



# Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 10:39 AM JST

PDB ID : 8WG9 / pdb\_00008wg9  
EMDB ID : EMD-37506  
Title : mGlu2-mGlu4 heterodimer bound mGlu4 agonist E7P  
Authors : Zhang, Y.; Liu, J.  
Deposited on : 2023-09-20  
Resolution : 4.46 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

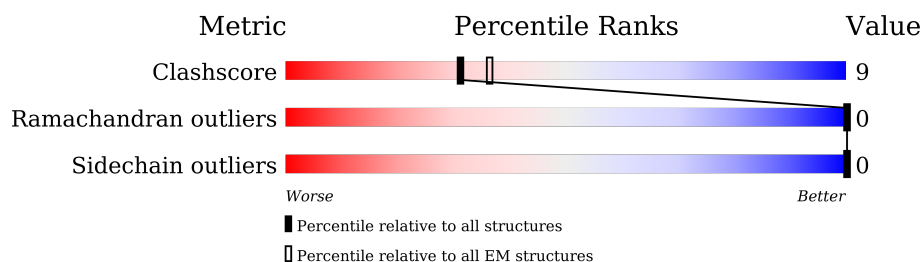
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	B	880	<div> <div>9%</div> <div>77%</div> <div>10%</div> <div>12%</div> </div>
2	C	854	<div> <div>8%</div> <div>73%</div> <div>12%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11806 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.

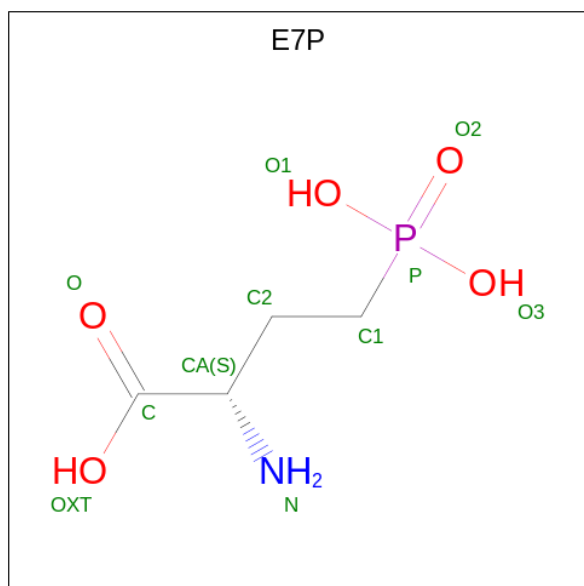
- Molecule 1 is a protein called Metabotropic glutamate receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	773	6062	3876	1047	1099	40	0	0

- Molecule 2 is a protein called Metabotropic glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	738	5733	3669	993	1032	39	0	0

- Molecule 3 is (2S)-2-amino-4-phosphonobutanoic acid (CCD ID: E7P) (formula: C<sub>4</sub>H<sub>10</sub>NO<sub>5</sub>P) (labeled as "Ligand of Interest" by depositor).

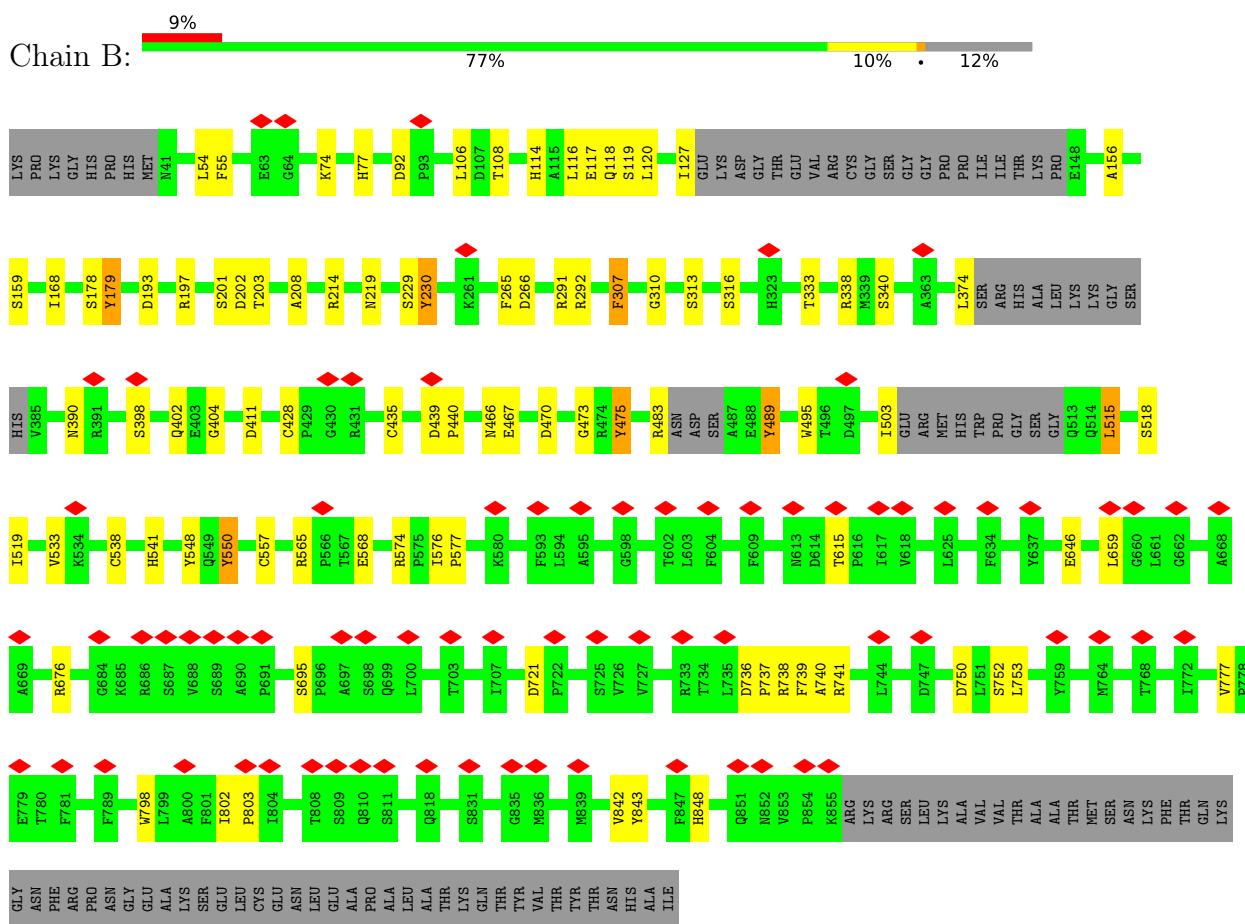


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	B	1	11	4	1	5	1	0

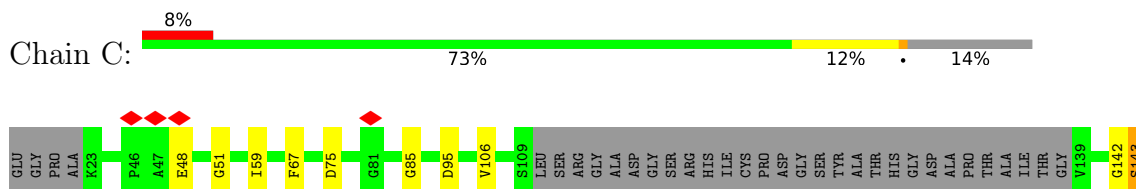
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Metabotropic glutamate receptor 4



#### • Molecule 2: Metabotropic glutamate receptor 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.950	Depositor
Minimum map value	-0.746	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.209	Depositor
Map size ( $\text{\AA}$ )	386.88, 386.88, 386.88	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.93, 0.93, 0.93	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E7P

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	0.97	4/6197 (0.1%)	1.36	34/8406 (0.4%)
2	C	1.02	2/5869 (0.0%)	1.42	64/7974 (0.8%)
All	All	0.99	6/12066 (0.0%)	1.39	98/16380 (0.6%)

