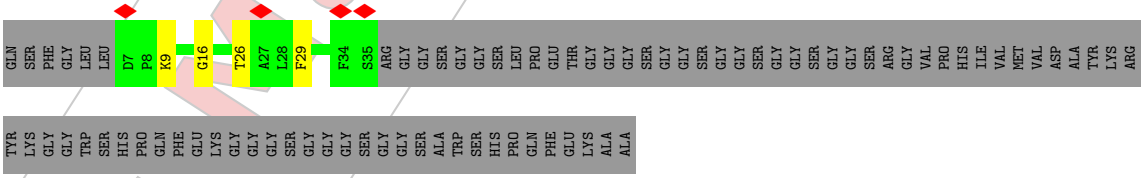
• Molecule 5: T-cell surface glycoprotein CD3 epsilon chain



• Molecule 6: T-cell surface glycoprotein CD3 zeta chain



• Molecule 6: T-cell surface glycoprotein CD3 zeta chain



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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119559	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.049	Depositor
Minimum map value	-3.842	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

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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, CLR

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	0.10	0/1931	0.24	0/2612
2	B	0.10	0/2305	0.27	0/3136
3	C	0.09	0/917	0.23	0/1233
4	D	0.11	0/853	0.32	0/1159
5	E	0.32	0/999	0.45	0/1356
5	e	0.12	0/1008	0.25	0/1367
6	Z	0.07	0/281	0.23	0/379
6	z	0.32	0/240	0.49	0/324
All	All	0.15	0/8534	0.30	0/11566

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1859	13	0
2	B	2247	0	2171	18	0
3	C	899	0	892	13	0
4	D	840	0	845	8	0
5	E	978	0	938	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	987	0	951	7	0
6	Z	275	0	298	3	0
6	z	235	0	253	4	0
7	A	70	0	65	1	0
7	B	28	0	26	1	0
7	C	14	0	13	0	0
7	D	28	0	26	0	0
8	C	28	0	46	3	0
All	All	8527	0	8383	59	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 3.

All (59) 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)
8:C:202:CLR:H221	6:z:16:GLY:HA3	1.73	0.69
5:E:35:ILE:HD11	5:E:76:CYS:HB2	1.78	0.63
1:A:117:PRO:HB2	1:A:196:THR:HG22	1.84	0.60
4:D:49:ILE:HD11	5:E:13:PRO:HB3	1.85	0.58
6:Z:29:PHE:HB2	6:z:29:PHE:HB2	1.84	0.58
2:B:14:ARG:HG3	2:B:20:VAL:HB	1.85	0.58
2:B:256:LEU:HD21	3:C:84:ASN:HA	1.85	0.58
3:C:7:HIS:HA	3:C:73:LYS:HB2	1.85	0.58
3:C:34:PHE:HE1	3:C:66:LYS:HB2	1.70	0.56
5:e:65:PHE:HB3	5:e:96:VAL:HG11	1.89	0.55
3:C:12:TYR:HB3	3:C:21:LEU:HB2	1.89	0.54
1:A:39:ASN:HB2	1:A:42:ARG:HE	1.73	0.53
1:A:130:LYS:HE3	2:B:147:THR:HG21	1.91	0.52
2:B:87:THR:HG23	2:B:111:THR:HA	1.92	0.52
4:D:101:VAL:HG21	5:E:123:LEU:HG	1.91	0.52
1:A:122:LEU:HD22	2:B:129:PRO:HA	1.93	0.50
4:D:20:ILE:HD13	4:D:52:CYS:HB2	1.93	0.50
5:e:18:ILE:HG12	5:e:23:VAL:HG13	1.94	0.49
2:B:254:GLY:HA2	8:C:202:CLR:H21	1.94	0.49
3:C:76:GLN:HE21	3:C:77:VAL:N	2.11	0.48
1:A:34:GLN:HG2	1:A:46:HIS:HE1	1.79	0.47
1:A:248:LEU:HD21	2:B:280:VAL:HB	1.98	0.47
4:D:72:CYS:HB3	4:D:75:CYS:HB2	1.79	0.46
2:B:206:HIS:HE2	2:B:237:GLU:HB3	1.80	0.46
5:e:56:ASP:HB3	5:e:59:HIS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:GLN:NE2	3:C:77:VAL:H	2.15	0.45
1:A:63:ARG:HE	1:A:76:LEU:HD22	1.82	0.45
4:D:12:VAL:HB	4:D:39:LEU:HB2	1.98	0.45
2:B:32:ALA:HA	2:B:69:ARG:HH12	1.82	0.44
3:C:34:PHE:HB2	3:C:64:GLN:HB2	1.99	0.44
3:C:76:GLN:HE21	3:C:77:VAL:H	1.63	0.44
2:B:9:PRO:HG2	2:B:23:SER:H	1.83	0.44
2:B:37:ARG:HB3	2:B:47:ILE:HD11	2.00	0.43
3:C:7:HIS:O	3:C:9:VAL:HG23	2.18	0.43
5:E:18:ILE:HG12	5:E:23:VAL:HG22	1.99	0.43
3:C:86:ILE:O	5:e:100:CYS:HB2	2.18	0.43
4:D:58:TYR:HD2	4:D:61:LYS:HE2	1.83	0.43
1:A:26:TYR:HB3	1:A:92:THR:HG21	2.00	0.43
2:B:139:LYS:HB3	2:B:194:ARG:HD2	2.00	0.43
3:C:86:ILE:HD12	5:e:103:MET:HG3	2.01	0.43
1:A:48:ILE:HD13	1:A:62:LEU:HB3	2.00	0.42
1:A:192:ILE:HG12	1:A:196:THR:HG21	2.01	0.42
7:A:304:NAG:O7	7:A:304:NAG:C1	2.68	0.42
7:B:402:NAG:O7	7:B:402:NAG:H3	2.19	0.42
8:C:202:CLR:H3	6:z:9:LYS:HG2	2.01	0.42
4:D:64:THR:HG23	5:E:88:PHE:CD1	2.54	0.42
2:B:182:LEU:HD23	2:B:184:ASP:H	1.85	0.42
5:E:52:ASN:HA	5:E:63:LYS:HB2	2.00	0.42
1:A:61:ARG:NH1	1:A:81:ARG:HE	2.18	0.41
2:B:38:GLN:HB2	2:B:44:LEU:HD23	2.03	0.41
2:B:271:LEU:HD22	5:e:116:ILE:HG23	2.03	0.41
5:E:116:ILE:HG13	6:Z:17:ILE:HD13	2.03	0.41
2:B:163:LYS:HE2	2:B:163:LYS:HB2	1.93	0.41
1:A:100:PHE:HB2	2:B:44:LEU:HB2	2.03	0.40
2:B:268:LYS:HB3	3:C:107:LEU:HD11	2.03	0.40
1:A:117:PRO:HG3	1:A:138:PHE:HA	2.04	0.40
6:Z:25:LEU:HD11	6:z:26:THR:HG23	2.02	0.40
3:C:4:LYS:HZ3	5:e:89:TYR:HE2	1.69	0.40
4:D:59:LYS:HE3	4:D:59:LYS:HB2	1.91	0.40

There are no symmetry-related clashes.

