



Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 10:18 AM JST

PDB ID : 9VB4 / pdb_00009vb4
EMDB ID : EMD-64915
Title : Cryo-EM structure of the human neurotensin receptor 1 (hNTSR1)-Gi1 complex in the GDP-bound, AHD-closed C state 1, plunge-frozen 15 seconds after GDP addition
Authors : Kobayashi, K.; Matsui, T.E.; Fukuda, M.; Kawakami, K.; Yamashita, K.; Kato, H.E.
Deposited on : 2025-06-04
Resolution : 2.85 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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:

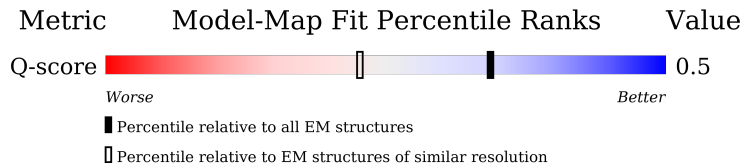
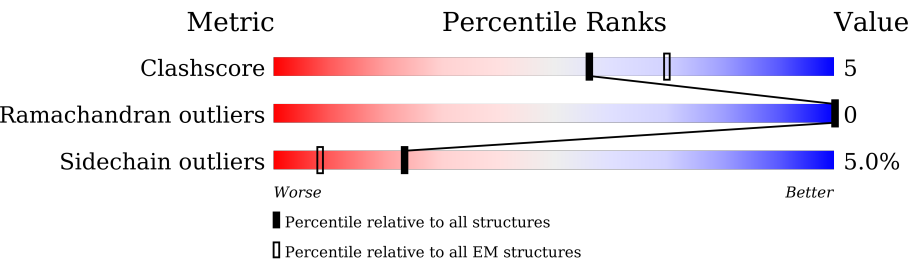
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

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	R	436	
2	L	6	
3	A	354	
4	B	358	

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Mol	Chain	Length	Quality of chain
5	C	71	<div><div></div><div>70%</div><div></div><div>25%</div></div>
6	D	259	<div><div></div><div>78%</div><div>10%</div><div>11%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10066 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 Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	309	Total	C	N	O	S	0	0
			2442	1602	410	415	15		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-11	MET	-	initiating methionine	UNP P30989
R	-10	GLY	-	expression tag	UNP P30989
R	-9	GLN	-	expression tag	UNP P30989
R	-8	PRO	-	expression tag	UNP P30989
R	-7	GLY	-	expression tag	UNP P30989
R	-6	ASN	-	expression tag	UNP P30989
R	-5	GLY	-	expression tag	UNP P30989
R	-4	SER	-	expression tag	UNP P30989
R	-3	ALA	-	expression tag	UNP P30989
R	-2	PHE	-	expression tag	UNP P30989
R	-1	LEU	-	expression tag	UNP P30989
R	0	LEU	-	expression tag	UNP P30989
R	1	ALA	-	expression tag	UNP P30989
R	2	PRO	-	expression tag	UNP P30989
R	3	ASN	-	expression tag	UNP P30989
R	4	ARG	-	expression tag	UNP P30989
R	5	SER	-	expression tag	UNP P30989
R	6	HIS	-	expression tag	UNP P30989
R	7	ALA	-	expression tag	UNP P30989
R	8	PRO	-	expression tag	UNP P30989
R	9	ASP	-	expression tag	UNP P30989
R	10	HIS	-	expression tag	UNP P30989
R	11	ASP	-	expression tag	UNP P30989
R	12	VAL	-	expression tag	UNP P30989
R	13	GLU	-	expression tag	UNP P30989
R	14	ASN	-	expression tag	UNP P30989
R	15	LEU	-	expression tag	UNP P30989
R	16	TYR	-	expression tag	UNP P30989

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Chain	Residue	Modelled	Actual	Comment	Reference
R	17	PHE	-	expression tag	UNP P30989
R	18	GLN	-	expression tag	UNP P30989
R	19	GLY	-	expression tag	UNP P30989
R	85	LEU	ALA	engineered mutation	UNP P30989
R	419	LEU	-	expression tag	UNP P30989
R	420	GLU	-	expression tag	UNP P30989
R	421	VAL	-	expression tag	UNP P30989
R	422	LEU	-	expression tag	UNP P30989
R	423	PHE	-	expression tag	UNP P30989
R	424	GLN	-	expression tag	UNP P30989

- Molecule 2 is a protein called JMV449.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	6	Total	C	N	O	0	0
			53	38	8	7		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	351	Total	C	N	O	S	0	0
			2793	1765	473	539	16		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	338	Total	C	N	O	S	0	0
			2584	1595	462	506	21		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

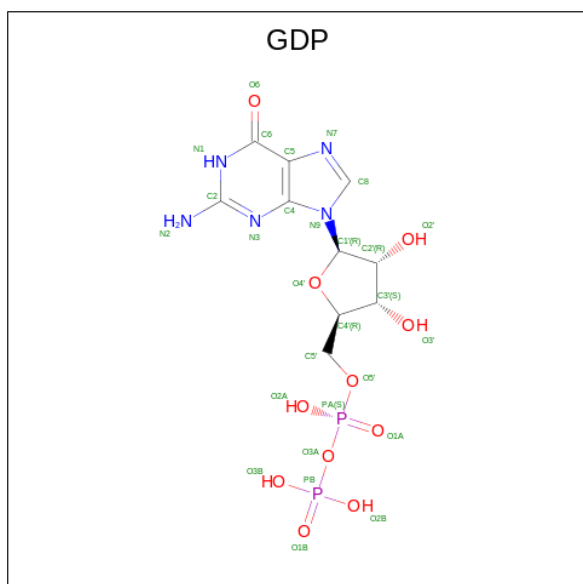
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	53	Total	C	N	O	S	0	0
			404	256	70	75	3		

- Molecule 6 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	231	Total	C	N	O	S	0	0
			1762	1121	294	337	10		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).

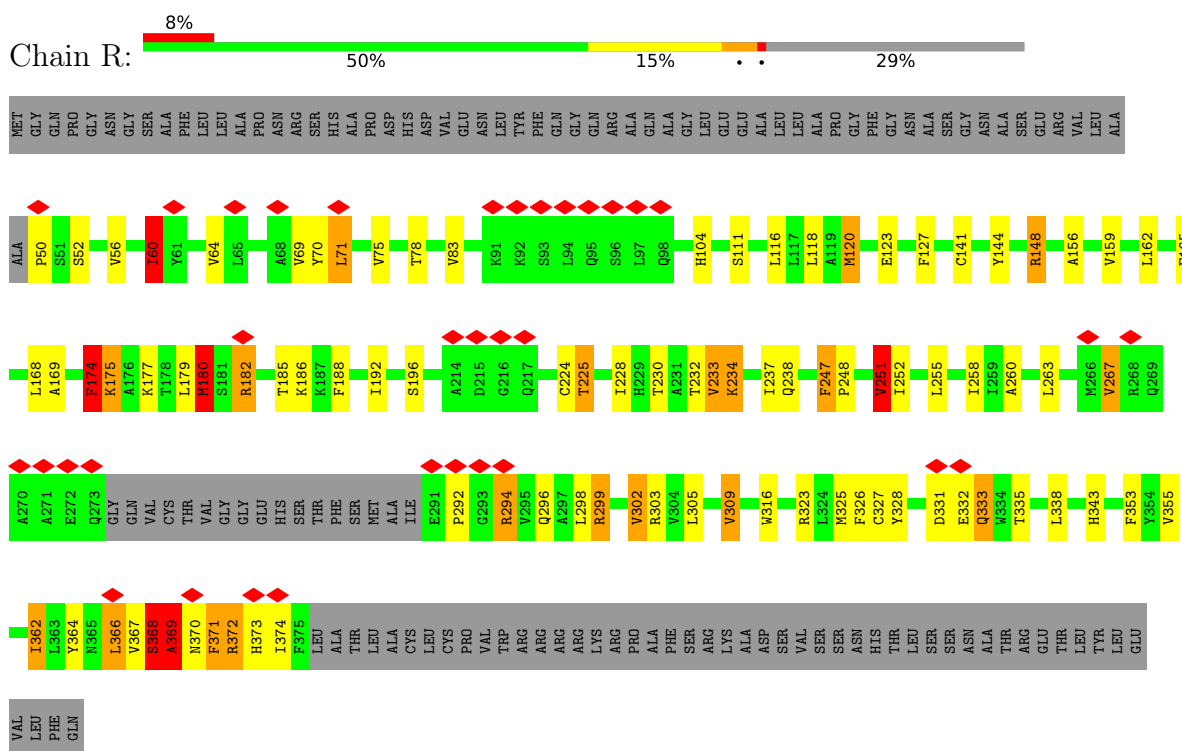


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	28	10	5	11	2	0

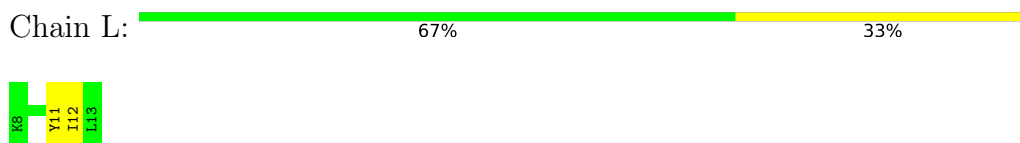
3 Residue-property plots [i](#)

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.