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	B	0	6
2	C	0	3
All	All	0	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	LEU	CB-CG	7.51	1.68	1.53
2	C	674	ILE	CB-CG1	6.53	1.66	1.53
1	B	483	ARG	NE-CZ	6.28	1.40	1.33
1	B	503	ILE	CB-CG1	6.04	1.65	1.53
2	C	395	MET	SD-CE	-5.84	1.65	1.79
1	B	127	ILE	CB-CG1	5.53	1.64	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	745	TYR	N-CA-C	-12.73	98.25	114.04
2	C	335	ASP	CA-C-N	10.40	130.01	119.82
2	C	335	ASP	C-N-CA	10.40	130.01	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	471	VAL	N-CA-C	-10.17	103.06	111.81
2	C	476	GLU	N-CA-C	-10.12	99.26	114.64
1	B	721	ASP	CA-C-N	9.37	129.94	119.92
1	B	721	ASP	C-N-CA	9.37	129.94	119.92
1	B	265	PHE	CA-CB-CG	-8.45	105.35	113.80
2	C	106	VAL	N-CA-C	-7.98	104.03	111.45
2	C	489	SER	N-CA-C	-7.69	100.75	109.60
1	B	77	HIS	CA-CB-CG	7.52	121.32	113.80
2	C	777	LEU	CA-C-N	7.48	127.19	119.56
2	C	777	LEU	C-N-CA	7.48	127.19	119.56
1	B	411	ASP	CA-CB-CG	7.40	120.00	112.60
2	C	51	GLY	CA-C-N	7.20	127.16	120.03
2	C	51	GLY	C-N-CA	7.20	127.16	120.03
2	C	419	TYR	N-CA-C	7.13	118.70	111.07
2	C	644	SER	N-CA-C	-7.08	103.56	111.71
1	B	777	VAL	CA-C-N	6.79	126.76	120.03
1	B	777	VAL	C-N-CA	6.79	126.76	120.03
2	C	493	GLY	CA-C-N	6.78	126.96	120.31
2	C	493	GLY	C-N-CA	6.78	126.96	120.31
2	C	485	ILE	CA-C-N	6.70	126.39	119.56
2	C	485	ILE	C-N-CA	6.70	126.39	119.56
2	C	342	ASN	CA-C-N	6.64	126.78	119.87
2	C	342	ASN	C-N-CA	6.64	126.78	119.87
2	C	400	CYS	CA-C-N	6.63	126.25	119.56
2	C	400	CYS	C-N-CA	6.63	126.25	119.56
2	C	621	PHE	CA-CB-CG	-6.58	107.22	113.80
1	B	515	LEU	N-CA-CB	-6.54	104.56	111.29
2	C	437	THR	N-CA-C	6.47	117.98	108.86
2	C	717	VAL	N-CA-C	6.42	117.36	108.12
2	C	271	ARG	NE-CZ-NH2	6.34	124.91	119.20
2	C	353	PHE	CA-C-N	-6.30	111.96	122.17
2	C	353	PHE	C-N-CA	-6.30	111.96	122.17
2	C	478	LEU	N-CA-C	6.28	120.06	109.76
2	C	740	ALA	N-CA-C	6.24	118.88	111.71
1	B	428	CYS	CA-C-N	6.15	125.77	119.56
1	B	428	CYS	C-N-CA	6.15	125.77	119.56
2	C	353	PHE	N-CA-C	-6.09	99.78	109.59
1	B	398	SER	CA-C-N	6.08	129.03	120.28
1	B	398	SER	C-N-CA	6.08	129.03	120.28
2	C	623	PHE	CA-CB-CG	6.04	119.83	113.80
1	B	659	LEU	N-CA-C	-6.02	104.72	111.28
1	B	615	THR	CA-C-N	5.97	126.39	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	THR	C-N-CA	5.97	126.39	119.47
2	C	48	GLU	CA-C-N	-5.96	111.83	120.29
2	C	48	GLU	C-N-CA	-5.96	111.83	120.29
2	C	495	LEU	CA-C-N	5.91	126.24	119.92
2	C	495	LEU	C-N-CA	5.91	126.24	119.92
1	B	193	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	736	ASP	CA-C-N	5.86	127.16	119.84
1	B	736	ASP	C-N-CA	5.86	127.16	119.84
2	C	595	THR	CA-C-N	5.78	126.17	119.47
2	C	595	THR	C-N-CA	5.78	126.17	119.47
2	C	414	ASN	N-CA-C	5.74	120.41	113.17
2	C	300	LEU	CA-C-N	5.71	128.72	120.38
2	C	300	LEU	C-N-CA	5.71	128.72	120.38
2	C	262	SER	N-CA-C	-5.69	105.45	112.90
1	B	266	ASP	N-CA-C	-5.68	105.07	112.23
2	C	142	GLY	N-CA-C	-5.67	99.74	113.18
2	C	59	ILE	N-CA-C	5.66	115.85	110.53
2	C	207	VAL	N-CA-C	5.66	115.68	107.88
2	C	158	PHE	CA-CB-CG	-5.65	108.15	113.80
1	B	676	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	739	PHE	CA-CB-CG	-5.63	108.17	113.80
2	C	627	PRO	N-CA-C	5.55	119.57	111.03
2	C	67	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	848	HIS	CA-C-N	5.41	125.74	119.47
1	B	848	HIS	C-N-CA	5.41	125.74	119.47
1	B	695	SER	CA-C-N	5.39	125.05	119.56
1	B	695	SER	C-N-CA	5.39	125.05	119.56
2	C	626	LYS	CA-C-N	5.38	125.64	119.83
2	C	626	LYS	C-N-CA	5.38	125.64	119.83
2	C	266	ALA	N-CA-C	5.37	116.44	108.60
1	B	92	ASP	CA-C-N	5.32	124.99	119.56
1	B	92	ASP	C-N-CA	5.32	124.99	119.56
2	C	75	ASP	CA-C-N	5.31	124.93	119.56
2	C	75	ASP	C-N-CA	5.31	124.93	119.56
1	B	646	GLU	CA-C-N	5.30	125.22	119.76
1	B	646	GLU	C-N-CA	5.30	125.22	119.76
2	C	781	TYR	N-CA-C	-5.30	107.47	114.04
1	B	202	ASP	CA-CB-CG	-5.29	107.31	112.60
2	C	648	SER	N-CA-C	5.29	117.79	111.71
1	B	435	CYS	CA-C-N	5.22	126.37	119.84
1	B	435	CYS	C-N-CA	5.22	126.37	119.84
2	C	411	ARG	NE-CZ-NH1	-5.22	116.28	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	85	GLY	N-CA-C	-5.22	105.42	112.57
2	C	143	SER	N-CA-C	-5.21	99.70	110.80
2	C	314	ALA	N-CA-C	5.16	116.91	109.07
1	B	168	ILE	N-CA-C	-5.16	107.72	111.90
2	C	570	GLY	CA-C-N	5.15	124.94	119.28
2	C	570	GLY	C-N-CA	5.15	124.94	119.28
2	C	614	PHE	CA-CB-CG	-5.11	108.69	113.80
2	C	165	TYR	N-CA-C	-5.06	107.79	114.31
1	B	798	TRP	CA-CB-CG	-5.06	103.99	113.60
2	C	160	ILE	CA-C-N	5.01	124.91	119.85
2	C	160	ILE	C-N-CA	5.01	124.91	119.85

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	179	TYR	Sidechain
1	B	230	TYR	Sidechain
1	B	307	PHE	Sidechain
1	B	475	TYR	Sidechain
1	B	489	TYR	Sidechain
1	B	550	TYR	Sidechain
2	C	189	PHE	Sidechain
2	C	458	TYR	Sidechain
2	C	530	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6062	0	6057	119	0
2	C	5733	0	5677	83	0
3	B	11	0	0	2	0
All	All	11806	0	11734	202	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 9.

