



Full wwPDB EM Validation Report ⓘ

Sep 29, 2022 – 05:11 pm BST

PDB ID : 7YZI
EMDB ID : EMD-14388
Title : Structure of Mycobacterium tuberculosis adenylyl cyclase Rv1625c / Cya
Authors : Mehta, V.; Khanppnavar, B.; Korkhov, V.M.
Deposited on : 2022-02-20
Resolution : 3.83 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

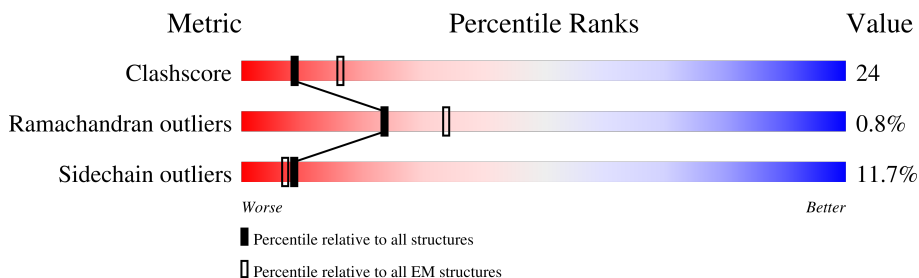
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.83 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	472	
1	B	472	
2	C	128	
2	D	128	
2	E	128	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16929 atoms, of which 8413 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 Adenylate cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	378	Total	C	H	N	O	S	1	0
			5775	1855	2902	489	520	9		
1	B	378	Total	C	H	N	O	S	1	0
			5775	1855	2902	489	520	9		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP P9WQ35
A	-24	GLY	-	expression tag	UNP P9WQ35
A	-23	SER	-	expression tag	UNP P9WQ35
A	-22	ALA	-	expression tag	UNP P9WQ35
A	-21	TRP	-	expression tag	UNP P9WQ35
A	-20	SER	-	expression tag	UNP P9WQ35
A	-19	HIS	-	expression tag	UNP P9WQ35
A	-18	PRO	-	expression tag	UNP P9WQ35
A	-17	GLN	-	expression tag	UNP P9WQ35
A	-16	PHE	-	expression tag	UNP P9WQ35
A	-15	GLU	-	expression tag	UNP P9WQ35
A	-14	LYS	-	expression tag	UNP P9WQ35
A	-13	GLY	-	expression tag	UNP P9WQ35
A	-12	SER	-	expression tag	UNP P9WQ35
A	-11	GLY	-	expression tag	UNP P9WQ35
A	-10	LEU	-	expression tag	UNP P9WQ35
A	-9	GLU	-	expression tag	UNP P9WQ35
A	-8	VAL	-	expression tag	UNP P9WQ35
A	-7	LEU	-	expression tag	UNP P9WQ35
A	-6	PHE	-	expression tag	UNP P9WQ35
A	-5	GLN	-	expression tag	UNP P9WQ35
A	-4	GLY	-	expression tag	UNP P9WQ35
A	-3	PRO	-	expression tag	UNP P9WQ35
A	-2	SER	-	expression tag	UNP P9WQ35
A	-1	GLY	-	expression tag	UNP P9WQ35
A	0	HIS	-	expression tag	UNP P9WQ35

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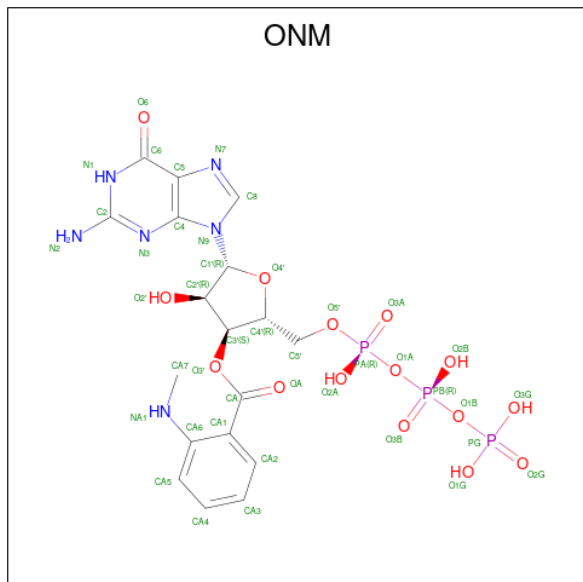
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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ALA	-	expression tag	UNP P9WQ35
A	445	ALA	-	expression tag	UNP P9WQ35
A	446	ALA	-	expression tag	UNP P9WQ35
B	-25	MET	-	initiating methionine	UNP P9WQ35
B	-24	GLY	-	expression tag	UNP P9WQ35
B	-23	SER	-	expression tag	UNP P9WQ35
B	-22	ALA	-	expression tag	UNP P9WQ35
B	-21	TRP	-	expression tag	UNP P9WQ35
B	-20	SER	-	expression tag	UNP P9WQ35
B	-19	HIS	-	expression tag	UNP P9WQ35
B	-18	PRO	-	expression tag	UNP P9WQ35
B	-17	GLN	-	expression tag	UNP P9WQ35
B	-16	PHE	-	expression tag	UNP P9WQ35
B	-15	GLU	-	expression tag	UNP P9WQ35
B	-14	LYS	-	expression tag	UNP P9WQ35
B	-13	GLY	-	expression tag	UNP P9WQ35
B	-12	SER	-	expression tag	UNP P9WQ35
B	-11	GLY	-	expression tag	UNP P9WQ35
B	-10	LEU	-	expression tag	UNP P9WQ35
B	-9	GLU	-	expression tag	UNP P9WQ35
B	-8	VAL	-	expression tag	UNP P9WQ35
B	-7	LEU	-	expression tag	UNP P9WQ35
B	-6	PHE	-	expression tag	UNP P9WQ35
B	-5	GLN	-	expression tag	UNP P9WQ35
B	-4	GLY	-	expression tag	UNP P9WQ35
B	-3	PRO	-	expression tag	UNP P9WQ35
B	-2	SER	-	expression tag	UNP P9WQ35
B	-1	GLY	-	expression tag	UNP P9WQ35
B	0	HIS	-	expression tag	UNP P9WQ35
B	444	ALA	-	expression tag	UNP P9WQ35
B	445	ALA	-	expression tag	UNP P9WQ35
B	446	ALA	-	expression tag	UNP P9WQ35

- Molecule 2 is a protein called Nanobody Nb4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	C	117	Total	C	H	N	O	S	4	0
			1752	552	858	161	177	4		
2	D	117	Total	C	H	N	O	S	4	0
			1752	552	858	161	177	4		
2	E	117	Total	C	H	N	O	S	4	0
			1749	552	855	161	177	4		

- Molecule 3 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: ONM) (formula: $C_{18}H_{23}N_6O_{15}P_3$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
3	A	1	61	18	19	6	15	3	0
3	B	1	61	18	19	6	15	3	0

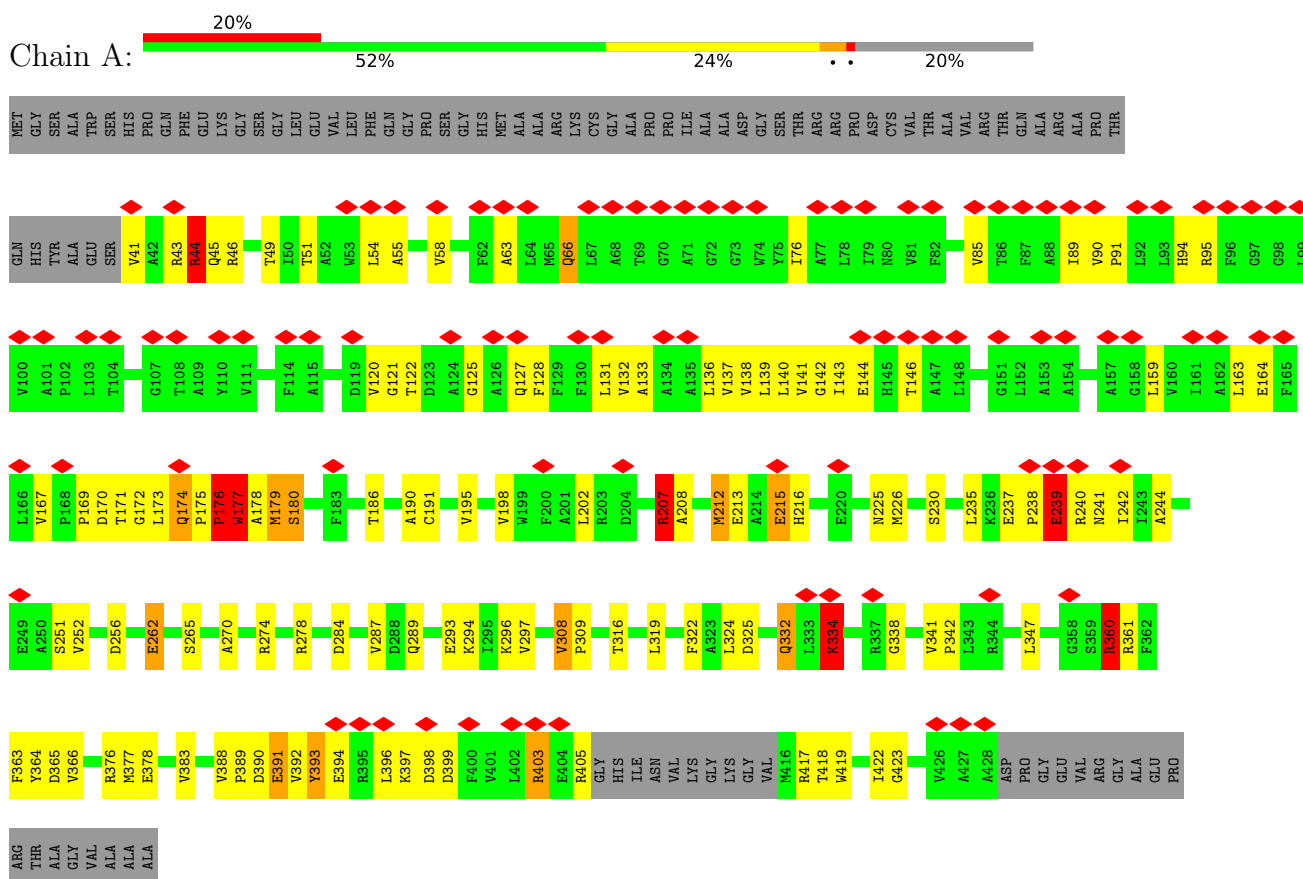
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
4	A	2	2	2	0
4	B	2	2	2	0

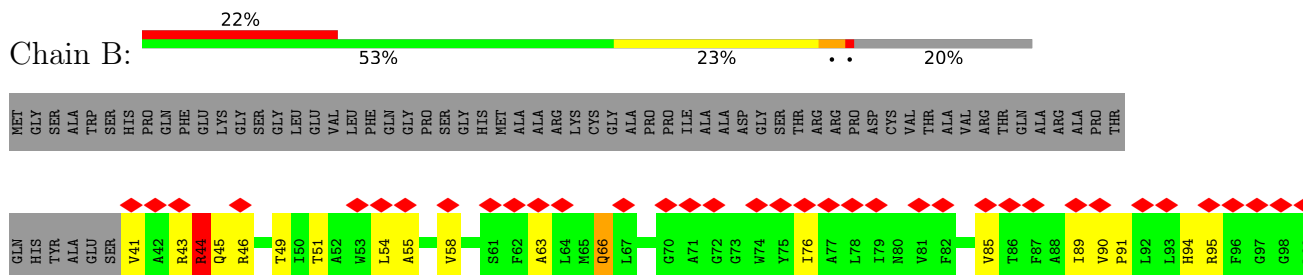
3 Residue-property plots

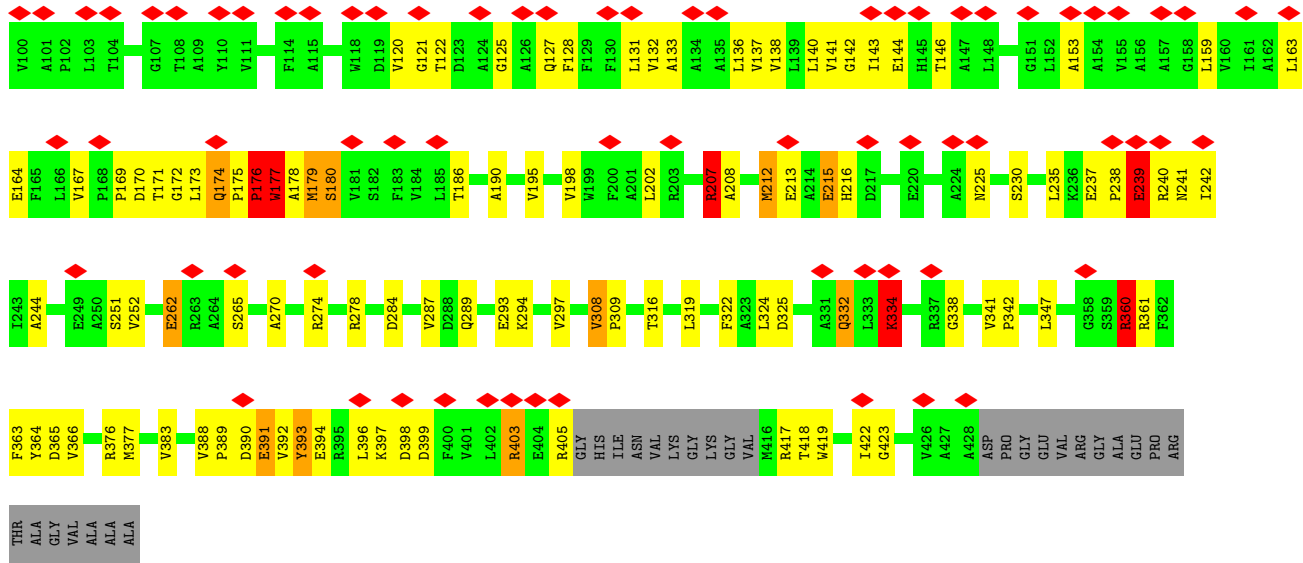
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Adenylate cyclase

