



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 08:55 AM JST

PDB ID : 7XO5
EMDB ID : EMD-33337
Title : SARS-CoV-2 Omicron BA.1 Variant Spike Trimer with one mouse ACE2 Bound
Authors : Xu, Y.; Wu, C.; Liu, H.; Yin, W.; Xu, H.E.
Deposited on : 2022-05-01
Resolution : 3.13 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
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) : 2.39

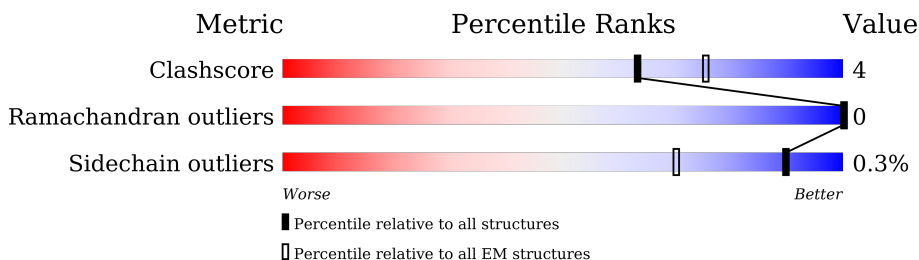
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1205	
1	B	1205	
1	C	1205	
2	D	805	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28503 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0
			7763	4968	1294	1467	34		
1	B	1022	Total	C	N	O	S	0	0
			7700	4958	1275	1432	35		
1	C	1022	Total	C	N	O	S	0	0
			7703	4959	1276	1433	35		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	210A	ILE	LEU	variant	UNP P0DTC2
A	210D	GLU	-	insertion	UNP P0DTC2
A	210E	PRO	-	insertion	UNP P0DTC2
A	210F	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	210A	ILE	LEU	variant	UNP P0DTC2
B	210D	GLU	-	insertion	UNP P0DTC2
B	210E	PRO	-	insertion	UNP P0DTC2
B	210F	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	210A	ILE	LEU	variant	UNP P0DTC2
C	210D	GLU	-	insertion	UNP P0DTC2
C	210E	PRO	-	insertion	UNP P0DTC2
C	210F	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	591	Total	C	N	O	S	0	0
			4818	3070	808	911	29		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

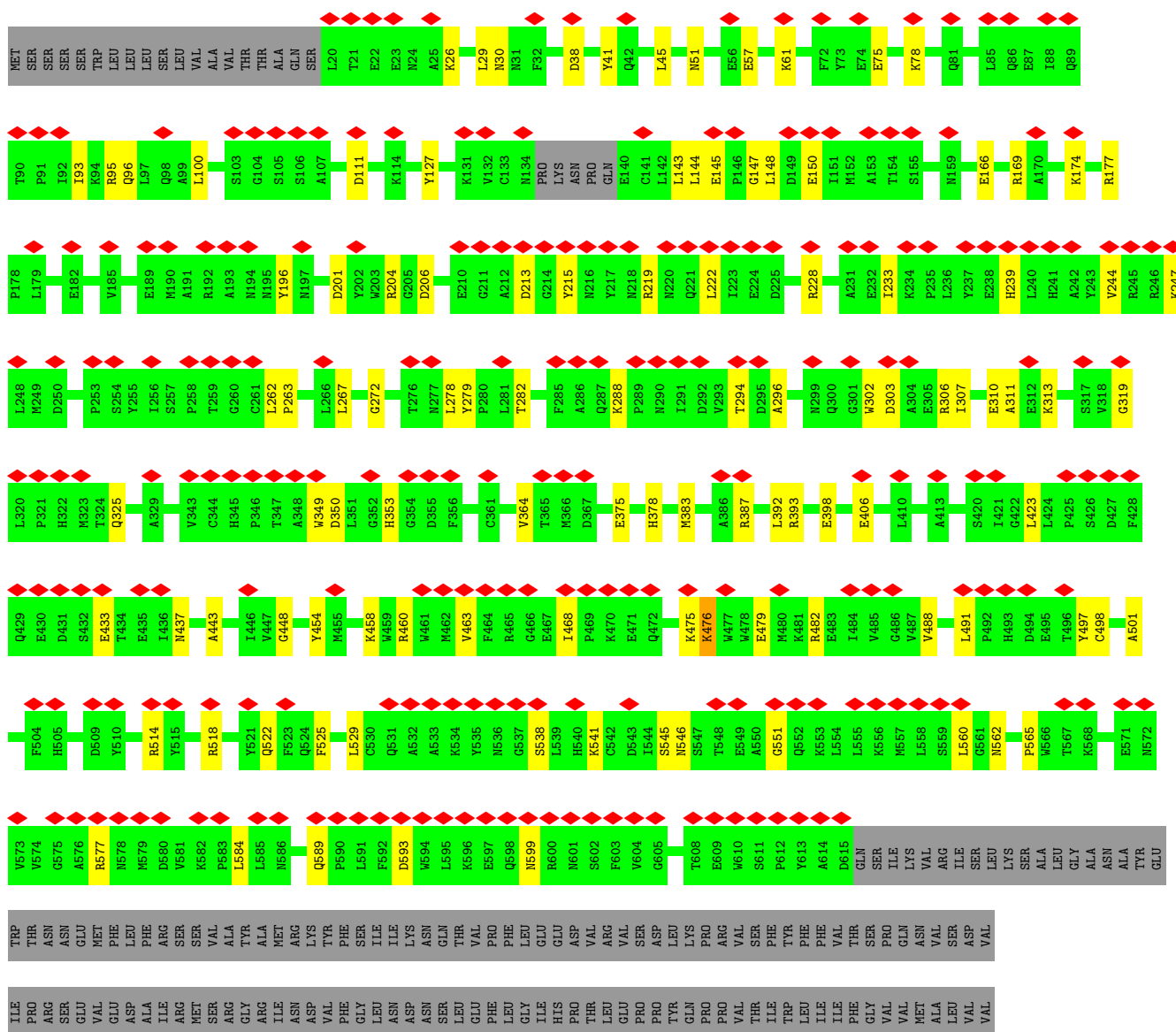
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Zn	0
			1	1	



- Molecule 2: Angiotensin-converting enzyme 2



VAL
GLY
ILE
ILE
ILE
LEU
ILE
VAL
THR
GLY
ILE
LYS
GLY
ARG
LYS
LYS
LYS
ASN
GLU
THR
LYS
ARG
GLU
GLU
ASN
PRO
TYR
ASP
SER
MET
ASP
ILE
GLY
LYS
GLY
GLU
SER
ASN
ALA
GLY
PHE
GLN
ASN
SER
ASP
ASP
ALA
GLN
THR
SER
PHE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227749	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.917	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.824, 0.824, 0.824	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: ZN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/7945	0.55	3/10846 (0.0%)
1	B	0.29	0/7884	0.58	5/10767 (0.0%)
1	C	0.28	0/7887	0.54	1/10771 (0.0%)
2	D	0.31	0/4950	0.62	5/6718 (0.1%)
All	All	0.29	0/28666	0.57	14/39102 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	CYS	CA-CB-SG	9.52	131.13	114.00
2	D	529	LEU	CA-CB-CG	6.11	129.34	115.30
1	A	455	LEU	CA-CB-CG	5.89	128.85	115.30
2	D	278	LEU	CA-CB-CG	5.67	128.34	115.30
2	D	45	LEU	CA-CB-CG	5.63	128.24	115.30
2	D	100	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	709	ASN	CB-CA-C	-5.59	99.23	110.40
1	A	117	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	709	ASN	N-CA-CB	5.50	120.49	110.60
1	B	1024	LEU	CA-CB-CG	5.21	127.27	115.30
1	C	765	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	A	533	LEU	CA-CB-CG	5.08	126.97	115.30
1	B	455	LEU	CA-CB-CG	5.05	126.92	115.30
2	D	560	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7763	0	7345	55	0
1	B	7700	0	7280	60	0
1	C	7703	0	7282	51	0
2	D	4818	0	4589	65	0
3	A	168	0	156	1	0
3	B	168	0	156	0	0
3	C	154	0	140	1	0
3	D	28	0	26	0	0
4	D	1	0	0	0	0
All	All	28503	0	26974	220	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.