All (202) 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:565:ARG:NH1	1:B:577:PRO:CD	1.72	1.53
1:B:340:SER:HB3	1:B:402:GLN:NE2	1.13	1.42
1:B:565:ARG:CD	1:B:740:ALA:HB3	1.49	1.42
1:B:565:ARG:HD3	1:B:740:ALA:CB	1.46	1.42
1:B:565:ARG:HG3	1:B:576:ILE:CD1	1.58	1.34
2:C:319:LEU:HG	2:C:453:TYR:CE1	1.63	1.33
1:B:340:SER:CB	1:B:402:GLN:NE2	1.92	1.32
1:B:565:ARG:CD	1:B:737:PRO:O	1.80	1.29
1:B:338:ARG:CD	1:B:404:GLY:O	1.82	1.26
1:B:565:ARG:NH1	1:B:577:PRO:HD3	1.37	1.24
2:C:811:ALA:O	2:C:815:HIS:CD2	1.94	1.21
1:B:338:ARG:HD2	1:B:404:GLY:O	1.34	1.20
1:B:475:TYR:CE1	1:B:495:TRP:CE3	2.32	1.18
1:B:197:ARG:NH1	1:B:470:ASP:OD1	1.75	1.17
1:B:159:SER:HB2	1:B:229:SER:OG	1.46	1.16
1:B:466:ASN:OD1	1:B:467:GLU:OE1	1.64	1.16
2:C:319:LEU:CG	2:C:453:TYR:HE1	1.59	1.16
1:B:565:ARG:HH22	1:B:741:ARG:NH2	1.42	1.15
1:B:338:ARG:CZ	1:B:404:GLY:O	1.94	1.14
1:B:338:ARG:NE	1:B:404:GLY:O	1.79	1.14
2:C:190:PHE:CE1	2:C:453:TYR:CE2	2.39	1.10
1:B:565:ARG:NH1	1:B:577:PRO:HD2	1.64	1.10
2:C:319:LEU:HA	2:C:453:TYR:CD1	1.87	1.09
2:C:319:LEU:HA	2:C:453:TYR:HD1	0.98	1.08
1:B:114:HIS:NE2	1:B:118:GLN:NE2	2.03	1.06
1:B:201:SER:OG	1:B:203:THR:HG22	1.53	1.05
1:B:208:ALA:HB2	1:B:475:TYR:OH	1.58	1.04
1:B:565:ARG:CG	1:B:576:ILE:HD13	1.86	1.04
1:B:565:ARG:HD2	1:B:737:PRO:O	0.85	1.02
1:B:208:ALA:CB	1:B:475:TYR:OH	2.09	0.99
1:B:340:SER:HB3	1:B:402:GLN:HE21	1.23	0.99
1:B:475:TYR:HE1	1:B:495:TRP:CE3	1.70	0.99
2:C:708:GLU:CD	2:C:722:ASN:HD21	1.71	0.98
2:C:190:PHE:CZ	2:C:453:TYR:CE2	2.52	0.97
2:C:319:LEU:CG	2:C:453:TYR:CE1	2.40	0.96
1:B:565:ARG:HH21	1:B:740:ALA:N	1.64	0.96
1:B:475:TYR:HH	1:B:495:TRP:CG	1.84	0.94
1:B:565:ARG:HG3	1:B:576:ILE:HD13	0.95	0.94
1:B:568:GLU:OE1	1:B:574:ARG:NH2	2.00	0.93
1:B:473:GLY:O	1:B:475:TYR:HD1	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ARG:HH22	1:B:741:ARG:HH22	1.14	0.91
2:C:190:PHE:CE1	2:C:453:TYR:CD2	2.58	0.91
1:B:565:ARG:HD2	1:B:737:PRO:C	1.97	0.90
1:B:565:ARG:NH1	1:B:577:PRO:CG	2.36	0.89
2:C:811:ALA:C	2:C:815:HIS:CD2	2.52	0.86
1:B:475:TYR:HE1	1:B:495:TRP:CZ3	1.93	0.86
2:C:202:PHE:C	2:C:204:TRP:H	1.81	0.85
1:B:565:ARG:NH2	1:B:741:ARG:NH2	2.24	0.85
1:B:565:ARG:CG	1:B:576:ILE:CD1	2.49	0.85
2:C:208:SER:HB2	2:C:257:LEU:CD1	2.06	0.85
1:B:466:ASN:CG	1:B:467:GLU:OE1	2.20	0.84
1:B:338:ARG:NH2	1:B:404:GLY:O	2.11	0.84
2:C:427:LYS:HE2	2:C:442:ARG:CD	2.06	0.83
1:B:159:SER:HB2	1:B:229:SER:HG	1.43	0.83
1:B:340:SER:CB	1:B:402:GLN:HE21	1.78	0.82
1:B:74:LYS:HA	3:B:1001:E7P:O2	1.79	0.82
2:C:427:LYS:HG2	2:C:442:ARG:HG2	1.62	0.82
2:C:319:LEU:CA	2:C:453:TYR:HD1	1.89	0.80
1:B:310:GLY:N	1:B:333:THR:HG22	1.96	0.79
1:B:473:GLY:O	1:B:475:TYR:CD1	2.34	0.79
1:B:475:TYR:OH	1:B:495:TRP:CD2	2.34	0.79
1:B:159:SER:CB	1:B:229:SER:OG	2.30	0.79
2:C:202:PHE:C	2:C:204:TRP:N	2.40	0.77
1:B:197:ARG:HH11	1:B:470:ASP:CG	1.90	0.77
2:C:319:LEU:HG	2:C:453:TYR:CD1	2.19	0.76
1:B:475:TYR:CE1	1:B:495:TRP:HE3	1.96	0.76
1:B:565:ARG:HH22	1:B:741:ARG:HH21	1.34	0.76
2:C:186:PRO:HG2	2:C:453:TYR:OH	1.85	0.76
1:B:565:ARG:NH2	1:B:740:ALA:O	2.19	0.75
1:B:114:HIS:CE1	1:B:118:GLN:NE2	2.53	0.75
2:C:319:LEU:CD1	2:C:453:TYR:HE1	1.98	0.74
1:B:208:ALA:HB1	1:B:475:TYR:OH	1.87	0.74
1:B:565:ARG:HH21	1:B:740:ALA:H	1.33	0.74
2:C:190:PHE:CZ	2:C:453:TYR:CZ	2.76	0.73
2:C:708:GLU:OE2	2:C:722:ASN:ND2	2.21	0.73
1:B:548:TYR:HE2	1:B:565:ARG:HG2	1.52	0.73
1:B:340:SER:HB3	1:B:402:GLN:HE22	0.91	0.73
2:C:708:GLU:CD	2:C:722:ASN:ND2	2.45	0.72
1:B:565:ARG:CZ	1:B:577:PRO:HD2	2.20	0.71
1:B:475:TYR:CZ	1:B:495:TRP:CE3	2.79	0.70
1:B:106:LEU:HD13	1:B:118:GLN:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ARG:CZ	1:B:577:PRO:CD	2.69	0.67
1:B:340:SER:HB2	1:B:402:GLN:NE2	2.00	0.67
1:B:116:LEU:O	1:B:117:GLU:C	2.36	0.66
1:B:116:LEU:O	1:B:119:SER:N	2.28	0.66
1:B:310:GLY:CA	1:B:333:THR:HG22	2.25	0.66
1:B:565:ARG:NH2	1:B:740:ALA:N	2.42	0.66
1:B:338:ARG:NH2	1:B:404:GLY:HA2	2.12	0.65
2:C:190:PHE:HE1	2:C:453:TYR:CD2	2.16	0.64
2:C:426:VAL:O	2:C:427:LYS:HG2	1.96	0.64
2:C:427:LYS:HE2	2:C:442:ARG:HD2	1.78	0.64
1:B:106:LEU:CD1	1:B:118:GLN:HB3	2.27	0.64
2:C:208:SER:CB	2:C:257:LEU:CD1	2.76	0.64
1:B:338:ARG:CZ	1:B:404:GLY:C	2.71	0.64
2:C:144:TYR:HE1	2:C:146:ASP:CG	2.08	0.61
1:B:338:ARG:CZ	1:B:404:GLY:HA2	2.31	0.61
1:B:565:ARG:HG3	1:B:576:ILE:HD11	1.70	0.61
1:B:55:PHE:CE2	1:B:179:TYR:CE2	2.89	0.60
2:C:427:LYS:CE	2:C:442:ARG:CD	2.79	0.60
2:C:319:LEU:CA	2:C:453:TYR:CD1	2.73	0.59
2:C:812:PRO:HA	2:C:815:HIS:HD2	1.67	0.59
2:C:811:ALA:C	2:C:815:HIS:HD2	2.07	0.59
2:C:208:SER:HB2	2:C:257:LEU:HD13	1.84	0.58
1:B:565:ARG:CZ	1:B:740:ALA:O	2.51	0.58
2:C:708:GLU:CD	2:C:708:GLU:H	2.12	0.57
1:B:197:ARG:CZ	1:B:470:ASP:OD1	2.50	0.57