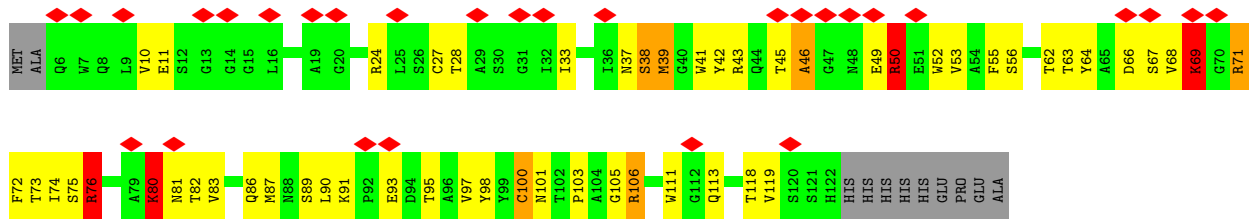


- Molecule 1: Adenylate cyclase

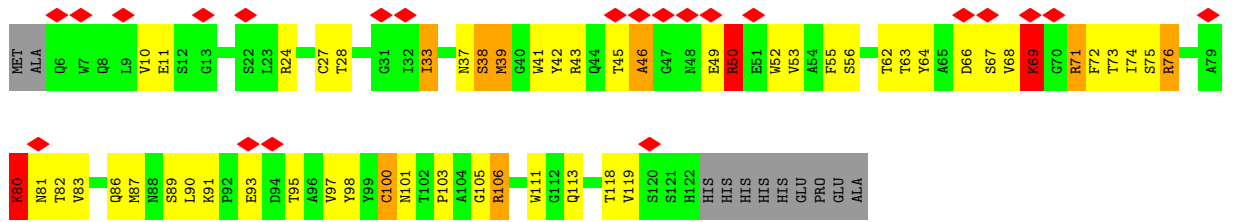




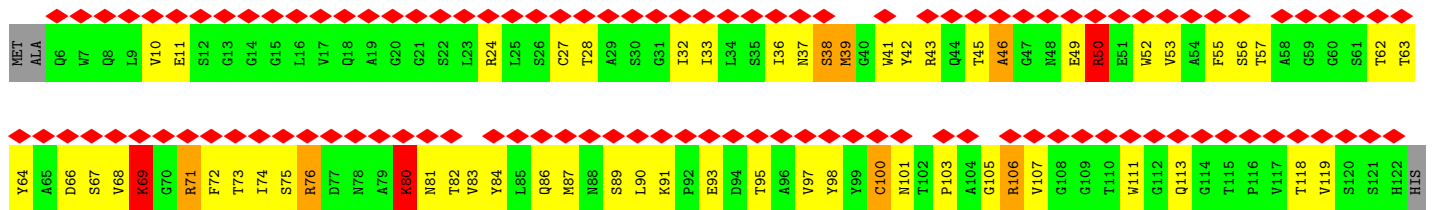
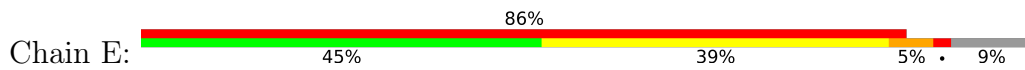
• Molecule 2: Nanobody Nb4



• Molecule 2: Nanobody Nb4



• Molecule 2: Nanobody Nb4



HIS
HIS
HIS
HIS
GLU
PRO
GLU
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	646042	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.020	Depositor
Minimum map value	-0.009	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00626	Depositor
Map size (\AA)	264.0, 264.0, 264.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.66, 0.66, 0.66	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: ONM, MN

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	0.46	1/2942 (0.0%)	0.87	14/4018 (0.3%)
1	B	0.46	1/2942 (0.0%)	0.87	14/4018 (0.3%)
2	C	0.51	1/928 (0.1%)	0.91	6/1260 (0.5%)
2	D	0.51	1/928 (0.1%)	0.91	6/1260 (0.5%)
2	E	0.51	1/928 (0.1%)	0.91	6/1260 (0.5%)
All	All	0.48	5/8668 (0.1%)	0.89	46/11816 (0.4%)

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	A	0	7
1	B	0	7
2	C	0	3
2	D	0	3
2	E	0	3
All	All	0	23

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	TYR	CD2-CE2	-5.45	1.31	1.39
1	B	393	TYR	CD2-CE2	-5.44	1.31	1.39
2	E	100	CYS	CB-SG	-5.10	1.73	1.81
2	C	100	CYS	CB-SG	-5.09	1.73	1.81
2	D	100	CYS	CB-SG	-5.08	1.73	1.81

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	LYS	CD-CE-NZ	14.78	145.70	111.70
1	A	334	LYS	CD-CE-NZ	14.76	145.65	111.70
1	A	44	ARG	CG-CD-NE	12.07	137.15	111.80
1	B	44	ARG	CG-CD-NE	12.05	137.11	111.80
1	B	44	ARG	CB-CA-C	-11.46	87.49	110.40
1	A	44	ARG	CB-CA-C	-11.45	87.49	110.40
1	A	44	ARG	CA-CB-CG	9.71	134.77	113.40
1	B	44	ARG	CA-CB-CG	9.71	134.75	113.40
1	B	44	ARG	CB-CG-CD	9.71	136.83	111.60
1	A	44	ARG	CB-CG-CD	9.69	136.78	111.60
2	E	80	LYS	CD-CE-NZ	8.29	130.77	111.70
2	C	80	LYS	CD-CE-NZ	8.28	130.74	111.70
2	D	80	LYS	CD-CE-NZ	8.27	130.72	111.70
1	A	207	ARG	CG-CD-NE	8.08	128.76	111.80
1	B	207	ARG	CG-CD-NE	8.06	128.74	111.80
1	B	95	ARG	CG-CD-NE	7.32	127.16	111.80
1	A	95	ARG	CG-CD-NE	7.29	127.11	111.80
1	A	177	TRP	CD1-CG-CD2	-7.25	100.50	106.30
1	B	177	TRP	CD1-CG-CD2	-7.20	100.54	106.30
2	D	39	MET	CB-CG-SD	6.90	133.09	112.40
2	C	39	MET	CB-CG-SD	6.89	133.08	112.40
2	E	39	MET	CB-CG-SD	6.89	133.07	112.40
1	B	44	ARG	N-CA-CB	6.64	122.55	110.60
1	A	44	ARG	N-CA-CB	6.63	122.54	110.60
1	B	239	GLU	CA-CB-CG	6.29	127.25	113.40
1	A	239	GLU	CA-CB-CG	6.29	127.23	113.40
2	E	39	MET	CG-SD-CE	-5.99	90.62	100.20
2	D	39	MET	CG-SD-CE	-5.97	90.64	100.20
2	C	39	MET	CG-SD-CE	-5.97	90.65	100.20
1	B	179	MET	CG-SD-CE	-5.88	90.78	100.20
1	A	179	MET	CG-SD-CE	-5.87	90.80	100.20
1	A	393	TYR	CB-CG-CD2	-5.74	117.55	121.00
2	E	80	LYS	CB-CG-CD	5.73	126.51	111.60
2	D	80	LYS	CB-CG-CD	5.73	126.50	111.60
2	C	80	LYS	CG-CD-CE	-5.72	94.73	111.90
2	D	80	LYS	CG-CD-CE	-5.71	94.76	111.90
2	E	80	LYS	CG-CD-CE	-5.71	94.77	111.90
2	C	80	LYS	CB-CG-CD	5.71	126.45	111.60
1	B	393	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	308	VAL	CG1-CB-CG2	5.45	119.63	110.90
1	B	308	VAL	CG1-CB-CG2	5.43	119.58	110.90
2	D	69	LYS	CB-CG-CD	5.27	125.31	111.60
2	C	69	LYS	CB-CG-CD	5.27	125.30	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	69	LYS	CB-CG-CD	5.26	125.28	111.60
1	A	177	TRP	CD1-NE1-CE2	-5.12	104.39	109.00
1	B	177	TRP	CD1-NE1-CE2	-5.11	104.41	109.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	PRO	Peptide
1	A	207	ARG	Sidechain
1	A	238	PRO	Peptide
1	A	360	ARG	Sidechain
1	A	403	ARG	Sidechain
1	A	405	ARG	Sidechain
1	A	44	ARG	Sidechain
1	B	176	PRO	Peptide
1	B	207	ARG	Sidechain
1	B	238	PRO	Peptide
1	B	360	ARG	Sidechain
1	B	403	ARG	Sidechain
1	B	405	ARG	Sidechain
1	B	44	ARG	Sidechain
2	C	50	ARG	Sidechain
2	C	71	ARG	Sidechain
2	C	76	ARG	Sidechain
2	D	50	ARG	Sidechain
2	D	71	ARG	Sidechain
2	D	76	ARG	Sidechain
2	E	50	ARG	Sidechain
2	E	71	ARG	Sidechain
2	E	76	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	A	2873	2902	2893	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2873	2902	2893	124	0
2	C	894	858	841	55	0
2	D	894	858	841	50	0
2	E	894	855	841	111	0
3	A	42	19	19	1	0
3	B	42	19	19	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	8516	8413	8347	398	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 24.

