



## Full wwPDB EM Validation Report ⓘ

Apr 28, 2024 – 08:04 am BST

PDB ID : 3ZYS  
EMDB ID : EMD-1949  
Title : Human dynamin 1 deltaPRD polymer stabilized with GMPPCP  
Authors : Chappie, J.S.; Mears, J.A.; Fang, S.; Leonard, M.; Schmid, S.L.; Milligan, R.A.; Hinshaw, J.E.; Dyda, F.  
Deposited on : 2011-08-24  
Resolution : 12.20 Å (reported)  
Based on initial models : 3LJB, 2X2E, 1DYN

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

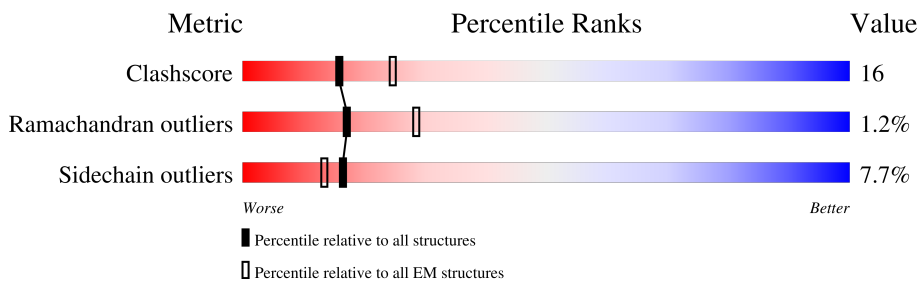
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	353	
1	D	353	
2	B	662	
2	E	662	
3	C	113	
3	F	113	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10677 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 DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	330	2573	1618	454	491	10	0	0
1	D	330	2573	1618	454	491	10	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	LYS	-	linker	UNP Q05193
A	322	HIS	-	linker	UNP Q05193
A	323	GLY	-	linker	UNP Q05193
A	324	THR	-	linker	UNP Q05193
A	325	ASP	-	linker	UNP Q05193
A	326	SER	-	linker	UNP Q05193
A	327	ARG	-	linker	UNP Q05193
A	328	VAL	-	linker	UNP Q05193
A	744	ASN	ASP	variant	UNP Q05193
D	321	LYS	-	linker	UNP Q05193
D	322	HIS	-	linker	UNP Q05193
D	323	GLY	-	linker	UNP Q05193
D	324	THR	-	linker	UNP Q05193
D	325	ASP	-	linker	UNP Q05193
D	326	SER	-	linker	UNP Q05193
D	327	ARG	-	linker	UNP Q05193
D	328	VAL	-	linker	UNP Q05193
D	744	ASN	ASP	variant	UNP Q05193

- Molecule 2 is a protein called INTERFERON-INDUCED GTP-BINDING PROTEIN MX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	211	1781	1135	308	330	8	0	0

*Continued on next page...*

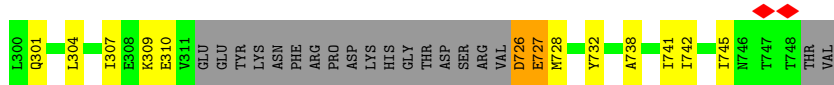
*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	219	1858	1187	318	344	9	0	0

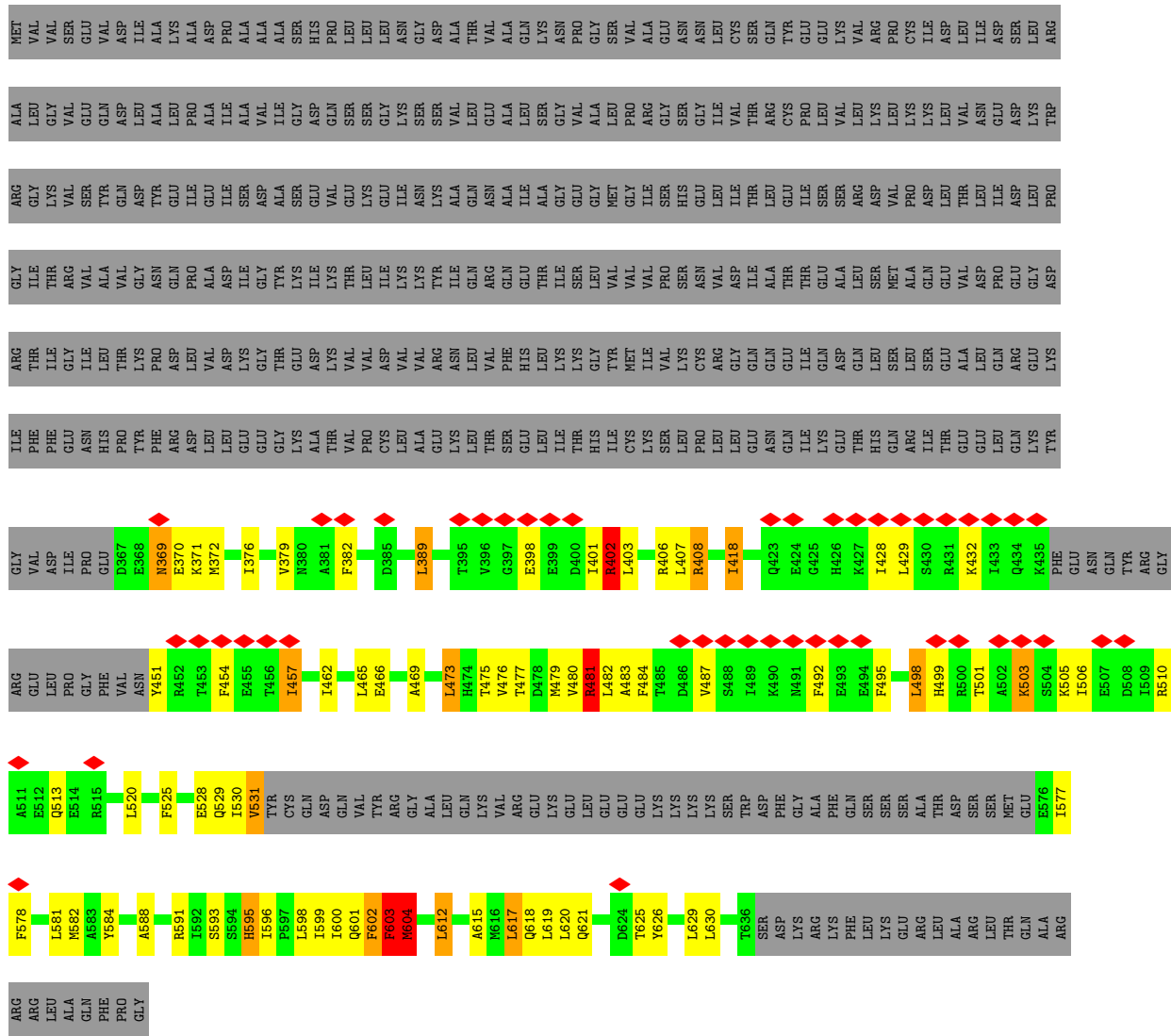
- Molecule 3 is a protein called DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	113	946	609	158	175	4	0	0
3	F	113	946	609	158	175	4	0	0

