



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2026 – 10:12 PM JST

PDB ID : 24XZ / pdb_000024xz
EMDB ID : EMD-69905
Title : P2Y14R-Gi complex bound to UDP
Authors : Oshima, H.S.; Akasaka, H.; Sano, F.K.; Nureki, O.
Deposited on : 2026-03-24
Resolution : 2.93 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

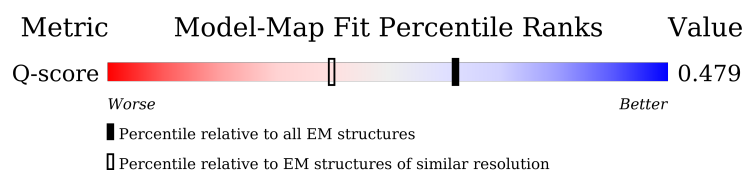
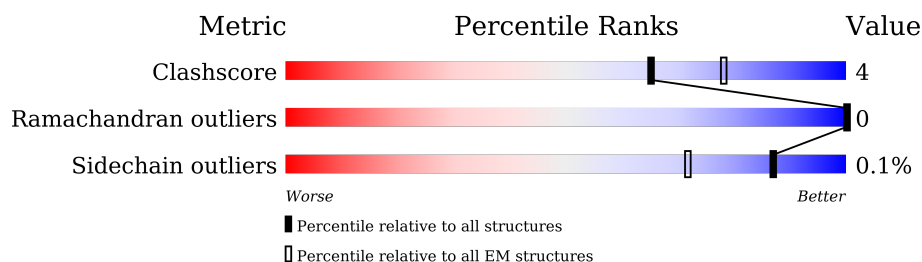
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 2.93 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	13037 (2.43 - 3.43)

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	B	375	
2	A	433	
2	G	433	
3	R	919	

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Mol	Chain	Length	Quality of chain
4	S	260	 81%8%11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9002 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 Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	336	2583	1593	465	504	21	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P62871
B	-3	GLY	-	expression tag	UNP P62871
B	-2	SER	-	expression tag	UNP P62871
B	-1	LEU	-	expression tag	UNP P62871
B	0	LEU	-	expression tag	UNP P62871
B	1	GLN	-	expression tag	UNP P62871
B	341	GLY	-	expression tag	UNP P62871
B	342	ALA	-	expression tag	UNP P62871
B	343	SER	-	expression tag	UNP P62871
B	344	GLY	-	expression tag	UNP P62871
B	345	GLY	-	expression tag	UNP P62871
B	346	GLY	-	expression tag	UNP P62871
B	347	SER	-	expression tag	UNP P62871
B	348	GLY	-	expression tag	UNP P62871
B	349	GLY	-	expression tag	UNP P62871
B	350	ASN	-	expression tag	UNP P62871
B	351	SER	-	expression tag	UNP P62871
B	352	GLY	-	expression tag	UNP P62871
B	353	SER	-	expression tag	UNP P62871
B	354	SER	-	expression tag	UNP P62871
B	355	GLY	-	expression tag	UNP P62871
B	356	GLY	-	expression tag	UNP P62871
B	357	SER	-	expression tag	UNP P62871
B	358	SER	-	expression tag	UNP P62871
B	359	GLY	-	expression tag	UNP P62871
B	360	VAL	-	expression tag	UNP P62871
B	361	SER	-	expression tag	UNP P62871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	362	GLY	-	expression tag	UNP P62871
B	363	TRP	-	expression tag	UNP P62871
B	364	ARG	-	expression tag	UNP P62871
B	365	LEU	-	expression tag	UNP P62871
B	366	PHE	-	expression tag	UNP P62871
B	367	LYS	-	expression tag	UNP P62871
B	368	LYS	-	expression tag	UNP P62871
B	369	ILE	-	expression tag	UNP P62871
B	370	SER	-	expression tag	UNP P62871