All (398) 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:170:ASP:CB	2:E:37:ASN:OD1	1.65	1.44
1:B:170:ASP:CG	2:E:37:ASN:OD1	1.72	1.27
1:A:176:PRO:CB	2:E:106:ARG:HH12	1.56	1.17
1:B:170:ASP:HB3	2:E:37:ASN:OD1	1.38	1.14
1:A:176:PRO:HB3	2:E:106:ARG:NH2	1.59	1.13
1:A:176:PRO:HB3	2:E:106:ARG:NH1	1.62	1.13
1:A:180:SER:OG	2:E:107:VAL:O	1.65	1.12
1:A:176:PRO:HB3	2:E:106:ARG:CZ	1.79	1.12
1:B:289:GLN:OE1	2:C:55:PHE:CE1	2.05	1.09
1:B:289:GLN:OE1	2:C:55:PHE:CD1	2.07	1.08
1:B:172:GLY:N	2:E:33:ILE:HD13	1.70	1.07
1:A:180:SER:HA	2:E:107:VAL:HG22	1.35	1.07
1:B:393:TYR:OH	1:B:419:TRP:N	1.90	1.05
1:B:172:GLY:H	2:E:33:ILE:HD13	0.92	1.04
1:B:172:GLY:H	2:E:33:ILE:CD1	1.70	1.03
1:A:393:TYR:OH	1:A:419:TRP:N	1.90	1.03
1:A:180:SER:HA	2:E:107:VAL:CG2	1.90	1.00
1:A:176:PRO:CB	2:E:106:ARG:HH22	1.72	1.00
1:A:176:PRO:HB3	2:E:106:ARG:HH22	1.16	0.98
1:A:176:PRO:HB3	2:E:106:ARG:HH12	1.19	0.96
1:B:41:VAL:HG22	1:B:44:ARG:HG2	1.48	0.93
1:A:176:PRO:CB	2:E:106:ARG:NH1	2.25	0.92
1:A:41:VAL:HG22	1:A:44:ARG:HG2	1.48	0.92
2:C:50:ARG:HD2	2:C:111:TRP:HZ3	1.37	0.90
2:E:50:ARG:HD2	2:E:111:TRP:HZ3	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:HB2	2:E:106:ARG:HH12	1.37	0.89
2:D:50:ARG:HD2	2:D:111:TRP:HZ3	1.37	0.88
1:A:170:ASP:OD2	2:E:103:PRO:CG	2.24	0.86
1:A:44:ARG:HA	1:A:44:ARG:NH1	1.91	0.84
1:B:44:ARG:HA	1:B:44:ARG:NH1	1.91	0.84
1:A:169:PRO:O	2:E:55:PHE:CE2	2.31	0.84
1:B:169:PRO:O	2:E:32:ILE:CG2	2.24	0.84
1:A:170:ASP:OD2	2:E:103:PRO:HG2	1.79	0.83
1:A:170:ASP:CG	2:E:103:PRO:HG3	1.99	0.83
1:B:170:ASP:CB	2:E:37:ASN:CG	2.48	0.82
1:A:180:SER:CA	2:E:107:VAL:CG2	2.58	0.81
1:A:180:SER:CA	2:E:107:VAL:HG22	2.09	0.81
1:A:170:ASP:CG	2:E:103:PRO:CG	2.51	0.79
1:A:172:GLY:O	2:E:52:TRP:NE1	2.15	0.79
1:B:325:ASP:OD2	2:C:38:SER:OG	2.00	0.78
1:A:170:ASP:HB2	2:E:55:PHE:CZ	2.18	0.78
1:B:91:PRO:O	1:B:94:HIS:ND1	2.17	0.77
1:A:91:PRO:O	1:A:94:HIS:ND1	2.17	0.77
2:D:33:ILE:O	2:D:37:ASN:ND2	2.19	0.76
2:E:33:ILE:O	2:E:37:ASN:ND2	2.19	0.75
2:C:33:ILE:O	2:C:37:ASN:ND2	2.19	0.75
1:A:176:PRO:CB	2:E:106:ARG:NH2	2.37	0.75
2:C:43:ARG:HD3	2:C:53:VAL:HG11	1.69	0.75
2:C:50:ARG:HD2	2:C:111:TRP:CZ3	2.22	0.74
2:D:43:ARG:HD3	2:D:53:VAL:HG11	1.69	0.74
2:D:50:ARG:HD2	2:D:111:TRP:CZ3	2.22	0.73
1:A:170:ASP:OD2	2:E:103:PRO:HG3	1.89	0.73
1:B:170:ASP:HB3	2:E:36:ILE:HG13	1.71	0.73
2:E:43:ARG:HD3	2:E:53:VAL:HG11	1.69	0.72
1:A:215:GLU:OE1	1:B:216:HIS:CE1	2.42	0.72
2:E:50:ARG:HD2	2:E:111:TRP:CZ3	2.22	0.71
1:B:54:LEU:HD11	1:B:136:LEU:HD21	1.73	0.71
1:A:54:LEU:HD11	1:A:136:LEU:HD21	1.73	0.71
1:B:169:PRO:O	2:E:32:ILE:HG22	1.92	0.69
1:A:325:ASP:OD2	2:D:38:SER:OG	2.09	0.69
1:B:393:TYR:CZ	1:B:419:TRP:HB2	2.28	0.69
1:A:180:SER:N	2:E:107:VAL:HG23	2.06	0.69
2:C:66:ASP:HA	2:C:69:LYS:HD2	1.75	0.69
1:A:241:ASN:OD1	1:A:242:ILE:N	2.26	0.69
1:A:334:LYS:NZ	1:A:338:GLY:O	2.24	0.69
1:B:390:ASP:HA	1:B:393:TYR:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:OD1	1:B:360:ARG:HD2	1.94	0.68
1:A:393:TYR:CZ	1:A:419:TRP:HB2	2.28	0.68
1:B:241:ASN:OD1	1:B:242:ILE:N	2.26	0.68
1:A:390:ASP:HA	1:A:393:TYR:CD2	2.29	0.67
2:E:66:ASP:HA	2:E:69:LYS:HD2	1.75	0.67
2:D:66:ASP:HA	2:D:69:LYS:HD2	1.75	0.67
1:B:169:PRO:O	2:E:32:ILE:HG21	1.93	0.67
2:C:24[A]:ARG:NH1	2:C:86:GLN:OE1	2.28	0.66
2:C:72:PHE:HD2	2:C:87:MET:HG2	1.61	0.66
2:E:72:PHE:HD2	2:E:87:MET:HG2	1.61	0.66
1:B:284:ASP:OD1	1:B:294:LYS:NZ	2.25	0.65
2:E:24[A]:ARG:NH1	2:E:86:GLN:OE1	2.30	0.65
1:B:334:LYS:NZ	1:B:338:GLY:O	2.24	0.65
2:D:24[A]:ARG:NH1	2:D:86:GLN:OE1	2.28	0.65
1:B:127:GLN:NE2	1:B:164:GLU:OE1	2.29	0.65
1:A:128:PHE:CD2	1:B:131:LEU:HD22	2.32	0.65
2:D:72:PHE:HD2	2:D:87:MET:HG2	1.61	0.65
1:A:127:GLN:NE2	1:A:164:GLU:OE1	2.30	0.64
1:B:341:VAL:HG13	1:B:341:VAL:O	1.98	0.64
2:C:72:PHE:CD2	2:C:87:MET:HG2	2.34	0.63
1:A:176:PRO:CB	2:E:106:ARG:CZ	2.66	0.63
1:B:393:TYR:CE1	1:B:419:TRP:HB2	2.33	0.63
2:E:72:PHE:CD2	2:E:87:MET:HG2	2.34	0.63
1:A:393:TYR:CE1	1:A:419:TRP:HB2	2.33	0.63
1:A:341:VAL:HG13	1:A:341:VAL:O	1.98	0.63
2:D:72:PHE:CD2	2:D:87:MET:HG2	2.34	0.62
1:A:180:SER:N	2:E:107:VAL:CG2	2.63	0.61
1:B:169:PRO:HD2	2:E:32:ILE:HG21	1.83	0.61
1:A:41:VAL:CG2	1:A:44:ARG:HG2	2.27	0.61
1:A:284:ASP:OD1	1:A:294:LYS:NZ	2.25	0.61
1:A:393:TYR:HH	1:A:419:TRP:H	1.50	0.60
1:B:163:LEU:HD12	1:B:167:VAL:HG21	1.84	0.60
1:A:131:LEU:HD21	1:B:132:VAL:HG23	1.84	0.60
1:B:41:VAL:CG2	1:B:44:ARG:HG2	2.27	0.59
1:B:198:VAL:O	1:B:202:LEU:HD23	2.02	0.59
2:E:64:TYR:OH	2:E:74:ILE:N	2.36	0.59
2:C:105:GLY:O	2:C:111:TRP:NE1	2.34	0.59
1:B:170:ASP:HB2	2:E:37:ASN:OD1	1.90	0.59
1:A:198:VAL:O	1:A:202:LEU:HD23	2.02	0.58
2:E:105:GLY:O	2:E:111:TRP:NE1	2.34	0.58
2:C:64:TYR:OH	2:C:74:ILE:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:OD2	2:E:37:ASN:OD1	2.20	0.58
1:A:216:HIS:CE1	1:B:215:GLU:OE1	2.57	0.58
2:D:64:TYR:OH	2:D:74:ILE:N	2.36	0.58
2:C:39:MET:HG2	2:C:83:VAL:HG21	1.86	0.58
2:D:39:MET:HG2	2:D:83:VAL:HG21	1.86	0.58
2:E:101:ASN:ND2	2:E:111:TRP:CD1	2.72	0.58
2:D:101:ASN:ND2	2:D:111:TRP:CD1	2.72	0.58
2:C:101:ASN:ND2	2:C:111:TRP:CD1	2.72	0.57
1:A:163:LEU:HD12	1:A:167:VAL:HG21	1.84	0.57
1:A:170:ASP:OD1	2:E:103:PRO:HB3	2.04	0.57
2:D:105:GLY:O	2:D:111:TRP:NE1	2.34	0.57
1:A:237:GLU:O	1:A:240:ARG:NH2	2.37	0.56
2:E:39:MET:HG2	2:E:83:VAL:HG21	1.86	0.56
2:D:68:VAL:HB	2:D:72:PHE:CE1	2.41	0.56
2:D:68:VAL:HB	2:D:72:PHE:CD1	2.41	0.56
1:B:316:THR:HG22	1:B:396:LEU:HD21	1.88	0.56
1:B:44:ARG:HA	1:B:44:ARG:HH11	1.70	0.56
1:B:172:GLY:H	2:E:33:ILE:CG1	2.18	0.55
1:B:237:GLU:O	1:B:240:ARG:NH2	2.37	0.55
1:B:289:GLN:OE1	2:C:55:PHE:CZ	2.58	0.55
2:C:68:VAL:HB	2:C:72:PHE:CE1	2.41	0.55
2:E:68:VAL:HB	2:E:72:PHE:CD1	2.41	0.55
2:C:68:VAL:HB	2:C:72:PHE:CD1	2.41	0.55
2:E:68:VAL:HB	2:E:72:PHE:CE1	2.40	0.55
1:B:393:TYR:HH	1:B:419:TRP:H	1.52	0.55
2:D:39:MET:O	2:D:55:PHE:CD1	2.60	0.55
1:A:174:GLN:CB	1:A:175:PRO:CD	2.85	0.54
1:A:316:THR:HG22	1:A:396:LEU:HD21	1.88	0.54
2:C:39:MET:O	2:C:55:PHE:CD1	2.60	0.54
2:E:39:MET:O	2:E:55:PHE:CD1	2.60	0.54
1:A:169:PRO:CD	2:E:57:THR:HG21	2.36	0.54
1:B:170:ASP:HB2	2:E:37:ASN:CG	2.26	0.54
2:C:38:SER:HB2	2:C:55:PHE:CZ	2.43	0.54
2:E:39:MET:HE1	2:E:100:CYS:SG	2.48	0.54
2:C:45:THR:O	2:C:46:ALA:HB2	2.08	0.54
1:B:174:GLN:CB	1:B:175:PRO:CD	2.85	0.54
2:D:38:SER:HB2	2:D:55:PHE:CZ	2.43	0.54
2:E:38:SER:HB2	2:E:55:PHE:CZ	2.43	0.54
2:E:45:THR:O	2:E:46:ALA:HB2	2.08	0.53
2:D:45:THR:O	2:D:46:ALA:HB2	2.08	0.53
2:D:39:MET:HE1	2:D:100:CYS:SG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:ARG:HB3	2:E:98:TYR:CD1	2.44	0.53
1:A:391:GLU:O	1:A:393:TYR:N	2.42	0.52
1:B:347:LEU:HB2	1:B:388:VAL:HG12	1.90	0.52
2:C:43:ARG:HB3	2:C:98:TYR:CD1	2.44	0.52
1:A:347:LEU:HB2	1:A:388:VAL:HG12	1.90	0.52
1:B:391:GLU:O	1:B:393:TYR:N	2.42	0.52
1:A:44:ARG:HA	1:A:44:ARG:HH11	1.70	0.52
1:A:251:SER:OG	1:A:319:LEU:HD22	2.10	0.51
1:B:170:ASP:O	2:E:33:ILE:N	2.27	0.51
2:C:28:THR:HA	2:C:82:THR:HG22	1.92	0.51
2:D:28:THR:HA	2:D:82:THR:HG22	1.93	0.51
2:D:43:ARG:HB3	2:D:98:TYR:CD1	2.44	0.51
1:A:41:VAL:O	1:A:41:VAL:HG13	2.10	0.51
1:A:51:THR:OG1	1:A:140:LEU:HD11	2.11	0.51
1:B:51:THR:OG1	1:B:140:LEU:HD11	2.11	0.51
1:B:170:ASP:HB3	2:E:37:ASN:CG	2.19	0.51
1:B:251:SER:OG	1:B:319:LEU:HD22	2.10	0.51
2:C:42:TYR:CE2	2:C:106:ARG:HG3	2.46	0.51
1:A:176:PRO:CG	2:E:106:ARG:HH22	2.23	0.51
1:B:174:GLN:HB3	1:B:175:PRO:HD3	1.93	0.51
2:D:42:TYR:CE2	2:D:106:ARG:HG3	2.46	0.50
2:E:42:TYR:OH	2:E:106:ARG:HG3	2.12	0.50
2:E:42:TYR:CE2	2:E:106:ARG:HG3	2.46	0.50
1:A:133:ALA:O	1:A:137:VAL:HG23	2.12	0.50
2:C:106:ARG:HA	2:C:111:TRP:CZ2	2.47	0.50
1:B:133:ALA:O	1:B:137:VAL:HG23	2.12	0.50
1:A:176:PRO:CA	2:E:106:ARG:NH2	2.74	0.50
1:B:41:VAL:O	1:B:41:VAL:HG13	2.11	0.50
2:C:95:THR:HG23	2:C:118:THR:HA	1.94	0.50
2:C:42:TYR:OH	2:C:106:ARG:HG3	2.12	0.49
1:A:169:PRO:CD	2:E:57:THR:CG2	2.90	0.49
2:C:64:TYR:OH	2:C:73:THR:HA	2.12	0.49
2:D:95:THR:HG23	2:D:118:THR:HA	1.94	0.49
1:A:131:LEU:HD21	1:B:132:VAL:CG2	2.41	0.49
2:E:28:THR:HA	2:E:82:THR:HG22	1.93	0.49
2:E:64:TYR:OH	2:E:73:THR:HA	2.13	0.49
2:E:101:ASN:ND2	2:E:111:TRP:NE1	2.61	0.49
2:E:106:ARG:HA	2:E:111:TRP:CZ2	2.47	0.49
1:A:174:GLN:HB3	1:A:175:PRO:HD3	1.93	0.49
2:D:64:TYR:OH	2:D:73:THR:HA	2.13	0.49
2:E:87:MET:HE2	2:E:90:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:HA	2:E:36:ILE:HD11	1.93	0.49
2:D:106:ARG:HA	2:D:111:TRP:CZ2	2.47	0.49
2:D:42:TYR:OH	2:D:106:ARG:HG3	2.12	0.49
1:A:244:ALA:CB	1:B:274:ARG:NH1	2.76	0.48
2:C:39:MET:CE	2:C:100:CYS:SG	3.01	0.48
2:D:63:THR:HG22	2:D:64:TYR:N	2.28	0.48
2:D:101:ASN:ND2	2:D:111:TRP:NE1	2.61	0.48
2:C:101:ASN:ND2	2:C:111:TRP:NE1	2.61	0.48
2:D:87:MET:HE2	2:D:90:LEU:HD21	1.94	0.48
2:D:39:MET:CE	2:D:100:CYS:SG	3.01	0.48
2:C:39:MET:HE1	2:C:100:CYS:SG	2.52	0.48
2:E:39:MET:CE	2:E:100:CYS:SG	3.01	0.48
2:E:95:THR:HG23	2:E:118:THR:HA	1.94	0.48
1:A:176:PRO:HD2	1:A:177:TRP:CD1	2.49	0.48
1:B:170:ASP:HB2	2:E:37:ASN:ND2	2.28	0.48
1:A:138:VAL:HG21	1:B:195:VAL:HG13	1.96	0.47
1:B:176:PRO:HD2	1:B:177:TRP:CD1	2.49	0.47
2:C:63:THR:HG22	2:C:64:TYR:N	2.28	0.47
