



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:55 PM UTC

PDB ID : 7WKK / pdb_00007wkk
EMDB ID : EMD-32566
Title : Cryo-EM structure of the IR subunit from *X. laevis* NPC
Authors : Huang, G.; Zhan, X.; Shi, Y.
Deposited on : 2022-01-10
Resolution : 4.20 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:

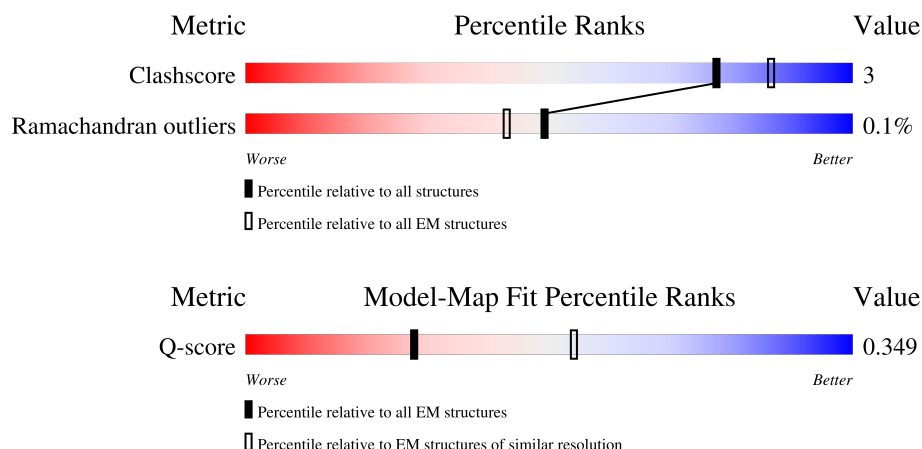
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.20 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.



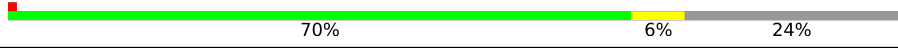
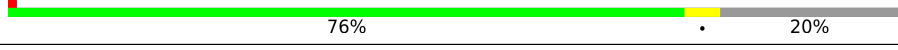
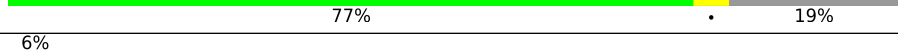
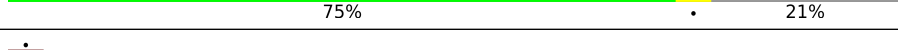
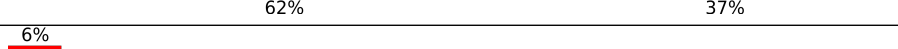
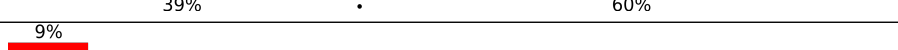
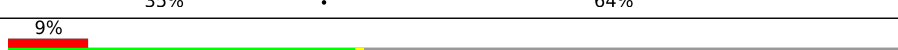
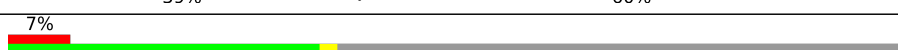
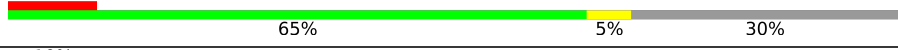
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	2011	 80% 16%
1	a	2011	 79% 17%
2	B	1739	 83% 15%
2	b	1739	 84% 15%
3	C	820	 5% 75% 23%

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Mol	Chain	Length	Quality of chain
3	E	820	
3	c	820	
3	e	820	
4	D	1388	
4	F	1388	
4	M	1388	
4	d	1388	
4	f	1388	
4	m	1388	
5	G	535	
5	J	535	
5	g	535	
5	j	535	
6	H	547	
6	L	547	
6	h	547	
6	l	547	
7	I	599	
7	K	599	
7	i	599	
7	k	599	
8	O	523	
8	o	523	
9	N	660	
9	n	660	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 92821 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 MGC83295 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1684	Total	C	N	O	0	0
			8339	4971	1684	1684		
1	a	1669	Total	C	N	O	0	0
			8268	4930	1669	1669		

- Molecule 2 is a protein called Nup188 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	1482	Total	C	N	O	0	0
			7347	4383	1482	1482		
2	b	1482	Total	C	N	O	0	0
			7347	4383	1482	1482		

- Molecule 3 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	633	Total	C	N	O	0	0
			3144	1878	633	633		
3	E	625	Total	C	N	O	0	0
			3105	1855	625	625		
3	c	633	Total	C	N	O	0	0
			3144	1878	633	633		
3	e	625	Total	C	N	O	0	0
			3105	1855	625	625		

- Molecule 4 is a protein called Nup155-prov protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	1115	Total	C	N	O	0	0
			5524	3294	1115	1115		
4	F	1094	Total	C	N	O	0	0
			5417	3229	1094	1094		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	869	Total	C	N	O	0	0
			4296	2558	869	869		
4	d	1123	Total	C	N	O	0	0
			5563	3317	1123	1123		
4	f	1097	Total	C	N	O	0	0
			5432	3238	1097	1097		
4	m	869	Total	C	N	O	0	0
			4296	2558	869	869		

- Molecule 5 is a protein called Nup54.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	215	Total	C	N	O	0	0
			1063	633	215	215		
5	J	195	Total	C	N	O	0	0
			963	573	195	195		
5	g	215	Total	C	N	O	0	0
			1063	633	215	215		
5	j	195	Total	C	N	O	0	0
			963	573	195	195		

- Molecule 6 is a protein called IL4I1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	163	Total	C	N	O	0	0
			813	487	163	163		
6	L	156	Total	C	N	O	0	0
			778	466	156	156		
6	h	163	Total	C	N	O	0	0
			813	487	163	163		
6	l	156	Total	C	N	O	0	0
			778	466	156	156		

- Molecule 7 is a protein called MGC84997 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	171	Total	C	N	O	0	0
			853	511	171	171		
7	K	166	Total	C	N	O	0	0
			829	497	166	166		
7	i	171	Total	C	N	O	0	0
			853	511	171	171		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	k	166	Total	C	N	O	0	0
			829	497	166	166		

- Molecule 8 is a protein called Aaas-prov protein.

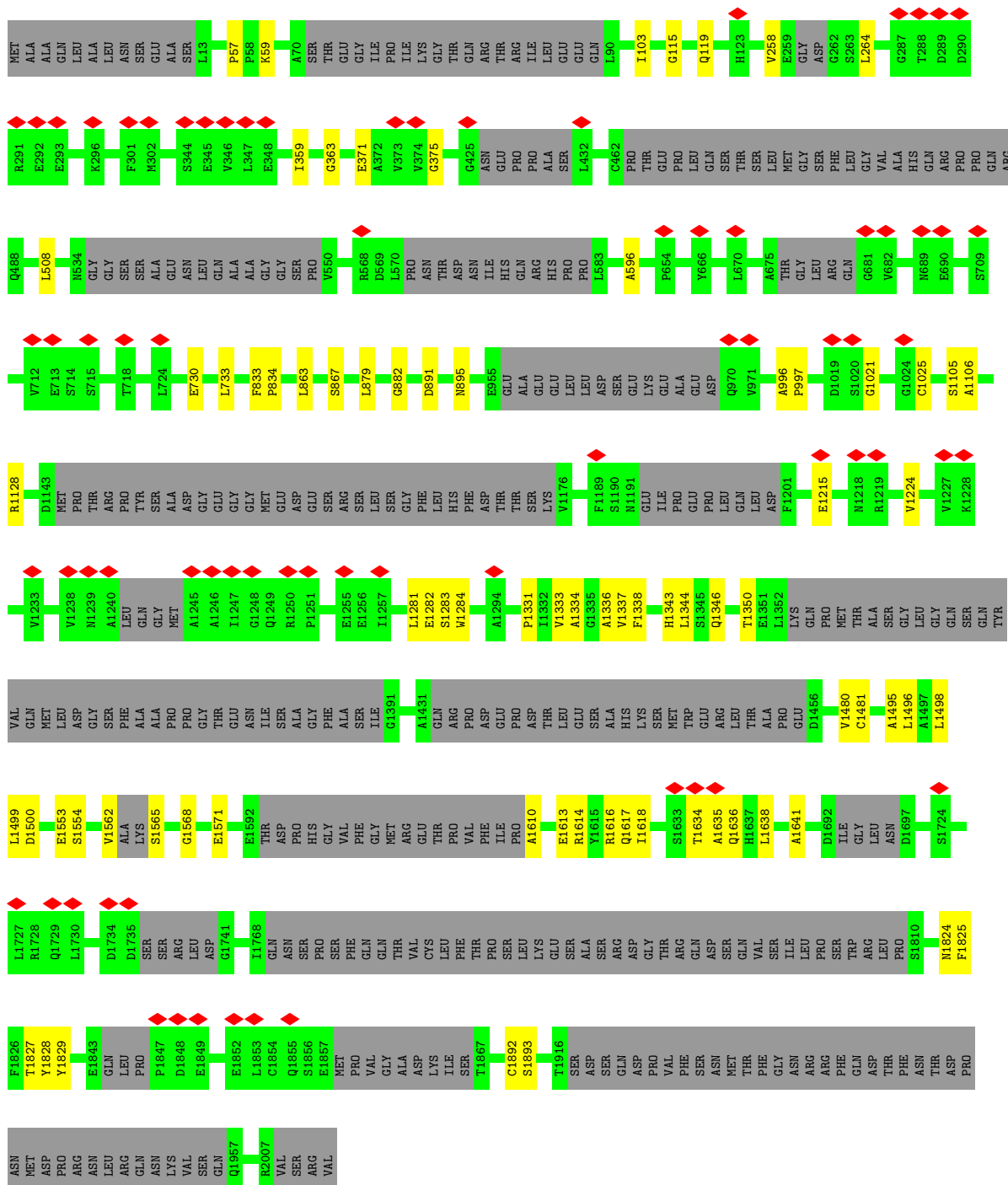
Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	367	Total	C	N	O	0	0
			1805	1071	367	367		
8	o	367	Total	C	N	O	0	0
			1805	1071	367	367		

- Molecule 9 is a protein called Nucleoporin NDC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	431	Total	C	N	O	0	0
			2143	1281	431	431		
9	n	431	Total	C	N	O	0	0
			2143	1281	431	431		



Chain a:



Chain B:

83% 15%

1.5
1.0
0.5
0

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100

NET
ALA
ALA
ALA
GLY
SER
LEU
TYR
TRP
ARG
T11
K50
K59
N63
D84
S288
D289
K290
Q293
A325
L329
K337
E405
Q409
A413
F440
T474
D483
I484
E490
W493
K494
R495
Q496
T497
P498

G505
L506
G507
L518
D524
E525
W532
T578
P606
P607
M608
G637
PHE
LEU
PRO
PHE
GLY
ALA
ASN
VAL
SER
GLY
HIS
LEU
ILE
SER
THR
GLU
GLY
MET
ASN
ALA
G659
L743
CYS
PRO
GLU
GLU
GLU
GLY
SER
SER
SER
PRO
CYS
GLN
THR
GLN
VAL
GLN
PRO
GLN
VAL
SER
SER
ALA
SER
L756
K822
PRO
PRO
SER

SER
GLY
SER
P830
W832
LEU
GLU
ALA
LYS
ASP
THR
GLN
GLY
SER
LYS
GLU
TYR
PHE
LEU
GLY
TRP
S951
D961
SER
GLN
ASP
PRO
GLU
SER
SER
W969
A1044
VAL
ARG
GLY
SER
LEU
GLY
S1052
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E1063
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SER
N1088
A1111
L1116
SER

R1141
SER
V1143
L1167
ALA
F1170
V1246
PRO
ALA
SER
ASP
THR
SER
GLU
ASP
LYS
ASP
SER
MET
GLN
THR
GLU
GLU
ASP
THR
THR
ILE
ARG
Q1268
G1293
Q1297
S1316
K1320
Q1364
LEU
SER
SER
ASN
GLY
ALA
GLY
SER
VAL
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LEU
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Q1422
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V1432
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GLN
S1437
S1489
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THR
PRO
ALA
ALA
GLU
SER
ASP
ALA
S1595
K1617
ASP
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SER
ARG
ALA
LEU
VAL
SER
GLN
SER
ASN
ASN
THR
GLY
E1633

P1663
R1693
ARG
GLY
GLY
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PRO
SER
SER
PRO
ALA
ALA
GLY
GLY
LEU
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MET
PRO
PRO
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SER
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GLN
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LYS
GLY
ALA
ALA
SER
ALA
ALA
LYS
VAL
VAL
PRO
GLU
GLU
ALA
GLN
GLU
P1725
V1734
Q1738
ARG

Chain b:

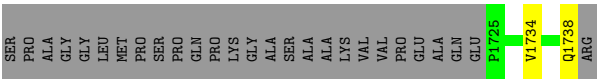
84% 15%

Met Ala Ala Ala Gly Ser Leu Tyr Arg Trp
T11
K59
A62 N63 K64
V262 E263
G266 Y267
K290 I291 E292 Q293
E299
A325 I329
K337 V338
E405
Q409
F440
T474
H479
W493 K494 R495 Q496 T497
G505 L506 G507
L518

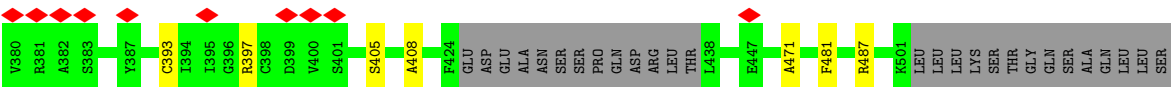
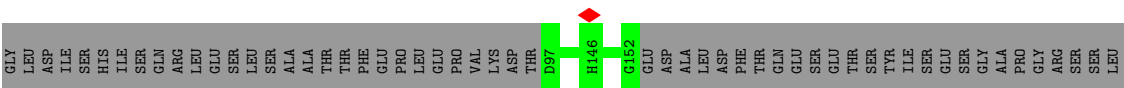
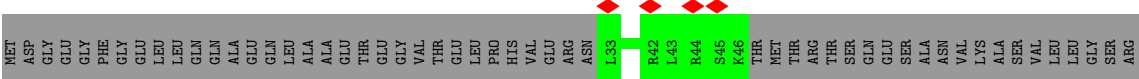
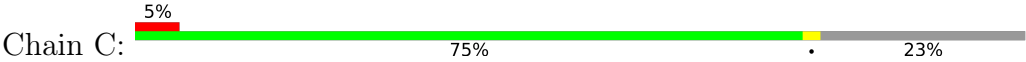
A523 D524 E525 N526 G527
W532
M604 N605 P606 P607 M608
G637 PHE LEU PRO PHE ALA ASN VAL SER HIS ILE SER THR GLU MET ASN ALA
G859 L678
L743 CYS PRO GLU GLU GLU GLY SER SER ALA PRO ASN L756
K822 PRO SER SER

GLY VAL SER P830
H841
N932
GLU ALA LYS ASP THR ASN GLY GLY SER LYS GLU TYR SER LEU GLY TRP
I951
D961
SER GLN ASP PRO GLU SER Y969
A1044 VAL ARG GLY SER LEU GLY ASP S1052
G1085 THR CYS H1088
A1111
L1116
R1141 SER Y1143

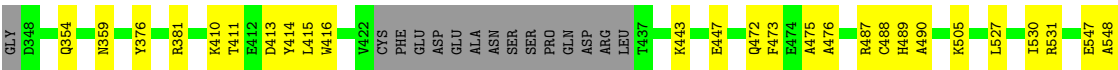
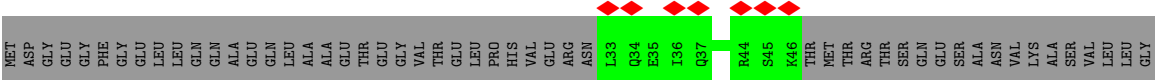
L1187
ALA P1170
V1246
PRO ALA SER ASP THR SER GLU ASP LYS LEU ASP MET SER LEU GLN HIS TYR LEU GLN ILE ASP THR ASN GLY GLU ILE SER MET MET SER SER THR ALA
Q1268
G1293
Q1297
S1316
K1320
Q1364
LEU SER ASN SER ALA GLY SER GLN VAL GLN PRO ALA VAL SER LEU ARG L1531
F1557
PRO ASP

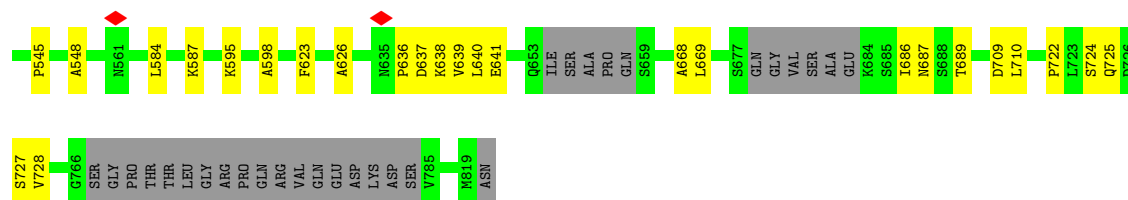


• Molecule 3: Nuclear pore complex protein Nup93



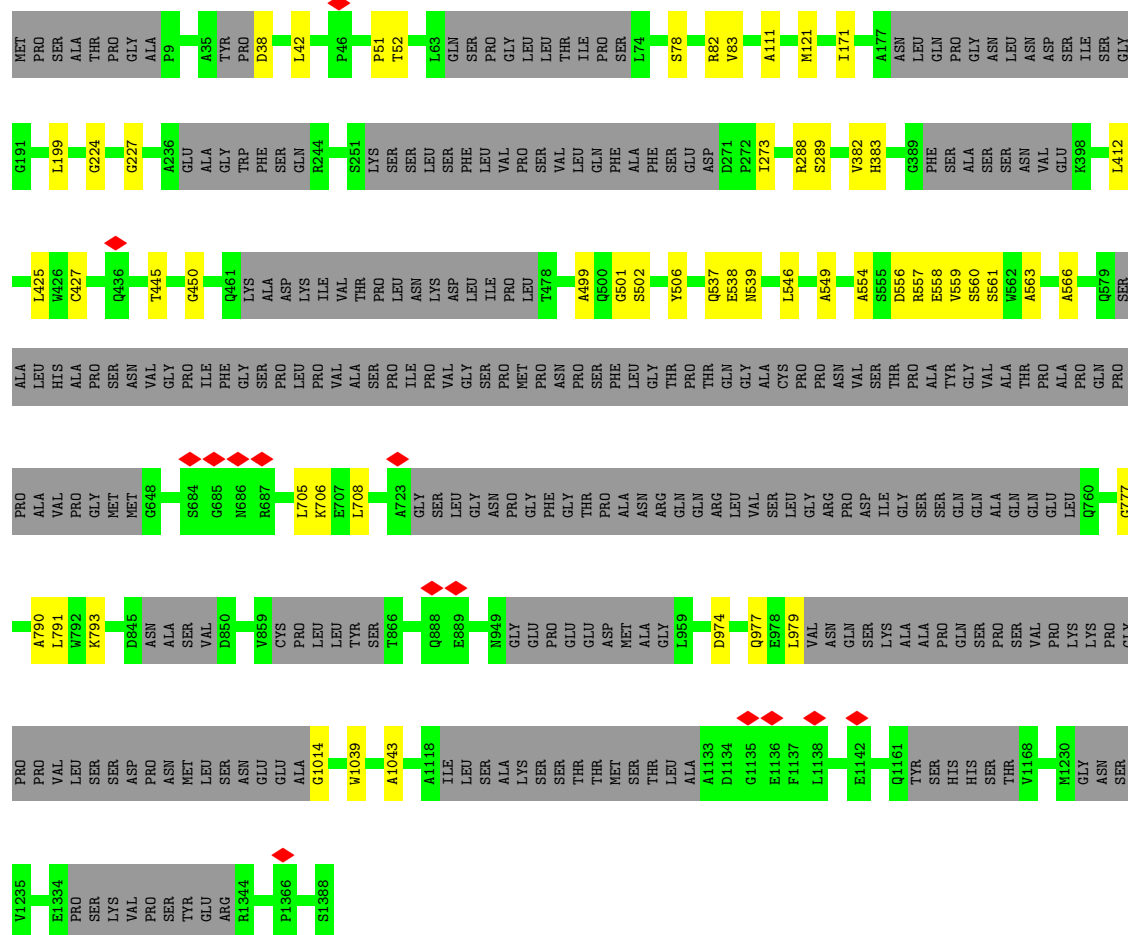
• Molecule 3: Nuclear pore complex protein Nup93