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	53	Total	C	N	O	S	0	0
			407	257	70	77	3		
2	A	223	Total	C	N	O	S	0	0
			1799	1143	298	345	13		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P63096
G	2	ALA	-	expression tag	UNP P63096
G	3	SER	-	expression tag	UNP P63096
G	4	ASN	-	expression tag	UNP P63096
G	5	ASN	-	expression tag	UNP P63096
G	6	THR	-	expression tag	UNP P63096
G	7	ALA	-	expression tag	UNP P63096
G	8	SER	-	expression tag	UNP P63096
G	9	ILE	-	expression tag	UNP P63096
G	10	ALA	-	expression tag	UNP P63096
G	11	GLN	-	expression tag	UNP P63096
G	12	ALA	-	expression tag	UNP P63096
G	13	ARG	-	expression tag	UNP P63096
G	14	LYS	-	expression tag	UNP P63096
G	15	LEU	-	expression tag	UNP P63096
G	16	VAL	-	expression tag	UNP P63096
G	17	GLU	-	expression tag	UNP P63096
G	18	GLN	-	expression tag	UNP P63096
G	19	LEU	-	expression tag	UNP P63096
G	20	LYS	-	expression tag	UNP P63096
G	21	MET	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
G	22	GLU	-	expression tag	UNP P63096
G	23	ALA	-	expression tag	UNP P63096
G	24	ASN	-	expression tag	UNP P63096
G	25	ILE	-	expression tag	UNP P63096
G	26	ASP	-	expression tag	UNP P63096
G	27	ARG	-	expression tag	UNP P63096
G	28	ILE	-	expression tag	UNP P63096
G	29	LYS	-	expression tag	UNP P63096
G	30	VAL	-	expression tag	UNP P63096
G	31	SER	-	expression tag	UNP P63096
G	32	LYS	-	expression tag	UNP P63096
G	33	ALA	-	expression tag	UNP P63096
G	34	ALA	-	expression tag	UNP P63096
G	35	ALA	-	expression tag	UNP P63096
G	36	ASP	-	expression tag	UNP P63096
G	37	LEU	-	expression tag	UNP P63096
G	38	MET	-	expression tag	UNP P63096
G	39	ALA	-	expression tag	UNP P63096
G	40	TYR	-	expression tag	UNP P63096
G	41	CYS	-	expression tag	UNP P63096
G	42	GLU	-	expression tag	UNP P63096
G	43	ALA	-	expression tag	UNP P63096
G	44	HIS	-	expression tag	UNP P63096
G	45	ALA	-	expression tag	UNP P63096
G	46	LYS	-	expression tag	UNP P63096
G	47	GLU	-	expression tag	UNP P63096
G	48	ASP	-	expression tag	UNP P63096
G	49	PRO	-	expression tag	UNP P63096
G	50	LEU	-	expression tag	UNP P63096
G	51	LEU	-	expression tag	UNP P63096
G	52	THR	-	expression tag	UNP P63096
G	53	PRO	-	expression tag	UNP P63096
G	54	VAL	-	expression tag	UNP P63096
G	55	PRO	-	expression tag	UNP P63096
G	56	ALA	-	expression tag	UNP P63096
G	57	SER	-	expression tag	UNP P63096
G	58	GLU	-	expression tag	UNP P63096
G	59	ASN	-	expression tag	UNP P63096
G	60	PRO	-	expression tag	UNP P63096
G	61	PHE	-	expression tag	UNP P63096
G	62	ARG	-	expression tag	UNP P63096
G	63	GLU	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
G	64	LYS	-	expression tag	UNP P63096
G	65	LYS	-	expression tag	UNP P63096
G	66	PHE	-	expression tag	UNP P63096
G	67	PHE	-	expression tag	UNP P63096
G	68	CYS	-	expression tag	UNP P63096
G	69	ALA	-	expression tag	UNP P63096
G	70	ILE	-	expression tag	UNP P63096
G	71	LEU	-	expression tag	UNP P63096
G	72	GLY	-	expression tag	UNP P63096
G	73	SER	-	expression tag	UNP P63096
G	74	ALA	-	expression tag	UNP P63096
G	75	GLY	-	expression tag	UNP P63096
G	76	SER	-	expression tag	UNP P63096
G	77	ALA	-	expression tag	UNP P63096
G	78	GLY	-	expression tag	UNP P63096
G	79	SER	-	expression tag	UNP P63096
G	80	ALA	-	expression tag	UNP P63096
G	81	MET	-	expression tag	UNP P63096
A	-78	MET	-	initiating methionine	UNP P63096
A	-77	ALA	-	expression tag	UNP P63096
A	-76	SER	-	expression tag	UNP P63096
A	-75	ASN	-	expression tag	UNP P63096
A	-74	ASN	-	expression tag	UNP P63096
A	-73	THR	-	expression tag	UNP P63096
A	-72	ALA	-	expression tag	UNP P63096
A	-71	SER	-	expression tag	UNP P63096
A	-70	ILE	-	expression tag	UNP P63096
A	-69	ALA	-	expression tag	UNP P63096
A	-68	GLN	-	expression tag	UNP P63096
A	-67	ALA	-	expression tag	UNP P63096
A	-66	ARG	-	expression tag	UNP P63096
A	-65	LYS	-	expression tag	UNP P63096
A	-64	LEU	-	expression tag	UNP P63096
A	-63	VAL	-	expression tag	UNP P63096
A	-62	GLU	-	expression tag	UNP P63096
A	-61	GLN	-	expression tag	UNP P63096
A	-60	LEU	-	expression tag	UNP P63096
A	-59	LYS	-	expression tag	UNP P63096
A	-58	MET	-	expression tag	UNP P63096
A	-57	GLU	-	expression tag	UNP P63096
A	-56	ALA	-	expression tag	UNP P63096
A	-55	ASN	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-54	ILE	-	expression tag	UNP P63096
A	-53	ASP	-	expression tag	UNP P63096
A	-52	ARG	-	expression tag	UNP P63096
A	-51	ILE	-	expression tag	UNP P63096
A	-50	LYS	-	expression tag	UNP P63096
A	-49	VAL	-	expression tag	UNP P63096
A	-48	SER	-	expression tag	UNP P63096
A	-47	LYS	-	expression tag	UNP P63096
A	-46	ALA	-	expression tag	UNP P63096
A	-45	ALA	-	expression tag	UNP P63096
A	-44	ALA	-	expression tag	UNP P63096
A	-43	ASP	-	expression tag	UNP P63096
A	-42	LEU	-	expression tag	UNP P63096
A	-41	MET	-	expression tag	UNP P63096
A	-40	ALA	-	expression tag	UNP P63096
A	-39	TYR	-	expression tag	UNP P63096
A	-38	CYS	-	expression tag	UNP P63096
A	-37	GLU	-	expression tag	UNP P63096
A	-36	ALA	-	expression tag	UNP P63096
A	-35	HIS	-	expression tag	UNP P63096
A	-34	ALA	-	expression tag	UNP P63096
A	-33	LYS	-	expression tag	UNP P63096
A	-32	GLU	-	expression tag	UNP P63096
A	-31	ASP	-	expression tag	UNP P63096
A	-30	PRO	-	expression tag	UNP P63096
A	-29	LEU	-	expression tag	UNP P63096
A	-28	LEU	-	expression tag	UNP P63096
A	-27	THR	-	expression tag	UNP P63096
A	-26	PRO	-	expression tag	UNP P63096
A	-25	VAL	-	expression tag	UNP P63096
A	-24	PRO	-	expression tag	UNP P63096
A	-23	ALA	-	expression tag	UNP P63096
A	-22	SER	-	expression tag	UNP P63096
A	-21	GLU	-	expression tag	UNP P63096
A	-20	ASN	-	expression tag	UNP P63096
A	-19	PRO	-	expression tag	UNP P63096
A	-18	PHE	-	expression tag	UNP P63096
A	-17	ARG	-	expression tag	UNP P63096
A	-16	GLU	-	expression tag	UNP P63096
A	-15	LYS	-	expression tag	UNP P63096
A	-14	LYS	-	expression tag	UNP P63096
A	-13	PHE	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	PHE	-	expression tag	UNP P63096
A	-11	CYS	-	expression tag	UNP P63096
A	-10	ALA	-	expression tag	UNP P63096
A	-9	ILE	-	expression tag	UNP P63096
A	-8	LEU	-	expression tag	UNP P63096
A	-7	GLY	-	expression tag	UNP P63096
A	-6	SER	-	expression tag	UNP P63096
A	-5	ALA	-	expression tag	UNP P63096
A	-4	GLY	-	expression tag	UNP P63096
A	-3	SER	-	expression tag	UNP P63096
A	-2	ALA	-	expression tag	UNP P63096
A	-1	GLY	-	expression tag	UNP P63096
A	0	SER	-	expression tag	UNP P63096
A	1	ALA	-	expression tag	UNP P63096
A	2	MET	-	expression tag	UNP P63096

- Molecule 3 is a protein called Soluble cytochrome b562,P2Y purinoceptor 14,LgBiT tag,GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	293	Total	C	N	O	S	0	0
			2405	1625	376	390	14		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-128	MET	-	initiating methionine	UNP P0ABE7
R	-127	LYS	-	expression tag	UNP P0ABE7
R	-126	THR	-	expression tag	UNP P0ABE7
R	-125	ILE	-	expression tag	UNP P0ABE7
R	-124	ILE	-	expression tag	UNP P0ABE7
R	-123	ALA	-	expression tag	UNP P0ABE7
R	-122	LEU	-	expression tag	UNP P0ABE7
R	-121	SER	-	expression tag	UNP P0ABE7
R	-120	TYR	-	expression tag	UNP P0ABE7
R	-119	ILE	-	expression tag	UNP P0ABE7
R	-118	PHE	-	expression tag	UNP P0ABE7
R	-117	CYS	-	expression tag	UNP P0ABE7
R	-116	LEU	-	expression tag	UNP P0ABE7
R	-115	VAL	-	expression tag	UNP P0ABE7
R	-114	PHE	-	expression tag	UNP P0ABE7
R	-113	ALA	-	expression tag	UNP P0ABE7
R	-112	ASP	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-111	TYR	-	expression tag	UNP P0ABE7
R	-110	LYS	-	expression tag	UNP P0ABE7
R	-109	ASP	-	expression tag	UNP P0ABE7
R	-108	ASP	-	expression tag	UNP P0ABE7
R	-107	ASP	-	expression tag	UNP P0ABE7
R	-106	ASP	-	expression tag	UNP P0ABE7
R	-105	LYS	-	expression tag	UNP P0ABE7
R	-98	TRP	MET	engineered mutation	UNP P0ABE7
R	-3	ILE	HIS	engineered mutation	UNP P0ABE7
R	1	LEU	ARG	engineered mutation	UNP P0ABE7
R	510	SER	-	linker	UNP Q15391
R	511	GLY	-	linker	UNP Q15391
R	512	GLY	-	linker	UNP Q15391
R	513	SER	-	linker	UNP Q15391
R	514	GLY	-	linker	UNP Q15391
R	515	GLY	-	linker	UNP Q15391
R	516	GLY	-	linker	UNP Q15391
R	517	GLY	-	linker	UNP Q15391
R	518	SER	-	linker	UNP Q15391
R	519	GLY	-	linker	UNP Q15391
R	520	GLY	-	linker	UNP Q15391
R	521	SER	-	linker	UNP Q15391
R	522	SER	-	linker	UNP Q15391
R	523	SER	-	linker	UNP Q15391
R	524	GLY	-	linker	UNP Q15391
R	525	GLY	-	linker	UNP Q15391
R	526	LEU	-	linker	UNP Q15391
R	527	GLU	-	linker	UNP Q15391
R	528	VAL	-	linker	UNP Q15391
R	529	LEU	-	linker	UNP Q15391
R	530	PHE	-	linker	UNP Q15391
R	531	GLN	-	linker	UNP Q15391
R	532	GLY	-	linker	UNP Q15391
R	533	PRO	-	linker	UNP Q15391
R	534	GLY	-	linker	UNP Q15391
R	535	SER	-	linker	UNP Q15391
R	536	ALA	-	linker	UNP Q15391
R	537	ALA	-	linker	UNP Q15391
R	538	ALA	-	linker	UNP Q15391
R	539	ALA	-	linker	UNP Q15391
R	778	SER	-	expression tag	UNP A0A5P9VSM6
R	779	GLY	-	expression tag	UNP A0A5P9VSM6