All (220) 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)
2:D:127:TYR:O	2:D:144:LEU:CD1	1.80	1.29
2:D:127:TYR:O	2:D:144:LEU:HD12	1.48	1.12
2:D:127:TYR:O	2:D:144:LEU:HD11	1.54	1.07
2:D:148:LEU:HD13	2:D:148:LEU:O	1.75	0.85
2:D:148:LEU:HD13	2:D:148:LEU:C	2.03	0.77
1:A:373:PRO:HB2	1:A:436:TRP:HB2	1.75	0.68
1:A:345:THR:HG23	1:A:346:ARG:HE	1.60	0.67
1:C:977:LEU:HD11	1:C:1000:ARG:HH22	1.63	0.63
1:A:907:ASN:HD21	1:A:913:GLN:HE21	1.46	0.63
2:D:398:GLU:HB3	2:D:514:ARG:HD2	1.82	0.62
1:A:442:ASP:O	1:A:448:ASN:ND2	2.33	0.61
1:A:447:GLY:HA2	1:A:498:ARG:HH12	1.67	0.60
1:C:433:VAL:HG23	1:C:512:VAL:HG22	1.83	0.60
2:D:482:ARG:HD2	2:D:488:VAL:HG22	1.84	0.60
1:B:452:LEU:HB3	1:B:492:LEU:HB3	1.83	0.60
2:D:51:ASN:HD21	2:D:349:TRP:HE1	1.50	0.60
1:A:363:ALA:HB3	1:A:526:GLY:HA2	1.84	0.58
2:D:310:GLU:HA	2:D:313:LYS:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ARG:HB3	1:A:501:TYR:HB2	1.85	0.58
1:C:480:CYS:SG	1:C:481:ASN:ND2	2.76	0.58
1:A:353:TRP:O	1:A:466:ARG:NH2	2.37	0.57
1:B:393:THR:HG22	1:B:521:PRO:HD2	1.86	0.57
1:B:562:PHE:O	1:C:41:LYS:NZ	2.34	0.57
2:D:148:LEU:C	2:D:148:LEU:CD1	2.72	0.57
2:D:522:GLN:HA	2:D:525:PHE:HB2	1.87	0.57
1:A:403:ARG:HH22	1:A:501:TYR:HE1	1.53	0.56
1:B:575:ALA:HB1	1:B:584:ILE:HD11	1.87	0.56
2:D:392:LEU:HD23	2:D:562:ASN:HB3	1.87	0.56
2:D:143:LEU:HB3	2:D:145:GLU:HG2	1.88	0.56
2:D:244:VAL:HA	2:D:247:LYS:HZ1	1.71	0.56
1:A:909:ILE:HD13	1:A:1047:TYR:HB3	1.87	0.55
1:A:432:CYS:SG	1:A:433:VAL:N	2.80	0.55
1:C:371:LEU:HG	1:C:373:PRO:HD2	1.88	0.55
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.89	0.55
2:D:406:GLU:HG3	2:D:518:ARG:HD2	1.88	0.55
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.88	0.54
1:B:858:LEU:HD11	1:B:962:LEU:HD23	1.88	0.54
1:C:912:THR:H	1:C:1106:GLN:HE22	1.55	0.54
1:B:316:SER:OG	1:B:317:ASN:N	2.40	0.54
2:D:93:ILE:HA	2:D:96:GLN:HB3	1.89	0.54
1:B:403:ARG:HA	1:B:507:PRO:HA	1.89	0.54
2:D:239:HIS:O	2:D:599:ASN:ND2	2.41	0.54
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.88	0.54
1:C:136:CYS:SG	1:C:137:ASN:N	2.81	0.54
1:A:89:GLY:HA3	1:A:270:LEU:HD12	1.88	0.54
1:B:420:ASP:O	1:B:460:ASN:ND2	2.41	0.54
1:B:742:ILE:O	1:B:1000:ARG:NH2	2.41	0.54
1:C:644:GLN:HA	1:C:649:CYS:HA	1.90	0.53
1:A:316:SER:OG	1:A:317:ASN:N	2.41	0.53
1:B:442:ASP:OD2	1:B:509:ARG:NH2	2.41	0.53
1:B:34:ARG:NH2	1:B:219:GLY:O	2.41	0.53
2:D:233:ILE:HD12	2:D:584:LEU:HD23	1.90	0.53
1:C:316:SER:OG	1:C:317:ASN:N	2.42	0.53
1:A:552:LEU:HB3	1:A:585:LEU:HD13	1.90	0.52
1:B:498:ARG:HE	1:B:500:THR:H	1.57	0.52
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.91	0.52
1:B:349:SER:OG	1:B:350:VAL:N	2.42	0.52
1:C:759:PHE:HD2	1:C:1001:LEU:HD13	1.74	0.52
2:D:538:SER:HA	2:D:589:GLN:HE22	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:HD12	1:B:456:PHE:HB2	1.91	0.52
1:B:296:LEU:HD13	1:B:608:VAL:HG21	1.91	0.52
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.92	0.51
2:D:294:THR:HG22	2:D:364:VAL:HG13	1.90	0.51
1:B:742:ILE:HD12	1:B:753:LEU:HD11	1.92	0.51
1:A:896:ILE:HD12	1:A:897:PRO:HD2	1.93	0.51
1:B:433:VAL:HG12	1:B:512:VAL:HG12	1.93	0.51
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.93	0.51
1:A:985:ASP:OD1	1:A:985:ASP:N	2.41	0.50
1:B:551:VAL:HG23	1:B:590:CYS:HB3	1.93	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.93	0.50
1:B:406:GLU:O	1:B:409:GLN:NE2	2.44	0.50
2:D:302:TRP:HA	2:D:306:ARG:HG3	1.93	0.50
1:B:736:VAL:HG21	1:B:1004:LEU:HD11	1.93	0.50
1:A:914:ASN:HD21	1:C:1121:PHE:HE2	1.60	0.50
1:B:552:LEU:HG	1:B:587:ILE:HG12	1.93	0.50
1:B:708:SER:OG	1:B:709:ASN:N	2.45	0.50
1:A:167:THR:HG22	1:A:168:PHE:H	1.77	0.50
2:D:204:ARG:HD2	2:D:222:LEU:HB3	1.93	0.50
1:B:956:ALA:O	1:B:960:ASN:ND2	2.45	0.49
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.40	0.49
2:D:143:LEU:C	2:D:145:GLU:H	2.16	0.49
2:D:454:TYR:O	2:D:458:LYS:NZ	2.45	0.49
1:A:388:ASN:HB3	1:A:527:PRO:HG2	1.95	0.49
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.93	0.49
1:B:119:ILE:HG12	1:B:128:ILE:HG23	1.95	0.49
1:C:1086:LYS:HD2	1:C:1122:VAL:HG21	1.94	0.49
2:D:96:GLN:HA	2:D:392:LEU:HD11	1.95	0.49
1:A:107:GLY:H	1:A:235:ILE:HG23	1.78	0.49
1:C:276:LEU:HD13	1:C:301:CYS:HA	1.95	0.49
1:A:382:VAL:HG13	1:A:386:LYS:HE3	1.95	0.48
2:D:443:ALA:O	2:D:448:GLY:N	2.39	0.48
1:B:560:LEU:HB2	1:B:563:GLN:HE21	1.77	0.48
1:B:641:ASN:HD22	1:B:654:GLU:HA	1.79	0.48
1:A:142:ASP:OD2	1:A:157:PHE:N	2.46	0.48
1:A:656:VAL:HA	3:A:1307:NAG:H82	1.96	0.48
1:B:578:ASP:OD2	1:B:578:ASP:N	2.46	0.48
2:D:267:LEU:HD23	2:D:272:GLY:HA3	1.94	0.48
1:A:644:GLN:HA	1:A:649:CYS:HA	1.95	0.48
1:A:503:VAL:HG11	2:D:325:GLN:H	1.79	0.48
2:D:375:GLU:HA	2:D:378:HIS:HD2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:THR:O	1:B:586:ASP:N	2.40	0.48
2:D:26:LYS:HA	2:D:29:LEU:HD12	1.96	0.47
2:D:177:ARG:HD2	2:D:498:CYS:HB3	1.96	0.47
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.97	0.47
1:A:454:ARG:HH22	1:A:457:ARG:HB3	1.79	0.47
1:B:443:SER:HB3	1:B:499:PRO:HG3	1.95	0.47
1:A:414:GLN:O	1:A:424:LYS:NZ	2.48	0.47
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.97	0.47
1:B:1037:SER:H	1:B:1048:HIS:HD2	1.62	0.47
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.95	0.47
1:B:818:ILE:HB	1:B:1054:GLN:HE21	1.80	0.47
1:B:663:ASP:OD1	1:B:663:ASP:N	2.48	0.46
1:C:887:THR:HB	1:C:894:LEU:HD13	1.98	0.46
2:D:296:ALA:HB3	2:D:423:LEU:HG	1.98	0.46
1:B:131:CYS:HB2	1:B:166:CYS:HA	1.97	0.46
1:C:215:ASP:N	1:C:215:ASP:OD2	2.47	0.46
1:B:880:GLY:O	1:B:884:SER:OG	2.30	0.46
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.97	0.46
1:B:592:PHE:HZ	1:C:855:PHE:HB2	1.81	0.46
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.97	0.46
2:D:319:GLY:HA3	2:D:551:GLY:HA3	1.98	0.46
1:A:964:LYS:HA	1:C:570:ALA:HB2	1.97	0.45
1:A:1006:THR:HG21	1:B:1005:GLN:HE21	1.80	0.45
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.65	0.45
2:D:215:TYR:HE1	2:D:577:ARG:HH22	1.63	0.45
1:A:736:VAL:HG23	1:A:858:LEU:HG	1.97	0.45
2:D:111:ASP:OD1	2:D:111:ASP:N	2.47	0.45
1:A:739:THR:O	1:A:744:GLY:N	2.49	0.45
1:A:745:ASP:OD1	1:A:745:ASP:N	2.46	0.45
1:C:961:THR:HA	1:C:964:LYS:HG2	1.98	0.45
2:D:75:GLU:HA	2:D:78:LYS:HD2	1.99	0.45
1:B:669:GLY:N	1:C:864:LEU:O	2.49	0.45
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.98	0.45
1:A:86:PHE:N	1:A:236:THR:O	2.48	0.45
2:D:593:ASP:N	2:D:593:ASP:OD2	2.49	0.45
2:D:147:GLY:HA2	2:D:150:GLU:HB2	1.99	0.45
1:B:984:LEU:HB2	1:B:989:ALA:HB2	1.99	0.44
2:D:95:ARG:HH21	2:D:565:PRO:HA	1.83	0.44
1:B:406:GLU:HB2	1:B:409:GLN:HE22	1.82	0.44
1:B:644:GLN:HA	1:B:649:CYS:HA	1.99	0.44
1:C:119:ILE:HG23	1:C:128:ILE:HG13	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:OD1	1:B:334:ASN:N	2.50	0.44
1:C:819:GLU:HA	1:C:822:LEU:HD12	1.99	0.44
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.98	0.44
1:B:1074:ASN:ND2	1:C:895:GLN:OE1	2.51	0.44
1:C:298:GLU:HG2	1:C:315:THR:HB	1.99	0.44
1:C:574:ASP:O	1:C:587:ILE:N	2.41	0.44
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	1.99	0.44
1:A:643:PHE:O	1:A:650:LEU:N	2.50	0.44
1:A:966:LEU:O	1:A:975:SER:OG	2.34	0.44
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.95	0.44
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.98	0.44
1:C:470:THR:HG21	1:C:492:LEU:HG	2.00	0.44
2:D:279:TYR:OH	2:D:437:ASN:O	2.33	0.44
1:C:206:LYS:HB2	1:C:223:LEU:HA	2.00	0.44
2:D:166:GLU:HG3	2:D:491:LEU:HD22	1.99	0.44
1:A:327:VAL:HG12	1:A:542:ASN:HB3	2.00	0.43
1:B:709:ASN:H	1:B:709:ASN:HD22	1.65	0.43
2:D:498:CYS:HB2	2:D:501:ALA:HB3	2.00	0.43
1:A:191:GLU:HB2	1:A:223:LEU:HD11	2.00	0.43
2:D:350:ASP:O	2:D:393:ARG:NH2	2.50	0.43
1:A:972:ALA:HA	1:A:995:ARG:HH11	1.84	0.43
1:A:85:PRO:HA	1:A:237:ARG:HA	2.00	0.43
1:C:65:PHE:HE1	1:C:84:LEU:HD11	1.84	0.43
1:C:457:ARG:HA	1:C:457:ARG:HD3	1.81	0.43
2:D:174:LYS:HA	2:D:174:LYS:HD2	1.90	0.43
1:B:712:ILE:HD13	1:B:1094:VAL:HG11	2.00	0.43
1:C:456:PHE:HE1	1:C:489:TYR:HB2	1.84	0.43
2:D:196:TYR:HB3	2:D:201:ASP:HB3	2.00	0.43
2:D:468:ILE:HG21	2:D:476:LYS:HG2	1.99	0.43
1:A:371:LEU:HG	1:A:373:PRO:HD2	2.00	0.43
2:D:213:ASP:OD2	2:D:213:ASP:N	2.45	0.43
2:D:262:LEU:HD12	2:D:263:PRO:HD2	2.00	0.43
2:D:288:LYS:HE3	2:D:288:LYS:HB3	1.85	0.43
2:D:383:MET:O	2:D:387:ARG:NH1	2.50	0.43
1:C:435:ALA:HB2	1:C:510:VAL:HG23	2.00	0.42
2:D:433:GLU:O	2:D:437:ASN:ND2	2.52	0.42
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	1.98	0.42
1:A:880:GLY:O	1:A:884:SER:OG	2.28	0.42
2:D:38:ASP:OD1	2:D:38:ASP:N	2.52	0.42
1:B:417:ASN:OD1	1:B:418:ILE:N	2.52	0.42
1:C:50:SER:O	1:C:50:SER:OG	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:TYR:HE1	2:D:353:HIS:HB2	1.83	0.42
1:A:297:SER:HA	1:A:300:LYS:HE2	2.00	0.42
1:C:928:ASN:HA	1:C:931:ILE:HG22	2.00	0.42
2:D:460:ARG:HA	2:D:463:VAL:HG12	2.00	0.42
1:A:365:TYR:HA	1:A:368:LEU:HG	2.01	0.42
2:D:307:ILE:O	2:D:311:ALA:N	2.50	0.42
2:D:475:LYS:O	2:D:479:GLU:N	2.47	0.42
2:D:541:LYS:HE2	2:D:541:LYS:HB3	1.76	0.42
1:A:928:ASN:HA	1:A:931:ILE:HG22	2.01	0.42
2:D:206:ASP:OD1	2:D:206:ASP:N	2.53	0.42
2:D:279:TYR:HA	2:D:282:THR:HG22	2.01	0.42
1:A:424:LYS:HB3	1:A:463:PRO:HG3	2.00	0.42
1:A:378:LYS:HE2	1:C:493:ARG:HH12	1.84	0.41
1:C:612:TYR:HB3	1:C:615:VAL:HB	2.01	0.41
1:C:438:SER:O	1:C:438:SER:OG	2.36	0.41
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.53	0.41
1:A:105:ILE:HG13	1:A:241:LEU:HD21	2.03	0.41
1:B:466:ARG:HA	1:B:466:ARG:HD2	1.90	0.41
1:B:484:ALA:N	1:B:488:CYS:SG	2.86	0.41
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.96	0.41
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.03	0.41
1:C:726:ILE:HD13	1:C:945:LEU:HD13	2.02	0.41
1:B:424:LYS:HE2	1:B:463:PRO:HG3	2.03	0.41
1:B:709:ASN:N	1:B:709:ASN:HD22	2.18	0.41
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.54	0.41
2:D:57:GLU:O	2:D:61:LYS:NZ	2.53	0.41
2:D:303:ASP:OD1	2:D:303:ASP:N	2.49	0.41
1:A:222:ALA:HB2	1:A:285:ILE:HB	2.02	0.41
1:A:742:ILE:HG12	1:A:1000:ARG:HB3	2.02	0.41
1:C:818:ILE:HB	1:C:1054:GLN:HE21	1.86	0.41
2:D:545:SER:OG	2:D:546:ASN:N	2.51	0.40
1:B:567:ARG:HD2	1:B:571:ASP:HA	2.04	0.40
2:D:30:ASN:OD1	2:D:30:ASN:N	2.53	0.40
2:D:169:ARG:HG3	2:D:497:TYR:HE1	1.86	0.40
1:A:796:TYR:HB3	3:C:1309:NAG:H5	1.68	0.40
1:A:896:ILE:HD11	1:A:900:MET:HE2	2.03	0.40
1:A:993:ILE:HD13	1:A:993:ILE:HA	1.94	0.40
2:D:201:ASP:OD2	2:D:219:ARG:NH1	2.55	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	A	1008/1205 (84%)	969 (96%)	39 (4%)	0	100	100
1	B	1006/1205 (84%)	952 (95%)	54 (5%)	0	100	100
1	C	1006/1205 (84%)	949 (94%)	57 (6%)	0	100	100
2	D	587/805 (73%)	555 (94%)	32 (6%)	0	100	100
All	All	3607/4420 (82%)	3425 (95%)	182 (5%)	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	A	824/1053 (78%)	823 (100%)	1 (0%)	92	97
1	B	802/1053 (76%)	800 (100%)	2 (0%)	92	96
1	C	803/1053 (76%)	800 (100%)	3 (0%)	89	94
2	D	515/707 (73%)	513 (100%)	2 (0%)	89	94
All	All	2944/3866 (76%)	2936 (100%)	8 (0%)	90	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1039	ARG
1	B	378	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	709	ASN
1	C	44	ARG
1	C	102	ARG
1	C	886	TRP
2	D	228	ARG
2	D	476	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	409	GLN
1	A	417	ASN
1	A	487	ASN
1	A	607	GLN
1	A	644	GLN
1	A	755	GLN
1	A	872	GLN
1	A	913	GLN
1	A	914	ASN
1	A	919	ASN
1	A	920	GLN
1	A	949	GLN
1	A	953	ASN
1	A	955	ASN
1	A	960	ASN
1	A	1036	GLN
1	A	1054	GLN
1	A	1064	HIS
1	A	1083	HIS
1	A	1106	GLN
1	A	1113	GLN
1	B	218	GLN
1	B	314	GLN
1	B	317	ASN
1	B	437	ASN
1	B	460	ASN
1	B	519	HIS
1	B	563	GLN
1	B	641	ASN
1	B	644	GLN
1	B	784	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	824	ASN
1	B	913	GLN
1	B	960	ASN
1	B	1054	GLN
1	C	481	ASN
1	C	607	GLN
1	C	613	GLN
1	C	755	GLN
1	C	935	GLN
1	C	953	ASN
1	C	960	ASN
1	C	1023	ASN
1	C	1036	GLN
1	C	1054	GLN
1	C	1106	GLN
1	C	1113	GLN
2	D	117	ASN
2	D	216	ASN
2	D	300	GLN
2	D	378	HIS
2	D	437	ASN
2	D	472	GLN
2	D	536	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](#)