1:A:363:PHE:CE2	1:A:365:ASP:OD1	2.67	0.47
1:B:363:PHE:CE2	1:B:365:ASP:OD1	2.67	0.47
2:C:43:ARG:HD3	2:C:53:VAL:CG1	2.41	0.47
1:A:176:PRO:CA	2:E:106:ARG:HH22	2.26	0.47
2:E:63:THR:HG22	2:E:64:TYR:N	2.28	0.47
1:A:121:GLY:HA3	1:A:170:ASP:HA	1.96	0.47
1:B:121:GLY:HA3	1:B:170:ASP:HA	1.96	0.47
1:A:122:THR:H	1:A:170:ASP:H	1.62	0.47
1:B:390:ASP:HA	1:B:393:TYR:HD2	1.78	0.47
1:B:122:THR:H	1:B:170:ASP:H	1.62	0.47
1:A:278:ARG:NH2	1:A:334:LYS:O	2.40	0.47
1:A:289:GLN:OE1	2:D:55:PHE:CD1	2.67	0.47
1:A:388:VAL:HB	1:A:392:VAL:HB	1.97	0.47
2:C:105:GLY:C	2:C:111:TRP:HE1	2.17	0.47
1:B:63:ALA:O	1:B:66:GLN:HB2	2.15	0.46
2:C:45:THR:O	2:C:46:ALA:CB	2.63	0.46
2:D:45:THR:O	2:D:46:ALA:CB	2.63	0.46
1:A:170:ASP:HB2	2:E:55:PHE:CE1	2.49	0.46
1:B:45:GLN:NE2	1:B:49:THR:HG21	2.31	0.46
2:D:80:LYS:HG2	2:D:82:THR:HG23	1.98	0.46
2:D:72:PHE:HD2	2:D:87:MET:CG	2.28	0.46
1:B:90:VAL:HG13	1:B:91:PRO:HD3	1.98	0.46
1:B:391:GLU:O	1:B:392:VAL:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:LYS:HG2	2:C:82:THR:HG23	1.98	0.46
2:D:66:ASP:OD1	2:D:67:SER:N	2.48	0.46
1:B:237:GLU:C	1:B:239:GLU:H	2.19	0.46
2:D:43:ARG:HD3	2:D:53:VAL:CG1	2.41	0.46
2:E:45:THR:O	2:E:46:ALA:CB	2.63	0.46
2:E:80:LYS:HG2	2:E:82:THR:HG23	1.98	0.46
2:C:66:ASP:OD1	2:C:67:SER:N	2.48	0.46
2:C:87:MET:HE2	2:C:90:LEU:HD21	1.96	0.46
2:C:103:PRO:HA	2:C:106:ARG:HB3	1.98	0.46
2:E:80:LYS:O	2:E:81:ASN:CB	2.64	0.46
1:A:195:VAL:HG22	1:B:138:VAL:HG21	1.97	0.46
2:C:80:LYS:O	2:C:81:ASN:CB	2.64	0.46
1:A:63:ALA:O	1:A:66:GLN:HB2	2.15	0.46
1:B:377:MET:HE1	1:B:389:PRO:HB3	1.98	0.46
2:C:43:ARG:HB3	2:C:98:TYR:CE1	2.51	0.46
2:E:66:ASP:OD1	2:E:67:SER:N	2.48	0.46
1:A:287:VAL:HG22	1:A:322:PHE:CE1	2.51	0.46
1:A:377:MET:HE1	1:A:389:PRO:HB3	1.98	0.46
2:C:91:LYS:CA	2:C:119:VAL:HG11	2.46	0.46
2:D:43:ARG:HB3	2:D:98:TYR:CE1	2.51	0.46
1:A:391:GLU:O	1:A:392:VAL:C	2.54	0.45
2:C:66:ASP:HA	2:C:69:LYS:CD	2.44	0.45
2:D:91:LYS:CA	2:D:119:VAL:HG11	2.45	0.45
1:A:237:GLU:C	1:A:239:GLU:H	2.19	0.45
1:B:85:VAL:O	1:B:89:ILE:HG12	2.16	0.45
1:B:287:VAL:HG22	1:B:322:PHE:CE1	2.51	0.45
2:E:105:GLY:C	2:E:111:TRP:HE1	2.17	0.45
1:B:278:ARG:NH2	1:B:334:LYS:O	2.40	0.45
1:B:388:VAL:HB	1:B:392:VAL:HB	1.97	0.45
2:D:106:ARG:O	2:D:111:TRP:HZ2	1.99	0.45
2:E:106:ARG:O	2:E:111:TRP:HZ2	1.99	0.45
1:A:85:VAL:O	1:A:89:ILE:HG12	2.16	0.45
1:A:226:MET:O	1:B:361:ARG:CD	2.64	0.45
1:B:132:VAL:HG21	1:B:190:ALA:HB1	1.98	0.45
1:A:237:GLU:HB3	1:A:239:GLU:HB2	1.98	0.45
1:A:388:VAL:HG23	1:A:393:TYR:CE1	2.52	0.45
1:B:308:VAL:N	1:B:309:PRO:HD2	2.31	0.45
1:A:90:VAL:HG13	1:A:91:PRO:HD3	1.98	0.45
1:B:388:VAL:HG23	1:B:393:TYR:CE1	2.52	0.45
1:B:397:LYS:HG3	1:B:398:ASP:N	2.32	0.45
2:C:63:THR:HG22	2:C:64:TYR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:LYS:CA	2:E:119:VAL:HG11	2.45	0.45
1:A:45:GLN:NE2	1:A:49:THR:HG21	2.31	0.45
1:A:122:THR:OG1	1:A:127:GLN:OE1	2.33	0.45
1:A:262:GLU:O	1:A:265:SER:N	2.49	0.45
1:B:159:LEU:O	1:B:163:LEU:N	2.50	0.45
1:B:237:GLU:HB3	1:B:239:GLU:HB2	1.98	0.45
2:D:80:LYS:O	2:D:81:ASN:CB	2.64	0.45
1:A:308:VAL:N	1:A:309:PRO:HD2	2.32	0.45
1:A:390:ASP:HA	1:A:393:TYR:HD2	1.78	0.45
2:E:43:ARG:HB3	2:E:98:TYR:CE1	2.51	0.45
1:B:122:THR:OG1	1:B:127:GLN:OE1	2.34	0.45
1:B:262:GLU:O	1:B:265:SER:N	2.49	0.44
2:C:106:ARG:O	2:C:111:TRP:HZ2	1.99	0.44
1:A:397:LYS:HG3	1:A:398:ASP:N	2.32	0.44
1:B:43:ARG:HA	1:B:46:ARG:HE	1.83	0.44
1:A:389:PRO:HD2	1:A:392:VAL:CG2	2.47	0.44
2:E:43:ARG:HD3	2:E:53:VAL:CG1	2.41	0.44
2:E:90:LEU:C	2:E:91:LYS:HG3	2.38	0.44
1:A:324:LEU:HD11	1:A:423:GLY:HA2	1.99	0.44
1:B:143:ILE:HA	1:B:146:THR:HG23	1.99	0.44
2:E:63:THR:HG22	2:E:64:TYR:H	1.82	0.44
2:E:103:PRO:HA	2:E:106:ARG:HB3	1.98	0.44
1:B:393:TYR:O	1:B:394:GLU:C	2.56	0.44
1:B:43:ARG:O	1:B:44:ARG:C	2.57	0.44
1:B:389:PRO:HD2	1:B:392:VAL:CG2	2.47	0.44
1:A:169:PRO:HD2	2:E:57:THR:CG2	2.47	0.44
1:A:170:ASP:OD1	2:E:103:PRO:CB	2.66	0.44
1:B:141:VAL:HG12	1:B:142:GLY:N	2.33	0.44
1:A:132:VAL:HG21	1:A:190:ALA:HB1	1.99	0.44
2:D:63:THR:HG22	2:D:64:TYR:H	1.82	0.44
2:E:43:ARG:CD	2:E:53:VAL:HG11	2.43	0.44
1:B:393:TYR:HH	1:B:418:THR:HA	1.83	0.43
2:C:90:LEU:C	2:C:91:LYS:HG3	2.38	0.43
2:D:103:PRO:HA	2:D:106:ARG:HB3	1.98	0.43
2:E:72:PHE:HD2	2:E:87:MET:CG	2.28	0.43
1:A:169:PRO:O	2:E:55:PHE:CZ	2.71	0.43
2:D:90:LEU:C	2:D:91:LYS:HG3	2.38	0.43
2:E:27:CYS:HB2	2:E:41:TRP:CZ2	2.54	0.43
1:B:213:GLU:HA	1:B:213:GLU:OE1	2.19	0.43
1:B:270:ALA:O	1:B:274:ARG:HD3	2.19	0.43
1:B:417:ARG:HA	1:B:417:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:O	1:A:163:LEU:N	2.50	0.43
1:A:393:TYR:O	1:A:394:GLU:C	2.56	0.43
2:D:50:ARG:NH1	2:D:111:TRP:HE3	2.17	0.43
1:A:143:ILE:HA	1:A:146:THR:HG23	1.99	0.43
2:D:105:GLY:C	2:D:111:TRP:HE1	2.17	0.43
2:E:66:ASP:HA	2:E:69:LYS:CD	2.44	0.43
1:B:289:GLN:OE1	2:C:55:PHE:CG	2.64	0.43
2:C:72:PHE:HD2	2:C:87:MET:CG	2.28	0.43
1:A:297:VAL:O	1:A:297:VAL:HG13	2.19	0.43
2:D:66:ASP:HA	2:D:69:LYS:CD	2.44	0.43
1:B:297:VAL:O	1:B:297:VAL:HG13	2.19	0.43
1:B:324:LEU:HD11	1:B:423:GLY:HA2	1.99	0.43
1:A:43:ARG:O	1:A:44:ARG:C	2.56	0.43
1:A:125:GLY:HA3	1:A:186:THR:HG21	2.00	0.43
2:D:27:CYS:HB2	2:D:41:TRP:CZ2	2.54	0.43
1:B:170:ASP:CB	2:E:37:ASN:ND2	2.82	0.42
2:C:43:ARG:CD	2:C:53:VAL:HG11	2.43	0.42
1:A:270:ALA:O	1:A:274:ARG:HD3	2.19	0.42
1:A:296:LYS:NZ	3:B:501:ONM:HN1	2.17	0.42
1:A:417:ARG:NE	1:A:417:ARG:HA	2.34	0.42
2:E:10:VAL:HG12	2:E:28:THR:HG23	2.02	0.42
1:A:141:VAL:HG12	1:A:142:GLY:N	2.33	0.42
1:A:179:MET:O	1:A:179:MET:HG2	2.20	0.42
2:C:27:CYS:HB2	2:C:41:TRP:CZ2	2.54	0.42
1:A:163:LEU:HD12	1:A:167:VAL:CG2	2.48	0.42
1:B:341:VAL:O	1:B:341:VAL:CG1	2.66	0.42
2:C:10:VAL:HG12	2:C:28:THR:HG23	2.02	0.42
1:A:43:ARG:HA	1:A:46:ARG:HE	1.83	0.42
1:A:90:VAL:N	1:A:91:PRO:HD2	2.35	0.42
1:A:121:GLY:HA2	1:A:171:THR:H	1.85	0.42
2:C:50:ARG:NH1	2:C:111:TRP:HE3	2.17	0.42
2:E:50:ARG:NH1	2:E:111:TRP:HE3	2.17	0.42
1:A:55:ALA:O	1:A:58:VAL:HG22	2.20	0.42
1:A:274:ARG:NH1	1:B:244:ALA:CB	2.83	0.42
1:A:341:VAL:O	1:A:341:VAL:CG1	2.66	0.42
1:A:393:TYR:HH	1:A:418:THR:HA	1.84	0.42
1:B:55:ALA:O	1:B:58:VAL:HG22	2.20	0.42
1:B:125:GLY:HA3	1:B:186:THR:HG21	2.00	0.42
1:B:170:ASP:HA	2:E:36:ILE:CD1	2.49	0.42
1:B:207:ARG:HH11	1:B:207:ARG:HD2	1.74	0.42
1:A:195:VAL:HG13	1:B:138:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLY:HA2	1:B:171:THR:H	1.85	0.42
1:B:179:MET:O	1:B:179:MET:HG2	2.20	0.42
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.19	0.42
1:A:342:PRO:CB	1:A:383:VAL:HG13	2.50	0.42
1:B:90:VAL:N	1:B:91:PRO:HD2	2.35	0.42
1:B:388:VAL:HG23	1:B:393:TYR:HE1	1.85	0.42
1:B:163:LEU:HD12	1:B:167:VAL:CG2	2.48	0.41
1:A:169:PRO:HG2	2:E:57:THR:HG22	2.02	0.41
2:C:72:PHE:HD2	2:C:87:MET:CB	2.33	0.41
1:A:360:ARG:HD2	1:B:225:ASN:OD1	2.21	0.41
1:B:208:ALA:O	1:B:212:MET:HB2	2.20	0.41
1:B:332:GLN:CA	1:B:332:GLN:OE1	2.68	0.41
1:A:127:GLN:HB3	1:B:128:PHE:HZ	1.85	0.41
1:A:208:ALA:O	1:A:212:MET:HB2	2.20	0.41
2:D:10:VAL:HG12	2:D:28:THR:HG23	2.02	0.41
1:A:177:TRP:CD1	1:A:178:ALA:N	2.88	0.41
1:A:332:GLN:CA	1:A:332:GLN:OE1	2.68	0.41
1:B:391:GLU:C	1:B:393:TYR:N	2.72	0.41
2:C:42:TYR:CE1	2:C:52:TRP:HB3	2.56	0.41
2:E:42:TYR:CE1	2:E:52:TRP:HB3	2.56	0.41
1:A:207:ARG:HH11	1:A:207:ARG:HD2	1.74	0.41
2:C:76:ARG:HE	2:C:76:ARG:HB2	1.79	0.41
2:D:72:PHE:HD2	2:D:87:MET:CB	2.33	0.41
1:A:139:LEU:CD1	1:B:202:LEU:HD21	2.51	0.41
1:A:191:CYS:SG	1:B:153:ALA:HB1	2.60	0.41
1:B:177:TRP:O	1:B:180:SER:HB2	2.21	0.41
2:E:72:PHE:HD2	2:E:87:MET:CB	2.33	0.41
1:A:177:TRP:CD1	1:A:177:TRP:N	2.87	0.41
1:A:360:ARG:HG3	1:A:361:ARG:N	2.35	0.41
1:A:364:TYR:O	1:A:365:ASP:HB2	2.20	0.41
1:B:177:TRP:CD1	1:B:178:ALA:N	2.88	0.41
1:A:391:GLU:C	1:A:393:TYR:N	2.72	0.41
1:B:342:PRO:CB	1:B:383:VAL:HG13	2.50	0.41
1:B:364:TYR:O	1:B:365:ASP:HB2	2.20	0.40
1:A:174:GLN:HB3	1:A:175:PRO:CD	2.51	0.40
1:A:388:VAL:HG23	1:A:393:TYR:HE1	1.85	0.40
1:B:174:GLN:HB3	1:B:175:PRO:CD	2.50	0.40
2:D:42:TYR:CE1	2:D:52:TRP:HB3	2.56	0.40
1:B:172:GLY:HA3	2:E:33:ILE:HG21	2.02	0.40
1:A:256:ASP:HB3	1:A:378:GLU:OE2	2.21	0.40
2:E:24[B]:ARG:NH2	2:E:84:TYR:CE2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PRO:HG2	2:E:57:THR:CG2	2.51	0.40
1:A:175:PRO:HB2	1:A:177:TRP:NE1	2.37	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	A	375/472 (79%)	353 (94%)	19 (5%)	3 (1%)	19	56
1	B	375/472 (79%)	353 (94%)	19 (5%)	3 (1%)	19	56
2	C	119/128 (93%)	112 (94%)	6 (5%)	1 (1%)	19	56
2	D	119/128 (93%)	112 (94%)	6 (5%)	1 (1%)	19	56
2	E	119/128 (93%)	112 (94%)	6 (5%)	1 (1%)	19	56
All	All	1107/1328 (83%)	1042 (94%)	56 (5%)	9 (1%)	24	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	177	TRP
1	B	174	GLN
1	B	177	TRP
1	A	176	PRO
1	B	176	PRO
2	C	46	ALA
2	D	46	ALA
2	E	46	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/361 (82%)	269 (91%)	27 (9%)	9	36
1	B	296/361 (82%)	269 (91%)	27 (9%)	9	36
2	C	96/101 (95%)	79 (82%)	17 (18%)	2	12
2	D	96/101 (95%)	78 (81%)	18 (19%)	1	10
2	E	96/101 (95%)	79 (82%)	17 (18%)	2	12
All	All	880/1025 (86%)	774 (88%)	106 (12%)	9	25