1:B:118:GLN:C	1:B:120:LEU:N	2.61	0.56
1:B:310:GLY:HA3	1:B:333:THR:HG22	1.87	0.56
2:C:427:LYS:CE	2:C:442:ARG:HD3	2.35	0.56
1:B:340:SER:CB	1:B:402:GLN:HE22	1.83	0.56
1:B:114:HIS:NE2	1:B:118:GLN:CD	2.64	0.56
1:B:118:GLN:O	1:B:119:SER:C	2.47	0.56
2:C:186:PRO:CG	2:C:453:TYR:OH	2.52	0.56
1:B:548:TYR:CE2	1:B:565:ARG:HG2	2.36	0.55
2:C:318:GLU:HG3	2:C:319:LEU:O	2.06	0.55
1:B:118:GLN:O	1:B:120:LEU:N	2.39	0.55
1:B:565:ARG:NH2	1:B:738:ARG:O	2.39	0.55
2:C:427:LYS:HE2	2:C:442:ARG:CG	2.35	0.55
1:B:74:LYS:HA	3:B:1001:E7P:P	2.47	0.54
2:C:452:ARG:O	2:C:453:TYR:CD1	2.60	0.54
1:B:565:ARG:NH2	1:B:741:ARG:HH21	1.93	0.53
1:B:230:TYR:HE2	1:B:313:SER:OG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:411:ARG:N	2:C:412:PRO:HD2	2.24	0.52
1:B:338:ARG:CZ	1:B:404:GLY:CA	2.87	0.52
2:C:95:ASP:OD1	2:C:95:ASP:N	2.41	0.52
2:C:257:LEU:HD11	2:C:266:ALA:HB2	1.91	0.51
2:C:811:ALA:O	2:C:815:HIS:CG	2.58	0.51
2:C:211:ALA:HB2	2:C:221:ILE:HG13	1.92	0.51
2:C:427:LYS:HE2	2:C:442:ARG:HG2	1.91	0.51
1:B:230:TYR:CE2	1:B:313:SER:OG	2.64	0.50
2:C:301:GLU:H	2:C:301:GLU:CD	2.19	0.50
1:B:156:ALA:HB2	1:B:178:SER:HA	1.93	0.50
2:C:205:THR:O	2:C:233:ILE:HG23	2.12	0.50
2:C:213:GLU:HA	2:C:240:LYS:HE2	1.93	0.50
2:C:411:ARG:N	2:C:412:PRO:CD	2.74	0.50
2:C:181:PHE:C	2:C:181:PHE:CD2	2.87	0.49
2:C:319:LEU:CB	2:C:453:TYR:CE1	2.94	0.49
2:C:812:PRO:CA	2:C:815:HIS:HD2	2.25	0.49
2:C:295:ASP:HB2	2:C:318:GLU:OE1	2.13	0.49
1:B:307:PHE:CZ	1:B:515:LEU:HB2	2.47	0.48
2:C:651:LEU:HD23	2:C:655:ASN:ND2	2.29	0.48
1:B:565:ARG:NH1	1:B:577:PRO:HG2	2.25	0.48
2:C:571:PRO:HA	2:C:574:ILE:HG22	1.94	0.48
2:C:143:SER:HB3	2:C:165:TYR:OH	2.14	0.48
1:B:550:TYR:C	1:B:557:CYS:SG	2.98	0.47
1:B:565:ARG:CD	1:B:740:ALA:CB	2.38	0.47
1:B:439:ASP:HB3	1:B:440:PRO:HD3	1.97	0.47
1:B:475:TYR:CE1	1:B:495:TRP:CZ3	2.83	0.47
2:C:190:PHE:CZ	2:C:453:TYR:CD2	2.94	0.47
1:B:475:TYR:OH	1:B:495:TRP:CE3	2.65	0.47
2:C:427:LYS:C	2:C:428:PHE:CG	2.93	0.47
2:C:456:PHE:HB3	2:C:470:LYS:HA	1.96	0.47
1:B:466:ASN:CG	1:B:467:GLU:H	2.24	0.46
2:C:710:ALA:C	2:C:712:GLU:N	2.71	0.46
2:C:812:PRO:HA	2:C:815:HIS:CD2	2.49	0.46
1:B:54:LEU:C	1:B:55:PHE:CD1	2.93	0.45
2:C:390:HIS:CE1	2:C:428:PHE:CZ	3.04	0.45
1:B:565:ARG:CG	1:B:740:ALA:HB3	2.36	0.45
2:C:190:PHE:C	2:C:190:PHE:CD1	2.93	0.45
2:C:319:LEU:CD1	2:C:453:TYR:CE1	2.89	0.45
1:B:565:ARG:NH2	1:B:738:ARG:C	2.75	0.45
1:B:310:GLY:H	1:B:333:THR:HG22	1.77	0.45
1:B:750:ASP:OD1	1:B:750:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:PHE:O	2:C:204:TRP:N	2.51	0.44
1:B:208:ALA:CB	1:B:475:TYR:CZ	2.98	0.44
1:B:118:GLN:C	1:B:120:LEU:H	2.26	0.43
2:C:707:LYS:O	2:C:708:GLU:C	2.59	0.43
2:C:810:PHE:O	2:C:811:ALA:C	2.61	0.43
2:C:710:ALA:C	2:C:712:GLU:H	2.27	0.43
1:B:752:SER:O	1:B:753:LEU:C	2.61	0.43
1:B:54:LEU:HD11	1:B:108:THR:HG22	2.01	0.42
1:B:518:SER:N	1:B:519:ILE:HG23	2.34	0.42
1:B:475:TYR:CZ	1:B:495:TRP:HB3	2.55	0.42
2:C:439:ASN:O	2:C:440:GLU:C	2.63	0.42
1:B:390:ASN:OD1	1:B:390:ASN:N	2.51	0.42
2:C:647:TYR:CD1	2:C:647:TYR:C	2.98	0.42
2:C:214:GLY:HA3	2:C:216:TYR:CZ	2.54	0.42
2:C:257:LEU:CD1	2:C:266:ALA:HB2	2.50	0.42
2:C:427:LYS:O	2:C:428:PHE:CG	2.72	0.42
2:C:754:GLU:O	2:C:755:ASN:C	2.62	0.42
1:B:518:SER:C	1:B:519:ILE:HG23	2.44	0.42
1:B:565:ARG:HD3	1:B:740:ALA:CA	2.36	0.42
2:C:545:TRP:N	2:C:546:PRO:HD3	2.35	0.42
1:B:802:ILE:HB	1:B:803:PRO:HD3	2.02	0.41
2:C:345:PHE:O	2:C:346:ARG:C	2.58	0.41
2:C:319:LEU:HD12	2:C:453:TYR:HE1	1.80	0.41
1:B:219:ASN:HB3	1:B:538:CYS:HB2	2.02	0.41
2:C:202:PHE:HB3	2:C:204:TRP:CB	2.50	0.41
1:B:117:GLU:O	1:B:120:LEU:HB2	2.20	0.41
1:B:214:ARG:NH1	1:B:219:ASN:OD1	2.54	0.41
1:B:316:SER:HA	1:B:489:TYR:CD2	2.55	0.41
2:C:625:ALA:O	2:C:626:LYS:C	2.64	0.41
1:B:338:ARG:NH2	1:B:404:GLY:CA	2.83	0.41
1:B:475:TYR:OH	1:B:495:TRP:CG	2.62	0.41
1:B:533:VAL:HG22	1:B:541:HIS:CE1	2.56	0.41
1:B:338:ARG:NH2	1:B:404:GLY:C	2.78	0.41
2:C:811:ALA:O	2:C:815:HIS:HD2	1.81	0.41
1:B:291:ARG:O	1:B:292:ARG:C	2.62	0.40
2:C:143:SER:HA	2:C:166:ALA:HB3	2.02	0.40
2:C:337:TRP:CE3	2:C:357:PHE:CE1	3.09	0.40
1:B:842:VAL:O	1:B:843:TYR:C	2.62	0.40
2:C:408:ASP:HA	2:C:411:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	763/880 (87%)	722 (95%)	41 (5%)	0	100	100
2	C	730/854 (86%)	686 (94%)	44 (6%)	0	100	100
All	All	1493/1734 (86%)	1408 (94%)	85 (6%)	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	B	662/755 (88%)	662 (100%)	0	100	100
2	C	608/698 (87%)	608 (100%)	0	100	100
All	All	1270/1453 (87%)	1270 (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. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	118	GLN
1	B	252	GLN
1	B	302	GLN
1	B	305	HIS
1	B	402	GLN
1	B	424	HIS