Of 38 ligands modelled in this entry, 1 is monoatomic - leaving 37 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1303	1	14,14,15	0.32	0	17,19,21	0.47	0
3	NAG	B	1308	1	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
3	NAG	C	1303	1	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	B	1302	1	14,14,15	0.35	0	17,19,21	0.43	0
3	NAG	B	1304	1	14,14,15	0.40	0	17,19,21	0.50	0
3	NAG	B	1312	1	14,14,15	0.37	0	17,19,21	0.46	0
3	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.55	0
3	NAG	C	1304	1	14,14,15	0.43	0	17,19,21	0.44	0
3	NAG	D	903	2	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	B	1307	1	14,14,15	1.67	2 (14%)	17,19,21	1.75	1 (5%)
3	NAG	B	1310	1	14,14,15	0.58	1 (7%)	17,19,21	0.43	0
3	NAG	C	1301	1	14,14,15	0.40	0	17,19,21	0.52	0
3	NAG	B	1301	1	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	C	1306	1	14,14,15	0.37	0	17,19,21	0.48	0
3	NAG	B	1309	1	14,14,15	0.44	0	17,19,21	0.52	0
3	NAG	A	1307	1	14,14,15	0.41	0	17,19,21	0.46	0
3	NAG	A	1304	1	14,14,15	1.53	1 (7%)	17,19,21	1.40	1 (5%)
3	NAG	B	1311	1	14,14,15	0.36	0	17,19,21	0.48	0
3	NAG	B	1306	1	14,14,15	0.40	0	17,19,21	0.53	0
3	NAG	A	1310	1	14,14,15	0.39	0	17,19,21	0.53	0
3	NAG	A	1309	1	14,14,15	0.38	0	17,19,21	0.51	0
3	NAG	A	1311	1	14,14,15	2.51	2 (14%)	17,19,21	2.25	2 (11%)
3	NAG	A	1305	1	14,14,15	0.35	0	17,19,21	0.49	0
3	NAG	A	1308	1	14,14,15	0.42	0	17,19,21	0.49	0
3	NAG	C	1311	1	14,14,15	0.37	0	17,19,21	0.43	0
3	NAG	C	1308	1	14,14,15	0.43	0	17,19,21	0.56	0
3	NAG	A	1306	1	14,14,15	0.40	0	17,19,21	0.55	0
3	NAG	A	1302	1	14,14,15	0.35	0	17,19,21	0.50	0
3	NAG	A	1312	1	14,14,15	0.45	0	17,19,21	0.53	0
3	NAG	C	1307	1	14,14,15	0.62	0	17,19,21	0.56	0
3	NAG	D	902	2	14,14,15	0.40	0	17,19,21	0.52	0
3	NAG	A	1303	1	14,14,15	0.40	0	17,19,21	0.49	0
3	NAG	C	1310	1	14,14,15	0.35	0	17,19,21	0.48	0
3	NAG	B	1305	1	14,14,15	0.53	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1309	1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	C	1305	1	14,14,15	0.41	0	17,19,21	0.52	0
3	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.54	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
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	D	903	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	902	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1311	NAG	O5-C1	8.99	1.58	1.43
3	B	1307	NAG	O5-C1	5.82	1.53	1.43
3	A	1304	NAG	O5-C1	5.61	1.52	1.43
3	A	1311	NAG	C1-C2	2.54	1.56	1.52
3	B	1307	NAG	C1-C2	2.09	1.55	1.52
3	B	1310	NAG	C1-C2	2.02	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1311	NAG	C1-O5-C5	8.73	124.02	112.19
3	B	1307	NAG	C1-O5-C5	6.61	121.15	112.19
3	A	1304	NAG	C1-O5-C5	5.58	119.75	112.19
3	A	1311	NAG	C3-C4-C5	-2.48	105.81	110.24
3	B	1308	NAG	C1-O5-C5	2.15	115.11	112.19