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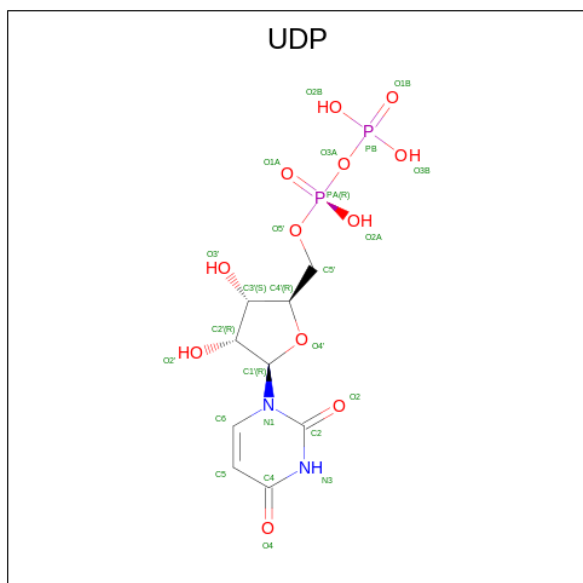
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Chain	Residue	Modelled	Actual	Comment	Reference
R	780	LEU	-	expression tag	UNP A0A5P9VSM6
R	781	ARG	-	expression tag	UNP A0A5P9VSM6
R	782	SER	-	expression tag	UNP A0A5P9VSM6
R	783	HIS	-	expression tag	UNP A0A5P9VSM6
R	784	HIS	-	expression tag	UNP A0A5P9VSM6
R	785	HIS	-	expression tag	UNP A0A5P9VSM6
R	786	HIS	-	expression tag	UNP A0A5P9VSM6
R	787	HIS	-	expression tag	UNP A0A5P9VSM6
R	788	HIS	-	expression tag	UNP A0A5P9VSM6
R	789	HIS	-	expression tag	UNP A0A5P9VSM6
R	790	HIS	-	expression tag	UNP A0A5P9VSM6

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	232	Total	C	N	O	S	0	0
			1783	1131	295	347	10		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).

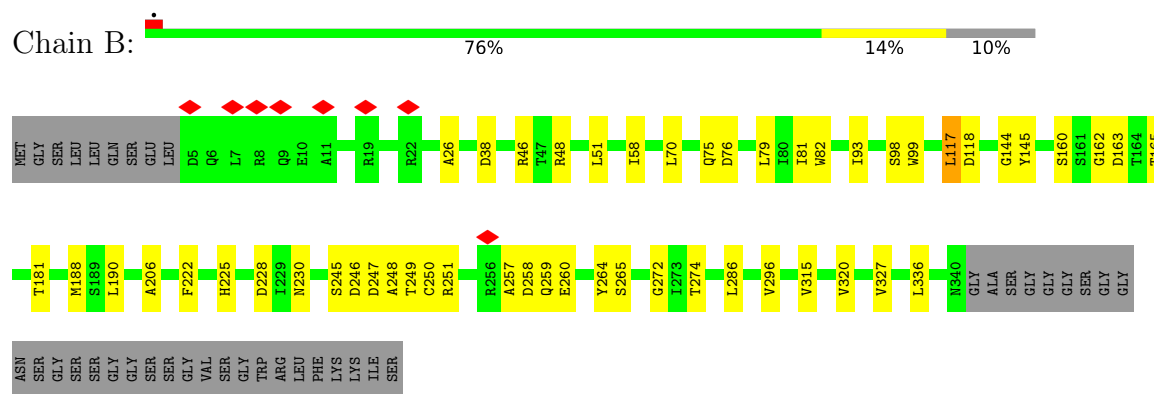


Mol	Chain	Residues	Atoms					AltConf
5	R	1	Total	C	N	O	P	0
			25	9	2	12	2	

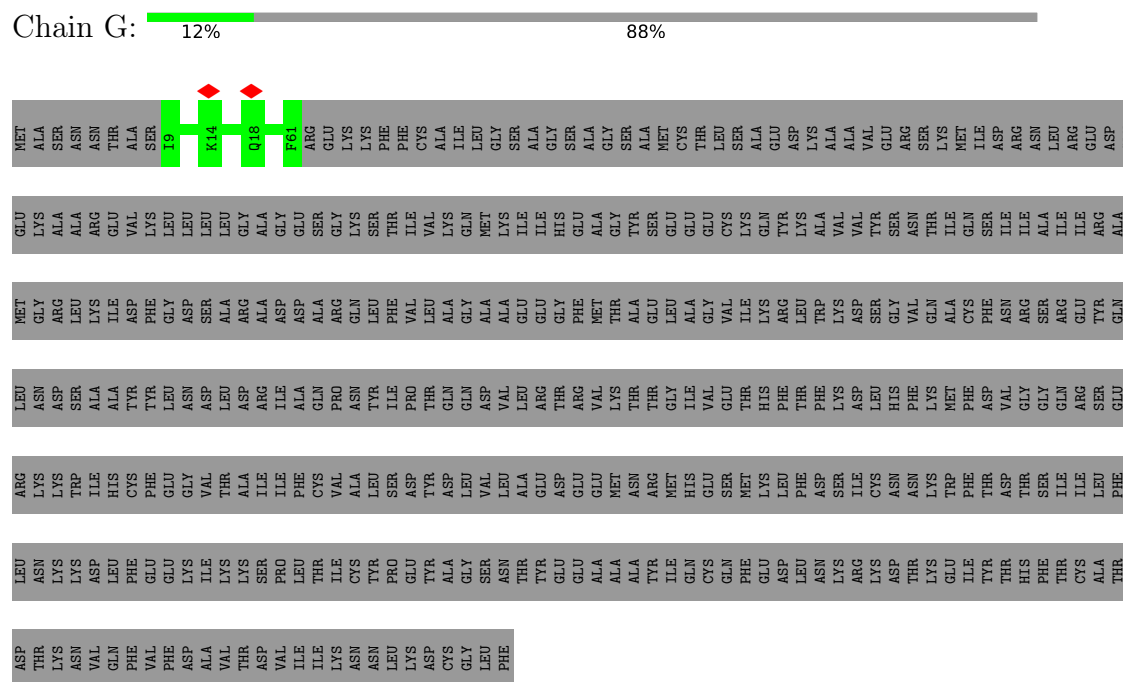
3 Residue-property plots

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.

