



Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 06:49 PM EDT

PDB ID : 7N6A
EMDB ID : EMD-24205
Title : Pre-fusion state 1 of EEEV with localized reconstruction
Authors : Chen, C.-L.; Kuhn, R.J.; Klose, T.
Deposited on : 2021-06-07
Resolution : 14.30 Å (reported)
Based on initial model : 6MX4

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

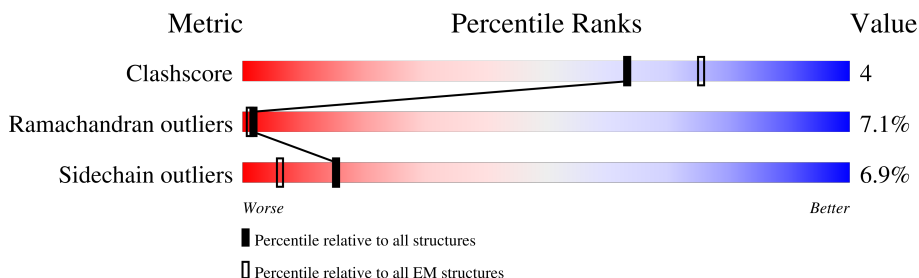
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.30 Å.

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







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

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

Mol	Chain	Length	Quality of chain
1	A	441	
1	C	441	
1	E	441	
1	G	441	
1	I	441	
1	K	441	
2	B	420	
2	D	420	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	420	
2	H	420	
2	J	420	
2	L	420	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 34962 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	C	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	E	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	G	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	I	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	K	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		

- Molecule 2 is a protein called Spike glycoprotein E2.

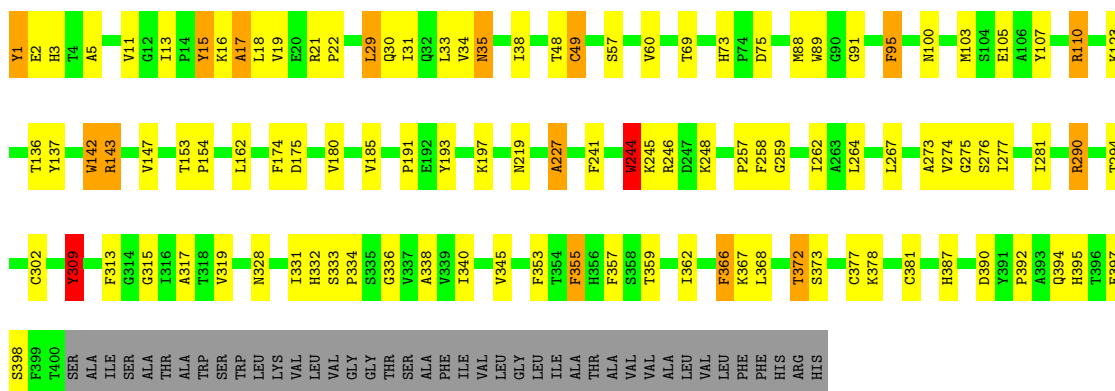
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	D	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	F	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	H	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	J	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		
2	L	351	Total	C	N	O	S	0	0
			2764	1734	510	504	16		

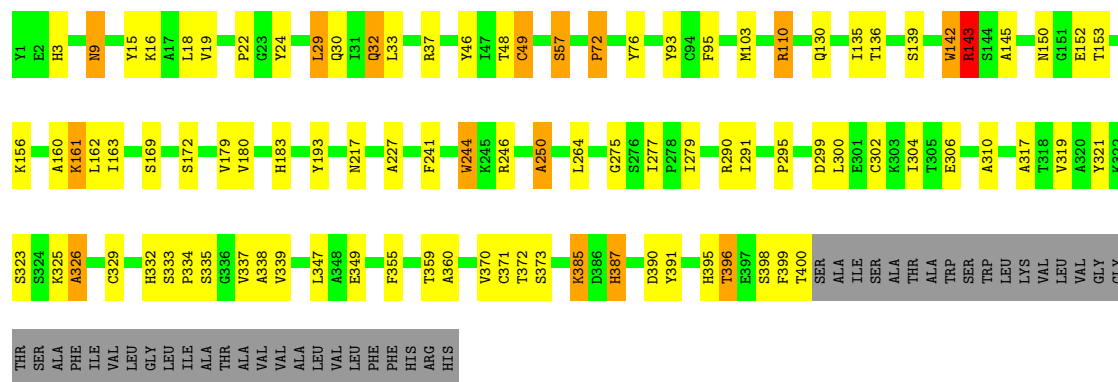
3 Residue-property plots [i](#)

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: Spike glycoprotein E1

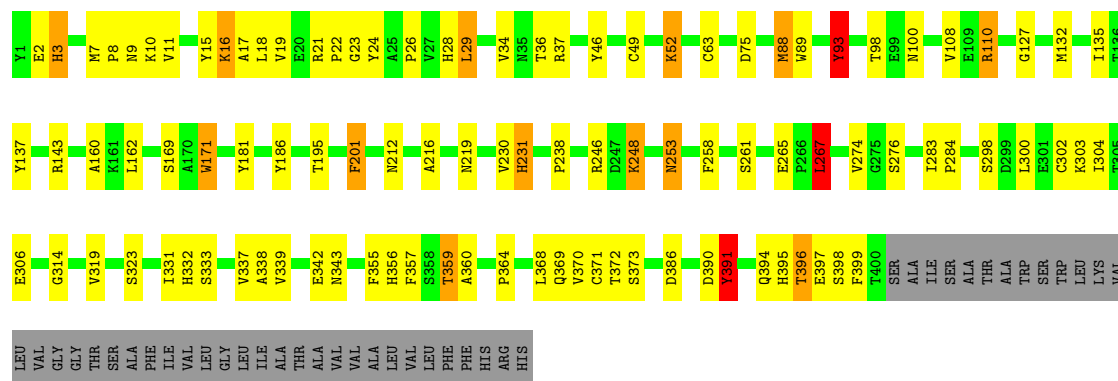
Chain A: 