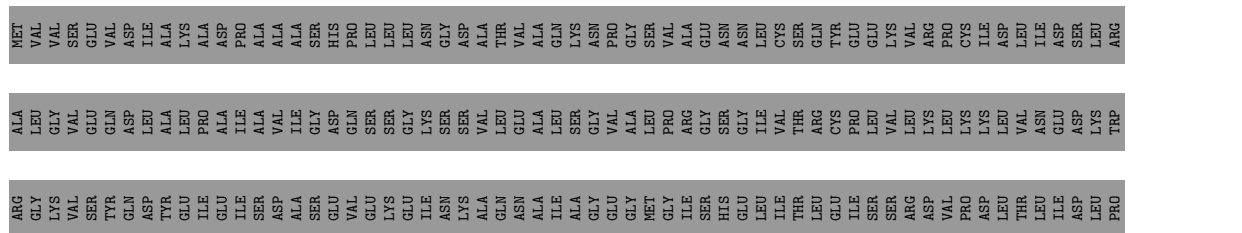


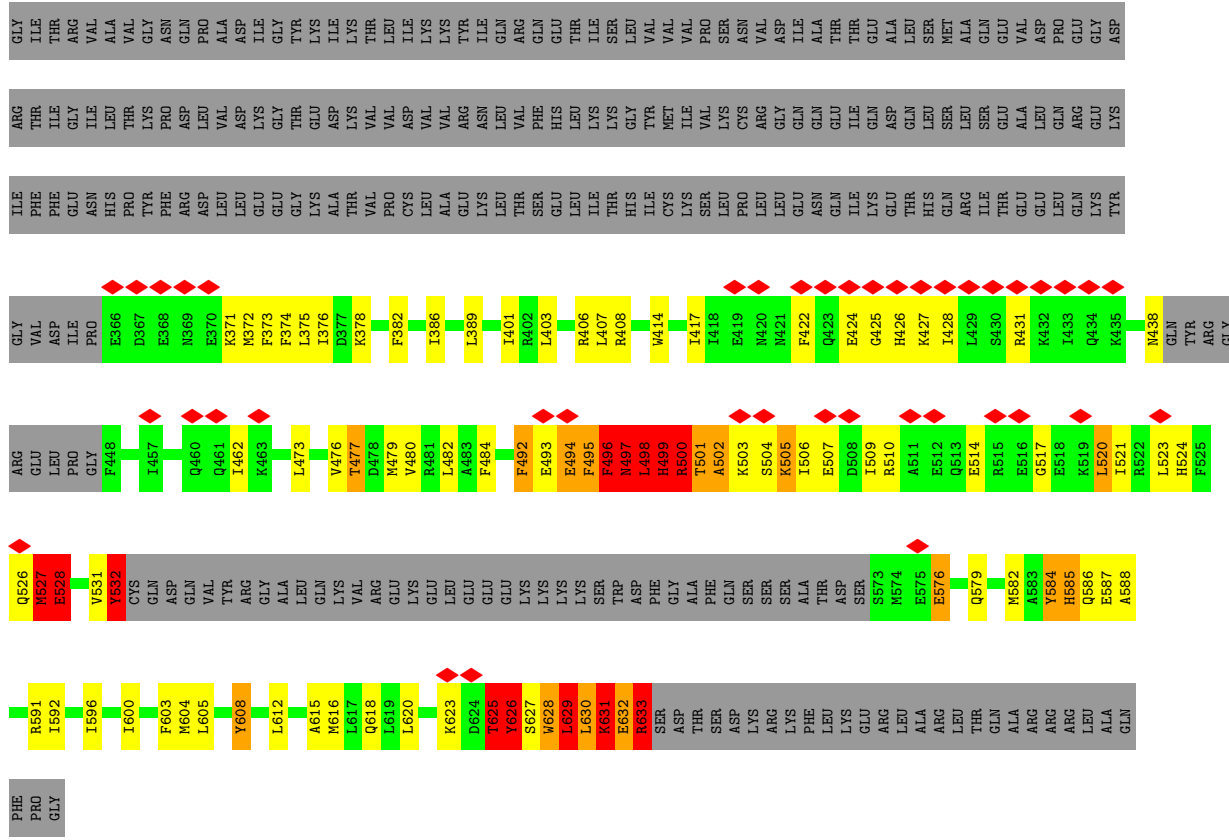


• Molecule 2: INTERFERON-INDUCED GTP-BINDING PROTEIN MX1

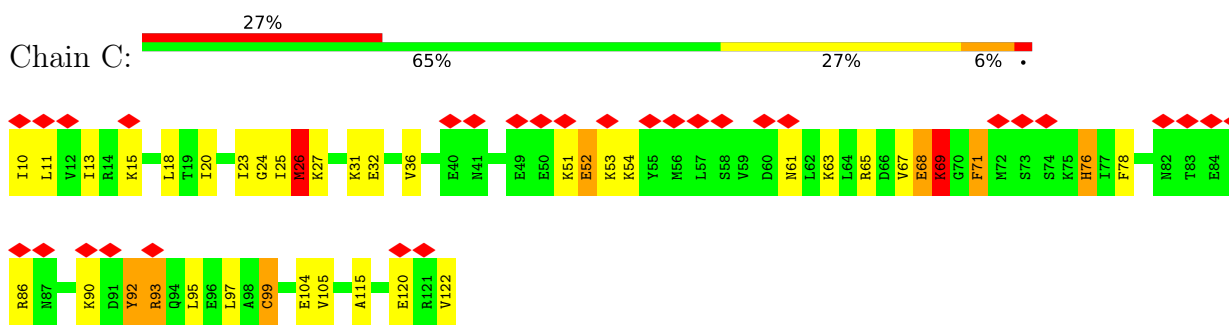


• Molecule 2: INTERFERON-INDUCED GTP-BINDING PROTEIN MX1

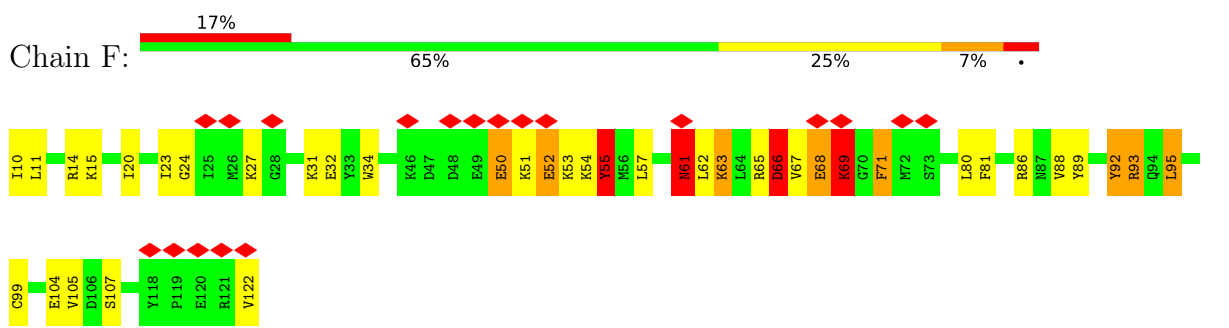




• Molecule 3: DYNAMIN-1



• Molecule 3: DYNAMIN-1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	4814	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL IMAGES USING ACE2	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	10	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	50000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	817.054	Depositor
Minimum map value	-749.478	Depositor
Average map value	37.001	Depositor
Map value standard deviation	200.731	Depositor
Recommended contour level	227.0	Depositor
Map size (Å)	452, 452, 452	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.26, 2.26, 2.26	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	0.72	1/2610 (0.0%)	1.29	29/3532 (0.8%)
1	D	0.79	5/2610 (0.2%)	1.28	31/3532 (0.9%)
2	B	0.81	1/1812 (0.1%)	1.27	16/2428 (0.7%)
2	E	1.25	16/1892 (0.8%)	2.67	105/2535 (4.1%)
3	C	0.76	1/966 (0.1%)	1.18	13/1298 (1.0%)
3	F	0.88	3/966 (0.3%)	1.42	18/1298 (1.4%)
All	All	0.88	27/10856 (0.2%)	1.61	212/14623 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	18
1	D	3	11
2	B	1	8
2	E	9	27
3	C	2	4
3	F	2	7
All	All	18	75

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	495	PHE	C-O	-14.80	0.95	1.23
2	E	497	ASN	C-O	-13.73	0.97	1.23
1	D	61	SER	CB-OG	-11.78	1.26	1.42
2	E	500	ARG	CD-NE	-9.87	1.29	1.46
2	E	496	PHE	C-O	-9.86	1.04	1.23
1	D	61	SER	CA-CB	9.01	1.66	1.52
2	E	496	PHE	CG-CD2	-6.98	1.28	1.38
1	D	115	ILE	N-CA	-6.89	1.32	1.46

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	SER	N-CA	-6.86	1.32	1.46
1	D	245	LYS	CA-CB	-6.83	1.39	1.53
3	F	61	ASN	CA-CB	-6.67	1.35	1.53
2	E	500	ARG	CB-CG	-6.66	1.34	1.52
2	E	504	SER	CB-OG	-6.24	1.34	1.42
2	E	498	LEU	C-N	-6.13	1.20	1.34
2	E	627	SER	CB-OG	-5.93	1.34	1.42
2	E	500	ARG	C-O	-5.88	1.12	1.23
3	F	66	ASP	CA-CB	-5.49	1.41	1.53
2	E	628	TRP	C-O	-5.41	1.13	1.23
2	B	603	PHE	CA-CB	-5.34	1.42	1.53
2	E	495	PHE	N-CA	-5.33	1.35	1.46
1	D	130	LEU	CA-CB	-5.27	1.41	1.53
2	E	500	ARG	N-CA	-5.26	1.35	1.46
3	F	53	LYS	N-CA	-5.25	1.35	1.46
2	E	579	GLN	CA-CB	-5.24	1.42	1.53
2	E	496	PHE	N-CA	-5.23	1.35	1.46
3	C	53	LYS	N-CA	-5.18	1.35	1.46
2	E	497	ASN	N-CA	-5.04	1.36	1.46

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	497	ASN	O-C-N	-36.57	64.19	122.70
2	E	500	ARG	NE-CZ-NH2	36.18	138.39	120.30
2	E	496	PHE	O-C-N	-33.97	68.35	122.70
2	E	495	PHE	O-C-N	-24.51	83.48	122.70
2	E	497	ASN	C-N-CA	21.47	175.38	121.70
2	E	500	ARG	CD-NE-CZ	20.40	152.17	123.60
2	E	498	LEU	O-C-N	-19.38	91.69	122.70
2	E	495	PHE	C-N-CA	17.31	164.97	121.70
2	E	498	LEU	C-N-CA	17.09	164.44	121.70
2	E	496	PHE	C-N-CA	16.64	163.29	121.70
1	A	67	ARG	NE-CZ-NH1	-16.54	112.03	120.30
2	E	496	PHE	CA-C-N	16.15	152.72	117.20
1	A	129	VAL	CA-CB-CG1	-15.90	87.06	110.90
2	E	498	LEU	CA-C-N	15.45	151.19	117.20
2	B	408	ARG	NE-CZ-NH1	-15.22	112.69	120.30
2	E	495	PHE	CA-C-N	14.51	149.13	117.20
2	E	498	LEU	CA-CB-CG	14.17	147.89	115.30
1	D	224	LEU	CB-CG-CD1	14.02	134.83	111.00
2	E	494	GLU	C-N-CA	13.99	156.69	121.70