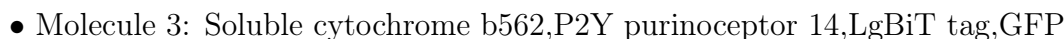
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1

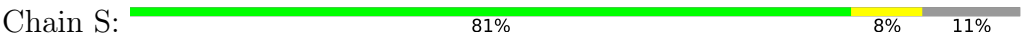


- Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1



LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	LEU	GLY	MET	ASP	GLU	LEU	TYR	LYS	SER	GLY	LEU	ARG	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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● Molecule 4: scFv16



ASP	Y2	S17	F68	Q82	M83	T91	Y94	G114	T118	S121	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S124	M128	S142	S149	L162	Y163	L166	Q167	P173	I204	Y215	Y216	C217	M218	G230	I235	LYS
-----	----	-----	-----	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

ALA	ALA	ALA	ALA	SER	SER	GLU	ASP	LEU	TYR	PHE	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.850	Depositor
Minimum map value	-46.935	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.174	Depositor
Recommended contour level	3	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8197531, 0.8197531, 0.8197531	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: UDP

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	B	0.31	0/2630	0.65	0/3566
2	A	0.31	0/1829	0.72	0/2452
2	G	0.23	0/413	0.52	0/558
3	R	0.47	0/2472	0.82	0/3352
4	S	0.27	0/1827	0.66	0/2477
All	All	0.35	0/9171	0.71	0/12405

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	B	2583	0	2486	33	0
2	A	1799	0	1785	9	0
2	G	407	0	418	0	0
3	R	2405	0	2525	18	0
4	S	1783	0	1717	12	0
5	R	25	0	11	0	0
All	All	9002	0	8942	71	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 4.

The worst 5 of 71 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:B:246:ASP:HA	1:B:272:GLY:HA3	1.68	0.75
1:B:228:ASP:O	1:B:245:SER:HB3	1.88	0.74
3:R:50:VAL:HG22	3:R:305:ILE:HD12	1.73	0.70
4:S:94:TYR:O	4:S:114:GLY:HA2	1.94	0.68
4:S:68:PHE:HA	4:S:82:GLN:O	1.97	0.64

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	B	334/375 (89%)	322 (96%)	12 (4%)	0	100	100
2	A	219/433 (51%)	216 (99%)	3 (1%)	0	100	100
2	G	51/433 (12%)	49 (96%)	2 (4%)	0	100	100
3	R	291/919 (32%)	281 (97%)	10 (3%)	0	100	100
4	S	228/260 (88%)	221 (97%)	7 (3%)	0	100	100
All	All	1123/2420 (46%)	1089 (97%)	34 (3%)	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	B	279/305 (92%)	278 (100%)	1 (0%)	84	92
2	A	198/366 (54%)	198 (100%)	0	100	100
2	G	43/366 (12%)	43 (100%)	0	100	100
3	R	274/801 (34%)	274 (100%)	0	100	100
4	S	197/209 (94%)	197 (100%)	0	100	100
All	All	991/2047 (48%)	990 (100%)	1 (0%)	87	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	S	159	ASN
2	A	346	ASN
2	A	22	ASN
3	R	184	HIS
2	A	255	ASN

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](#)

1 ligand is 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	$\# Z > 2$
5	UDP	R	801	-	24,26,26	0.42	0	37,40,40	0.48	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
5	UDP	R	801	-	-	0/16/32/32	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

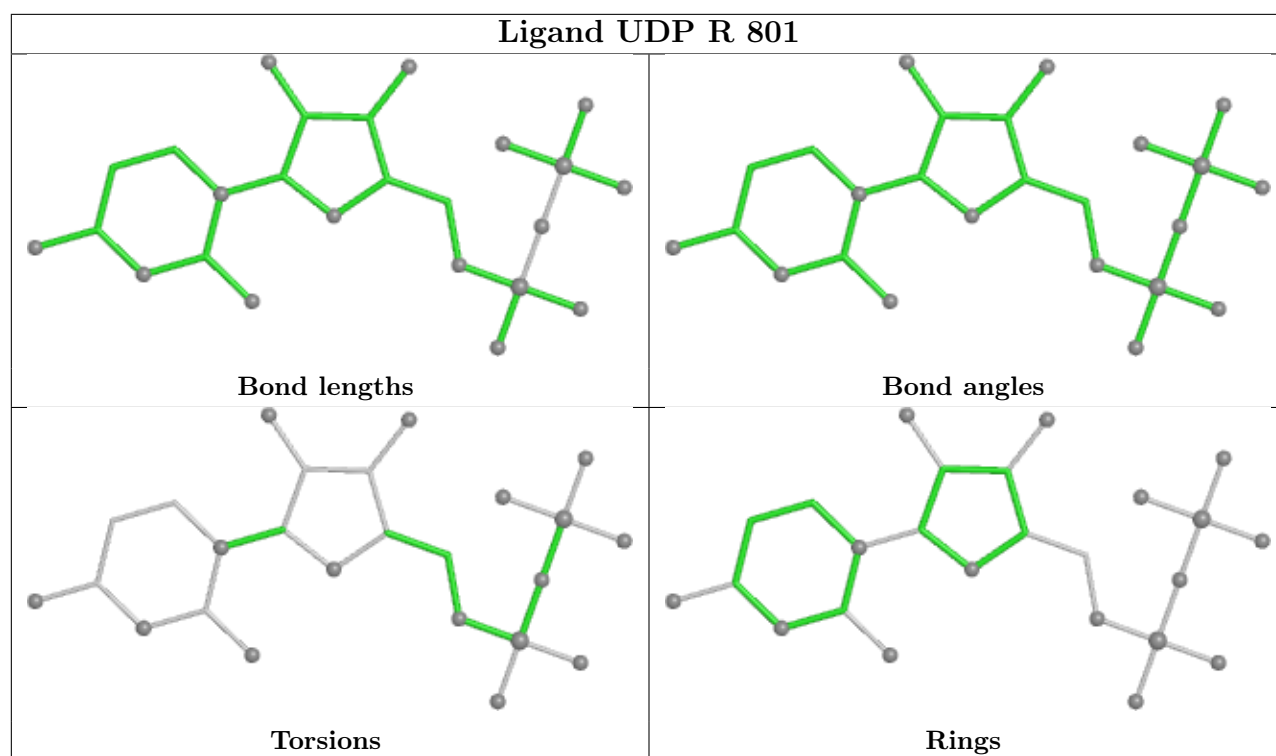
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

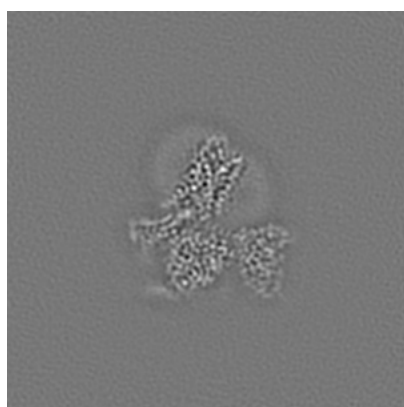
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69905. These allow visual inspection of the internal detail of the map and identification of artifacts.