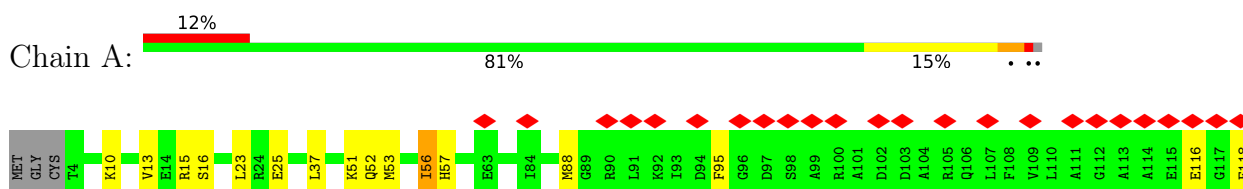
• Molecule 1: Neurotensin receptor type 1

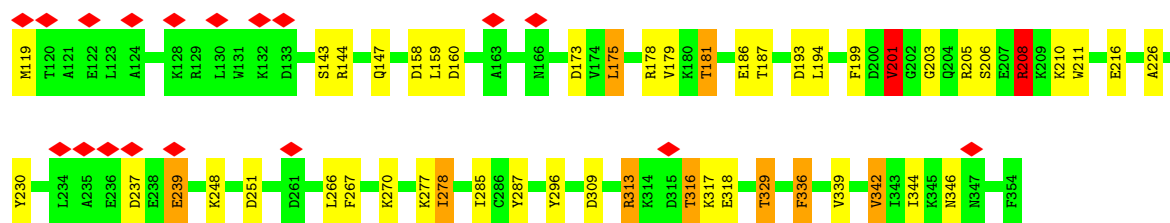


• Molecule 2: JMV449



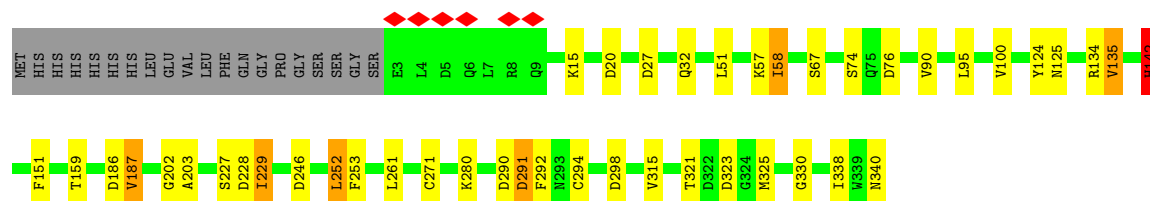
• Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-1





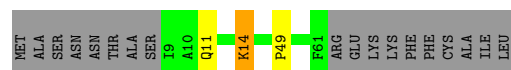
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 82% 11% 6%



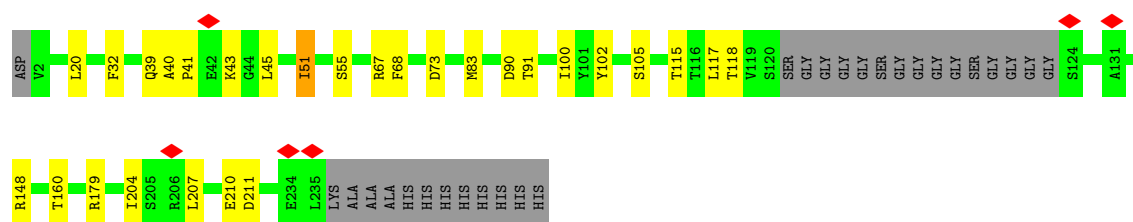
- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C: 70% 25%



- Molecule 6: scFv16

Chain D: 78% 10% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.643	Depositor
Minimum map value	-0.732	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.308	Depositor
Map size (\AA)	160.46666, 160.46666, 160.46666	wwPDB
Map dimensions	116, 116, 116	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3833333, 1.3833333, 1.3833333	Depositor

5 Model quality

5.1 Standard geometry

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

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	R	0.99	8/2506 (0.3%)	1.89	43/3419 (1.3%)
2	L	0.87	0/54	1.67	1/69 (1.4%)
3	A	0.72	0/2840	1.69	25/3825 (0.7%)
4	B	0.75	1/2631 (0.0%)	1.47	21/3569 (0.6%)
5	C	0.67	0/410	1.52	1/554 (0.2%)
6	D	0.73	0/1806	1.30	4/2450 (0.2%)
All	All	0.80	9/10247 (0.1%)	1.62	95/13886 (0.7%)

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	R	0	8
3	A	0	2
6	D	0	1
All	All	0	11

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	71	LEU	CG-CD1	19.84	2.18	1.52
1	R	71	LEU	CG-CD2	-11.03	1.16	1.52
1	R	174	PHE	CG-CD2	-9.14	1.19	1.38
1	R	118	LEU	CG-CD1	-7.91	1.26	1.52
1	R	332	GLU	CA-CB	-7.63	1.41	1.53
1	R	52	SER	CB-OG	-6.50	1.29	1.42
4	B	142	HIS	CE1-NE2	-6.35	1.26	1.32
1	R	60	ILE	CB-CG2	-6.13	1.32	1.52
1	R	186	LYS	CB-CG	5.69	1.69	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	174	PHE	CD1-CG-CD2	18.72	146.68	118.60
1	R	148	ARG	NE-CZ-NH1	-14.66	106.84	121.50
1	R	118	LEU	CD1-CG-CD2	14.31	142.29	110.80
1	R	174	PHE	CB-CG-CD2	-13.83	97.19	120.70
1	R	148	ARG	NE-CZ-NH2	12.00	130.00	119.20
1	R	71	LEU	CB-CG-CD2	11.75	145.96	110.70
3	A	346	ASN	CB-CA-C	-11.22	93.08	110.92
3	A	342	VAL	N-CA-CB	10.51	122.84	110.55
1	R	127	PHE	CB-CA-C	9.72	124.78	109.03
1	R	174	PHE	CG-CD1-CE1	-9.44	104.66	120.70
1	R	174	PHE	CG-CD2-CE2	-8.68	105.94	120.70
1	R	309	VAL	N-CA-CB	8.68	120.08	110.62
3	A	309	ASP	CA-CB-CG	8.60	121.20	112.60
1	R	71	LEU	CD1-CG-CD2	-8.59	91.91	110.80
6	D	211	ASP	CA-CB-CG	8.47	121.07	112.60
1	R	123	GLU	N-CA-CB	8.21	122.18	109.94
1	R	294	ARG	NE-CZ-NH1	-8.20	113.30	121.50
4	B	291	ASP	CB-CA-C	-7.99	93.87	110.17
1	R	75	VAL	N-CA-CB	7.68	119.53	110.55
1	R	233	VAL	N-CA-CB	7.64	120.94	110.54
1	R	188	PHE	CA-CB-CG	7.56	121.36	113.80
1	R	368	SER	N-CA-C	-7.44	94.89	107.99
1	R	186	LYS	CA-CB-CG	-7.37	99.37	114.10
3	A	208	ARG	NE-CZ-NH1	-7.25	114.25	121.50
3	A	208	ARG	NE-CZ-NH2	6.94	125.45	119.20
3	A	339	VAL	N-CA-CB	6.83	119.82	110.54
4	B	323	ASP	CA-CB-CG	6.82	119.42	112.60
4	B	291	ASP	CA-CB-CG	6.77	119.37	112.60
3	A	201	VAL	N-CA-C	-6.76	100.81	109.80
4	B	186	ASP	CA-CB-CG	6.71	119.31	112.60
1	R	141	CYS	CB-CA-C	-6.64	100.19	110.81
3	A	267	PHE	CA-CB-CG	6.56	120.36	113.80
3	A	118	PHE	CA-CB-CG	6.51	120.31	113.80
1	R	182	ARG	CA-CB-CG	-6.40	101.30	114.10
3	A	186	GLU	N-CA-CB	6.36	119.31	109.97
4	B	252	LEU	N-CA-CB	6.31	120.71	110.43
1	R	368	SER	N-CA-CB	6.29	119.73	110.35
1	R	353	PHE	CA-CB-CG	6.27	120.07	113.80
4	B	187	VAL	N-CA-CB	6.27	119.22	110.56
3	A	10	LYS	CB-CA-C	6.27	121.19	110.79
1	R	331	ASP	CA-CB-CG	6.25	118.85	112.60
3	A	116	GLU	CB-CG-CD	6.21	123.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	158	ASP	CA-CB-CG	6.19	118.79	112.60
3	A	336	PHE	N-CA-CB	6.15	118.92	110.01
4	B	290	ASP	CA-CB-CG	6.10	118.70	112.60
3	A	193	ASP	CA-CB-CG	6.06	118.66	112.60
3	A	56	ILE	CB-CA-C	6.06	116.86	111.71
1	R	251	VAL	N-CA-CB	6.02	116.94	110.62
1	R	326	PHE	CA-CB-CG	5.99	119.79	113.80
1	R	299	ARG	CB-CA-C	5.99	119.13	109.07
3	A	116	GLU	CB-CA-C	5.96	122.29	110.42
4	B	292	PHE	CA-CB-CG	5.96	119.76	113.80
4	B	57	LYS	CB-CG-CD	5.95	124.98	111.30
4	B	27	ASP	CA-CB-CG	5.94	118.54	112.60
1	R	71	LEU	CB-CG-CD1	-5.81	93.28	110.70
1	R	144	TYR	N-CA-CB	5.79	118.37	109.91
3	A	287	TYR	CB-CA-C	5.79	116.60	110.17
1	R	180	MET	CB-CA-C	-5.78	102.02	110.06
1	R	174	PHE	CB-CG-CD1	-5.78	110.88	120.70
1	R	247	PHE	CA-CB-CG	5.69	119.49	113.80
4	B	135	VAL	N-CA-CB	5.64	117.50	111.46
4	B	32	GLN	N-CA-CB	5.62	118.47	110.16
4	B	228	ASP	CB-CA-C	-5.60	100.68	109.70
3	A	216	GLU	CB-CA-C	5.56	118.90	109.84
1	R	185	THR	CA-CB-OG1	-5.55	101.27	109.60
1	R	355	VAL	N-CA-CB	5.54	118.08	110.54
1	R	50	PRO	CB-CA-C	5.52	120.59	110.10
1	R	371	PHE	CB-CA-C	-5.51	99.77	110.46
4	B	20	ASP	CA-CB-CG	5.50	118.10	112.60
4	B	227	SER	CA-C-N	5.47	128.61	120.90
4	B	227	SER	C-N-CA	5.47	128.61	120.90
1	R	369	ALA	N-CA-C	5.45	117.11	108.67
5	C	49	PRO	N-CA-C	5.43	120.98	113.65
3	A	201	VAL	CA-C-O	-5.41	116.02	121.59
2	L	12	ILE	CA-CB-CG1	5.37	119.53	110.40
1	R	294	ARG	NE-CZ-NH2	5.32	123.99	119.20
3	A	13	VAL	N-CA-CB	5.30	117.75	110.54
6	D	73	ASP	CA-CB-CG	5.30	117.90	112.60
3	A	160	ASP	CA-CB-CG	5.28	117.88	112.60
1	R	332	GLU	CB-CA-C	5.27	121.13	110.38
4	B	151	PHE	CA-CB-CG	5.27	119.07	113.80
1	R	323	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	R	332	GLU	N-CA-CB	-5.17	102.34	110.30
6	D	41	PRO	N-CA-C	5.15	121.28	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	69	VAL	N-CA-CB	5.14	116.56	110.55
4	B	291	ASP	N-CA-C	-5.13	106.86	113.01
4	B	298	ASP	CA-CB-CG	5.12	117.72	112.60
3	A	173	ASP	CA-CB-CG	5.10	117.70	112.60
3	A	251	ASP	CA-CB-CG	5.09	117.69	112.60
1	R	353	PHE	CB-CA-C	5.05	119.17	110.79
4	B	253	PHE	CA-CB-CG	5.05	118.85	113.80
6	D	68	PHE	CA-CB-CG	5.05	118.85	113.80
3	A	206	SER	CA-C-O	-5.04	116.03	121.38
4	B	246	ASP	CA-CB-CG	5.04	117.64	112.60
1	R	303	ARG	NE-CZ-NH2	5.04	123.73	119.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	208	ARG	Sidechain
3	A	313	ARG	Sidechain
6	D	210	GLU	Peptide
1	R	148	ARG	Sidechain
1	R	169	ALA	Mainchain
1	R	174	PHE	Sidechain
1	R	182	ARG	Sidechain
1	R	294	ARG	Sidechain
1	R	368	SER	Peptide
1	R	369	ALA	Peptide
1	R	372	ARG	Sidechain

