



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 03:31 AM UTC

PDB ID : 7LIH / pdb_00007lih
EMDB ID : EMD-23378
Title : CryoEM structure of Mayaro virus icosahedral subunit
Authors : Chmielewski, D.; Kaelber, J.T.; Jin, J.; Weaver, S.; Auguste, A.J.; Chiu, W.
Deposited on : 2021-01-27
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

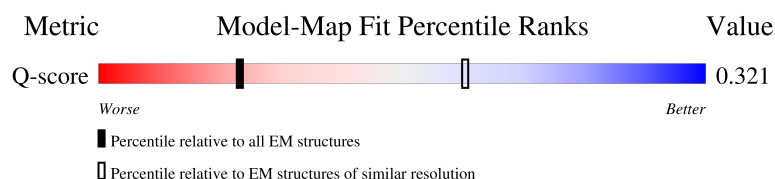
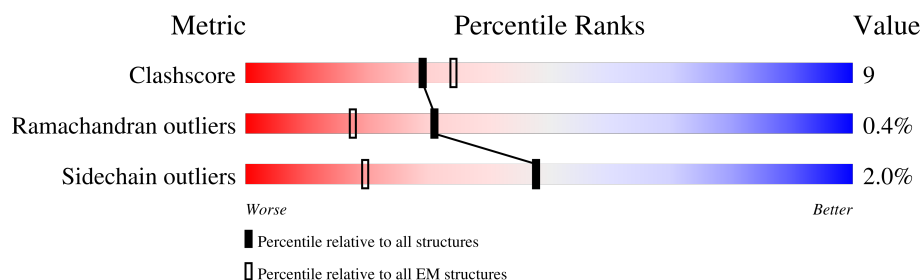
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



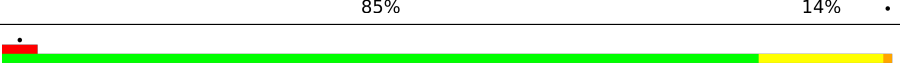
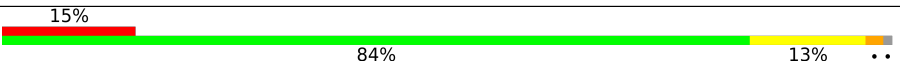
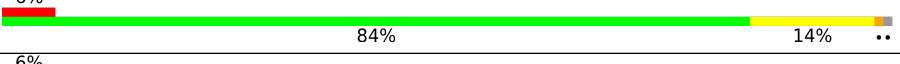
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	160	
1	B	160	
1	C	160	
1	F	160	

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Mol	Chain	Length	Quality of chain
2	H	435	
2	I	435	
2	J	435	
2	T	435	
3	D	410	
3	E	410	
3	G	410	
3	M	410	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 30856 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	160	Total	C	N	O	S	0	0
			1233	778	215	231	9		
1	A	160	Total	C	N	O	S	0	0
			1233	778	215	231	9		
1	B	160	Total	C	N	O	S	0	0
			1233	778	215	231	9		
1	C	160	Total	C	N	O	S	0	0
			1233	778	215	231	9		

- Molecule 2 is a protein called E1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	435	Total	C	N	O	S	0	0
			3309	2095	560	631	23		
2	H	435	Total	C	N	O	S	0	0
			3309	2095	560	631	23		
2	I	435	Total	C	N	O	S	0	0
			3309	2095	560	631	23		
2	J	435	Total	C	N	O	S	0	0
			3309	2095	560	631	23		

- Molecule 3 is a protein called E2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	407	Total	C	N	O	S	0	0
			3172	1996	562	592	22		
3	D	407	Total	C	N	O	S	0	0
			3172	1996	562	592	22		
3	E	407	Total	C	N	O	S	0	0
			3172	1996	562	592	22		
3	G	407	Total	C	N	O	S	0	0
			3172	1996	562	592	22		

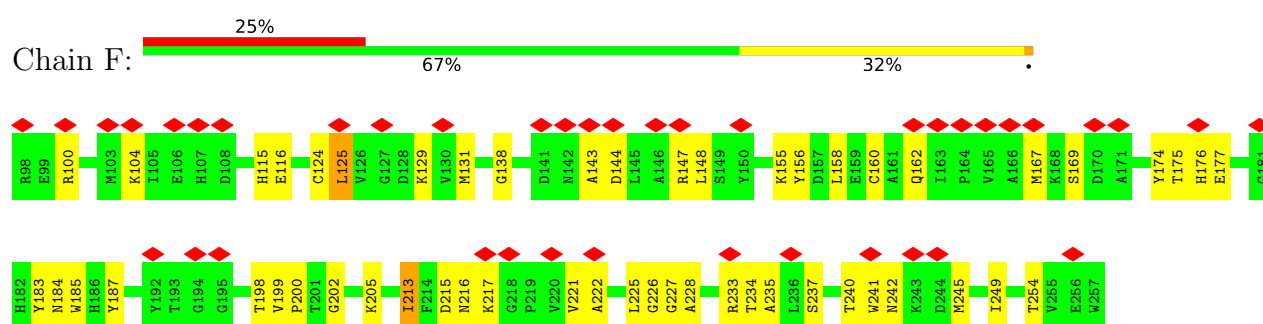
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	371	ILE	VAL	conflict	UNP A0A0P0BWJ4
M	372	ARG	ALA	conflict	UNP A0A0P0BWJ4
M	381	PHE	VAL	conflict	UNP A0A0P0BWJ4
M	393	THR	ASN	conflict	UNP A0A0P0BWJ4
D	371	ILE	VAL	conflict	UNP A0A0P0BWJ4
D	372	ARG	ALA	conflict	UNP A0A0P0BWJ4
D	381	PHE	VAL	conflict	UNP A0A0P0BWJ4
D	393	THR	ASN	conflict	UNP A0A0P0BWJ4
E	371	ILE	VAL	conflict	UNP A0A0P0BWJ4
E	372	ARG	ALA	conflict	UNP A0A0P0BWJ4
E	381	PHE	VAL	conflict	UNP A0A0P0BWJ4
E	393	THR	ASN	conflict	UNP A0A0P0BWJ4
G	371	ILE	VAL	conflict	UNP A0A0P0BWJ4
G	372	ARG	ALA	conflict	UNP A0A0P0BWJ4
G	381	PHE	VAL	conflict	UNP A0A0P0BWJ4
G	393	THR	ASN	conflict	UNP A0A0P0BWJ4

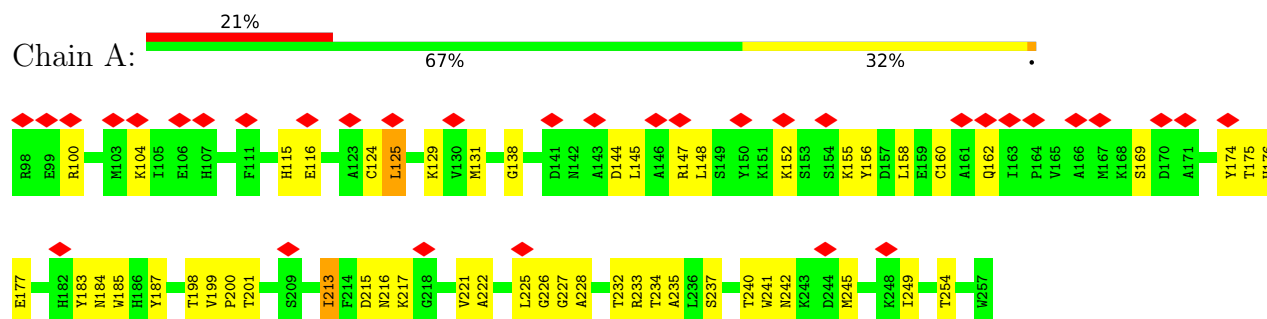
3 Residue-property plots

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.

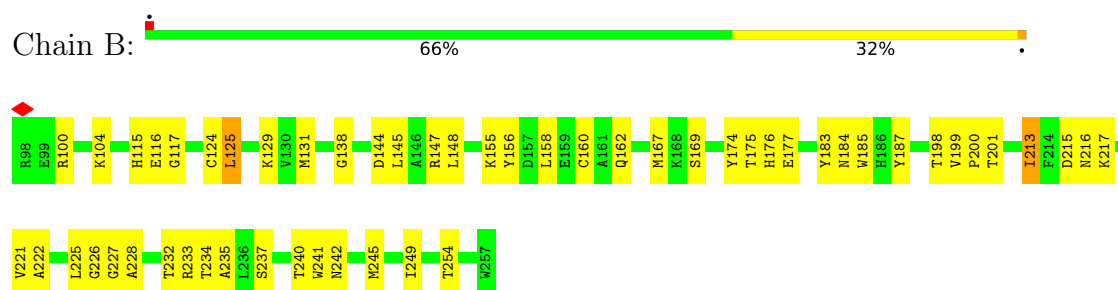
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

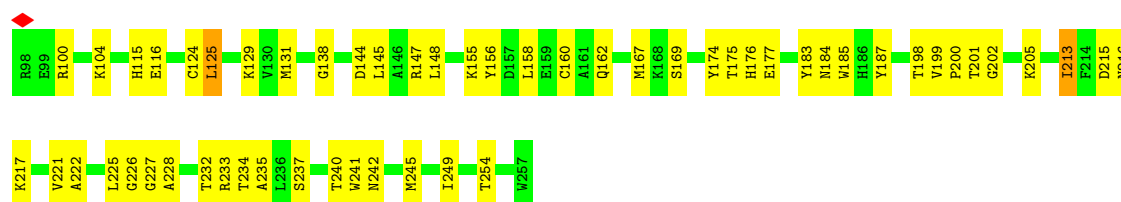


- Molecule 1: Capsid protein

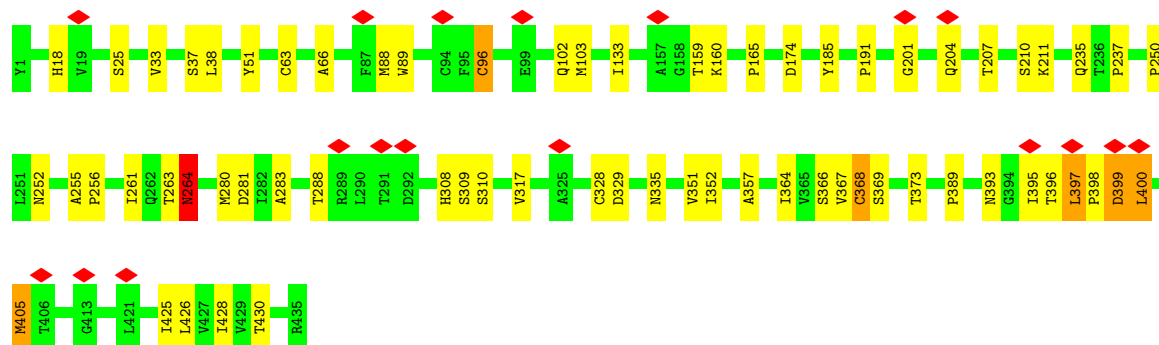
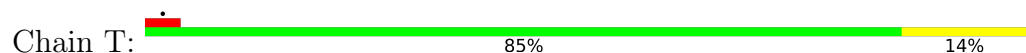


- Molecule 1: Capsid protein

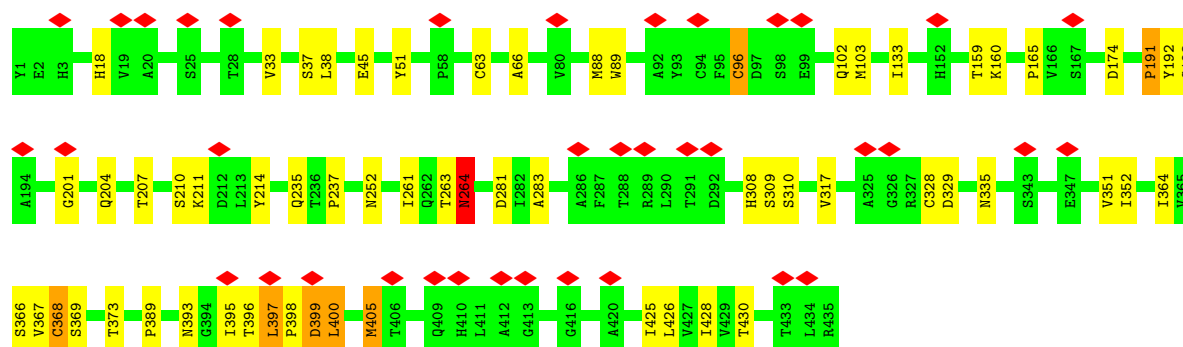
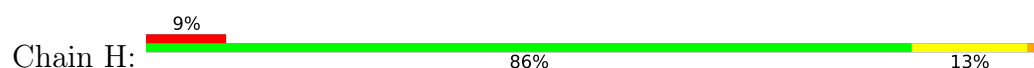




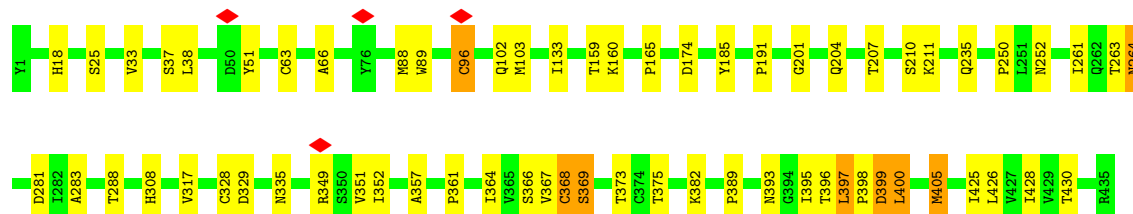
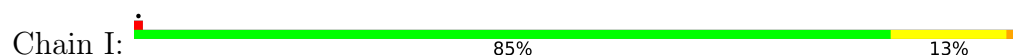
• Molecule 2: E1 protein