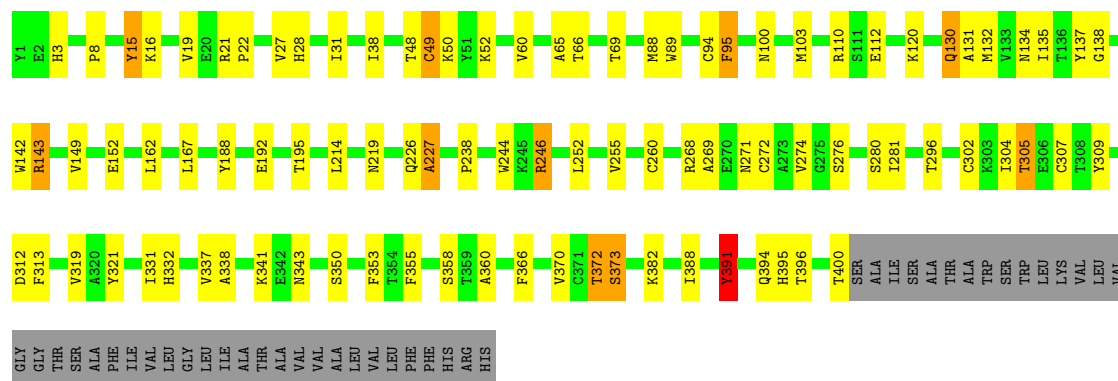
• Molecule 1: Spike glycoprotein E1

Chain G: 68% 20% 9%



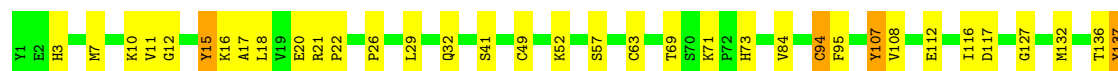
• Molecule 1: Spike glycoprotein E1

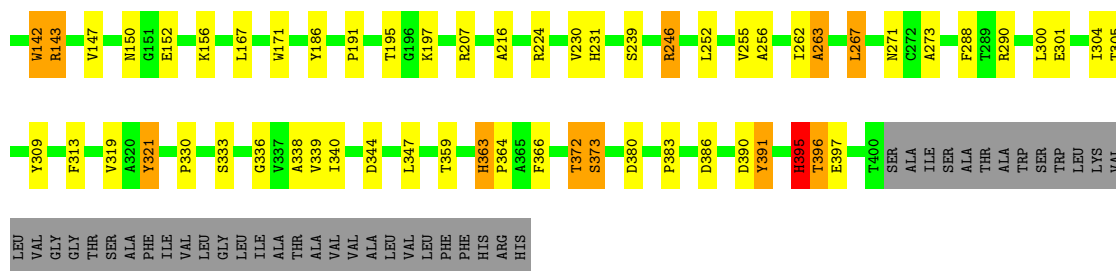
Chain I: 69% 19% 9%



• Molecule 1: Spike glycoprotein E1

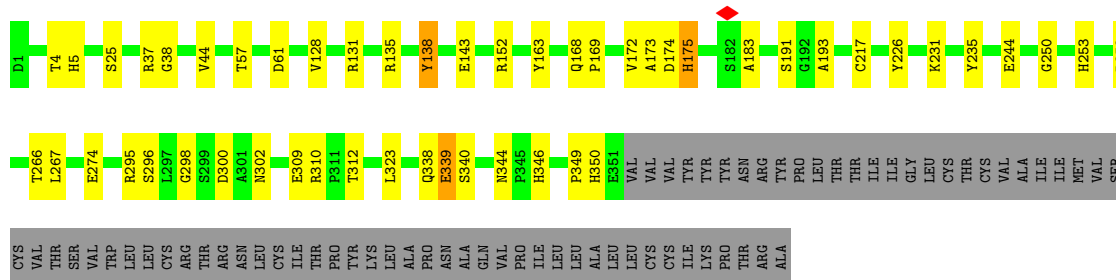
Chain K: 69% 18% 9%





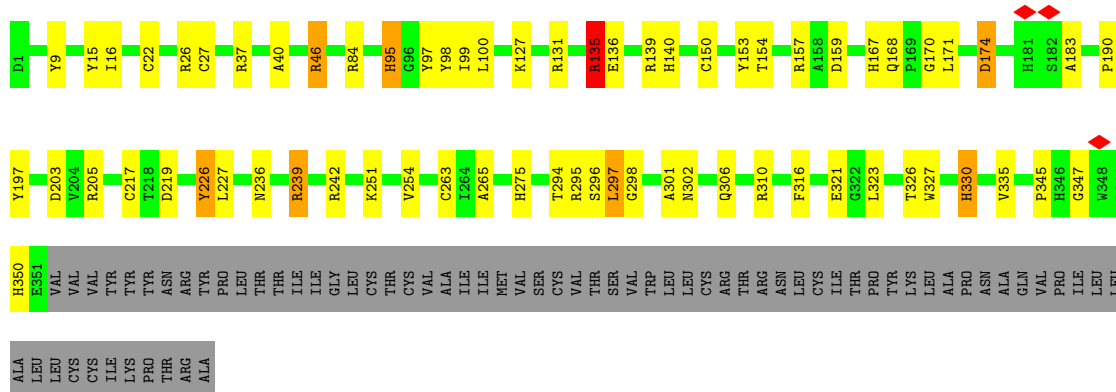
• Molecule 2: Spike glycoprotein E2

Chain B: 71% 11% 16%



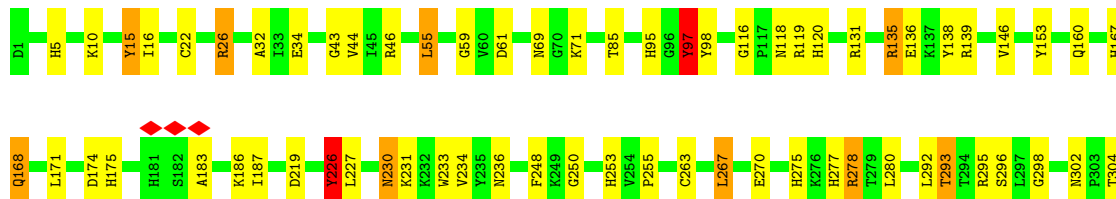
• Molecule 2: Spike glycoprotein E2

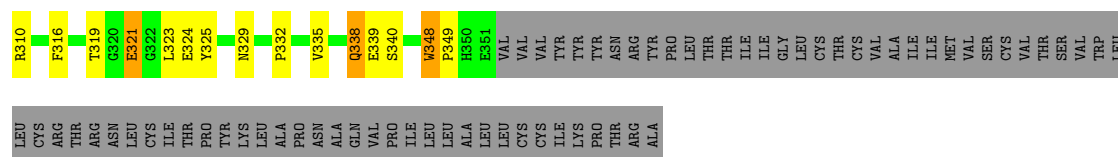
Chain D: 68% 14% 16%



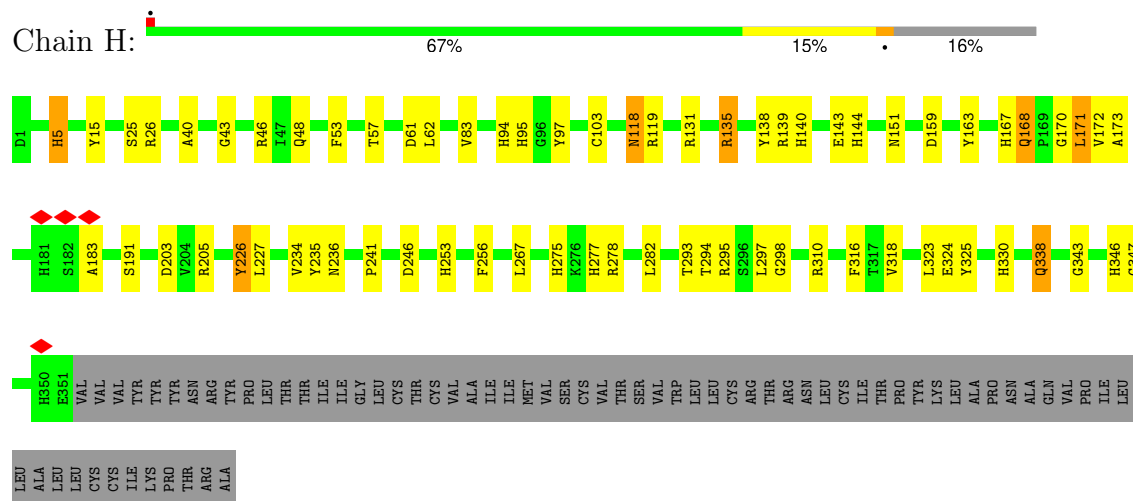
• Molecule 2: Spike glycoprotein E2

Chain F: 64% 16% 16%

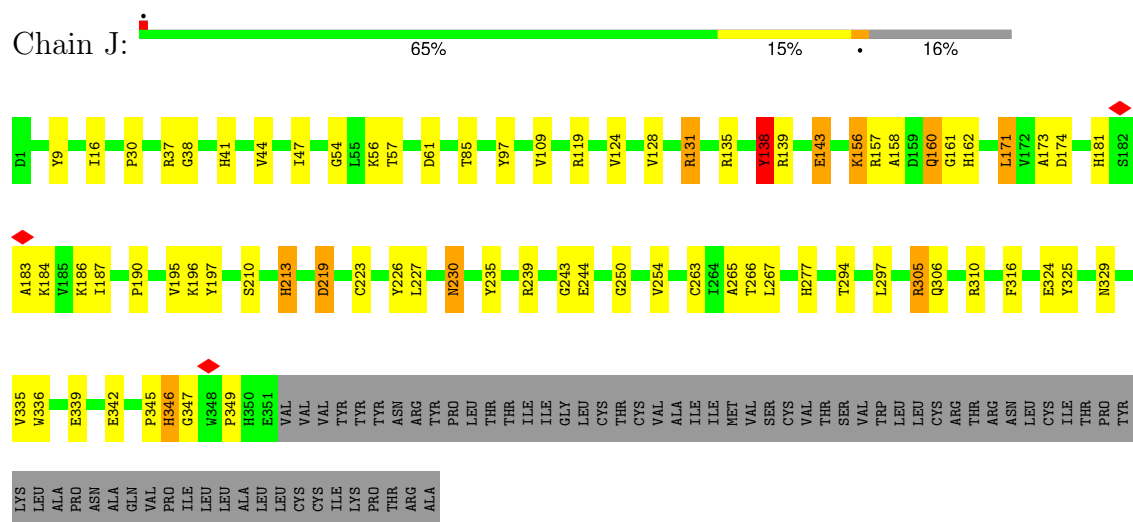




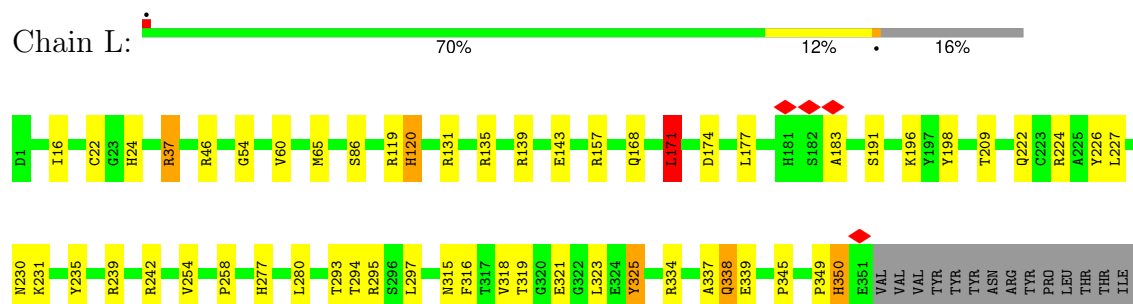
• Molecule 2: Spike glycoprotein E2



• Molecule 2: Spike glycoprotein E2



• Molecule 2: Spike glycoprotein E2



ILE
GLY
LEU
CYS
THR
CYS
VAL
ALA
ILE
ILE
MET
VAL
SER
CYS
VAL
THR
SER
VAL
TRP
LEU
LEU
CYS
ARG
THR
ARG
ASN
LEU
CYS
ILE
THR
PRO
TYR
LYS
LEU
ALA
PRO
ASN
ALA
GLN
VAL
PRO
ILE
LEU
LEU
ALA
LEU
LEU
CYS
CYS
ILE
LYS
PRO
THR
ARG
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.254	Depositor
Minimum map value	-5.570	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	573.696, 573.696, 573.696	wwPDB
Map dimensions	108, 108, 108	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	5.312, 5.312, 5.312	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	0.91	0/3147	1.23	11/4294 (0.3%)
1	C	0.90	0/3147	1.21	8/4294 (0.2%)
1	E	0.91	0/3147	1.21	9/4294 (0.2%)
1	G	0.92	0/3147	1.23	9/4294 (0.2%)
1	I	0.91	0/3147	1.20	7/4294 (0.2%)
1	K	0.92	0/3147	1.22	10/4294 (0.2%)
2	B	0.91	0/2847	1.13	2/3876 (0.1%)
2	D	0.91	0/2847	1.17	6/3876 (0.2%)
2	F	0.91	0/2847	1.20	6/3876 (0.2%)
2	H	0.91	0/2847	1.15	3/3876 (0.1%)
2	J	0.90	0/2847	1.18	8/3876 (0.2%)
2	L	0.91	0/2847	1.16	6/3876 (0.2%)
All	All	0.91	0/35964	1.19	85/49020 (0.2%)

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	2
1	C	0	5
1	E	0	5
1	G	0	4
1	I	0	2
1	K	0	5
2	B	0	3
2	D	0	5
2	F	0	9
2	H	0	5
2	J	0	4
2	L	0	6
All	All	0	55