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	66	GLN
1	A	76	ILE
1	A	120	VAL
1	A	144	GLU
1	A	173	LEU
1	A	177	TRP
1	A	180	SER
1	A	207	ARG
1	A	212	MET
1	A	215	GLU
1	A	230	SER
1	A	235	LEU
1	A	239	GLU
1	A	252	VAL
1	A	262	GLU
1	A	293	GLU
1	A	332	GLN
1	A	334	LYS
1	A	360	ARG
1	A	366[A]	VAL
1	A	366[B]	VAL
1	A	376	ARG

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Mol	Chain	Res	Type
1	A	391	GLU
1	A	399	ASP
1	A	403	ARG
1	A	422	ILE
1	B	44	ARG
1	B	66	GLN
1	B	76	ILE
1	B	120	VAL
1	B	144	GLU
1	B	173	LEU
1	B	177	TRP
1	B	180	SER
1	B	207	ARG
1	B	212	MET
1	B	215	GLU
1	B	230	SER
1	B	235	LEU
1	B	239	GLU
1	B	252	VAL
1	B	262	GLU
1	B	293	GLU
1	B	332	GLN
1	B	334	LYS
1	B	360	ARG
1	B	366[A]	VAL
1	B	366[B]	VAL
1	B	376	ARG
1	B	391	GLU
1	B	399	ASP
1	B	403	ARG
1	B	422	ILE
2	C	11	GLU
2	C	38	SER
2	C	49	GLU
2	C	50	ARG
2	C	56	SER
2	C	62	THR
2	C	69	LYS
2	C	71	ARG
2	C	75	SER
2	C	76	ARG
2	C	80	LYS

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Mol	Chain	Res	Type
2	C	89	SER
2	C	93[A]	GLU
2	C	93[B]	GLU
2	C	97	VAL
2	C	106	ARG
2	C	113	GLN
2	D	11	GLU
2	D	33	ILE
2	D	38	SER
2	D	49	GLU
2	D	50	ARG
2	D	56	SER
2	D	62	THR
2	D	69	LYS
2	D	71	ARG
2	D	75	SER
2	D	76	ARG
2	D	80	LYS
2	D	89	SER
2	D	93[A]	GLU
2	D	93[B]	GLU
2	D	97	VAL
2	D	106	ARG
2	D	113	GLN
2	E	11	GLU
2	E	38	SER
2	E	49	GLU
2	E	50	ARG
2	E	56	SER
2	E	62	THR
2	E	69	LYS
2	E	71	ARG
2	E	75	SER
2	E	76	ARG
2	E	80	LYS
2	E	89	SER
2	E	93[A]	GLU
2	E	93[B]	GLU
2	E	97	VAL
2	E	106	ARG
2	E	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	HIS
1	B	216	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ONM	B	501	4	37,45,45	4.27	18 (48%)	47,69,69	1.37	8 (17%)
3	ONM	A	501	4	37,45,45	4.27	18 (48%)	47,69,69	1.37	8 (17%)

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	ONM	B	501	4	-	4/28/48/48	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ONM	A	501	4	-	4/28/48/48	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ONM	O4'-C1'	14.72	1.61	1.41
3	A	501	ONM	O4'-C1'	14.68	1.61	1.41
3	B	501	ONM	C2'-C1'	-13.39	1.33	1.53
3	A	501	ONM	C2'-C1'	-13.38	1.33	1.53
3	A	501	ONM	O4'-C4'	-7.09	1.29	1.45
3	B	501	ONM	O4'-C4'	-7.04	1.29	1.45
3	B	501	ONM	C2-N3	5.41	1.46	1.33
3	A	501	ONM	C2-N3	5.40	1.46	1.33
3	B	501	ONM	C4-N3	5.21	1.50	1.37
3	A	501	ONM	C4-N3	5.21	1.50	1.37
3	A	501	ONM	O3'-C3'	-5.19	1.37	1.44
3	B	501	ONM	O3'-C3'	-5.16	1.37	1.44
3	B	501	ONM	C2-N2	4.92	1.45	1.34
3	A	501	ONM	C2-N2	4.91	1.45	1.34
3	A	501	ONM	O3'-CA	4.48	1.43	1.34
3	B	501	ONM	O3'-CA	4.47	1.43	1.34
3	B	501	ONM	CA1-CA	3.93	1.58	1.50
3	A	501	ONM	CA1-CA	3.90	1.58	1.50
3	A	501	ONM	C6-N1	3.79	1.43	1.37
3	B	501	ONM	C6-N1	3.77	1.43	1.37
3	B	501	ONM	C5-C6	3.32	1.54	1.47
3	A	501	ONM	C5-C6	3.30	1.54	1.47
3	B	501	ONM	CA6-NA1	3.04	1.43	1.37
3	A	501	ONM	O2'-C2'	3.04	1.50	1.43
3	B	501	ONM	O2'-C2'	3.03	1.50	1.43
3	A	501	ONM	CA6-NA1	3.01	1.43	1.37
3	A	501	ONM	C2-N1	2.80	1.44	1.37
3	B	501	ONM	C2-N1	2.79	1.44	1.37
3	A	501	ONM	C5-C4	-2.61	1.36	1.43
3	B	501	ONM	C5-C4	-2.60	1.36	1.43
3	A	501	ONM	C3'-C4'	2.48	1.59	1.52
3	B	501	ONM	C3'-C4'	2.47	1.59	1.52
3	B	501	ONM	CA7-NA1	2.25	1.49	1.45
3	A	501	ONM	CA7-NA1	2.23	1.49	1.45
3	A	501	ONM	O6-C6	-2.06	1.19	1.23
3	B	501	ONM	O6-C6	-2.04	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ONM	O3'-CA-CA1	4.07	118.03	111.69
3	B	501	ONM	O3'-CA-CA1	4.04	117.99	111.69
3	B	501	ONM	PB-O1B-PG	-3.43	121.07	132.83
3	A	501	ONM	PB-O1B-PG	-3.41	121.14	132.83
3	B	501	ONM	C5-C6-N1	3.27	119.73	113.95
3	A	501	ONM	C5-C6-N1	3.26	119.70	113.95
3	A	501	ONM	C2-N1-C6	-2.74	120.05	125.10
3	B	501	ONM	C2-N1-C6	-2.74	120.06	125.10
3	A	501	ONM	C8-N7-C5	2.53	107.82	102.99
3	B	501	ONM	C8-N7-C5	2.52	107.79	102.99
3	B	501	ONM	PB-O1A-PA	-2.35	124.75	132.83
3	A	501	ONM	PB-O1A-PA	-2.34	124.81	132.83
3	B	501	ONM	O6-C6-C5	-2.21	120.05	124.37
3	A	501	ONM	O6-C6-C5	-2.20	120.07	124.37
3	A	501	ONM	O4'-C1'-C2'	-2.03	103.96	106.93
3	B	501	ONM	O4'-C1'-C2'	-2.03	103.97	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ONM	PB-O1A-PA-O5'
3	A	501	ONM	PB-O1B-PG-O3G
3	B	501	ONM	PB-O1A-PA-O5'
3	B	501	ONM	PB-O1B-PG-O3G
3	A	501	ONM	PB-O1B-PG-O1G
3	B	501	ONM	PB-O1B-PG-O1G
3	A	501	ONM	PB-O1B-PG-O2G
3	B	501	ONM	PB-O1B-PG-O2G

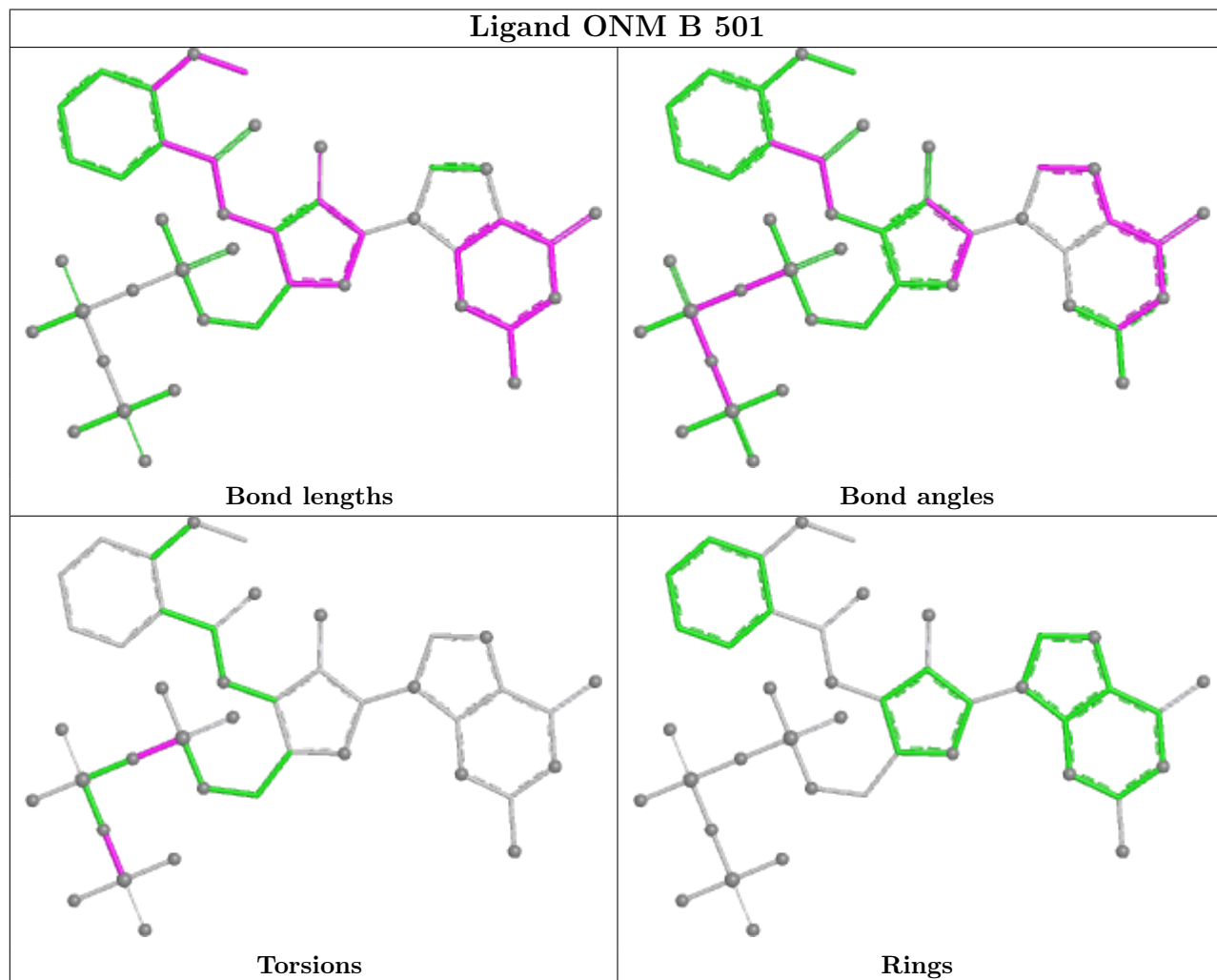
There are no ring outliers.