• Molecule 2: E1 protein



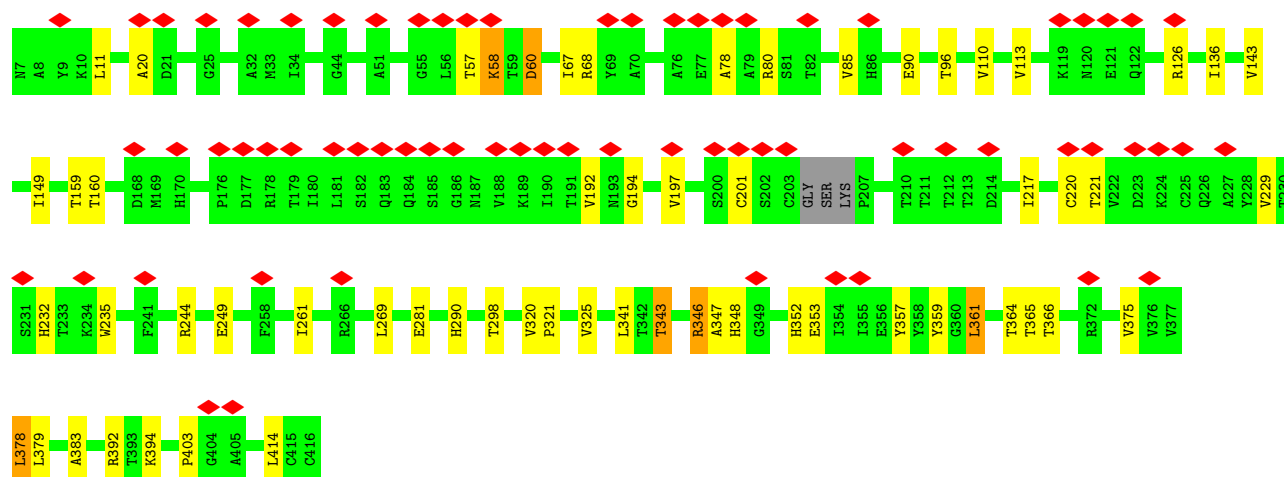
• Molecule 2: E1 protein



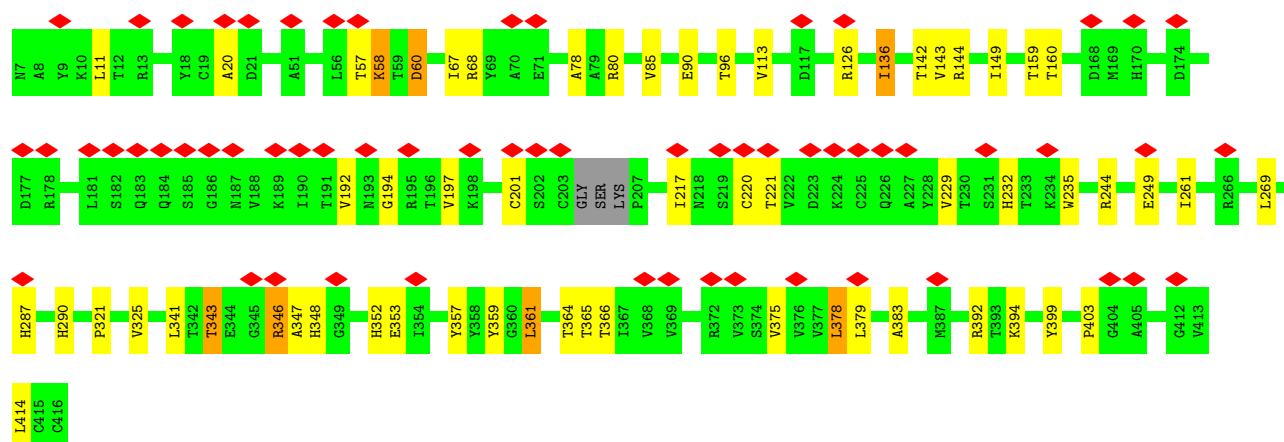
• Molecule 2: E1 protein

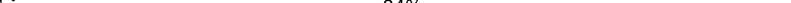
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Category 1	T261	10	Green	1261
	T262	20	Green	1262
	T263	30	Green	1263
	T264	40	Red	1264
	T265	50	Green	1265
	T266	60	Green	1266
	T267	70	Green	1267
	T268	80	Green	1268
	T269	90	Green	1269
	T270	100	Green	1270
Category 2	M280	10	Green	1280
	D281	20	Green	1281
	L282	30	Green	1282
	A283	40	Green	1283
	H308	50	Green	1308
	S309	60	Green	1309
	S310	70	Green	1310
	V317	80	Green	1317
	E323	90	Green	1323
	C328	100	Green	1328
Category 3	D329	10	Green	1329
	N335	20	Green	1335
	R349	30	Red	1349
	S350	40	Green	1350
	V351	50	Green	1351
	I352	60	Green	1352
	L364	70	Green	1364
	S366	80	Green	1366
	V367	90	Green	1367
	C368	100	Green	1368
Category 4	S369	10	Green	1369
	T373	20	Green	1373
	P389	30	Green	1389
	N393	40	Green	1393
	G394	50	Green	1394
	L395	60	Green	1395
	T396	70	Green	1396
	L397	80	Green	1397
	P398	90	Green	1398
	D399	100	Green	1399
Category 5	L400	10	Green	1400
	M405	20	Red	1405
	I425	30	Green	1425
	L426	40	Green	1426
	V427	50	Green	1427
	I428	60	Green	1428
	V429	70	Green	1429
	T430	80	Green	1430
	R435	90	Green	1435
	L436	100	Green	1436
Category 6	Y1	10	Green	1451
	H18	20	Green	1458
	R21	30	Green	1461
	V33	40	Green	1463
	S37	50	Green	1467
	L38	60	Green	1468
	D50	70	Red	1470
	Y51	80	Green	1471
	C63	90	Green	1473
	A66	100	Green	1476
Category 7	Y76	10	Green	1486
	H88	20	Green	1488
	H89	30	Green	1489
	C96	40	Red	1496
	Q102	50	Green	1502
	M103	60	Green	1503
	I133	70	Green	1513
	G150	80	Green	1515
	D151	90	Green	1516
	H152	100	Green	1517
Category 8	A153	10	Green	1518
	T159	20	Green	1519
	L160	30	Green	1520
	P165	40	Green	1525
	D174	50	Green	1527
	Y185	60	Green	1528
	P191	70	Green	1531
	G201	80	Green	1536
	Q204	90	Green	1539
	T207	100	Green	1542
Category 9	S210	10	Green	1547
	K211	20	Green	1548
	Q235	30	Green	1553
	P250	40	Green	1556
	L261	50	Green	1561
	V262	60	Green	1562
	L263	70	Green	1563
	L264	80	Green	1564
	L265	90	Green	1565
	L266	100	Green	1566

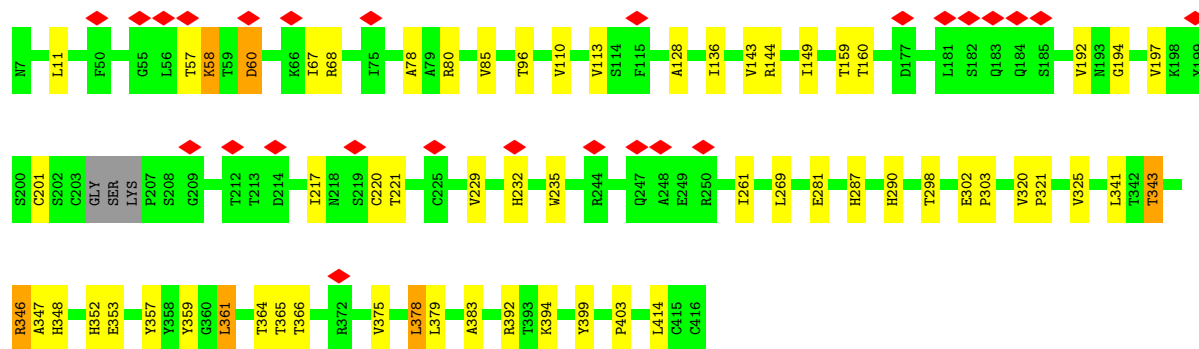
Chain M:  17% 84% 13%



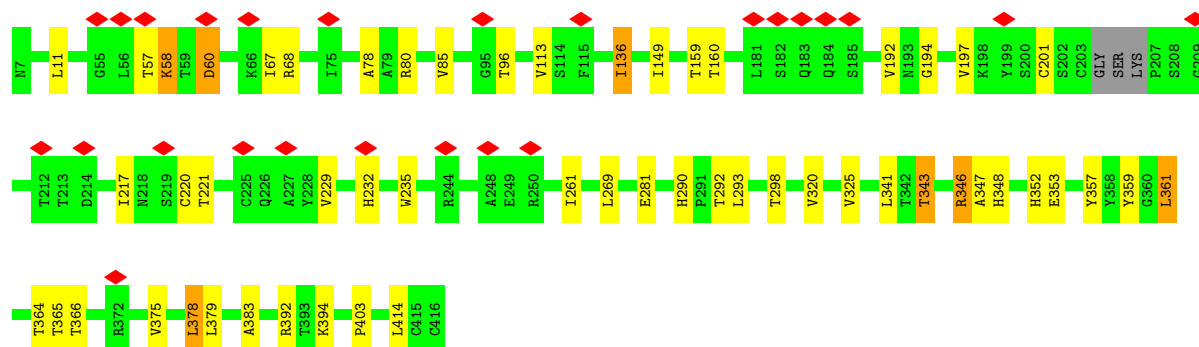
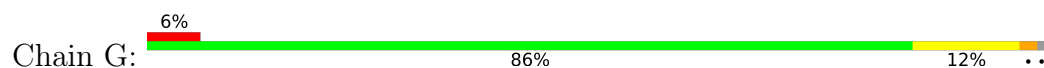
Chain D:  15% 84% 13%



Chain E:  6% 84% 14%



• Molecule 3: E2 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.760	Depositor
Minimum map value	-20.101	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.756	Depositor
Recommended contour level	3.96	Depositor
Map size ($\text{\AA}$)	924.48004, 924.48004, 924.48004	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.284, 1.284, 1.284	Depositor

5 Model quality

5.1 Standard geometry

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	0.58	0/1263	0.84	0/1708
1	B	0.58	0/1263	0.84	0/1708
1	C	0.58	0/1263	0.84	0/1708
1	F	0.58	0/1263	0.84	0/1708
2	H	0.38	0/3391	0.77	1/4631 (0.0%)
2	I	0.38	0/3391	0.77	1/4631 (0.0%)
2	J	0.38	0/3391	0.77	1/4631 (0.0%)
2	T	0.38	0/3391	0.77	1/4631 (0.0%)
3	D	0.41	1/3251 (0.0%)	0.76	0/4435
3	E	0.41	1/3251 (0.0%)	0.76	0/4435
3	G	0.41	1/3251 (0.0%)	0.76	0/4435
3	M	0.41	1/3251 (0.0%)	0.76	0/4435
All	All	0.43	4/31620 (0.0%)	0.78	4/43096 (0.0%)

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
2	H	0	10
2	I	0	10
2	J	0	10
2	T	0	10
3	D	0	3
3	E	0	3
3	G	0	3
3	M	0	3
All	All	0	52

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	232	HIS	CA-C	5.68	1.60	1.52
3	D	232	HIS	CA-C	5.66	1.60	1.52
3	M	232	HIS	CA-C	5.62	1.60	1.52
3	E	232	HIS	CA-C	5.60	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	405	MET	CG-SD-CE	-5.05	89.79	100.90
2	T	405	MET	CG-SD-CE	-5.04	89.80	100.90
2	I	405	MET	CG-SD-CE	-5.04	89.82	100.90
2	J	405	MET	CG-SD-CE	-5.03	89.83	100.90

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	290	HIS	Peptide
3	D	58	LYS	Peptide
3	D	60	ASP	Peptide
3	E	290	HIS	Peptide
3	E	58	LYS	Peptide
3	E	60	ASP	Peptide
3	G	290	HIS	Peptide
3	G	58	LYS	Peptide
3	G	60	ASP	Peptide
2	H	18	HIS	Peptide
2	H	207	THR	Peptide
2	H	263	THR	Peptide
2	H	264	ASN	Peptide
2	H	308	HIS	Peptide
2	H	366	SER	Peptide
2	H	367	VAL	Peptide
2	H	389	PRO	Peptide
2	H	66	ALA	Peptide
2	H	96	CYS	Peptide
2	I	18	HIS	Peptide
2	I	207	THR	Peptide
2	I	263	THR	Peptide
2	I	264	ASN	Peptide
2	I	308	HIS	Peptide
2	I	366	SER	Peptide

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Mol	Chain	Res	Type	Group
2	I	367	VAL	Peptide
2	I	389	PRO	Peptide
2	I	66	ALA	Peptide
2	I	96	CYS	Peptide
2	J	18	HIS	Peptide
2	J	207	THR	Peptide
2	J	263	THR	Peptide
2	J	264	ASN	Peptide
2	J	308	HIS	Peptide
2	J	366	SER	Peptide
2	J	367	VAL	Peptide
2	J	389	PRO	Peptide
2	J	66	ALA	Peptide
2	J	96	CYS	Peptide
3	M	290	HIS	Peptide
3	M	58	LYS	Peptide
3	M	60	ASP	Peptide
2	T	18	HIS	Peptide
2	T	207	THR	Peptide
2	T	263	THR	Peptide
2	T	264	ASN	Peptide
2	T	308	HIS	Peptide
2	T	366	SER	Peptide
2	T	367	VAL	Peptide
2	T	389	PRO	Peptide
2	T	66	ALA	Peptide
2	T	96	CYS	Peptide