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	93	TYR	CB-CG-CD1	-9.11	115.54	121.00
1	E	24	TYR	CB-CG-CD2	8.70	126.22	121.00
1	G	93	TYR	CB-CG-CD2	8.65	126.19	121.00
1	E	24	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	C	107	TYR	CB-CG-CD2	8.02	125.81	121.00
2	D	226	TYR	CB-CG-CD1	7.91	125.75	121.00
2	J	226	TYR	CB-CG-CD2	7.28	125.36	121.00
2	J	226	TYR	CB-CG-CD1	-7.27	116.64	121.00
2	D	226	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	G	391	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	G	391	TYR	CB-CG-CD1	7.03	125.22	121.00
1	E	76	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	1	TYR	CB-CG-CD1	-6.91	116.86	121.00
1	A	309	TYR	CB-CG-CD1	-6.84	116.90	121.00
1	E	76	TYR	CB-CG-CD1	6.72	125.03	121.00
1	G	201	PHE	CB-CG-CD2	6.70	125.49	120.80
2	F	135	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	C	107	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	C	186	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	I	15	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	C	338	ALA	N-CA-CB	6.35	118.99	110.10
1	G	201	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	A	1	TYR	CB-CG-CD2	6.32	124.79	121.00
1	K	7	MET	N-CA-C	-6.28	94.03	111.00
1	A	372	THR	N-CA-CB	6.28	122.23	110.30
2	F	248	PHE	CB-CG-CD1	6.26	125.18	120.80
1	E	143	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	J	138	TYR	CB-CG-CD2	5.96	124.57	121.00
1	A	143	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	E	326	ALA	N-CA-CB	5.92	118.39	110.10
2	J	138	TYR	CB-CG-CD1	-5.75	117.55	121.00
2	H	295	ARG	N-CA-CB	5.68	120.83	110.60
1	E	161	LYS	N-CA-C	-5.65	95.75	111.00
1	A	244	TRP	CB-CG-CD2	5.65	133.94	126.60
1	K	373	SER	N-CA-CB	5.62	118.93	110.50
1	I	15	TYR	CB-CG-CD1	5.60	124.36	121.00
2	L	239	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	174	ASP	N-CA-C	-5.58	95.93	111.00
2	B	172	VAL	N-CA-C	-5.57	95.97	111.00
1	G	132	MET	CG-SD-CE	-5.56	91.30	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	295	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	250	ALA	N-CA-CB	5.50	117.80	110.10
1	I	373	SER	N-CA-CB	5.49	118.74	110.50
2	H	298	GLY	N-CA-C	-5.48	99.40	113.10
1	C	310	ALA	N-CA-CB	5.47	117.76	110.10
2	D	37	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	I	280	SER	N-CA-C	-5.46	96.25	111.00
2	L	338	GLN	N-CA-CB	5.45	120.42	110.60
1	C	256	ALA	N-CA-CB	5.45	117.73	110.10
1	K	372	THR	N-CA-CB	5.45	120.65	110.30
1	K	107	TYR	CB-CG-CD1	5.39	124.23	121.00
1	K	107	TYR	CB-CG-CD2	-5.38	117.78	121.00
2	J	305	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	K	340	ILE	N-CA-C	-5.30	96.69	111.00
1	K	263	ALA	N-CA-CB	5.29	117.51	110.10
1	I	227	ALA	N-CA-CB	5.28	117.49	110.10
2	L	37	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	332	HIS	N-CA-CB	5.26	120.07	110.60
2	D	37	ARG	N-CA-C	-5.25	96.81	111.00
1	A	31	ILE	N-CA-C	-5.24	96.86	111.00
2	F	69	ASN	N-CA-C	-5.23	96.87	111.00
2	D	174	ASP	N-CA-CB	5.22	120.00	110.60
1	K	267	LEU	N-CA-CB	5.22	120.85	110.40
1	I	358	SER	N-CA-CB	5.20	118.30	110.50
1	A	244	TRP	CB-CG-CD1	-5.17	120.27	127.00
1	K	15	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	E	163	ILE	N-CA-C	-5.17	97.05	111.00
2	F	248	PHE	CB-CG-CD2	-5.17	117.18	120.80
2	J	54	GLY	N-CA-C	-5.15	100.22	113.10
1	G	137	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	I	372	THR	N-CA-CB	5.12	120.03	110.30
1	A	227	ALA	N-CA-CB	5.12	117.26	110.10
1	K	21	ARG	N-CA-C	-5.10	97.24	111.00
2	J	219	ASP	N-CA-CB	5.08	119.75	110.60
2	F	226	TYR	CB-CA-C	-5.08	100.24	110.40
2	L	54	GLY	N-CA-C	-5.07	100.42	113.10
1	C	137	TYR	CB-CG-CD1	-5.07	117.96	121.00
2	J	226	TYR	N-CA-CB	5.06	119.71	110.60
1	G	338	ALA	N-CA-C	-5.04	97.39	111.00
2	L	239	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	D	239	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	F	227	LEU	N-CA-C	-5.02	97.45	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	TYR	N-CA-CB	5.02	119.63	110.60
2	H	278	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	290	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	TYR	Sidechain
1	A	309	TYR	Sidechain
2	B	138	TYR	Sidechain
2	B	235	TYR	Sidechain
2	B	295	ARG	Sidechain
1	C	110	ARG	Sidechain
1	C	137	TYR	Sidechain
1	C	24	TYR	Sidechain
1	C	270	GLU	Peptide
1	C	76	TYR	Sidechain
2	D	197	TYR	Sidechain
2	D	295	ARG	Sidechain
2	D	9	TYR	Sidechain
2	D	97	TYR	Sidechain
2	D	98	TYR	Sidechain
1	E	355	PHE	Sidechain
1	E	385	LYS	Peptide
1	E	391	TYR	Sidechain
1	E	46	TYR	Sidechain
1	E	93	TYR	Sidechain
2	F	138	TYR	Sidechain
2	F	15	TYR	Sidechain
2	F	168	GLN	Peptide
2	F	226	TYR	Sidechain
2	F	263	CYS	Peptide
2	F	278	ARG	Sidechain
2	F	295	ARG	Sidechain
2	F	97	TYR	Sidechain
2	F	98	TYR	Sidechain
1	G	186	TYR	Sidechain
1	G	3	HIS	Sidechain
1	G	46	TYR	Sidechain
1	G	93	TYR	Sidechain
2	H	135	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	H	138	TYR	Sidechain
2	H	226	TYR	Sidechain
2	H	235	TYR	Sidechain
2	H	97	TYR	Sidechain
1	I	137	TYR	Sidechain
1	I	309	TYR	Sidechain
2	J	131	ARG	Sidechain
2	J	138	TYR	Sidechain
2	J	235	TYR	Sidechain
2	J	37	ARG	Sidechain
1	K	186	TYR	Sidechain
1	K	26	PRO	Mainchain
1	K	309	TYR	Sidechain
1	K	321	TYR	Sidechain
1	K	391	TYR	Sidechain
2	L	139	ARG	Sidechain
2	L	226	TYR	Sidechain
2	L	235	TYR	Sidechain
2	L	325	TYR	Sidechain
2	L	37	ARG	Sidechain
2	L	46	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3063	0	2950	41	0
1	C	3063	0	2950	29	0
1	E	3063	0	2950	32	0
1	G	3063	0	2950	37	0
1	I	3063	0	2950	26	0
1	K	3063	0	2950	33	0
2	B	2764	0	2679	10	0
2	D	2764	0	2679	23	0
2	F	2764	0	2679	21	0
2	H	2764	0	2679	19	0
2	J	2764	0	2679	20	0
2	L	2764	0	2679	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	34962	0	33774	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (275) 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:A:136:THR:HG23	1:A:142:TRP:H	1.51	0.75
1:A:136:THR:HG22	1:A:137:TYR:H	1.56	0.71
1:I:38:ILE:HD13	1:I:269:ALA:H	1.58	0.68
2:F:280:LEU:HD11	2:F:335:VAL:HG11	1.77	0.65
2:D:167:HIS:CG	2:D:168:GLN:H	2.15	0.64
1:E:33:LEU:HD22	1:E:277:ILE:HD12	1.80	0.62
1:G:110:ARG:HD3	1:G:110:ARG:H	1.65	0.62
1:G:337:VAL:HG12	2:H:346:HIS:CE1	2.35	0.61
1:A:17:ALA:HA	1:A:332:HIS:CD2	2.36	0.60
1:C:304:ILE:HG12	1:C:380:ASP:H	1.67	0.60
2:J:38:GLY:H	2:J:128:VAL:HG12	1.67	0.60
1:K:321:TYR:CD2	1:K:347:LEU:HD22	2.38	0.58
1:I:400:THR:HG23	2:J:345:PRO:HG2	1.86	0.57
1:A:11:VAL:HA	1:A:35:ASN:H	1.69	0.57
1:A:3:HIS:CE1	1:A:17:ALA:HB1	2.40	0.56
1:E:57:SER:H	2:F:236:ASN:HB3	1.70	0.56
1:A:274:VAL:HG22	1:A:275:GLY:H	1.70	0.55
1:A:17:ALA:HA	1:A:336:GLY:H	1.72	0.55
1:A:88:MET:HB2	2:B:173:ALA:H	1.71	0.55
2:H:275:HIS:HE1	2:H:338:GLN:H	1.55	0.54
1:A:331:ILE:HD12	1:A:368:LEU:HD21	1.88	0.54
1:I:400:THR:HG22	2:J:339:GLU:H	1.73	0.54
2:F:135:ARG:HH11	2:F:329:ASN:HA	1.72	0.54
1:K:304:ILE:HG23	1:K:380:ASP:H	1.73	0.54
1:I:302:CYS:SG	1:I:319:VAL:HG22	2.48	0.53
2:H:294:THR:HG22	2:H:325:TYR:HA	1.89	0.53
1:E:135:ILE:HB	1:E:143:ARG:HH11	1.73	0.53
1:E:48:THR:HG22	1:E:49:CYS:H	1.74	0.53
1:C:39:ILE:H	1:C:129:VAL:HG12	1.72	0.53
1:I:48:THR:HG22	1:I:49:CYS:H	1.74	0.53
1:E:387:HIS:CE1	2:F:278:ARG:HA	2.43	0.52
1:C:28:HIS:CD2	1:C:28:HIS:H	2.26	0.52
1:C:57:SER:H	2:D:242:ARG:HH21	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:THR:HA	2:F:338:GLN:HA	1.92	0.52
1:E:323:SER:H	1:E:349:GLU:HA	1.75	0.52
1:I:27:VAL:CG1	1:I:138:GLY:H	2.23	0.52
2:J:294:THR:HG21	2:J:316:PHE:CD2	2.45	0.52
1:I:394:GLN:HE22	1:I:400:THR:HG21	1.74	0.52
2:H:294:THR:HG21	2:H:316:PHE:CD2	2.44	0.52
1:I:112:GLU:HA	2:J:162:HIS:CD2	2.46	0.51
1:A:3:HIS:CE1	1:A:5:ALA:HB2	2.46	0.51
1:G:16:LYS:HB2	1:G:332:HIS:CE1	2.46	0.51
1:I:15:TYR:CD1	1:I:395:HIS:HB2	2.46	0.51
2:H:53:PHE:O	2:H:94:HIS:CD2	2.64	0.51
1:I:8:PRO:HA	1:I:276:SER:HA	1.93	0.51
1:K:16:LYS:H	1:K:339:VAL:HG22	1.75	0.51
1:C:180:VAL:HG13	1:C:185:VAL:HG22	1.93	0.51
1:K:17:ALA:HA	1:K:336:GLY:HA2	1.93	0.51
1:A:332:HIS:CD2	1:A:333:SER:O	2.64	0.51
1:E:332:HIS:CD2	1:E:333:SER:O	2.63	0.51
1:C:27:VAL:CG1	1:C:138:GLY:H	2.23	0.51
1:G:298:SER:H	1:G:323:SER:HA	1.76	0.51
1:E:15:TYR:CG	1:E:395:HIS:CD2	2.99	0.50
2:F:44:VAL:HG21	2:F:153:TYR:H	1.76	0.50
1:G:391:TYR:CZ	2:H:297:LEU:HD11	2.46	0.50
1:G:8:PRO:HA	1:G:276:SER:HA	1.94	0.50
1:I:319:VAL:HG11	1:I:321:TYR:CE1	2.46	0.50
1:G:302:CYS:SG	1:G:319:VAL:HG22	2.52	0.50
2:D:40:ALA:HB2	2:D:153:TYR:CE2	2.45	0.50
1:G:231:HIS:CD2	2:H:26:ARG:HH12	2.29	0.50
1:K:10:LYS:HD2	1:K:12:GLY:H	1.75	0.50
1:G:355:PHE:CZ	1:G:368:LEU:HD22	2.47	0.50
1:G:357:PHE:CD2	1:G:359:THR:HG23	2.46	0.50
1:G:17:ALA:HB3	1:G:29:LEU:HD23	1.94	0.50
1:K:136:THR:HA	1:K:142:TRP:H	1.77	0.50
2:F:298:GLY:H	2:F:319:THR:HG21	1.77	0.49
2:L:171:LEU:H	2:L:227:LEU:H	1.59	0.49
1:C:362:ILE:HD12	1:C:362:ILE:H	1.77	0.49
1:I:388:ILE:HA	2:J:335:VAL:HG23	1.95	0.49
1:I:332:HIS:CE1	1:I:338:ALA:O	2.66	0.49
1:A:110:ARG:H	1:A:110:ARG:HD3	1.78	0.48
1:G:16:LYS:HG3	1:G:28:HIS:CE1	2.48	0.48
1:A:16:LYS:HG3	1:A:340:ILE:H	1.79	0.48
2:F:187:ILE:HD11	2:F:226:TYR:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:333:SER:CB	1:K:338:ALA:H	2.26	0.48
2:L:198:TYR:HB3	2:L:224:ARG:HH21	1.77	0.48
2:H:282:LEU:HD13	2:H:325:TYR:CE1	2.48	0.48
1:C:185:VAL:HG11	1:C:267:LEU:HD11	1.95	0.48