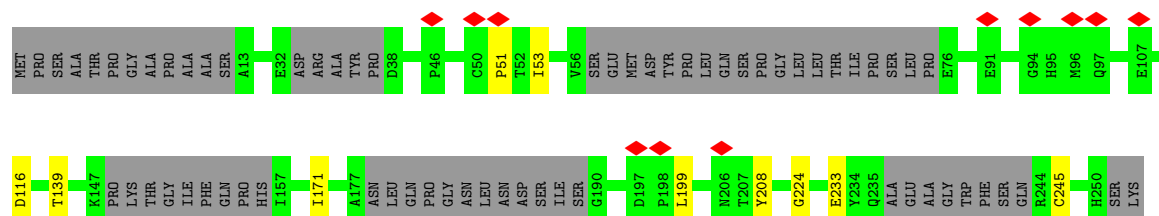
• Molecule 4: Nup155-prov protein

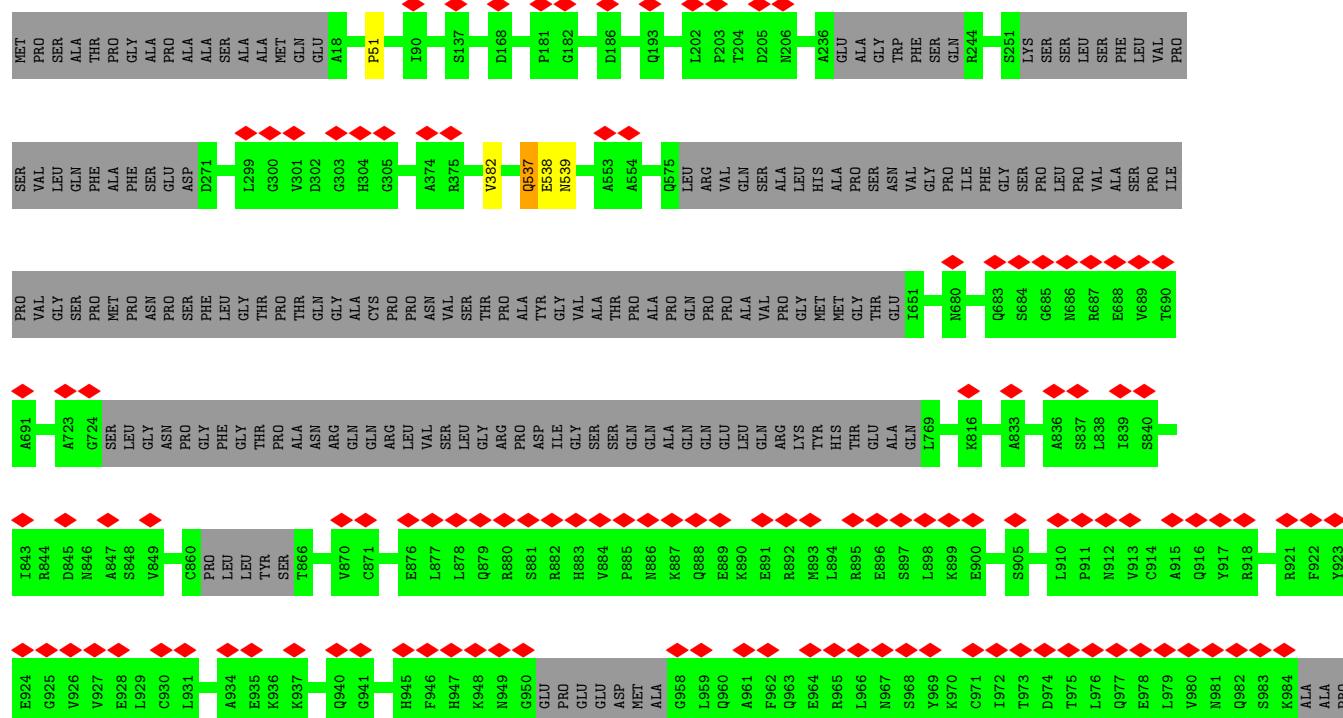
Chain D: 76% 20%

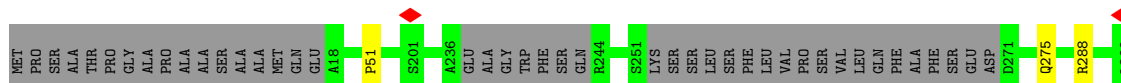


• Molecule 4: Nup155-prov protein

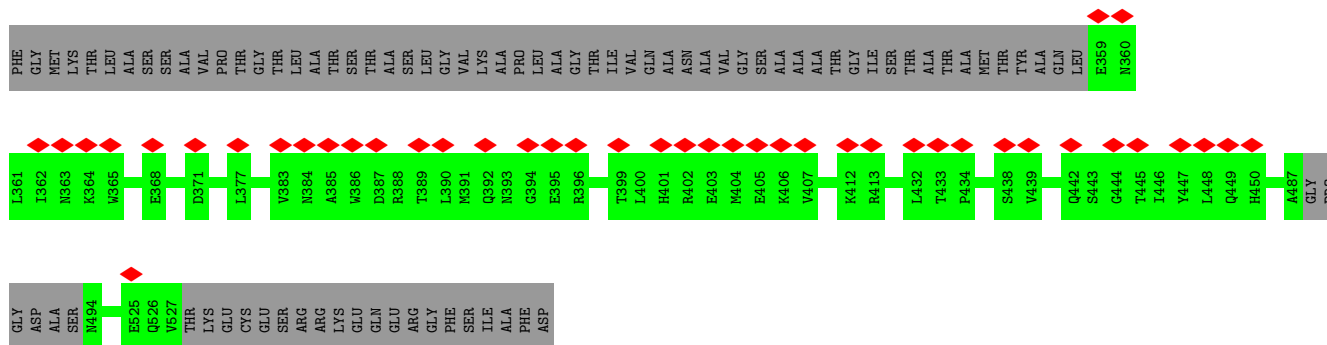
Chain F: 75% 21%



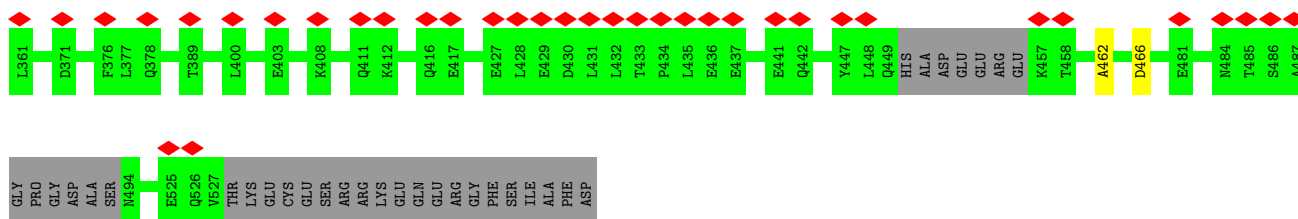
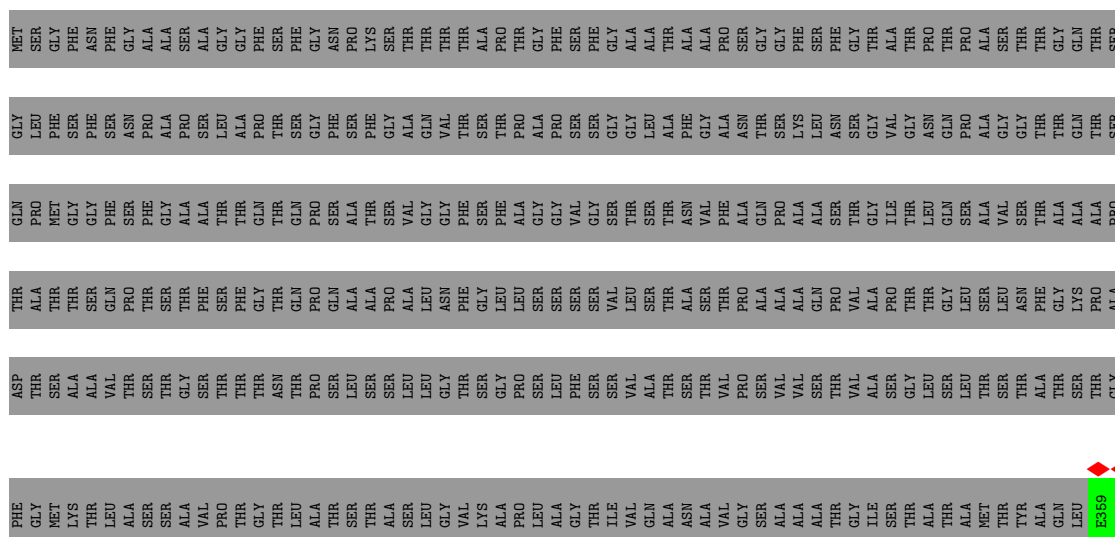




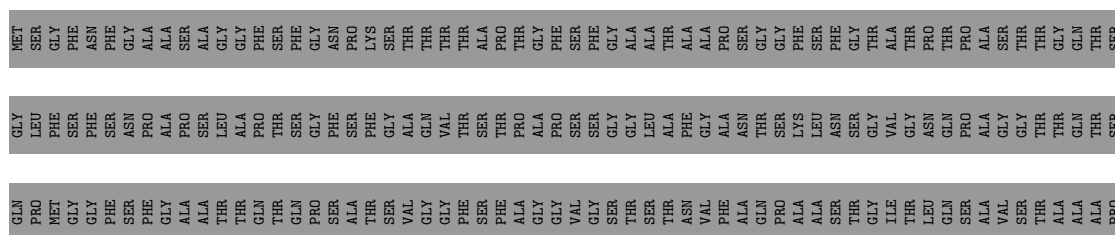


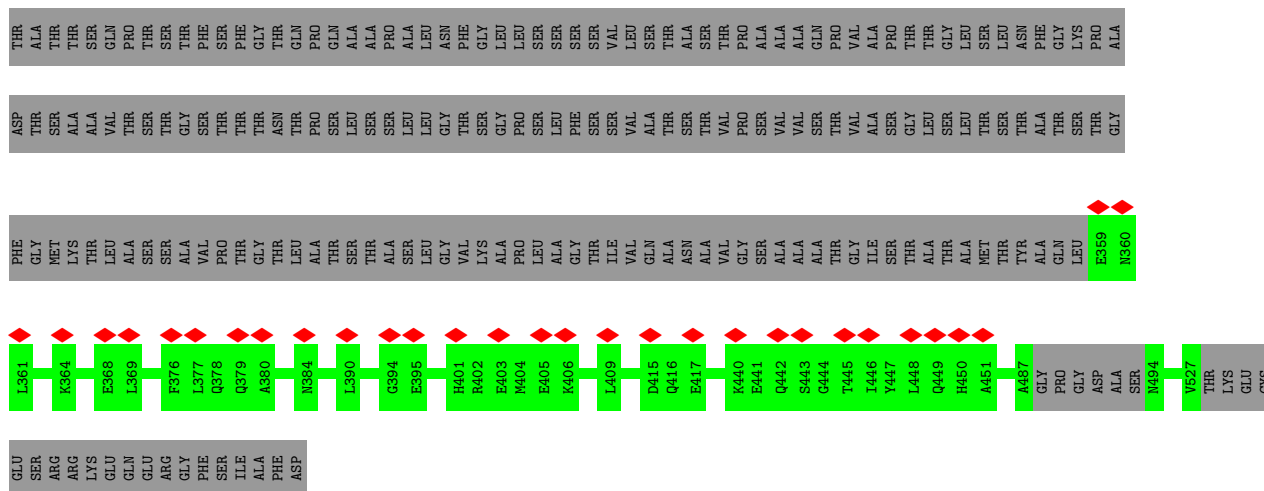


- Molecule 6: IL4I1 protein

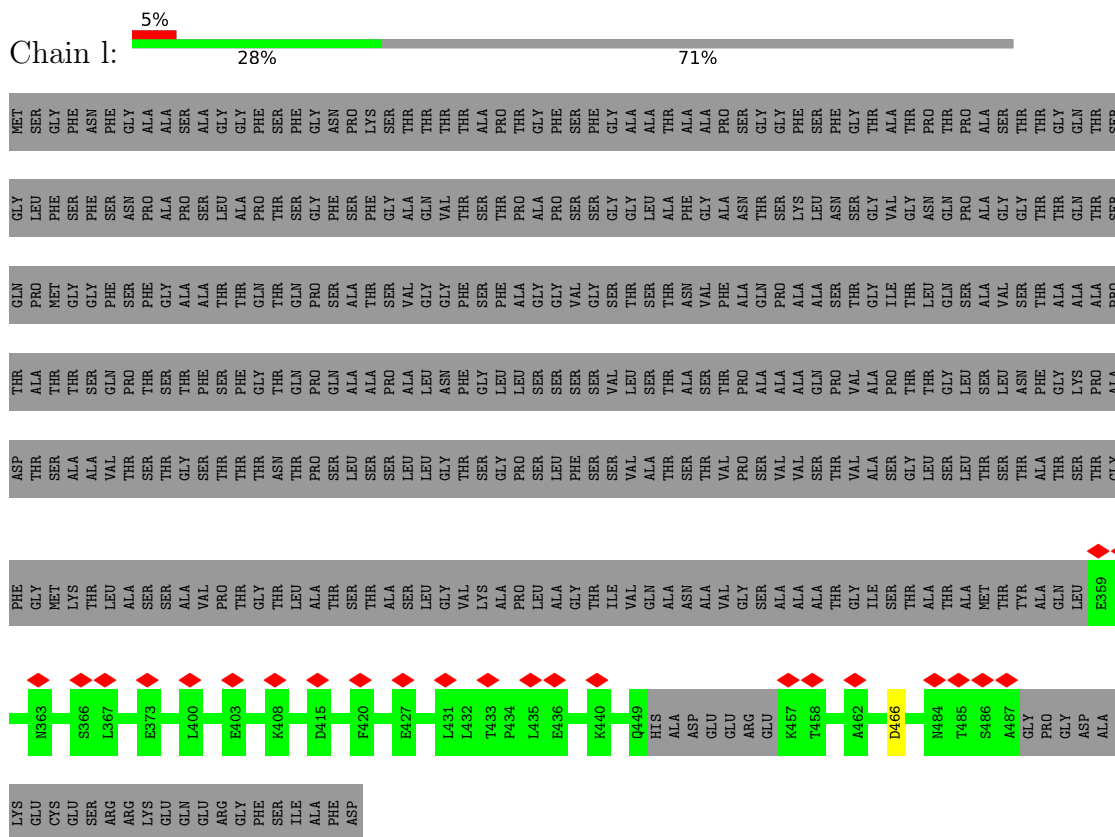


- Molecule 6: IL4I1 protein

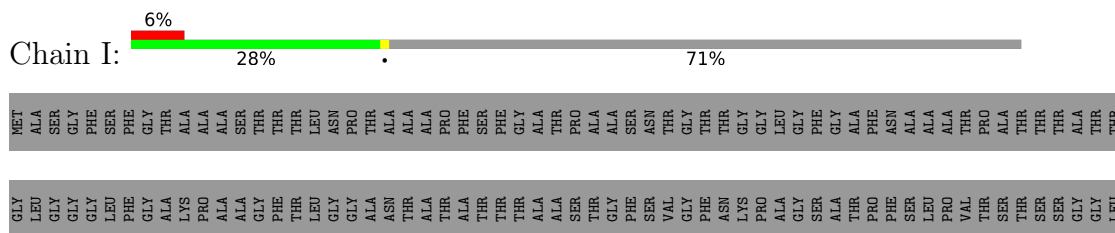




- Molecule 6: IL4I1 protein



- Molecule 7: MGC84997 protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2093631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	710.144, 710.144, 710.144	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.387, 1.387, 1.387	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.32	0/8318	0.46	0/11563
1	a	0.31	0/8246	0.46	0/11463
2	B	0.21	0/7330	0.37	0/10197
2	b	0.21	0/7330	0.37	0/10197
3	C	0.19	0/3134	0.36	0/4359
3	E	0.38	0/3093	0.46	0/4299
3	c	0.19	0/3134	0.37	0/4359
3	e	0.37	0/3093	0.47	0/4299
4	D	0.29	0/5506	0.45	0/7649
4	F	0.26	0/5399	0.42	0/7498
4	M	0.18	0/4288	0.38	0/5961
4	d	0.29	0/5545	0.46	0/7703
4	f	0.26	0/5414	0.42	0/7519
4	m	0.18	0/4288	0.38	0/5961
5	G	0.22	0/1059	0.43	0/1469
5	J	0.20	0/959	0.40	0/1329
5	g	0.20	0/1059	0.44	0/1469
5	j	0.20	0/959	0.43	0/1329
6	H	0.20	0/811	0.38	0/1131
6	L	0.40	0/775	0.58	0/1079
6	h	0.21	0/811	0.38	0/1131
6	l	0.39	0/775	0.59	0/1079
7	I	0.23	0/852	0.47	0/1190
7	K	0.38	1/827 (0.1%)	0.95	2/1154 (0.2%)
7	i	0.23	0/852	0.48	1/1190 (0.1%)
7	k	0.32	0/827	0.45	0/1154
8	O	0.23	0/1799	0.46	0/2491
8	o	0.23	0/1799	0.46	0/2491
9	N	0.21	0/2138	0.37	0/2978
9	n	0.21	0/2138	0.37	0/2978
All	All	0.26	1/92558 (0.0%)	0.43	3/128669 (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
1	A	0	1
4	F	0	1
4	M	0	1
4	f	0	1
4	m	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	415	SER	C-N	6.66	1.49	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	415	SER	CA-C-N	20.28	145.19	119.84
7	K	415	SER	C-N-CA	20.28	145.19	119.84
7	i	412	LEU	N-CA-C	-5.10	105.09	113.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1634	THR	Peptide
4	F	537	GLN	Peptide
4	M	537	GLN	Peptide
4	f	115	ILE	Peptide
4	m	537	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8339	0	3704	41	0
1	a	8268	0	3662	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7347	0	3233	16	0
2	b	7347	0	3233	14	0
3	C	3144	0	1401	8	0
3	E	3105	0	1386	37	0
3	c	3144	0	1401	15	0
3	e	3105	0	1386	30	0
4	D	5524	0	2437	30	0
4	F	5417	0	2406	27	0
4	M	4296	0	1901	2	0
4	d	5563	0	2457	28	0
4	f	5432	0	2415	28	0
4	m	4296	0	1901	3	0
5	G	1063	0	456	4	0
5	J	963	0	410	4	0
5	g	1063	0	456	3	0
5	j	963	0	410	6	0
6	H	813	0	351	0	0
6	L	778	0	333	2	0
6	h	813	0	351	0	0
6	l	778	0	333	2	0
7	I	853	0	387	2	0
7	K	829	0	375	6	0
7	i	853	0	387	1	0
7	k	829	0	375	1	0
8	O	1805	0	810	15	0
8	o	1805	0	810	14	0
9	N	2143	0	953	7	0
9	n	2143	0	953	4	0
All	All	92821	0	41073	383	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 3.