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	1233	0	1218	58	0
1	B	1233	0	1218	59	0
1	C	1233	0	1218	58	0
1	F	1233	0	1218	59	0
2	H	3309	0	3234	54	0
2	I	3309	0	3234	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	3309	0	3234	59	0
2	T	3309	0	3234	45	0
3	D	3172	0	3138	63	0
3	E	3172	0	3138	55	0
3	G	3172	0	3138	47	0
3	M	3172	0	3138	60	0
All	All	30856	0	30360	567	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (567) 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:129:LYS:NZ	1:B:162:GLN:HE21	1.05	1.48
1:C:155:LYS:HZ1	3:G:394:LYS:CE	1.27	1.46
1:B:155:LYS:HZ1	3:E:394:LYS:CE	1.29	1.44
1:A:129:LYS:NZ	1:A:162:GLN:HE21	1.05	1.44
1:C:129:LYS:NZ	1:C:162:GLN:HE21	1.05	1.43
1:F:129:LYS:NZ	1:F:162:GLN:HE21	1.05	1.42
1:A:155:LYS:NZ	3:D:394:LYS:HE3	1.08	1.40
1:A:155:LYS:HZ1	3:D:394:LYS:CE	1.32	1.40
1:F:155:LYS:NZ	3:M:394:LYS:CE	1.84	1.40
1:C:155:LYS:NZ	3:G:394:LYS:HE3	1.08	1.40
1:F:155:LYS:NZ	3:M:394:LYS:HE3	1.08	1.38
1:A:155:LYS:NZ	3:D:394:LYS:CE	1.84	1.37
1:B:155:LYS:NZ	3:E:394:LYS:HE3	1.08	1.35
3:E:352:HIS:CE1	3:E:353:GLU:HG3	1.62	1.34
3:G:352:HIS:CE1	3:G:353:GLU:HG3	1.62	1.34
3:D:352:HIS:CE1	3:D:353:GLU:HG3	1.62	1.34
3:M:352:HIS:CE1	3:M:353:GLU:HG3	1.62	1.33
1:C:155:LYS:NZ	3:G:394:LYS:CE	1.84	1.33
1:B:155:LYS:NZ	3:E:394:LYS:CE	1.84	1.33
1:A:129:LYS:NZ	1:A:162:GLN:NE2	1.78	1.32
1:B:129:LYS:NZ	1:B:162:GLN:NE2	1.77	1.31
1:C:129:LYS:NZ	1:C:162:GLN:NE2	1.77	1.30
2:H:192:TYR:CB	2:J:151:ASP:O	1.80	1.29
1:F:129:LYS:NZ	1:F:162:GLN:NE2	1.77	1.27
1:F:155:LYS:HZ1	3:M:394:LYS:CE	1.42	1.22
2:H:45:GLU:OE2	2:J:151:ASP:OD2	1.62	1.18
2:T:397:LEU:CD1	2:T:398:PRO:HD2	1.79	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:397:LEU:CD1	2:I:398:PRO:HD2	1.79	1.11
2:J:397:LEU:CD1	2:J:398:PRO:HD2	1.79	1.11
2:H:397:LEU:CD1	2:H:398:PRO:HD2	1.79	1.10
2:T:399:ASP:O	2:T:405:MET:HE1	1.54	1.07
2:I:399:ASP:O	2:I:405:MET:HE1	1.54	1.06
2:J:399:ASP:O	2:J:405:MET:HE1	1.54	1.06
2:H:399:ASP:O	2:H:405:MET:HE1	1.54	1.05
1:F:129:LYS:NZ	1:F:162:GLN:HG2	1.73	1.04
1:A:129:LYS:NZ	1:A:162:GLN:HG2	1.73	1.04
2:H:397:LEU:HD12	2:H:398:PRO:HD2	1.04	1.03
2:I:397:LEU:HD12	2:I:398:PRO:HD2	1.04	1.03
2:H:192:TYR:HB3	2:J:151:ASP:O	1.55	1.02
2:T:397:LEU:HD12	2:T:398:PRO:HD2	1.04	1.02
1:B:129:LYS:NZ	1:B:162:GLN:HG2	1.73	1.01
2:H:192:TYR:HB2	2:J:151:ASP:O	1.56	1.01
1:C:129:LYS:NZ	1:C:162:GLN:HG2	1.73	1.01
2:J:397:LEU:HD12	2:J:398:PRO:HD2	1.04	1.00
1:F:155:LYS:HZ3	3:M:394:LYS:CE	1.61	0.99
3:D:352:HIS:CE1	3:D:353:GLU:CG	2.46	0.99
3:G:352:HIS:CE1	3:G:353:GLU:CG	2.46	0.98
3:M:352:HIS:CE1	3:M:353:GLU:CG	2.46	0.97
3:E:352:HIS:CE1	3:E:353:GLU:CG	2.46	0.97
1:C:129:LYS:HZ2	1:C:162:GLN:CG	1.78	0.97
1:A:155:LYS:HZ3	3:D:394:LYS:CE	1.71	0.96
1:A:129:LYS:NZ	1:A:162:GLN:CG	2.29	0.95
2:H:397:LEU:HD12	2:H:398:PRO:CD	1.96	0.95
1:B:129:LYS:NZ	1:B:162:GLN:CG	2.29	0.95
3:M:126:ARG:HB3	3:D:143:VAL:HG11	1.47	0.95
1:C:129:LYS:NZ	1:C:162:GLN:CG	2.29	0.95
2:H:399:ASP:C	2:H:405:MET:HE1	1.92	0.95
2:J:399:ASP:C	2:J:405:MET:HE1	1.92	0.95
1:F:129:LYS:NZ	1:F:162:GLN:CG	2.29	0.94
2:I:397:LEU:HD12	2:I:398:PRO:CD	1.97	0.94
2:I:399:ASP:C	2:I:405:MET:HE1	1.92	0.94
2:H:191:PRO:HB3	2:J:151:ASP:HA	1.51	0.93
2:T:399:ASP:C	2:T:405:MET:HE1	1.92	0.93
1:B:129:LYS:HZ3	1:B:162:GLN:HG2	1.28	0.92
1:B:155:LYS:HZ3	3:E:394:LYS:CE	1.74	0.92
1:B:129:LYS:HZ2	1:B:162:GLN:HE21	1.17	0.92
1:C:155:LYS:CE	3:G:394:LYS:HE3	2.00	0.92
1:C:155:LYS:HZ3	3:G:394:LYS:CE	1.77	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:397:LEU:HD12	2:J:398:PRO:CD	1.97	0.91
1:B:155:LYS:CE	3:E:394:LYS:HE3	2.00	0.91
1:A:129:LYS:HZ2	1:A:162:GLN:CG	1.84	0.91
1:F:155:LYS:CE	3:M:394:LYS:HE3	2.00	0.90
2:T:397:LEU:HD12	2:T:398:PRO:CD	1.97	0.90
1:B:129:LYS:HZ3	1:B:162:GLN:CG	1.85	0.90
1:A:155:LYS:CE	3:D:394:LYS:HE3	2.00	0.89
3:M:20:ALA:HB1	3:D:144:ARG:O	1.74	0.87
1:C:129:LYS:HZ3	1:C:162:GLN:NE2	1.70	0.86
1:F:129:LYS:HZ2	1:F:162:GLN:CG	1.88	0.86
3:M:346:ARG:HD2	3:M:353:GLU:OE1	1.77	0.85
1:C:129:LYS:NZ	1:C:162:GLN:CD	2.35	0.85
1:F:129:LYS:HZ2	1:F:162:GLN:HE21	1.22	0.85
3:G:346:ARG:HD2	3:G:353:GLU:OE1	1.77	0.85
1:F:129:LYS:NZ	1:F:162:GLN:CD	2.35	0.84
1:A:129:LYS:NZ	1:A:162:GLN:CD	2.35	0.84
1:B:129:LYS:NZ	1:B:162:GLN:CD	2.35	0.83
1:B:131:MET:SD	1:B:160:CYS:SG	2.76	0.83
3:D:346:ARG:HD2	3:D:353:GLU:OE1	1.77	0.83
3:E:346:ARG:HD2	3:E:353:GLU:OE1	1.77	0.83
1:A:129:LYS:HZ3	1:A:162:GLN:NE2	1.71	0.83
1:B:129:LYS:HZ1	1:B:162:GLN:HE21	0.83	0.83
1:A:131:MET:SD	1:A:160:CYS:SG	2.76	0.83
1:C:131:MET:SD	1:C:160:CYS:SG	2.76	0.83
1:F:155:LYS:HZ3	3:M:394:LYS:HE2	1.40	0.82
1:F:129:LYS:HZ3	1:F:162:GLN:NE2	1.72	0.82
1:F:131:MET:SD	1:F:160:CYS:SG	2.76	0.82
2:T:237:PRO:CG	3:D:287:HIS:HB3	2.09	0.82
1:B:129:LYS:HZ3	1:B:162:GLN:NE2	1.73	0.82
1:A:129:LYS:HZ2	1:A:162:GLN:HE21	1.23	0.82
1:B:129:LYS:HZ1	1:B:162:GLN:NE2	1.61	0.81
1:F:129:LYS:HZ3	1:F:162:GLN:HG2	1.42	0.81
1:F:129:LYS:HZ1	1:F:162:GLN:HE21	0.80	0.80
2:I:399:ASP:O	2:I:405:MET:CE	2.31	0.79
2:T:399:ASP:O	2:T:405:MET:CE	2.31	0.79
1:A:129:LYS:HZ1	1:A:162:GLN:HE21	0.80	0.79
2:H:191:PRO:CB	2:J:151:ASP:HA	2.13	0.79
1:A:129:LYS:HZ3	1:A:162:GLN:HG2	1.46	0.79
2:J:399:ASP:O	2:J:405:MET:CE	2.31	0.79
2:H:399:ASP:O	2:H:405:MET:CE	2.31	0.79
1:F:129:LYS:HZ1	1:F:162:GLN:NE2	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HZ2	1:B:162:GLN:NE2	1.76	0.78
1:B:129:LYS:HZ3	1:B:162:GLN:CD	1.91	0.78
1:C:129:LYS:HZ1	1:C:162:GLN:HE21	0.79	0.77
3:M:341:LEU:HD11	3:M:361:LEU:HD21	1.68	0.76
2:J:397:LEU:CD1	2:J:398:PRO:CD	2.61	0.76
3:D:341:LEU:HD11	3:D:361:LEU:HD21	1.68	0.76
3:E:341:LEU:HD11	3:E:361:LEU:HD21	1.68	0.75
3:G:341:LEU:HD11	3:G:361:LEU:HD21	1.67	0.75
1:C:129:LYS:HZ2	1:C:162:GLN:HE21	1.26	0.75
1:C:129:LYS:HZ2	1:C:162:GLN:NE2	1.78	0.74
3:M:110:VAL:CG1	3:D:142:THR:OG1	2.36	0.73
1:A:155:LYS:HZ3	3:D:394:LYS:HE2	1.51	0.73
2:H:192:TYR:N	2:J:151:ASP:O	2.21	0.73
2:T:397:LEU:CD1	2:T:398:PRO:CD	2.61	0.73
3:D:341:LEU:HD11	3:D:361:LEU:CD2	2.19	0.73
3:E:341:LEU:HD11	3:E:361:LEU:CD2	2.19	0.73
1:F:155:LYS:NZ	3:M:394:LYS:CD	2.53	0.72
2:H:192:TYR:CA	2:J:151:ASP:O	2.38	0.72
3:M:341:LEU:HD11	3:M:361:LEU:CD2	2.19	0.72
1:C:129:LYS:HZ3	1:C:162:GLN:HG2	1.53	0.72
1:C:129:LYS:HZ1	1:C:162:GLN:NE2	1.62	0.72
1:B:129:LYS:HZ2	1:B:162:GLN:CG	2.02	0.72
1:A:129:LYS:HZ1	1:A:162:GLN:NE2	1.62	0.71
1:B:155:LYS:NZ	3:E:394:LYS:CD	2.53	0.71
1:F:129:LYS:HZ3	1:F:162:GLN:CG	1.98	0.71
1:C:155:LYS:NZ	3:G:394:LYS:CD	2.53	0.71
3:G:341:LEU:HD11	3:G:361:LEU:CD2	2.19	0.71
1:F:129:LYS:HZ2	1:F:162:GLN:NE2	1.77	0.71
2:I:397:LEU:CD1	2:I:398:PRO:CD	2.61	0.71
2:J:335:ASN:ND2	2:J:393:ASN:OD1	2.24	0.71
2:H:335:ASN:ND2	2:H:393:ASN:OD1	2.24	0.71
1:A:155:LYS:NZ	3:D:394:LYS:CD	2.53	0.70
2:H:192:TYR:HB3	2:J:152:HIS:HA	1.71	0.70
2:I:335:ASN:ND2	2:I:393:ASN:OD1	2.24	0.70
3:M:352:HIS:NE2	3:M:353:GLU:HG3	2.07	0.70
3:M:346:ARG:NH1	3:M:346:ARG:HB3	2.07	0.70
2:I:349:ARG:NE	2:J:323:GLU:HB3	2.05	0.70
2:H:397:LEU:CD1	2:H:398:PRO:CD	2.61	0.70
3:D:352:HIS:NE2	3:D:353:GLU:HG3	2.07	0.69
3:D:346:ARG:HB3	3:D:346:ARG:NH1	2.07	0.69
2:T:335:ASN:ND2	2:T:393:ASN:OD1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:THR:HG21	3:D:357:TYR:CD1	2.27	0.69
3:M:343:THR:HG21	3:M:357:TYR:CD1	2.27	0.69
3:E:343:THR:HG21	3:E:357:TYR:CD1	2.27	0.69
3:E:346:ARG:NH1	3:E:346:ARG:HB3	2.07	0.69
3:G:192:VAL:HG12	3:G:194:GLY:H	1.58	0.69
3:G:346:ARG:HB3	3:G:346:ARG:NH1	2.07	0.69
1:C:155:LYS:HZ3	3:G:394:LYS:HE2	1.56	0.69
3:G:343:THR:HG21	3:G:357:TYR:CD1	2.27	0.69
1:B:155:LYS:HZ3	3:E:394:LYS:HE2	1.53	0.69
3:E:192:VAL:HG12	3:E:194:GLY:H	1.58	0.68
3:G:352:HIS:NE2	3:G:353:GLU:HG3	2.07	0.68
3:D:192:VAL:HG12	3:D:194:GLY:H	1.58	0.68
1:C:155:LYS:HZ1	3:G:394:LYS:CD	2.04	0.68
1:A:155:LYS:HZ1	3:D:394:LYS:CD	2.06	0.68
3:M:143:VAL:CG2	3:E:128:ALA:HB2	2.24	0.68
3:M:192:VAL:HG12	3:M:194:GLY:H	1.58	0.67
1:A:129:LYS:HZ3	1:A:162:GLN:CD	1.99	0.67
1:C:124:CYS:SG	1:C:125:LEU:N	2.67	0.67
1:F:124:CYS:SG	1:F:125:LEU:N	2.67	0.67
1:B:124:CYS:SG	1:B:125:LEU:N	2.67	0.67
1:A:124:CYS:SG	1:A:125:LEU:N	2.67	0.67
1:F:129:LYS:HZ3	1:F:162:GLN:CD	1.97	0.67
2:T:33:VAL:HG12	2:T:133:ILE:HG12	1.77	0.67
2:T:237:PRO:HD2	3:D:287:HIS:CB	2.24	0.67
2:T:237:PRO:CD	3:D:287:HIS:HB3	2.25	0.66
3:E:352:HIS:NE2	3:E:353:GLU:HG3	2.07	0.66
2:H:33:VAL:HG12	2:H:133:ILE:HG12	1.77	0.66
2:J:33:VAL:HG12	2:J:133:ILE:HG12	1.77	0.65
1:A:242:ASN:HB3	1:A:245:MET:H	1.62	0.65
1:F:242:ASN:HB3	1:F:245:MET:H	1.62	0.65
3:M:90:GLU:OE2	3:D:90:GLU:OE2	2.15	0.65
2:I:33:VAL:HG12	2:I:133:ILE:HG12	1.77	0.65
1:C:242:ASN:HB3	1:C:245:MET:H	1.62	0.64
1:A:129:LYS:HZ3	1:A:162:GLN:CG	2.02	0.64
1:B:242:ASN:HB3	1:B:245:MET:H	1.62	0.64
2:I:349:ARG:CZ	2:J:323:GLU:HB3	2.28	0.63
2:I:328:CYS:SG	2:I:329:ASP:N	2.72	0.63
1:C:129:LYS:HZ3	1:C:162:GLN:CD	2.02	0.63
2:T:328:CYS:SG	2:T:329:ASP:N	2.72	0.62
1:C:129:LYS:HZ2	1:C:162:GLN:CD	2.04	0.62
2:H:214:TYR:HE1	2:J:160:LYS:NZ	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:HZ1	3:E:394:LYS:CD	2.05	0.62
2:H:328:CYS:SG	2:H:329:ASP:N	2.72	0.61
1:F:155:LYS:HZ1	3:M:394:LYS:CD	2.09	0.61
1:A:129:LYS:HZ2	1:A:162:GLN:NE2	1.77	0.61
3:D:126:ARG:HB3	3:E:143:VAL:HG11	1.83	0.61
3:E:392:ARG:NH2	3:E:414:LEU:O	2.34	0.60
3:G:392:ARG:NH2	3:G:414:LEU:O	2.34	0.60
2:J:396:THR:O	2:J:396:THR:HG22	2.02	0.60
3:M:392:ARG:NH2	3:M:414:LEU:O	2.34	0.60
2:J:395:ILE:O	2:J:395:ILE:HG23	2.01	0.60
3:D:392:ARG:NH2	3:D:414:LEU:O	2.34	0.60
3:D:359:TYR:HA	3:D:366:THR:HG21	1.84	0.60
1:A:129:LYS:CD	1:A:162:GLN:HG2	2.32	0.60
2:T:237:PRO:HG3	3:D:287:HIS:HB3	1.84	0.60
3:M:126:ARG:CB	3:D:143:VAL:HG11	2.26	0.60
3:E:352:HIS:ND1	3:E:353:GLU:HG3	2.15	0.60
3:M:359:TYR:HA	3:M:366:THR:HG21	1.83	0.59
3:E:359:TYR:HA	3:E:366:THR:HG21	1.84	0.59
1:C:129:LYS:CD	1:C:162:GLN:HG2	2.32	0.59
1:F:129:LYS:CD	1:F:162:GLN:HG2	2.32	0.59
1:B:129:LYS:CD	1:B:162:GLN:HG2	2.32	0.59
2:I:395:ILE:HG23	2:I:395:ILE:O	2.01	0.59
2:I:396:THR:HG22	2:I:396:THR:O	2.02	0.59
3:G:359:TYR:HA	3:G:366:THR:HG21	1.84	0.59
2:T:395:ILE:O	2:T:395:ILE:HG23	2.01	0.59
3:M:90:GLU:OE2	3:D:90:GLU:CD	2.45	0.59
1:F:155:LYS:HZ1	3:M:394:LYS:HE3	0.59	0.59
2:H:395:ILE:HG23	2:H:395:ILE:O	2.01	0.59
2:H:193:GLY:HA3	2:J:153:ALA:HB3	1.85	0.59
2:H:396:THR:HG22	2:H:396:THR:O	2.02	0.58
1:C:228:ALA:HB3	1:C:235:ALA:HB3	1.85	0.58
2:H:214:TYR:HE1	2:J:160:LYS:HZ1	1.51	0.58
1:B:175:THR:OG1	1:B:177:GLU:OE1	2.22	0.58
1:B:228:ALA:HB3	1:B:235:ALA:HB3	1.85	0.58
2:T:237:PRO:CD	3:D:287:HIS:CB	2.80	0.58
1:F:175:THR:OG1	1:F:177:GLU:OE1	2.22	0.58
3:E:57:THR:O	3:E:68:ARG:NH2	2.37	0.58
1:A:240:THR:OG1	1:A:241:TRP:N	2.37	0.58
1:C:240:THR:OG1	1:C:241:TRP:N	2.37	0.58
1:B:240:THR:OG1	1:B:241:TRP:N	2.37	0.58
1:A:228:ALA:HB3	1:A:235:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:328:CYS:SG	2:J:329:ASP:N	2.72	0.58
1:F:226:GLY:N	1:F:237:SER:OG	2.35	0.57
2:T:159:THR:HG22	2:T:283:ALA:H	1.69	0.57
3:M:110:VAL:HG13	3:D:142:THR:OG1	2.04	0.57
3:D:57:THR:O	3:D:68:ARG:NH2	2.37	0.57
2:H:159:THR:HG22	2:H:283:ALA:H	1.69	0.57
2:I:159:THR:HG22	2:I:283:ALA:H	1.70	0.57
2:T:396:THR:HG22	2:T:396:THR:O	2.02	0.57
3:M:57:THR:O	3:M:68:ARG:NH2	2.37	0.57
1:C:175:THR:OG1	1:C:177:GLU:OE1	2.22	0.57
1:A:213:ILE:HD12	1:A:221:VAL:HB	1.87	0.57
1:C:213:ILE:HD12	1:C:221:VAL:HB	1.87	0.57
2:J:159:THR:HG22	2:J:283:ALA:H	1.69	0.57
1:B:226:GLY:N	1:B:237:SER:OG	2.35	0.57
1:C:129:LYS:HZ3	1:C:162:GLN:CG	2.09	0.57
1:A:175:THR:OG1	1:A:177:GLU:OE1	2.22	0.57
3:G:352:HIS:NE2	3:G:353:GLU:CG	2.66	0.57
2:I:252:ASN:HD21	2:I:261:ILE:HB	1.70	0.57
2:J:252:ASN:HD21	2:J:261:ILE:HB	1.70	0.57
1:F:213:ILE:HD12	1:F:221:VAL:HB	1.87	0.57
3:M:346:ARG:HB3	3:M:346:ARG:HH11	1.70	0.57
3:G:57:THR:O	3:G:68:ARG:NH2	2.37	0.57
3:G:346:ARG:HB3	3:G:346:ARG:HH11	1.70	0.57
1:F:228:ALA:HB3	1:F:235:ALA:HB3	1.85	0.56
2:T:252:ASN:HD21	2:T:261:ILE:HB	1.70	0.56
1:B:213:ILE:HD12	1:B:221:VAL:HB	1.87	0.56
1:F:129:LYS:CE	1:F:162:GLN:HG2	2.36	0.56
1:A:129:LYS:CE	1:A:162:GLN:HG2	2.36	0.56
1:A:155:LYS:HZ1	3:D:394:LYS:HE3	0.48	0.56
3:D:352:HIS:NE2	3:D:353:GLU:CG	2.66	0.56
3:E:352:HIS:NE2	3:E:353:GLU:CG	2.66	0.56
1:B:129:LYS:CE	1:B:162:GLN:HG2	2.36	0.56
1:A:226:GLY:N	1:A:237:SER:OG	2.35	0.55
3:E:346:ARG:HB3	3:E:346:ARG:HH11	1.70	0.55
3:M:379:LEU:O	3:M:383:ALA:N	2.39	0.55
1:C:167:MET:SD	1:C:167:MET:N	2.76	0.55
3:D:379:LEU:O	3:D:383:ALA:N	2.39	0.55
3:E:220:CYS:SG	3:E:221:THR:N	2.80	0.55
3:G:379:LEU:O	3:G:383:ALA:N	2.39	0.55
2:H:210:SER:OG	2:H:211:LYS:N	2.40	0.55
2:I:210:SER:OG	2:I:211:LYS:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:210:SER:OG	2:J:211:LYS:N	2.40	0.55
3:D:346:ARG:HB3	3:D:346:ARG:HH11	1.70	0.54
3:D:352:HIS:ND1	3:D:353:GLU:HG3	2.15	0.54
3:G:220:CYS:SG	3:G:221:THR:N	2.80	0.54
1:B:199:VAL:O	1:B:234:THR:N	2.35	0.54
3:M:143:VAL:HG11	3:E:110:VAL:CG1	2.38	0.54
3:M:220:CYS:SG	3:M:221:THR:N	2.80	0.54
2:H:252:ASN:HD21	2:H:261:ILE:HB	1.70	0.54
3:M:352:HIS:NE2	3:M:353:GLU:CG	2.66	0.54
1:C:129:LYS:CE	1:C:162:GLN:HG2	2.36	0.54
3:D:220:CYS:SG	3:D:221:THR:N	2.80	0.54
2:T:210:SER:OG	2:T:211:LYS:N	2.40	0.54
1:C:155:LYS:NZ	3:G:394:LYS:HE2	2.05	0.54
1:F:175:THR:OG1	1:F:176:HIS:N	2.41	0.54