2:H:316:PHE:HB3	2:H:323:LEU:HD11	1.96	0.48
1:K:15:TYR:HA	1:K:339:VAL:HG11	1.95	0.48
1:A:33:LEU:HD13	1:A:277:ILE:H	1.79	0.48
1:A:332:HIS:CE1	1:A:338:ALA:HB3	2.49	0.48
1:G:110:ARG:H	1:G:110:ARG:CD	2.27	0.48
1:C:321:TYR:CE1	1:C:370:VAL:HG11	2.48	0.48
1:E:15:TYR:CE2	1:E:395:HIS:CE1	3.02	0.47
2:H:171:LEU:HB3	2:H:226:TYR:CD1	2.48	0.47
1:I:260:CYS:HA	1:I:272:CYS:HA	1.96	0.47
2:D:22:CYS:HB3	2:D:27:CYS:H	1.79	0.47
2:H:15:TYR:CE2	2:H:234:VAL:HG21	2.50	0.47
2:B:296:SER:HA	2:B:323:LEU:HA	1.95	0.47
1:K:338:ALA:HB2	1:K:366:PHE:CD2	2.49	0.47
2:D:294:THR:HG21	2:D:316:PHE:CG	2.49	0.47
2:D:327:TRP:H	2:D:330:HIS:CE1	2.33	0.47
1:I:130:GLN:HA	1:I:149:VAL:H	1.78	0.47
1:A:180:VAL:HG13	1:A:185:VAL:HG22	1.97	0.47
1:A:345:VAL:HG11	1:A:355:PHE:HB3	1.96	0.47
2:D:167:HIS:CG	2:D:168:GLN:N	2.83	0.47
2:F:171:LEU:H	2:F:171:LEU:HD23	1.80	0.47
2:H:167:HIS:CE1	2:H:236:ASN:HA	2.50	0.47
1:C:183:HIS:H	1:C:183:HIS:CD2	2.32	0.46
1:C:332:HIS:CD2	1:C:340:ILE:HB	2.50	0.46
1:C:360:ALA:HB2	1:C:394:GLN:HG3	1.98	0.46
1:G:21:ARG:HG3	1:G:24:TYR:H	1.80	0.46
1:I:31:ILE:HA	1:I:134:ASN:O	2.15	0.46
1:C:33:LEU:HD13	1:C:277:ILE:H	1.80	0.46
1:A:273:ALA:HB3	2:B:298:GLY:H	1.80	0.46
2:D:297:LEU:H	2:D:323:LEU:HA	1.81	0.46
1:E:302:CYS:SG	1:E:319:VAL:HG22	2.55	0.46
2:D:347:GLY:HA2	1:G:23:GLY:HA2	1.96	0.46
1:G:3:HIS:HA	1:G:19:VAL:HG13	1.98	0.46
1:K:167:LEU:H	1:K:167:LEU:HD22	1.80	0.46
1:I:88:MET:HB2	2:J:173:ALA:HB2	1.97	0.46
2:J:190:PRO:HD3	2:J:227:LEU:HD22	1.98	0.46
1:K:252:LEU:HA	1:K:255:VAL:HG22	1.97	0.46
2:J:47:ILE:HG23	2:J:109:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:TYR:CE1	1:E:370:VAL:HG11	2.51	0.46
2:F:5:HIS:CD2	2:F:253:HIS:CE1	3.03	0.46
2:F:323:LEU:O	2:F:335:VAL:HG22	2.16	0.46
1:A:91:GLY:H	2:B:175:HIS:CD2	2.33	0.46
1:C:16:LYS:H	1:C:339:VAL:HG22	1.80	0.46
1:G:342:GLU:HG2	1:G:356:HIS:H	1.80	0.46
1:A:21:ARG:HH21	1:I:382:LYS:CG	2.29	0.46
1:C:156:LYS:HA	1:C:161:LYS:HA	1.97	0.46
1:E:15:TYR:CE2	1:E:32:GLN:HA	2.51	0.46
1:K:330:PRO:HA	1:K:344:ASP:HA	1.97	0.46
1:C:16:LYS:CG	1:C:332:HIS:CE1	3.00	0.45
1:C:394:GLN:O	1:C:395:HIS:CG	2.70	0.45
1:G:337:VAL:HG13	1:G:399:PHE:CZ	2.51	0.45
1:I:3:HIS:CG	1:I:19:VAL:HG13	2.51	0.45
2:F:296:SER:H	2:F:302:ASN:HB3	1.80	0.45
2:L:294:THR:HG21	2:L:316:PHE:CG	2.51	0.45
2:H:171:LEU:HA	2:H:227:LEU:H	1.82	0.45
1:A:13:ILE:HD11	1:A:395:HIS:HA	1.98	0.45
1:E:329:CYS:HB2	1:E:347:LEU:HD11	1.99	0.45
1:K:3:HIS:CD2	1:K:20:GLU:H	2.34	0.45
1:K:363:HIS:CG	1:K:364:PRO:HD2	2.51	0.45
1:E:110:ARG:H	1:E:110:ARG:CD	2.30	0.45
1:A:16:LYS:HA	1:A:30:GLN:HA	1.98	0.45
1:A:143:ARG:HH22	1:A:162:LEU:HD13	1.82	0.45
2:H:346:HIS:CG	2:H:347:GLY:N	2.85	0.45
2:J:16:ILE:HB	2:J:173:ALA:H	1.82	0.45
1:K:363:HIS:CG	1:K:364:PRO:CD	3.00	0.45
1:E:3:HIS:HB2	1:E:19:VAL:HG22	1.99	0.45
1:C:16:LYS:HG2	1:C:332:HIS:CE1	2.52	0.45
1:E:16:LYS:HB2	1:E:332:HIS:CE1	2.52	0.44
1:A:366:PHE:CE2	1:A:368:LEU:HD13	2.52	0.44
1:C:183:HIS:CD2	2:D:135:ARG:HH22	2.35	0.44
1:K:333:SER:HB2	1:K:338:ALA:H	1.82	0.44
1:G:265:GLU:C	1:G:267:LEU:H	2.21	0.44
2:J:16:ILE:HG23	2:J:30:PRO:HA	1.99	0.44
2:B:37:ARG:HH12	2:B:258:PRO:HD3	1.83	0.44
2:F:95:HIS:CD2	2:F:255:PRO:HG3	2.52	0.44
2:B:38:GLY:HA3	2:B:128:VAL:HG13	1.99	0.44
2:J:187:ILE:HG13	2:J:227:LEU:HD21	1.98	0.44
1:A:19:VAL:CG2	1:A:29:LEU:HD21	2.48	0.44
2:D:171:LEU:HA	2:D:227:LEU:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:THR:HA	1:E:142:TRP:H	1.82	0.44
1:G:331:ILE:HG22	1:G:370:VAL:HA	1.98	0.44
1:A:91:GLY:H	2:B:175:HIS:CG	2.36	0.44
1:A:366:PHE:CZ	1:A:368:LEU:HD13	2.53	0.44
2:D:171:LEU:HD22	2:D:226:TYR:CE1	2.52	0.44
1:K:41:SER:H	1:K:127:GLY:HA3	1.82	0.44
2:B:138:TYR:CG	2:B:266:THR:HG21	2.53	0.44
2:F:292:LEU:HD21	2:F:316:PHE:CE2	2.53	0.44
1:I:16:LYS:HZ2	1:I:343:ASN:HA	1.82	0.44
2:J:196:LYS:HZ2	2:J:243:GLY:HA2	1.83	0.44
1:A:294:THR:HA	1:A:328:ASN:O	2.18	0.43
1:A:332:HIS:HE1	1:A:338:ALA:O	2.01	0.43
2:L:171:LEU:H	2:L:227:LEU:N	2.14	0.43
2:B:163:TYR:HA	2:B:253:HIS:HA	2.00	0.43
2:F:10:LYS:HA	2:F:55:LEU:HD21	2.00	0.43
2:F:135:ARG:HH22	2:F:332:PRO:HG3	1.82	0.43
1:I:60:VAL:HG13	1:I:103:MET:H	1.83	0.43
1:I:331:ILE:HG22	1:I:370:VAL:HA	2.00	0.43
2:F:277:HIS:HA	2:F:340:SER:H	1.83	0.43
1:K:363:HIS:CD2	1:K:364:PRO:HD3	2.54	0.43
1:C:362:ILE:HG21	2:D:350:HIS:H	1.84	0.43
1:E:360:ALA:HB1	1:E:396:THR:HG22	2.01	0.43
1:G:28:HIS:O	1:G:29:LEU:HD13	2.18	0.43
1:K:108:VAL:H	1:K:216:ALA:HB1	1.84	0.43
2:D:100:LEU:HD11	2:D:153:TYR:HB2	2.01	0.43
1:G:88:MET:HB2	2:H:173:ALA:H	1.84	0.43
1:G:108:VAL:H	1:G:216:ALA:HB1	1.82	0.43
2:J:181:HIS:CG	2:J:181:HIS:O	2.72	0.43
1:K:11:VAL:HG23	1:K:271:ASN:HA	2.00	0.43
2:L:319:THR:O	2:L:337:ALA:HB2	2.18	0.43
1:A:309:TYR:CE1	1:A:315:GLY:HA3	2.54	0.43
1:K:112:GLU:CG	2:L:254:VAL:HG21	2.49	0.43
1:K:143:ARG:HH12	1:K:147:VAL:HG12	1.84	0.43
2:F:97:TYR:CD1	2:F:234:VAL:HA	2.53	0.43
1:G:332:HIS:CE1	1:G:339:VAL:HA	2.54	0.43
2:H:163:TYR:HA	2:H:253:HIS:HA	2.01	0.42
2:L:198:TYR:CB	2:L:224:ARG:HH21	2.32	0.42
1:E:304:ILE:HA	1:E:317:ALA:HA	2.01	0.42
2:F:116:GLY:HA3	2:F:120:HIS:CD2	2.54	0.42
2:F:348:TRP:H	2:F:349:PRO:CD	2.32	0.42
1:A:302:CYS:SG	1:A:317:ALA:HB1	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LYS:HA	1:E:161:LYS:HA	2.01	0.42
2:D:95:HIS:CD2	2:D:157:ARG:HE	2.37	0.42
2:D:297:LEU:HD13	2:D:298:GLY:H	1.84	0.42
1:E:180:VAL:HG12	1:E:264:LEU:HA	2.02	0.42
1:E:332:HIS:HE1	1:E:339:VAL:HA	1.83	0.42
1:K:17:ALA:H	1:K:29:LEU:HB2	1.85	0.42
1:A:362:ILE:HG21	2:B:344:ASN:H	1.83	0.42
1:G:253:ASN:HA	1:G:261:SER:HA	2.02	0.42
1:K:71:LYS:HG3	2:L:168:GLN:HE22	1.84	0.42
2:L:294:THR:HG22	2:L:325:TYR:HA	2.01	0.42
1:A:16:LYS:O	1:A:332:HIS:CG	2.72	0.42
1:C:27:VAL:HG11	1:C:138:GLY:H	1.83	0.42
1:C:255:VAL:HA	2:D:301:ALA:HB1	2.02	0.42
1:A:357:PHE:CG	1:A:366:PHE:CZ	3.08	0.42
1:K:363:HIS:CD2	2:L:349:PRO:HA	2.54	0.42
2:L:277:HIS:HB2	2:L:350:HIS:CG	2.55	0.42
2:D:46:ARG:HH22	2:D:254:VAL:HB	1.85	0.42
1:G:29:LEU:HG	1:G:135:ILE:HG21	2.02	0.42
2:L:318:VAL:HA	2:L:323:LEU:HB2	2.02	0.42
1:E:29:LEU:CD1	1:E:135:ILE:HG23	2.50	0.41
1:G:9:ASN:HD22	1:G:274:VAL:HG12	1.85	0.41
1:K:112:GLU:HB2	2:L:258:PRO:HD2	2.02	0.41
1:K:112:GLU:CB	2:L:258:PRO:HD2	2.50	0.41
1:A:3:HIS:CE1	1:A:29:LEU:HD23	2.56	0.41
1:C:302:CYS:SG	1:C:319:VAL:HG22	2.60	0.41
1:C:331:ILE:O	1:C:332:HIS:CD2	2.72	0.41
1:E:9:ASN:HB2	1:E:277:ILE:HD11	2.02	0.41
1:E:295:PRO:HB3	1:E:325:LYS:H	1.85	0.41
1:A:332:HIS:HD1	1:A:340:ILE:HG12	1.85	0.41
2:J:195:VAL:H	2:J:210:SER:HA	1.85	0.41
1:K:15:TYR:CE1	1:K:32:GLN:HA	2.54	0.41
2:D:150:CYS:SG	2:D:265:ALA:HB2	2.60	0.41
1:E:33:LEU:HD21	1:E:279:ILE:HG12	2.02	0.41
1:G:28:HIS:CD2	1:G:343:ASN:HA	2.55	0.41
2:H:318:VAL:HA	2:H:323:LEU:HB2	2.03	0.41
1:E:319:VAL:HG11	1:E:321:TYR:CE1	2.55	0.41
1:G:15:TYR:HB2	1:G:395:HIS:CE1	2.55	0.41
1:G:332:HIS:CD2	1:G:333:SER:O	2.73	0.41
2:J:263:CYS:SG	2:J:265:ALA:HB2	2.61	0.41
2:F:293:THR:HA	2:F:304:THR:HB	2.03	0.41
1:G:19:VAL:HG23	1:G:29:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:HIS:CD2	2:H:95:HIS:HE1	2.39	0.41
2:J:184:LYS:HB3	2:J:213:HIS:CE1	2.56	0.41
1:K:319:VAL:HB	1:K:321:TYR:CD2	2.56	0.41
1:K:395:HIS:CD2	1:K:396:THR:HG22	2.56	0.41
1:G:52:LYS:HA	1:G:52:LYS:HE2	2.02	0.41
1:C:259:GLY:HA2	2:D:298:GLY:O	2.21	0.41
2:D:170:GLY:HA3	2:D:242:ARG:HA	2.02	0.41
2:D:275:HIS:CE1	2:D:335:VAL:HG22	2.55	0.41
2:D:296:SER:HB2	2:D:302:ASN:HD22	1.86	0.41
1:E:15:TYR:CD2	1:E:395:HIS:CG	3.08	0.41
1:G:7:MET:SD	1:G:17:ALA:HA	2.61	0.41
1:I:8:PRO:HB2	1:I:396:THR:HA	2.03	0.41
1:E:143:ARG:HH21	1:E:145:ALA:HB3	1.86	0.41
1:K:11:VAL:HG11	2:L:297:LEU:HD12	2.03	0.41
1:A:48:THR:HG22	1:A:49:CYS:H	1.86	0.40
1:A:180:VAL:HG11	1:A:264:LEU:HA	2.03	0.40
1:C:9:ASN:HD22	1:C:272:CYS:HB3	1.86	0.40
1:C:297:VAL:HG21	1:C:370:VAL:HG12	2.03	0.40
2:L:297:LEU:H	2:L:323:LEU:HA	1.86	0.40
1:A:244:TRP:H	1:A:248:LYS:HA	1.87	0.40
1:A:332:HIS:HD1	1:A:340:ILE:CG1	2.33	0.40
1:E:290:ARG:HH11	1:E:290:ARG:HA	1.86	0.40
1:G:332:HIS:HE1	1:G:339:VAL:HA	1.87	0.40
1:G:337:VAL:HG13	1:G:399:PHE:CE1	2.56	0.40
2:H:118:ASN:H	2:H:118:ASN:HD22	1.69	0.40
1:K:273:ALA:HB1	2:L:321:GLU:CB	2.51	0.40
1:A:60:VAL:HG23	1:A:103:MET:H	1.86	0.40
1:E:18:LEU:HB3	1:E:335:SER:H	1.86	0.40
1:G:171:TRP:CZ2	1:G:258:PHE:HB3	2.56	0.40
1:I:391:TYR:CE1	2:J:297:LEU:CD1	3.04	0.40
1:C:143:ARG:HH12	1:C:145:ALA:H	1.70	0.40
1:C:243:ARG:HB2	1:C:244:TRP:H	1.75	0.40
1:I:135:ILE:HB	1:I:143:ARG:HE	1.87	0.40
2:J:230:ASN:H	2:J:230:ASN:HD22	1.68	0.40
1:K:29:LEU:HD13	1:K:137:TYR:HA	2.04	0.40
1:G:359:THR:HG21	1:G:364:PRO:HB2	2.04	0.40
1:I:95:PHE:HB3	2:J:223:CYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/441 (90%)	313 (79%)	47 (12%)	38 (10%)	0	8
1	C	398/441 (90%)	322 (81%)	47 (12%)	29 (7%)	1	10
1	E	398/441 (90%)	315 (79%)	48 (12%)	35 (9%)	0	9
1	G	398/441 (90%)	299 (75%)	63 (16%)	36 (9%)	0	8
1	I	398/441 (90%)	310 (78%)	55 (14%)	33 (8%)	0	9
1	K	398/441 (90%)	308 (77%)	56 (14%)	34 (8%)	0	9
2	B	349/420 (83%)	280 (80%)	50 (14%)	19 (5%)	1	15
2	D	349/420 (83%)	291 (83%)	46 (13%)	12 (3%)	3	21
2	F	349/420 (83%)	276 (79%)	50 (14%)	23 (7%)	1	12
2	H	349/420 (83%)	277 (79%)	51 (15%)	21 (6%)	1	13
2	J	349/420 (83%)	284 (81%)	45 (13%)	20 (6%)	1	14
2	L	349/420 (83%)	291 (83%)	40 (12%)	18 (5%)	1	15
All	All	4482/5166 (87%)	3566 (80%)	598 (13%)	318 (7%)	2	11