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Mol	Chain	Res	Type
1	B	513	GLN
1	B	569	ASN
2	C	87	HIS
2	C	507	ASN
2	C	722	ASN
2	C	815	HIS

### 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	$\# Z  > 2$
3	E7P	B	1001	-	9,10,10	2.37	3 (33%)	12,14,14	2.00	1 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	E7P	B	1001	-	-	3/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	E7P	P-C1	5.69	1.84	1.78
3	B	1001	E7P	P-O1	-2.59	1.49	1.54
3	B	1001	E7P	P-O3	-2.05	1.50	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	E7P	P-C1-C2	-5.62	107.95	114.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

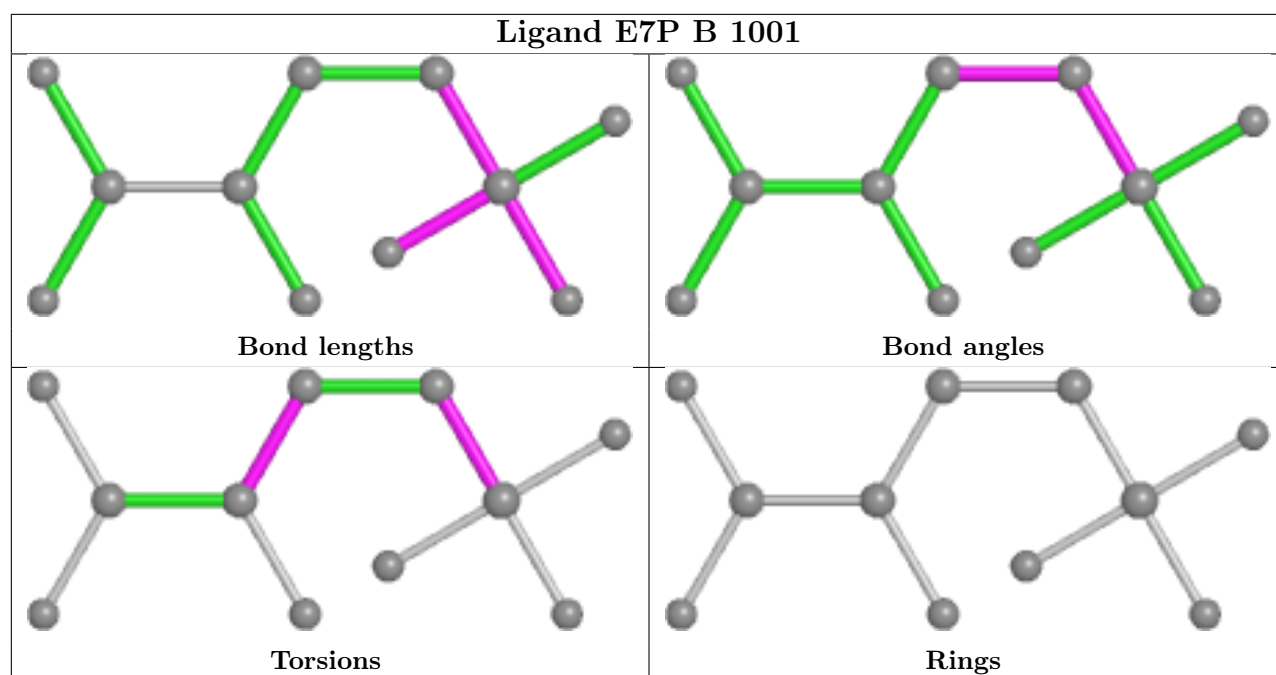
Mol	Chain	Res	Type	Atoms
3	B	1001	E7P	C1-C2-CA-N
3	B	1001	E7P	C1-C2-CA-C
3	B	1001	E7P	C2-C1-P-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	E7P	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

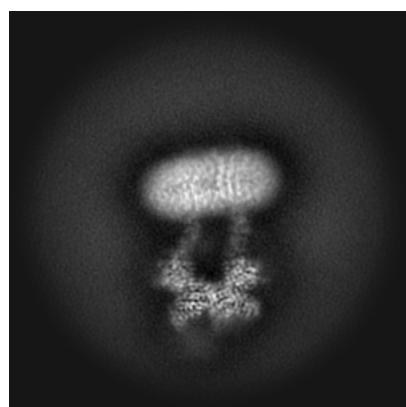
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37506. These allow visual inspection of the internal detail of the map and identification of artifacts.

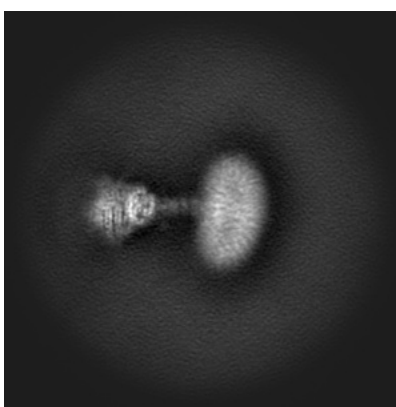
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

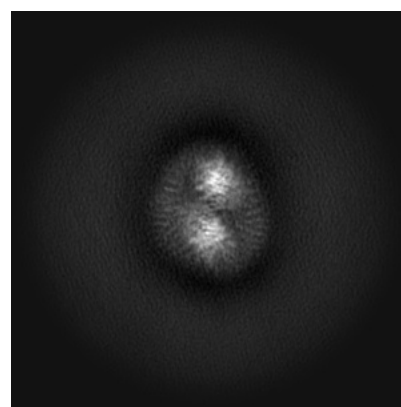
#### 6.1.1 Primary map



X



Y

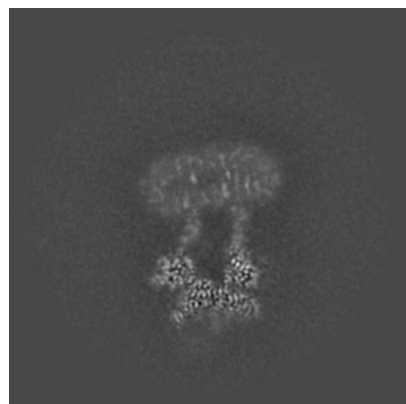


Z

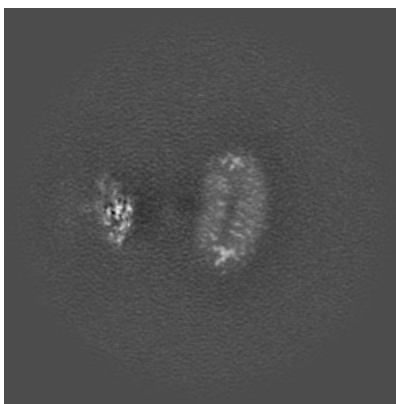
The images above show the map projected in three orthogonal directions.

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

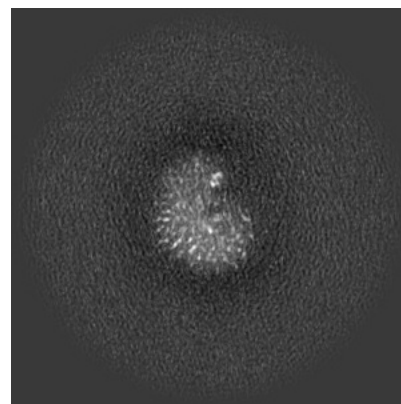
#### 6.2.1 Primary map



X Index: 208



Y Index: 208

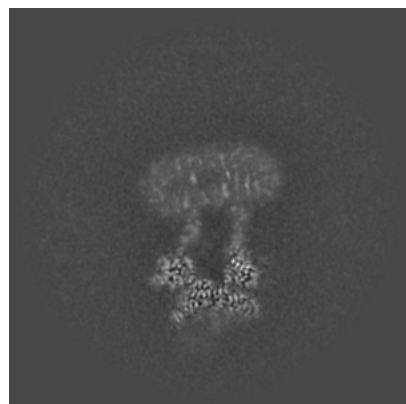


Z Index: 208

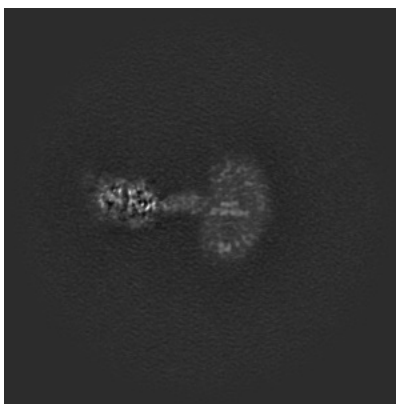
The images above show central slices of the map in three orthogonal directions.