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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	241/251 (96%)	239 (99%)	2 (1%)	0	100	100
2	B	282/318 (89%)	277 (98%)	5 (2%)	0	100	100
3	C	112/145 (77%)	109 (97%)	3 (3%)	0	100	100
4	D	106/135 (78%)	99 (93%)	7 (7%)	0	100	100
5	E	121/158 (77%)	118 (98%)	3 (2%)	0	100	100
5	e	122/158 (77%)	120 (98%)	2 (2%)	0	100	100
6	Z	32/110 (29%)	32 (100%)	0	0	100	100
6	z	27/110 (24%)	27 (100%)	0	0	100	100
All	All	1043/1385 (75%)	1021 (98%)	22 (2%)	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	220/227 (97%)	220 (100%)	0	100	100
2	B	245/271 (90%)	245 (100%)	0	100	100
3	C	96/120 (80%)	96 (100%)	0	100	100
4	D	95/114 (83%)	95 (100%)	0	100	100
5	E	111/135 (82%)	111 (100%)	0	100	100
5	e	112/135 (83%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Z	30/76 (40%)	30 (100%)	0	100	100
6	z	26/76 (34%)	26 (100%)	0	100	100
All	All	935/1154 (81%)	935 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
7	NAG	A	305	1	14,14,15	0.74	0	17,19,21	0.72	0
7	NAG	A	303	1	14,14,15	0.72	0	17,19,21	0.76	0
7	NAG	A	302	1	14,14,15	0.62	0	17,19,21	0.55	0
7	NAG	B	402	2	14,14,15	0.61	0	17,19,21	0.61	0
7	NAG	A	304	1	14,14,15	0.62	0	17,19,21	0.65	0

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	301	1	14,14,15	0.74	0	17,19,21	0.77	0
7	NAG	D	202	4	14,14,15	0.72	0	17,19,21	0.76	0
7	NAG	C	201	3	14,14,15	0.74	0	17,19,21	0.79	0
7	NAG	B	401	2	14,14,15	0.72	0	17,19,21	0.77	0
8	CLR	C	202	-	31,31,31	0.35	0	48,48,48	0.54	0
7	NAG	D	201	4	14,14,15	0.39	0	17,19,21	0.75	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
7	NAG	A	305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	303	1	-	0/6/23/26	0/1/1/1
7	NAG	A	302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	402	2	-	1/6/23/26	0/1/1/1
7	NAG	A	304	1	-	1/6/23/26	0/1/1/1
7	NAG	A	301	1	-	0/6/23/26	0/1/1/1
7	NAG	D	202	4	-	0/6/23/26	0/1/1/1
7	NAG	C	201	3	-	0/6/23/26	0/1/1/1
7	NAG	B	401	2	-	1/6/23/26	0/1/1/1
8	CLR	C	202	-	-	7/10/68/68	0/4/4/4
7	NAG	D	201	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	304	NAG	C1-C2-N2-C7
8	C	202	CLR	C20-C22-C23-C24
8	C	202	CLR	C23-C24-C25-C26
8	C	202	CLR	C22-C23-C24-C25
8	C	202	CLR	C23-C24-C25-C27
7	B	401	NAG	O5-C5-C6-O6
7	A	302	NAG	C1-C2-N2-C7
7	B	402	NAG	C3-C2-N2-C7
8	C	202	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
8	C	202	CLR	C13-C17-C20-C21
8	C	202	CLR	C16-C17-C20-C22
7	A	302	NAG	C3-C2-N2-C7
7	D	201	NAG	C4-C5-C6-O6

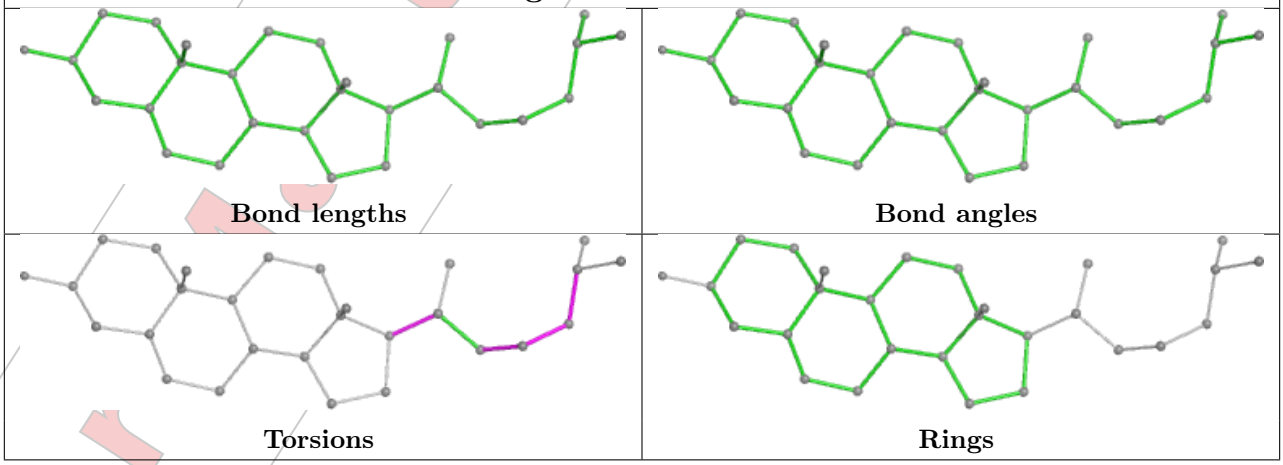
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	402	NAG	1	0
7	A	304	NAG	1	0
8	C	202	CLR	3	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 then 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.

Ligand CLR C 202



5.7 Other polymers (i)

There are no such residues in this entry.