2:H:191:PRO:O	2:J:151:ASP:HB2	2.08	0.54
1:B:175:THR:OG1	1:B:176:HIS:N	2.41	0.54
1:A:129:LYS:HZ2	1:A:162:GLN:CD	2.08	0.53
3:M:352:HIS:ND1	3:M:353:GLU:HG3	2.15	0.53
1:A:199:VAL:O	1:A:234:THR:N	2.35	0.53
2:H:192:TYR:CB	2:J:152:HIS:HA	2.39	0.53
3:D:20:ALA:HB1	3:E:144:ARG:O	2.08	0.53
1:C:175:THR:OG1	1:C:176:HIS:N	2.41	0.53
1:C:200:PRO:HA	1:C:233:ARG:HA	1.91	0.53
3:E:379:LEU:O	3:E:383:ALA:N	2.39	0.53
1:A:200:PRO:HA	1:A:233:ARG:HA	1.91	0.53
3:G:352:HIS:ND1	3:G:353:GLU:HG3	2.15	0.53
1:C:226:GLY:N	1:C:237:SER:OG	2.35	0.53
3:M:90:GLU:OE2	3:D:90:GLU:OE1	2.27	0.52
1:C:169:SER:O	1:C:169:SER:OG	2.25	0.52
1:B:200:PRO:HA	1:B:233:ARG:HA	1.91	0.52
2:H:160:LYS:HB2	2:H:281:ASP:HB3	1.92	0.52
3:M:143:VAL:HG11	3:E:110:VAL:HG11	1.92	0.52
1:A:175:THR:OG1	1:A:176:HIS:N	2.41	0.52
1:F:240:THR:OG1	1:F:241:TRP:N	2.37	0.52
1:B:184:ASN:OD1	1:B:184:ASN:N	2.43	0.52
2:T:160:LYS:HB2	2:T:281:ASP:HB3	1.92	0.52
2:J:160:LYS:HB2	2:J:281:ASP:HB3	1.92	0.52
1:F:200:PRO:HA	1:F:233:ARG:HA	1.91	0.51
2:T:357:ALA:O	2:T:396:THR:OG1	2.28	0.51
1:A:129:LYS:HZ2	1:A:162:GLN:HG2	1.55	0.51
2:I:160:LYS:HB2	2:I:281:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:264:ASN:OD1	2:T:264:ASN:N	2.44	0.50
2:J:201:GLY:O	2:J:204:GLN:NE2	2.45	0.50
2:H:201:GLY:O	2:H:204:GLN:NE2	2.45	0.50
2:I:201:GLY:O	2:I:204:GLN:NE2	2.45	0.50
2:J:174:ASP:OD1	2:J:174:ASP:N	2.44	0.50
3:G:364:THR:OG1	3:G:365:THR:N	2.45	0.50
2:H:102:GLN:NE2	2:H:103:MET:O	2.46	0.49
2:T:102:GLN:NE2	2:T:103:MET:O	2.45	0.49
2:I:102:GLN:NE2	2:I:103:MET:O	2.46	0.49
2:T:201:GLY:O	2:T:204:GLN:NE2	2.45	0.49
1:A:184:ASN:OD1	1:A:184:ASN:N	2.42	0.49
3:D:364:THR:OG1	3:D:365:THR:N	2.45	0.49
1:B:169:SER:O	1:B:169:SER:OG	2.25	0.49
1:B:155:LYS:HZ1	3:E:394:LYS:HE3	0.45	0.49
2:J:317:VAL:HG12	2:J:351:VAL:HG12	1.95	0.49
1:A:213:ILE:HD11	1:A:222:ALA:HB3	1.95	0.49
2:J:102:GLN:NE2	2:J:103:MET:O	2.46	0.49
2:T:317:VAL:HG12	2:T:351:VAL:HG12	1.95	0.49
2:H:192:TYR:HB3	2:J:152:HIS:CA	2.43	0.49
2:H:317:VAL:HG12	2:H:351:VAL:HG12	1.95	0.49
3:E:364:THR:OG1	3:E:365:THR:N	2.45	0.49
1:C:199:VAL:O	1:C:234:THR:N	2.35	0.48
1:F:169:SER:O	1:F:169:SER:OG	2.25	0.48
2:I:174:ASP:OD1	2:I:174:ASP:N	2.44	0.48
1:A:201:THR:OG1	1:A:232:THR:O	2.26	0.48
2:H:264:ASN:OD1	2:H:264:ASN:N	2.44	0.48
3:E:375:VAL:HA	3:E:378:LEU:HD22	1.95	0.48
3:G:375:VAL:HA	3:G:378:LEU:HD22	1.96	0.48
3:M:364:THR:OG1	3:M:365:THR:N	2.45	0.48
1:C:184:ASN:OD1	1:C:184:ASN:N	2.42	0.48
2:T:174:ASP:OD1	2:T:174:ASP:N	2.44	0.48
2:H:191:PRO:C	2:J:151:ASP:O	2.56	0.48
2:H:399:ASP:O	2:H:405:MET:SD	2.72	0.48
3:M:375:VAL:HA	3:M:378:LEU:HD22	1.96	0.48
2:I:357:ALA:O	2:I:396:THR:OG1	2.28	0.48
1:B:144:ASP:OD1	1:B:147:ARG:NH1	2.47	0.48
2:J:399:ASP:O	2:J:405:MET:SD	2.72	0.48
1:F:183:TYR:HD1	1:F:215:ASP:HA	1.79	0.47
1:A:144:ASP:OD1	1:A:147:ARG:NH1	2.47	0.47
1:F:129:LYS:HZ2	1:F:162:GLN:CD	2.10	0.47
3:D:375:VAL:HA	3:D:378:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ASP:OD1	1:F:147:ARG:NH1	2.47	0.47
1:F:199:VAL:O	1:F:234:THR:N	2.35	0.47
2:T:399:ASP:O	2:T:405:MET:SD	2.72	0.47
1:B:183:TYR:HD1	1:B:215:ASP:HA	1.79	0.47
1:C:213:ILE:HD11	1:C:222:ALA:HB3	1.95	0.47
1:F:227:GLY:O	1:F:254:THR:OG1	2.30	0.47
1:C:183:TYR:HD1	1:C:215:ASP:HA	1.79	0.47
1:B:213:ILE:HD11	1:B:222:ALA:HB3	1.95	0.47
1:F:184:ASN:N	1:F:184:ASN:OD1	2.43	0.47
2:I:399:ASP:O	2:I:405:MET:SD	2.72	0.47
1:C:227:GLY:O	1:C:254:THR:OG1	2.30	0.47
3:M:67:ILE:HD11	3:M:78:ALA:HB3	1.97	0.47
1:A:174:TYR:OH	3:D:403:PRO:O	2.27	0.47
1:A:225:LEU:N	1:A:237:SER:O	2.48	0.47
1:B:167:MET:SD	1:B:167:MET:N	2.76	0.47
1:B:225:LEU:N	1:B:237:SER:O	2.48	0.47
2:I:317:VAL:HG12	2:I:351:VAL:HG12	1.95	0.47
1:C:144:ASP:OD1	1:C:147:ARG:NH1	2.47	0.47
1:F:213:ILE:HD11	1:F:222:ALA:HB3	1.95	0.47
1:A:169:SER:O	1:A:169:SER:OG	2.25	0.47
3:D:67:ILE:HD11	3:D:78:ALA:HB3	1.96	0.47
3:D:149:ILE:HG12	3:D:269:LEU:HD12	1.97	0.47
1:B:201:THR:OG1	1:B:232:THR:O	2.26	0.46
3:G:60:ASP:OD1	3:G:60:ASP:N	2.49	0.46
2:H:214:TYR:CE1	2:J:160:LYS:NZ	2.74	0.46
1:B:227:GLY:O	1:B:254:THR:OG1	2.30	0.46
1:F:225:LEU:N	1:F:237:SER:O	2.48	0.46
3:M:57:THR:OG1	3:M:58:LYS:N	2.49	0.46
3:M:60:ASP:OD1	3:M:60:ASP:N	2.49	0.46
1:A:222:ALA:HA	1:A:241:TRP:HZ3	1.81	0.46
1:C:174:TYR:OH	3:G:403:PRO:O	2.27	0.46
3:M:11:LEU:O	3:M:235:TRP:N	2.45	0.46
3:M:143:VAL:HG23	3:E:128:ALA:HB2	1.98	0.46
1:B:222:ALA:HA	1:B:241:TRP:HZ3	1.81	0.46
2:T:328:CYS:SG	2:T:368:CYS:N	2.89	0.46
3:M:149:ILE:HG12	3:M:269:LEU:HD12	1.97	0.46
3:D:341:LEU:HD11	3:D:361:LEU:HD23	1.96	0.46
2:I:400:LEU:HD13	2:I:400:LEU:HA	1.79	0.46
1:A:183:TYR:HD1	1:A:215:ASP:HA	1.79	0.46
3:D:60:ASP:N	3:D:60:ASP:OD1	2.49	0.46
3:E:67:ILE:HD11	3:E:78:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LYS:HZ1	3:G:394:LYS:HE3	0.42	0.46
3:G:341:LEU:HD11	3:G:361:LEU:HD23	1.96	0.46
2:I:368:CYS:HB3	2:I:369:SER:H	1.64	0.46
1:F:222:ALA:HA	1:F:241:TRP:HZ3	1.81	0.46
2:H:237:PRO:CG	3:E:287:HIS:HB3	2.46	0.46
3:E:149:ILE:HG12	3:E:269:LEU:HD12	1.97	0.46
3:E:11:LEU:O	3:E:235:TRP:N	2.45	0.45
3:G:67:ILE:HD11	3:G:78:ALA:HB3	1.97	0.45
1:F:100:ARG:O	1:F:104:LYS:NZ	2.50	0.45
1:A:100:ARG:O	1:A:104:LYS:NZ	2.50	0.45
2:J:328:CYS:SG	2:J:368:CYS:N	2.89	0.45
3:G:11:LEU:O	3:G:235:TRP:N	2.45	0.45
3:G:149:ILE:HG12	3:G:269:LEU:HD12	1.97	0.45
2:H:63:CYS:HB3	2:H:96:CYS:HB3	1.63	0.45
3:D:57:THR:OG1	3:D:58:LYS:N	2.49	0.45
3:E:85:VAL:HG12	3:E:113:VAL:HG22	1.99	0.45
3:M:197:VAL:HG22	3:M:229:VAL:HG22	1.99	0.45
2:I:328:CYS:SG	2:I:368:CYS:N	2.89	0.45
3:E:57:THR:OG1	3:E:58:LYS:N	2.49	0.45
1:C:100:ARG:O	1:C:104:LYS:NZ	2.50	0.45
1:C:222:ALA:HA	1:C:241:TRP:HZ3	1.81	0.45
1:C:225:LEU:N	1:C:237:SER:O	2.48	0.45
2:J:364:ILE:HG22	2:J:373:THR:HB	1.99	0.45
3:G:85:VAL:HG12	3:G:113:VAL:HG22	1.99	0.45
2:J:397:LEU:HD13	2:J:398:PRO:CD	2.46	0.45
2:T:405:MET:H	2:T:405:MET:HG2	1.64	0.45
3:D:197:VAL:HG22	3:D:229:VAL:HG22	1.99	0.45
3:M:85:VAL:HG12	3:M:113:VAL:HG22	1.99	0.45
2:T:364:ILE:HG22	2:T:373:THR:HB	1.99	0.45
2:H:328:CYS:SG	2:H:368:CYS:N	2.88	0.45
2:I:364:ILE:HG22	2:I:373:THR:HB	1.99	0.45
3:E:60:ASP:OD1	3:E:60:ASP:N	2.49	0.45
2:H:364:ILE:HG22	2:H:373:THR:HB	1.99	0.45
1:B:185:TRP:CZ2	1:B:187:TYR:HB2	2.52	0.45
1:F:185:TRP:CZ2	1:F:187:TYR:HB2	2.52	0.45
2:H:397:LEU:HD13	2:H:398:PRO:CD	2.46	0.45
3:M:346:ARG:HB2	3:M:347:ALA:H	1.61	0.44
1:A:115:HIS:HB2	1:A:138:GLY:HA2	2.00	0.44
1:B:100:ARG:O	1:B:104:LYS:NZ	2.50	0.44
1:F:129:LYS:HD3	1:F:162:GLN:HG2	2.00	0.44
1:A:185:TRP:CZ2	1:A:187:TYR:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:TYR:OH	2:H:235:GLN:NE2	2.51	0.44
3:D:11:LEU:O	3:D:235:TRP:N	2.45	0.44
2:I:51:TYR:OH	2:I:235:GLN:NE2	2.51	0.44
1:F:115:HIS:HB2	1:F:138:GLY:HA2	1.99	0.44
2:H:174:ASP:OD1	2:H:174:ASP:N	2.44	0.44
3:D:85:VAL:HG12	3:D:113:VAL:HG22	1.98	0.44
2:I:397:LEU:HD13	2:I:398:PRO:CD	2.46	0.44
3:E:341:LEU:HD11	3:E:361:LEU:HD23	1.96	0.44
1:A:129:LYS:HD3	1:A:162:GLN:HG2	2.00	0.44
1:F:143:ALA:HB1	1:B:117:GLY:HA3	2.00	0.44
1:C:129:LYS:HD3	1:C:162:GLN:HG2	2.00	0.44
1:C:185:TRP:CZ2	1:C:187:TYR:HB2	2.52	0.44
2:H:309:SER:OG	2:H:310:SER:N	2.51	0.44
2:J:63:CYS:HB3	2:J:96:CYS:HB3	1.63	0.44
2:T:51:TYR:OH	2:T:235:GLN:NE2	2.51	0.44
3:G:57:THR:OG1	3:G:58:LYS:N	2.48	0.44
3:G:197:VAL:HG22	3:G:229:VAL:HG22	1.99	0.44
3:D:126:ARG:CB	3:E:143:VAL:HG11	2.46	0.43
3:M:352:HIS:CE1	3:M:353:GLU:CD	2.96	0.43
3:E:197:VAL:HG22	3:E:229:VAL:HG22	1.99	0.43
2:T:237:PRO:HD2	3:D:287:HIS:CG	2.53	0.43
2:J:400:LEU:HA	2:J:400:LEU:HD13	1.79	0.43
1:A:198:THR:HG23	1:A:233:ARG:HH21	1.84	0.43
1:B:198:THR:HG23	1:B:233:ARG:HH21	1.84	0.43
2:J:280:MET:HE3	2:J:280:MET:HB3	1.92	0.43
2:T:309:SER:OG	2:T:310:SER:N	2.51	0.43
1:B:174:TYR:OH	3:E:403:PRO:O	2.27	0.43
2:J:51:TYR:OH	2:J:235:GLN:NE2	2.51	0.43
2:J:264:ASN:OD1	2:J:264:ASN:N	2.44	0.43
3:M:341:LEU:HD11	3:M:361:LEU:HD23	1.96	0.43
1:C:115:HIS:HB2	1:C:138:GLY:HA2	2.00	0.43
1:C:198:THR:HG23	1:C:233:ARG:HH21	1.84	0.43
1:C:202:GLY:O	1:C:205:LYS:NZ	2.52	0.43
1:F:167:MET:SD	1:F:167:MET:N	2.76	0.43
3:E:346:ARG:HB2	3:E:347:ALA:H	1.61	0.43
1:F:198:THR:HG23	1:F:233:ARG:HH21	1.84	0.43
2:T:397:LEU:HD13	2:T:398:PRO:CD	2.46	0.43
2:I:382:LYS:NZ	2:J:21:ARG:O	2.51	0.43
3:M:159:THR:HG22	3:M:160:THR:H	1.84	0.42
2:H:37:SER:OG	2:H:38:LEU:N	2.52	0.42
3:D:352:HIS:CE1	3:D:353:GLU:CD	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:159:THR:HG22	3:G:160:THR:H	1.84	0.42
2:H:426:LEU:O	2:H:430:THR:OG1	2.33	0.42
3:D:136:ILE:H	3:D:136:ILE:HG13	1.73	0.42
3:E:80:ARG:NH2	3:E:96:THR:OG1	2.53	0.42
1:C:201:THR:OG1	1:C:232:THR:O	2.26	0.42
3:G:80:ARG:NH2	3:G:96:THR:OG1	2.53	0.42
1:A:227:GLY:O	1:A:254:THR:OG1	2.30	0.42
1:B:115:HIS:HB2	1:B:138:GLY:HA2	2.00	0.42
3:E:159:THR:HG22	3:E:160:THR:H	1.84	0.42
2:T:63:CYS:HB3	2:T:96:CYS:HB3	1.63	0.42
1:F:202:GLY:O	1:F:205:LYS:NZ	2.52	0.42
1:A:152:LYS:HA	1:A:152:LYS:HD2	1.90	0.42
3:D:159:THR:HG22	3:D:160:THR:H	1.84	0.42
1:F:156:TYR:HB3	1:F:158:LEU:HD13	2.02	0.42
3:M:80:ARG:NH2	3:M:96:THR:OG1	2.53	0.42
2:H:192:TYR:O	2:J:153:ALA:HB2	2.20	0.42
1:B:129:LYS:HD3	1:B:162:GLN:HG2	2.00	0.42
1:F:226:GLY:H	1:F:237:SER:HG	1.65	0.42
3:D:80:ARG:NH2	3:D:96:THR:OG1	2.53	0.42
2:I:37:SER:OG	2:I:38:LEU:N	2.53	0.42
2:I:63:CYS:HB3	2:I:96:CYS:HB3	1.63	0.42
2:I:425:ILE:HA	2:I:428:ILE:HG12	2.02	0.42
3:E:347:ALA:O	3:E:348:HIS:CG	2.73	0.42
3:E:352:HIS:CE1	3:E:353:GLU:CD	2.96	0.42
2:T:37:SER:OG	2:T:38:LEU:N	2.53	0.42
2:H:400:LEU:HD13	2:H:400:LEU:HA	1.79	0.42
2:J:37:SER:OG	2:J:38:LEU:N	2.52	0.42
2:J:309:SER:OG	2:J:310:SER:N	2.51	0.41
2:T:88:MET:HG2	2:T:89:TRP:H	1.85	0.41
1:A:156:TYR:HB3	1:A:158:LEU:HD13	2.02	0.41
2:J:397:LEU:HD13	2:J:397:LEU:HA	1.83	0.41
3:G:136:ILE:H	3:G:136:ILE:HG13	1.73	0.41
3:G:343:THR:HG21	3:G:357:TYR:CE1	2.55	0.41
1:F:216:ASN:OD1	1:F:217:LYS:N	2.53	0.41
3:G:347:ALA:O	3:G:348:HIS:CG	2.73	0.41
3:M:347:ALA:O	3:M:348:HIS:CG	2.73	0.41
1:B:104:LYS:HB2	1:B:104:LYS:HE2	1.80	0.41
2:J:88:MET:HG2	2:J:89:TRP:H	1.85	0.41
1:A:216:ASN:OD1	1:A:217:LYS:N	2.53	0.41
2:H:191:PRO:HB3	2:J:150:GLY:O	2.21	0.41
3:D:347:ALA:O	3:D:348:HIS:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:TYR:OH	3:M:403:PRO:O	2.27	0.41
2:T:25:SER:HG	2:T:288:THR:HG1	1.67	0.41
2:T:425:ILE:HA	2:T:428:ILE:HG12	2.02	0.41
2:H:425:ILE:HA	2:H:428:ILE:HG12	2.02	0.41
1:B:226:GLY:H	1:B:237:SER:HG	1.66	0.41
1:C:216:ASN:OD1	1:C:217:LYS:N	2.53	0.41
2:J:425:ILE:HA	2:J:428:ILE:HG12	2.02	0.41
3:M:343:THR:HG21	3:M:357:TYR:CE1	2.55	0.41
3:D:244:ARG:HH22	3:D:249:GLU:HG3	1.86	0.41
1:B:216:ASN:OD1	1:B:217:LYS:N	2.53	0.41
2:T:426:LEU:O	2:T:430:THR:OG1	2.34	0.41
3:M:110:VAL:HG11	3:D:143:VAL:HG13	2.02	0.41
3:M:298:THR:HA	3:M:325:VAL:HG12	2.02	0.41
2:I:361:PRO:O	2:I:375:THR:OG1	2.30	0.41
2:I:426:LEU:O	2:I:430:THR:OG1	2.33	0.41
1:F:245:MET:HE2	1:F:245:MET:HB2	1.95	0.41
2:T:255:ALA:HA	2:T:256:PRO:HD3	1.91	0.41
2:T:280:MET:HE3	2:T:280:MET:HB3	1.92	0.41
2:I:185:TYR:HE1	2:I:250:PRO:HB3	1.86	0.41
3:E:302:GLU:HA	3:E:303:PRO:HD3	1.90	0.41
1:C:145:LEU:HA	1:C:148:LEU:HD23	2.03	0.41
2:J:426:LEU:O	2:J:430:THR:OG1	2.34	0.41
3:M:244:ARG:HH22	3:M:249:GLU:HG3	1.86	0.41
3:M:281:GLU:HA	3:M:320:VAL:HG12	2.03	0.41
2:H:397:LEU:HD13	2:H:397:LEU:HA	1.83	0.41
1:B:145:LEU:HA	1:B:148:LEU:HD23	2.03	0.41
2:T:400:LEU:HD13	2:T:400:LEU:HA	1.79	0.40
3:D:321:PRO:HD2	3:D:325:VAL:HG13	2.03	0.40
1:B:245:MET:HE1	3:E:399:TYR:CZ	2.56	0.40
2:J:425:ILE:HG13	2:J:428:ILE:HD11	2.03	0.40
1:F:148:LEU:HD13	1:F:148:LEU:HA	1.91	0.40
2:T:185:TYR:HE1	2:T:250:PRO:HB3	1.86	0.40
2:H:88:MET:HG2	2:H:89:TRP:H	1.85	0.40
1:B:156:TYR:HB3	1:B:158:LEU:HD13	2.02	0.40
3:E:298:THR:HA	3:E:325:VAL:HG12	2.02	0.40
1:C:156:TYR:HB3	1:C:158:LEU:HD13	2.02	0.40
2:J:185:TYR:HE1	2:J:250:PRO:HB3	1.86	0.40
3:G:352:HIS:CE1	3:G:353:GLU:CD	2.96	0.40
3:E:321:PRO:HD2	3:E:325:VAL:HG13	2.03	0.40
3:G:281:GLU:HA	3:G:320:VAL:HG12	2.03	0.40
3:G:298:THR:HA	3:G:325:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:321:PRO:HD2	3:M:325:VAL:HG13	2.03	0.40
1:A:245:MET:HE1	3:D:399:TYR:CZ	2.56	0.40
2:I:25:SER:HG	2:I:288:THR:HG1	1.64	0.40
2:I:88:MET:HG2	2:I:89:TRP:H	1.85	0.40
3:G:292:THR:HG22	3:G:293:LEU:H	1.87	0.40
1:A:145:LEU:HA	1:A:148:LEU:HD23	2.03	0.40
3:E:281:GLU:HA	3:E:320:VAL:HG12	2.03	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	158/160 (99%)	141 (89%)	17 (11%)	0	100	100
1	B	158/160 (99%)	141 (89%)	17 (11%)	0	100	100
1	C	158/160 (99%)	141 (89%)	17 (11%)	0	100	100
1	F	158/160 (99%)	141 (89%)	17 (11%)	0	100	100
2	H	433/435 (100%)	356 (82%)	73 (17%)	4 (1%)	14	49
2	I	433/435 (100%)	356 (82%)	73 (17%)	4 (1%)	14	49
2	J	433/435 (100%)	356 (82%)	73 (17%)	4 (1%)	14	49
2	T	433/435 (100%)	357 (82%)	72 (17%)	4 (1%)	14	49
3	D	403/410 (98%)	330 (82%)	73 (18%)	0	100	100
3	E	403/410 (98%)	331 (82%)	72 (18%)	0	100	100
3	G	403/410 (98%)	330 (82%)	73 (18%)	0	100	100
3	M	403/410 (98%)	330 (82%)	73 (18%)	0	100	100
All	All	3976/4020 (99%)	3310 (83%)	650 (16%)	16 (0%)	31	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	T	368	CYS
2	H	368	CYS
2	I	368	CYS
2	J	368	CYS
2	T	369	SER
2	H	369	SER
2	I	369	SER
2	J	369	SER
2	T	191	PRO
2	H	191	PRO
2	I	191	PRO
2	J	191	PRO
2	T	165	PRO
2	H	165	PRO
2	I	165	PRO
2	J	165	PRO