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	ARG	NE-CZ-NH1	-13.81	113.39	120.30
1	D	67	ARG	NE-CZ-NH1	-13.80	113.40	120.30
2	E	625	THR	CA-CB-CG2	13.69	131.57	112.40
2	E	500	ARG	CG-CD-NE	13.64	140.44	111.80
2	E	497	ASN	CA-C-N	13.51	146.92	117.20
2	E	532	TYR	CB-CG-CD2	-13.22	113.07	121.00
2	B	603	PHE	N-CA-CB	13.09	134.16	110.60
2	E	625	THR	O-C-N	-13.05	101.83	122.70
2	E	579	GLN	N-CA-CB	13.02	134.03	110.60
2	E	501	THR	CA-CB-CG2	12.80	130.32	112.40
2	E	500	ARG	O-C-N	-12.58	102.57	122.70
1	D	114	GLY	C-N-CA	12.21	152.23	121.70
2	E	498	LEU	CB-CG-CD2	12.19	131.72	111.00
2	B	604	MET	N-CA-CB	12.13	132.44	110.60
1	A	60	GLY	C-N-CA	11.99	151.67	121.70
1	D	67	ARG	NE-CZ-NH2	11.52	126.06	120.30
3	F	61	ASN	CA-CB-CG	11.41	138.51	113.40
2	E	497	ASN	CA-C-O	11.38	144.00	120.10
2	E	527	MET	CG-SD-CE	-11.27	82.17	100.20
2	E	499	HIS	C-N-CA	11.27	149.87	121.70
1	A	125	TYR	CB-CG-CD2	-11.21	114.27	121.00
2	E	496	PHE	N-CA-C	11.19	141.20	111.00
2	E	497	ASN	N-CA-C	11.19	141.21	111.00
2	E	527	MET	O-C-N	-11.17	104.83	122.70
2	E	496	PHE	CZ-CE2-CD2	-11.05	106.84	120.10
2	E	576	GLU	CA-CB-CG	11.00	137.61	113.40
2	E	499	HIS	O-C-N	-10.96	105.16	122.70
3	F	50	GLU	CA-CB-CG	10.83	137.22	113.40
2	E	500	ARG	CB-CG-CD	10.75	139.54	111.60
2	E	500	ARG	NH1-CZ-NH2	-10.54	107.80	119.40
2	E	527	MET	CA-CB-CG	10.31	130.82	113.30
1	A	61	SER	N-CA-CB	10.28	125.92	110.50
2	E	495	PHE	CB-CA-C	10.28	130.96	110.40
2	E	532	TYR	CA-C-O	10.27	141.67	120.10
2	E	628	TRP	O-C-N	-10.19	106.39	122.70
2	E	505	LYS	CD-CE-NZ	10.04	134.79	111.70
1	D	72	GLN	CB-CA-C	9.70	129.80	110.40
2	E	631	LYS	CA-CB-CG	9.63	134.59	113.40
2	E	633	ARG	NE-CZ-NH2	9.59	125.09	120.30
2	B	601	GLN	CA-CB-CG	9.58	134.48	113.40
1	A	72	GLN	CB-CA-C	9.55	129.50	110.40
1	D	61	SER	CA-CB-OG	-9.53	85.46	111.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	THR	N-CA-CB	9.51	128.37	110.30
1	A	131	ASN	C-N-CA	9.48	145.41	121.70
1	A	212	GLU	CA-CB-CG	9.45	134.18	113.40
2	E	498	LEU	N-CA-CB	9.44	129.28	110.40
1	D	212	GLU	CA-CB-CG	9.33	133.93	113.40
2	E	629	LEU	CA-C-N	9.31	137.69	117.20
1	D	90	LYS	C-N-CA	9.30	144.96	121.70
2	B	602	PHE	O-C-N	-9.16	108.05	122.70
2	E	499	HIS	CB-CA-C	9.11	128.62	110.40
3	F	66	ASP	CB-CG-OD1	-8.89	110.30	118.30
1	A	125	TYR	CB-CG-CD1	8.73	126.24	121.00
1	D	130	LEU	N-CA-CB	8.57	127.54	110.40
2	B	603	PHE	CA-C-O	8.51	137.97	120.10
1	A	129	VAL	C-N-CA	8.38	142.64	121.70
2	E	495	PHE	CB-CG-CD1	8.28	126.60	120.80
2	E	532	TYR	CB-CG-CD1	8.22	125.93	121.00
2	B	402	ARG	NE-CZ-NH1	-8.22	116.19	120.30
2	E	631	LYS	CB-CG-CD	8.20	132.93	111.60
1	A	73	LEU	N-CA-CB	8.16	126.71	110.40
2	E	629	LEU	O-C-N	-8.14	109.67	122.70
2	E	438	ASN	CA-C-O	-8.11	103.08	120.10
2	E	626	TYR	N-CA-CB	8.09	125.16	110.60
1	A	140	MET	CA-CB-CG	7.92	126.77	113.30
1	D	130	LEU	CA-CB-CG	7.91	133.49	115.30
1	A	130	LEU	N-CA-CB	7.89	126.18	110.40
2	E	495	PHE	CD1-CG-CD2	-7.81	108.14	118.30
3	C	52	GLU	C-N-CA	7.80	141.21	121.70
1	A	134	LEU	CB-CG-CD2	7.79	124.24	111.00
1	D	201	ILE	CG1-CB-CG2	-7.69	94.48	111.40
2	E	527	MET	CA-C-O	7.68	136.24	120.10
2	E	496	PHE	CB-CA-C	-7.68	95.04	110.40
2	E	499	HIS	CA-C-N	7.65	134.03	117.20
3	F	66	ASP	N-CA-CB	7.56	124.21	110.60
3	F	52	GLU	C-N-CA	7.56	140.59	121.70
2	E	631	LYS	CG-CD-CE	7.44	134.22	111.90
1	D	245	LYS	CB-CG-CD	-7.36	92.45	111.60
1	D	90	LYS	O-C-N	-7.34	110.96	122.70
2	E	628	TRP	CZ3-CH2-CZ2	-7.30	112.83	121.60
2	E	493	GLU	N-CA-CB	7.25	123.66	110.60
1	A	130	LEU	CA-CB-CG	7.25	131.97	115.30
1	A	59	ARG	O-C-N	-7.24	110.89	123.20
1	D	91	PHE	N-CA-CB	7.22	123.60	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	ARG	CD-NE-CZ	7.20	133.68	123.60
2	B	602	PHE	C-N-CA	7.19	139.67	121.70
2	E	500	ARG	N-CA-CB	7.17	123.50	110.60
2	E	507	GLU	O-C-N	-7.16	111.25	122.70
1	D	131	ASN	C-N-CA	7.12	139.50	121.70
2	E	576	GLU	N-CA-CB	7.11	123.39	110.60
1	D	115	ILE	N-CA-CB	7.11	127.14	110.80
3	C	69	LYS	C-N-CA	7.10	137.22	122.30
2	B	621	GLN	CG-CD-OE1	-7.07	107.46	121.60
2	E	633	ARG	N-CA-C	7.02	129.96	111.00
3	F	61	ASN	CB-CG-OD1	7.02	135.64	121.60
3	C	26	MET	N-CA-CB	6.98	123.17	110.60
2	E	501	THR	O-C-N	-6.98	111.53	122.70
2	E	626	TYR	CE1-CZ-CE2	-6.95	108.69	119.80
3	F	61	ASN	CB-CA-C	6.90	124.20	110.40
3	F	55	TYR	N-CA-CB	6.87	122.96	110.60
1	D	272	MET	C-N-CA	6.80	136.58	122.30
3	F	53	LYS	N-CA-CB	6.79	122.81	110.60
2	B	603	PHE	O-C-N	-6.74	111.92	122.70
1	D	123	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	131	ASN	O-C-N	-6.69	112.00	122.70
3	F	61	ASN	CB-CG-ND2	-6.67	100.70	116.70
2	E	626	TYR	CZ-CE2-CD2	-6.66	113.81	119.80
2	E	497	ASN	CB-CA-C	-6.62	97.16	110.40
1	A	129	VAL	CA-C-N	6.61	131.74	117.20
2	E	629	LEU	CB-CG-CD2	6.59	122.21	111.00
3	C	53	LYS	N-CA-CB	6.58	122.44	110.60
3	F	93	ARG	C-N-CA	6.56	138.10	121.70
1	A	223	LYS	CD-CE-NZ	6.55	126.76	111.70
2	B	529	GLN	O-C-N	-6.52	112.27	122.70
1	A	67	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	E	503	LYS	O-C-N	-6.48	112.34	122.70
2	E	498	LEU	CB-CG-CD1	-6.44	100.05	111.00
1	A	125	TYR	N-CA-CB	6.43	122.18	110.60
2	E	628	TRP	CG-CD2-CE3	6.39	139.66	133.90
2	E	492	PHE	N-CA-CB	6.38	122.08	110.60
1	A	221	GLU	OE1-CD-OE2	-6.37	115.65	123.30
3	F	69	LYS	C-N-CA	6.36	135.65	122.30
2	E	495	PHE	CG-CD1-CE1	6.33	127.76	120.80
3	C	25	ILE	C-N-CA	6.28	137.39	121.70
2	E	503	LYS	CA-CB-CG	6.24	127.12	113.40
2	E	626	TYR	CD1-CE1-CZ	-6.23	114.19	119.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	502	ALA	N-CA-CB	6.21	118.80	110.10
3	C	76	HIS	N-CA-CB	6.19	121.75	110.60
1	D	91	PHE	O-C-N	-6.19	112.80	122.70
2	E	527	MET	N-CA-CB	6.17	121.70	110.60
2	E	497	ASN	N-CA-CB	6.12	121.62	110.60
2	E	494	GLU	O-C-N	-6.10	112.94	122.70
2	E	633	ARG	CG-CD-NE	6.09	124.59	111.80
2	E	633	ARG	CD-NE-CZ	6.04	132.05	123.60
3	C	93	ARG	C-N-CA	6.03	136.79	121.70
1	A	228	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	E	492	PHE	O-C-N	-5.98	113.13	122.70
2	B	617	LEU	C-N-CA	5.98	136.65	121.70
1	A	73	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	A	67	ARG	CD-NE-CZ	5.96	131.94	123.60
3	F	51	LYS	C-N-CA	5.95	136.56	121.70
3	C	51	LYS	C-N-CA	5.92	136.49	121.70
2	B	603	PHE	CB-CG-CD1	5.87	124.91	120.80
2	E	527	MET	C-N-CA	5.87	136.36	121.70
2	B	481	ARG	NE-CZ-NH1	-5.84	117.38	120.30
2	E	495	PHE	CG-CD2-CE2	5.84	127.23	120.80
1	D	245	LYS	N-CA-CB	5.81	121.05	110.60
2	E	500	ARG	CA-C-N	5.80	129.95	117.20
1	A	130	LEU	CB-CA-C	5.77	121.16	110.20
2	E	625	THR	OG1-CB-CG2	5.74	123.21	110.00
3	C	52	GLU	N-CA-CB	5.74	120.92	110.60
3	F	93	ARG	O-C-N	-5.73	113.54	122.70
1	D	201	ILE	CA-CB-CG1	-5.70	100.16	111.00
2	E	502	ALA	O-C-N	-5.69	113.60	122.70
2	E	628	TRP	CH2-CZ2-CE2	-5.67	111.73	117.40
1	D	270	ASP	C-N-CA	5.65	135.83	121.70
3	C	93	ARG	O-C-N	-5.62	113.71	122.70
2	E	626	TYR	CG-CD2-CE2	-5.61	116.82	121.30
3	F	67	VAL	C-N-CA	5.58	135.66	121.70
2	E	510	ARG	CD-NE-CZ	5.55	131.38	123.60
1	D	178	ASN	C-N-CA	5.52	135.50	121.70
2	E	386	ILE	CB-CG1-CD1	-5.52	98.45	113.90
1	D	270	ASP	O-C-N	-5.47	113.95	122.70
1	D	61	SER	N-CA-CB	-5.46	102.31	110.50
3	C	92	TYR	N-CA-C	5.45	125.72	111.00
2	E	528	GLU	O-C-N	-5.45	113.98	122.70
2	E	502	ALA	C-N-CA	5.44	135.30	121.70
2	E	417	ILE	CA-CB-CG1	5.43	121.31	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	92	TYR	N-CA-C	5.39	125.56	111.00
1	D	115	ILE	CA-CB-CG1	-5.39	100.76	111.00
2	E	630	LEU	N-CA-C	5.38	125.53	111.00
2	E	625	THR	CA-C-O	5.35	131.34	120.10
2	E	496	PHE	CB-CG-CD1	5.34	124.54	120.80
1	D	224	LEU	CB-CA-C	5.33	120.34	110.20
2	E	417	ILE	CB-CG1-CD1	5.32	128.80	113.90
2	B	621	GLN	CG-CD-NE2	5.32	129.46	116.70
1	A	60	GLY	O-C-N	-5.30	114.21	122.70
3	F	52	GLU	N-CA-C	5.28	125.27	111.00
1	A	272	MET	C-N-CA	5.25	133.33	122.30
1	D	224	LEU	N-CA-CB	5.23	120.86	110.40
1	A	223	LYS	N-CA-CB	5.21	119.97	110.60
2	B	601	GLN	N-CA-CB	5.17	119.91	110.60
1	D	272	MET	O-C-N	-5.17	114.41	123.20
2	E	496	PHE	CD1-CG-CD2	-5.15	111.60	118.30
2	E	584	TYR	CB-CG-CD1	5.12	124.08	121.00
2	E	579	GLN	CA-CB-CG	5.12	124.66	113.40
3	F	69	LYS	O-C-N	-5.12	114.50	123.20
1	D	130	LEU	CB-CA-C	5.11	119.90	110.20
3	C	69	LYS	O-C-N	-5.07	114.58	123.20
2	E	386	ILE	CA-CB-CG2	5.04	120.98	110.90
3	C	67	VAL	C-N-CA	5.02	134.25	121.70
2	E	500	ARG	C-N-CA	5.01	134.22	121.70
2	E	507	GLU	C-N-CA	5.00	134.21	121.70

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	ASP	CA
2	B	435	LYS	CA
3	C	26	MET	CA
3	C	52	GLU	CA
1	D	91	PHE	CA
1	D	92	THR	CB,CA
2	E	495	PHE	CA
2	E	497	ASN	CA
2	E	500	ARG	CA
2	E	528	GLU	CA
2	E	573	SER	CA
2	E	579	GLN	CA
2	E	625	THR	CB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
2	E	626	TYR	CA
2	E	633	ARG	CA
3	F	52	GLU	CA
3	F	55	TYR	CA

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Mainchain
1	A	130	LEU	Mainchain
1	A	132	LEU	Mainchain
1	A	177	ALA	Mainchain
1	A	197	GLY	Mainchain
1	A	206	LYS	Mainchain
1	A	221	GLU	Sidechain
1	A	228	ARG	Sidechain
1	A	231	TYR	Sidechain
1	A	290	ARG	Sidechain
1	A	41	SER	Mainchain
1	A	5	SER	Mainchain
1	A	59	ARG	Peptide
1	A	60	GLY	Peptide
1	A	67	ARG	Sidechain
1	A	7	GLU	Mainchain
1	A	72	GLN	Mainchain
1	A	728	MET	Mainchain
2	B	369	ASN	Sidechain
2	B	402	ARG	Sidechain
2	B	408	ARG	Sidechain
2	B	492	PHE	Mainchain
2	B	595	HIS	Sidechain
2	B	602	PHE	Sidechain
2	B	620	LEU	Mainchain
2	B	626	TYR	Sidechain
3	C	24	GLY	Mainchain
3	C	61	ASN	Mainchain
3	C	68	GLU	Mainchain
3	C	99	CYS	Mainchain
1	D	113	LYS	Peptide,Mainchain
1	D	114	GLY	Mainchain
1	D	197	GLY	Mainchain
1	D	43	GLY	Mainchain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	D	62	GLY	Mainchain
1	D	7	GLU	Mainchain
1	D	72	GLN	Mainchain
1	D	726	ASP	Mainchain
1	D	90	LYS	Peptide
1	D	91	PHE	Mainchain
2	E	373	PHE	Sidechain
2	E	494	GLU	Peptide,Mainchain
2	E	495	PHE	Peptide,Sidechain,Mainchain
2	E	496	PHE	Peptide,Sidechain,Mainchain
2	E	497	ASN	Mainchain
2	E	498	LEU	Peptide
2	E	499	HIS	Sidechain,Mainchain
2	E	502	ALA	Mainchain
2	E	532	TYR	Sidechain
2	E	585	HIS	Sidechain
2	E	587	GLU	Sidechain
2	E	608	TYR	Sidechain
2	E	616	MET	Mainchain
2	E	620	LEU	Mainchain
2	E	625	THR	Mainchain
2	E	626	TYR	Sidechain,Mainchain
2	E	629	LEU	Peptide,Mainchain
2	E	632	GLU	Mainchain
2	E	633	ARG	Sidechain
3	F	24	GLY	Mainchain
3	F	55	TYR	Sidechain,Mainchain
3	F	61	ASN	Sidechain,Mainchain
3	F	68	GLU	Mainchain
3	F	69	LYS	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2573	0	2631	75	0
1	D	2573	0	2630	134	0
2	B	1781	0	1770	52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1858	0	1824	98	0
3	C	946	0	937	20	0
3	F	946	0	937	24	0
All	All	10677	0	10729	345	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 16.