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5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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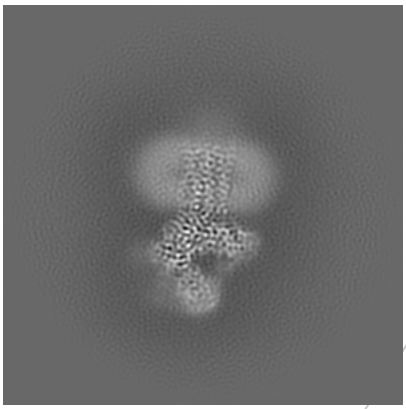
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-56497. These allow visual inspection of the internal detail of the map and identification of artifacts.

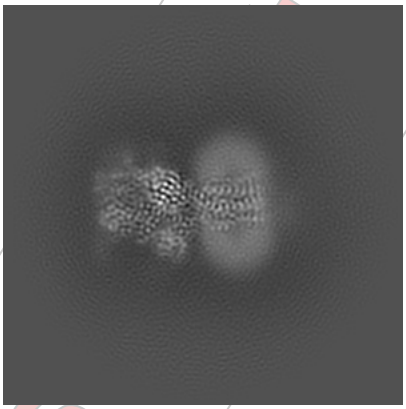
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

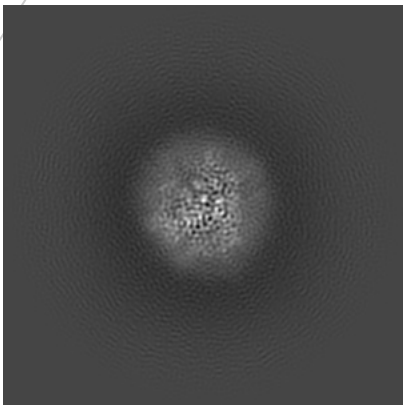
6.1.1 Primary map



X

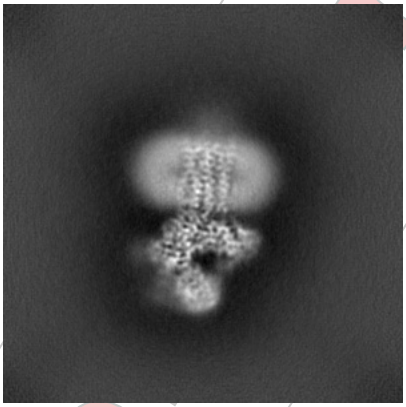


Y

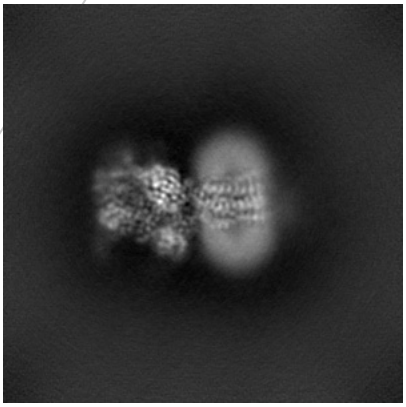


Z

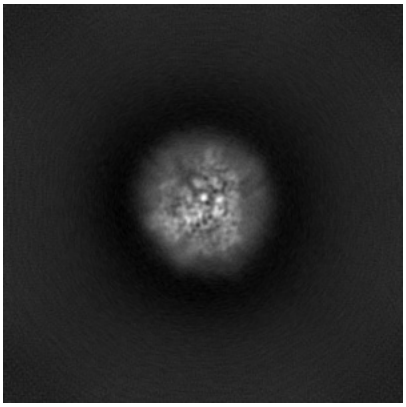
6.1.2 Raw map



X



Y



Z

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

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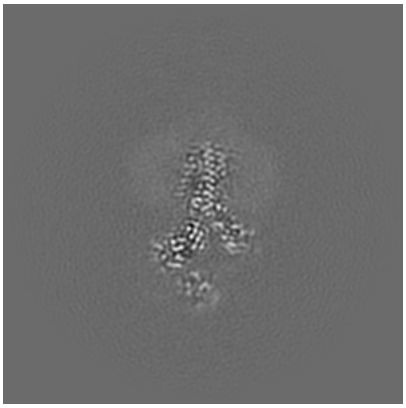
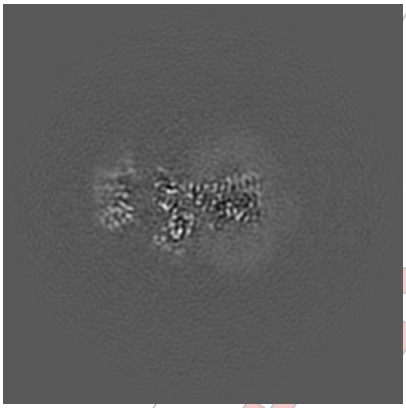
6.2 Central slices (i)

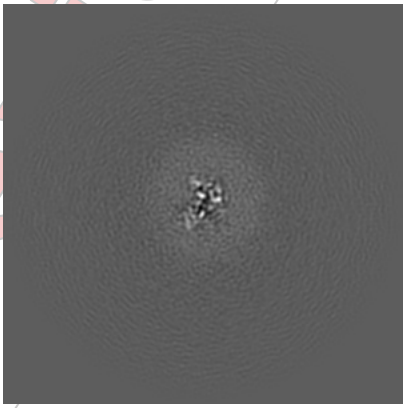
6.2.1 Primary map



X Index: 150

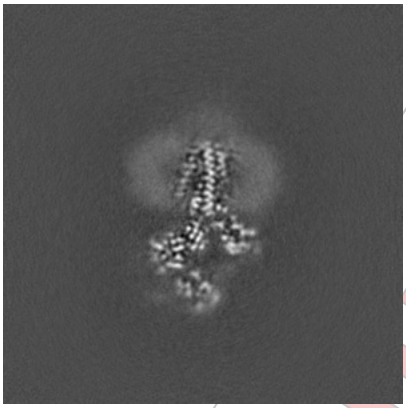


Y Index: 150

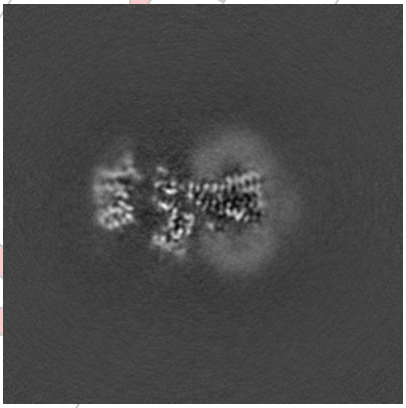


Z Index: 150

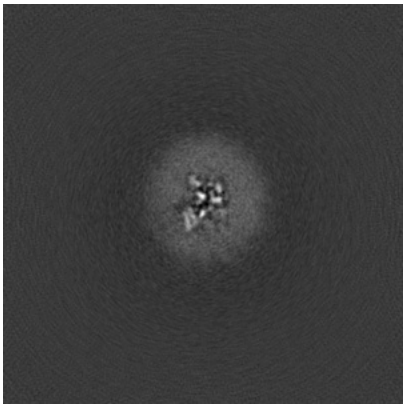
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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