All (383) 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)
4:D:51:PRO:HA	4:D:382:VAL:O	1.68	0.93
4:d:51:PRO:HA	4:d:382:VAL:O	1.73	0.87
4:F:537:GLN:O	4:F:539:ASN:N	2.16	0.79
3:e:494:ALA:O	3:e:498:PHE:N	2.17	0.78
1:A:1634:THR:O	1:A:1636:GLN:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:171:ILE:O	4:D:199:LEU:N	2.19	0.76
4:d:273:ILE:HA	4:d:289:SER:HA	1.70	0.73
1:A:1021:GLY:N	1:A:1025:CYS:O	2.14	0.73
2:b:1293:GLY:O	2:b:1297:GLN:N	2.23	0.71
4:F:51:PRO:HA	4:F:382:VAL:O	1.90	0.71
8:o:2:CYS:O	8:o:384:ASP:N	2.23	0.71
8:O:2:CYS:O	8:O:384:ASP:N	2.23	0.70
2:B:1293:GLY:O	2:B:1297:GLN:N	2.23	0.70
1:a:1634:THR:O	1:a:1636:GLN:N	2.27	0.68
4:m:537:GLN:O	4:m:539:ASN:N	2.27	0.68
4:M:537:GLN:O	4:M:539:ASN:N	2.27	0.68
1:a:1333:VAL:O	1:a:1336:ALA:HB3	1.94	0.68
1:A:1331:PRO:O	1:A:1334:ALA:HB3	1.94	0.68
5:G:186:ASN:HA	5:G:350:LEU:HA	1.76	0.67
1:a:863:LEU:O	1:a:867:SER:CB	2.43	0.67
3:E:618:GLU:O	3:E:621:GLY:N	2.28	0.65
1:a:1021:GLY:N	1:a:1025:CYS:O	2.23	0.65
4:f:273:ILE:HA	4:f:289:SER:HA	1.77	0.65
3:E:584:LEU:HA	3:E:598:ALA:HB3	1.78	0.64
6:L:466:ASP:HA	7:K:387:PHE:CB	2.28	0.64
4:d:563:ALA:O	4:d:566:ALA:HB3	1.98	0.63
3:C:728:VAL:HA	3:C:796:PHE:HA	1.81	0.62
4:F:233:GLU:O	4:F:245:CYS:HA	2.00	0.62
6:L:462:ALA:HB1	7:K:384:VAL:CB	2.29	0.62
1:A:263:SER:HA	1:A:372:ALA:HA	1.81	0.62
4:D:1039:TRP:O	4:D:1043:ALA:N	2.26	0.61
7:I:407:THR:O	7:I:411:THR:N	2.34	0.61
4:f:412:LEU:O	4:f:427:CYS:HA	2.01	0.61
3:c:728:VAL:HA	3:c:796:PHE:HA	1.82	0.60
4:d:537:GLN:O	4:d:539:ASN:N	2.34	0.60
8:O:261:GLY:HA3	9:N:629:TYR:CB	2.32	0.60
5:G:175:PHE:O	5:G:177:GLY:N	2.35	0.60
1:A:1218:ASN:N	1:A:1222:GLN:O	2.31	0.59
8:o:141:GLU:O	8:o:145:ALA:N	2.33	0.59
1:A:1271:LEU:O	1:A:1274:LEU:N	2.34	0.59
4:D:546:LEU:HA	4:D:549:ALA:HB3	1.84	0.59
4:F:983:SER:HA	4:F:1010:ASN:O	2.03	0.59
3:E:410:LYS:O	3:E:413:ASP:N	2.35	0.58
3:e:34:GLN:CB	6:l:504:ASN:HA	2.33	0.58
4:D:537:GLN:O	4:D:539:ASN:N	2.37	0.58
4:D:52:THR:O	4:D:383:HIS:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:GLU:O	1:A:1293:THR:CB	2.52	0.57
4:d:716:ASP:O	4:d:719:SER:N	2.34	0.57
1:A:1391:GLY:O	1:A:1394:SER:N	2.33	0.57
3:c:444:GLN:O	3:c:449:TYR:N	2.29	0.57
7:K:410:ASN:C	7:K:412:LEU:H	2.13	0.56
4:f:917:TYR:O	4:f:922:PHE:N	2.35	0.56
3:E:443:LYS:O	3:E:447:GLU:N	2.30	0.56
3:e:97:ASP:O	3:e:101:PHE:N	2.31	0.56
8:o:300:SER:N	8:o:305:LYS:O	2.38	0.56
4:D:78:SER:H	4:D:506:TYR:H	1.52	0.56
8:O:300:SER:N	8:O:305:LYS:O	2.38	0.56
1:A:836:LYS:O	1:A:839:LEU:N	2.38	0.56
4:F:1039:TRP:O	4:F:1043:ALA:N	2.37	0.55
4:f:1064:MET:O	4:f:1068:ASP:N	2.40	0.55
3:C:725:GLN:N	3:C:792:ALA:HB1	2.22	0.55
4:D:425:LEU:O	4:D:445:THR:HA	2.07	0.55
4:d:669:GLY:O	4:d:672:TRP:N	2.28	0.55
2:b:59:LYS:O	2:b:63:ASN:N	2.40	0.55
4:f:1040:LEU:HA	4:f:1043:ALA:HB3	1.89	0.55
4:F:1202:ILE:O	4:F:1205:CYS:N	2.40	0.55
1:a:1562:VAL:O	1:a:1565:SER:N	2.40	0.55
1:a:59:LYS:HA	1:a:103:ILE:C	2.32	0.54
4:d:353:LEU:HA	4:d:362:PHE:O	2.07	0.54
2:b:493:TRP:O	2:b:518:LEU:HA	2.08	0.54
4:f:537:GLN:O	4:f:539:ASN:N	2.40	0.54
2:B:493:TRP:O	2:B:518:LEU:HA	2.08	0.54
2:b:405:GLU:O	2:b:409:GLN:N	2.40	0.53
3:E:647:LEU:O	3:E:650:VAL:N	2.41	0.53
4:f:549:ALA:HA	4:f:560:SER:HA	1.89	0.53
2:B:262:VAL:O	2:B:266:GLY:N	2.38	0.53
1:a:1495:ALA:O	1:a:1498:LEU:N	2.41	0.53
4:d:361:ARG:O	4:d:385:ARG:N	2.31	0.53
1:a:258:VAL:HA	1:a:264:LEU:HA	1.90	0.53
1:a:1346:GLN:O	1:a:1350:THR:N	2.42	0.53
3:e:264:GLU:CB	3:e:330:GLY:HA3	2.38	0.53
1:A:1687:VAL:O	1:A:1690:GLU:N	2.39	0.53
8:o:407:CYS:O	8:o:416:ALA:N	2.38	0.53
2:b:1111:ALA:O	2:b:1116:LEU:N	2.34	0.52
4:d:52:THR:O	4:d:383:HIS:HA	2.09	0.52
8:O:407:CYS:O	8:O:416:ALA:N	2.38	0.52
2:b:263:GLU:O	2:b:267:TYR:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:701:ASP:O	3:c:705:ALA:CB	2.56	0.52
4:F:287:THR:O	4:F:294:ILE:HA	2.10	0.52
9:n:555:SER:CB	9:n:627:ALA:HB1	2.40	0.52
2:B:59:LYS:O	2:B:63:ASN:N	2.40	0.52
3:e:587:LYS:O	3:e:595:LYS:N	2.43	0.52
4:d:450:GLY:HA3	4:d:499:ALA:HB3	1.92	0.52
1:A:1634:THR:C	1:A:1636:GLN:H	2.16	0.52
2:B:263:GLU:O	2:B:267:TYR:N	2.38	0.52
1:A:57:PRO:O	1:A:103:ILE:HA	2.10	0.52
2:B:405:GLU:O	2:B:409:GLN:N	2.40	0.52
3:E:560:ASP:N	3:E:564:GLU:O	2.31	0.51
3:c:589:GLU:N	3:c:593:SER:O	2.31	0.51
4:f:1068:ASP:C	4:f:1070:ASN:H	2.18	0.51
4:f:1202:ILE:O	4:f:1205:CYS:N	2.43	0.51
8:o:318:TRP:HA	8:o:324:THR:O	2.11	0.51
3:c:481:PHE:HA	3:c:487:ARG:HA	1.93	0.51
9:N:555:SER:CB	9:N:627:ALA:HB1	2.40	0.51
1:a:1824:ASN:O	1:a:1827:THR:N	2.44	0.51
2:b:1734:VAL:O	2:b:1738:GLN:N	2.44	0.51
5:J:175:PHE:O	5:J:177:GLY:N	2.42	0.51
2:B:1734:VAL:O	2:B:1738:GLN:N	2.44	0.51
8:O:405:SER:O	8:O:418:LEU:N	2.39	0.51
4:d:718:TYR:O	4:d:721:PHE:N	2.44	0.51
8:O:141:GLU:O	8:O:145:ALA:N	2.33	0.51
3:e:636:PRO:O	3:e:639:VAL:N	2.43	0.50
4:F:539:ASN:HA	4:F:655:GLY:O	2.12	0.50
3:E:674:ARG:O	3:E:677:SER:N	2.44	0.50
4:d:111:ALA:O	4:d:121:MET:HA	2.12	0.50
3:e:545:PRO:O	3:e:548:ALA:N	2.45	0.50
8:O:318:TRP:HA	8:O:324:THR:O	2.11	0.50
1:A:156:LYS:H	1:A:238:GLN:HA	1.77	0.50
4:D:450:GLY:HA3	4:D:499:ALA:HB3	1.93	0.50
4:d:83:VAL:O	4:d:501:GLY:HA3	2.12	0.50
8:o:407:CYS:N	8:o:416:ALA:O	2.43	0.50
4:F:171:ILE:O	4:F:199:LEU:N	2.44	0.49
1:A:1657:ALA:O	1:A:1660:ARG:N	2.45	0.49
4:F:273:ILE:HA	4:F:289:SER:HA	1.95	0.49
4:d:676:VAL:N	4:d:818:THR:O	2.35	0.49
8:o:272:ALA:HA	8:o:286:LEU:O	2.13	0.49
3:E:472:GLN:O	3:E:475:ALA:N	2.46	0.49
4:M:51:PRO:HA	4:M:382:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:879:LEU:O	1:a:882:GLY:N	2.38	0.49
1:A:1123:ILE:O	1:A:1126:LEU:N	2.45	0.49
4:f:220:ILE:O	4:f:231:GLU:HA	2.13	0.49
4:m:51:PRO:HA	4:m:382:VAL:O	2.13	0.49
3:E:569:ARG:O	3:E:572:SER:N	2.46	0.48
4:f:674:GLY:O	4:f:820:PHE:N	2.37	0.48
4:D:790:ALA:O	4:D:793:LYS:N	2.47	0.48
4:F:116:ASP:O	4:F:139:THR:HA	2.13	0.48
1:a:57:PRO:O	1:a:103:ILE:HA	2.12	0.48
2:B:325:ALA:O	2:B:329:LEU:N	2.36	0.48
3:e:278:ASN:O	3:e:281:GLN:N	2.40	0.48
3:e:415:LEU:O	3:e:416:TRP:C	2.56	0.48
8:O:272:ALA:HA	8:O:286:LEU:O	2.13	0.48
8:o:405:SER:O	8:o:418:LEU:N	2.39	0.48
9:n:15:ALA:O	9:n:19:ALA:HB2	2.13	0.48
4:F:533:PHE:HA	4:F:541:ALA:HB2	1.95	0.48
9:N:15:ALA:O	9:N:19:ALA:HB2	2.13	0.48
2:b:1316:SER:O	2:b:1320:LYS:N	2.46	0.48
8:O:407:CYS:N	8:O:416:ALA:O	2.43	0.48
3:E:376:TYR:O	3:E:381:ARG:N	2.42	0.48
1:a:1331:PRO:O	1:a:1334:ALA:HB3	2.14	0.48
1:a:1568:GLY:O	1:a:1571:GLU:N	2.47	0.48
2:B:1316:SER:O	2:B:1320:LYS:N	2.46	0.47
3:c:629:LEU:O	3:c:633:ALA:N	2.42	0.47
3:E:415:LEU:O	3:E:416:TRP:C	2.57	0.47
2:b:262:VAL:O	2:b:266:GLY:N	2.38	0.47
1:A:1140:LEU:HA	1:A:1179:LYS:CB	2.45	0.47
3:e:584:LEU:HA	3:e:598:ALA:HB3	1.96	0.47
4:f:539:ASN:HA	4:f:655:GLY:O	2.15	0.47
1:A:1283:SER:O	1:A:1284:TRP:C	2.57	0.47
1:A:1495:ALA:O	1:A:1498:LEU:N	2.47	0.47
4:D:563:ALA:O	4:D:566:ALA:HB3	2.14	0.47
1:a:508:LEU:HA	1:a:596:ALA:CB	2.45	0.47
1:a:1215:GLU:HA	1:a:1224:VAL:O	2.13	0.47
1:a:1616:ARG:O	1:a:1618:ILE:N	2.48	0.47
3:c:497:LEU:O	3:c:501:LYS:N	2.48	0.47
3:e:722:PRO:CB	3:e:728:VAL:HA	2.45	0.47
4:f:1136:GLU:O	4:f:1139:HIS:N	2.48	0.47
2:b:325:ALA:O	2:b:329:LEU:N	2.36	0.47
3:c:252:GLN:HA	3:c:471:ALA:HB2	1.96	0.47
3:e:443:LYS:O	3:e:447:GLU:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:408:TRP:HA	8:O:415:LEU:HA	1.97	0.47
1:a:115:GLY:O	1:a:119:GLN:N	2.47	0.46
1:a:1610:ALA:O	1:a:1613:GLU:N	2.48	0.46
8:o:408:TRP:HA	8:o:415:LEU:HA	1.97	0.46
4:D:38:ASP:O	4:D:42:LEU:N	2.45	0.46
4:D:705:LEU:O	4:D:708:LEU:N	2.48	0.46
3:e:638:LYS:O	3:e:639:VAL:C	2.56	0.46
1:A:1337:VAL:O	1:A:1338:PHE:C	2.56	0.46
5:J:173:GLN:HA	5:J:176:TRP:CB	2.45	0.46
1:a:1337:VAL:O	1:a:1338:PHE:C	2.59	0.46
3:E:97:ASP:O	3:E:101:PHE:N	2.41	0.46
4:F:355:VAL:HA	4:F:360:VAL:O	2.16	0.46
5:j:346:ASP:O	5:j:350:LEU:N	2.48	0.46
2:b:1418:VAL:O	2:b:1422:GLN:N	2.49	0.46
2:B:1418:VAL:O	2:B:1422:GLN:N	2.49	0.46
7:K:410:ASN:C	7:K:412:LEU:N	2.74	0.46
7:K:408:GLN:HA	7:K:411:THR:CB	2.46	0.46
1:A:1405:PHE:O	1:A:1408:LYS:N	2.49	0.46
3:E:413:ASP:O	3:E:414:TYR:C	2.59	0.46
3:e:668:ALA:O	3:e:669:LEU:C	2.59	0.46
2:B:1111:ALA:O	2:B:1116:LEU:N	2.34	0.46
9:n:12:TRP:O	9:n:15:ALA:HB3	2.16	0.46
4:D:412:LEU:O	4:D:427:CYS:HA	2.16	0.45
1:a:996:ALA:HB1	1:a:997:PRO:HA	1.99	0.45
4:F:574:ALA:HB2	4:F:771:GLU:CB	2.46	0.45
4:F:1056:PHE:O	4:F:1060:HIS:N	2.33	0.45
1:a:371:GLU:O	1:a:375:GLY:HA3	2.15	0.45
3:c:701:ASP:O	3:c:705:ALA:HB3	2.16	0.45
4:d:979:LEU:O	4:d:1013:ALA:HB1	2.16	0.45
1:A:1339:THR:O	1:A:1340:LEU:C	2.60	0.45
4:D:554:ALA:O	4:D:556:ASP:N	2.49	0.45
8:o:339:CYS:O	8:o:348:LEU:N	2.38	0.45
3:c:584:LEU:HA	3:c:598:ALA:HB3	1.99	0.45
3:e:640:LEU:O	3:e:641:GLU:C	2.59	0.45
3:e:686:ILE:O	3:e:687:ASN:C	2.59	0.45
3:E:587:LYS:O	3:E:595:LYS:N	2.47	0.45
9:N:12:TRP:O	9:N:15:ALA:HB3	2.16	0.45
4:F:983:SER:HA	4:F:1010:ASN:HA	1.99	0.45
1:a:1480:VAL:O	1:a:1481:CYS:C	2.58	0.45
4:f:537:GLN:O	4:f:540:GLN:N	2.48	0.45