All (345) 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:D:309:LYS:CE	2:E:374:PHE:HD1	1.31	1.40
1:D:309:LYS:CE	2:E:374:PHE:CD1	2.07	1.38
1:D:726:ASP:HB3	2:E:633:ARG:N	1.39	1.34
1:D:726:ASP:OD1	2:E:632:GLU:HG2	1.23	1.33
1:D:726:ASP:CG	2:E:632:GLU:CG	1.97	1.33
1:D:726:ASP:OD1	2:E:632:GLU:CG	1.76	1.31
1:D:726:ASP:HB3	2:E:633:ARG:CA	1.58	1.31
1:D:309:LYS:HE2	2:E:374:PHE:CD1	1.63	1.30
1:D:726:ASP:OD2	2:E:632:GLU:HG3	1.34	1.28
1:D:726:ASP:CB	2:E:633:ARG:N	1.98	1.24
1:A:311:VAL:HG13	2:B:370:GLU:CD	1.60	1.20
1:D:726:ASP:CG	2:E:632:GLU:HG2	1.60	1.18
1:A:311:VAL:HG13	2:B:370:GLU:OE1	1.40	1.16
1:D:726:ASP:HB3	2:E:633:ARG:HA	1.27	1.15
1:D:726:ASP:CA	2:E:633:ARG:H	1.61	1.14
1:D:309:LYS:HE3	2:E:374:PHE:HD1	1.10	1.11
1:D:726:ASP:HA	2:E:632:GLU:H	1.01	1.11
1:D:726:ASP:CG	2:E:632:GLU:HG3	1.62	1.10
1:D:309:LYS:HE2	2:E:374:PHE:CG	1.94	1.02
1:D:726:ASP:OD2	2:E:632:GLU:CG	2.08	0.96
2:E:375:LEU:HB2	2:E:630:LEU:HD21	1.47	0.96
1:D:726:ASP:HA	2:E:632:GLU:N	1.80	0.95
1:A:311:VAL:CG1	2:B:370:GLU:OE1	2.16	0.94
1:A:73:LEU:HD22	1:A:129:VAL:HG11	1.49	0.93
1:D:310:GLU:OE2	2:E:632:GLU:OE1	1.79	0.91
1:A:311:VAL:CG1	2:B:370:GLU:CD	2.40	0.90
1:D:727:GLU:HG3	2:E:631:LYS:HD2	1.54	0.90
1:D:309:LYS:HE2	2:E:374:PHE:HB2	1.55	0.88
1:D:309:LYS:HE2	2:E:374:PHE:CB	2.04	0.87
1:D:199:ARG:HB3	1:D:284:GLN:HG3	1.55	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:ILE:HG12	2:B:612:LEU:HD11	1.56	0.87
1:D:9:LEU:HD11	1:D:289:ILE:HD12	1.58	0.85
1:D:309:LYS:NZ	2:E:374:PHE:CD1	2.43	0.84
1:D:726:ASP:CB	2:E:633:ARG:H	1.74	0.84
1:D:42:ALA:HA	1:D:206:LYS:HE2	1.58	0.84
1:A:34:ILE:HG12	1:A:170:LEU:HB2	1.60	0.83
2:E:477:THR:HG21	2:E:514:GLU:HG3	1.62	0.82
1:A:207:LEU:HB2	1:A:235:VAL:HG22	1.61	0.82
1:D:310:GLU:HB3	2:E:632:GLU:OE2	1.81	0.81
1:D:16:LEU:HD21	1:D:293:LEU:HD21	1.63	0.80
1:A:232:ILE:HD11	1:A:280:VAL:HG21	1.63	0.79
1:A:31:LEU:HB3	1:A:132:LEU:HD23	1.63	0.79
1:D:235:VAL:HB	1:D:255:GLU:HA	1.64	0.79
2:B:403:LEU:HD21	2:B:480:VAL:HG22	1.64	0.78
1:D:29:LEU:HD23	1:D:289:ILE:HG23	1.65	0.78
1:D:170:LEU:HD13	1:D:281:LEU:HB3	1.64	0.78
1:D:84:LEU:HB2	1:D:121:ASN:HB2	1.66	0.78
1:A:23:ILE:HG12	1:A:734:ALA:HB1	1.68	0.76
2:B:501:THR:HB	2:B:619:LEU:HD21	1.67	0.76
1:D:138:PRO:HB2	1:D:156:ILE:HG23	1.67	0.75
2:E:531:VAL:HG13	2:E:584:TYR:HB2	1.68	0.75
1:A:138:PRO:HB2	1:A:156:ILE:HG23	1.69	0.75
1:A:232:ILE:HG21	1:A:277:LEU:HB2	1.69	0.74
1:D:201:ILE:HG23	1:D:232:ILE:HD13	1.69	0.74
2:B:403:LEU:HA	2:B:406:ARG:HD3	1.67	0.74
1:A:63:ILE:HG21	1:A:148:GLN:HE22	1.52	0.74
1:D:727:GLU:HB2	2:E:631:LYS:HG3	1.70	0.74
1:D:12:LEU:HD23	1:D:745:ILE:HA	1.68	0.73
1:D:63:ILE:HG23	1:D:66:ARG:HD3	1.70	0.73
1:D:232:ILE:HG23	1:D:272:MET:HA	1.70	0.73
3:F:65:ARG:HB2	3:F:122:VAL:HA	1.71	0.73
1:D:310:GLU:OE2	2:E:374:PHE:CE2	2.42	0.73
2:B:498:LEU:HG	2:B:629:LEU:HD22	1.69	0.72
1:D:726:ASP:HA	2:E:633:ARG:H	1.52	0.72
1:D:13:VAL:HG13	1:D:29:LEU:HD22	1.70	0.72
2:E:427:LYS:HE2	2:E:431:ARG:HD2	1.72	0.71
1:A:177:ALA:HB1	1:A:210:MET:HG2	1.72	0.71
2:B:473:LEU:HA	2:B:600:ILE:HG12	1.73	0.71
3:C:10:ILE:HG13	3:C:11:LEU:H	1.56	0.71
2:B:588:ALA:HA	2:B:591:ARG:HH21	1.56	0.70
2:B:418:ILE:HD13	2:B:465:LEU:HD13	1.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:HB1	1:D:186:ALA:HB1	1.72	0.70
1:D:181:LEU:HD11	1:D:204:ILE:HD12	1.74	0.70
1:D:726:ASP:CB	2:E:633:ARG:HA	2.14	0.70
1:D:726:ASP:C	2:E:633:ARG:H	1.91	0.69
3:C:27:LYS:HE3	3:C:54:LYS:HE2	1.74	0.68
3:F:10:ILE:HG13	3:F:11:LEU:H	1.59	0.68
1:D:59:ARG:HA	1:D:64:VAL:HG13	1.77	0.67
1:D:109:THR:HB	1:D:114:GLY:HA2	1.77	0.67
1:A:29:LEU:HD23	1:A:289:ILE:HG23	1.75	0.66
2:E:403:LEU:HD21	2:E:480:VAL:HG22	1.77	0.66
3:F:14:ARG:HH12	3:F:107:SER:HB2	1.59	0.66
1:A:39:GLY:HA2	1:A:140:MET:HG3	1.78	0.66
3:F:23:ILE:HD12	3:F:27:LYS:HD3	1.77	0.65
1:A:16:LEU:HA	1:A:741:ILE:HG21	1.78	0.65
3:F:62:LEU:HD13	3:F:80:LEU:HD13	1.78	0.65
1:D:309:LYS:HE3	2:E:374:PHE:CD1	2.02	0.65
1:D:39:GLY:HA3	1:D:176:PRO:HG3	1.79	0.64
1:A:132:LEU:HD21	1:A:285:LEU:HD11	1.78	0.64
2:E:371:LYS:HG3	2:E:630:LEU:HD12	1.79	0.64
1:D:137:LEU:HD13	1:D:160:LEU:HB2	1.80	0.64
1:D:727:GLU:CG	2:E:631:LYS:HD2	2.26	0.64
2:B:505:LYS:HD2	2:B:615:ALA:HB1	1.79	0.62
3:F:20:ILE:HD13	3:F:95:LEU:HD21	1.80	0.62
1:D:726:ASP:CA	2:E:633:ARG:N	2.37	0.62
2:B:477:THR:HG23	2:B:604:MET:HG3	1.82	0.61
1:D:42:ALA:HB3	1:D:44:LYS:HG3	1.82	0.61
1:D:61:SER:HA	1:D:239:GLN:HE22	1.66	0.61
1:D:726:ASP:CB	2:E:632:GLU:C	2.67	0.61
1:A:132:LEU:HD21	1:A:285:LEU:HD21	1.83	0.61
2:B:371:LYS:HE3	2:B:630:LEU:HD12	1.81	0.61
2:B:379:VAL:HG11	2:B:617:LEU:HD23	1.82	0.61
1:D:310:GLU:HB3	2:E:632:GLU:CD	2.21	0.61
1:D:174:VAL:HG13	1:D:205:THR:HG21	1.83	0.60
2:B:462:ILE:HG21	2:B:528:GLU:HB3	1.83	0.60
2:E:407:LEU:HD11	2:E:476:VAL:HG13	1.82	0.60
1:A:16:LEU:HB2	1:A:745:ILE:HD11	1.84	0.60
2:B:418:ILE:HG21	2:B:593:SER:HB2	1.83	0.60
3:C:10:ILE:HG13	3:C:11:LEU:N	2.16	0.60
3:F:71:PHE:HD1	3:F:71:PHE:N	2.00	0.59
3:F:99:CYS:HB2	3:F:105:VAL:HG23	1.83	0.59
2:B:389:LEU:HD11	2:B:483:ALA:HB1	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:ILE:HG13	3:F:11:LEU:N	2.16	0.59
1:D:23:ILE:HD11	1:D:738:ALA:HB2	1.83	0.59
1:D:140:MET:HG3	1:D:160:LEU:HD21	1.84	0.58
2:B:498:LEU:HD22	2:B:619:LEU:HD13	1.85	0.58
3:F:99:CYS:HB3	3:F:104:GLU:HB3	1.84	0.58
1:D:246:LYS:HE3	1:D:250:ALA:HB1	1.84	0.58
1:A:48:LEU:HD22	1:A:134:LEU:HD13	1.87	0.57
3:C:71:PHE:N	3:C:71:PHE:CD1	2.72	0.57
3:C:71:PHE:N	3:C:71:PHE:HD1	2.03	0.57
1:D:310:GLU:CB	2:E:632:GLU:OE2	2.51	0.57
1:D:297:ARG:NH2	1:D:298:ASN:HB2	2.20	0.56
3:F:71:PHE:N	3:F:71:PHE:CD1	2.71	0.56
1:D:255:GLU:HG3	1:D:259:PHE:HE2	1.71	0.56
1:A:10:ILE:HG12	1:A:130:LEU:HD12	1.88	0.55
1:A:297:ARG:NH2	1:A:298:ASN:HB2	2.20	0.55
1:A:19:ALA:HB2	1:A:741:ILE:HG13	1.89	0.55
2:B:429:LEU:HB2	2:B:457:ILE:HD11	1.87	0.55
2:E:372:MET:HG3	2:E:376:ILE:HD12	1.89	0.55
3:C:15:LYS:HE2	3:C:36:VAL:HG13	1.88	0.55
1:D:76:ALA:HB3	1:D:125:TYR:HB3	1.87	0.55
1:A:304:LEU:HD13	1:A:732:TYR:HA	1.88	0.55
1:D:170:LEU:HD22	1:D:281:LEU:HD22	1.88	0.55
2:E:505:LYS:HD3	2:E:615:ALA:HB1	1.89	0.55
1:D:727:GLU:HG3	2:E:631:LYS:CD	2.34	0.54
1:D:130:LEU:HD23	1:D:132:LEU:HG	1.88	0.54
2:E:477:THR:HG22	2:E:604:MET:HG3	1.90	0.53
1:D:310:GLU:CB	2:E:632:GLU:CD	2.74	0.53
1:D:297:ARG:HB2	1:D:742:ILE:HG21	1.90	0.53
2:B:451:TYR:HE1	2:B:581:LEU:HD11	1.74	0.53
1:D:36:VAL:HG23	1:D:172:LEU:HB3	1.89	0.53
2:E:623:LYS:HA	2:E:626:TYR:CD2	2.43	0.53
1:A:161:MET:HA	1:A:164:VAL:HG22	1.91	0.53
2:B:429:LEU:HD11	2:B:454:PHE:HB3	1.91	0.53
1:D:19:ALA:HB2	1:D:741:ILE:HG13	1.90	0.53
1:A:205:THR:HA	1:A:234:VAL:HG23	1.90	0.53
2:B:429:LEU:HG	2:B:578:PHE:CE1	2.44	0.53
2:B:401:ILE:HD12	2:B:402:ARG:H	1.73	0.52
2:E:521:ILE:HG23	2:E:596:ILE:HD12	1.90	0.52
1:A:132:LEU:HD11	1:A:285:LEU:HD21	1.91	0.52
1:D:40:GLN:HA	1:D:139:GLY:HA3	1.90	0.52
2:E:389:LEU:HD13	2:E:484:PHE:CD1	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:GLU:OE1	2:B:398:GLU:N	2.42	0.52
2:E:424:GLU:HG2	2:E:428:ILE:HD11	1.92	0.52
3:F:66:ASP:H	3:F:122:VAL:HG12	1.75	0.52
1:D:80:TYR:HB3	1:D:92:THR:HG21	1.91	0.52
1:D:201:ILE:HG21	1:D:277:LEU:HD13	1.91	0.52
3:C:13:ILE:HD12	3:C:115:ALA:HB2	1.91	0.51
1:A:235:VAL:H	1:A:255:GLU:HG3	1.75	0.51
1:D:310:GLU:OE2	2:E:374:PHE:HE2	1.93	0.51
3:F:69:LYS:HE3	3:F:69:LYS:H	1.75	0.51
1:D:15:ARG:HG3	1:D:15:ARG:HH11	1.76	0.51
1:D:726:ASP:OD1	2:E:632:GLU:HG3	1.74	0.51
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.76	0.50
1:A:170:LEU:HD21	1:A:284:GLN:HE21	1.76	0.50
3:C:99:CYS:HB3	3:C:104:GLU:HB3	1.93	0.50
1:D:310:GLU:HG2	2:E:630:LEU:O	2.11	0.50
1:D:10:ILE:HG12	1:D:130:LEU:HD12	1.94	0.50
2:E:403:LEU:HD23	2:E:605:LEU:HD13	1.94	0.50
2:E:531:VAL:HA	2:E:584:TYR:CD1	2.46	0.50
1:A:45:SER:HB2	1:A:59:ARG:HG2	1.93	0.50
2:B:531:VAL:HA	2:B:584:TYR:CZ	2.47	0.50
1:A:16:LEU:HD22	1:A:745:ILE:HD12	1.93	0.50
1:D:134:LEU:N	1:D:134:LEU:HD12	2.27	0.50
3:F:54:LYS:O	3:F:55:TYR:HB3	2.12	0.50
1:A:58:PRO:HG3	1:A:98:ARG:HG2	1.94	0.50
2:E:378:LYS:HB3	2:E:492:PHE:HE1	1.76	0.50
3:C:18:LEU:HD13	3:C:97:LEU:HD22	1.94	0.49
1:D:205:THR:HG22	1:D:234:VAL:HG23	1.94	0.49
1:D:309:LYS:CE	2:E:374:PHE:HB2	2.36	0.49
2:E:426:HIS:HA	2:E:582:MET:CE	2.42	0.49
1:D:218:ASP:HB3	1:D:224:LEU:HB2	1.94	0.49
1:D:220:LEU:HD13	1:D:265:TYR:CE1	2.48	0.49
2:B:406:ARG:HG2	2:B:406:ARG:HH11	1.77	0.49
1:D:304:LEU:HD11	1:D:732:TYR:CD1	2.47	0.49
1:D:727:GLU:C	2:E:633:ARG:HG2	2.23	0.49
3:C:69:LYS:HE3	3:C:69:LYS:H	1.78	0.48
1:A:58:PRO:HA	1:A:98:ARG:HD2	1.95	0.48
1:A:304:LEU:HB2	1:A:735:LEU:CD1	2.43	0.48
1:D:69:LEU:HD12	1:D:120:ILE:HB	1.94	0.48
1:D:207:LEU:HB3	1:D:258:PHE:CE2	2.48	0.48
1:D:309:LYS:NZ	1:D:309:LYS:HB3	2.28	0.48
1:A:170:LEU:HD21	1:A:284:GLN:HG3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:PHE:HB3	2:B:498:LEU:HB2	1.94	0.48
2:E:528:GLU:HG2	2:E:591:ARG:NH1	2.28	0.48
1:A:29:LEU:HD12	1:A:29:LEU:N	2.28	0.48
1:A:12:LEU:HD23	1:A:745:ILE:HA	1.95	0.48
1:A:221:GLU:HB3	1:A:223:LYS:HE3	1.94	0.48
2:B:407:LEU:HD11	2:B:476:VAL:HG13	1.94	0.48
3:C:54:LYS:HB3	3:C:90:LYS:NZ	2.29	0.48
1:A:63:ILE:HD13	1:A:148:GLN:NE2	2.28	0.48
2:B:513:GLN:HB2	2:B:604:MET:CE	2.44	0.48
1:A:309:LYS:NZ	1:A:309:LYS:HB3	2.28	0.48
3:F:63:LYS:HB3	3:F:81:PHE:CZ	2.49	0.48
1:A:106:ASP:HB3	1:A:111:THR:HG22	1.95	0.48
1:D:23:ILE:HD11	1:D:738:ALA:CB	2.43	0.48
1:A:67:ARG:HD3	1:A:105:THR:HA	1.95	0.48
1:D:37:VAL:HG11	1:D:164:VAL:HG11	1.95	0.48
1:D:29:LEU:HD12	1:D:29:LEU:N	2.29	0.47
2:B:599:ILE:HG23	2:B:603:PHE:CD1	2.49	0.47
2:E:403:LEU:HD11	2:E:480:VAL:HG22	1.96	0.47
1:A:311:VAL:HA	1:A:726:ASP:N	2.29	0.47
2:E:625:THR:HA	2:E:628:TRP:HB3	1.94	0.47
1:D:113:LYS:HG3	1:D:146:GLY:HA3	1.95	0.47
1:A:52:VAL:HG22	1:A:73:LEU:HD21	1.97	0.47
2:B:429:LEU:HG	2:B:578:PHE:HE1	1.79	0.47
1:D:726:ASP:OD1	2:E:632:GLU:CD	2.51	0.47
1:D:36:VAL:HG23	1:D:172:LEU:CB	2.45	0.47
1:A:23:ILE:HD11	1:A:738:ALA:HB2	1.97	0.47
2:E:425:GLY:HA2	2:E:428:ILE:HD12	1.96	0.47
1:A:9:LEU:HD21	1:A:289:ILE:HD12	1.97	0.47
1:A:10:ILE:HG12	1:A:130:LEU:CD1	2.45	0.47
2:B:499:HIS:NE2	2:B:503:LYS:HE2	2.30	0.47
1:D:59:ARG:HA	1:D:64:VAL:CG1	2.44	0.47
1:A:6:MET:SD	1:A:279:LYS:HA	2.55	0.46
1:D:40:GLN:HE22	1:D:145:VAL:HG21	1.79	0.46
1:A:49:GLU:HB3	1:A:57:LEU:HD12	1.97	0.46
1:A:227:LEU:HD22	1:A:231:TYR:CZ	2.50	0.46
3:C:23:ILE:HD12	3:C:27:LYS:HD3	1.97	0.46
3:F:71:PHE:HD1	3:F:71:PHE:H	1.61	0.46
1:D:190:ALA:HB1	1:D:200:THR:CG2	2.45	0.46
2:E:425:GLY:HA3	2:E:585:HIS:CE1	2.50	0.46
1:D:34:ILE:HG12	1:D:170:LEU:HB2	1.97	0.46
1:D:205:THR:HG22	1:D:234:VAL:CG2	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:CD2	1:A:745:ILE:HA	2.46	0.46
2:E:372:MET:CG	2:E:376:ILE:HD12	2.44	0.46
1:D:232:ILE:HG12	1:D:276:TYR:HD2	1.81	0.46
2:E:403:LEU:CD2	2:E:605:LEU:HD13	2.45	0.46
1:D:180:ASP:HB2	1:D:183:ASN:ND2	2.31	0.46
2:E:588:ALA:HA	2:E:591:ARG:NH1	2.31	0.46
1:D:36:VAL:HB	1:D:48:LEU:HG	1.98	0.46
2:B:466:GLU:HG3	2:B:525:PHE:CD2	2.51	0.45
2:B:505:LYS:CD	2:B:615:ALA:HB1	2.46	0.45
1:D:304:LEU:HD11	1:D:732:TYR:HD1	1.80	0.45
2:E:473:LEU:HD12	2:E:600:ILE:HG12	1.98	0.45
1:A:220:LEU:HD13	1:A:272:MET:SD	2.56	0.45
2:E:473:LEU:HA	2:E:600:ILE:HG12	1.98	0.45
1:D:79:GLU:HB3	1:D:94:PHE:CZ	2.52	0.45
3:F:57:LEU:CD2	3:F:62:LEU:HD11	2.46	0.45
1:A:63:ILE:HD13	1:A:148:GLN:HE22	1.80	0.45
1:A:235:VAL:HB	1:A:255:GLU:HA	1.98	0.45
2:B:625:THR:O	2:B:625:THR:HG22	2.17	0.45
2:E:532:TYR:HA	2:E:584:TYR:HA	1.99	0.45
1:D:171:ILE:HD13	1:D:189:VAL:HG12	1.98	0.45
3:F:23:ILE:HG23	3:F:27:LYS:HD3	1.98	0.45
3:C:31:LYS:HG2	3:C:32:GLU:H	1.82	0.44
1:D:140:MET:CG	1:D:160:LEU:HD21	2.45	0.44
2:E:506:ILE:HG13	2:E:612:LEU:HD11	1.99	0.44
1:A:23:ILE:CD1	1:A:738:ALA:HB2	2.46	0.44
1:A:83:PHE:CD2	1:A:122:LEU:HD13	2.53	0.44
1:A:299:LYS:HD3	1:A:299:LYS:C	2.38	0.44
1:D:727:GLU:N	2:E:633:ARG:HG2	1.65	0.44
2:E:517:GLY:HA2	2:E:603:PHE:CD2	2.52	0.44
2:B:372:MET:HG2	2:B:376:ILE:HD12	2.00	0.44
2:B:389:LEU:HD23	2:B:484:PHE:HD1	1.82	0.44
3:C:54:LYS:HE3	3:C:90:LYS:HZ1	1.83	0.44
1:D:72:GLN:HE22	1:D:74:VAL:HG22	1.81	0.44
2:B:429:LEU:HD23	2:B:582:MET:SD	2.57	0.43
2:B:469:ALA:HB1	2:B:596:ILE:HG13	2.00	0.43
2:B:520:LEU:HB3	2:B:599:ILE:HD11	1.99	0.43
2:B:451:TYR:CE1	2:B:581:LEU:HD11	2.53	0.43
2:E:422:PHE:HE1	2:E:586:GLN:HA	1.82	0.43
1:A:83:PHE:HZ	1:A:101:ILE:HG13	1.83	0.43
1:D:12:LEU:HD23	1:D:745:ILE:HG12	1.99	0.43
1:D:262:HIS:CE1	1:D:264:SER:HB2	2.52	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:31:LYS:HG2	3:F:32:GLU:H	1.84	0.43
3:C:20:ILE:CG2	3:C:23:ILE:HG12	2.49	0.43
3:C:71:PHE:HD1	3:C:71:PHE:H	1.63	0.43
1:A:202:GLY:HA3	1:A:231:TYR:CD2	2.54	0.43
3:C:92:TYR:O	3:C:93:ARG:HB2	2.18	0.43
2:E:406:ARG:NH2	2:E:479:MET:HG2	2.33	0.43
2:E:509:ILE:HG22	2:E:608:TYR:CD1	2.53	0.43
1:D:726:ASP:HB3	2:E:633:ARG:CB	2.41	0.43
3:F:15:LYS:HB3	3:F:34:TRP:CZ2	2.53	0.43
1:A:72:GLN:HE22	1:A:74:VAL:HG22	1.84	0.42
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.93	0.42
1:D:299:LYS:HD3	1:D:299:LYS:C	2.39	0.42
3:F:92:TYR:O	3:F:93:ARG:HB2	2.18	0.42
1:A:83:PHE:CE2	1:A:122:LEU:HD13	2.55	0.42
3:C:54:LYS:HB3	3:C:90:LYS:HZ1	1.84	0.42
3:F:20:ILE:CG2	3:F:23:ILE:HG12	2.49	0.42
1:D:137:LEU:HD13	1:D:160:LEU:CB	2.47	0.42
1:A:66:ARG:NH2	1:A:102:GLU:HG3	2.34	0.42
2:B:389:LEU:HD23	2:B:484:PHE:CD1	2.54	0.42
2:E:520:LEU:HG	2:E:603:PHE:CZ	2.54	0.42
1:A:44:LYS:HE3	1:A:139:GLY:HA2	2.02	0.42
2:E:498:LEU:HD13	2:E:629:LEU:HD22	2.01	0.42
1:A:262:HIS:HA	1:A:263:PRO:HD2	1.89	0.42
1:A:274:THR:HB	1:A:275:PRO:HD3	2.01	0.42
1:A:60:GLY:HA2	1:A:64:VAL:HG21	2.01	0.42
1:D:310:GLU:O	2:E:630:LEU:O	2.37	0.42
1:D:727:GLU:HB2	2:E:631:LYS:HD2	2.02	0.42
1:A:311:VAL:HG13	2:B:370:GLU:OE2	2.14	0.42
2:B:382:PHE:CD2	2:B:487:VAL:HG12	2.55	0.42
1:D:59:ARG:HB3	1:D:242:ILE:HG23	2.00	0.42
1:D:190:ALA:HB1	1:D:200:THR:HG21	2.01	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.85	0.41
2:B:481:ARG:HG3	2:B:510:ARG:HH11	1.84	0.41
2:E:631:LYS:HD2	2:E:633:ARG:NE	2.35	0.41
1:D:310:GLU:O	2:E:630:LEU:C	2.58	0.41
1:D:727:GLU:CB	2:E:631:LYS:HD2	2.50	0.41
2:E:498:LEU:CD1	2:E:629:LEU:HD22	2.51	0.41
2:E:524:HIS:HA	2:E:527:MET:HG3	2.02	0.41
3:C:78:PHE:CD1	3:C:105:VAL:HG13	2.55	0.41
1:D:63:ILE:CG2	1:D:113:LYS:HA	2.50	0.41
1:D:174:VAL:HG13	1:D:205:THR:CG2	2.49	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ILE:HG23	1:D:726:ASP:N	2.35	0.41
1:A:262:HIS:CE1	1:A:264:SER:HB2	2.56	0.41
3:C:65:ARG:HB2	3:C:122:VAL:HG12	2.02	0.41
1:D:79:GLU:HB3	1:D:94:PHE:HZ	1.86	0.41
3:F:20:ILE:CD1	3:F:95:LEU:HD21	2.48	0.41
1:D:274:THR:HB	1:D:275:PRO:HD3	2.02	0.41
1:D:232:ILE:HG12	1:D:276:TYR:CD2	2.55	0.41
1:D:726:ASP:HA	2:E:633:ARG:N	2.21	0.41
1:D:728:MET:N	2:E:633:ARG:HG2	2.36	0.41
2:E:462:ILE:HG23	2:E:592:ILE:HD11	2.01	0.41
1:A:177:ALA:CB	1:A:210:MET:HG2	2.44	0.41
1:A:297:ARG:HH22	1:A:298:ASN:HB2	1.86	0.41
3:F:88:VAL:HG13	3:F:89:TYR:HD1	1.86	0.41
1:A:138:PRO:HB2	1:A:156:ILE:CG2	2.45	0.41
2:B:469:ALA:CB	2:B:596:ILE:HG13	2.51	0.41
2:B:506:ILE:HG13	2:B:612:LEU:HD21	2.02	0.41
2:E:414:TRP:NE1	2:E:596:ILE:HB	2.36	0.41
2:E:523:LEU:HD12	2:E:526:GLN:HE21	1.86	0.41
2:B:428:ILE:HG22	2:B:457:ILE:HD12	2.03	0.40
2:B:473:LEU:HA	2:B:600:ILE:CG1	2.47	0.40
2:E:401:ILE:CG2	2:E:406:ARG:HG3	2.51	0.40
2:B:595:HIS:HE1	2:B:598:LEU:HD23	1.85	0.40
2:E:509:ILE:HG22	2:E:608:TYR:HD1	1.86	0.40
1:D:12:LEU:HB3	1:D:745:ILE:HG12	2.03	0.40
1:D:297:ARG:HH22	1:D:298:ASN:HB2	1.87	0.40
1:D:63:ILE:HG22	1:D:113:LYS:HA	2.03	0.40
2:E:382:PHE:HZ	2:E:612:LEU:HD21	1.85	0.40
1:D:46:SER:HB3	1:D:237:ARG:HH21	1.87	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	326/353 (92%)	315 (97%)	11 (3%)	0	100	100
1	D	326/353 (92%)	314 (96%)	9 (3%)	3 (1%)	17	57
2	B	205/662 (31%)	197 (96%)	7 (3%)	1 (0%)	29	69
2	E	213/662 (32%)	198 (93%)	10 (5%)	5 (2%)	6	34
3	C	111/113 (98%)	94 (85%)	13 (12%)	4 (4%)	3	25
3	F	111/113 (98%)	95 (86%)	13 (12%)	3 (3%)	5	31
All	All	1292/2256 (57%)	1213 (94%)	63 (5%)	16 (1%)	17	50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	MET
3	C	68	GLU
1	D	91	PHE
1	D	92	THR
1	D	115	ILE
2	E	498	LEU
2	E	499	HIS
2	E	500	ARG
2	E	501	THR
3	F	68	GLU
2	B	604	MET
2	E	626	TYR
3	C	69	LYS
3	C	120	GLU
3	F	55	TYR
3	F	69	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/309 (93%)	268 (93%)	20 (7%)	15	40
1	D	288/309 (93%)	269 (93%)	19 (7%)	16	41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	196/588 (33%)	177 (90%)	19 (10%)	8	27
2	E	204/588 (35%)	189 (93%)	15 (7%)	13	38
3	C	102/102 (100%)	94 (92%)	8 (8%)	12	36
3	F	102/102 (100%)	92 (90%)	10 (10%)	8	26
All	All	1180/1998 (59%)	1089 (92%)	91 (8%)	16	37