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	132/132 (100%)	128 (97%)	4 (3%)	36	57
1	B	132/132 (100%)	128 (97%)	4 (3%)	36	57
1	C	132/132 (100%)	128 (97%)	4 (3%)	36	57
1	F	132/132 (100%)	128 (97%)	4 (3%)	36	57
2	H	362/362 (100%)	357 (99%)	5 (1%)	59	71
2	I	362/362 (100%)	357 (99%)	5 (1%)	59	71
2	J	362/362 (100%)	357 (99%)	5 (1%)	59	71
2	T	362/362 (100%)	357 (99%)	5 (1%)	59	71
3	D	357/359 (99%)	349 (98%)	8 (2%)	45	64
3	E	357/359 (99%)	349 (98%)	8 (2%)	45	64
3	G	357/359 (99%)	349 (98%)	8 (2%)	45	64
3	M	357/359 (99%)	349 (98%)	8 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3404/3412 (100%)	3336 (98%)	68 (2%)	48 66

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	116	GLU
1	F	125	LEU
1	F	213	ILE
1	F	249	ILE
2	T	264	ASN
2	T	352	ILE
2	T	397	LEU
2	T	399	ASP
2	T	400	LEU
3	M	136	ILE
3	M	201	CYS
3	M	217	ILE
3	M	261	ILE
3	M	343	THR
3	M	346	ARG
3	M	361	LEU
3	M	378	LEU
1	A	116	GLU
1	A	125	LEU
1	A	213	ILE
1	A	249	ILE
2	H	264	ASN
2	H	352	ILE
2	H	397	LEU
2	H	399	ASP
2	H	400	LEU
3	D	136	ILE
3	D	201	CYS
3	D	217	ILE
3	D	261	ILE
3	D	343	THR
3	D	346	ARG
3	D	361	LEU
3	D	378	LEU
1	B	116	GLU
1	B	125	LEU
1	B	213	ILE