All (318) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	22	PRO
1	A	100	ASN
1	A	142	TRP
1	A	227	ALA
1	A	244	TRP
1	A	258	PHE
1	A	267	LEU
1	A	390	ASP
2	B	57	THR
2	B	183	ALA
2	B	191	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	300	ASP
2	B	339	GLU
2	B	346	HIS
1	C	73	HIS
1	C	150	ASN
1	C	168	SER
1	C	169	SER
1	C	267	LEU
1	C	310	ALA
1	C	395	HIS
2	D	135	ARG
2	D	174	ASP
2	D	219	ASP
2	D	321	GLU
1	E	57	SER
1	E	72	PRO
1	E	130	GLN
1	E	152	GLU
1	E	244	TRP
1	E	250	ALA
1	E	306	GLU
1	E	310	ALA
1	E	326	ALA
1	E	387	HIS
1	E	390	ASP
1	E	396	THR
1	E	398	SER
2	F	136	GLU
2	F	174	ASP
2	F	219	ASP
2	F	230	ASN
2	F	321	GLU
2	F	339	GLU
2	F	348	TRP
1	G	2	GLU
1	G	11	VAL
1	G	89	TRP
1	G	169	SER
1	G	231	HIS
1	G	386	ASP
1	G	394	GLN
1	G	398	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	5	HIS
2	H	25	SER
2	H	40	ALA
2	H	57	THR
2	H	140	HIS
2	H	143	GLU
2	H	168	GLN
2	H	203	ASP
2	H	246	ASP
2	H	267	LEU
2	H	277	HIS
1	I	65	ALA
1	I	100	ASN
1	I	192	GLU
1	I	255	VAL
1	I	274	VAL
1	I	360	ALA
1	I	373	SER
2	J	139	ARG
2	J	158	ALA
2	J	171	LEU
2	J	174	ASP
2	J	219	ASP
1	K	73	HIS
1	K	117	ASP
1	K	263	ALA
1	K	267	LEU
1	K	372	THR
1	K	383	PRO
1	K	386	ASP
1	K	390	ASP
1	K	396	THR
2	L	22	CYS
2	L	60	VAL
2	L	143	GLU
2	L	338	GLN
1	A	89	TRP
1	A	175	ASP
1	A	245	LYS
1	A	372	THR
2	B	193	ALA
2	B	340	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	350	HIS
1	C	11	VAL
1	C	49	CYS
1	C	142	TRP
1	C	167	LEU
1	C	227	ALA
1	C	276	SER
1	C	299	ASP
1	C	306	GLU
1	C	372	THR
1	C	386	ASP
1	C	396	THR
2	D	203	ASP
1	E	22	PRO
1	E	49	CYS
1	E	160	ALA
1	E	172	SER
1	E	337	VAL
1	E	338	ALA
1	E	372	THR
2	F	26	ARG
2	F	160	GLN
2	F	168	GLN
2	F	183	ALA
2	F	338	GLN
1	G	34	VAL
1	G	230	VAL
1	G	248	LYS
1	G	267	LEU
1	G	300	LEU
1	G	306	GLU
1	G	360	ALA
1	G	372	THR
1	G	390	ASP
2	H	241	PRO
2	H	338	GLN
1	I	49	CYS
1	I	89	TRP
1	I	142	TRP
1	I	227	ALA
1	I	350	SER
1	I	372	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	61	ASP
2	J	156	LYS
2	J	157	ARG
2	J	213	HIS
2	J	346	HIS
1	K	63	CYS
1	K	231	HIS
1	K	373	SER
2	L	174	ASP
2	L	183	ALA
2	L	242	ARG
2	L	339	GLU
2	L	345	PRO
1	A	38	ILE
1	A	49	CYS
1	A	69	THR
1	A	75	ASP
1	A	95	PHE
1	A	191	PRO
1	A	219	ASN
1	A	241	PHE
1	A	276	SER
2	B	25	SER
2	B	143	GLU
2	B	244	GLU
2	B	338	GLN
1	C	152	GLU
1	C	170	ALA
1	C	322	LYS
2	D	154	THR
2	D	159	ASP
2	D	183	ALA
1	E	139	SER
1	E	183	HIS
1	E	373	SER
2	F	43	GLY
2	F	59	GLY
2	F	267	LEU
1	G	22	PRO
1	G	49	CYS
1	G	63	CYS
1	G	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	127	GLY
1	G	160	ALA
1	G	195	THR
1	G	219	ASN
1	G	314	GLY
1	G	396	THR
2	H	43	GLY
2	H	170	GLY
2	H	183	ALA
2	H	343	GLY
1	I	22	PRO
1	I	131	ALA
1	I	132	MET
1	I	152	GLU
1	I	246	ARG
1	I	307	CYS
1	I	313	PHE
2	J	161	GLY
2	J	183	ALA
2	J	244	GLU
2	J	250	GLY
2	J	347	GLY
1	K	49	CYS
1	K	94	CYS
1	K	152	GLU
1	K	230	VAL
1	K	246	ARG
1	K	288	PHE
1	K	395	HIS
1	K	397	GLU
2	L	24	HIS
2	L	86	SER
2	L	171	LEU
2	L	231	LYS
2	L	350	HIS
1	A	35	ASN
1	A	57	SER
1	A	246	ARG
1	A	313	PHE
1	A	373	SER
1	A	381	CYS
1	A	387	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	398	SER
1	C	22	PRO
1	C	75	ASP
1	C	117	ASP
1	C	244	TRP
2	D	136	GLU
1	E	193	TYR
1	E	241	PHE
1	E	275	GLY
1	E	299	ASP
1	E	371	CYS
1	E	399	PHE
2	F	32	ALA
2	F	55	LEU
2	F	233	TRP
1	G	238	PRO
1	G	371	CYS
1	G	373	SER
2	H	256	PHE
1	I	66	THR
1	I	69	THR
1	I	195	THR
1	I	271	ASN
1	I	312	ASP
2	J	57	THR
1	K	57	SER
1	K	191	PRO
1	K	239	SER
1	K	391	TYR
2	L	16	ILE
2	L	222	GLN
1	A	73	HIS
1	A	257	PRO
1	A	334	PRO
1	A	397	GLU
2	B	61	ASP
2	B	169	PRO
1	C	88	MET
1	E	30	GLN
1	E	142	TRP
1	E	153	THR
1	E	169	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	22	CYS
2	F	61	ASP
2	F	231	LYS
1	G	88	MET
1	G	304	ILE
2	H	61	ASP
1	I	219	ASN
1	I	244	TRP
1	I	305	THR
2	J	143	GLU
2	J	160	GLN
2	J	342	GLU
1	K	142	TRP
1	K	150	ASN
1	K	195	THR
1	K	207	ARG
2	L	120	HIS
2	L	191	SER
1	A	193	TYR
2	B	168	GLN
2	B	250	GLY
1	C	89	TRP
1	C	238	PRO
1	C	324	SER
2	D	345	PRO
1	E	227	ALA
1	E	334	PRO
1	G	75	ASP
1	G	98	THR
2	H	159	ASP
2	H	191	SER
1	I	238	PRO
1	I	304	ILE
2	J	349	PRO
1	K	116	ILE
1	K	137	TYR
1	K	313	PHE
1	I	337	VAL
1	A	154	PRO
2	D	190	PRO
1	G	391	TYR
1	I	21	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	391	TYR
1	K	22	PRO
1	K	84	VAL
2	B	302	ASN
2	F	250	GLY
1	G	284	PRO
1	K	256	ALA
1	A	153	THR
2	B	349	PRO
2	F	270	GLU
1	A	259	GLY
2	D	140	HIS