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	48	LEU
1	A	54	ARG
1	A	69	LEU
1	A	73	LEU
1	A	75	ASN
1	A	84	LEU
1	A	125	TYR
1	A	128	HIS
1	A	129	VAL
1	A	130	LEU
1	A	140	MET
1	A	172	LEU
1	A	212	GLU
1	A	240	LYS
1	A	252	LEU
1	A	285	LEU
1	A	299	LYS
1	A	301	GLN
1	A	727	GLU
2	B	369	ASN
2	B	389	LEU
2	B	418	ILE
2	B	432	LYS
2	B	457	ILE
2	B	473	LEU
2	B	475	THR
2	B	479	MET
2	B	481	ARG
2	B	482	LEU
2	B	498	LEU
2	B	503	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	530	ILE
2	B	531	VAL
2	B	577	ILE
2	B	603	PHE
2	B	604	MET
2	B	612	LEU
2	B	618	GLN
3	C	26	MET
3	C	52	GLU
3	C	63	LYS
3	C	69	LYS
3	C	71	PHE
3	C	76	HIS
3	C	86	ARG
3	C	95	LEU
1	D	31	LEU
1	D	48	LEU
1	D	54	ARG
1	D	61	SER
1	D	69	LEU
1	D	75	ASN
1	D	84	LEU
1	D	130	LEU
1	D	172	LEU
1	D	175	SER
1	D	201	ILE
1	D	212	GLU
1	D	240	LYS
1	D	245	LYS
1	D	252	LEU
1	D	285	LEU
1	D	299	LYS
1	D	301	GLN
1	D	727	GLU
2	E	408	ARG
2	E	477	THR
2	E	482	LEU
2	E	496	PHE
2	E	497	ASN
2	E	498	LEU
2	E	500	ARG
2	E	520	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	527	MET
2	E	528	GLU
2	E	532	TYR
2	E	576	GLU
2	E	618	GLN
2	E	631	LYS
2	E	633	ARG
3	F	50	GLU
3	F	52	GLU
3	F	55	TYR
3	F	61	ASN
3	F	63	LYS
3	F	66	ASP
3	F	69	LYS
3	F	71	PHE
3	F	86	ARG
3	F	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	75	ASN
1	A	85	HIS
1	A	148	GLN
1	A	168	ASN
1	A	236	ASN
1	A	282	ASN
1	A	284	GLN
1	A	301	GLN
1	A	746	ASN
2	B	384	GLN
2	B	434	GLN
2	B	526	GLN
2	B	595	HIS
3	C	94	GLN
1	D	75	ASN
1	D	85	HIS
1	D	168	ASN
1	D	239	GLN
1	D	284	GLN
1	D	301	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	746	ASN
2	E	499	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	498:LEU	C	499:HIS	N	1.19