1:A:521:PRO:HA	1:A:607:TRP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:273:ILE:HA	4:D:289:SER:HA	1.98	0.45
3:e:355:GLU:HA	3:e:359:ASN:O	2.17	0.45
7:i:407:THR:O	7:i:411:THR:N	2.50	0.45
1:A:1470:GLU:O	1:A:1473:GLY:N	2.41	0.45
4:F:1089:SER:O	4:F:1092:ALA:HB3	2.17	0.45
4:f:550:CYS:O	4:f:710:GLY:HA3	2.18	0.44
5:j:347:PRO:HA	5:j:350:LEU:O	2.16	0.44
3:E:668:ALA:O	3:E:669:LEU:C	2.57	0.44
3:e:636:PRO:O	3:e:637:ASP:C	2.59	0.44
8:O:43:VAL:O	8:O:45:ILE:N	2.50	0.44
3:C:481:PHE:HA	3:C:487:ARG:HA	1.99	0.44
3:E:672:ALA:O	3:E:673:GLU:C	2.61	0.44
3:E:686:ILE:O	3:E:687:ASN:C	2.60	0.44
3:e:724:SER:O	3:e:725:GLN:C	2.59	0.44
4:D:705:LEU:O	4:D:706:LYS:C	2.61	0.44
5:j:175:PHE:O	5:j:177:GLY:N	2.51	0.44
1:a:508:LEU:HA	1:a:596:ALA:HB3	1.98	0.44
1:a:1105:SER:O	1:a:1106:ALA:C	2.60	0.44
1:a:1281:LEU:O	1:a:1282:GLU:C	2.61	0.44
4:d:681:THR:HA	4:d:690:THR:HA	2.00	0.44
1:A:1007:GLU:H	1:A:1015:THR:CB	2.31	0.44
4:F:53:ILE:HA	4:F:384:VAL:O	2.17	0.44
3:c:493:VAL:O	3:c:496:ALA:HB3	2.18	0.44
3:e:623:PHE:O	3:e:626:ALA:N	2.51	0.44
3:e:727:SER:O	3:e:728:VAL:C	2.60	0.44
4:f:1283:THR:O	4:f:1284:TYR:C	2.60	0.44
4:D:224:GLY:O	4:D:227:GLY:N	2.46	0.44
3:E:629:LEU:O	3:E:632:LEU:N	2.51	0.44
9:N:305:PHE:O	9:N:309:SER:N	2.51	0.44
4:f:979:LEU:O	4:f:1013:ALA:HB1	2.18	0.44
5:g:356:ILE:H	5:g:360:GLU:CB	2.31	0.44
4:D:273:ILE:HA	4:D:288:ARG:O	2.18	0.43
2:b:518:LEU:O	2:b:532:TRP:HA	2.18	0.43
1:A:508:LEU:HA	1:A:596:ALA:HB3	1.99	0.43
1:a:1283:SER:O	1:a:1284:TRP:C	2.59	0.43
2:b:440:PHE:O	2:b:474:THR:N	2.45	0.43
6:l:466:ASP:HA	7:k:387:PHE:CB	2.48	0.43
8:O:341:SER:N	8:O:346:ARG:O	2.49	0.43
1:A:1333:VAL:O	1:A:1336:ALA:HB3	2.18	0.43
4:d:123:ASN:O	4:d:127:GLY:N	2.46	0.43
1:a:359:ILE:O	1:a:363:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1310:TRP:O	4:d:1313:ARG:N	2.52	0.43
8:O:339:CYS:O	8:O:348:LEU:N	2.38	0.43
9:n:305:PHE:O	9:n:309:SER:N	2.51	0.43
7:K:313:ALA:O	7:K:316:LYS:N	2.51	0.43
3:c:190:TYR:HA	3:c:550:GLN:O	2.18	0.43
4:d:482:VAL:O	4:d:486:GLN:N	2.52	0.43
4:f:1118:ALA:O	4:f:1119:ILE:C	2.62	0.43
3:E:638:LYS:O	3:E:639:VAL:C	2.61	0.43
1:A:14:TRP:HA	1:A:138:GLY:HA2	2.00	0.43
2:B:518:LEU:O	2:B:532:TRP:HA	2.18	0.43
4:D:51:PRO:CA	4:D:382:VAL:O	2.55	0.43
3:E:530:ILE:O	3:E:531:ARG:C	2.62	0.43
3:e:219:LYS:O	3:e:220:ASN:C	2.62	0.43
3:e:528:ASN:O	3:e:532:LEU:N	2.47	0.43
5:g:175:PHE:O	5:g:177:GLY:N	2.51	0.43
1:A:1105:SER:O	1:A:1106:ALA:C	2.61	0.43
5:G:358:PHE:CB	7:I:303:GLN:HA	2.49	0.43
1:a:1614:ARG:O	1:a:1617:GLN:N	2.52	0.43
3:e:709:ASP:O	3:e:710:LEU:C	2.62	0.43
4:m:275:GLN:O	4:m:288:ARG:N	2.47	0.43
3:C:393:CYS:O	3:C:397:ARG:N	2.52	0.43
3:E:584:LEU:O	3:E:599:ILE:N	2.36	0.43
3:E:740:ASP:O	3:E:743:ARG:N	2.52	0.43
4:F:1136:GLU:O	4:F:1139:HIS:N	2.52	0.43
5:J:186:ASN:HA	5:J:350:LEU:HA	2.01	0.43
1:a:730:GLU:O	1:a:733:LEU:N	2.50	0.43
4:d:366:THR:HA	4:d:378:MET:O	2.19	0.43
3:C:252:GLN:HA	3:C:471:ALA:HB2	2.01	0.42
4:D:111:ALA:O	4:D:121:MET:HA	2.19	0.42
3:E:472:GLN:O	3:E:473:PHE:C	2.62	0.42
1:a:1892:CYS:O	1:a:1893:SER:C	2.62	0.42
3:E:688:SER:O	3:E:689:THR:C	2.62	0.42
4:F:979:LEU:O	4:F:1013:ALA:HB1	2.19	0.42
8:o:341:SER:N	8:o:346:ARG:O	2.49	0.42
1:A:460:TYR:HA	1:A:491:LEU:CB	2.49	0.42
4:D:82:ARG:HA	4:D:502:SER:O	2.19	0.42
5:g:157:LEU:O	5:g:160:ASP:N	2.52	0.42
3:E:505:LYS:HA	3:E:527:LEU:O	2.19	0.42
1:A:1475:ALA:O	1:A:1478:GLU:N	2.52	0.42
3:E:487:ARG:O	3:E:488:CYS:C	2.62	0.42
3:E:666:ASN:O	3:E:669:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:670:ASN:O	4:F:674:GLY:N	2.35	0.42
3:e:686:ILE:O	3:e:689:THR:N	2.53	0.42
3:E:670:ALA:O	3:E:671:ILE:C	2.62	0.42
1:a:1495:ALA:O	1:a:1496:LEU:C	2.62	0.42
8:O:387:GLU:HA	8:O:400:GLY:HA3	2.02	0.42
1:A:1271:LEU:O	1:A:1272:GLN:C	2.61	0.42
4:D:790:ALA:O	4:D:791:LEU:C	2.61	0.42
1:a:1343:HIS:O	1:a:1344:LEU:C	2.63	0.42
1:a:1499:LEU:O	1:a:1500:ASP:C	2.61	0.42
4:d:53:ILE:HA	4:d:384:VAL:O	2.20	0.42
4:f:670:ASN:O	4:f:674:GLY:N	2.53	0.42
1:a:833:PHE:O	1:a:834:PRO:C	2.62	0.42
1:A:882:GLY:O	1:A:890:ALA:HA	2.20	0.42
4:D:979:LEU:O	4:D:1014:GLY:N	2.53	0.42
4:D:556:ASP:O	4:D:557:ARG:C	2.62	0.41
3:E:410:LYS:O	3:E:411:THR:C	2.63	0.41
3:E:569:ARG:O	3:E:570:CYS:C	2.63	0.41
4:D:777:GLY:O	4:D:778:ILE:C	2.61	0.41
4:f:298:ASP:N	4:f:307:SER:O	2.45	0.41
4:f:1136:GLU:O	4:f:1137:PHE:C	2.62	0.41
8:o:43:VAL:O	8:o:45:ILE:N	2.50	0.41
1:A:535:GLY:HA2	1:A:553:ASP:CB	2.51	0.41
3:e:486:THR:O	3:e:487:ARG:C	2.63	0.41
1:A:1495:ALA:O	1:A:1496:LEU:C	2.63	0.41
2:B:50:LYS:O	2:B:84:ASP:N	2.47	0.41
4:F:819:THR:O	4:F:822:ASP:N	2.52	0.41
4:d:171:ILE:O	4:d:199:LEU:N	2.53	0.41
4:f:692:ILE:O	4:f:801:SER:HA	2.19	0.41
2:B:1059:LYS:O	2:B:1063:GLU:N	2.48	0.41
4:D:83:VAL:O	4:D:501:GLY:HA3	2.21	0.41
4:F:533:PHE:HA	4:F:541:ALA:CB	2.51	0.41
4:F:1115:ILE:O	4:F:1118:ALA:HB3	2.20	0.41
1:a:1638:LEU:O	1:a:1641:ALA:HB3	2.21	0.41
4:d:777:GLY:O	4:d:778:ILE:C	2.63	0.41
5:j:168:LYS:O	5:j:177:GLY:N	2.54	0.41
8:o:304:SER:O	8:o:320:THR:N	2.52	0.41
8:o:387:GLU:HA	8:o:400:GLY:HA3	2.01	0.41
3:C:728:VAL:CA	3:C:796:PHE:HA	2.50	0.41
4:F:1136:GLU:O	4:F:1137:PHE:C	2.62	0.41
3:c:726:ASP:C	3:c:728:VAL:N	2.78	0.41
3:e:219:LYS:O	3:e:222:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:PRO:O	2:B:608:MET:N	2.54	0.41
3:E:354:GLN:O	3:E:359:ASN:N	2.51	0.41
3:c:730:GLU:O	3:c:731:ARG:C	2.64	0.41
5:j:177:GLY:C	5:j:179:GLY:H	2.28	0.41
1:A:882:GLY:HA2	5:J:402:GLN:CB	2.51	0.41
1:A:1568:GLY:O	1:A:1571:GLU:N	2.54	0.41
3:C:405:SER:HA	3:C:408:ALA:O	2.21	0.41
3:E:666:ASN:O	3:E:667:MET:C	2.63	0.41
2:b:606:PRO:O	2:b:608:MET:N	2.54	0.41
4:d:784:LYS:O	4:d:787:GLN:N	2.54	0.41
4:f:983:SER:HA	4:f:1010:ASN:O	2.20	0.41
1:A:980:THR:O	1:A:981:LYS:C	2.63	0.41
1:A:1065:TYR:O	1:A:1068:CYS:N	2.53	0.41
3:C:289:GLY:O	3:C:293:LEU:N	2.37	0.41
4:D:558:GLU:O	4:D:559:VAL:C	2.64	0.41
3:E:285:GLY:O	9:N:568:GLY:HA3	2.21	0.41
3:E:475:ALA:O	3:E:476:ALA:C	2.64	0.41
1:a:1553:GLU:O	1:a:1554:SER:C	2.63	0.41
1:a:1828:TYR:O	1:a:1829:TYR:C	2.62	0.41
4:d:321:ALA:O	4:d:325:ALA:N	2.30	0.41
3:e:33:LEU:O	3:e:37:GLN:N	2.52	0.41
5:j:329:LEU:O	5:j:331:GLY:N	2.53	0.41
1:A:836:LYS:O	1:A:837:LYS:C	2.63	0.41
2:B:440:PHE:O	2:B:474:THR:N	2.45	0.41
4:D:974:ASP:O	4:D:977:GLN:N	2.54	0.41
3:E:547:GLU:O	3:E:548:ALA:C	2.64	0.41
4:F:208:TYR:O	4:F:224:GLY:HA2	2.21	0.41
4:f:819:THR:O	4:f:822:ASP:N	2.54	0.41
1:a:1824:ASN:O	1:a:1825:PHE:C	2.62	0.40
3:e:254:ALA:O	3:e:255:PHE:C	2.64	0.40
4:f:682:PHE:O	4:f:688:GLU:HA	2.21	0.40
3:e:487:ARG:O	3:e:488:CYS:C	2.64	0.40
4:f:355:VAL:HA	4:f:360:VAL:O	2.21	0.40
4:D:560:SER:O	4:D:561:SER:C	2.62	0.40
3:E:724:SER:O	3:E:725:GLN:C	2.64	0.40
4:F:298:ASP:N	4:F:307:SER:O	2.51	0.40
1:a:891:ASP:O	1:a:895:ASN:N	2.31	0.40
3:c:582:ASP:HA	3:c:586:GLY:O	2.20	0.40
9:N:544:ALA:HB1	9:N:620:LEU:CB	2.52	0.40
1:A:1971:GLY:O	1:A:1974:LEU:N	2.55	0.40
3:E:489:HIS:O	3:E:490:ALA:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1616:ARG:C	1:a:1618:ILE:N	2.78	0.40
4:f:297:TYR:HA	4:f:308:ARG:HA	2.03	0.40
4:f:1149:ARG:O	4:f:1150:ILE:C	2.64	0.40
1:A:1636:GLN:O	1:A:1638:LEU:N	2.54	0.40
5:G:167:ALA:HB1	5:G:174:ALA:HB3	2.02	0.40
4:d:40:SER:O	4:d:43:LEU:N	2.55	0.40
4:d:169:ILE:O	4:d:201:SER:HA	2.22	0.40
4:d:675:SER:HA	4:d:819:THR:HA	2.03	0.40
8:O:406:MET:HA	8:O:417:VAL:HA	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	1642/2011 (82%)	1523 (93%)	116 (7%)	3 (0%)	43	77
1	a	1625/2011 (81%)	1509 (93%)	114 (7%)	2 (0%)	48	82
2	B	1448/1739 (83%)	1406 (97%)	42 (3%)	0	100	100
2	b	1448/1739 (83%)	1407 (97%)	41 (3%)	0	100	100
3	C	613/820 (75%)	593 (97%)	20 (3%)	0	100	100
3	E	601/820 (73%)	542 (90%)	59 (10%)	0	100	100
3	c	613/820 (75%)	592 (97%)	21 (3%)	0	100	100
3	e	601/820 (73%)	547 (91%)	54 (9%)	0	100	100
4	D	1079/1388 (78%)	1020 (94%)	58 (5%)	1 (0%)	48	82
4	F	1058/1388 (76%)	1018 (96%)	39 (4%)	1 (0%)	48	82
4	M	853/1388 (62%)	823 (96%)	29 (3%)	1 (0%)	48	82
4	d	1087/1388 (78%)	1029 (95%)	56 (5%)	2 (0%)	43	77
4	f	1061/1388 (76%)	1014 (96%)	46 (4%)	1 (0%)	48	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	m	853/1388 (62%)	823 (96%)	29 (3%)	1 (0%)	48	82
5	G	207/535 (39%)	193 (93%)	14 (7%)	0	100	100
5	J	187/535 (35%)	178 (95%)	7 (4%)	2 (1%)	11	45
5	g	207/535 (39%)	192 (93%)	15 (7%)	0	100	100
5	j	187/535 (35%)	174 (93%)	12 (6%)	1 (0%)	24	62
6	H	159/547 (29%)	154 (97%)	5 (3%)	0	100	100
6	L	150/547 (27%)	150 (100%)	0	0	100	100
6	h	159/547 (29%)	153 (96%)	6 (4%)	0	100	100
6	l	150/547 (27%)	148 (99%)	2 (1%)	0	100	100
7	I	169/599 (28%)	162 (96%)	7 (4%)	0	100	100
7	K	162/599 (27%)	154 (95%)	6 (4%)	2 (1%)	10	42
7	i	169/599 (28%)	159 (94%)	10 (6%)	0	100	100
7	k	162/599 (27%)	156 (96%)	4 (2%)	2 (1%)	10	42
8	O	355/523 (68%)	339 (96%)	16 (4%)	0	100	100
8	o	355/523 (68%)	339 (96%)	16 (4%)	0	100	100
9	N	421/660 (64%)	412 (98%)	9 (2%)	0	100	100
9	n	421/660 (64%)	412 (98%)	9 (2%)	0	100	100
All	All	18202/28198 (65%)	17321 (95%)	862 (5%)	19 (0%)	49	82