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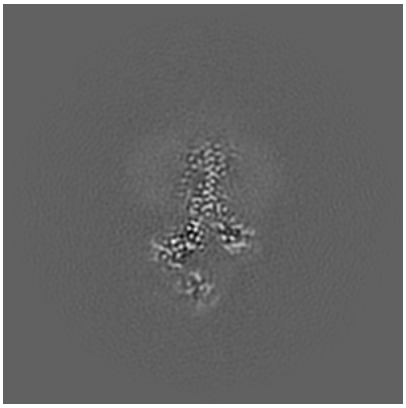
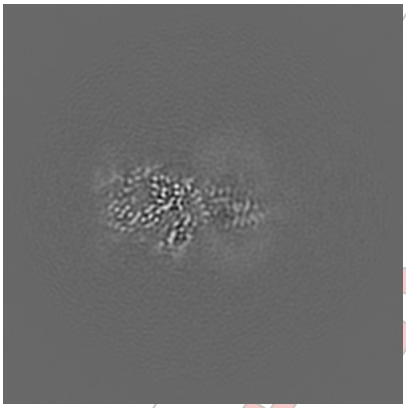
6.3 Largest variance slices (i)

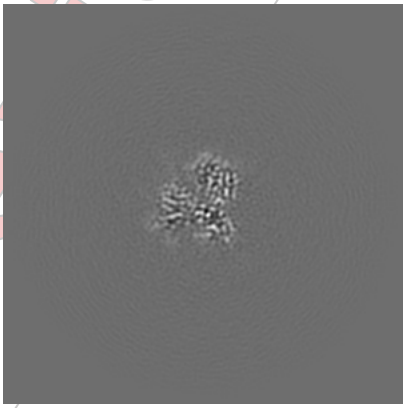
6.3.1 Primary map



X Index: 151

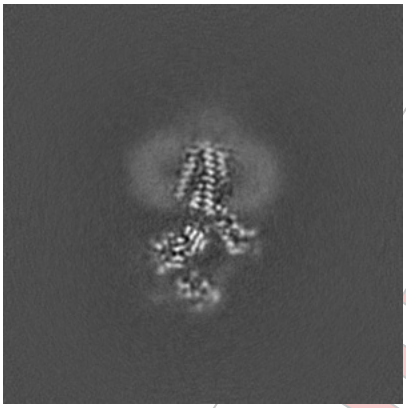


Y Index: 140

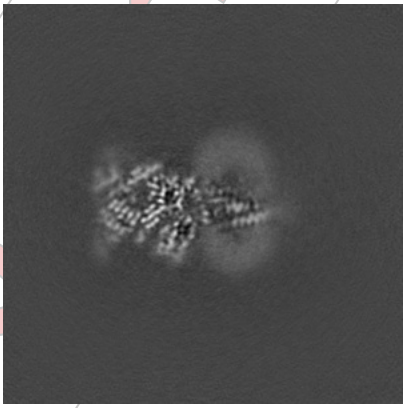


Z Index: 127

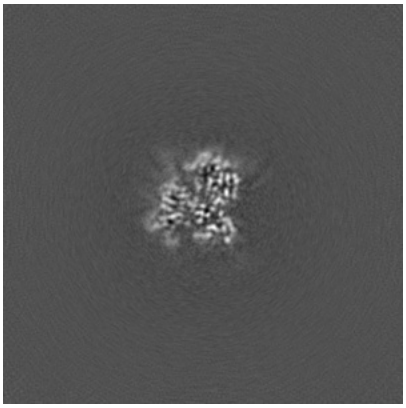
6.3.2 Raw map



X Index: 149



Y Index: 139



Z Index: 127

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

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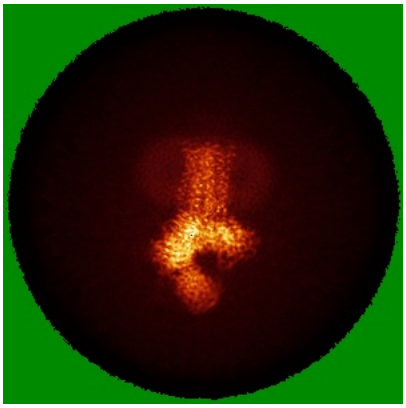
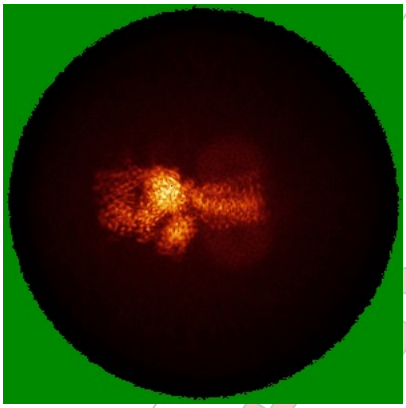
6.4 Orthogonal standard-deviation projections (False-color)