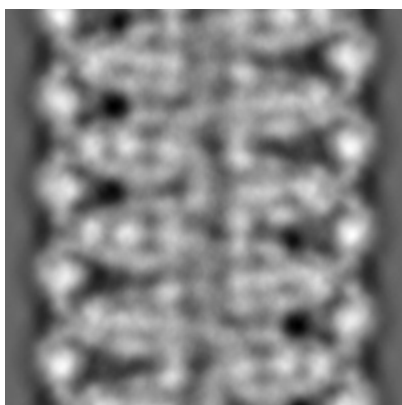
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1949. These allow visual inspection of the internal detail of the map and identification of artifacts.

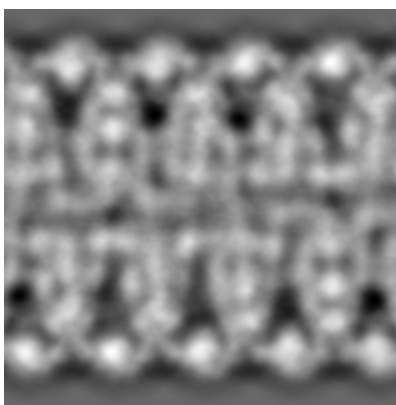
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

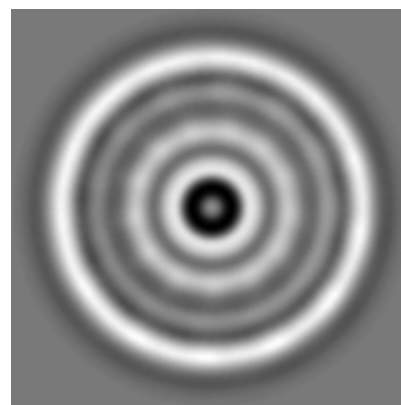
#### 6.1.1 Primary map



X



Y

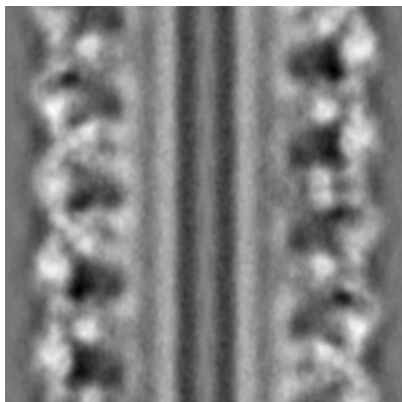


Z

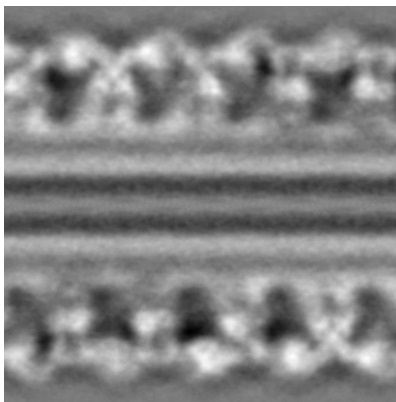
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 100