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

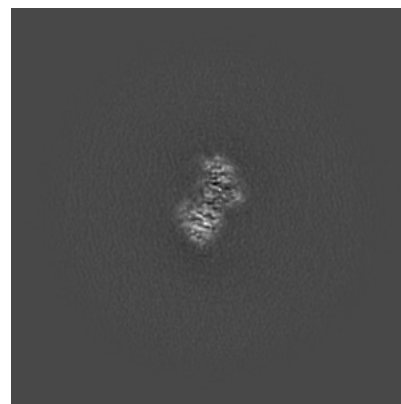
### 6.3.1 Primary map



X Index: 208



Y Index: 238

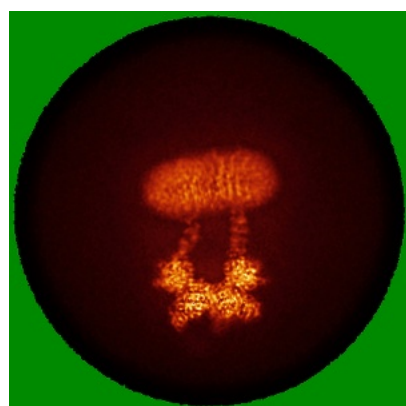


Z Index: 110

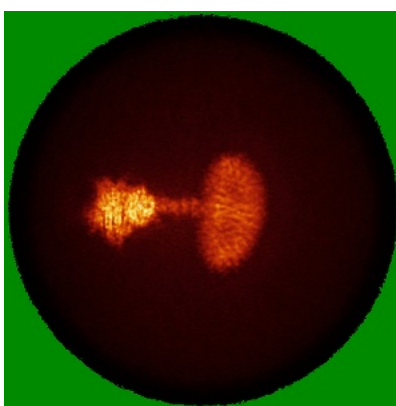
The images above show the largest variance slices of the map in three orthogonal directions.

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

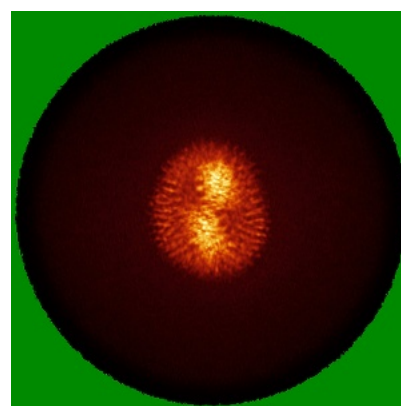
### 6.4.1 Primary map



X



Y

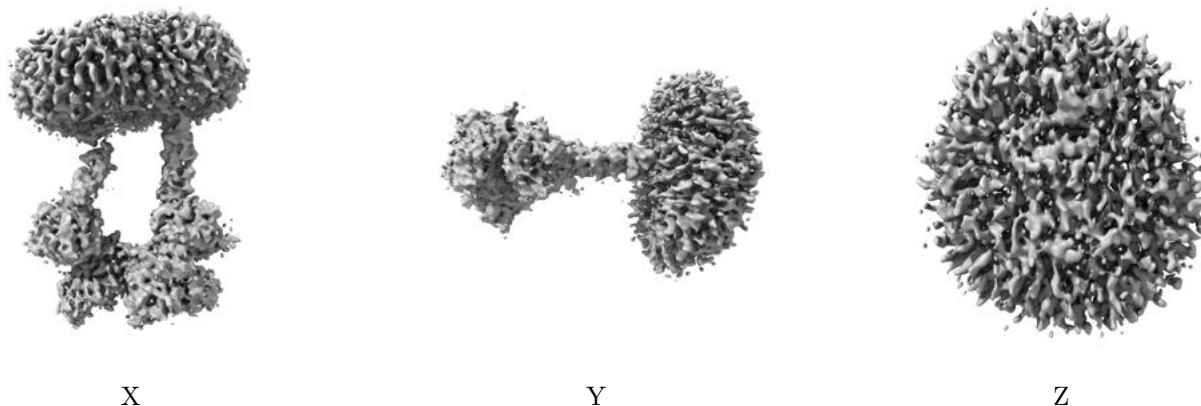


Z

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

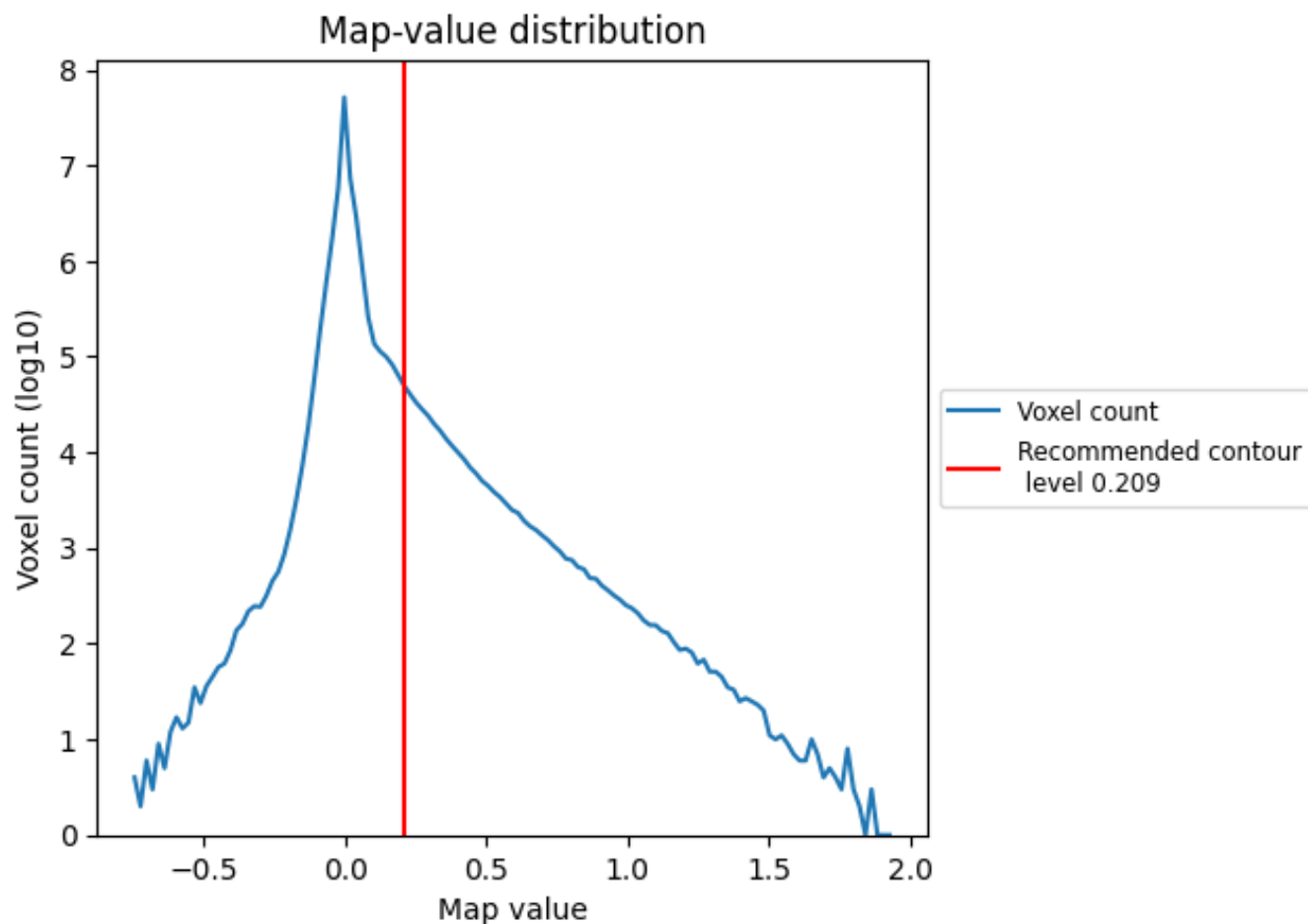
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