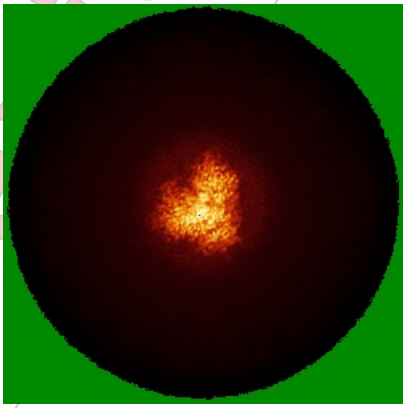
6.4.1 Primary map



X

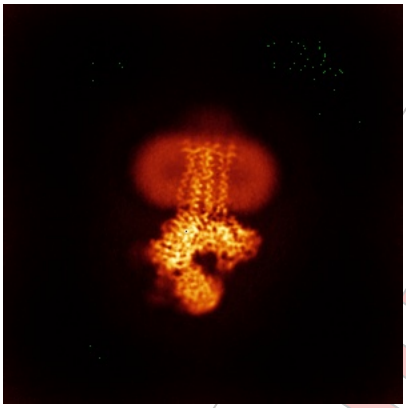


Y

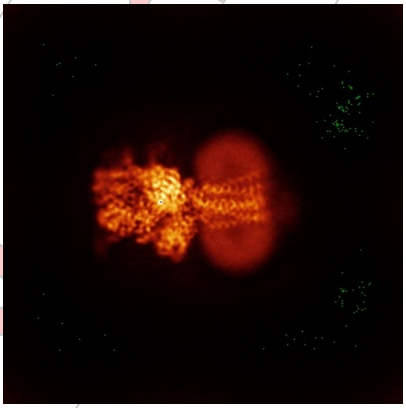


Z

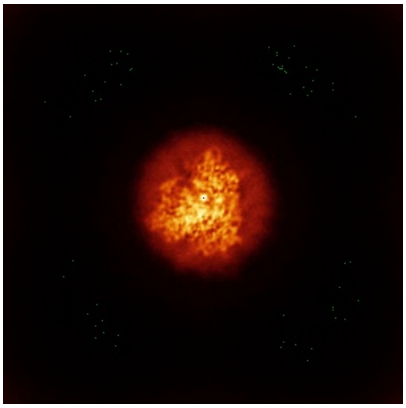
6.4.2 Raw map



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.

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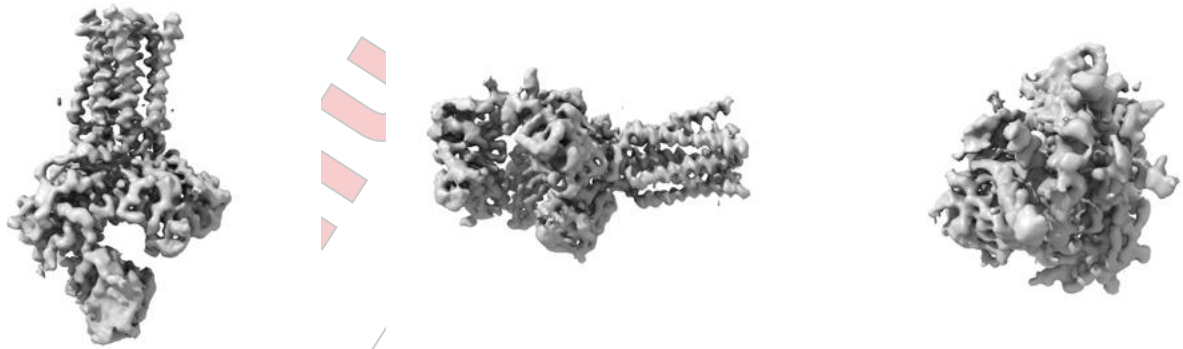
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

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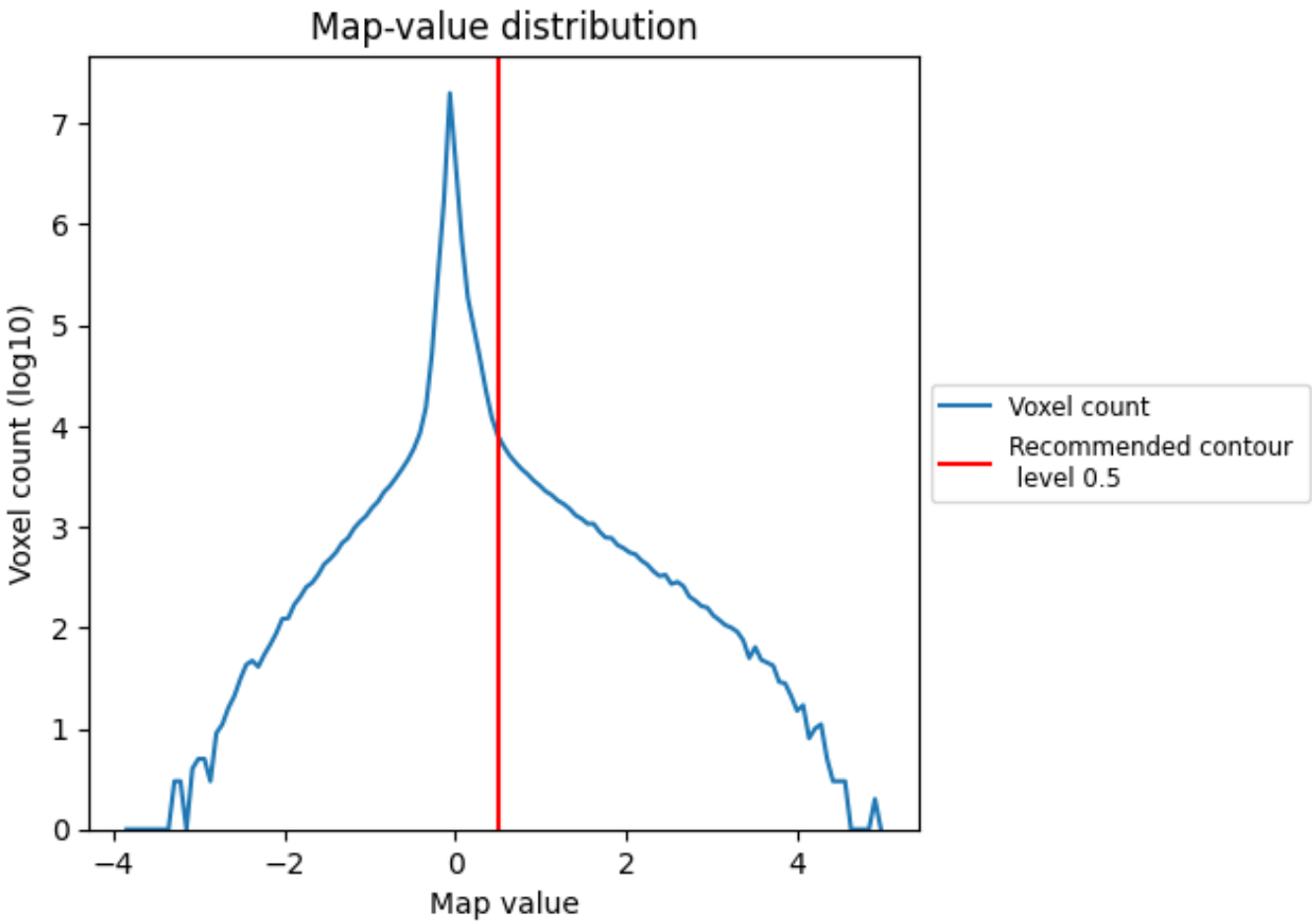
7 Map analysis

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

7.1 Map-value distribution



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.