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	R	2442	0	2476	48	0
2	L	53	0	63	1	0
3	A	2793	0	2739	26	0
4	B	2584	0	2473	16	0
5	C	404	0	416	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1762	0	1694	11	0
7	A	28	0	12	0	0
All	All	10066	0	9873	97	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 5.

All (97) 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:R:71:LEU:CD1	1:R:71:LEU:CG	2.18	1.22
3:A:52:GLN:HE21	3:A:329:THR:HG23	1.13	1.14
1:R:174:PHE:CE2	3:A:344:ILE:HG13	2.05	0.91
3:A:313:ARG:HB2	3:A:316:THR:HG22	1.53	0.89
1:R:71:LEU:CD1	1:R:71:LEU:CD2	2.50	0.89
3:A:56:ILE:HD11	3:A:329:THR:HG22	1.57	0.84
3:A:119:MET:HE1	3:A:159:LEU:HD11	1.64	0.79
1:R:251:VAL:HG13	1:R:255:LEU:HD12	1.65	0.77
3:A:52:GLN:HE21	3:A:329:THR:CG2	1.99	0.73
1:R:71:LEU:CD1	1:R:71:LEU:HD22	2.21	0.69
3:A:52:GLN:NE2	3:A:329:THR:HG23	1.97	0.67
3:A:52:GLN:OE1	3:A:175:LEU:HG	1.94	0.67
6:D:83:MET:HE1	6:D:117:LEU:HD13	1.77	0.66
3:A:56:ILE:CD1	3:A:329:THR:HG22	2.25	0.65
1:R:71:LEU:CD1	1:R:71:LEU:CB	2.73	0.65
1:R:237:ILE:HD12	1:R:327:CYS:SG	2.39	0.63
1:R:260:ALA:HB1	1:R:302:VAL:HG13	1.83	0.60
3:A:15:ARG:NH1	4:B:90:VAL:O	2.35	0.60
4:B:90:VAL:HG13	6:D:102:TYR:HB2	1.85	0.58
3:A:144:ARG:HH12	3:A:285:ILE:HG21	1.70	0.56
3:A:181:THR:HG22	3:A:203:GLY:HA3	1.88	0.56
1:R:369:ALA:HB1	1:R:372:ARG:H	1.70	0.55
4:B:58:ILE:HD11	4:B:330:GLY:HA3	1.89	0.55
6:D:105:SER:O	6:D:179:ARG:NH2	2.40	0.55
1:R:228:ILE:HD12	1:R:232:THR:HG23	1.89	0.54
6:D:91:THR:HG23	6:D:118:THR:HA	1.90	0.54
1:R:104:HIS:CE1	1:R:165:GLU:HG3	2.44	0.53
1:R:230:THR:HA	1:R:233:VAL:HG12	1.91	0.53
1:R:116:LEU:HD22	1:R:120:MET:HE3	1.91	0.53
1:R:371:PHE:O	1:R:374:ILE:N	2.42	0.52
4:B:74:SER:OG	4:B:76:ASP:OD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:296:GLN:HA	1:R:299:ARG:HE	1.75	0.51
3:A:56:ILE:HG22	3:A:57:HIS:CD2	2.46	0.51
4:B:95:LEU:HD13	4:B:100:VAL:HG21	1.91	0.51
1:R:370:ASN:O	1:R:373:HIS:N	2.44	0.51
1:R:159:VAL:HG12	1:R:252:ILE:HG21	1.93	0.50
1:R:369:ALA:O	1:R:372:ARG:HB2	2.11	0.50
4:B:142:HIS:HE1	4:B:159:THR:OG1	1.95	0.49
1:R:233:VAL:HG13	1:R:327:CYS:SG	2.52	0.49
1:R:366:LEU:O	1:R:369:ALA:HB2	2.13	0.49
1:R:60:ILE:O	1:R:64:VAL:HG23	2.13	0.49
1:R:263:LEU:O	1:R:267:VAL:HG23	2.12	0.48
6:D:204:ILE:HG21	6:D:207:LEU:HD23	1.94	0.48
1:R:156:ALA:HB2	1:R:316:TRP:HZ3	1.78	0.48
3:A:56:ILE:CG1	3:A:329:THR:HG22	2.43	0.48
1:R:177:LYS:HG2	3:A:194:LEU:HD11	1.94	0.48
1:R:175:LYS:HB2	1:R:175:LYS:HE2	1.51	0.47
1:R:267:VAL:HG22	1:R:298:LEU:HB3	1.95	0.47
3:A:230:TYR:OH	3:A:277:LYS:HB3	2.14	0.47
1:R:238:GLN:NE2	1:R:328:TYR:OH	2.47	0.47
4:B:202:GLY:HA2	4:B:229:ILE:HD11	1.96	0.47
3:A:208:ARG:HG2	3:A:211:TRP:CH2	2.51	0.46
1:R:371:PHE:CA	1:R:374:ILE:HG22	2.45	0.46
3:A:15:ARG:O	3:A:16:SER:C	2.58	0.46
4:B:271:CYS:SG	4:B:291:ASP:OD1	2.66	0.46
3:A:53:MET:HE1	3:A:336:PHE:CD1	2.50	0.46
5:C:11:GLN:HA	5:C:14:LYS:HE3	1.97	0.46
1:R:333:GLN:O	1:R:335:THR:HG23	2.16	0.45
1:R:371:PHE:O	1:R:372:ARG:C	2.58	0.45
1:R:333:GLN:O	1:R:338:LEU:HD12	2.15	0.45
1:R:174:PHE:CE2	3:A:344:ILE:CG1	2.90	0.45
4:B:125:ASN:HD22	4:B:134:ARG:HH11	1.64	0.45
3:A:88:MET:HE1	3:A:95:PHE:CE1	2.52	0.45
1:R:56:VAL:HG11	1:R:343:HIS:CD2	2.53	0.44
1:R:247:PHE:HB3	1:R:248:PRO:HD3	2.00	0.44
1:R:180:MET:HE3	1:R:180:MET:HB3	1.62	0.44
6:D:67:ARG:HH22	6:D:90:ASP:CG	2.25	0.43
3:A:37:LEU:HD12	3:A:199:PHE:O	2.18	0.43
1:R:224:CYS:O	1:R:225:THR:HG23	2.18	0.43
1:R:162:LEU:HD13	1:R:364:TYR:CE1	2.53	0.43
1:R:252:ILE:O	1:R:309:VAL:HG22	2.18	0.43
4:B:67:SER:HB2	4:B:321:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:VAL:HG21	3:A:211:TRP:CZ3	2.53	0.43
3:A:278:ILE:HD11	3:A:296:TYR:HA	2.00	0.43
4:B:187:VAL:HG12	4:B:203:ALA:HB2	2.00	0.43
6:D:20:LEU:HD22	6:D:115:THR:HG21	2.00	0.43
1:R:70:TYR:O	1:R:120:MET:HE1	2.18	0.42
4:B:325:MET:O	4:B:340:ASN:ND2	2.53	0.42
1:R:366:LEU:HD12	1:R:371:PHE:H	1.84	0.42
4:B:252:LEU:HD11	4:B:261:LEU:HD23	2.01	0.42
6:D:51:ILE:HG22	6:D:55:SER:HA	2.02	0.42
3:A:237:ASP:HB3	3:A:239:GLU:HG3	2.01	0.42
4:B:51:LEU:HD11	4:B:338:ILE:HD11	2.01	0.42
4:B:124:TYR:CE1	4:B:135:VAL:HG22	2.55	0.42
6:D:32:PHE:CD1	6:D:100:ILE:HB	2.55	0.42
1:R:369:ALA:HB3	1:R:372:ARG:HE	1.85	0.42
1:R:156:ALA:HB1	1:R:248:PRO:HG2	2.01	0.41
1:R:83:VAL:HG13	1:R:374:ILE:HG12	2.02	0.41
1:R:371:PHE:HA	1:R:374:ILE:HG22	2.03	0.41
1:R:234:LYS:HA	1:R:327:CYS:SG	2.61	0.41
3:A:226:ALA:HB2	3:A:270:LYS:HE3	2.03	0.41
6:D:40:ALA:HB3	6:D:43:LYS:HB2	2.03	0.41
1:R:362:ILE:O	1:R:367:VAL:HG23	2.20	0.41
6:D:39:GLN:HB2	6:D:45:LEU:HD23	2.03	0.41
1:R:225:THR:CG2	2:L:11:TYR:HB2	2.51	0.40
1:R:156:ALA:HB2	1:R:316:TRP:CZ3	2.56	0.40
4:B:294:CYS:SG	4:B:315:VAL:HG11	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	R	305/436 (70%)	287 (94%)	18 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	A	349/354 (99%)	329 (94%)	20 (6%)	0	100	100
4	B	336/358 (94%)	327 (97%)	9 (3%)	0	100	100
5	C	51/71 (72%)	51 (100%)	0	0	100	100
6	D	227/259 (88%)	221 (97%)	6 (3%)	0	100	100
All	All	1272/1484 (86%)	1218 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	265/368 (72%)	242 (91%)	23 (9%)	9	21
2	L	6/6 (100%)	6 (100%)	0	100	100
3	A	297/305 (97%)	275 (93%)	22 (7%)	13	26
4	B	277/298 (93%)	272 (98%)	5 (2%)	51	73
5	C	42/58 (72%)	41 (98%)	1 (2%)	43	67
6	D	191/209 (91%)	188 (98%)	3 (2%)	55	76
All	All	1078/1244 (87%)	1024 (95%)	54 (5%)	23	44