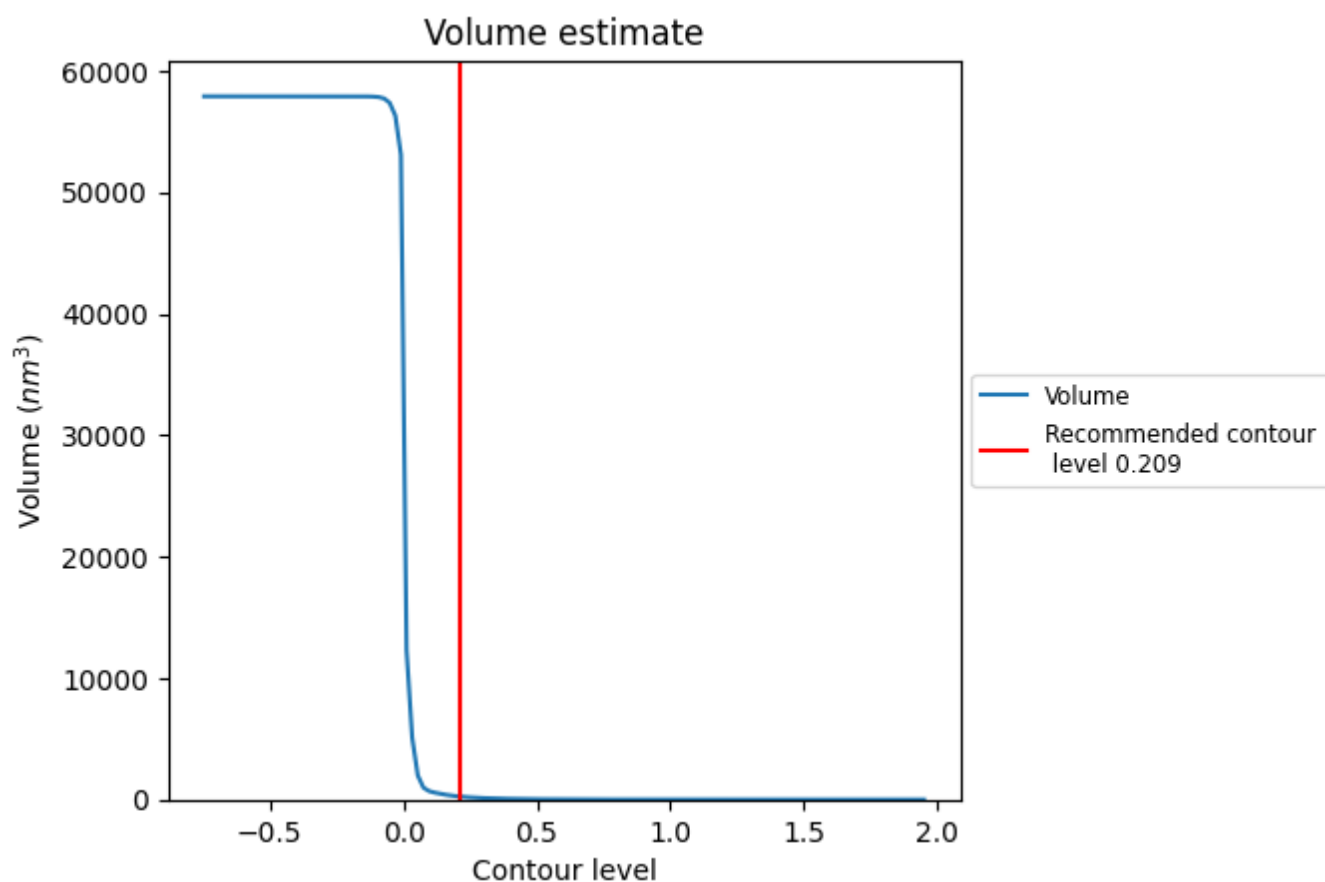
This section contains the results of statistical analysis of the map.

### 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](#)

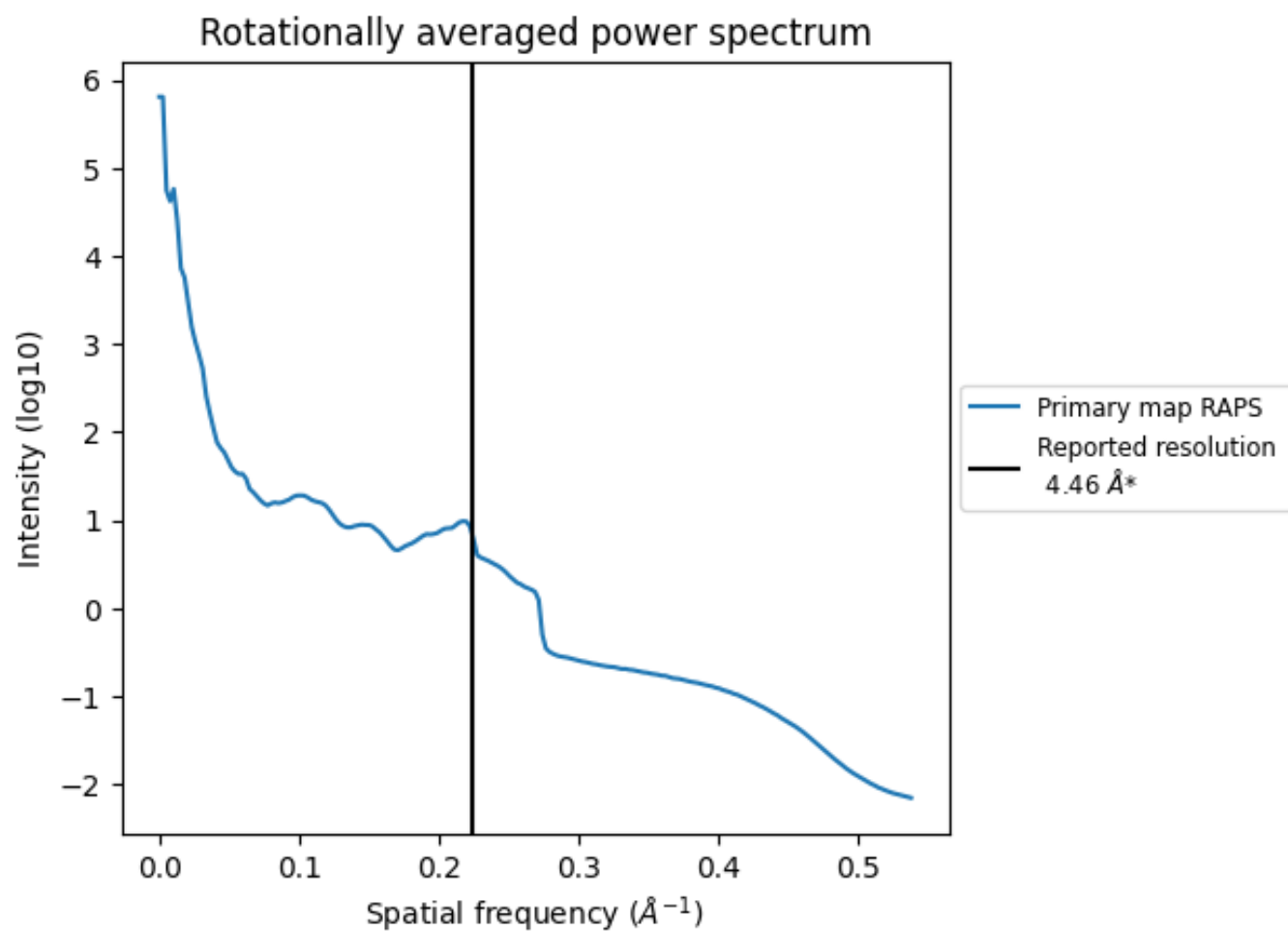


The volume at the recommended contour level is 252  $\text{nm}^3$ ; this corresponds to an approximate mass of 227 kDa.