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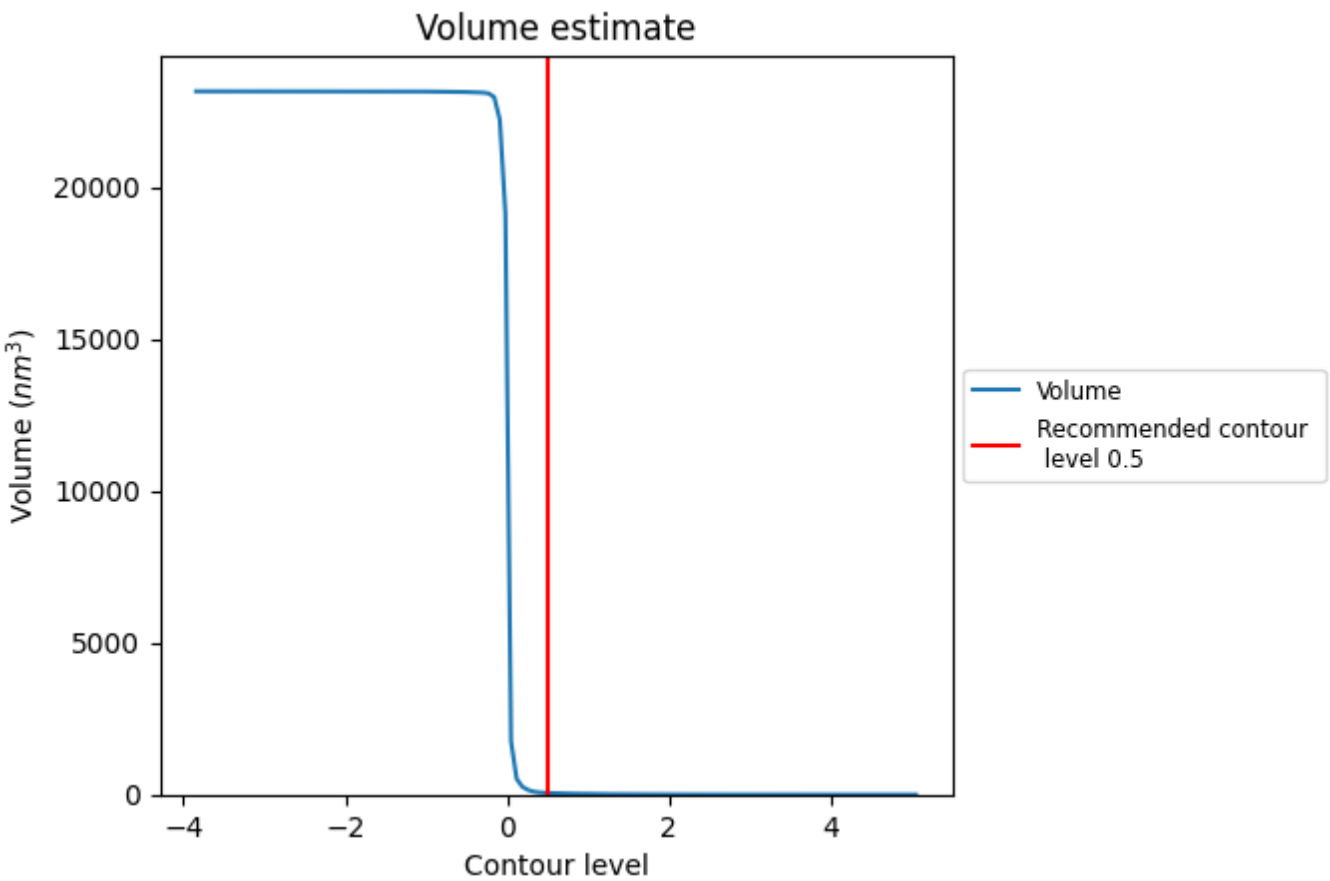
7.2 Volume estimate (i)



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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.

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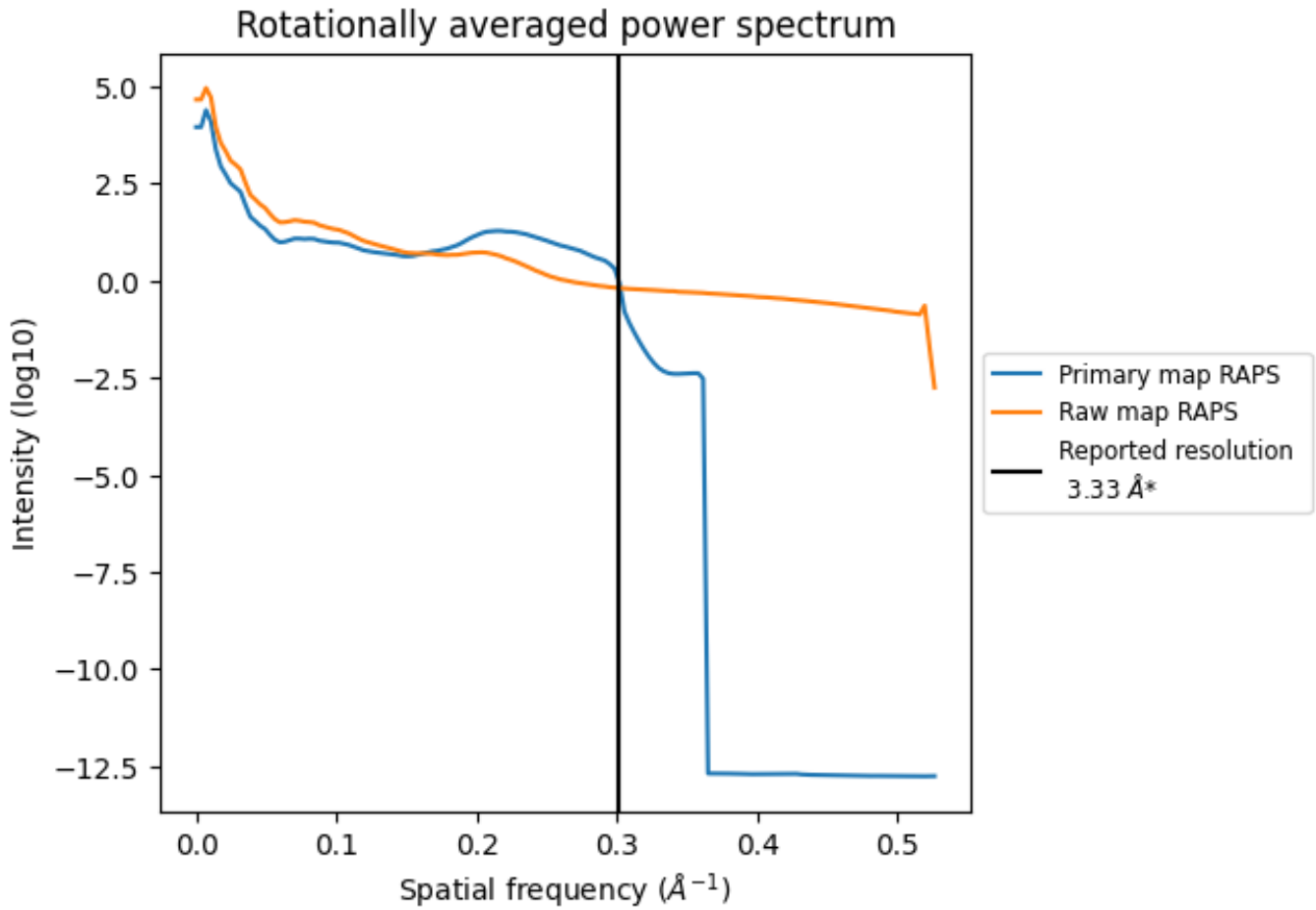
7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