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	60	ILE
1	R	78	THR
1	R	111	SER
1	R	120	MET
1	R	168	LEU
1	R	175	LYS
1	R	179	LEU
1	R	180	MET

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Mol	Chain	Res	Type
1	R	192	ILE
1	R	196	SER
1	R	225	THR
1	R	234	LYS
1	R	251	VAL
1	R	258	ILE
1	R	267	VAL
1	R	292	PRO
1	R	302	VAL
1	R	305	LEU
1	R	325	MET
1	R	333	GLN
1	R	362	ILE
1	R	366	LEU
1	R	368	SER
3	A	23	LEU
3	A	25	GLU
3	A	51	LYS
3	A	143	SER
3	A	147	GLN
3	A	175	LEU
3	A	178	ARG
3	A	179	VAL
3	A	181	THR
3	A	187	THR
3	A	201	VAL
3	A	205	ARG
3	A	210	LYS
3	A	239	GLU
3	A	248	LYS
3	A	266	LEU
3	A	278	ILE
3	A	316	THR
3	A	317	LYS
3	A	318	GLU
3	A	329	THR
3	A	342	VAL
4	B	15	LYS
4	B	58	ILE
4	B	142	HIS
4	B	229	ILE
4	B	280	LYS

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Mol	Chain	Res	Type
5	C	14	LYS
6	D	51	ILE
6	D	148	ARG
6	D	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	238	GLN
1	R	320	HIS
1	R	350	ASN
1	R	360	ASN
3	A	22	ASN
3	A	52	GLN
3	A	57	HIS
3	A	106	GLN
3	A	204	GLN
3	A	241	ASN
4	B	75	GLN
4	B	88	ASN
4	B	110	ASN
4	B	119	ASN
4	B	125	ASN
4	B	142	HIS
4	B	156	GLN
4	B	220	GLN
4	B	311	HIS
4	B	340	ASN
6	D	39	GLN
6	D	155	HIS
6	D	167	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
7	GDP	A	401	-	28,30,30	0.56	0	44,47,47	0.75	1 (2%)

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	GDP	A	401	-	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	GDP	C4'-O4'-C1'	-2.21	104.60	109.47

There are no chirality outliers.

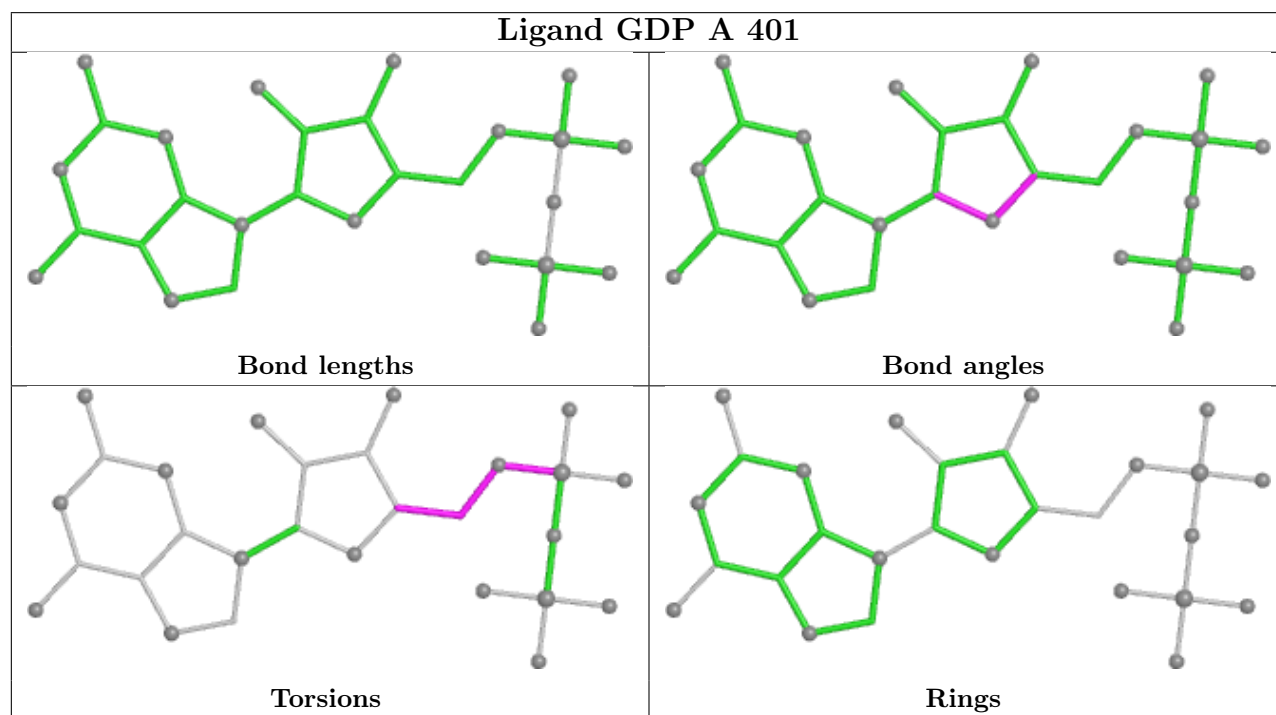
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	GDP	C5'-O5'-PA-O3A
7	A	401	GDP	O4'-C4'-C5'-O5'
7	A	401	GDP	C3'-C4'-C5'-O5'
7	A	401	GDP	C4'-C5'-O5'-PA
7	A	401	GDP	C5'-O5'-PA-O1A

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.

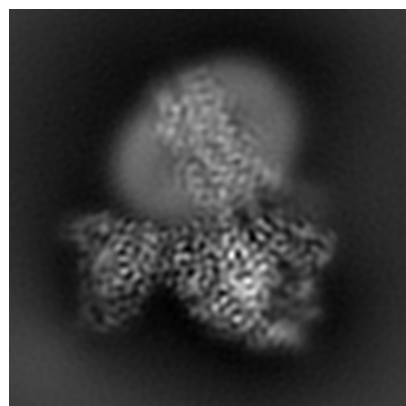
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64915. These allow visual inspection of the internal detail of the map and identification of artifacts.

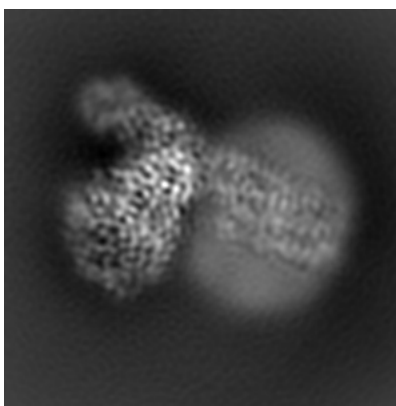
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

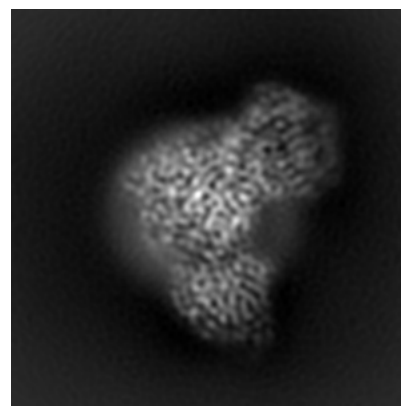
6.1.1 Primary map



X

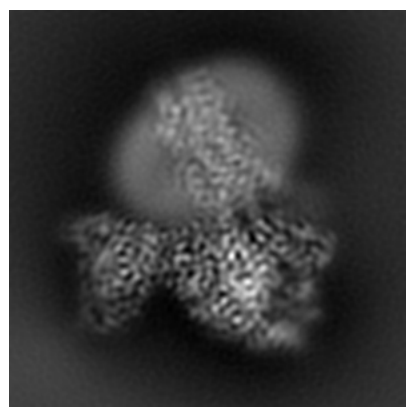


Y

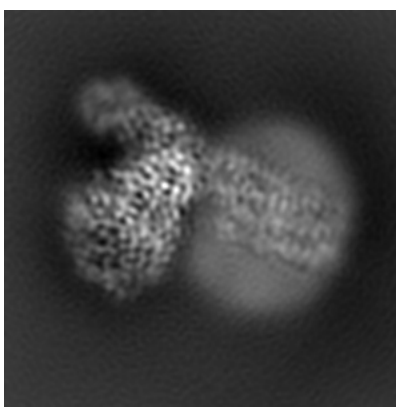


Z

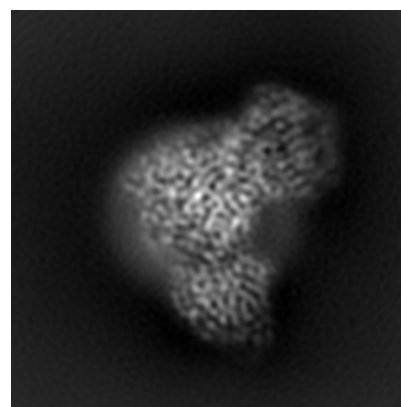
6.1.2 Raw map



X



Y

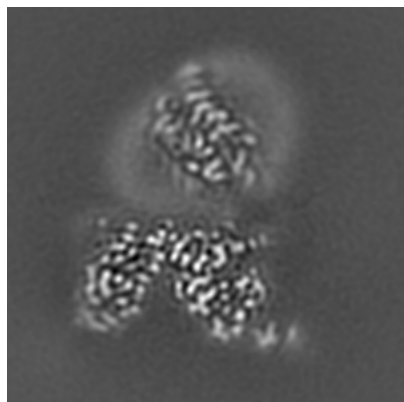


Z

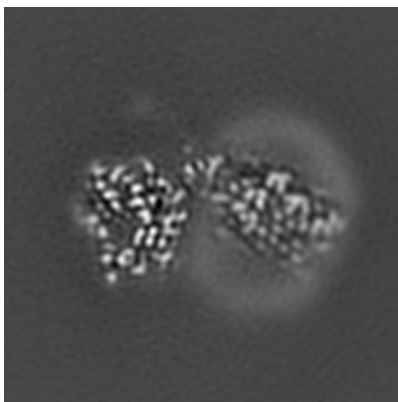
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