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	339/370 (92%)	312 (92%)	27 (8%)	10	29
1	C	339/370 (92%)	317 (94%)	22 (6%)	14	35
1	E	339/370 (92%)	320 (94%)	19 (6%)	17	38
1	G	339/370 (92%)	313 (92%)	26 (8%)	10	30
1	I	339/370 (92%)	314 (93%)	25 (7%)	11	31
1	K	339/370 (92%)	318 (94%)	21 (6%)	15	36
2	B	304/367 (83%)	288 (95%)	16 (5%)	19	40
2	D	304/367 (83%)	282 (93%)	22 (7%)	12	32
2	F	304/367 (83%)	280 (92%)	24 (8%)	10	29
2	H	304/367 (83%)	284 (93%)	20 (7%)	14	34
2	J	304/367 (83%)	273 (90%)	31 (10%)	6	20
2	L	304/367 (83%)	289 (95%)	15 (5%)	21	42
All	All	3858/4422 (87%)	3590 (93%)	268 (7%)	15	33

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	TYR
1	A	2	GLU
1	A	18	LEU
1	A	29	LEU
1	A	34	VAL
1	A	95	PHE
1	A	105	GLU
1	A	107	TYR
1	A	110	ARG
1	A	123	LYS
1	A	147	VAL
1	A	174	PHE
1	A	197	LYS
1	A	244	TRP
1	A	262	ILE
1	A	281	ILE
1	A	290	ARG
1	A	319	VAL
1	A	353	PHE
1	A	355	PHE
1	A	359	THR
1	A	366	PHE
1	A	367	LYS
1	A	377	CYS
1	A	378	LYS
1	A	392	PRO
1	A	394	GLN
2	B	4	THR
2	B	5	HIS
2	B	44	VAL
2	B	131	ARG
2	B	135	ARG
2	B	152	ARG
2	B	175	HIS
2	B	217	CYS
2	B	226	TYR
2	B	231	LYS
2	B	267	LEU
2	B	274	GLU
2	B	309	GLU
2	B	310	ARG
2	B	312	THR
2	B	339	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	10	LYS
1	C	16	LYS
1	C	34	VAL
1	C	52	LYS
1	C	53	THR
1	C	102	GLN
1	C	107	TYR
1	C	143	ARG
1	C	214	LEU
1	C	234	PHE
1	C	245	LYS
1	C	246	ARG
1	C	248	LYS
1	C	283	ILE
1	C	290	ARG
1	C	303	LYS
1	C	318	THR
1	C	334	PRO
1	C	341	LYS
1	C	354	THR
1	C	362	ILE
1	C	395	HIS
2	D	15	TYR
2	D	16	ILE
2	D	26	ARG
2	D	46	ARG
2	D	84	ARG
2	D	95	HIS
2	D	99	ILE
2	D	127	LYS
2	D	131	ARG
2	D	135	ARG
2	D	139	ARG
2	D	205	ARG
2	D	217	CYS
2	D	236	ASN
2	D	239	ARG
2	D	251	LYS
2	D	263	CYS
2	D	297	LEU
2	D	306	GLN
2	D	310	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	326	THR
2	D	330	HIS
1	E	9	ASN
1	E	29	LEU
1	E	32	GLN
1	E	37	ARG
1	E	72	PRO
1	E	95	PHE
1	E	103	MET
1	E	110	ARG
1	E	143	ARG
1	E	150	ASN
1	E	162	LEU
1	E	179	VAL
1	E	217	ASN
1	E	244	TRP
1	E	246	ARG
1	E	291	ILE
1	E	300	LEU
1	E	359	THR
1	E	385	LYS
2	F	15	TYR
2	F	16	ILE
2	F	26	ARG
2	F	34	GLU
2	F	46	ARG
2	F	71	LYS
2	F	85	THR
2	F	97	TYR
2	F	118	ASN
2	F	119	ARG
2	F	131	ARG
2	F	139	ARG
2	F	146	VAL
2	F	167	HIS
2	F	175	HIS
2	F	186	LYS
2	F	230	ASN
2	F	267	LEU
2	F	275	HIS
2	F	293	THR
2	F	310	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	321	GLU
2	F	324	GLU
2	F	325	TYR
1	G	10	LYS
1	G	16	LYS
1	G	18	LEU
1	G	26	PRO
1	G	29	LEU
1	G	36	THR
1	G	37	ARG
1	G	52	LYS
1	G	93	TYR
1	G	110	ARG
1	G	143	ARG
1	G	162	LEU
1	G	171	TRP
1	G	181	TYR
1	G	201	PHE
1	G	212	ASN
1	G	246	ARG
1	G	248	LYS
1	G	253	ASN
1	G	267	LEU
1	G	283	ILE
1	G	303	LYS
1	G	359	THR
1	G	369	GLN
1	G	396	THR
1	G	397	GLU
2	H	46	ARG
2	H	48	GLN
2	H	62	LEU
2	H	83	VAL
2	H	103	CYS
2	H	118	ASN
2	H	119	ARG
2	H	131	ARG
2	H	135	ARG
2	H	139	ARG
2	H	144	HIS
2	H	151	ASN
2	H	168	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	171	LEU
2	H	172	VAL
2	H	205	ARG
2	H	293	THR
2	H	310	ARG
2	H	324	GLU
2	H	330	HIS
1	I	28	HIS
1	I	50	LYS
1	I	52	LYS
1	I	94	CYS
1	I	95	PHE
1	I	110	ARG
1	I	120	LYS
1	I	130	GLN
1	I	143	ARG
1	I	162	LEU
1	I	167	LEU
1	I	188	TYR
1	I	214	LEU
1	I	226	GLN
1	I	246	ARG
1	I	252	LEU
1	I	268	ARG
1	I	281	ILE
1	I	296	THR
1	I	305	THR
1	I	341	LYS
1	I	353	PHE
1	I	355	PHE
1	I	366	PHE
1	I	391	TYR
2	J	9	TYR
2	J	41	HIS
2	J	44	VAL
2	J	56	LYS
2	J	85	THR
2	J	97	TYR
2	J	119	ARG
2	J	124	VAL
2	J	131	ARG
2	J	135	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	138	TYR
2	J	143	GLU
2	J	156	LYS
2	J	160	GLN
2	J	171	LEU
2	J	186	LYS
2	J	197	TYR
2	J	230	ASN
2	J	239	ARG
2	J	254	VAL
2	J	266	THR
2	J	267	LEU
2	J	277	HIS
2	J	305	ARG
2	J	306	GLN
2	J	310	ARG
2	J	324	GLU
2	J	325	TYR
2	J	329	ASN
2	J	336	TRP
2	J	346	HIS
1	K	18	LEU
1	K	52	LYS
1	K	69	THR
1	K	94	CYS
1	K	95	PHE
1	K	107	TYR
1	K	132	MET
1	K	143	ARG
1	K	156	LYS
1	K	171	TRP
1	K	197	LYS
1	K	224	ARG
1	K	246	ARG
1	K	262	ILE
1	K	290	ARG
1	K	300	LEU
1	K	301	GLU
1	K	305	THR
1	K	359	THR
1	K	363	HIS
1	K	395	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	65	MET
2	L	119	ARG
2	L	120	HIS
2	L	131	ARG
2	L	135	ARG
2	L	157	ARG
2	L	171	LEU
2	L	177	LEU
2	L	196	LYS
2	L	209	THR
2	L	230	ASN
2	L	280	LEU
2	L	293	THR
2	L	315	ASN
2	L	334	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	28	HIS
1	A	73	HIS
1	A	150	ASN
2	B	8	GLN
2	B	41	HIS
2	B	120	HIS
2	B	167	HIS
2	B	175	HIS
1	C	28	HIS
1	C	183	HIS
1	C	332	HIS
2	D	162	HIS
2	D	167	HIS
2	D	194	GLN
2	D	275	HIS
2	D	302	ASN
1	E	217	ASN
1	E	395	HIS
2	F	5	HIS
2	F	73	GLN
2	F	95	HIS
2	F	144	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	222	GLN
2	F	230	ASN
2	F	302	ASN
2	F	306	GLN
2	F	346	HIS
1	G	226	GLN
1	G	236	GLN
1	G	332	HIS
2	H	5	HIS
2	H	21	ASN
2	H	118	ASN
2	H	126	HIS
2	H	144	HIS
2	H	151	ASN
2	H	175	HIS
2	H	253	HIS
2	H	275	HIS
2	H	350	HIS
1	I	134	ASN
1	I	332	HIS
1	I	343	ASN
1	I	387	HIS
1	I	394	GLN
2	J	144	HIS
2	J	155	HIS
2	J	162	HIS
2	J	213	HIS
2	J	230	ASN
2	J	253	HIS
2	J	288	HIS
2	J	346	HIS
1	K	3	HIS
1	K	361	ASN
1	K	395	HIS
2	L	24	HIS
2	L	82	HIS
2	L	95	HIS
2	L	102	GLN
2	L	144	HIS
2	L	160	GLN
2	L	162	HIS
2	L	167	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	168	GLN
2	L	253	HIS
2	L	275	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.

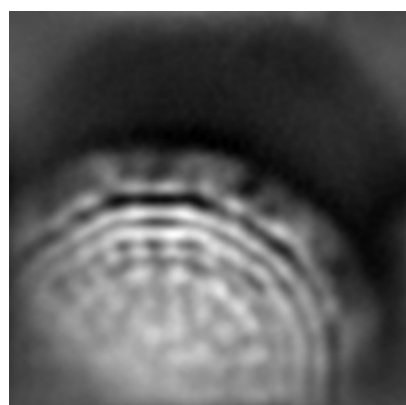
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24205. These allow visual inspection of the internal detail of the map and identification of artifacts.

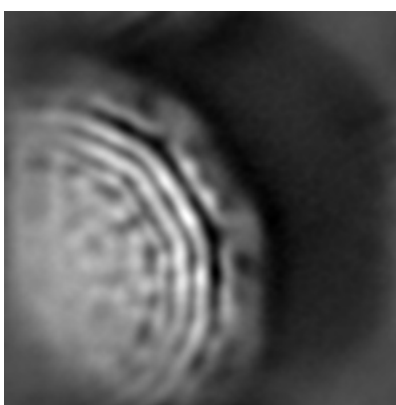
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

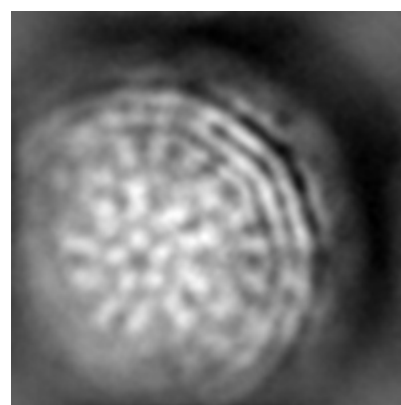
6.1.1 Primary map



X



Y

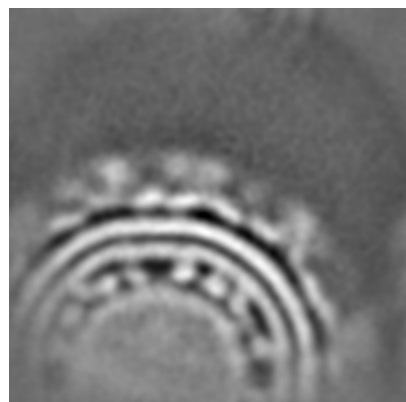


Z

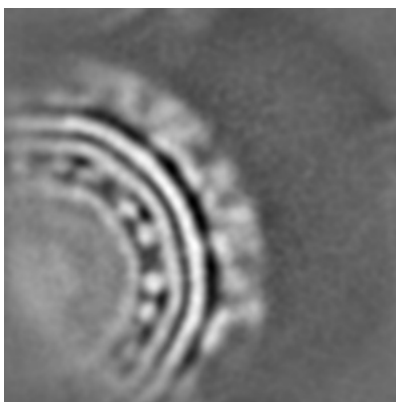
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

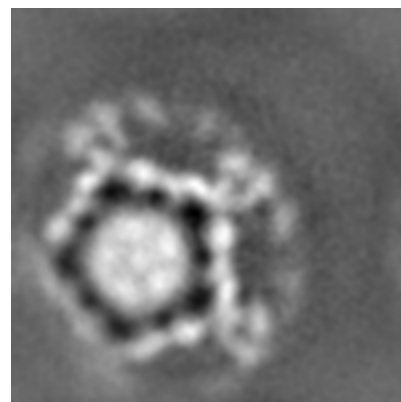
6.2.1 Primary map



X Index: 54



Y Index: 54

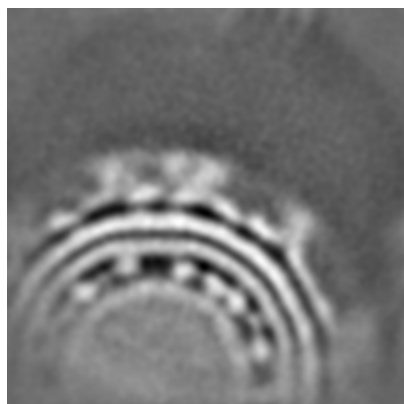


Z Index: 54

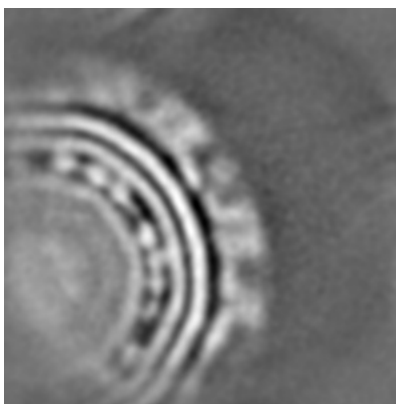
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

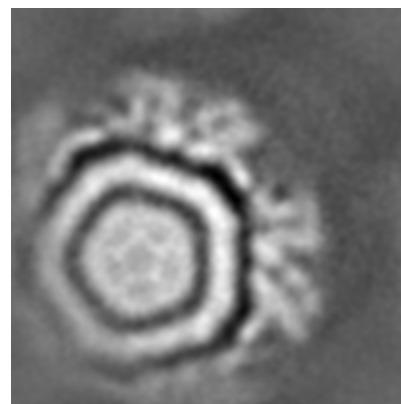
6.3.1 Primary map



X Index: 52



Y Index: 52

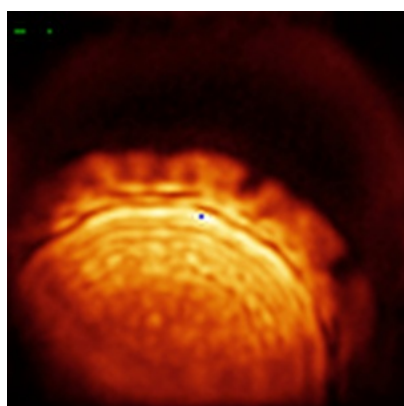


Z Index: 47

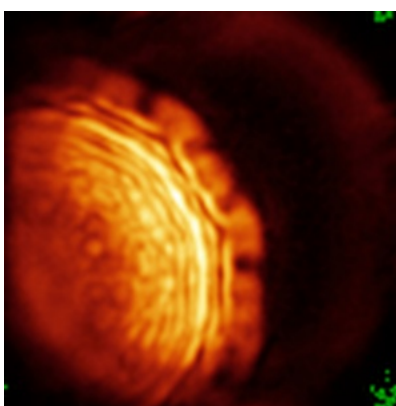
The images above show the largest variance slices of the map in three orthogonal directions.