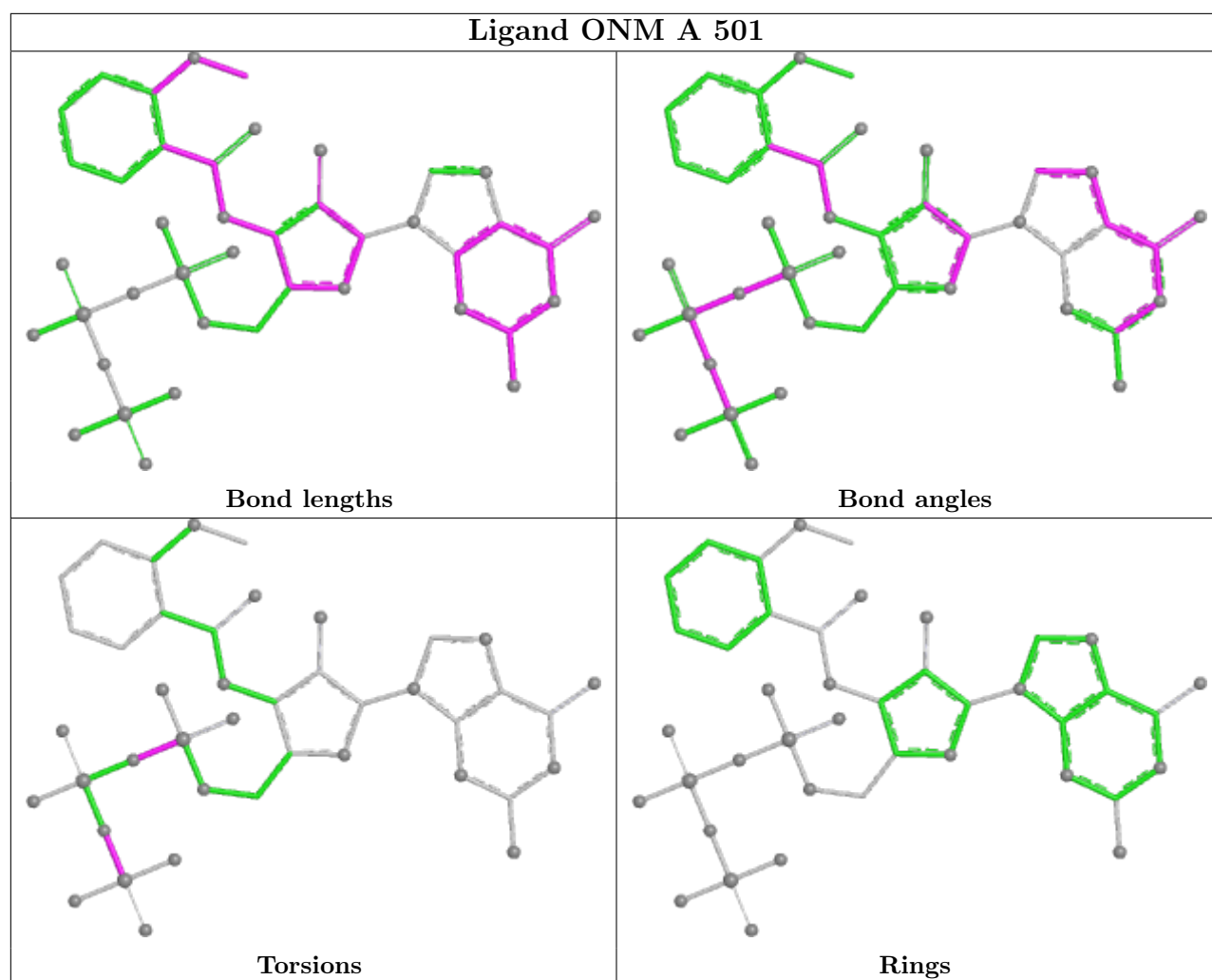
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	ONM	2	0
3	A	501	ONM	1	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.

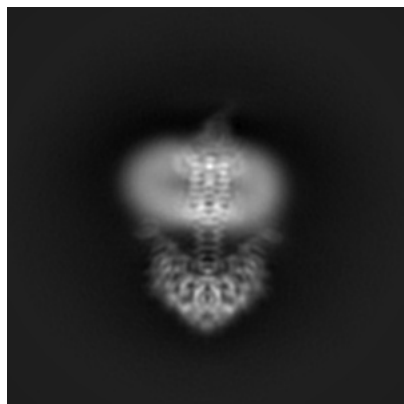
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14388. These allow visual inspection of the internal detail of the map and identification of artifacts.

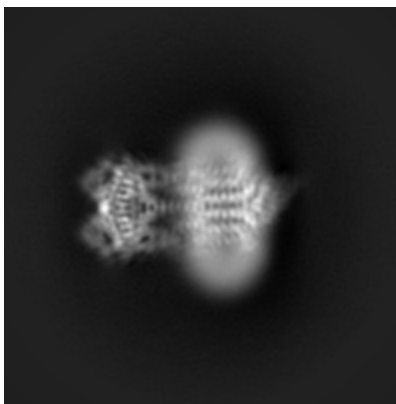
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

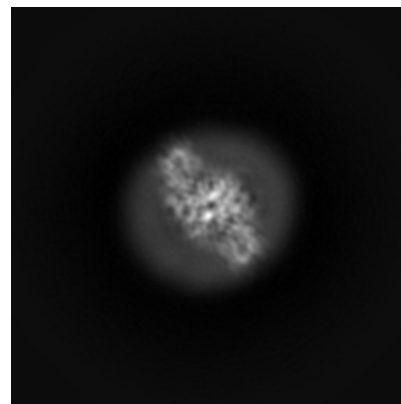
6.1.1 Primary map



X

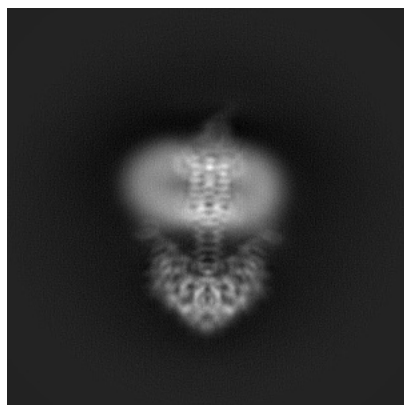


Y

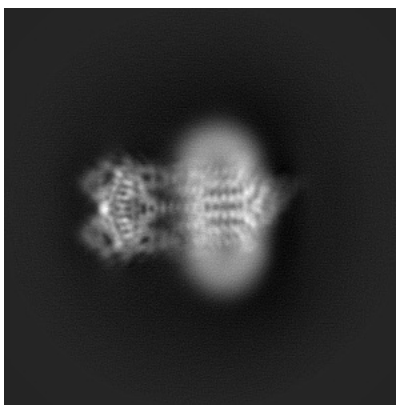


Z

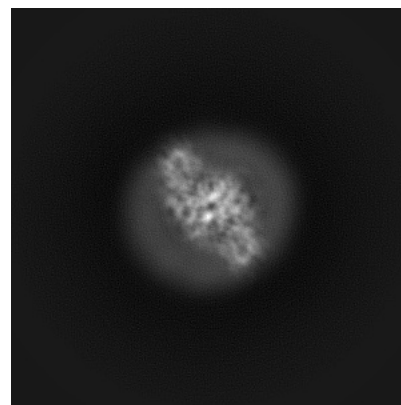
6.1.2 Raw map



X



Y

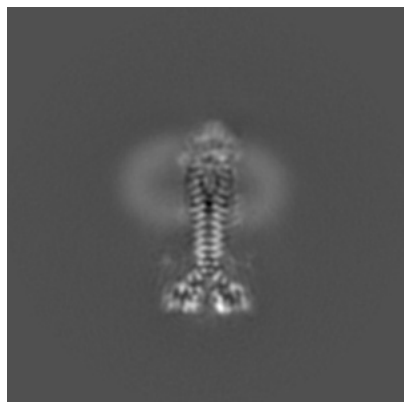


Z

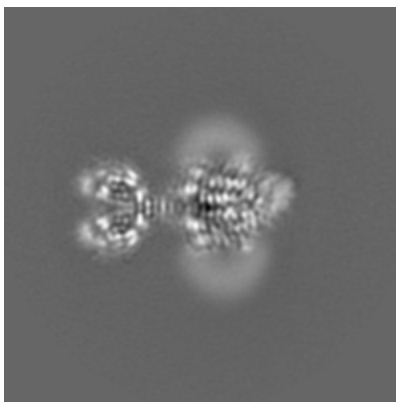
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

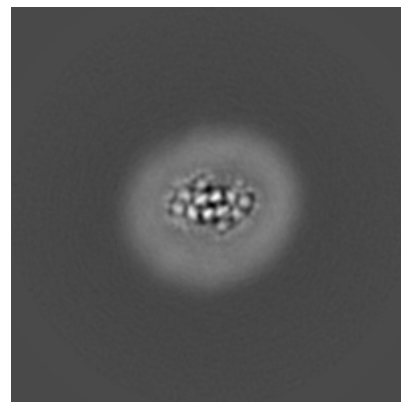
6.2.1 Primary map



X Index: 200

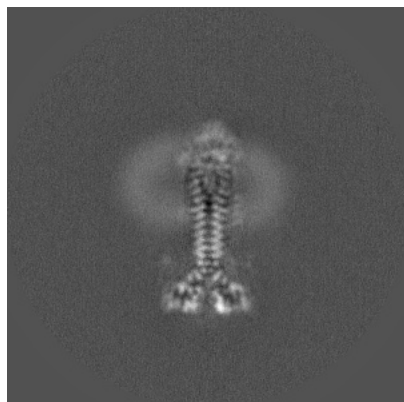


Y Index: 200

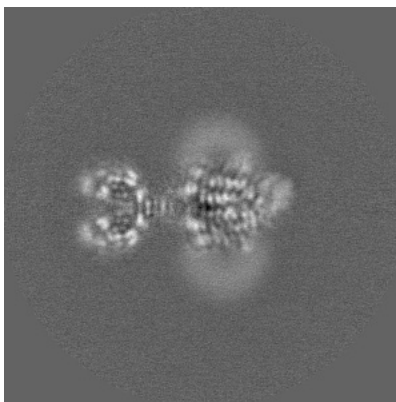


Z Index: 200

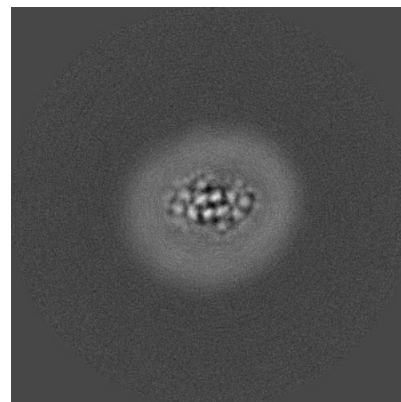
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

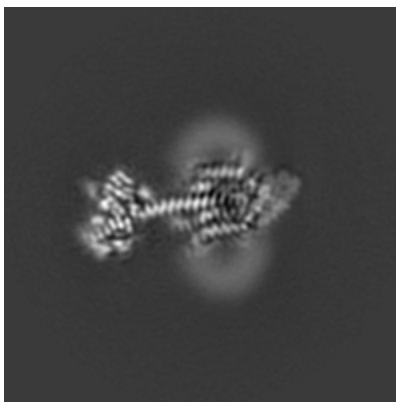
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