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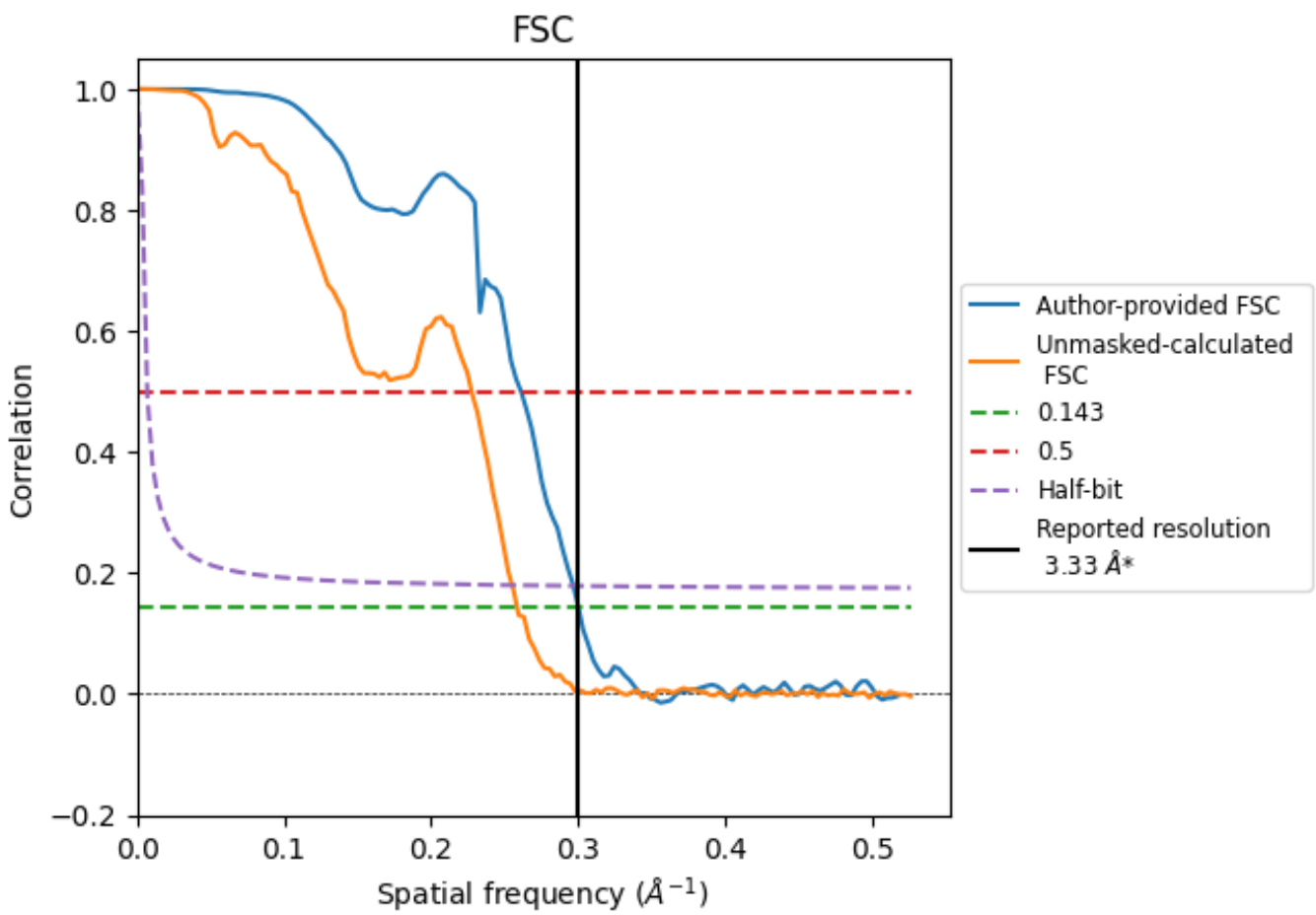
8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.83	3.37
Unmasked-calculated*	3.87	4.39	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.33 by more than 10 %

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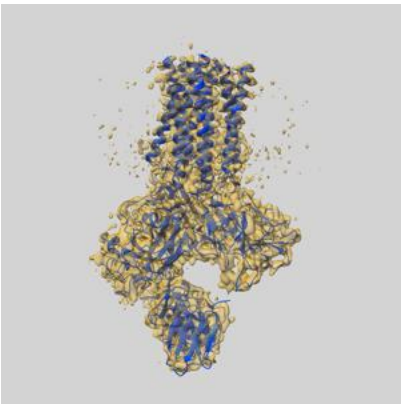
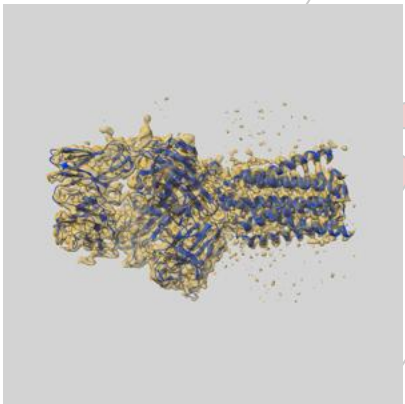
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-56497 and PDB model 9U0N. Per-residue inclusion information can be found in section 3 on page 13.