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1304	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1308	NAG	O5-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	A	1311	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1311	NAG	C8-C7-N2-C2
3	A	1311	NAG	O7-C7-N2-C2
3	A	1312	NAG	C8-C7-N2-C2
3	A	1312	NAG	O7-C7-N2-C2
3	B	1307	NAG	C8-C7-N2-C2
3	B	1307	NAG	O7-C7-N2-C2
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1307	NAG	C8-C7-N2-C2
3	C	1307	NAG	O7-C7-N2-C2
3	C	1310	NAG	C4-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1307	NAG	1	0
3	C	1309	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33337. These allow visual inspection of the internal detail of the map and identification of artifacts.

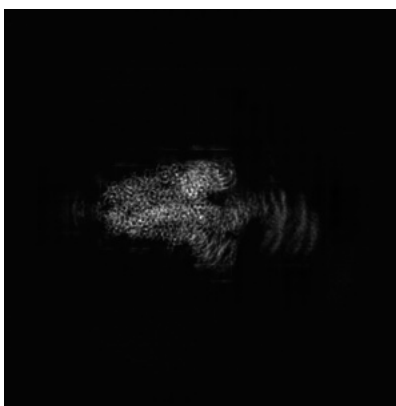
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

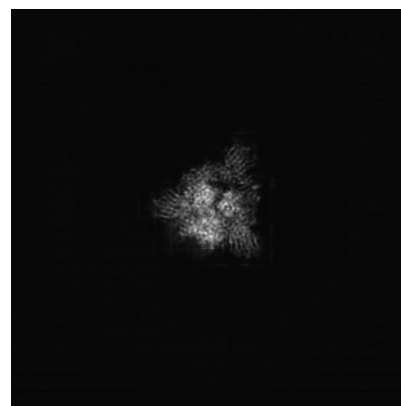
6.1.1 Primary map



X

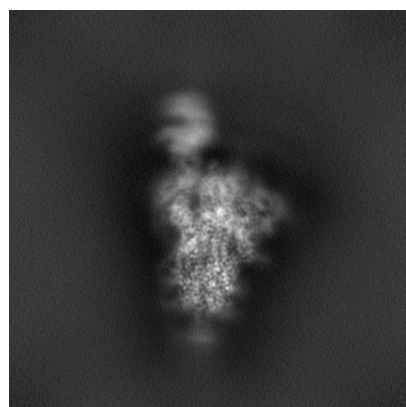


Y

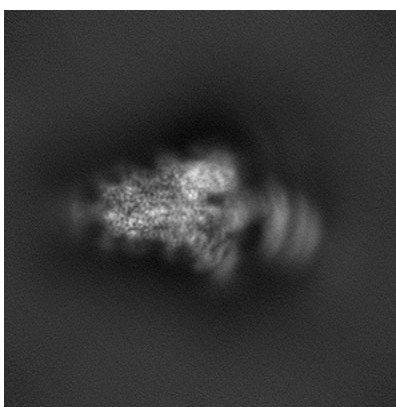


Z

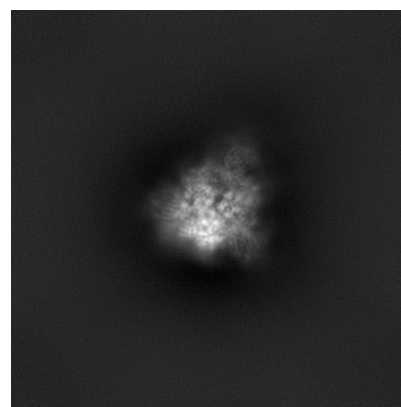
6.1.2 Raw map



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: 240



Y Index: 240

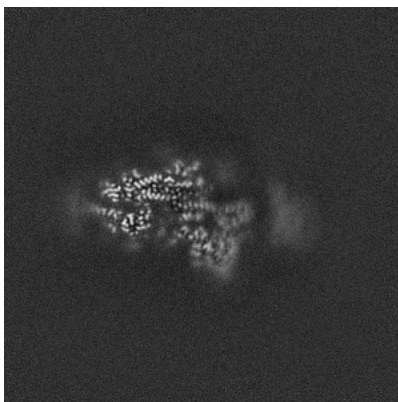


Z Index: 240

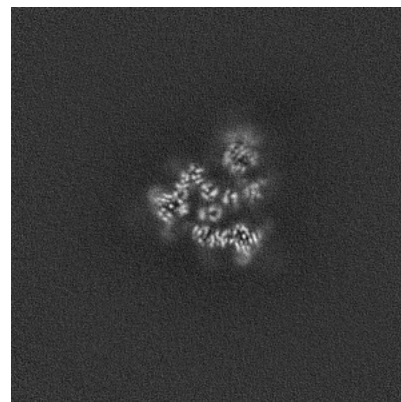
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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: 230