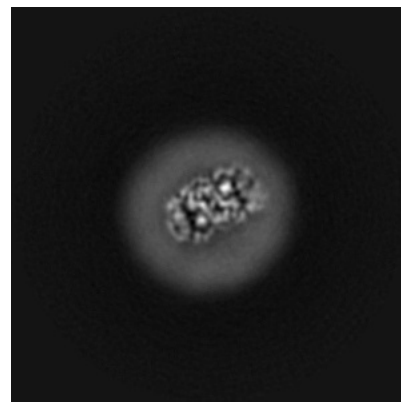
6.3.1 Primary map



X Index: 195

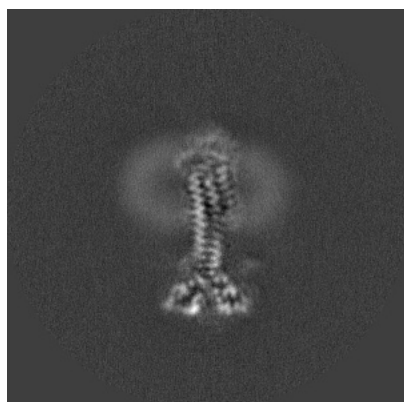


Y Index: 209

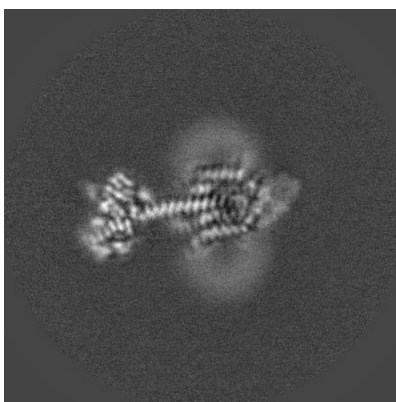


Z Index: 241

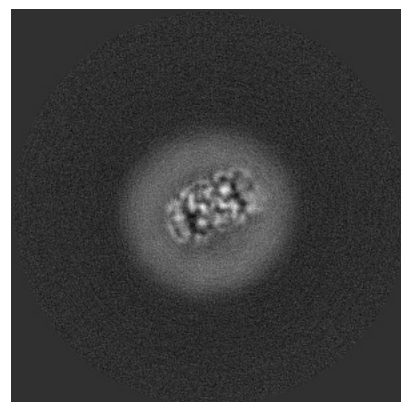
6.3.2 Raw map



X Index: 196



Y Index: 209

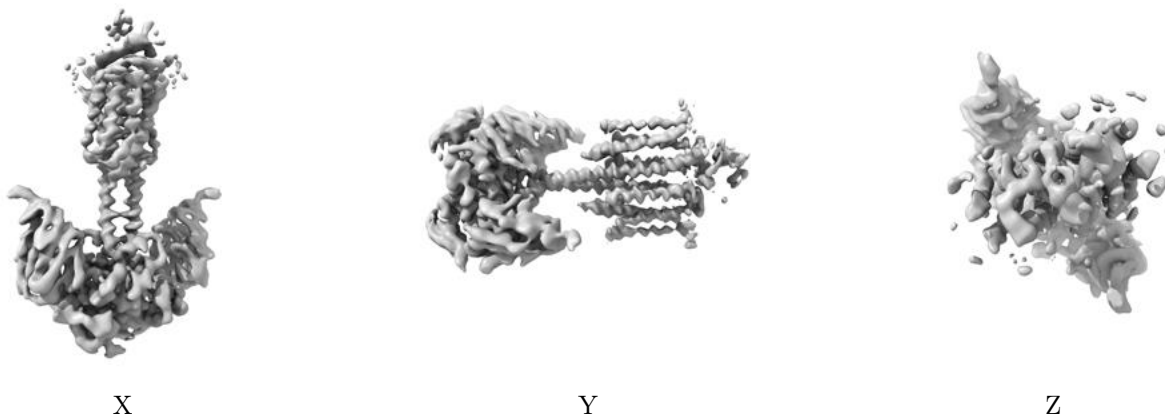


Z Index: 240

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

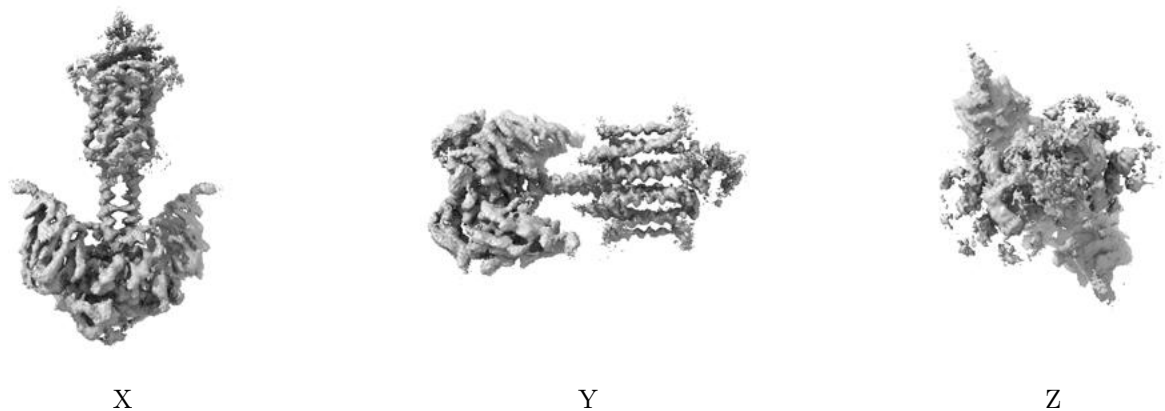
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00626. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

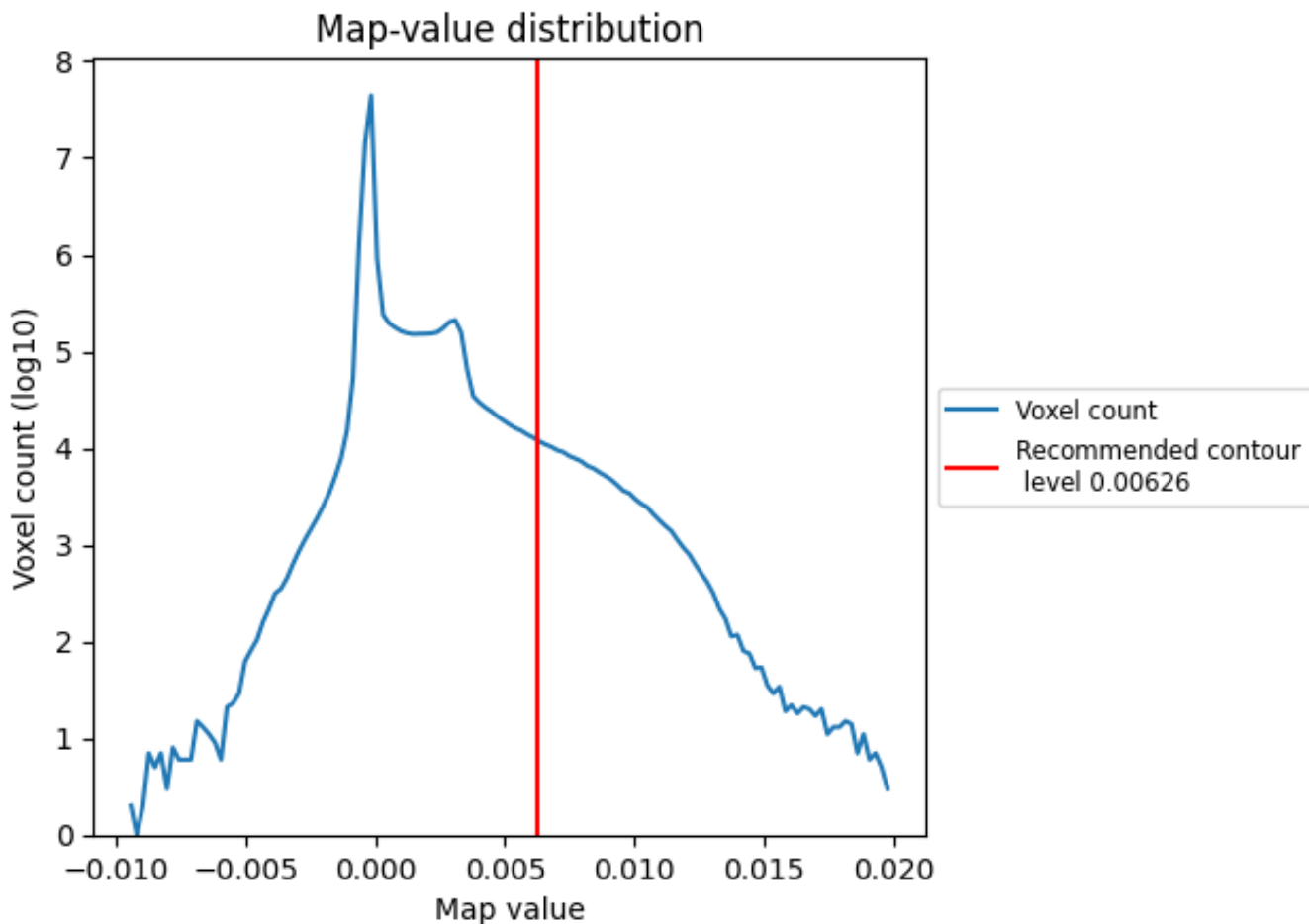
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

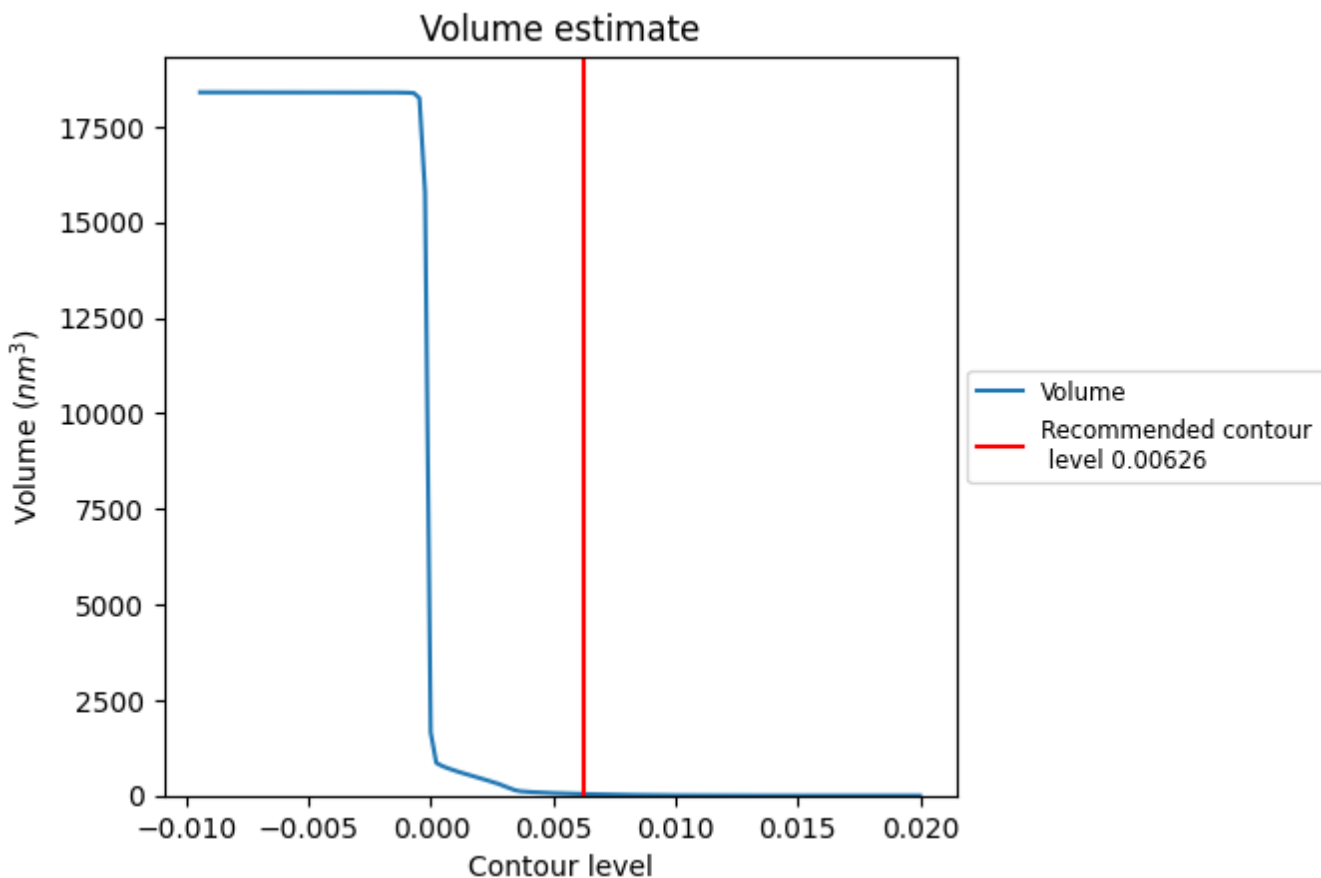
This section contains the results of statistical analysis of the map.

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.

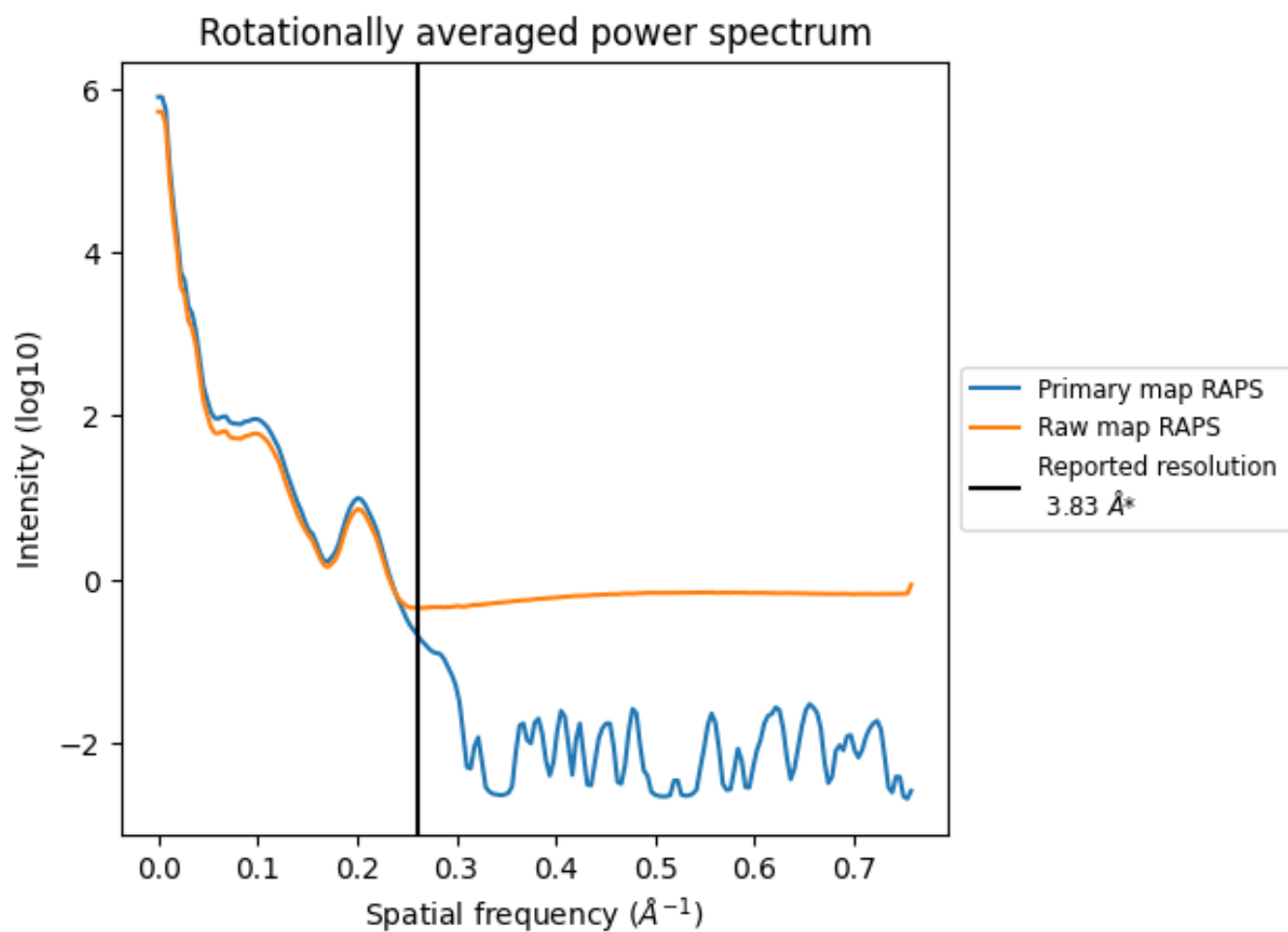
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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 [i](#)