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1635	ALA
1	a	1635	ALA
1	A	258	VAL
4	F	538	GLU
5	J	176	TRP
4	M	538	GLU
4	m	538	GLU
1	A	1128	ARG
4	D	538	GLU
7	K	411	THR
4	d	538	GLU
4	f	538	GLU
7	k	412	LEU
7	k	413	HIS

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Mol	Chain	Res	Type
7	K	416	PRO
1	a	1128	ARG
5	J	329	LEU
5	j	176	TRP
4	d	698	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

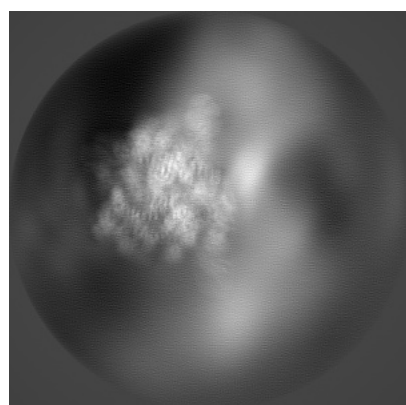
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32566. These allow visual inspection of the internal detail of the map and identification of artifacts.

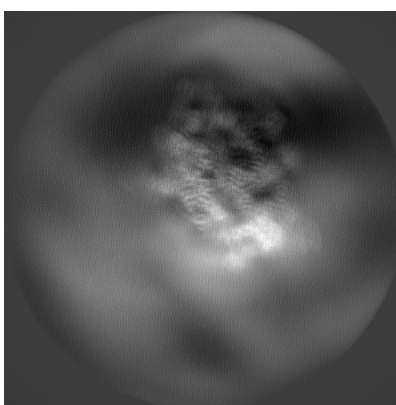
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

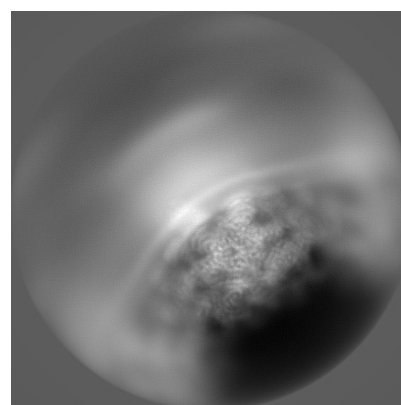
6.1.1 Primary map



X



Y

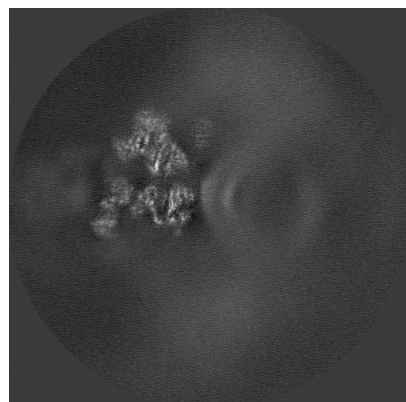


Z

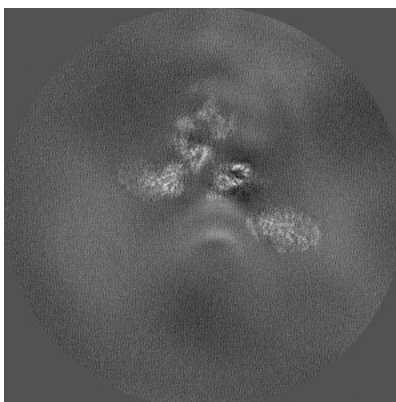
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