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Mol	Chain	Res	Type
1	B	249	ILE
2	I	264	ASN
2	I	352	ILE
2	I	397	LEU
2	I	399	ASP
2	I	400	LEU
3	E	136	ILE
3	E	201	CYS
3	E	217	ILE
3	E	261	ILE
3	E	343	THR
3	E	346	ARG
3	E	361	LEU
3	E	378	LEU
1	C	116	GLU
1	C	125	LEU
1	C	213	ILE
1	C	249	ILE
2	J	264	ASN
2	J	352	ILE
2	J	397	LEU
2	J	399	ASP
2	J	400	LEU
3	G	136	ILE
3	G	201	CYS
3	G	217	ILE
3	G	261	ILE
3	G	343	THR
3	G	346	ARG
3	G	361	LEU
3	G	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	115	HIS
1	F	162	GLN
2	T	18	HIS
2	T	142	GLN
2	T	252	ASN
2	T	335	ASN
2	T	353	HIS

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Mol	Chain	Res	Type
2	T	391	ASN
3	M	62	HIS
3	M	73	HIS
3	M	86	HIS
3	M	120	ASN
3	M	335	GLN
3	M	362	HIS
1	A	115	HIS
1	A	162	GLN
2	H	18	HIS
2	H	142	GLN
2	H	252	ASN
2	H	335	ASN
2	H	353	HIS
2	H	391	ASN
3	D	62	HIS
3	D	73	HIS
3	D	86	HIS
3	D	120	ASN
3	D	287	HIS
3	D	335	GLN
3	D	362	HIS
1	B	115	HIS
1	B	162	GLN
2	I	18	HIS
2	I	142	GLN
2	I	252	ASN
2	I	335	ASN
2	I	353	HIS
2	I	391	ASN
3	E	62	HIS
3	E	73	HIS
3	E	86	HIS
3	E	120	ASN
3	E	335	GLN
3	E	362	HIS
1	C	115	HIS
1	C	162	GLN
2	J	18	HIS
2	J	102	GLN
2	J	142	GLN
2	J	252	ASN

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Mol	Chain	Res	Type
2	J	335	ASN
2	J	353	HIS
2	J	391	ASN
3	G	62	HIS
3	G	73	HIS
3	G	86	HIS
3	G	120	ASN
3	G	335	GLN
3	G	362	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

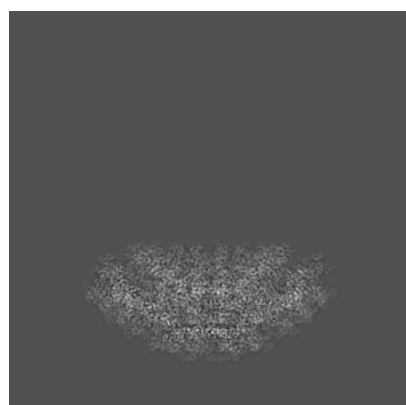
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23378. These allow visual inspection of the internal detail of the map and identification of artifacts.