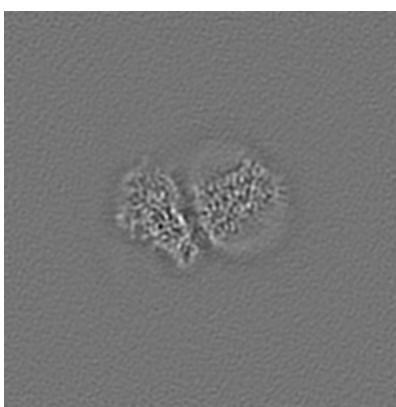
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

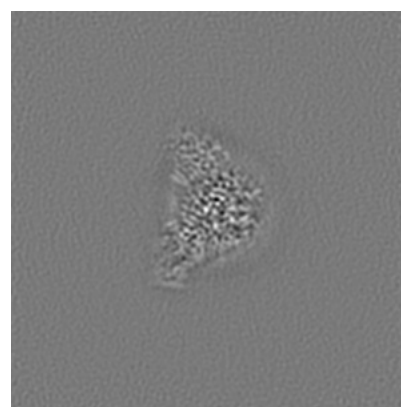
6.1.1 Primary map



X



Y

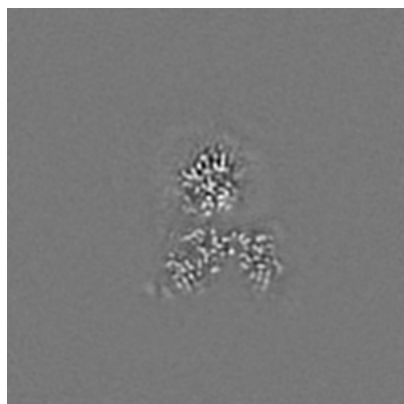


Z

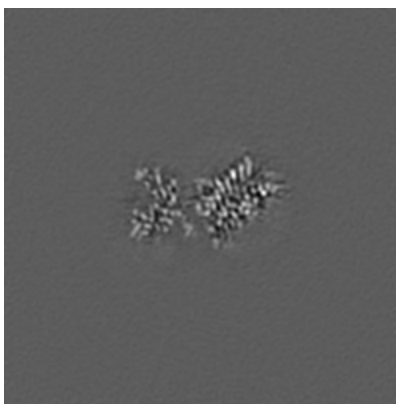
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

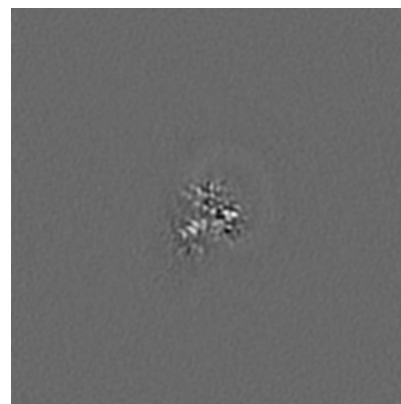
6.2.1 Primary map



X Index: 162



Y Index: 162

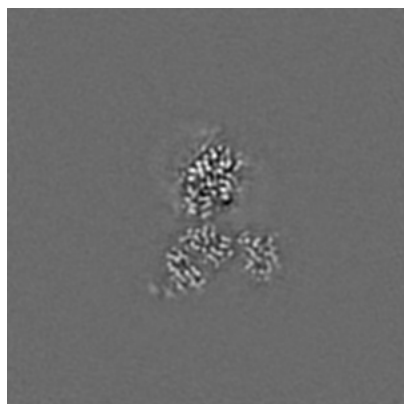


Z Index: 162

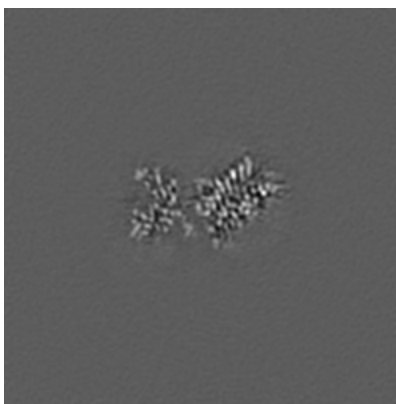
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

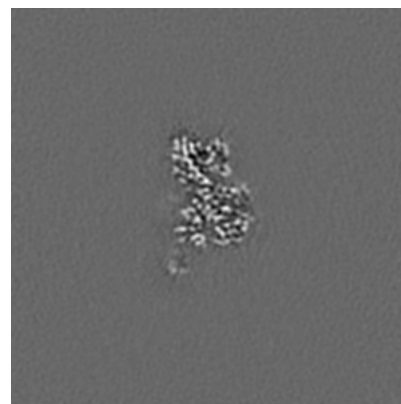
6.3.1 Primary map



X Index: 165



Y Index: 162

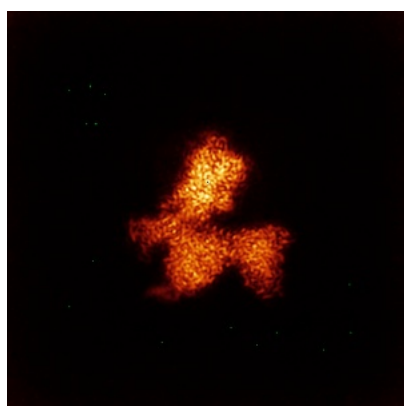


Z Index: 129

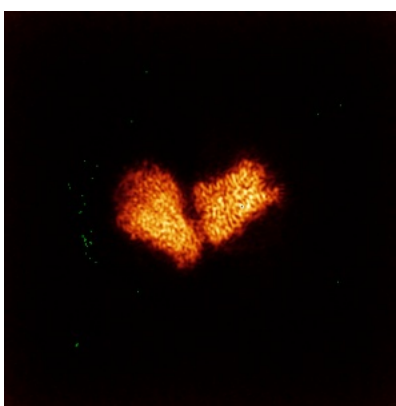
The images above show the largest variance slices of the map in three orthogonal directions.

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

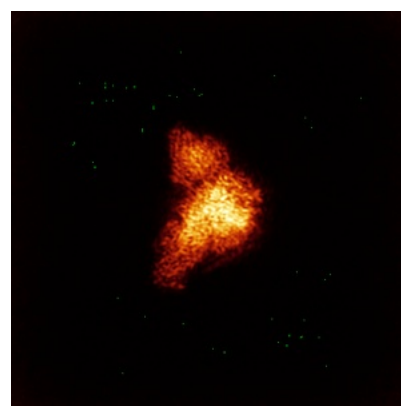
6.4.1 Primary map



X



Y

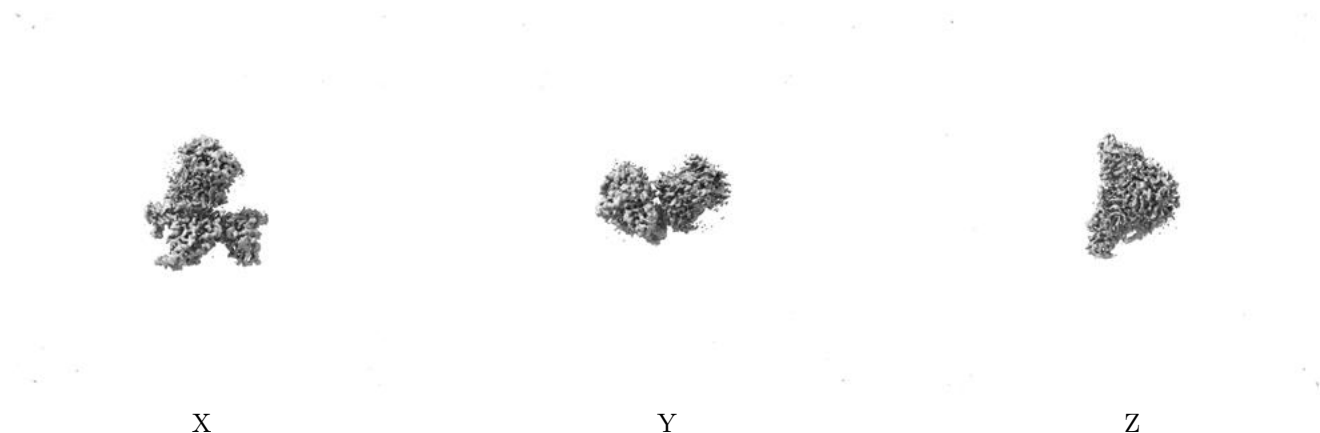


Z

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.