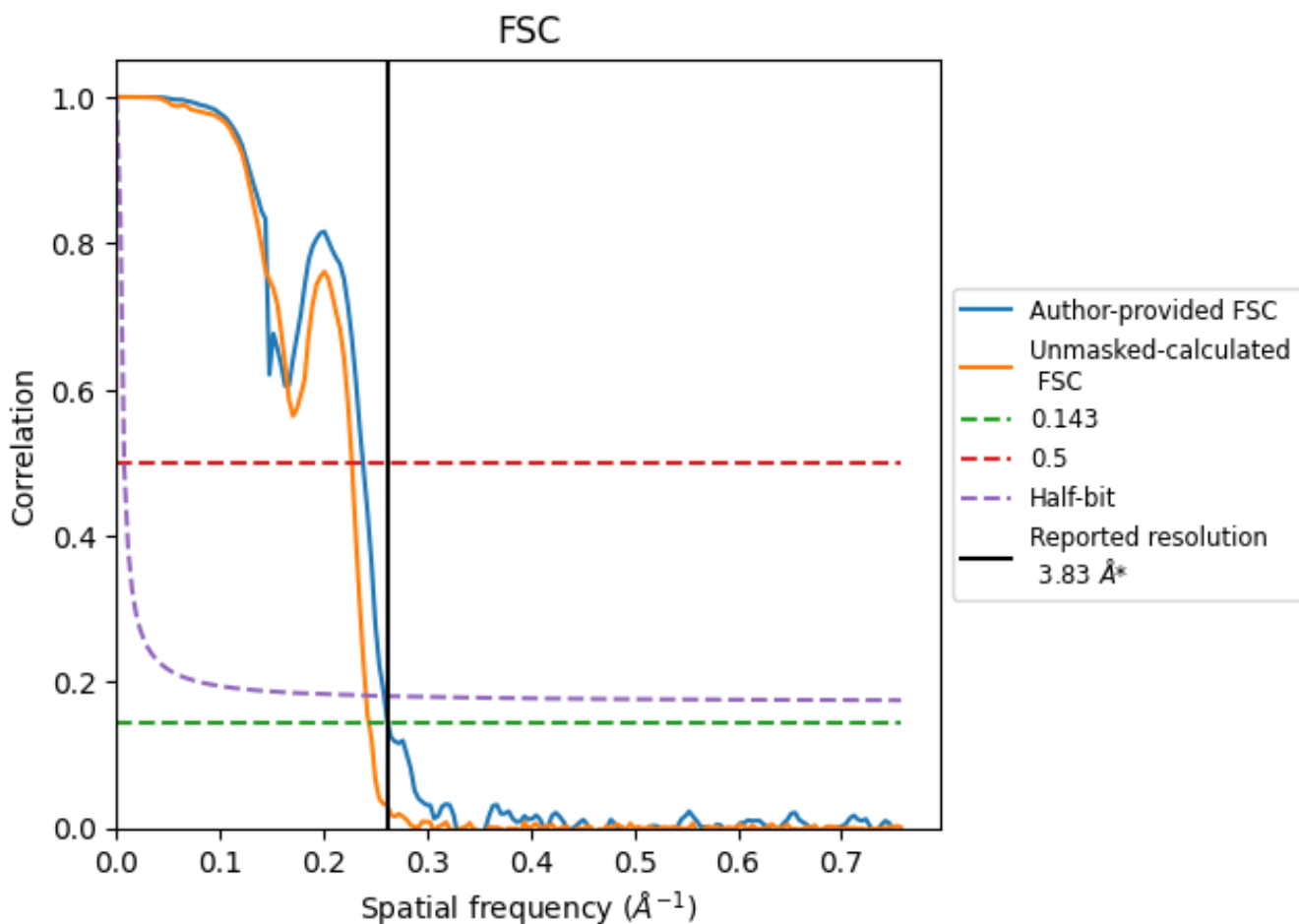


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

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 0.261\AA^{-1}

8.2 Resolution estimates [i](#)

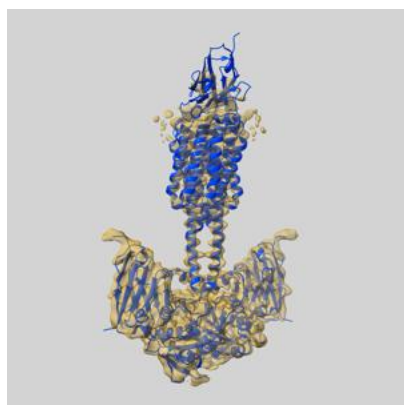
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.82	4.20	3.87
Unmasked-calculated*	4.10	4.40	4.15

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

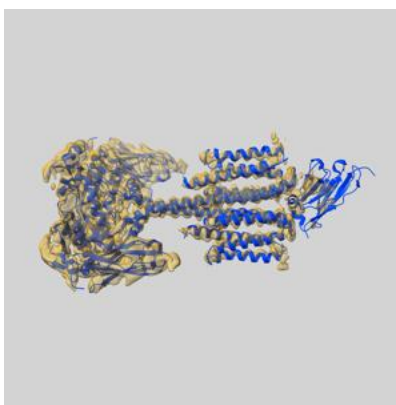
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14388 and PDB model 7YZI. Per-residue inclusion information can be found in section 3 on page 6.

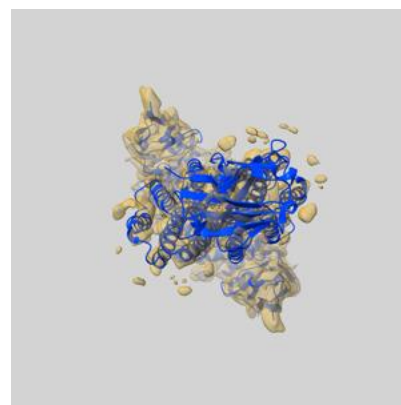
9.1 Map-model overlay [i](#)



X



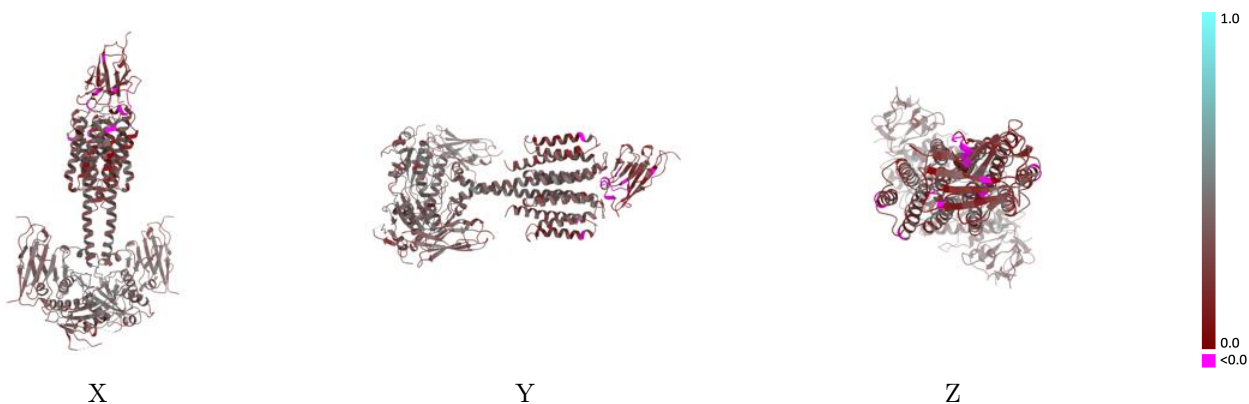
Y



Z

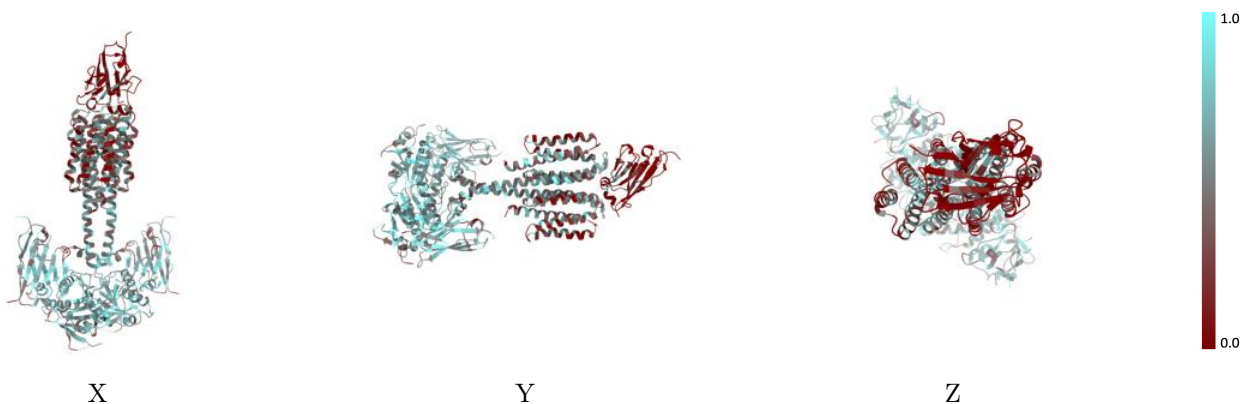
The images above show the 3D surface view of the map at the recommended contour level 0.00626 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



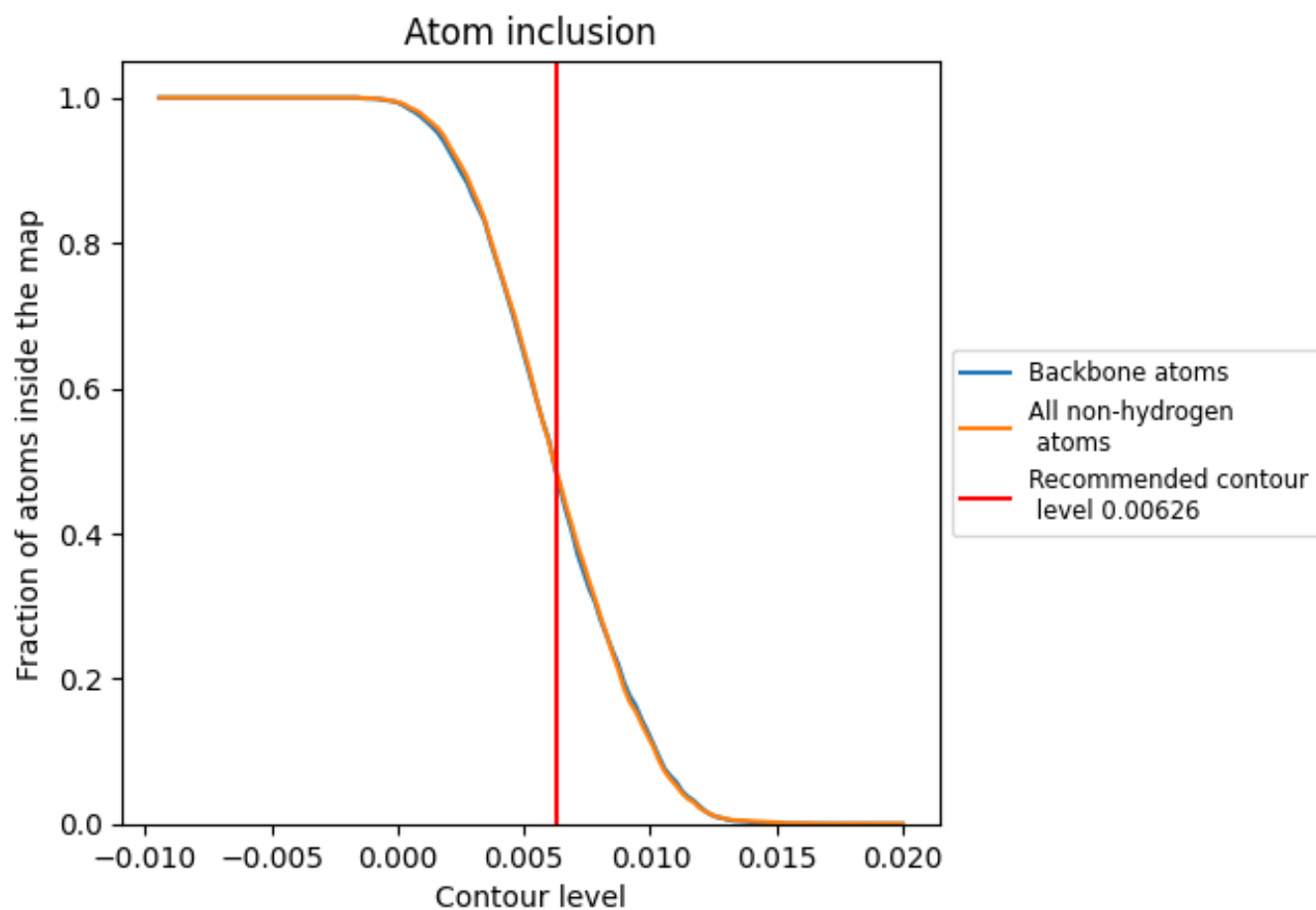
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00626).













9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 49% 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 (0.00626) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4884	 0.3320
A	 0.5431	 0.3500
B	 0.5371	 0.3530
C	 0.5920	 0.3560
D	 0.6026	 0.3410
E	 0.0891	 0.1690