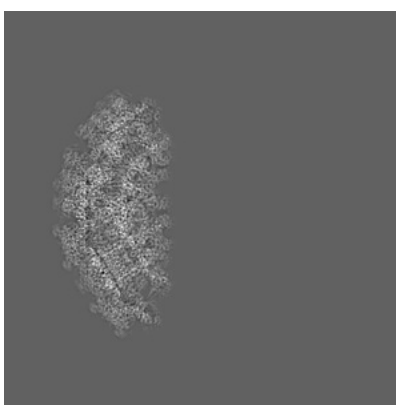
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

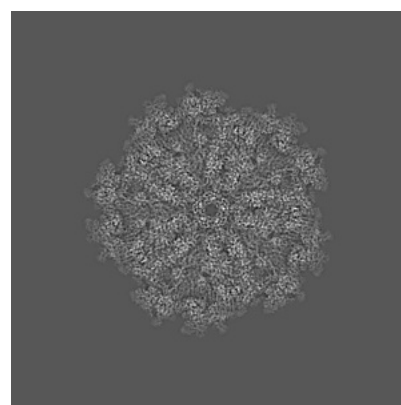
6.1.1 Primary map



X



Y



Z

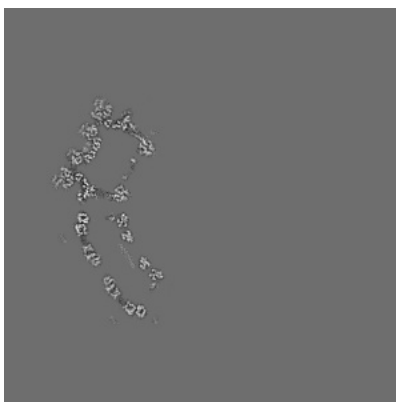
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

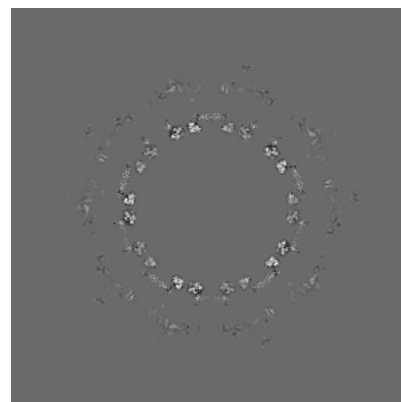
6.2.1 Primary map



X Index: 360



Y Index: 360

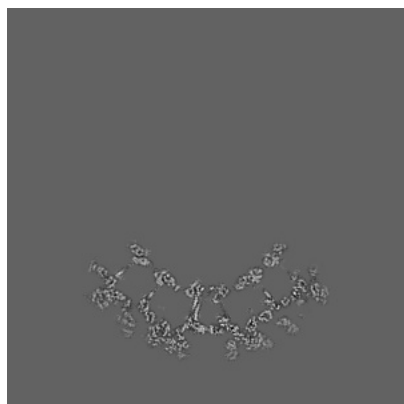


Z Index: 360

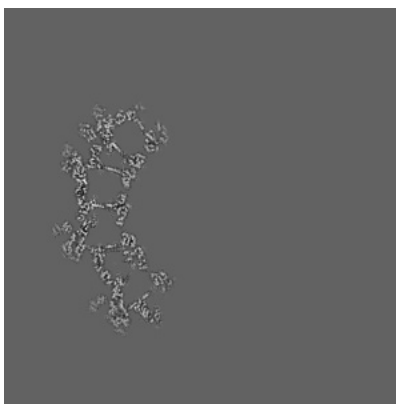
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 370



Y Index: 383

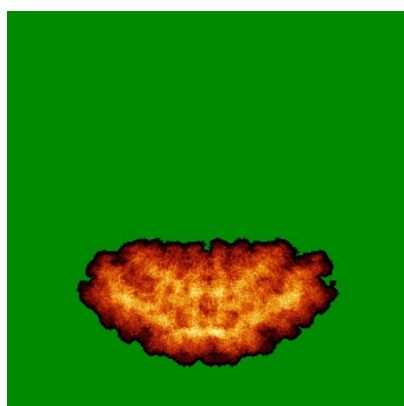


Z Index: 206

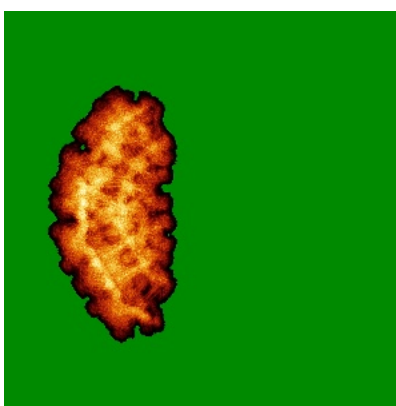
The images above show the largest variance slices of the map in three orthogonal directions.

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

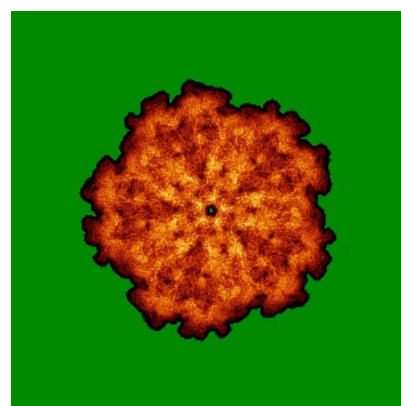
6.4.1 Primary map



X



Y

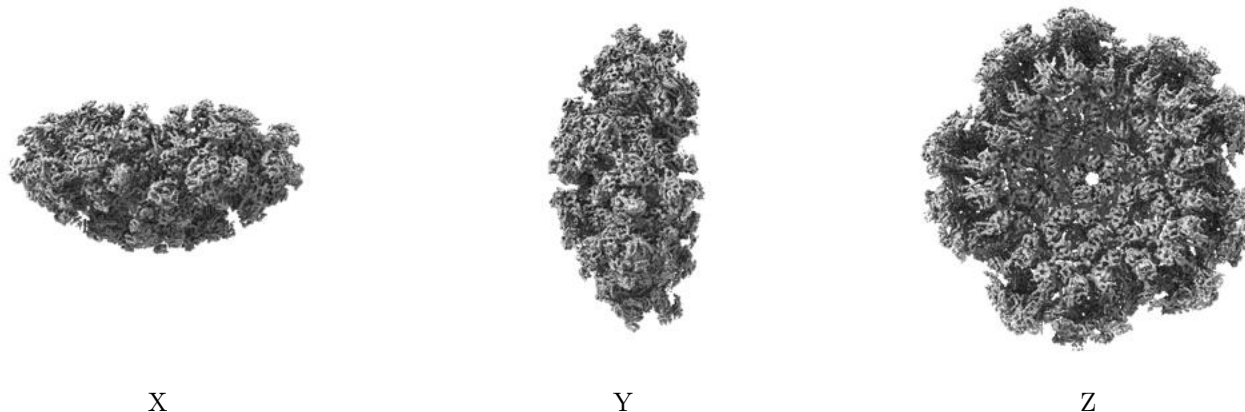


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.96. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

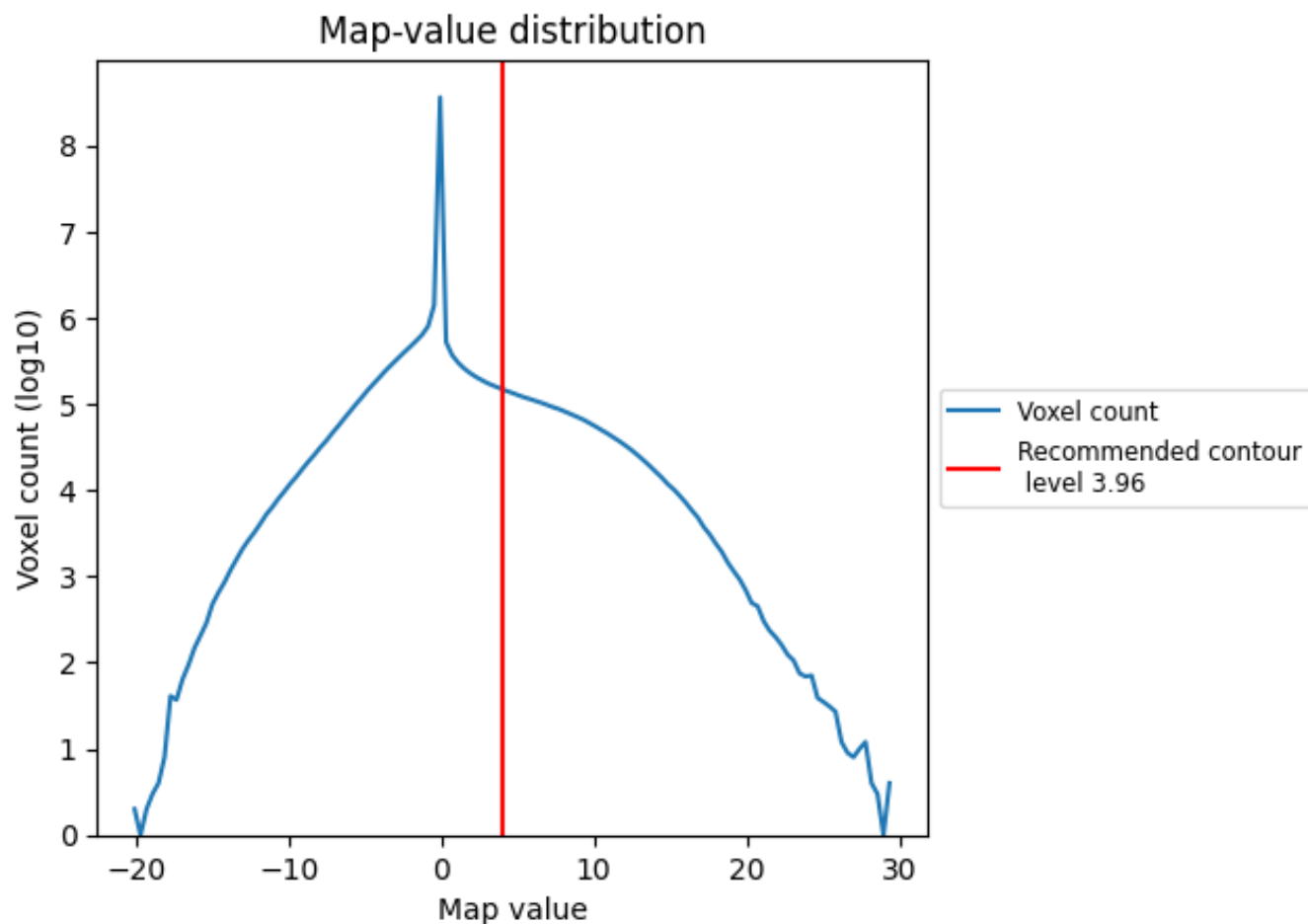
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

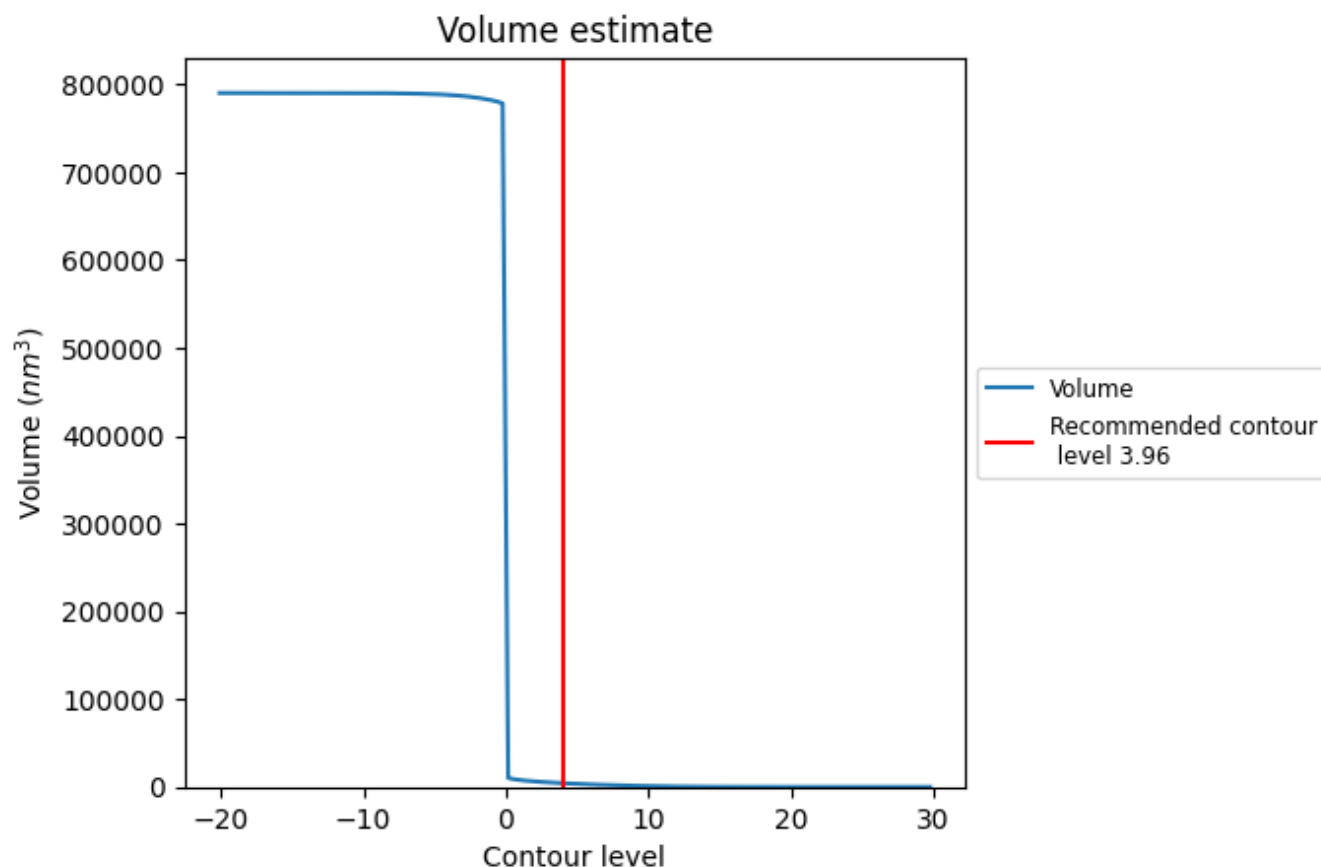
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