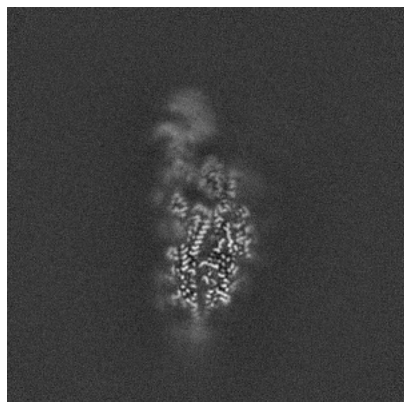


Y Index: 246

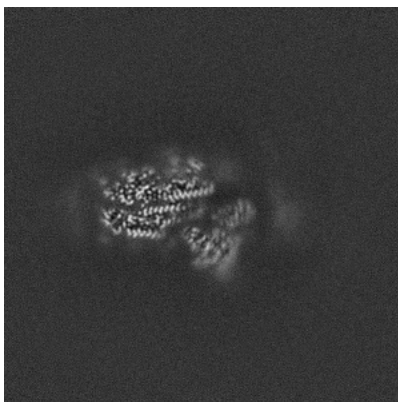


Z Index: 228

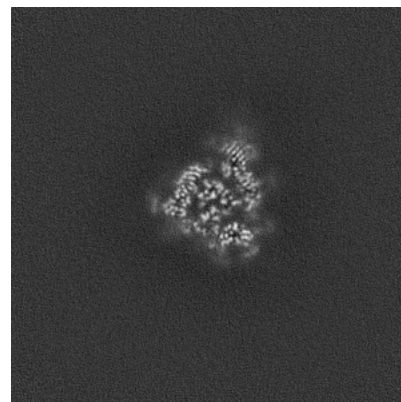
6.3.2 Raw map



X Index: 230



Y Index: 246

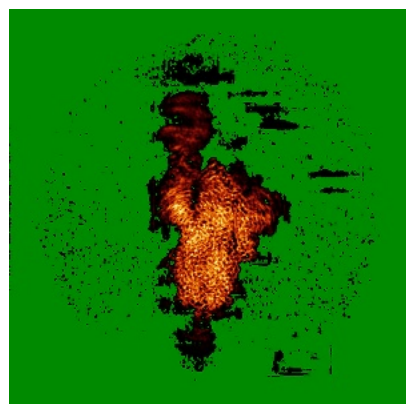


Z Index: 228

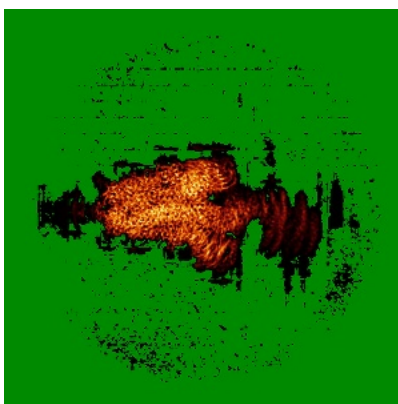
The images above show the largest variance slices of the map in three orthogonal directions.

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

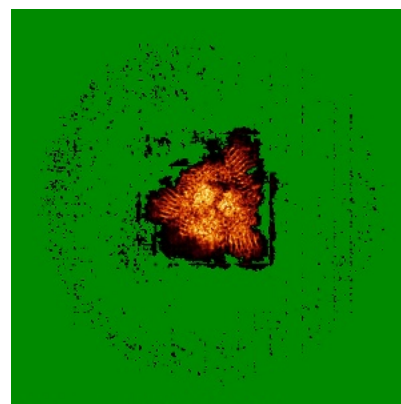
6.4.1 Primary map



X

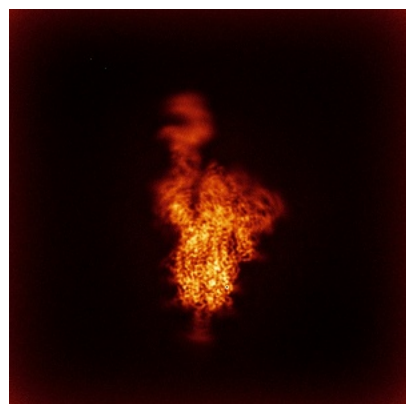


Y

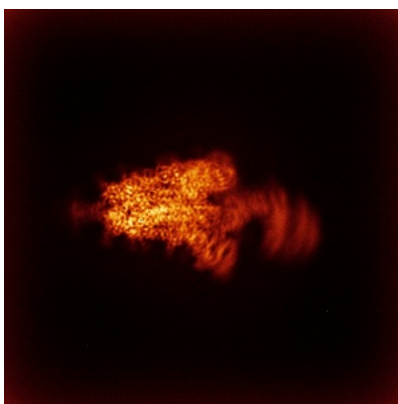


Z

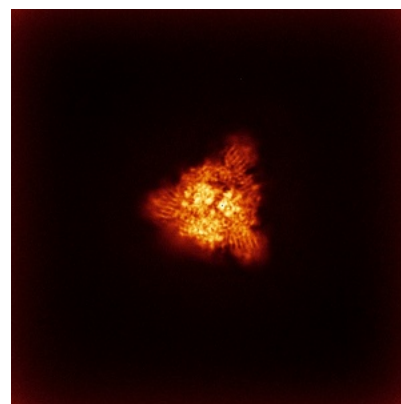
6.4.2 Raw map



X



Y

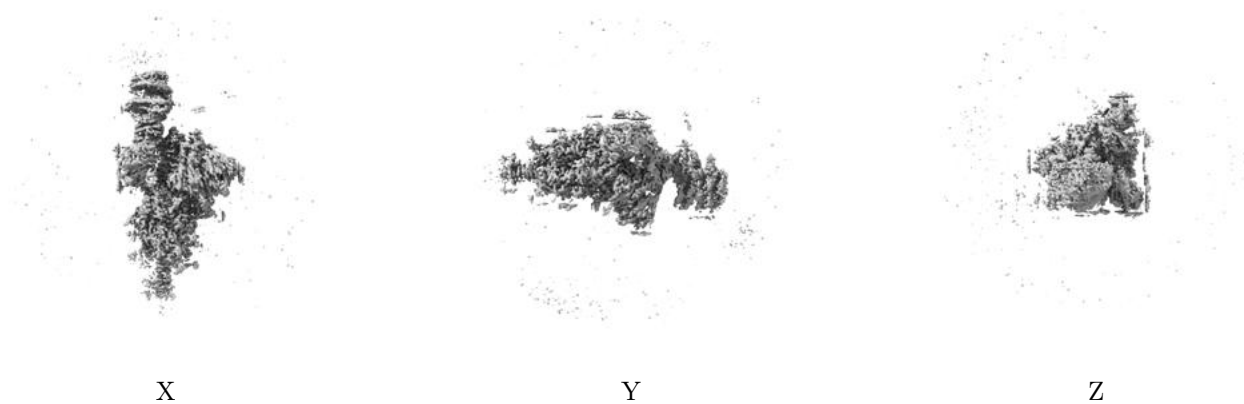


Z

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.