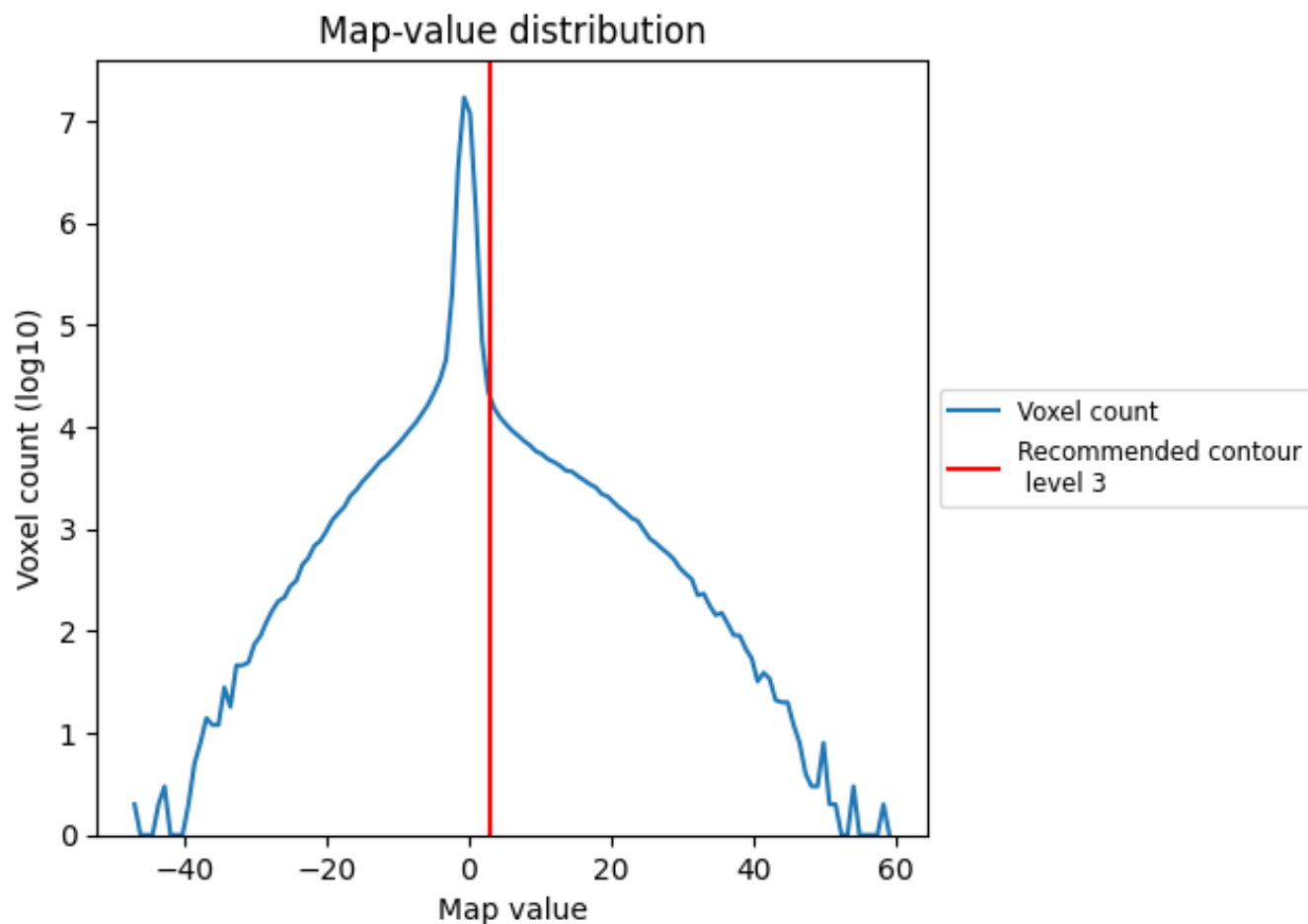
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

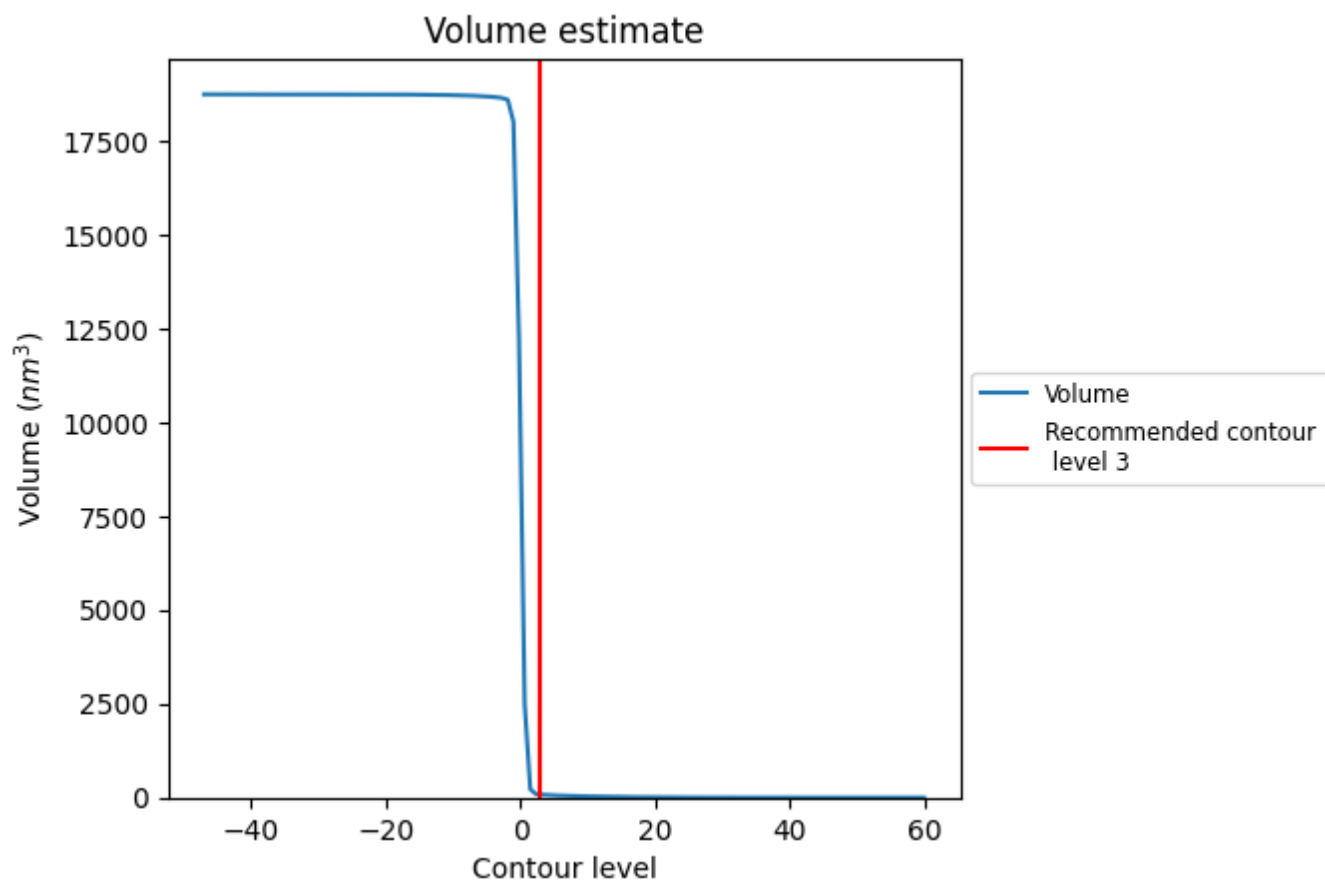
This section contains the results of statistical analysis of the map.