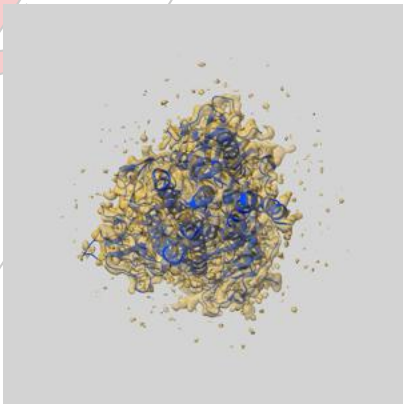
9.1 Map-model overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

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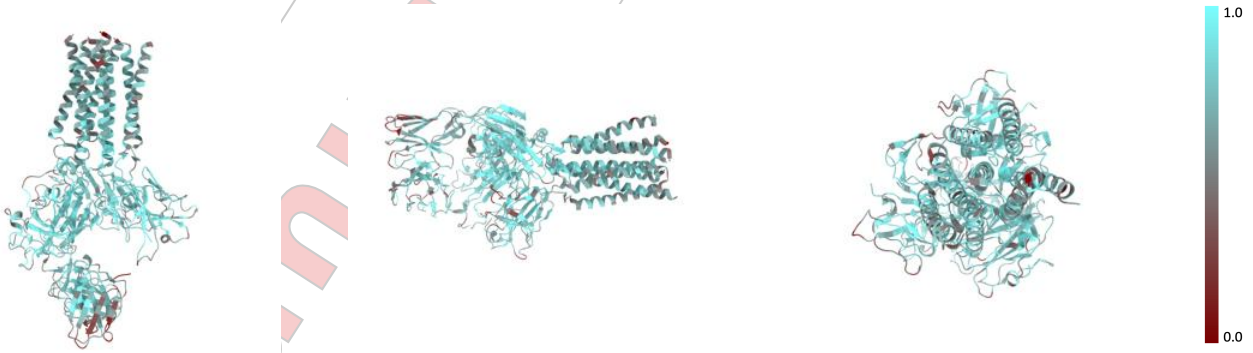
9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according 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)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

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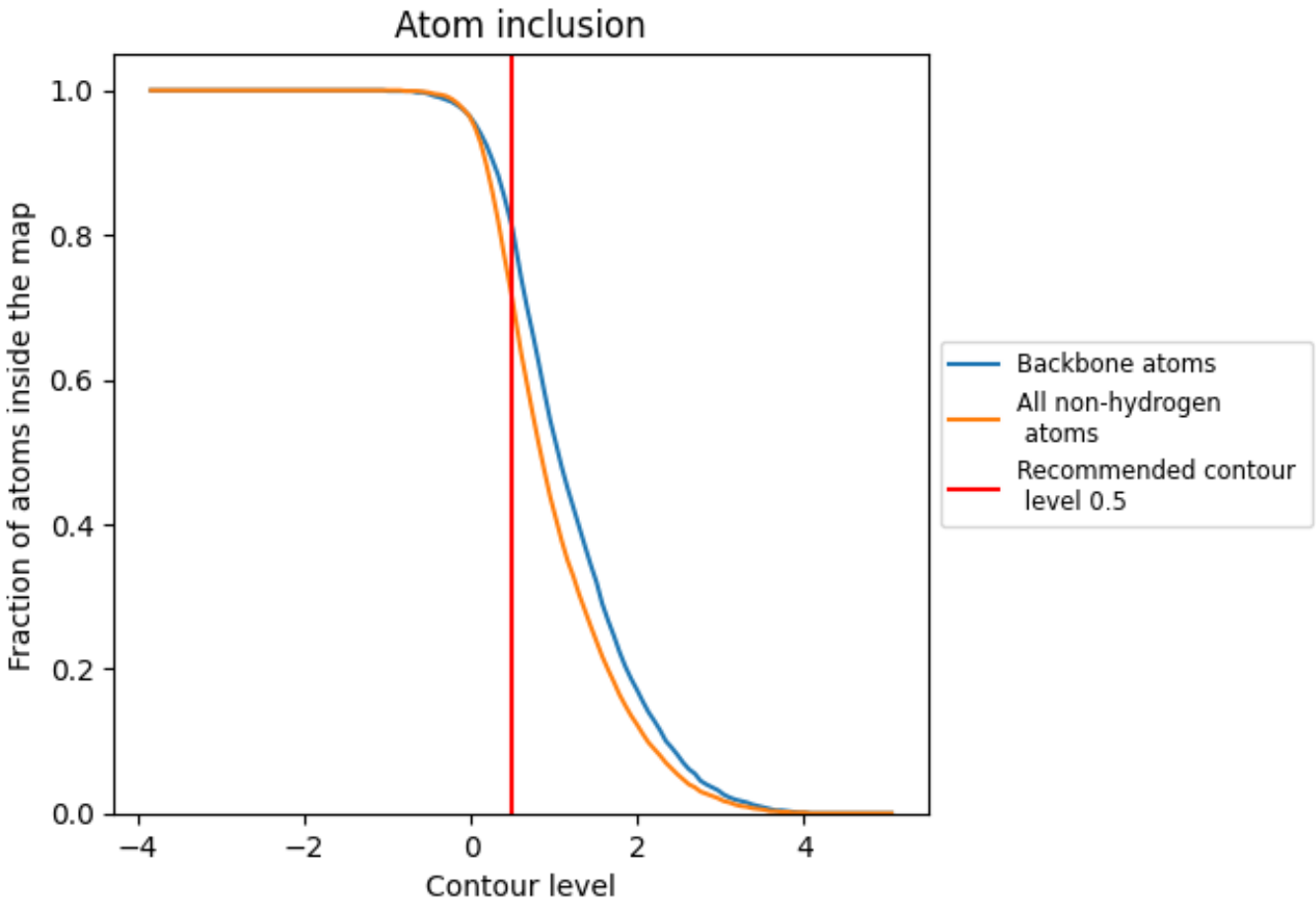
9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

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9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4440
A	0.6810	0.4400
B	0.7490	0.4600
C	0.6910	0.4310
D	0.7610	0.4670
E	0.7080	0.4480
Z	0.6970	0.4300
e	0.6750	0.4230
z	0.5970	0.3750

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