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

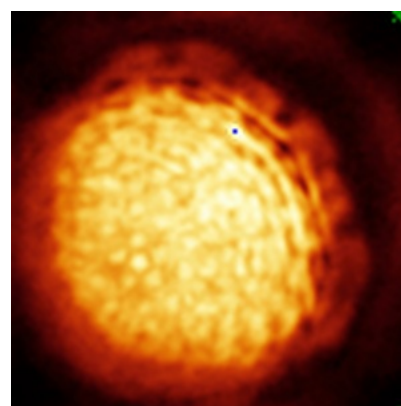
6.4.1 Primary map



X



Y

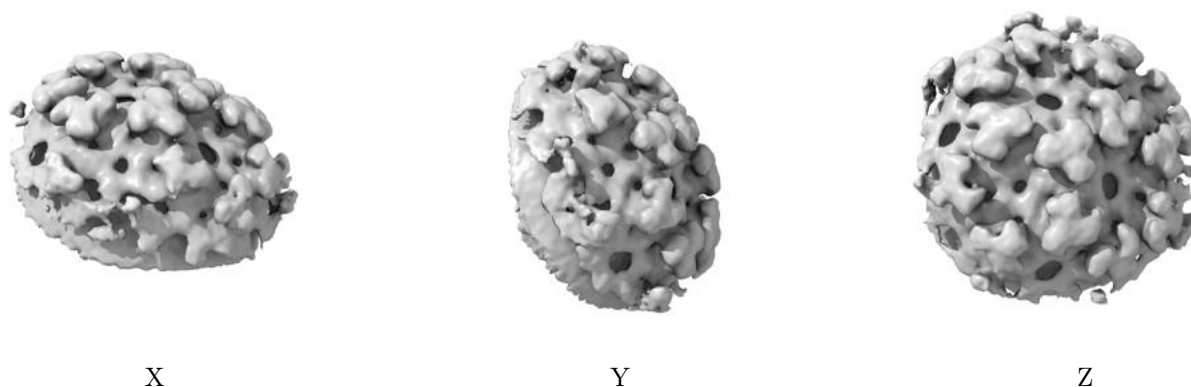


Z

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

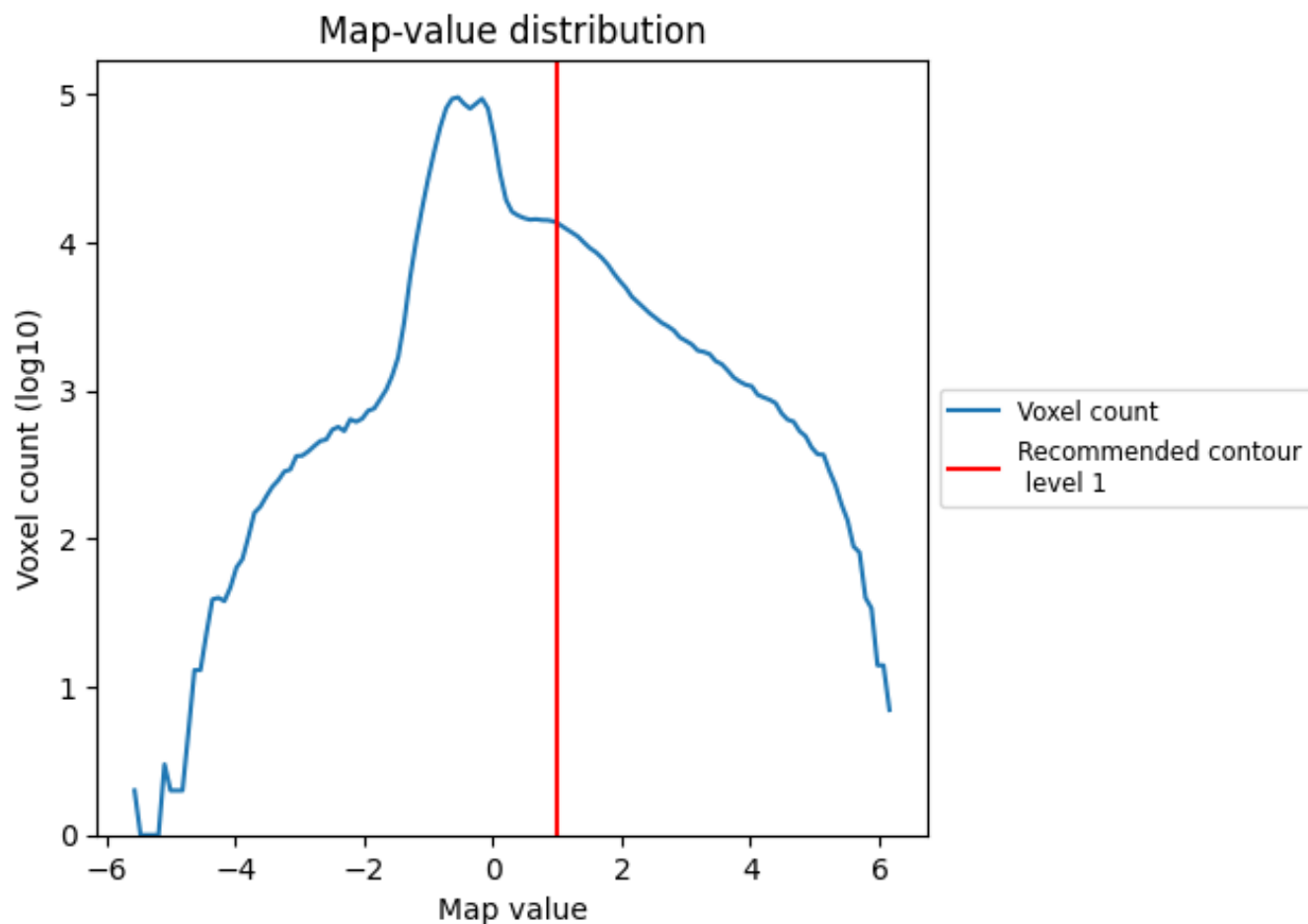
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

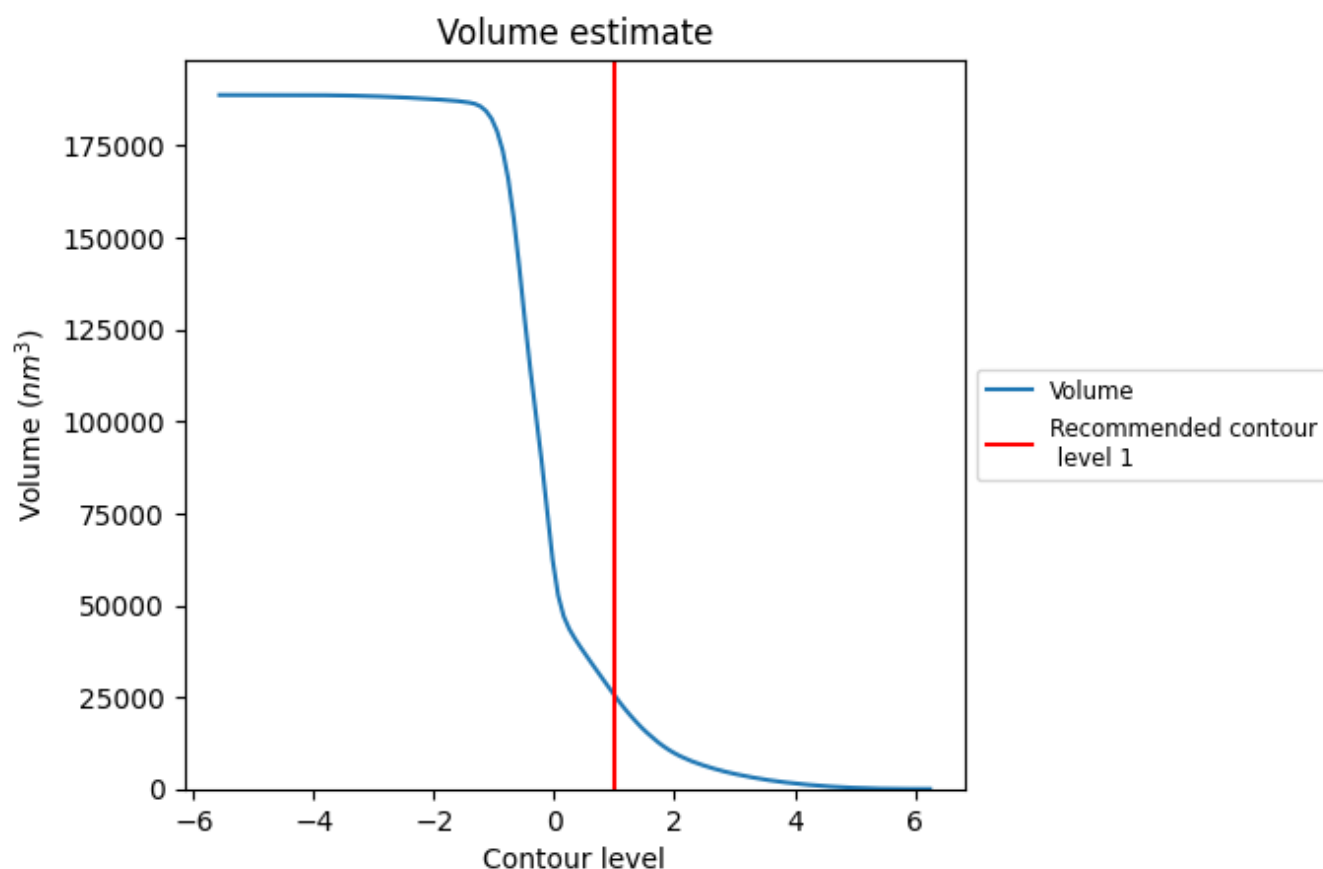
This section contains the results of statistical analysis of the map.

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.

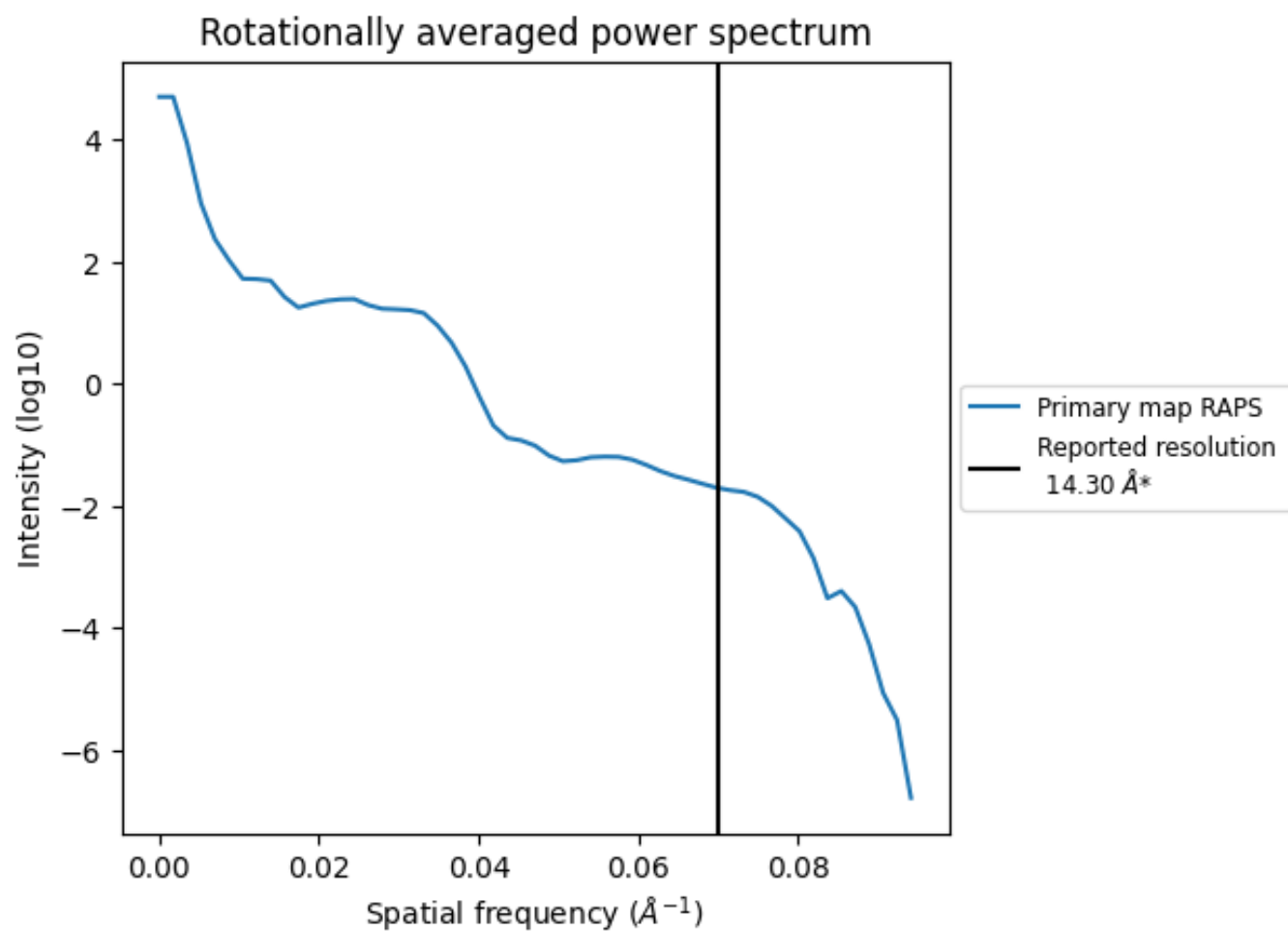
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25541 nm^3 ; this corresponds to an approximate mass of 23072 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 ⓘ