Y Index: 100



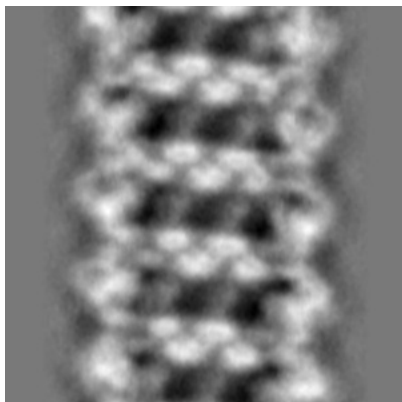
Z Index: 100



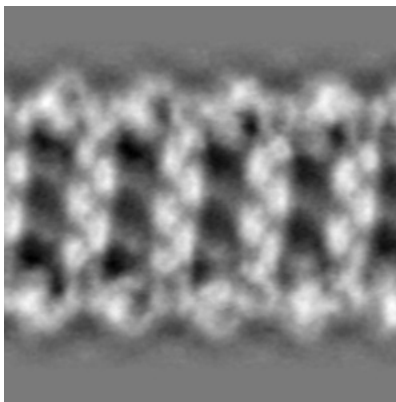
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

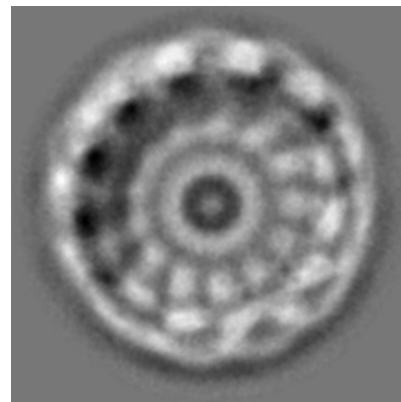
### 6.3.1 Primary map



X Index: 42



Y Index: 43

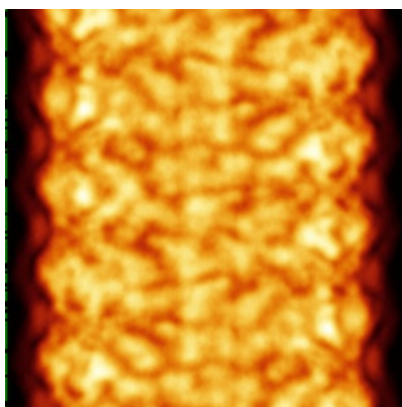


Z Index: 47

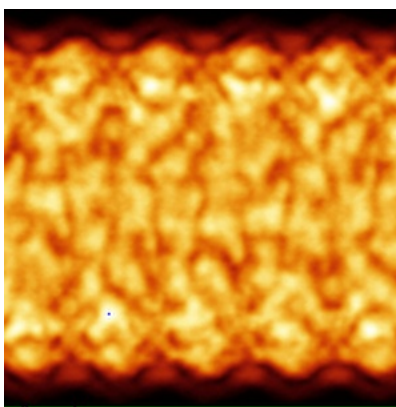
The images above show the largest variance slices of the map in three orthogonal directions.

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

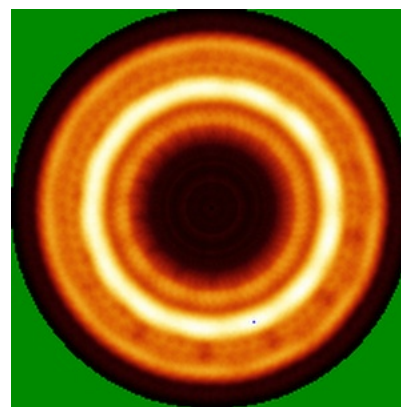
### 6.4.1 Primary map



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

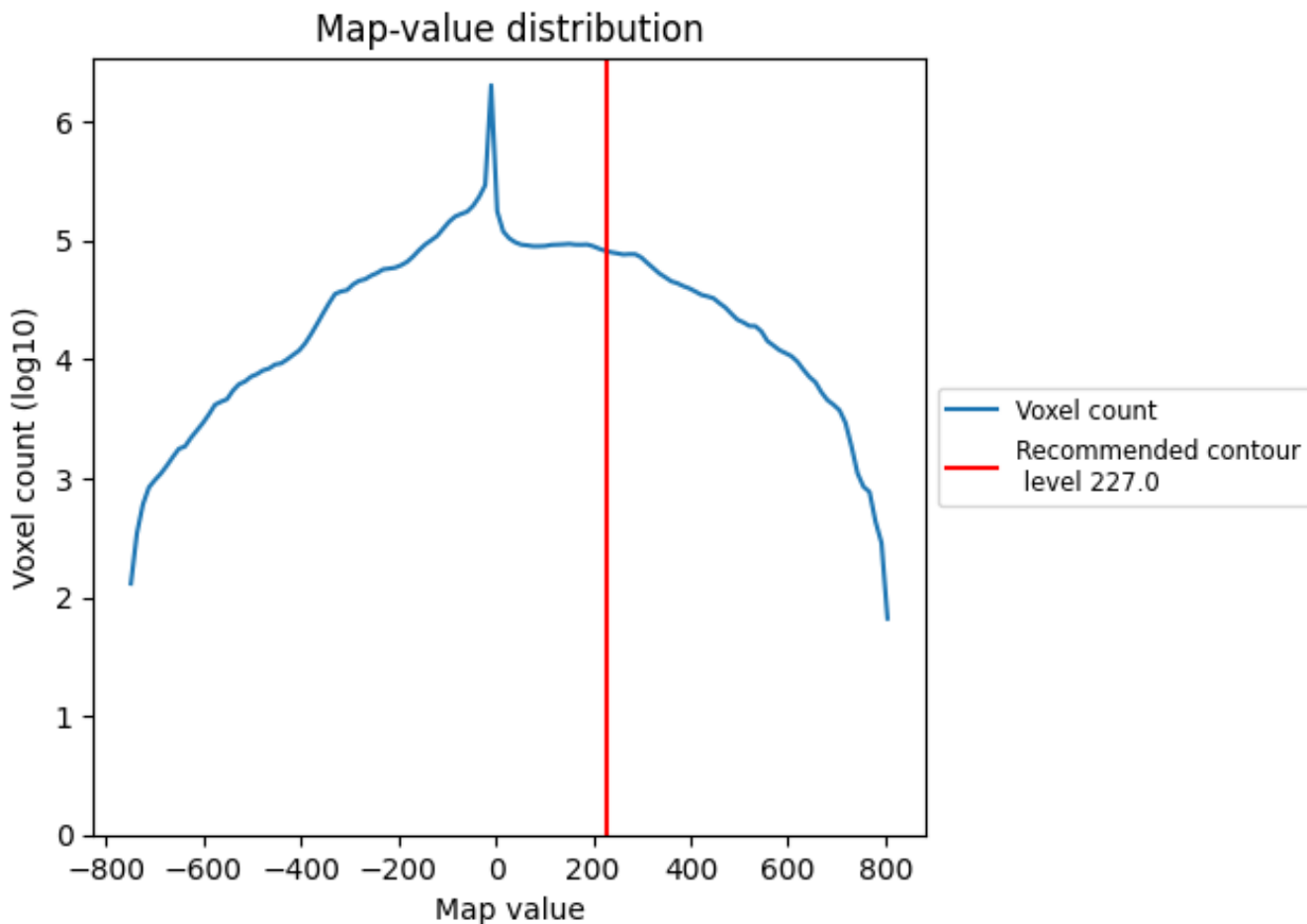
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

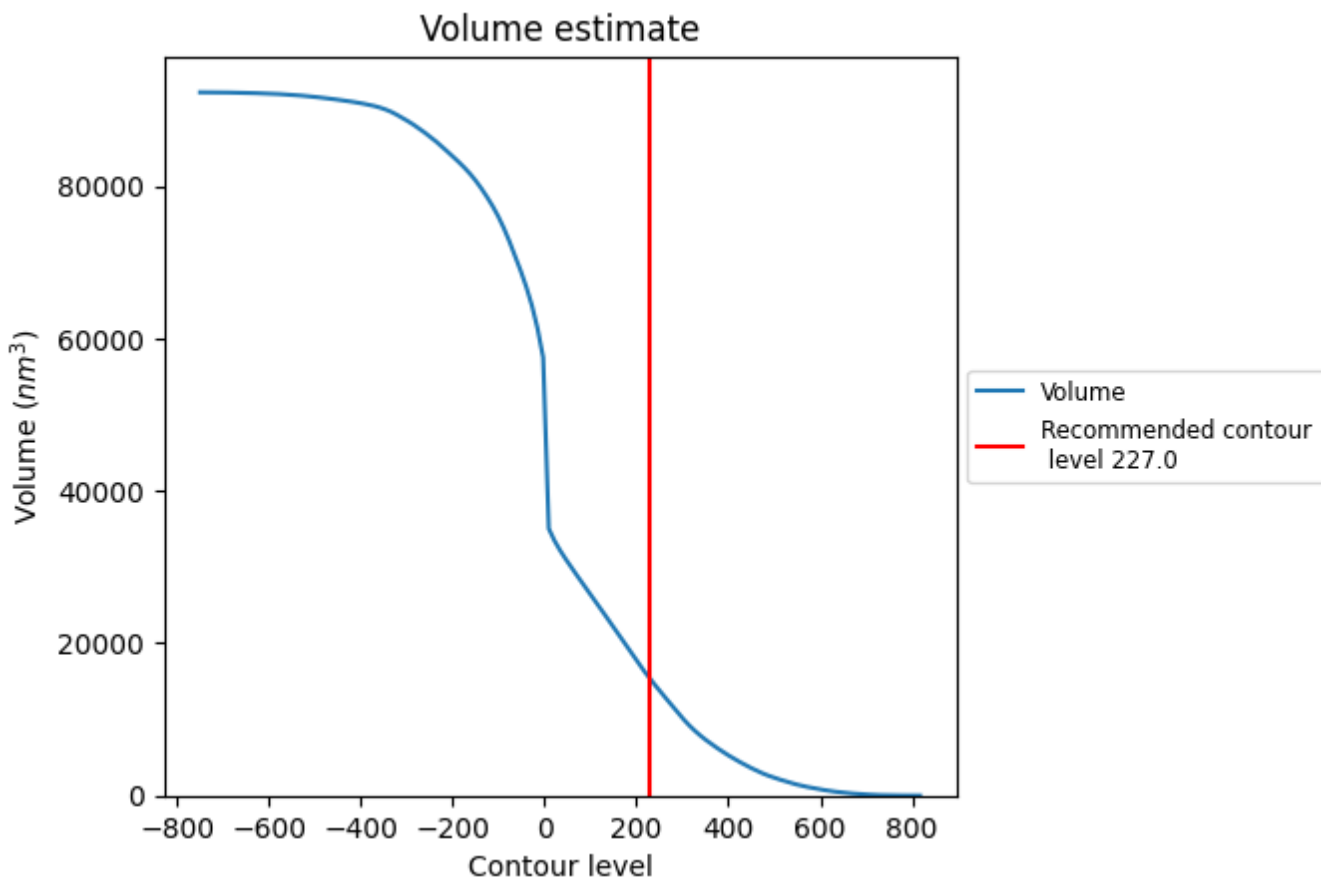
This section contains the results of statistical analysis of the map.