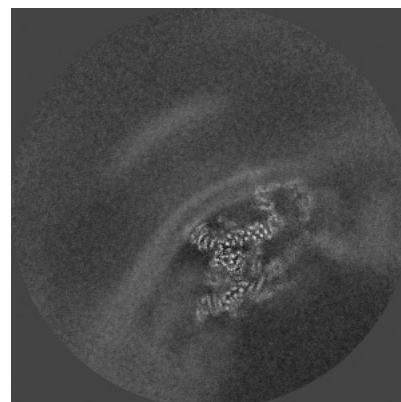
6.2.1 Primary map



X Index: 256



Y Index: 256

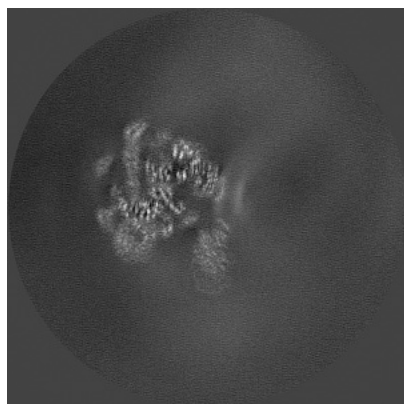


Z Index: 256

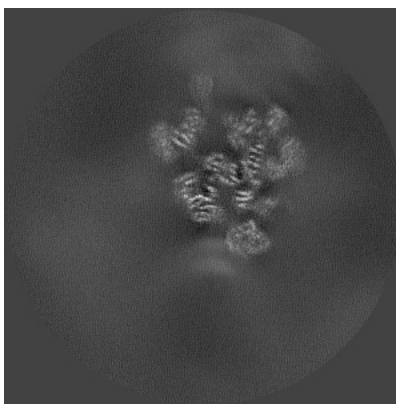
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

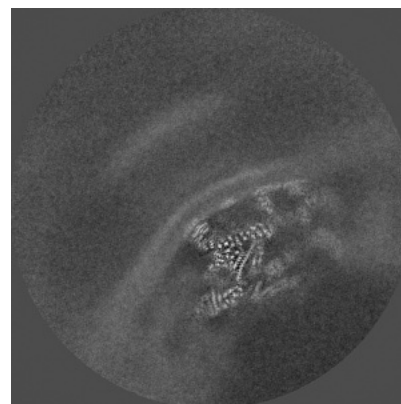
6.3.1 Primary map



X Index: 293



Y Index: 206

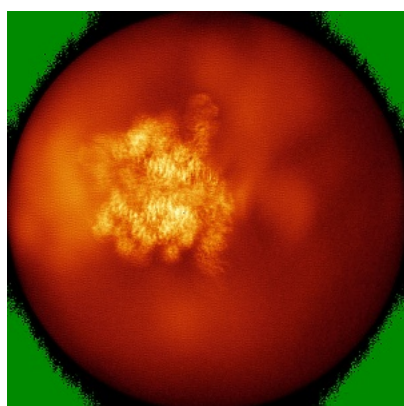


Z Index: 260

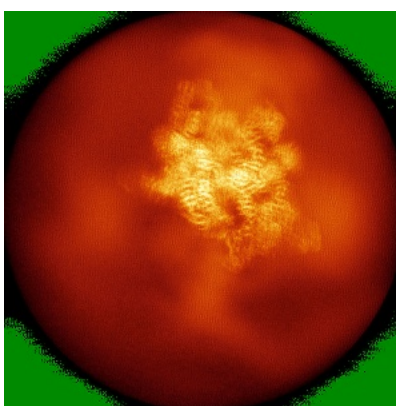
The images above show the largest variance slices of the map in three orthogonal directions.

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

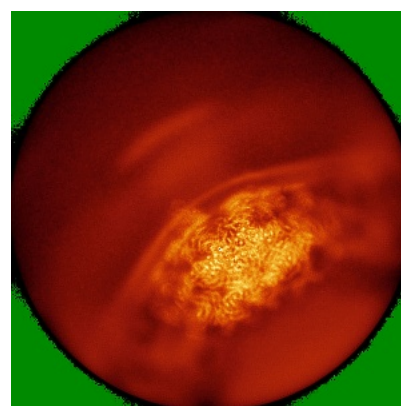
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

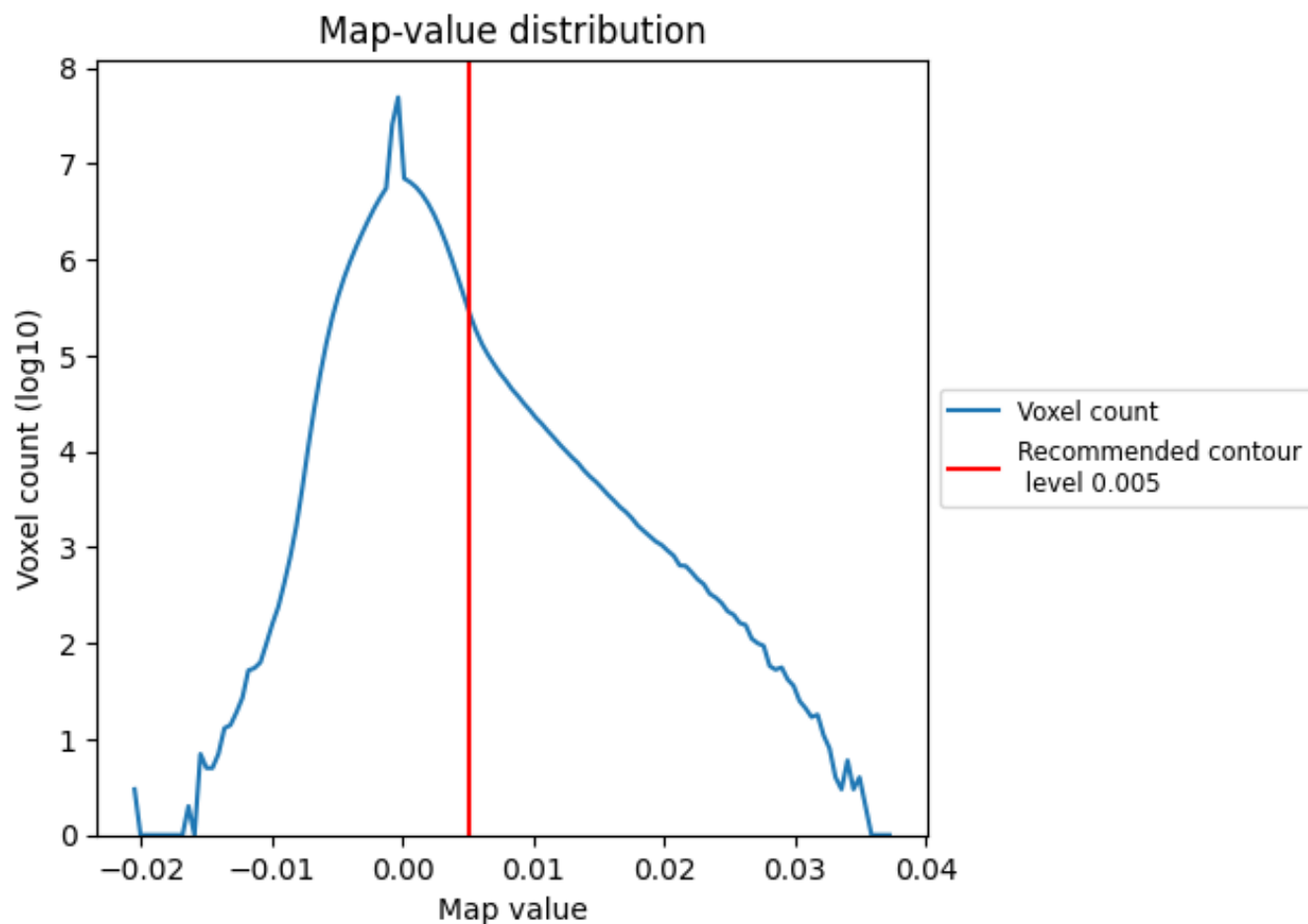
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

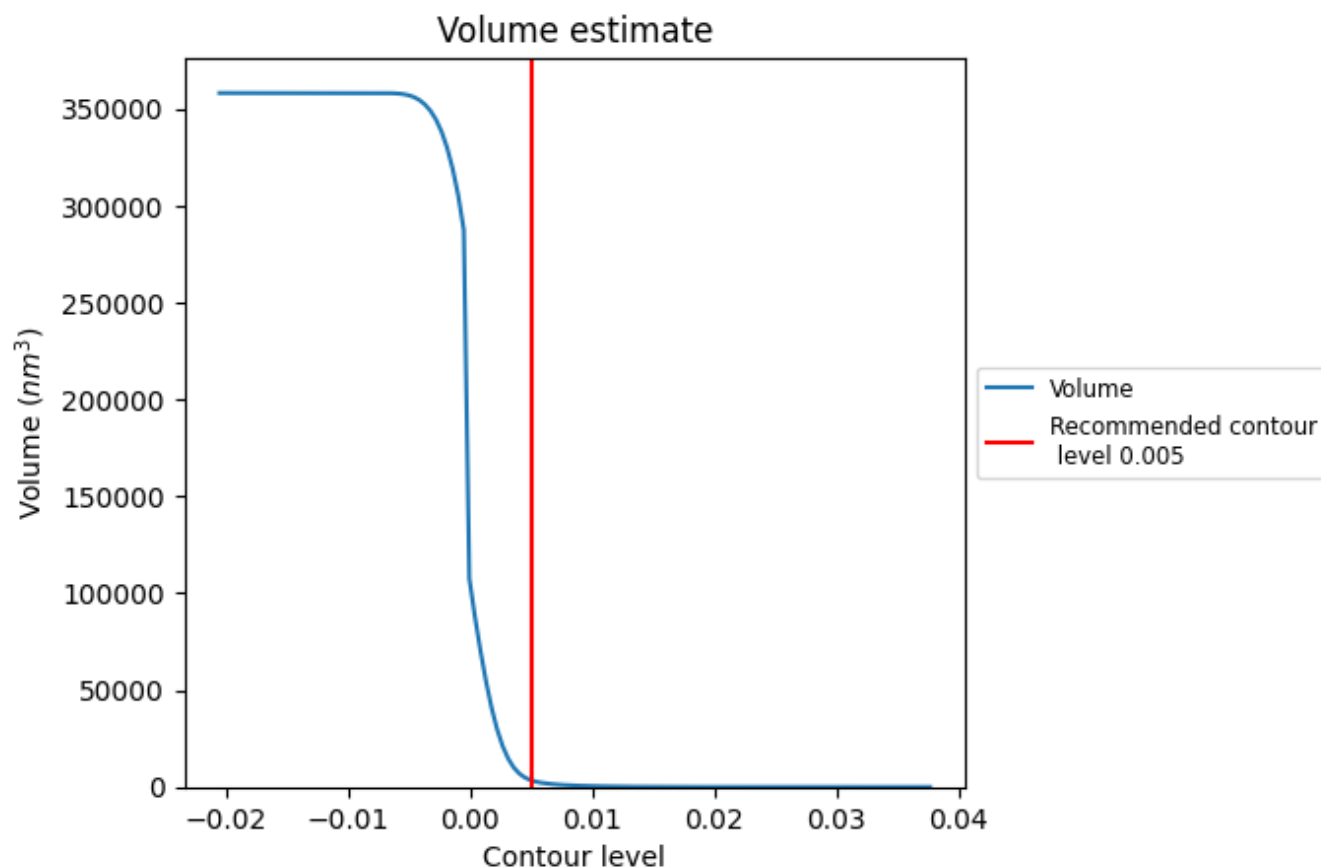
This section contains the results of statistical analysis of the map.

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.