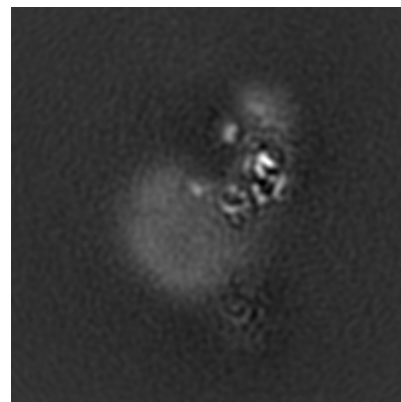
6.2.1 Primary map



X Index: 58

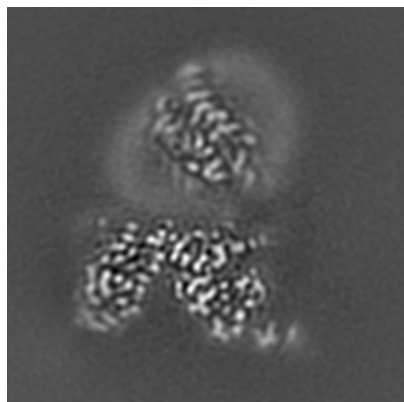


Y Index: 58

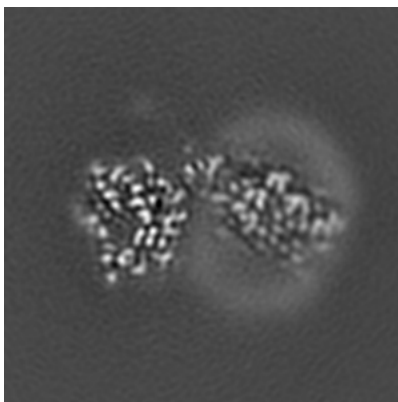


Z Index: 58

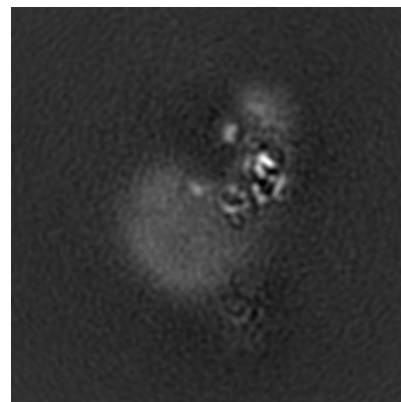
6.2.2 Raw map



X Index: 58



Y Index: 58

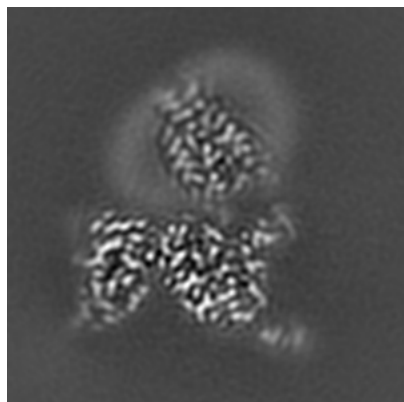


Z Index: 58

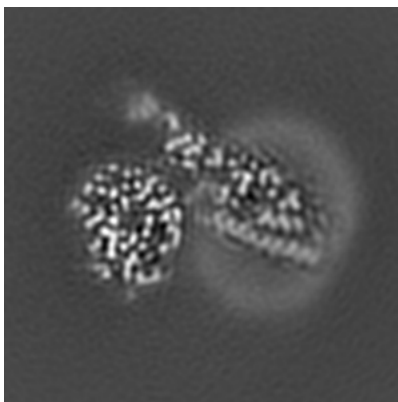
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

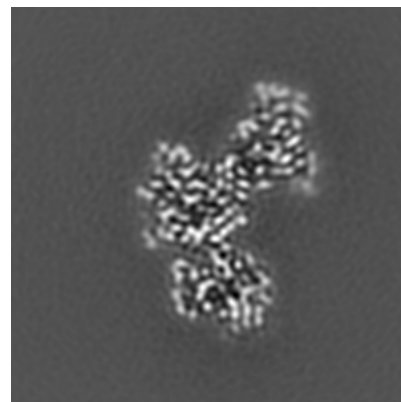
6.3.1 Primary map



X Index: 61

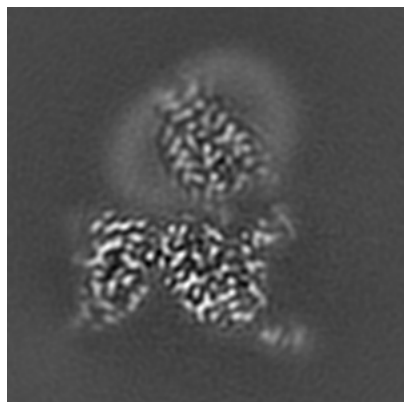


Y Index: 62

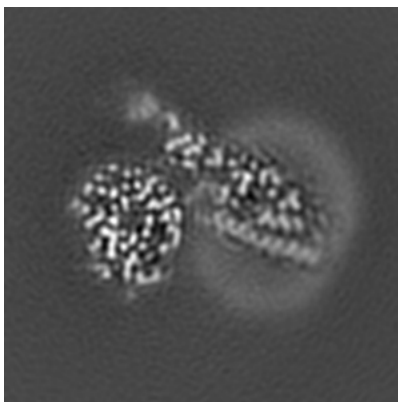


Z Index: 44

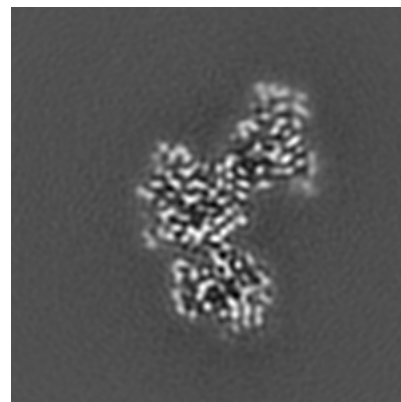
6.3.2 Raw map



X Index: 61



Y Index: 62

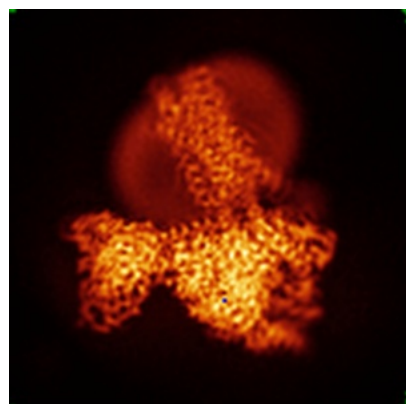


Z Index: 44

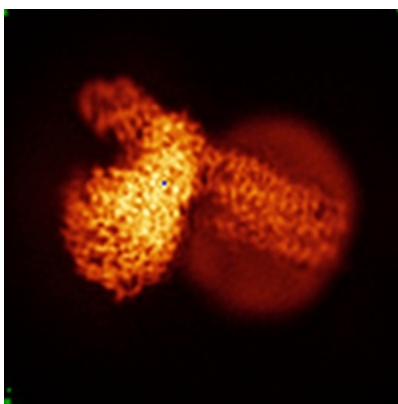
The images above show the largest variance slices of the map in three orthogonal directions.