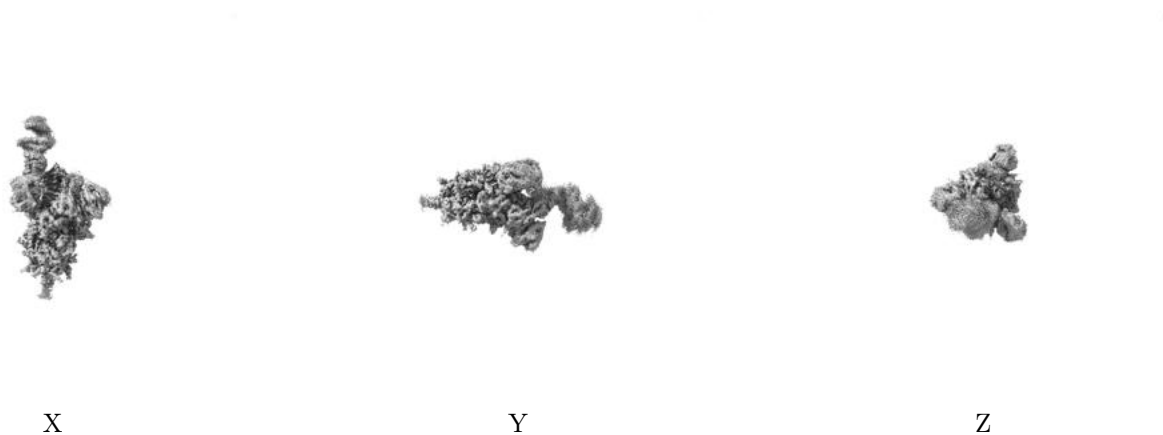
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

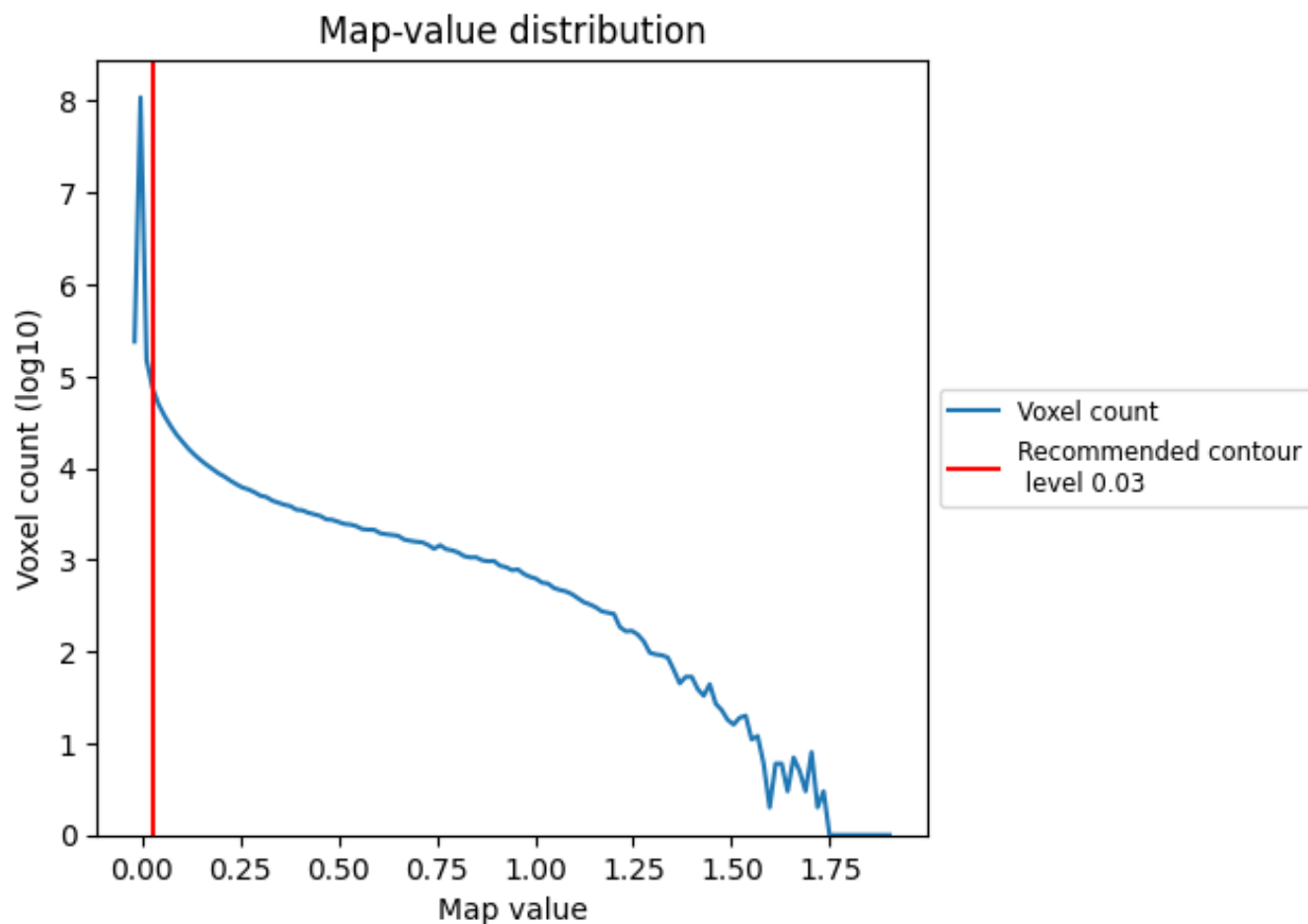
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

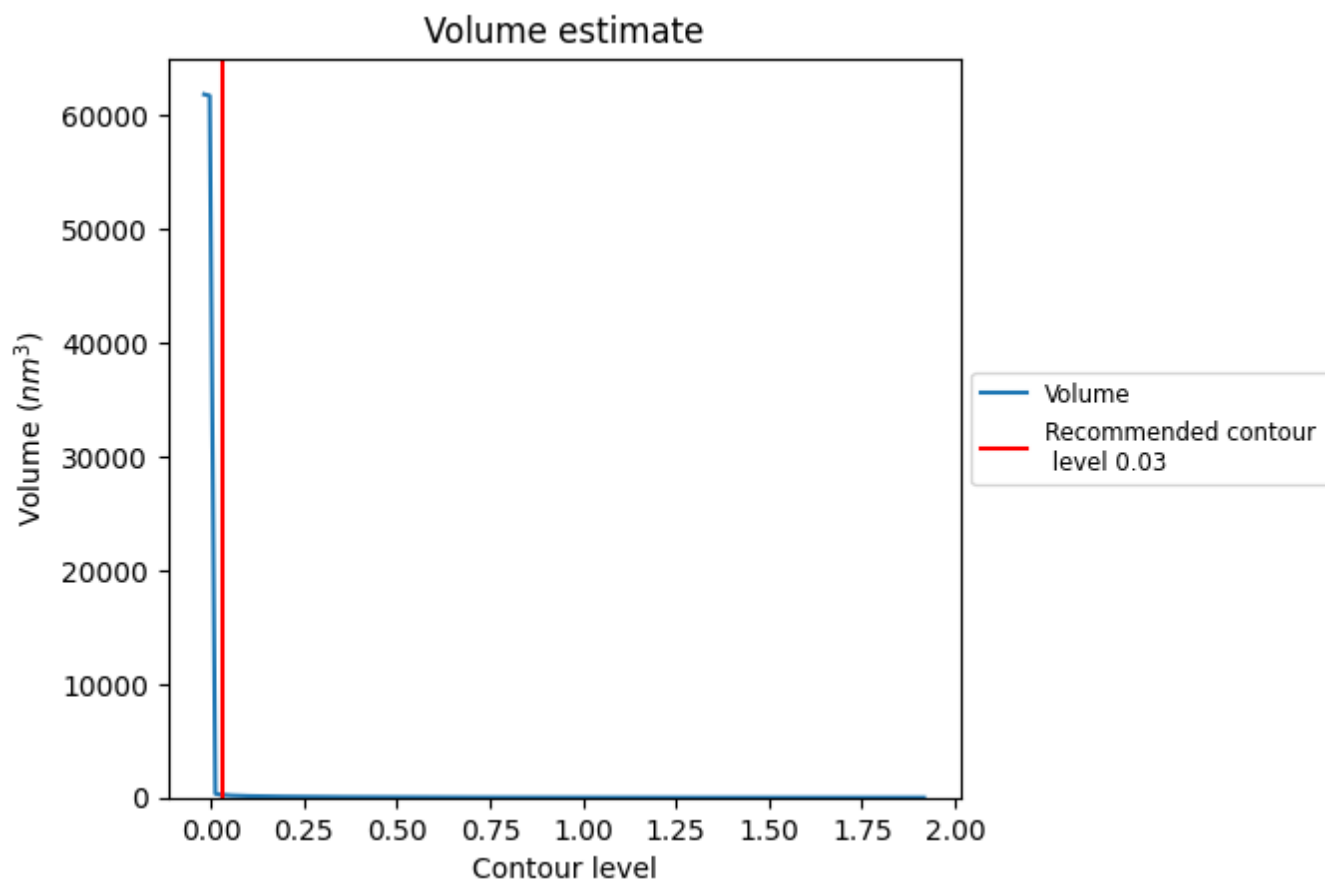
This section contains the results of statistical analysis of the map.