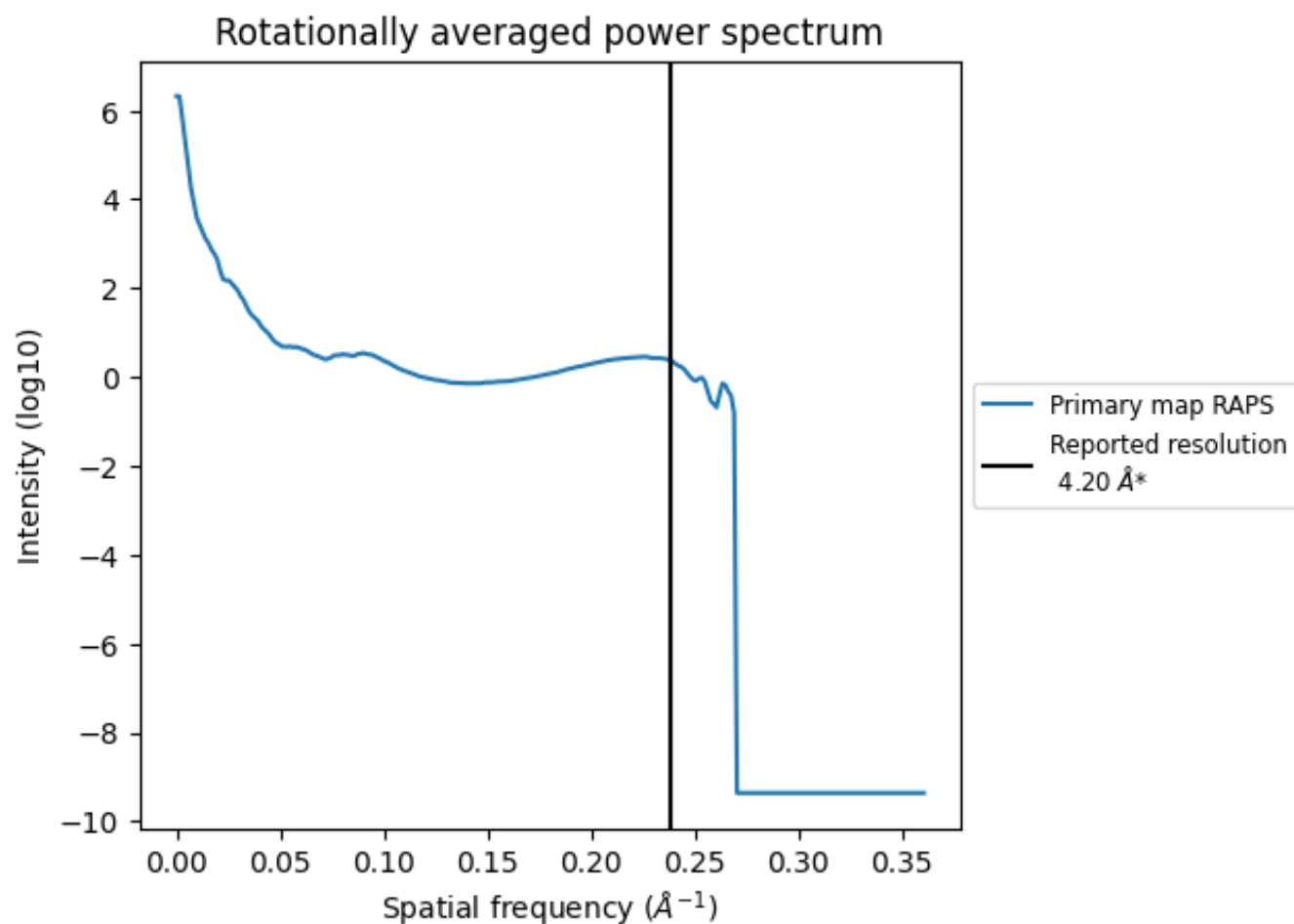
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3486 nm³; this corresponds to an approximate mass of 3149 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 0.238 Å⁻¹

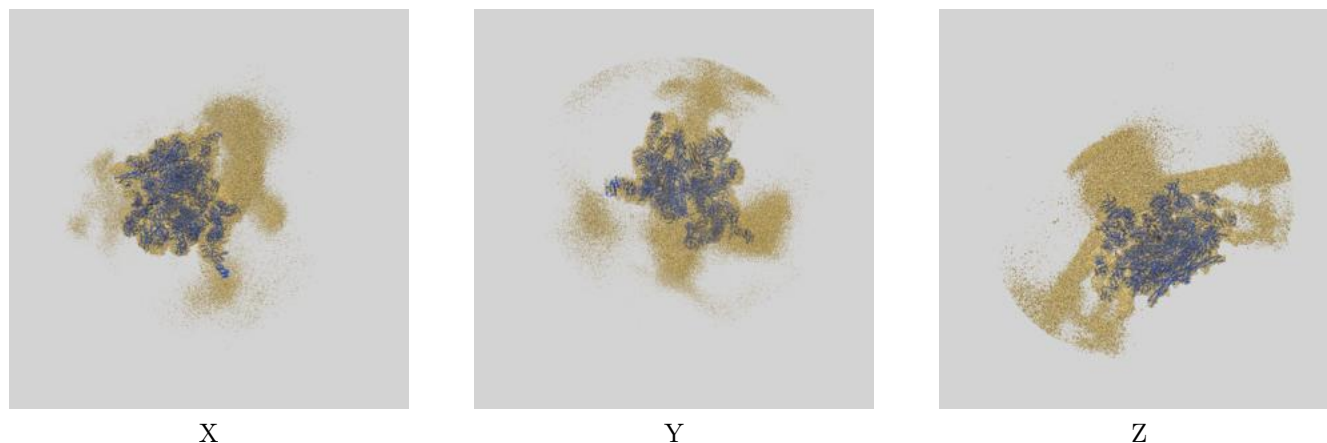
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

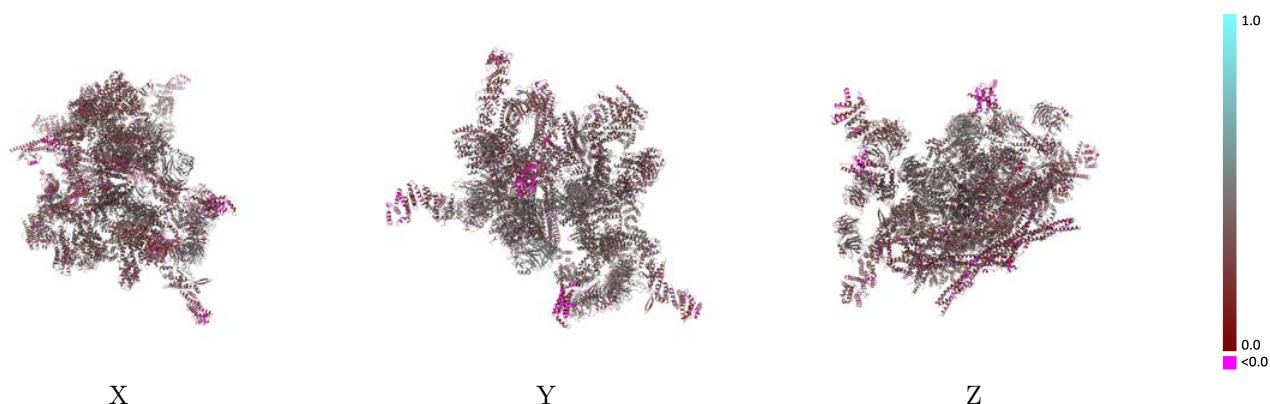
This section contains information regarding the fit between EMDB map EMD-32566 and PDB model 7WKK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



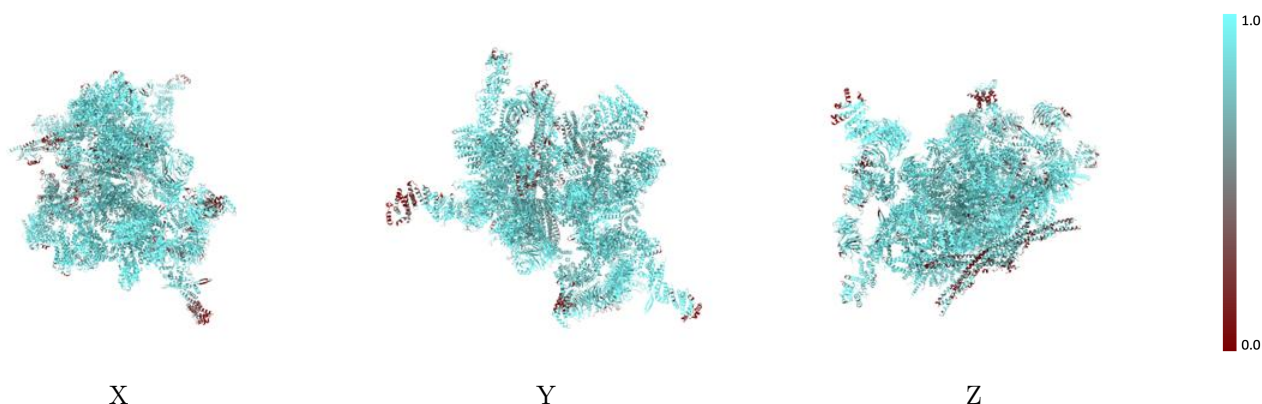
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



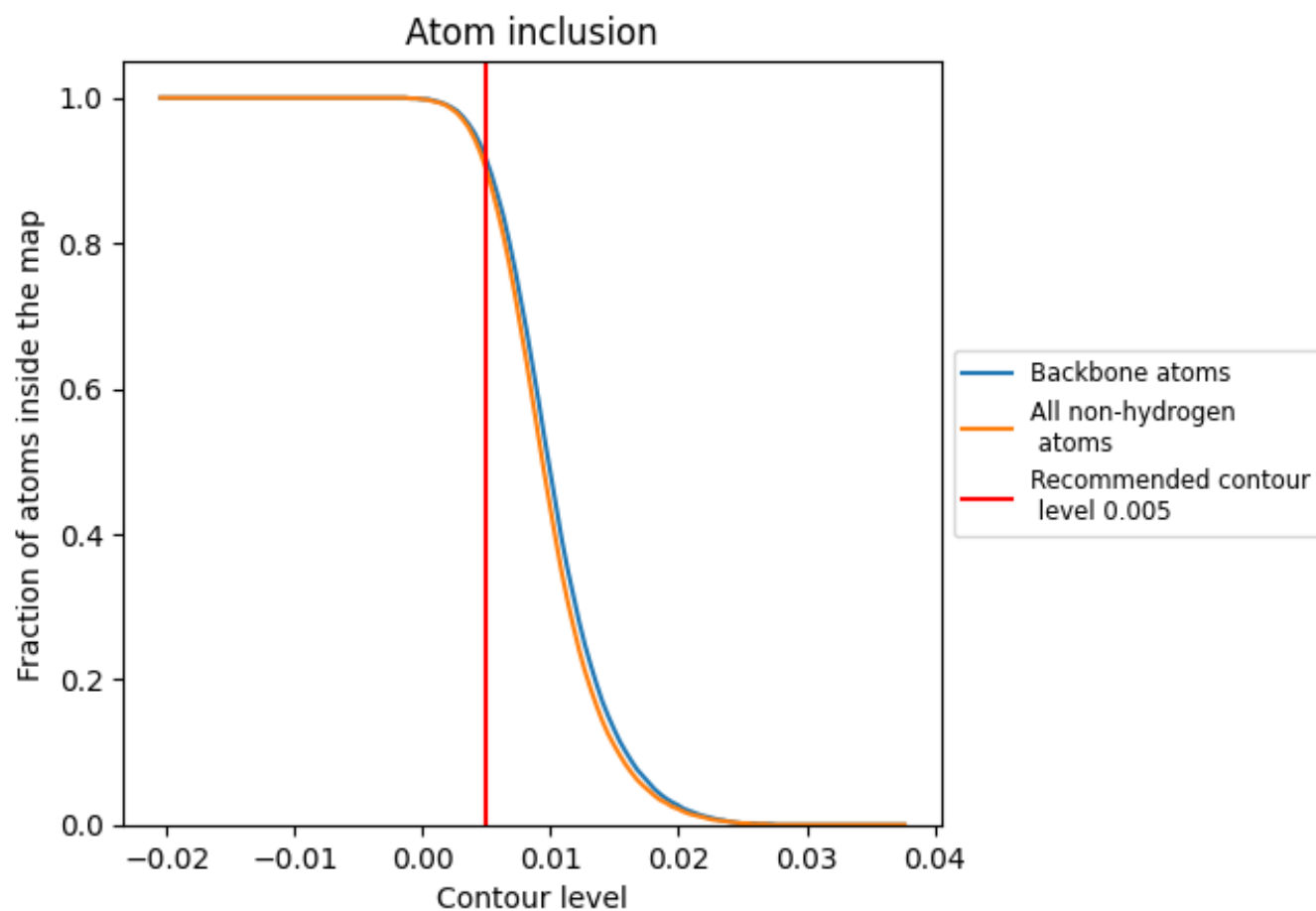
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.3490
A	 0.9400	 0.3610
B	 0.9650	 0.3500
C	 0.8980	 0.3010
D	 0.9710	 0.4130
E	 0.9760	 0.4020
F	 0.9220	 0.3760
G	 0.8070	 0.3160
H	 0.7170	 0.2640
I	 0.7690	 0.2870
J	 0.7300	 0.2680
K	 0.6790	 0.2380
L	 0.7200	 0.2520
M	 0.7910	 0.3620
N	 0.7640	 0.2400
O	 0.8340	 0.3690
a	 0.9270	 0.3590
b	 0.9640	 0.3420
c	 0.9170	 0.3040
d	 0.9540	 0.4020
e	 0.9720	 0.3950
f	 0.8950	 0.3660
g	 0.7290	 0.2720
h	 0.7470	 0.2870
i	 0.6920	 0.2760
j	 0.7590	 0.2820
k	 0.7370	 0.2500
l	 0.7760	 0.2530
m	 0.9230	 0.3720
n	 0.8090	 0.2360
o	 0.8260	 0.3550

