



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:04 PM UTC

PDB ID : 3ZYS / pdb_00003zys
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 : 1DYN, 3LJB, 2X2E

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

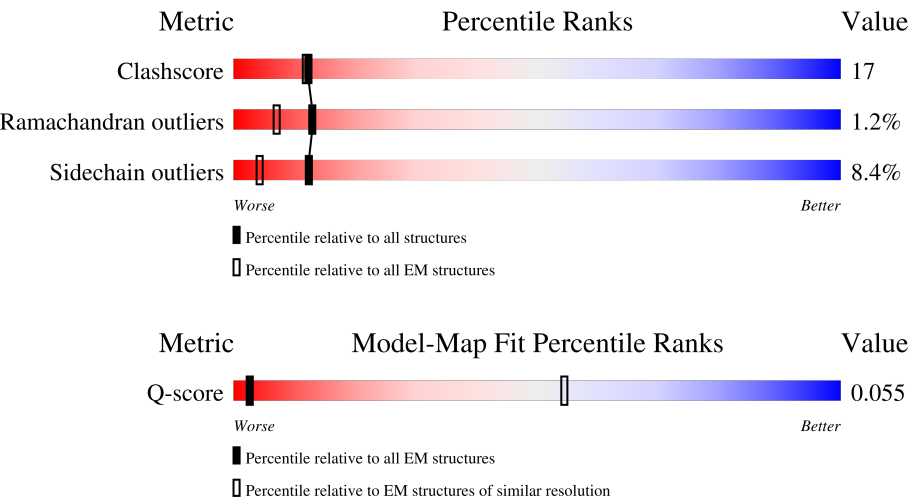
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	81 (11.70 - 12.70)

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

Mol	Chain	Length	Quality of chain
1	A	353	
1	D	353	
2	B	662	
2	E	662	

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Mol	Chain	Length	Quality of chain
3	C	113	27% 62% 30% 5%
3	F	113	17% 59% 30% 6%

2 Entry composition

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
1	A	330	Total	C	N	O	S	0	0
			2573	1618	454	491	10		
1	D	330	Total	C	N	O	S	0	0
			2573	1618	454	491	10		

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
2	B	211	Total	C	N	O	S	0	0
			1781	1135	308	330	8		

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

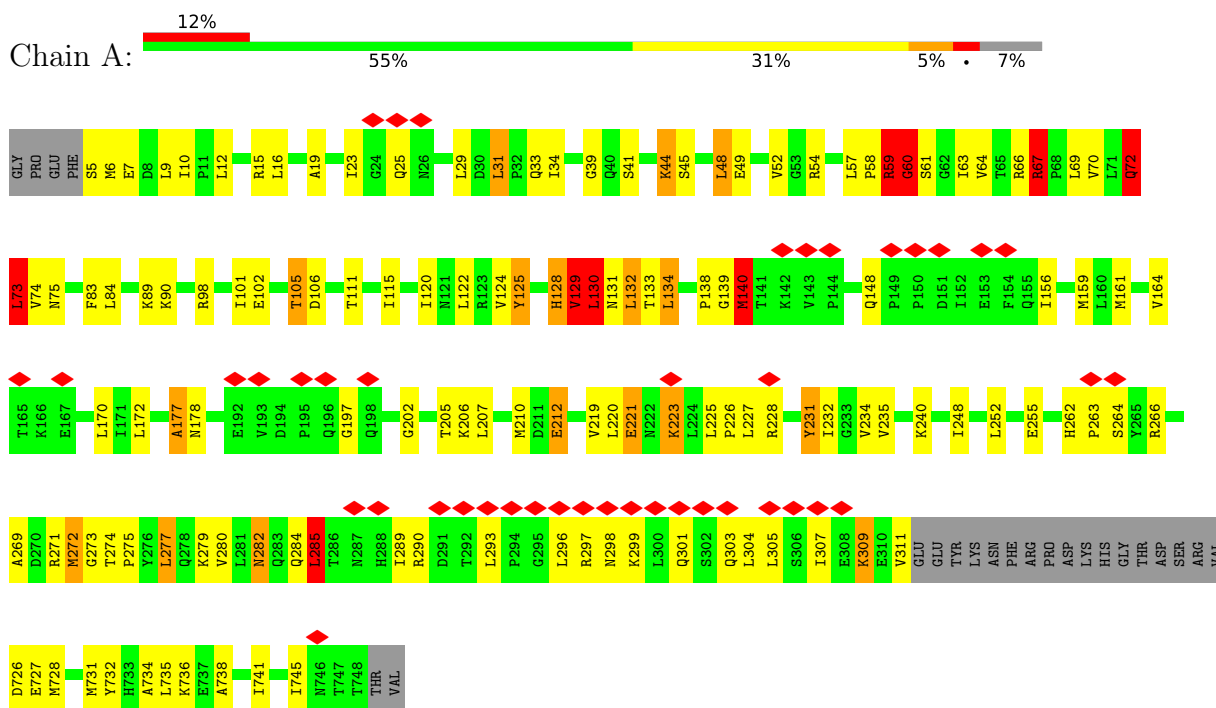
- Molecule 3 is a protein called DYNAMIN-1.