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 0.224 Å<sup>-1</sup>

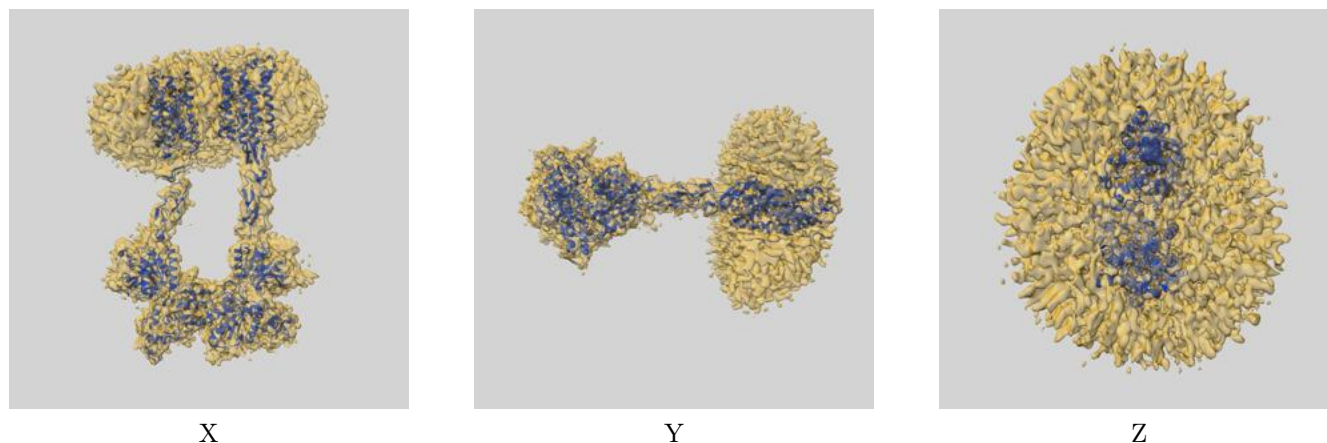
## 8 Fourier-Shell correlation

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

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

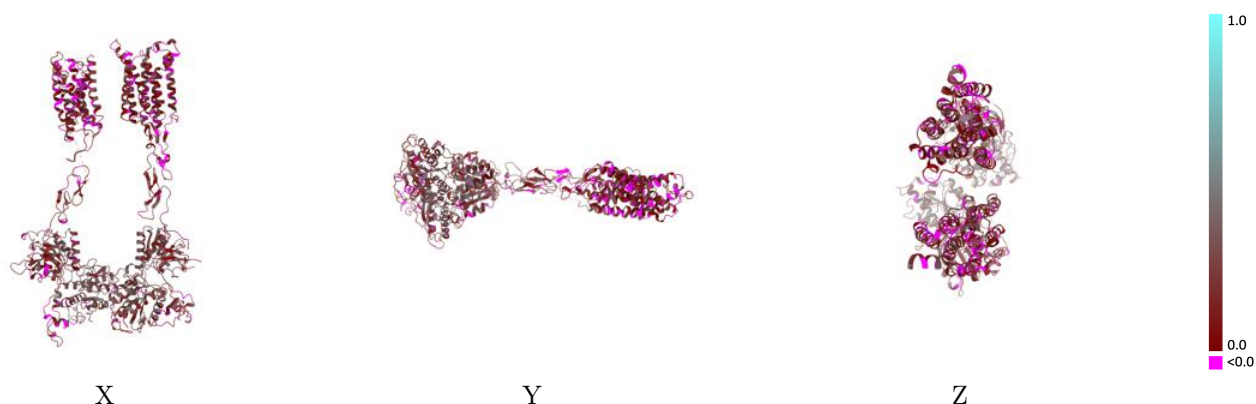
This section contains information regarding the fit between EMDB map EMD-37506 and PDB model 8WG9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



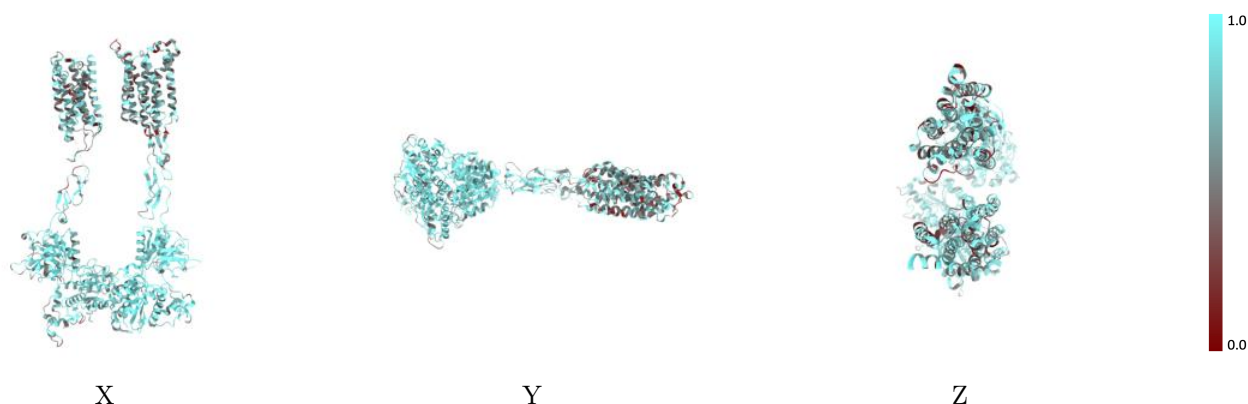
The images above show the 3D surface view of the map at the recommended contour level 0.209 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



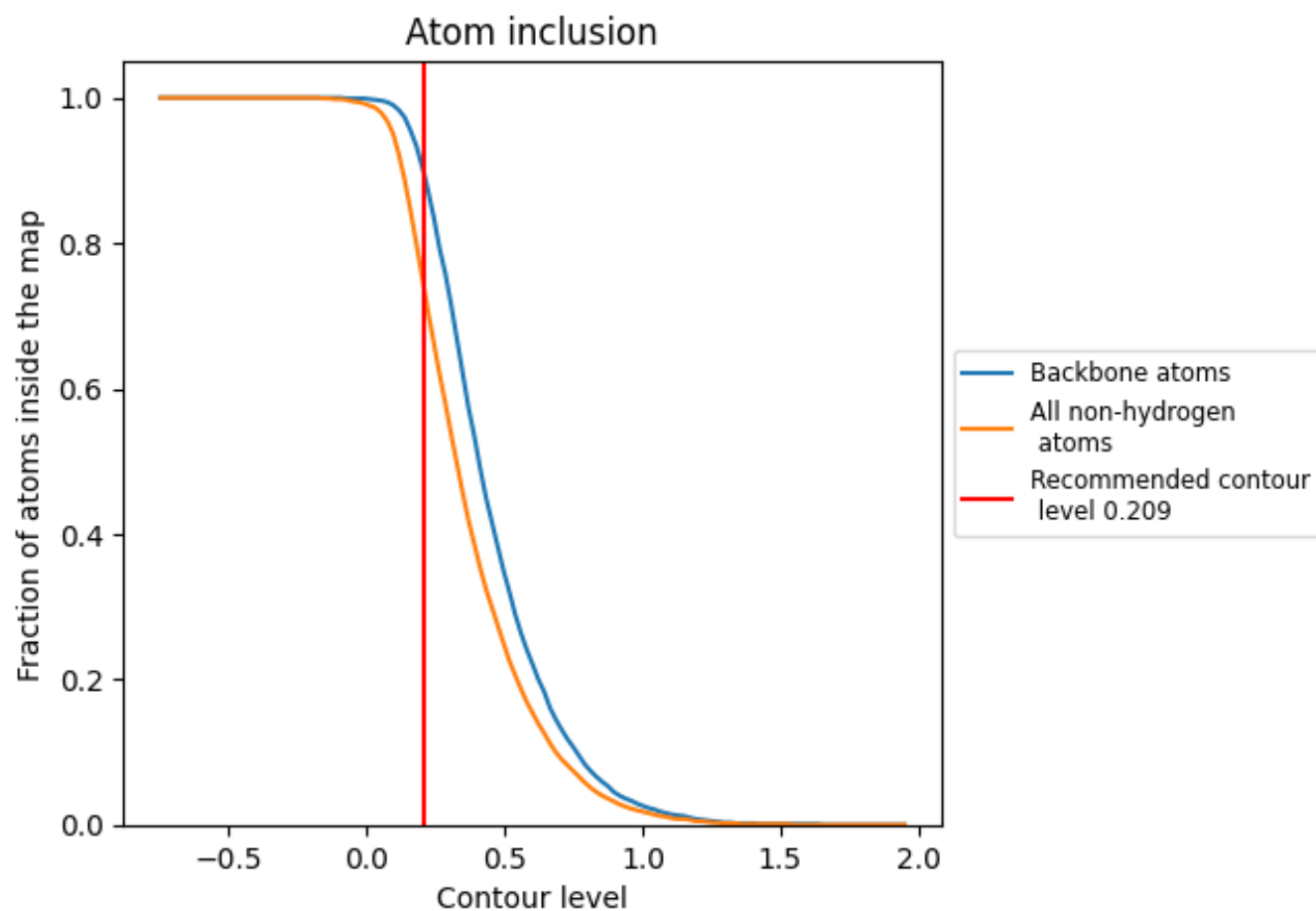
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.209).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 74% 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 (0.209) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.1860
B	<div></div> 0.7440	<div></div> 0.1920
C	<div></div> 0.7270	<div></div> 0.1800