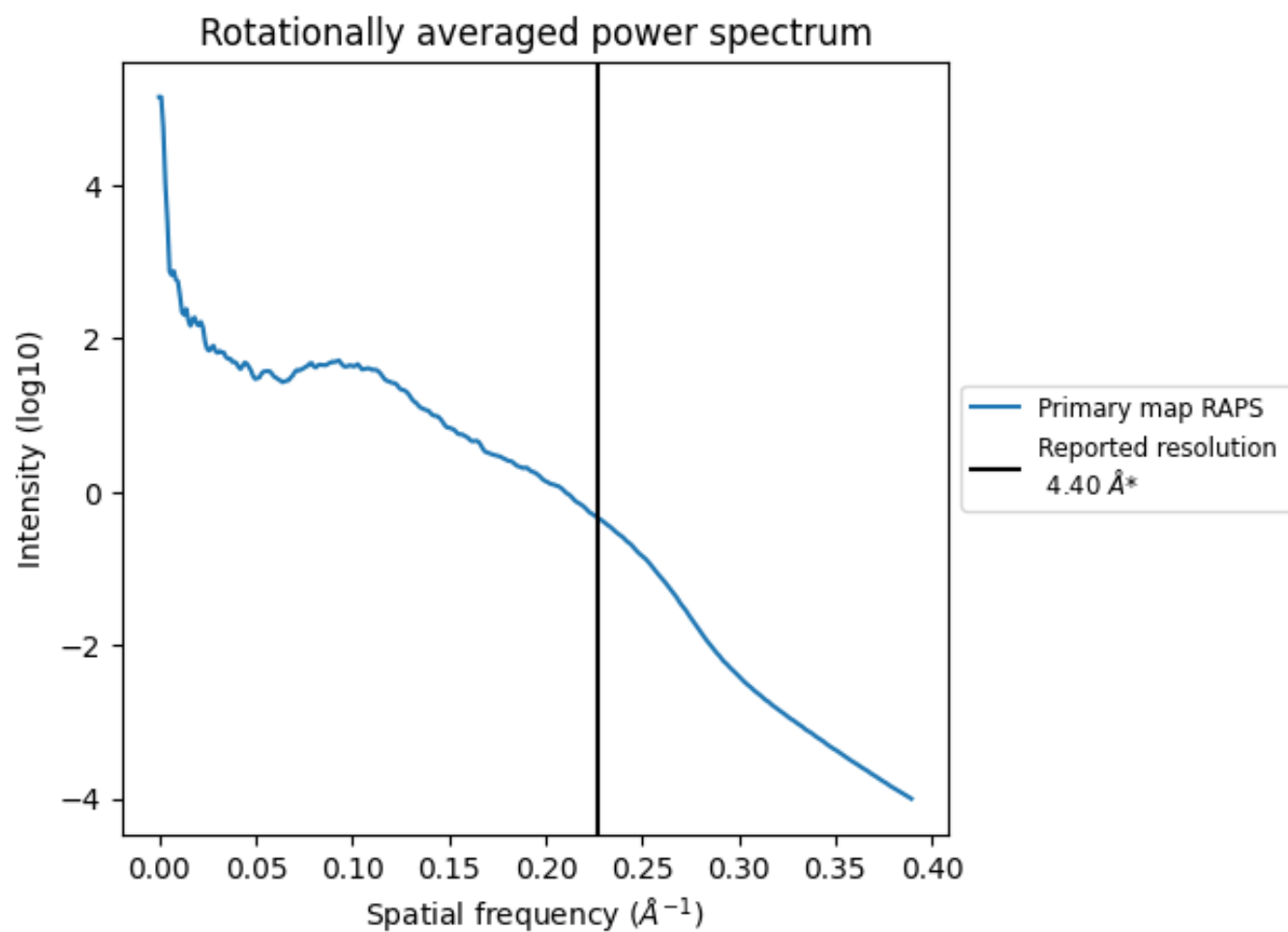
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4316 nm³; this corresponds to an approximate mass of 3899 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 0.227 Å⁻¹

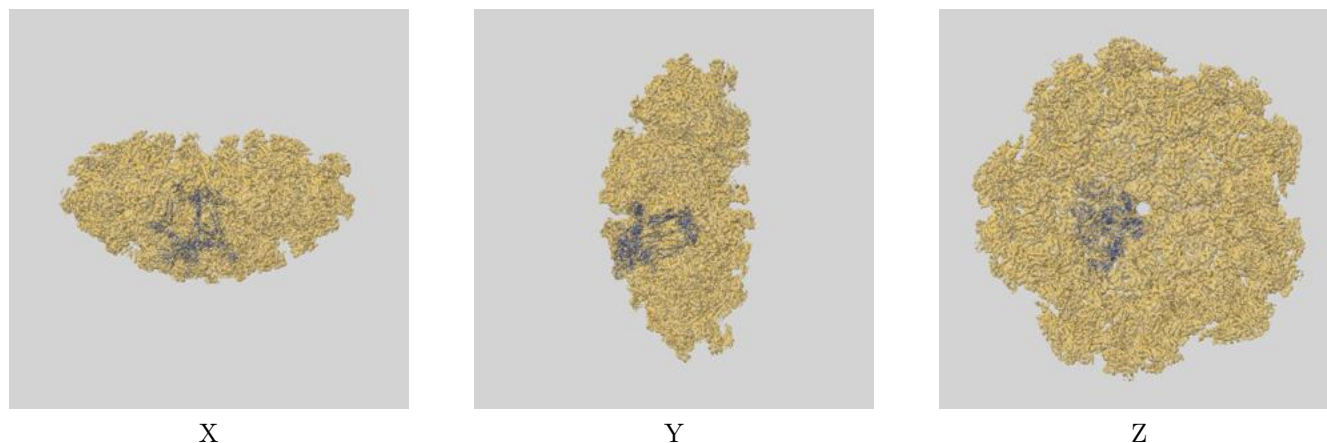
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

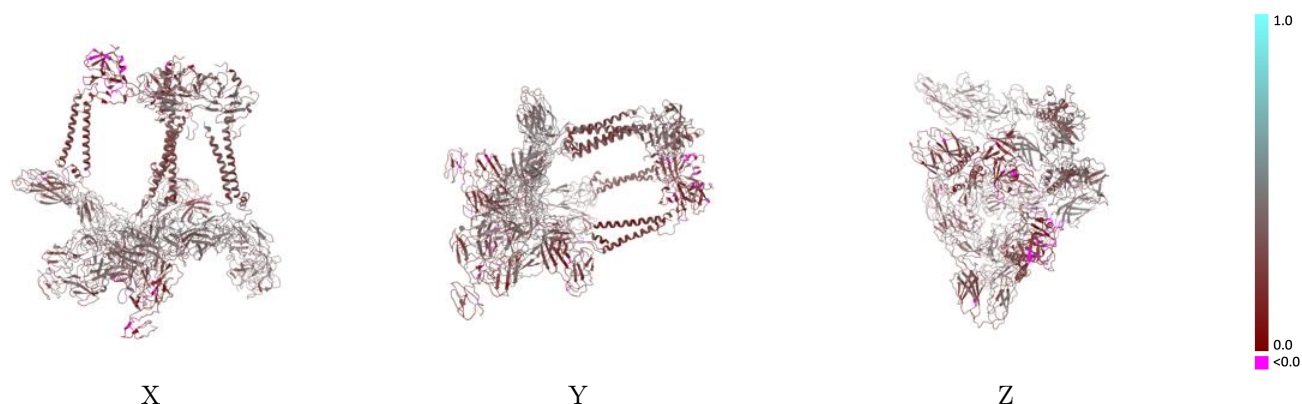
This section contains information regarding the fit between EMDB map EMD-23378 and PDB model 7LIH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



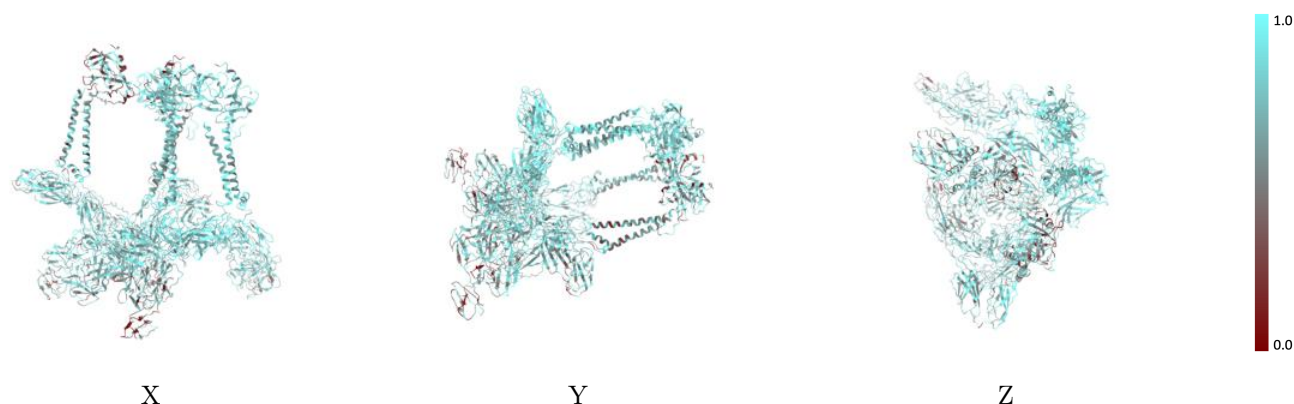
The images above show the 3D surface view of the map at the recommended contour level 3.96 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



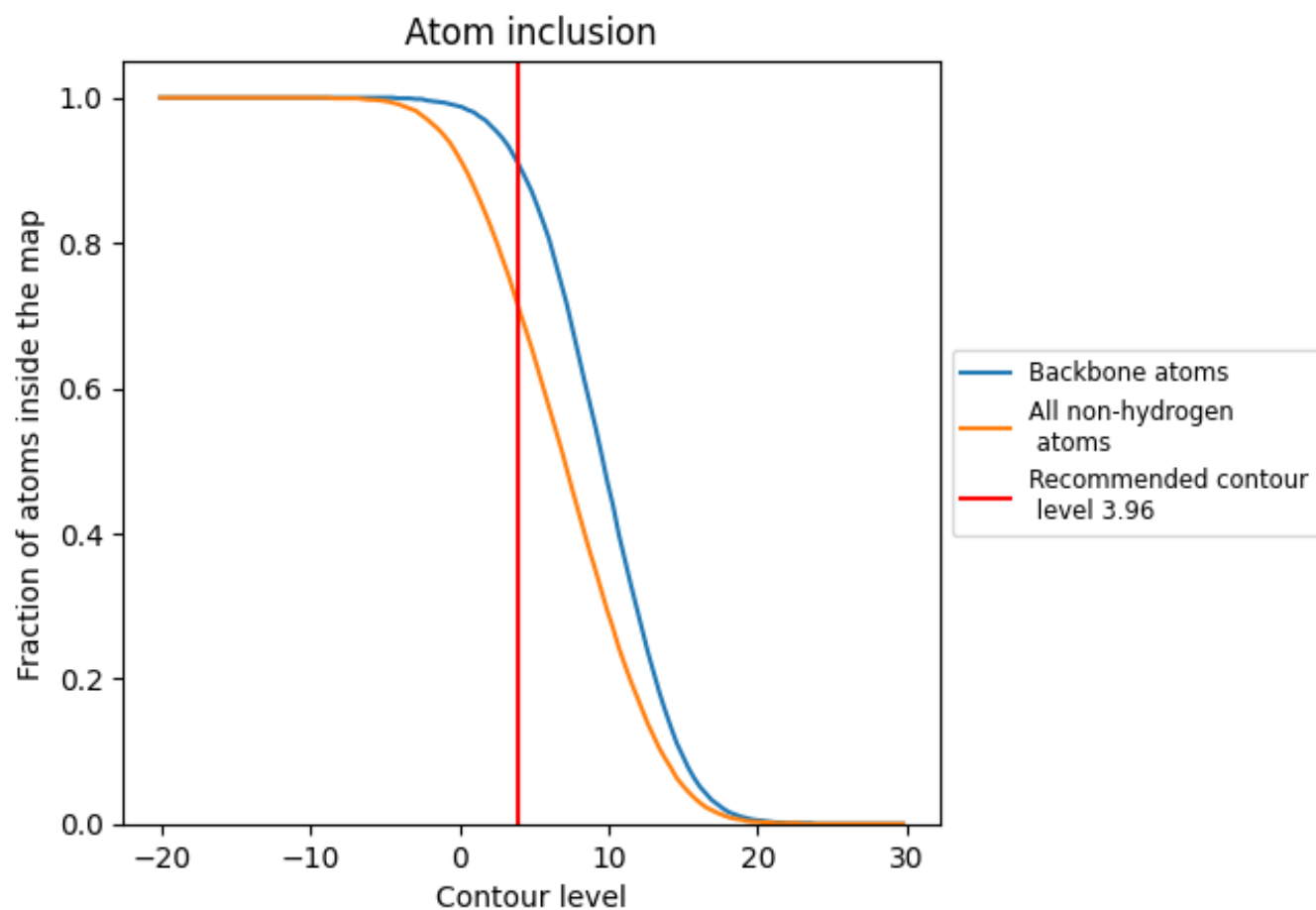
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.96).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.96) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.3210
A	0.6270	0.2000
B	0.7980	0.3700
C	0.7970	0.3650
D	0.6440	0.2800
E	0.7230	0.3600
F	0.5740	0.1570
G	0.7220	0.3570
H	0.6960	0.2850
I	0.7790	0.3850
J	0.7770	0.3870
M	0.6370	0.2720
T	0.7150	0.3120

1.0

0.0

<0.0