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

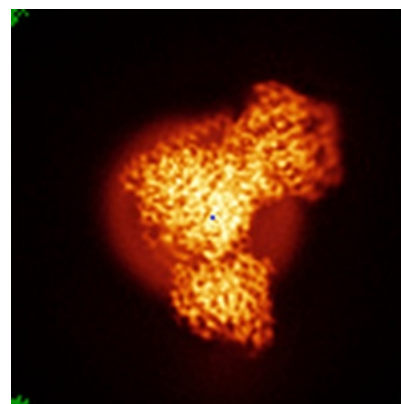
6.4.1 Primary map



X

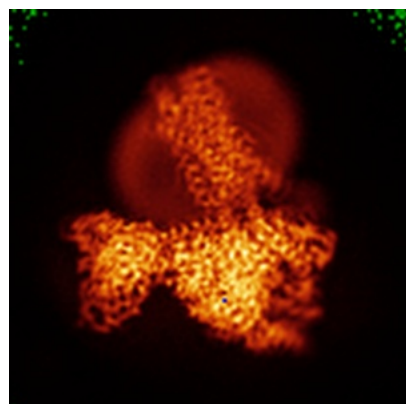


Y

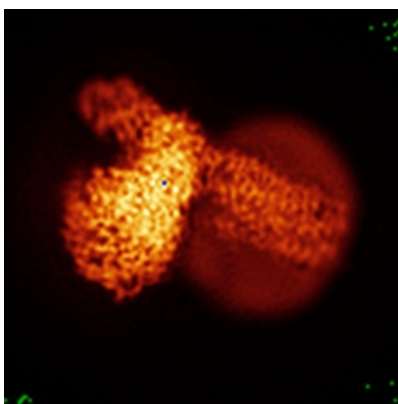


Z

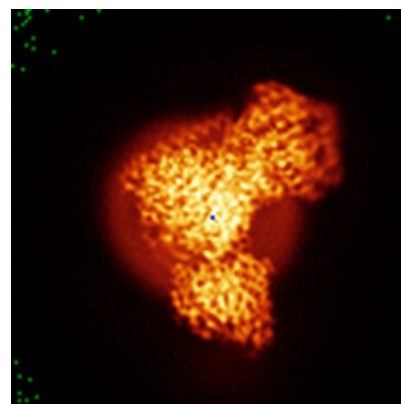
6.4.2 Raw map



X



Y

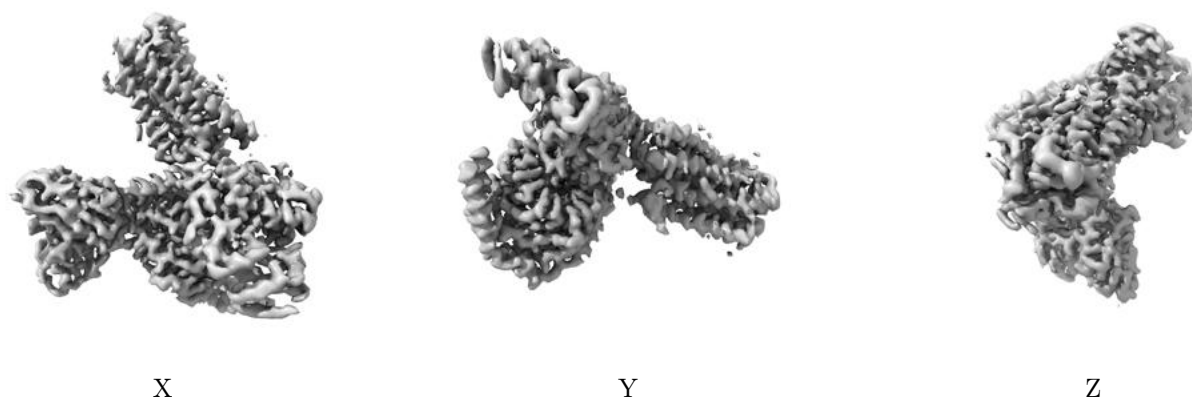


Z

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.

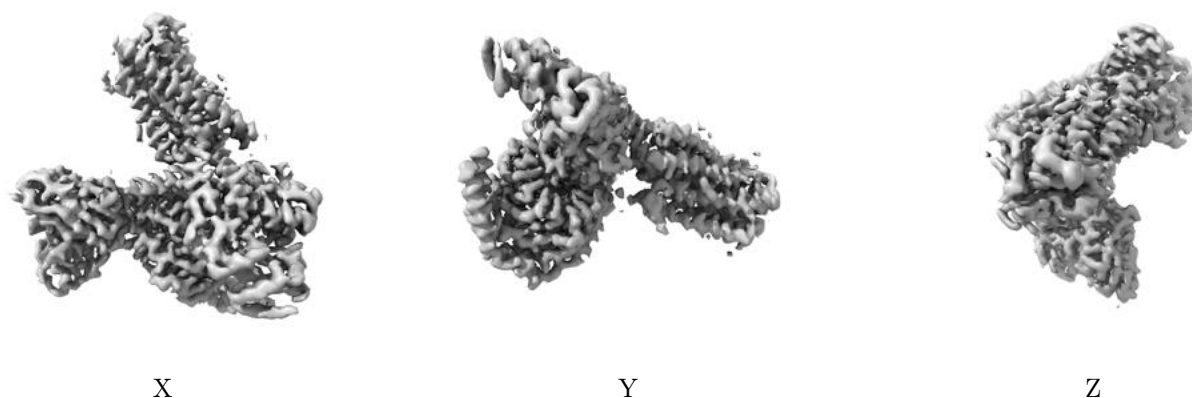
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.308. 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



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.

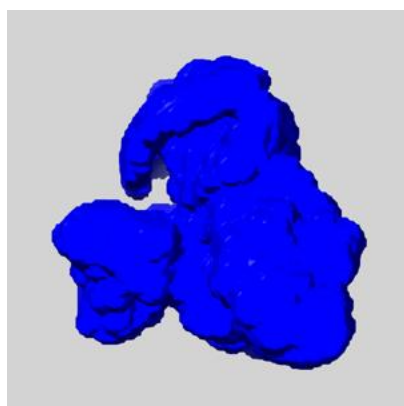
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

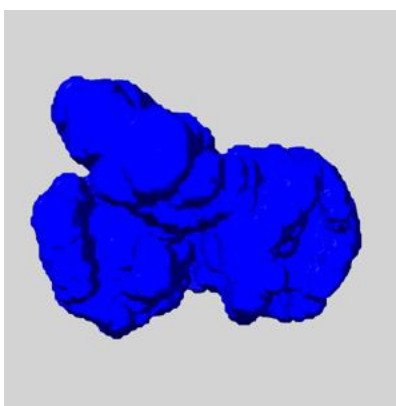
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

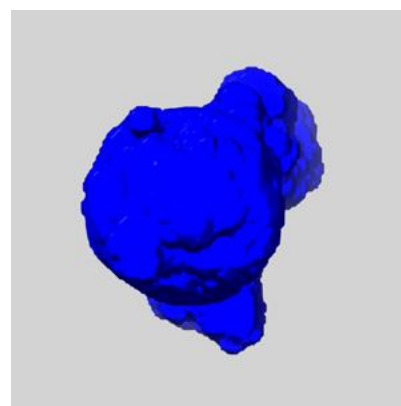
6.6.1 emd_64915_msk_1.map [i](#)