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.

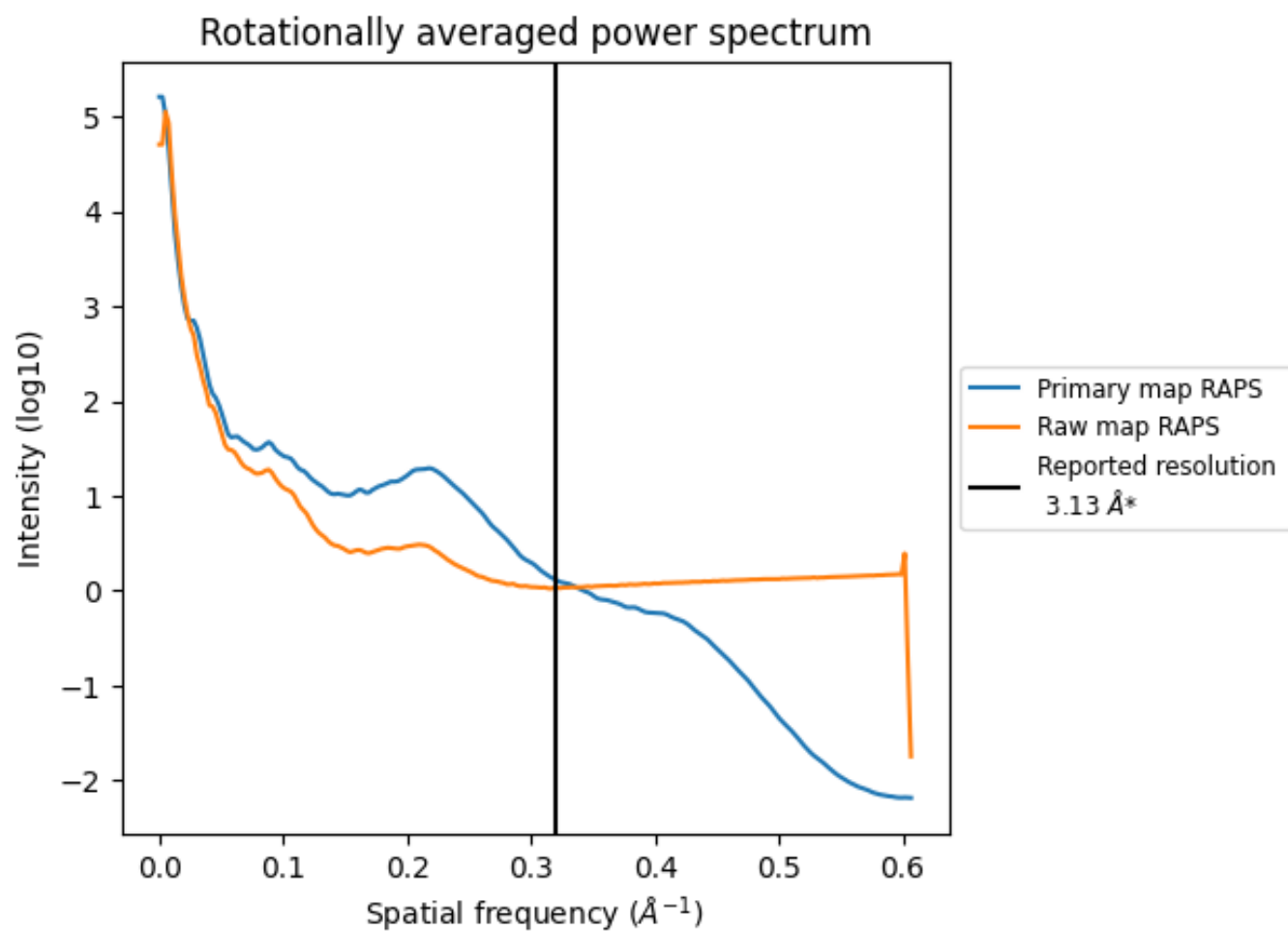
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm³; this corresponds to an approximate mass of 220 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 ⓘ

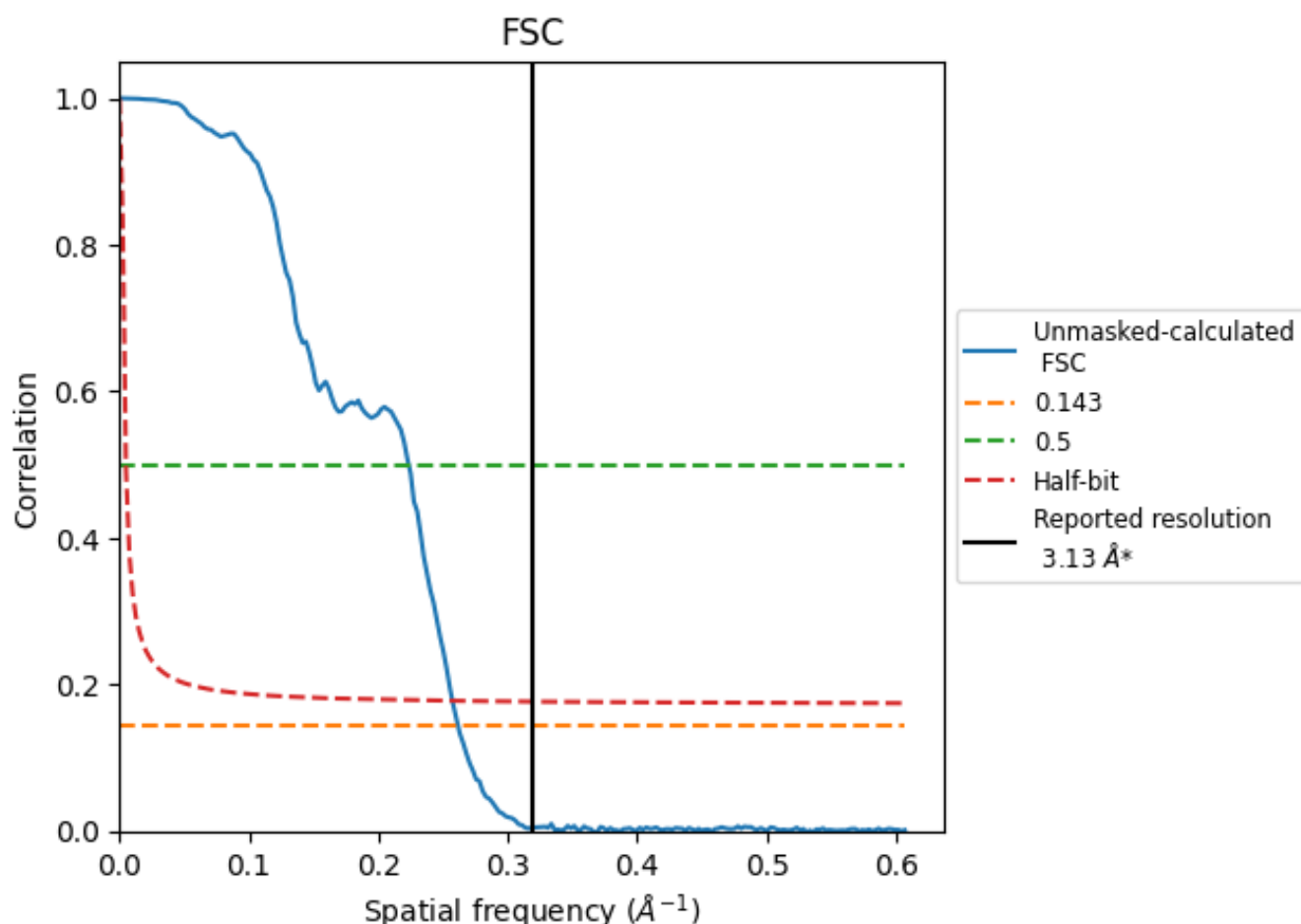


*Reported resolution corresponds to spatial frequency of 0.319 \AA^{-1}

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 0.319 Å⁻¹

8.2 Resolution estimates [i](#)

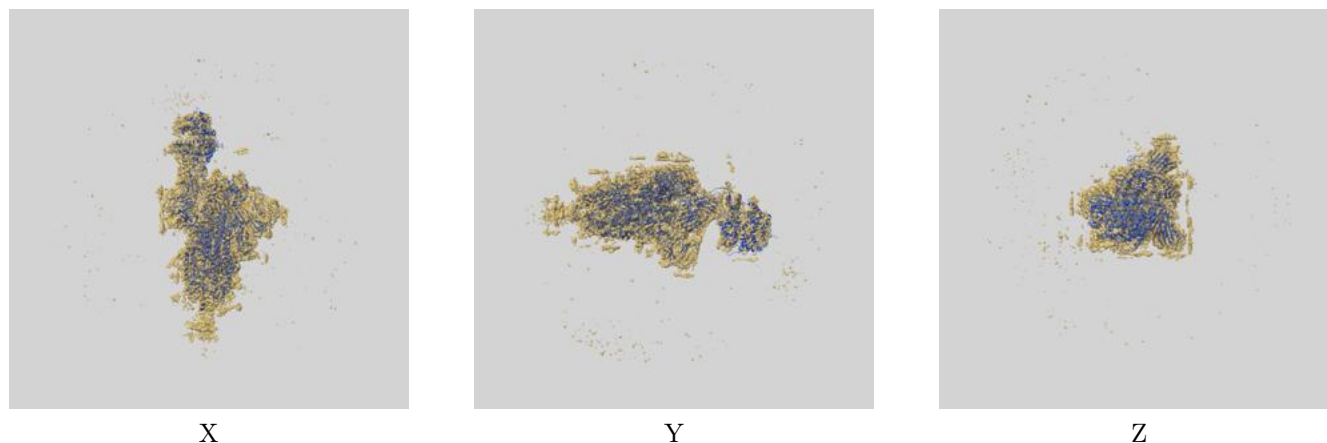
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.48	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