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.

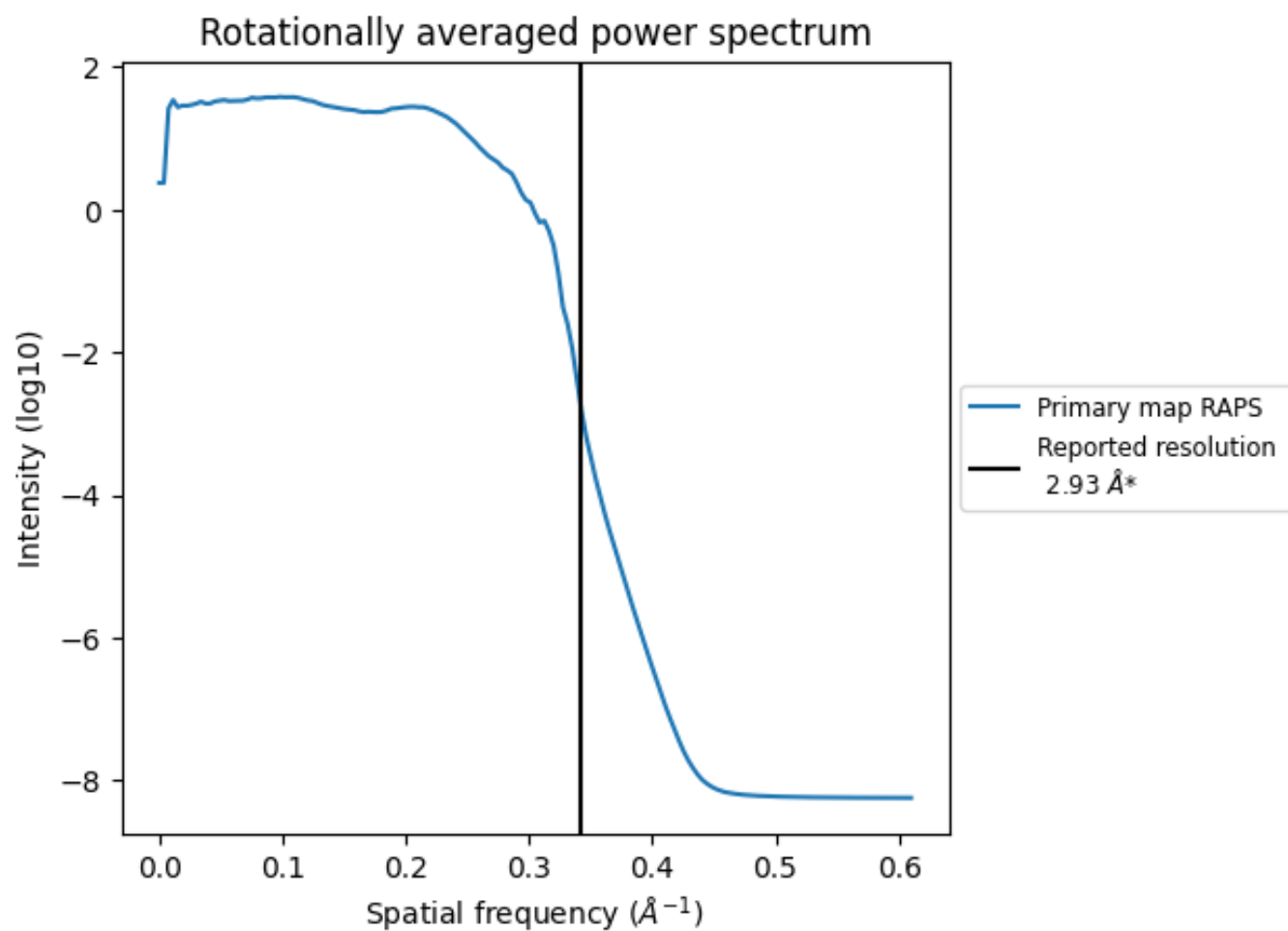
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 72 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 0.341 Å⁻¹

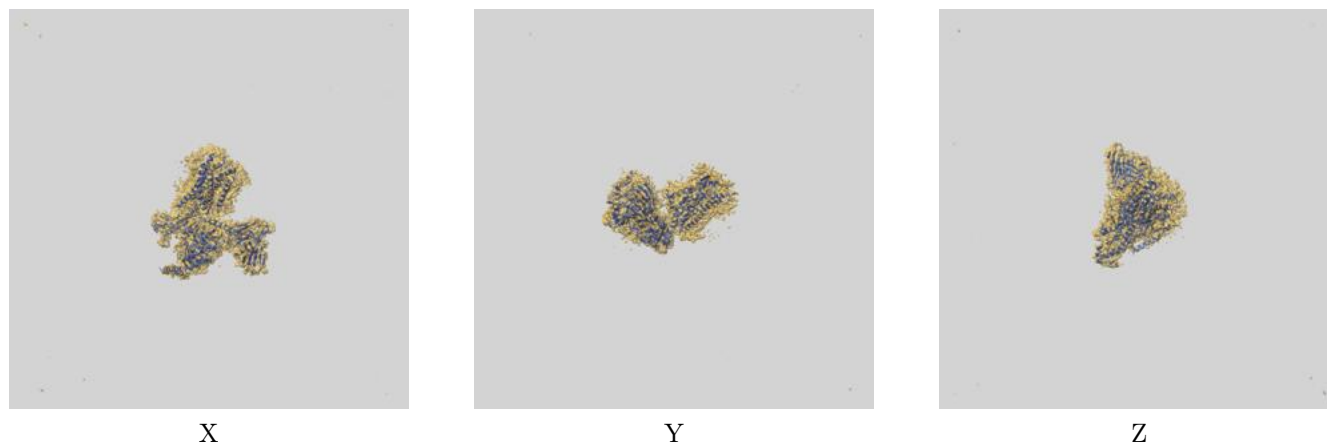
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