X



Y

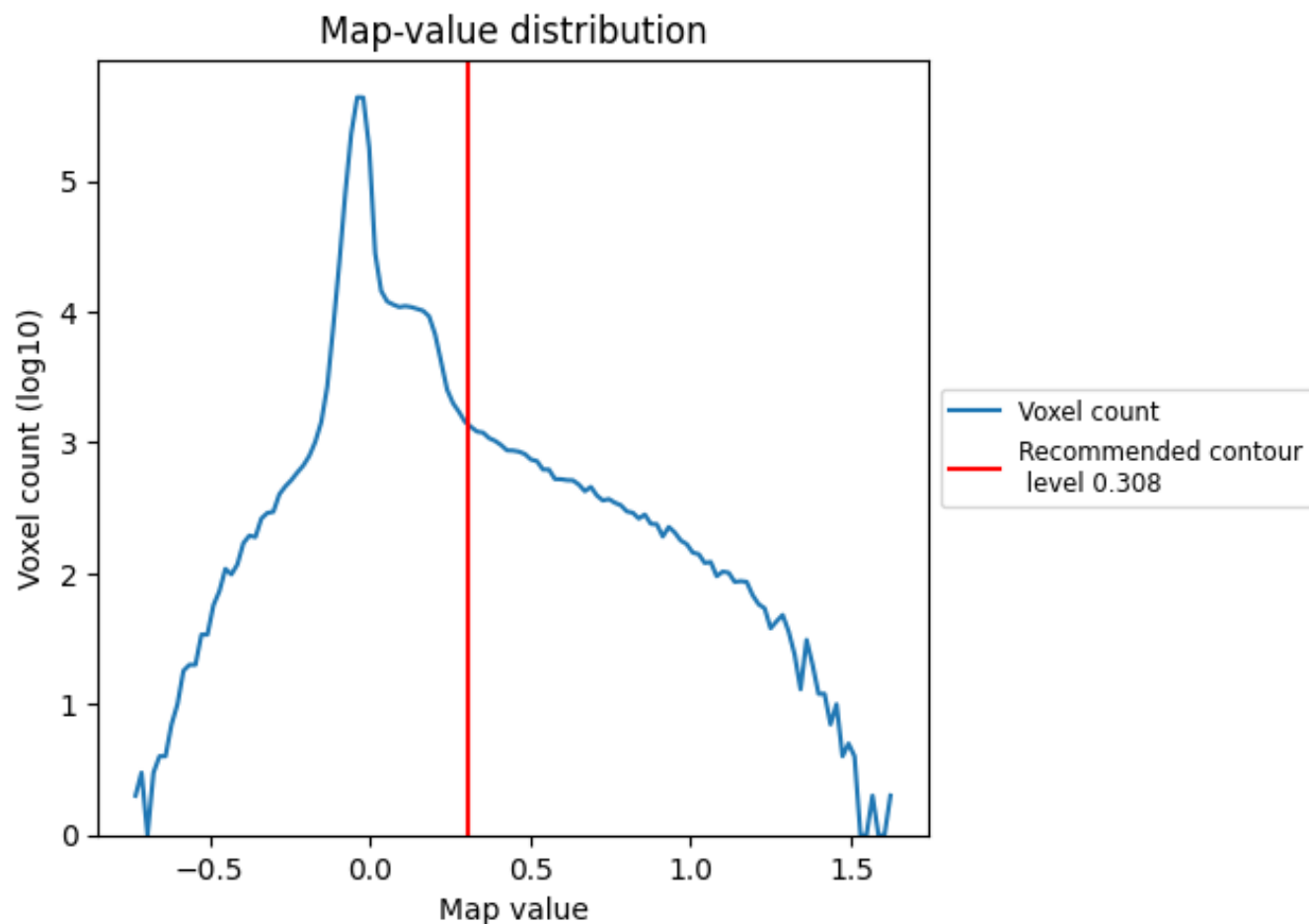


Z

7 Map analysis [i](#)

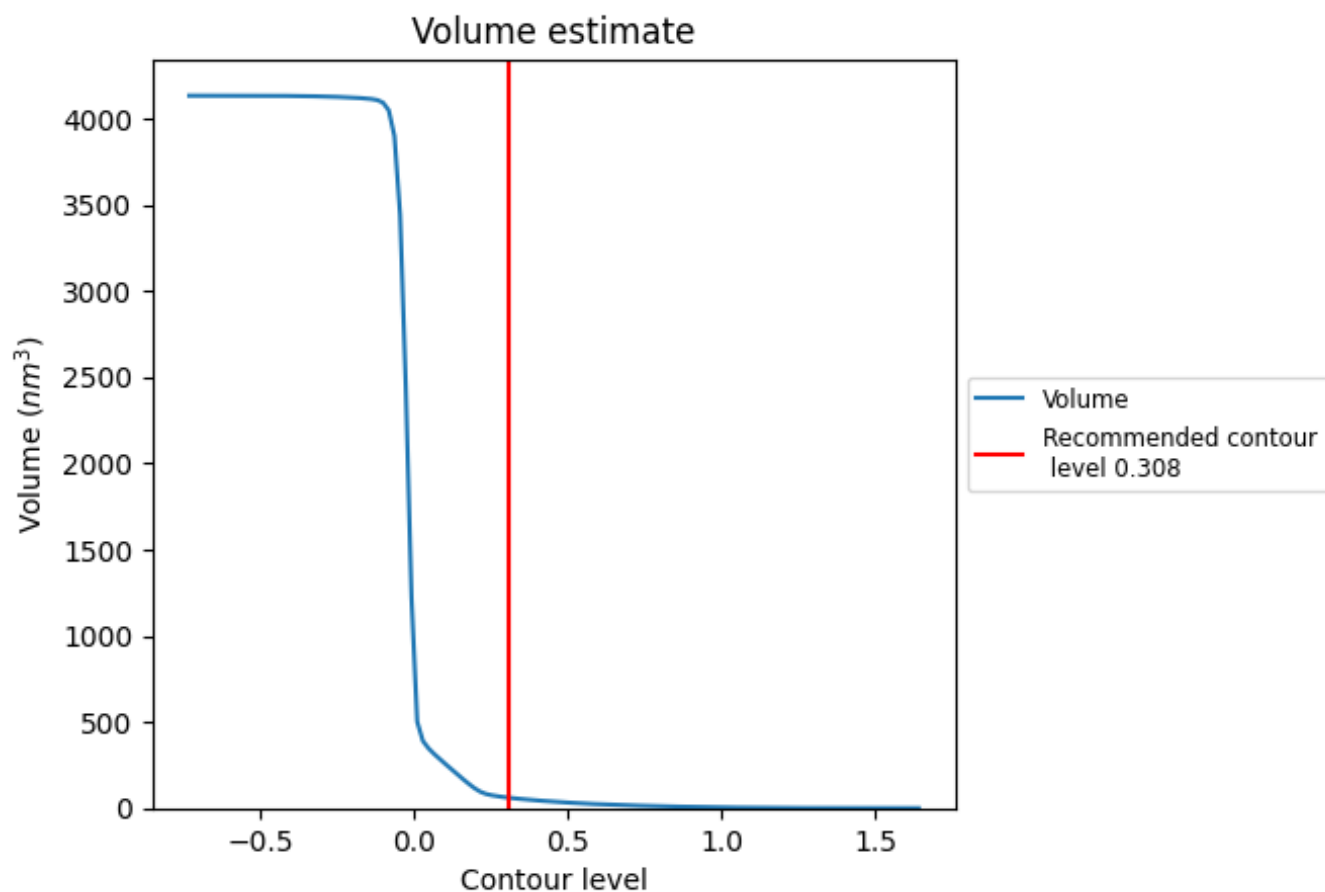
This section contains the results of statistical analysis of the map.

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.

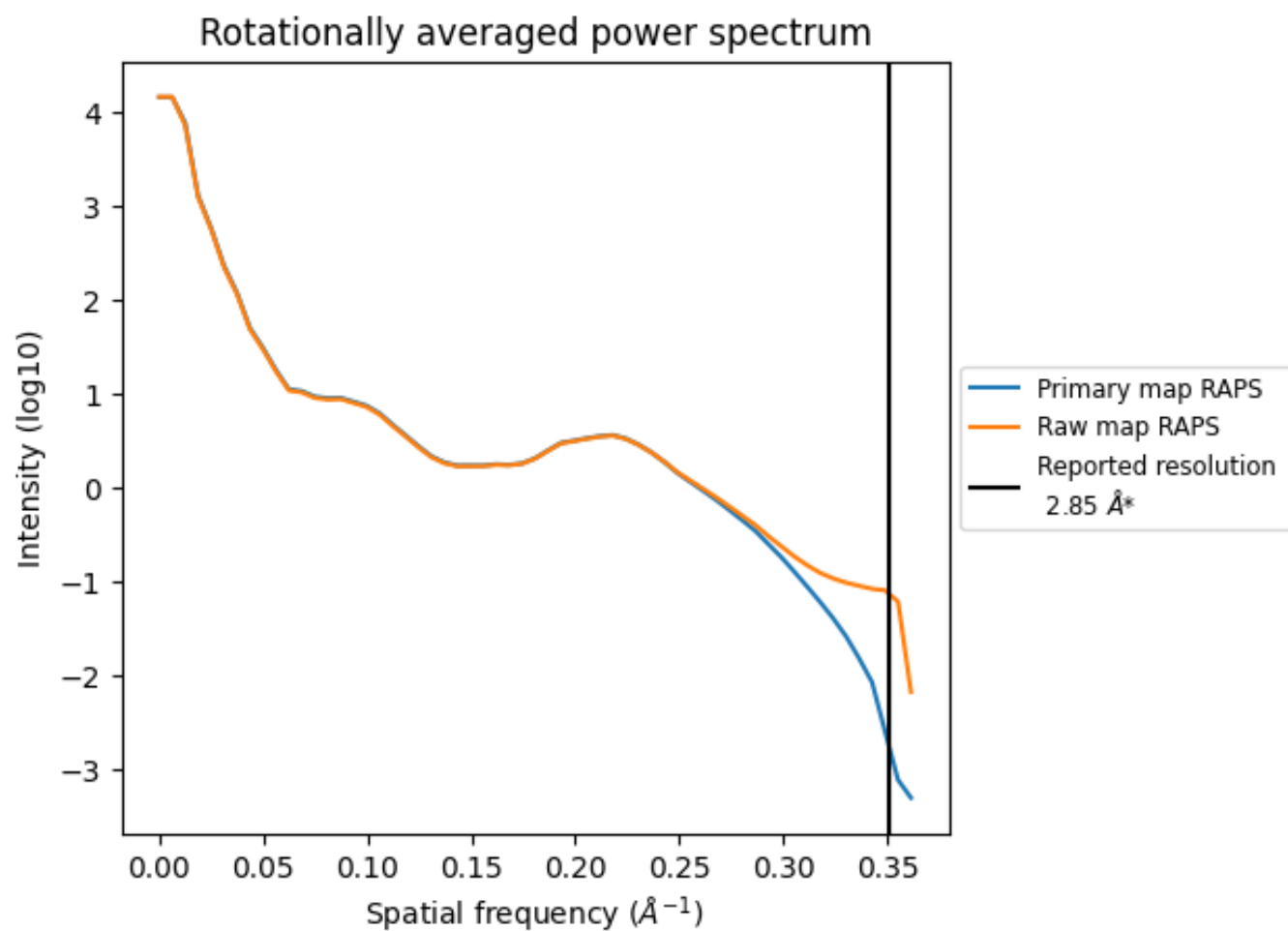
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 55 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 ⓘ

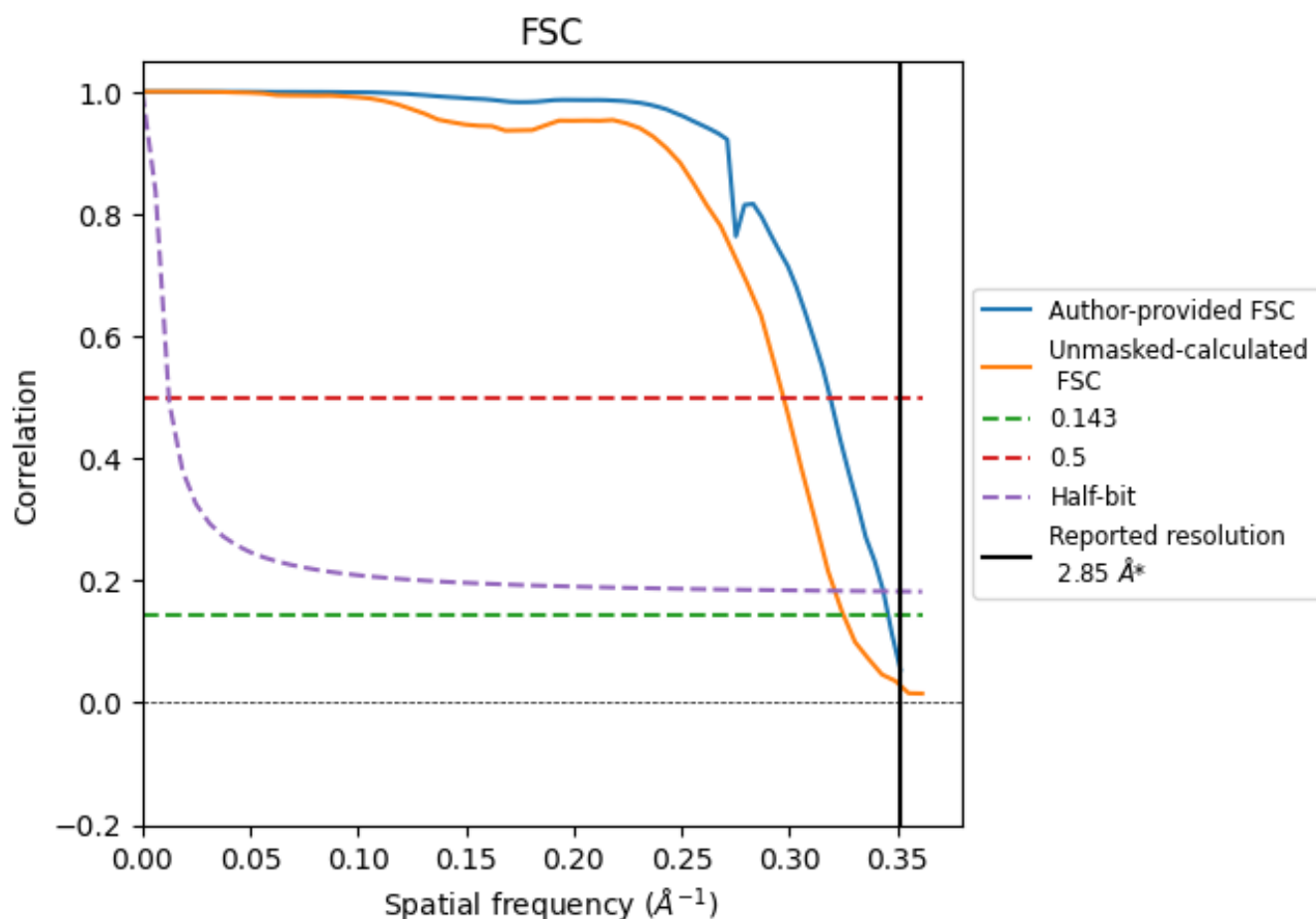


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

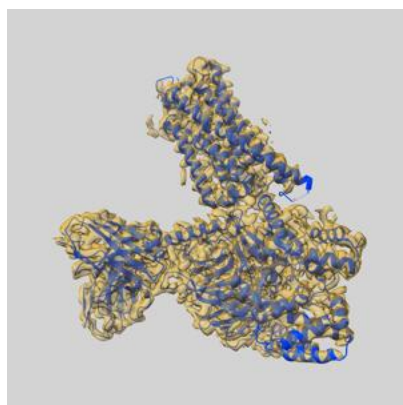
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.89	3.14	2.91
Unmasked-calculated*	3.08	3.37	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