### 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.

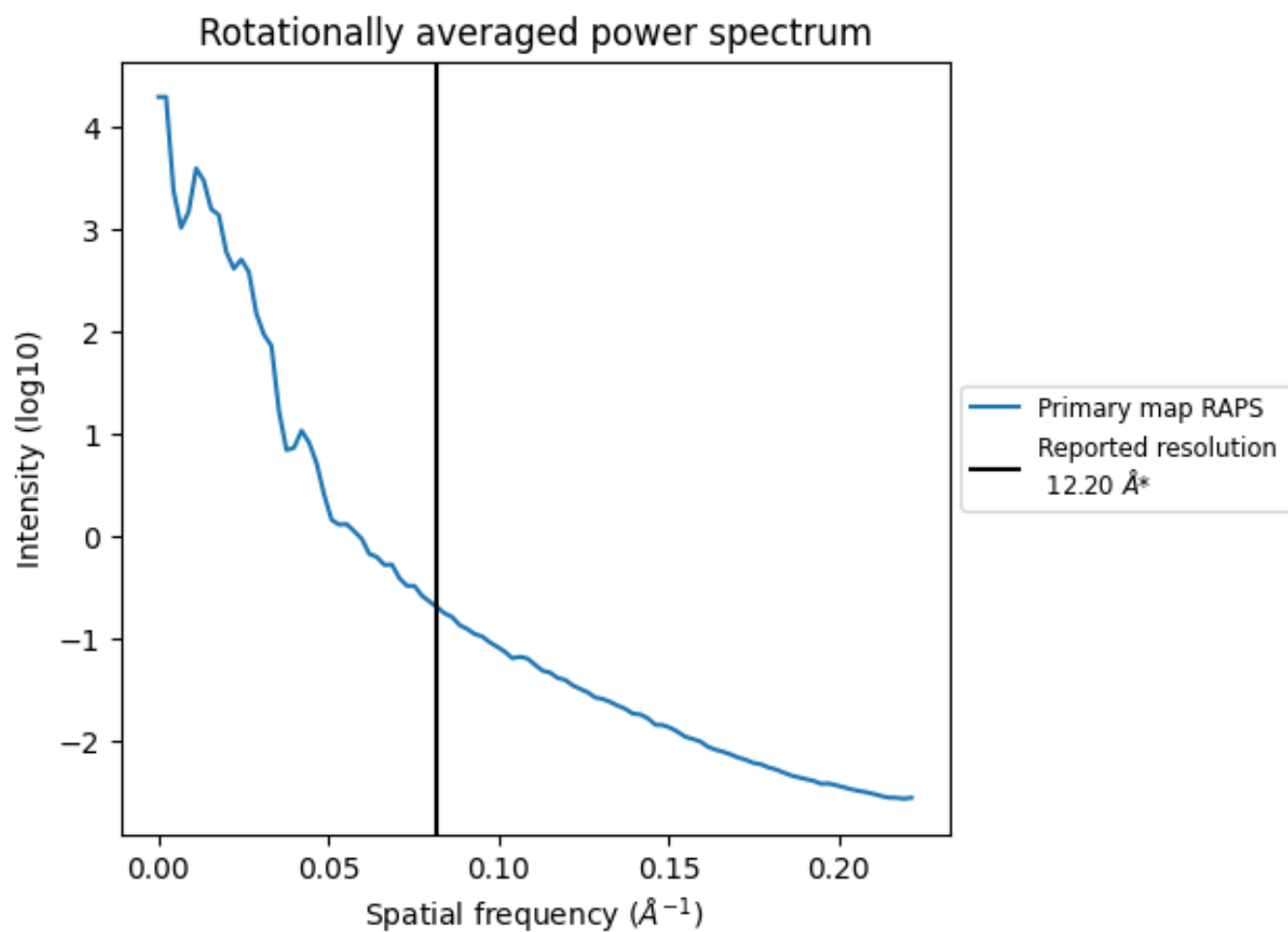
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15548 nm<sup>3</sup>; this corresponds to an approximate mass of 14045 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.082 \text{\AA}^{-1}$

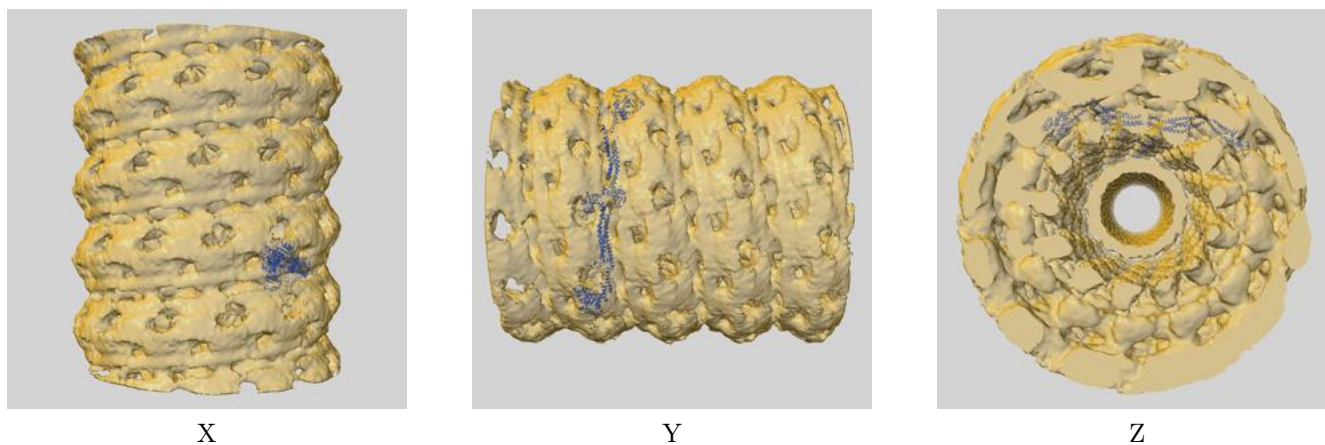
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

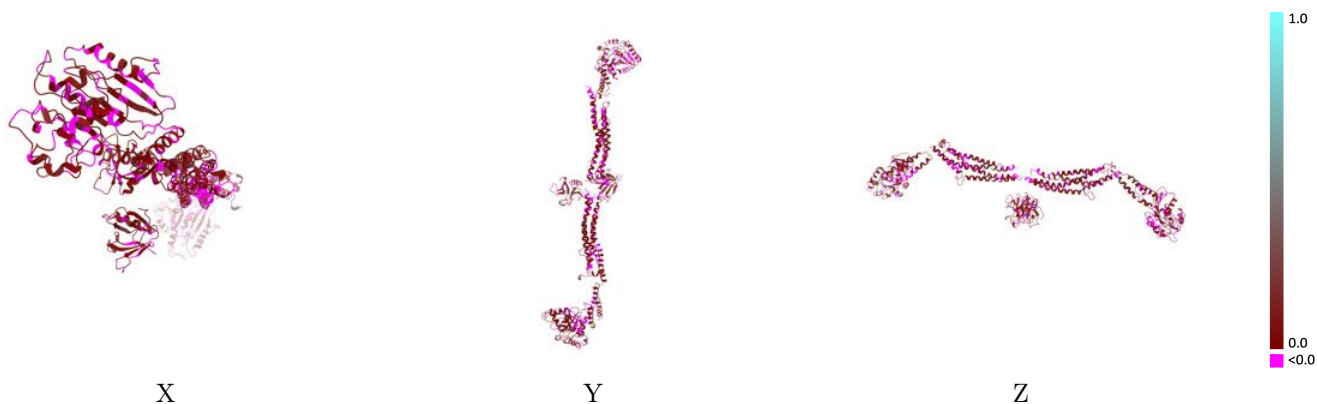
This section contains information regarding the fit between EMDB map EMD-1949 and PDB model 3ZYS. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



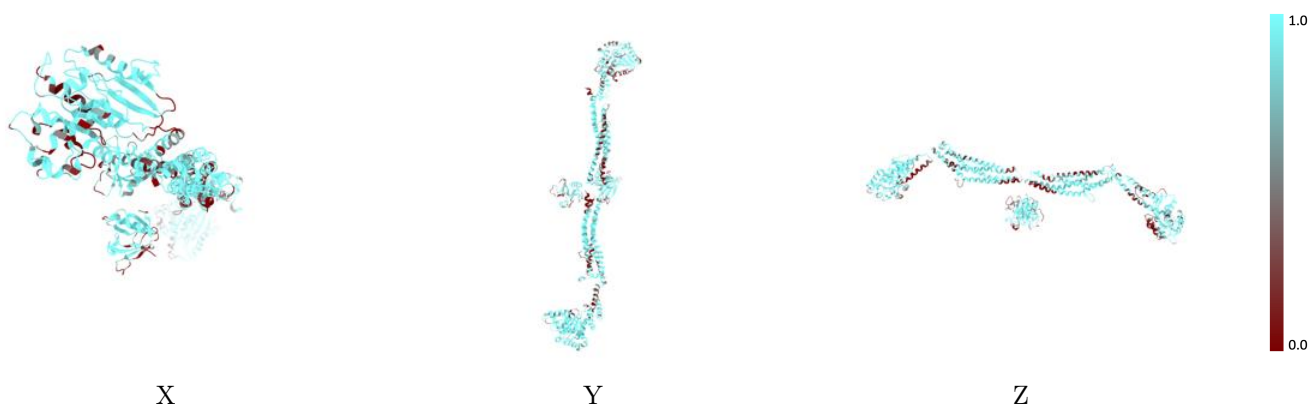
The images above show the 3D surface view of the map at the recommended contour level 227.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

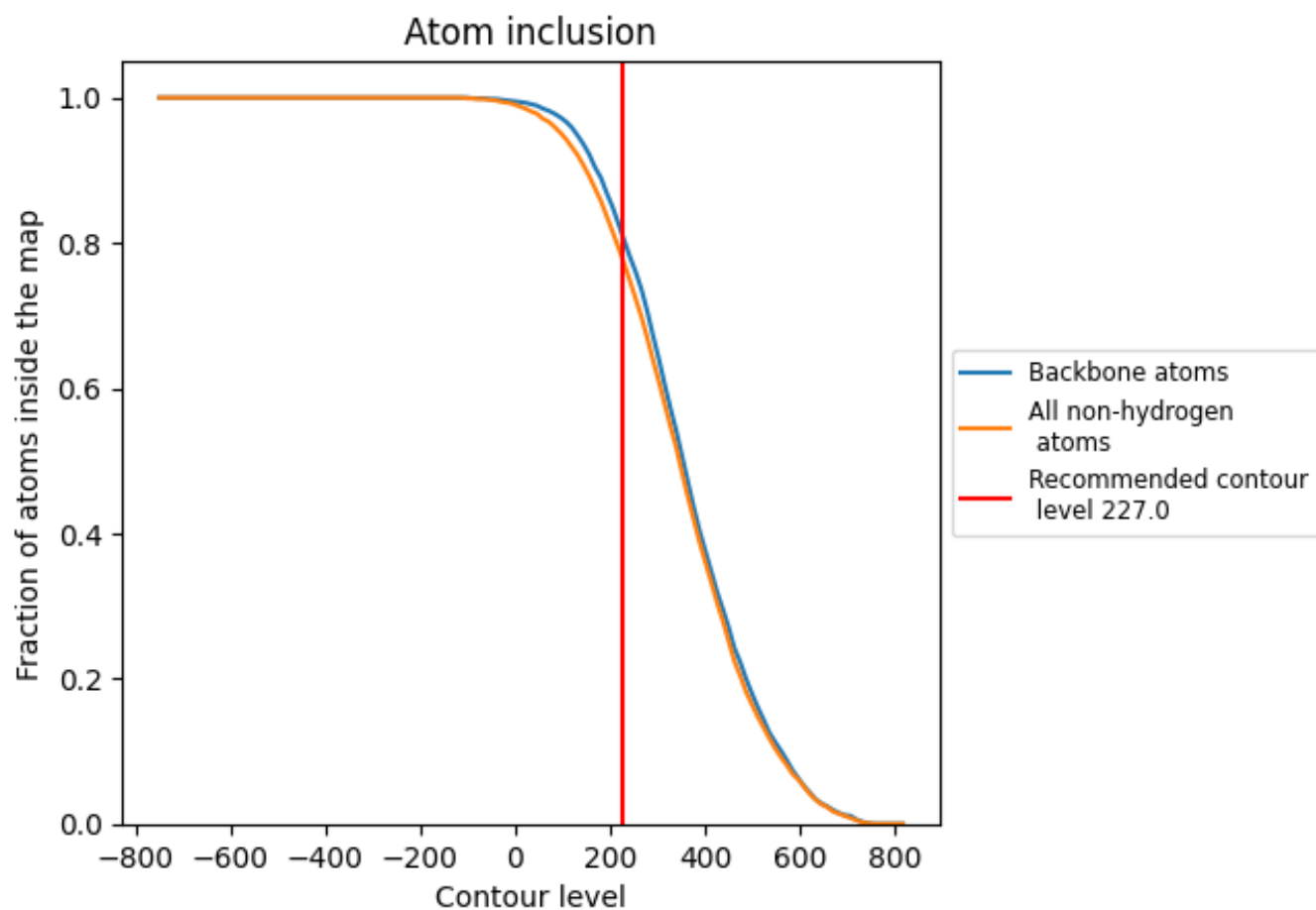
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (227.0).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (227.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.0550
A	 0.8500	 0.0630
B	 0.7490	 0.0530
C	 0.7170	 0.0620
D	 0.7630	 0.0460
E	 0.7600	 0.0480
F	 0.7670	 0.0660