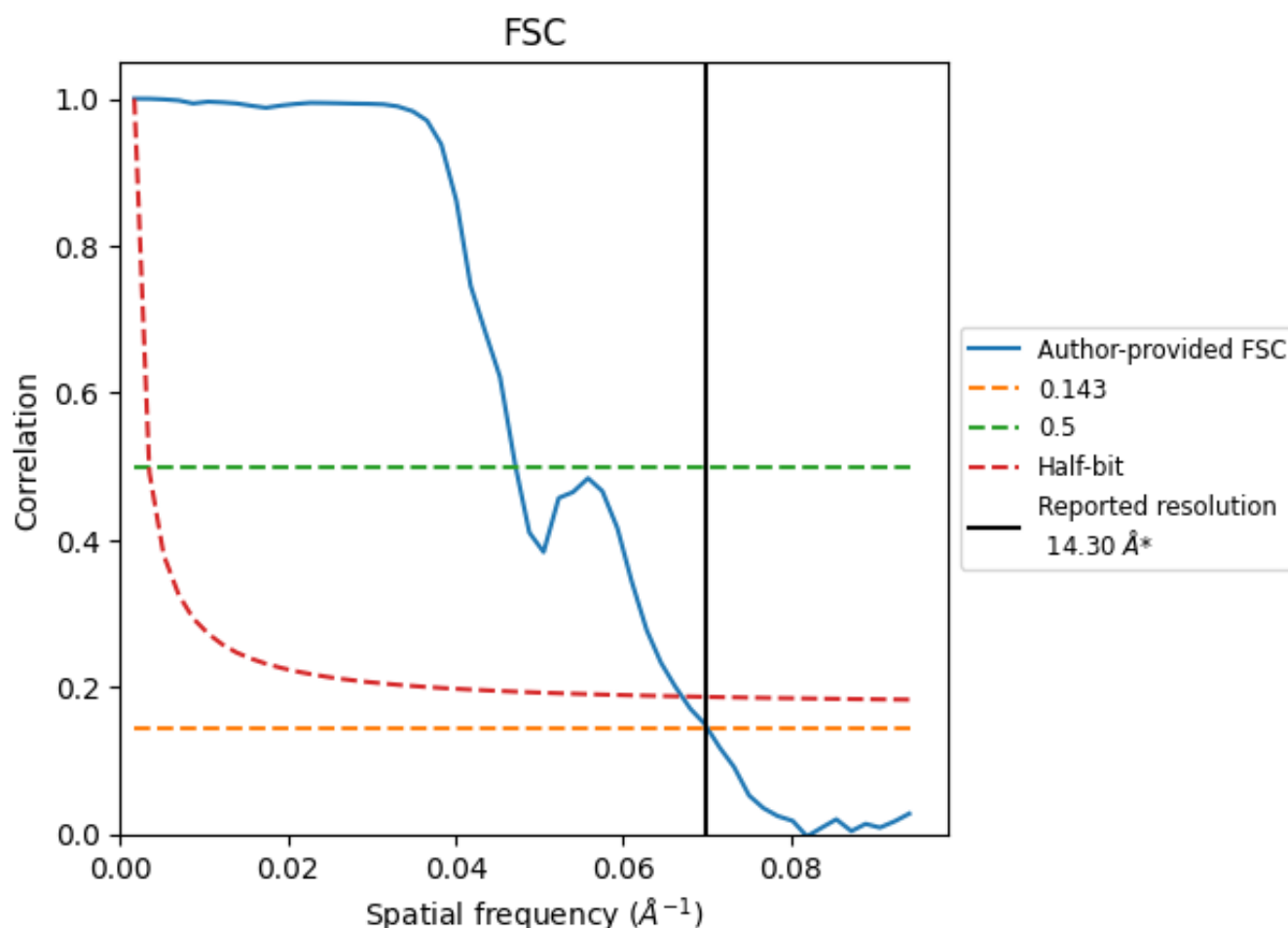


*Reported resolution corresponds to spatial frequency of 0.070 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.070 Å⁻¹

8.2 Resolution estimates [i](#)

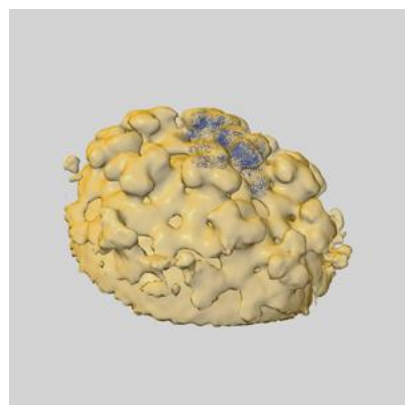
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.30	-	-
Author-provided FSC curve	14.27	21.23	14.93
Unmasked-calculated*	-	-	-

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

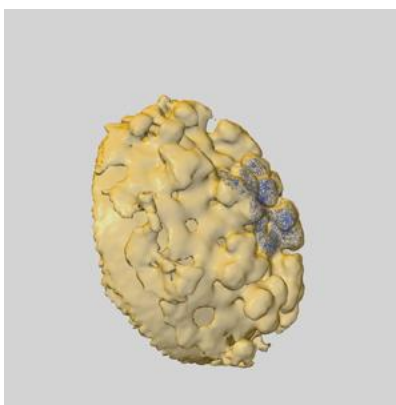
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24205 and PDB model 7N6A. Per-residue inclusion information can be found in section [3](#) on page [5](#).

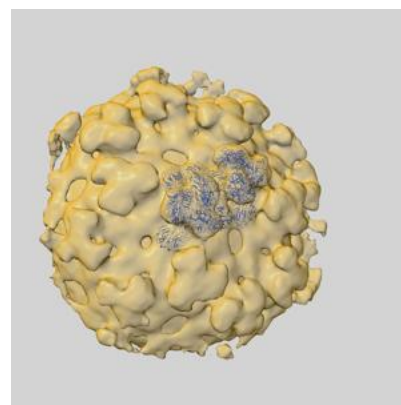
9.1 Map-model overlay [i](#)



X



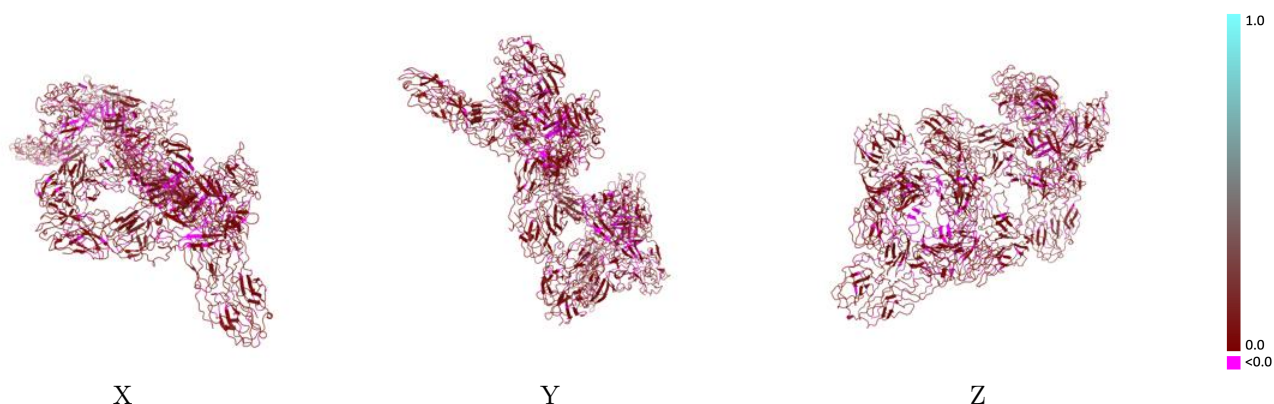
Y



Z

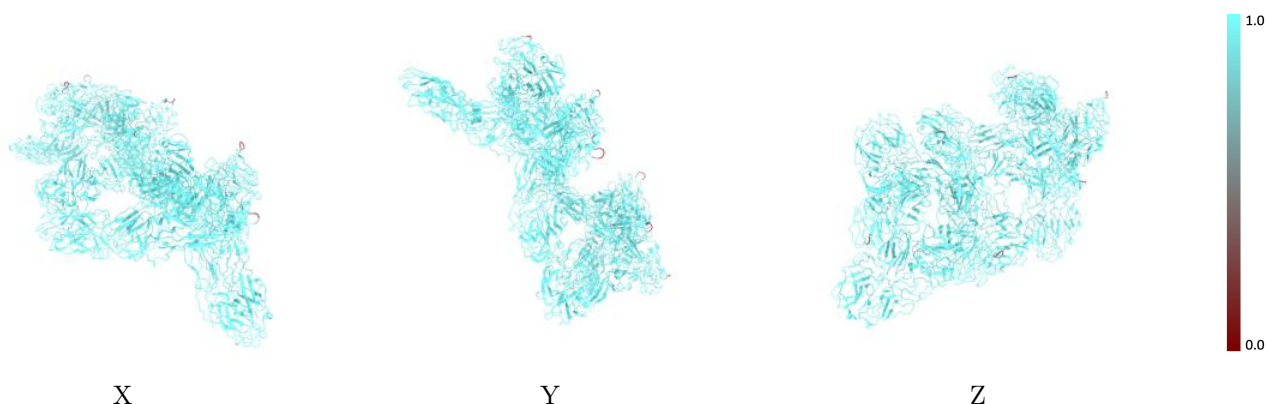
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



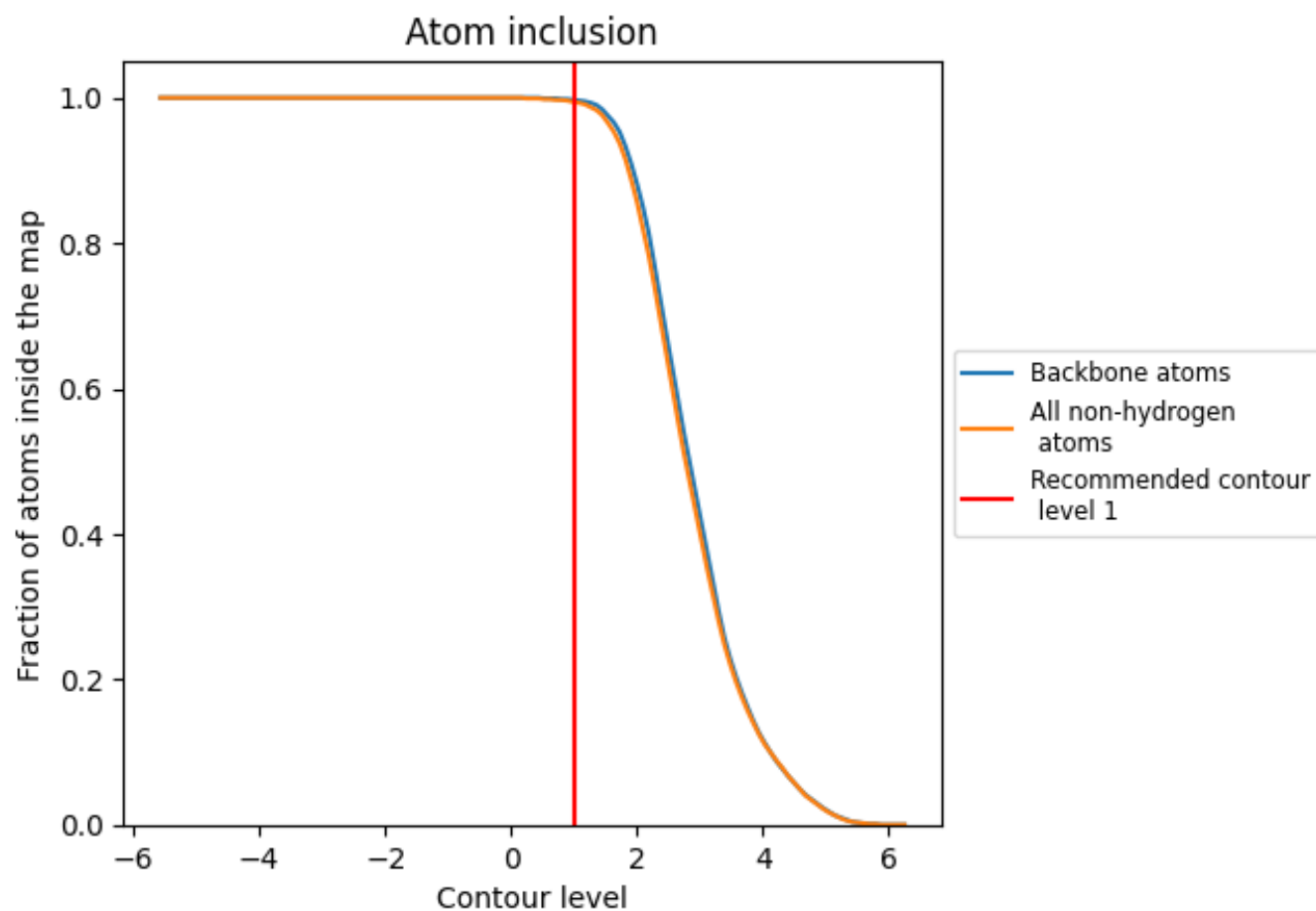
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9940	<div></div> 0.0660
A	<div></div> 1.0000	<div></div> 0.0740
B	<div></div> 0.9950	<div></div> 0.0620
C	<div></div> 0.9980	<div></div> 0.0680
D	<div></div> 0.9910	<div></div> 0.0710
E	<div></div> 0.9990	<div></div> 0.0660
F	<div></div> 0.9900	<div></div> 0.0660
G	<div></div> 0.9990	<div></div> 0.0660
H	<div></div> 0.9900	<div></div> 0.0640
I	<div></div> 0.9990	<div></div> 0.0690
J	<div></div> 0.9860	<div></div> 0.0550
K	<div></div> 0.9990	<div></div> 0.0620
L	<div></div> 0.9840	<div></div> 0.0590

1.0

0.0

<0.0