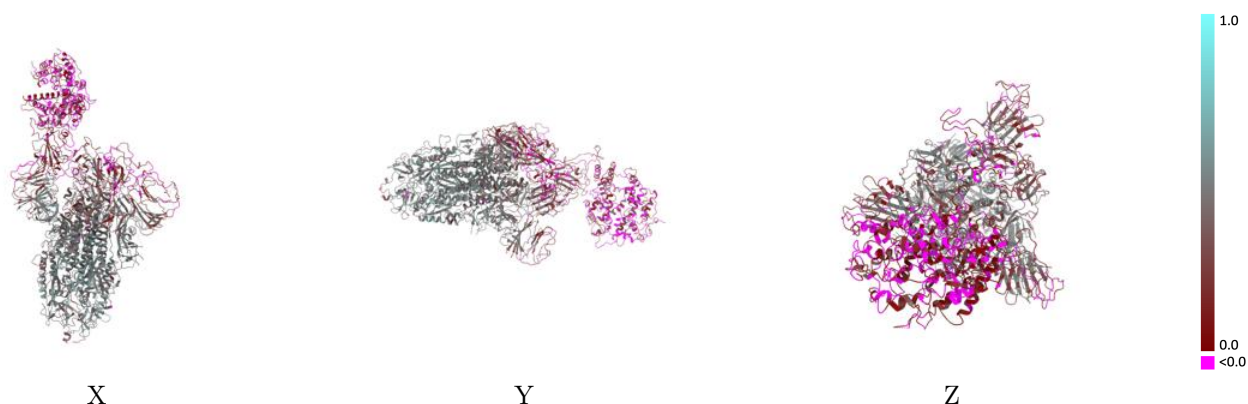
This section contains information regarding the fit between EMDB map EMD-33337 and PDB model 7XO5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



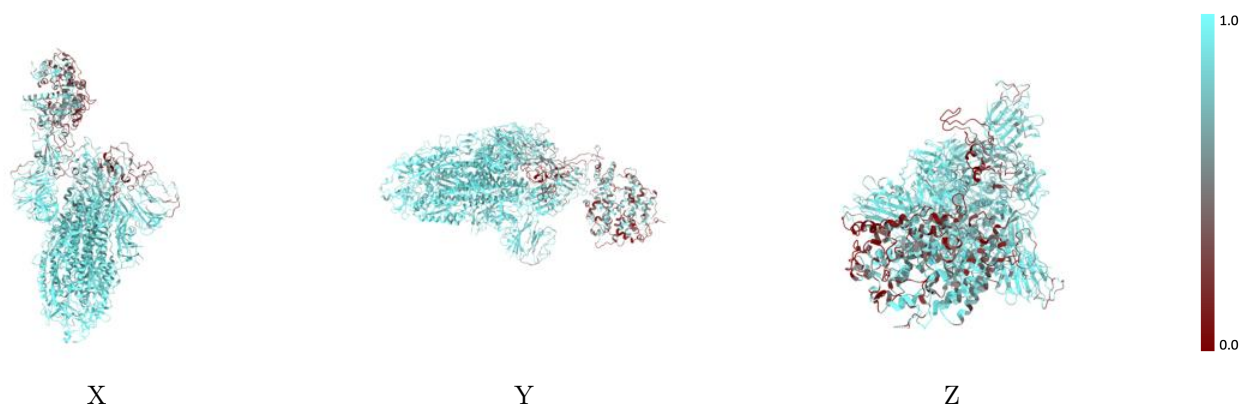
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



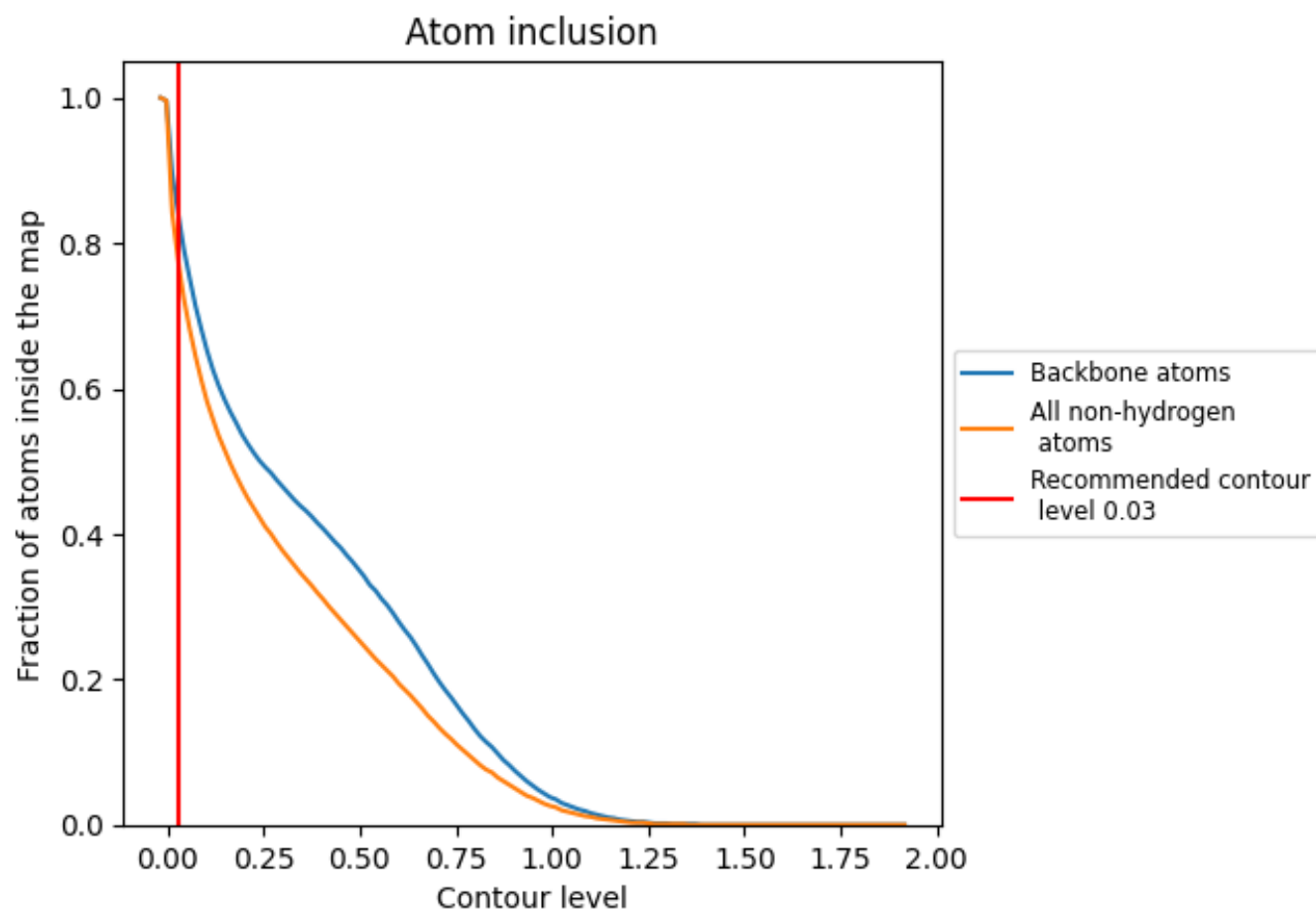
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7660	<div></div> 0.3150
A	<div></div> 0.8280	<div></div> 0.3710
B	<div></div> 0.7840	<div></div> 0.3570
C	<div></div> 0.8520	<div></div> 0.3820
D	<div></div> 0.4950	<div></div> 0.0470