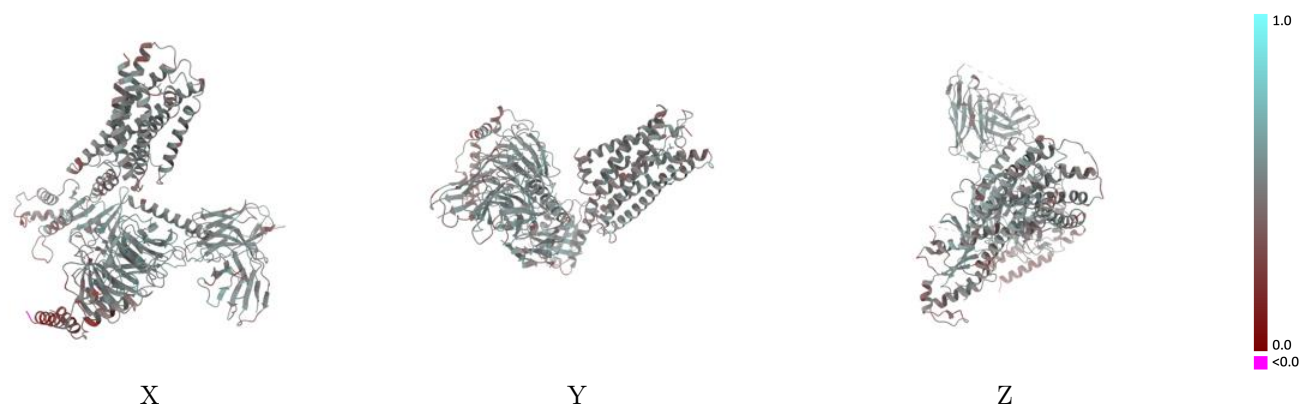
This section contains information regarding the fit between EMDB map EMD-69905 and PDB model 24XZ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



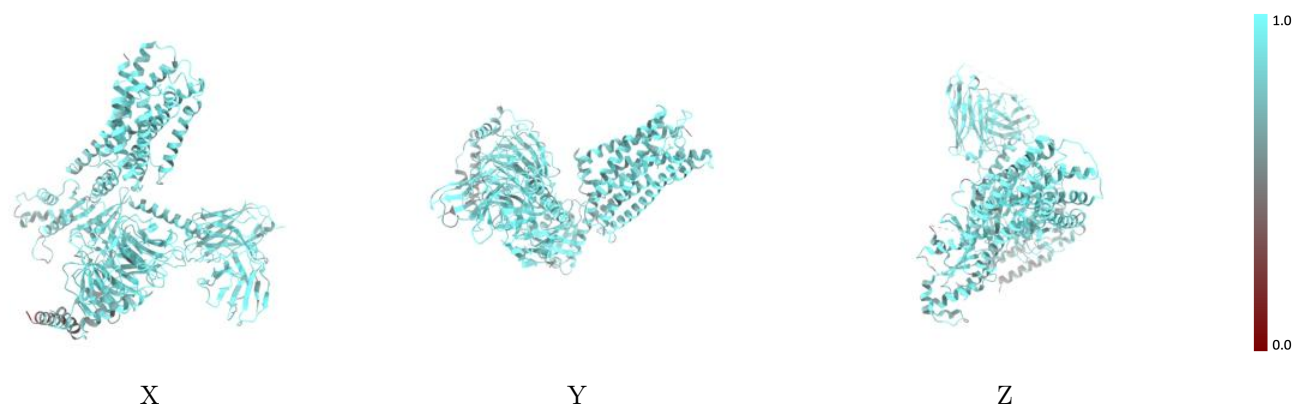
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



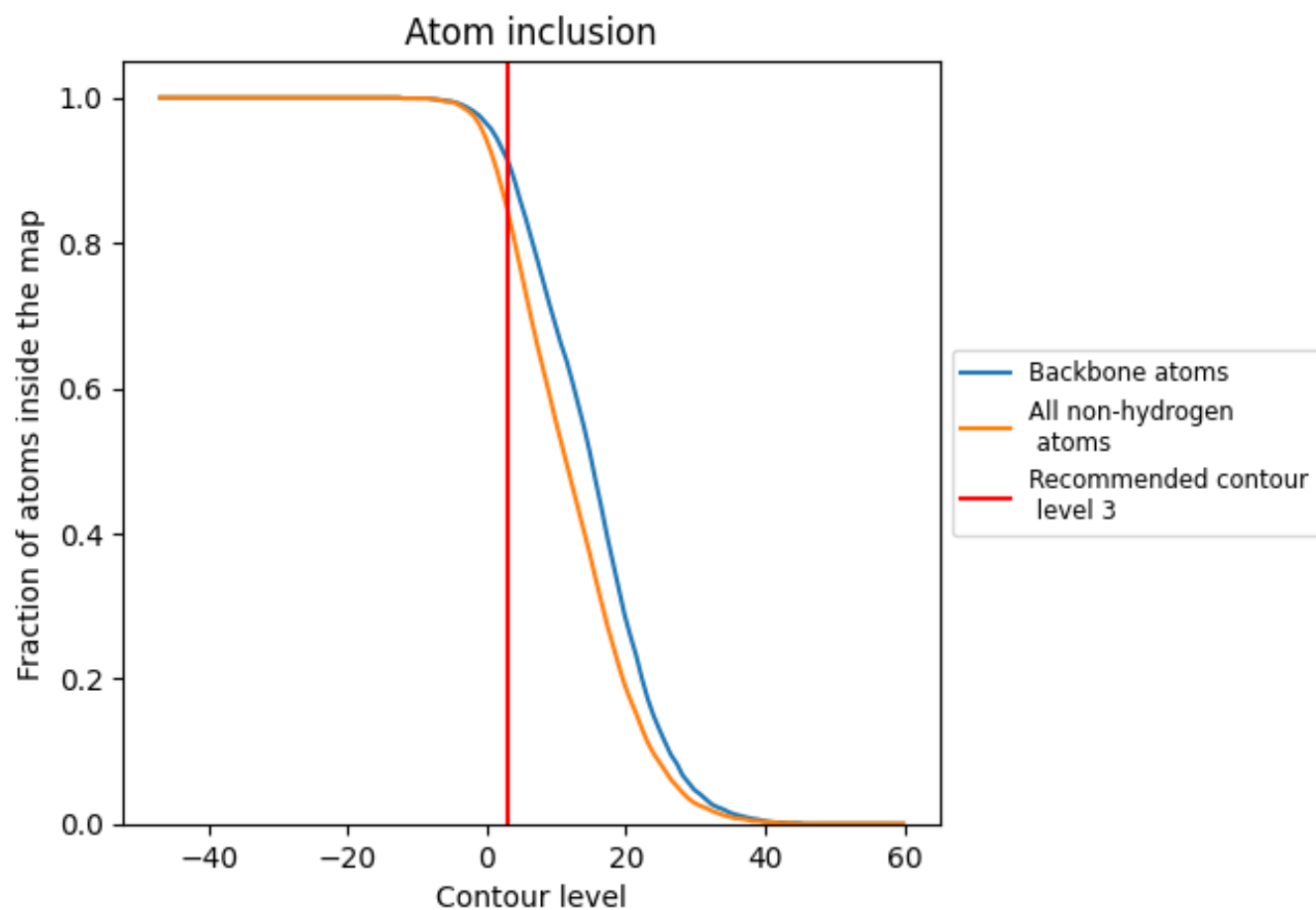
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 84% 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> 0.8450	<div></div> 0.4790
A	<div></div> 0.8080	<div></div> 0.4630
B	<div></div> 0.8500	<div></div> 0.4910
G	<div></div> 0.7040	<div></div> 0.3840
R	<div></div> 0.8690	<div></div> 0.4750
S	<div></div> 0.8730	<div></div> 0.5030