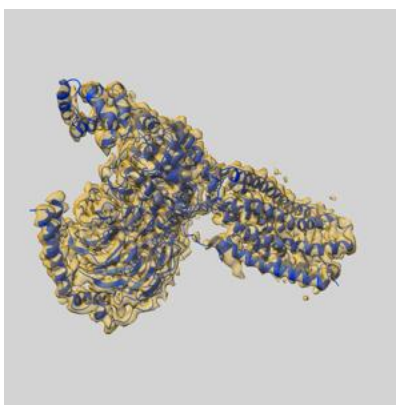
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64915 and PDB model 9VB4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

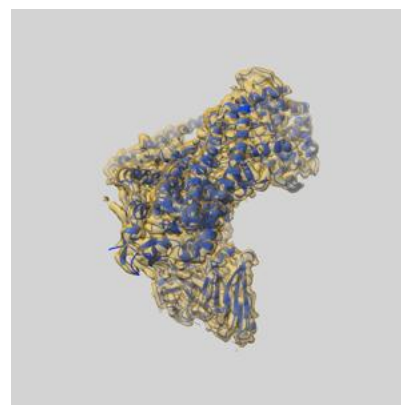
9.1 Map-model overlay [i](#)



X



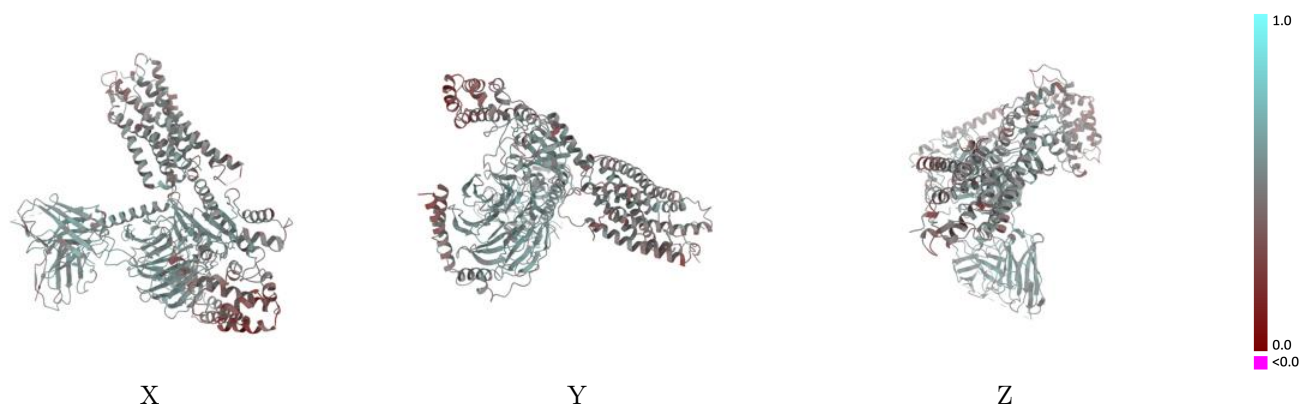
Y



Z

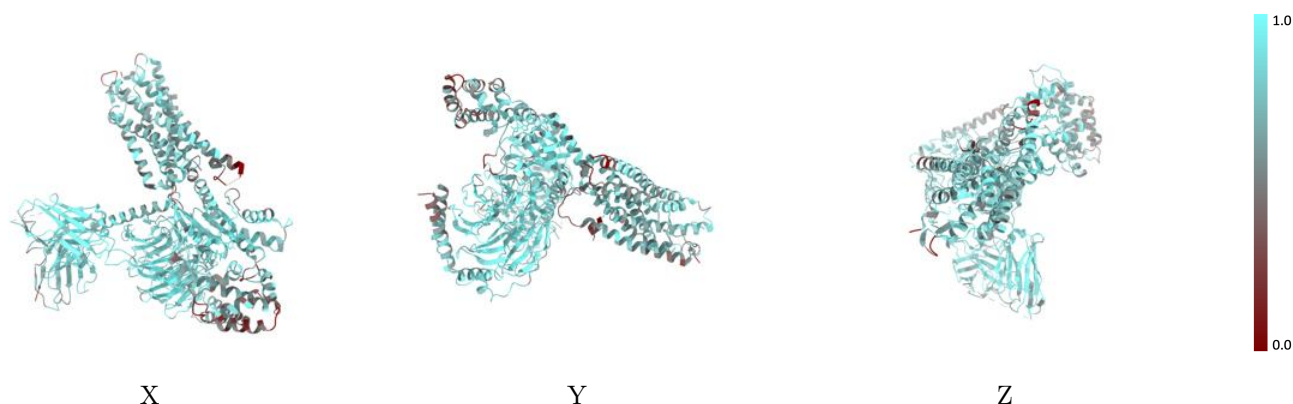
The images above show the 3D surface view of the map at the recommended contour level 0.308 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



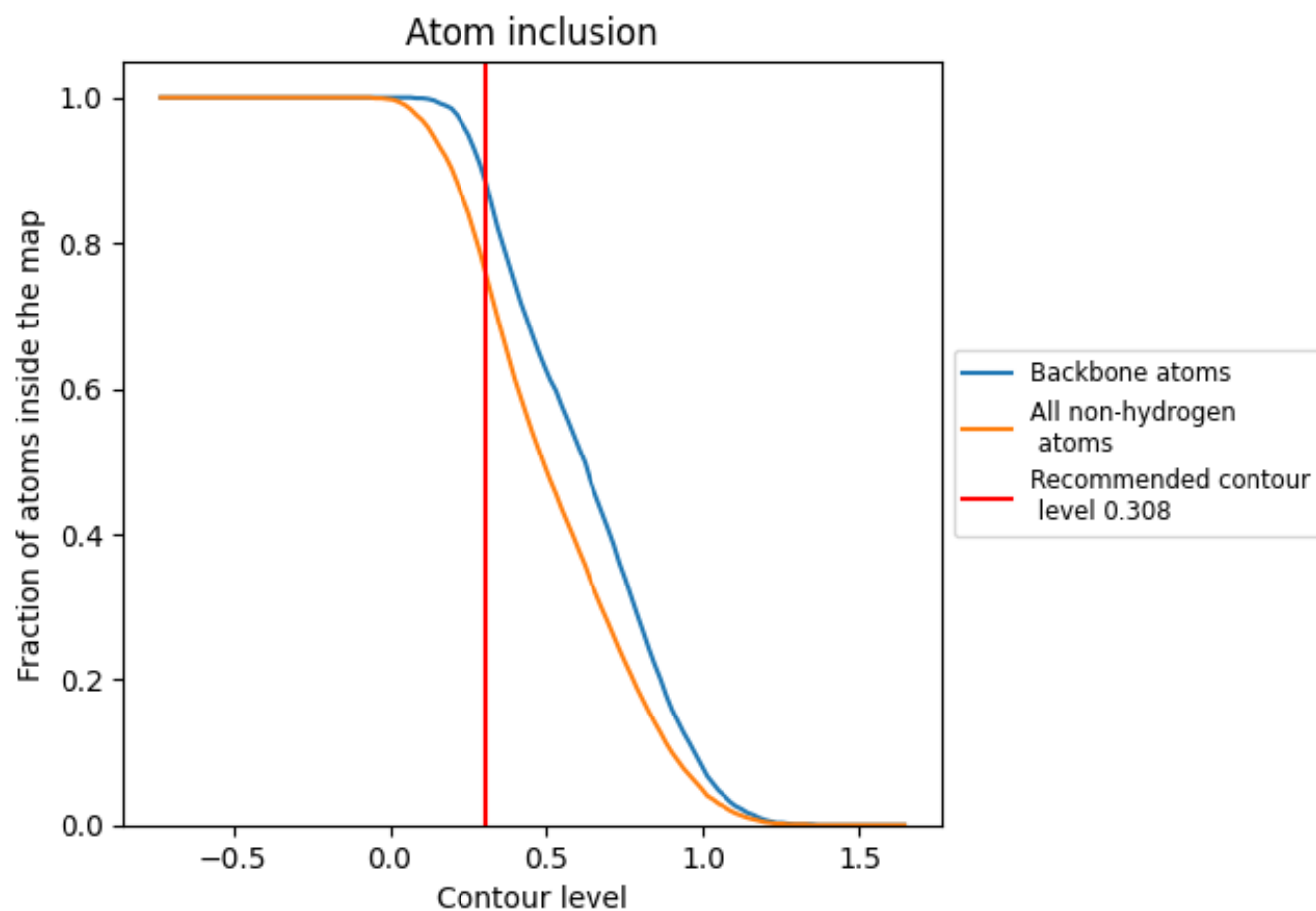
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.308).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7560	<div></div> 0.5000
A	<div></div> 0.7030	<div></div> 0.4690
B	<div></div> 0.8600	<div></div> 0.5440
C	<div></div> 0.7270	<div></div> 0.4760
D	<div></div> 0.8210	<div></div> 0.5440
L	<div></div> 0.7500	<div></div> 0.5190
R	<div></div> 0.6670	<div></div> 0.4590