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

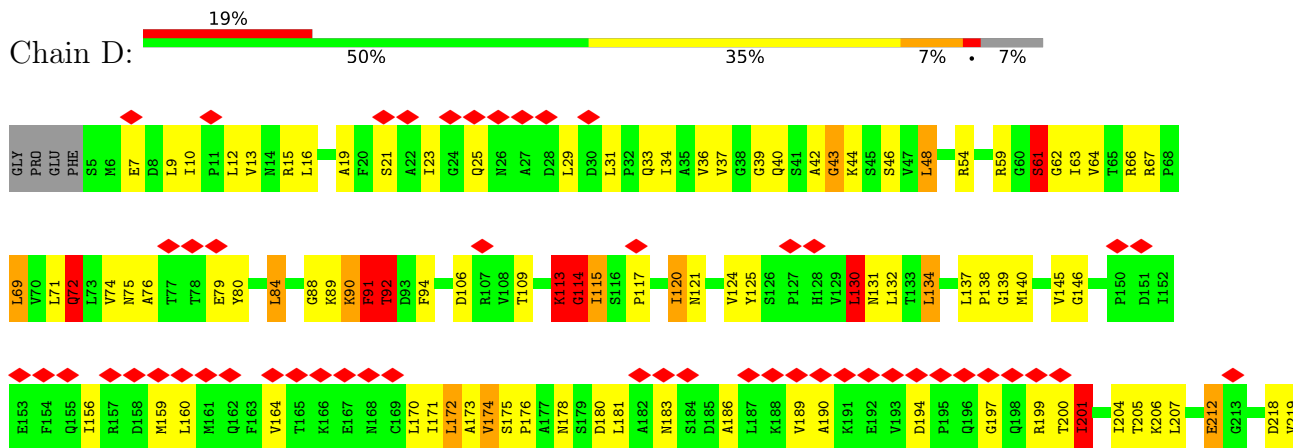
3 Residue-property plots

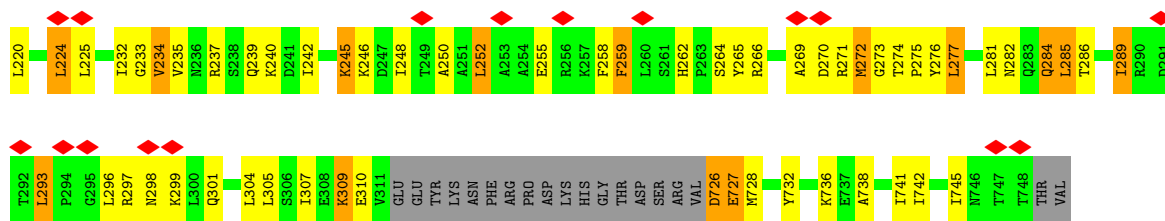
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DYNAMIN-1

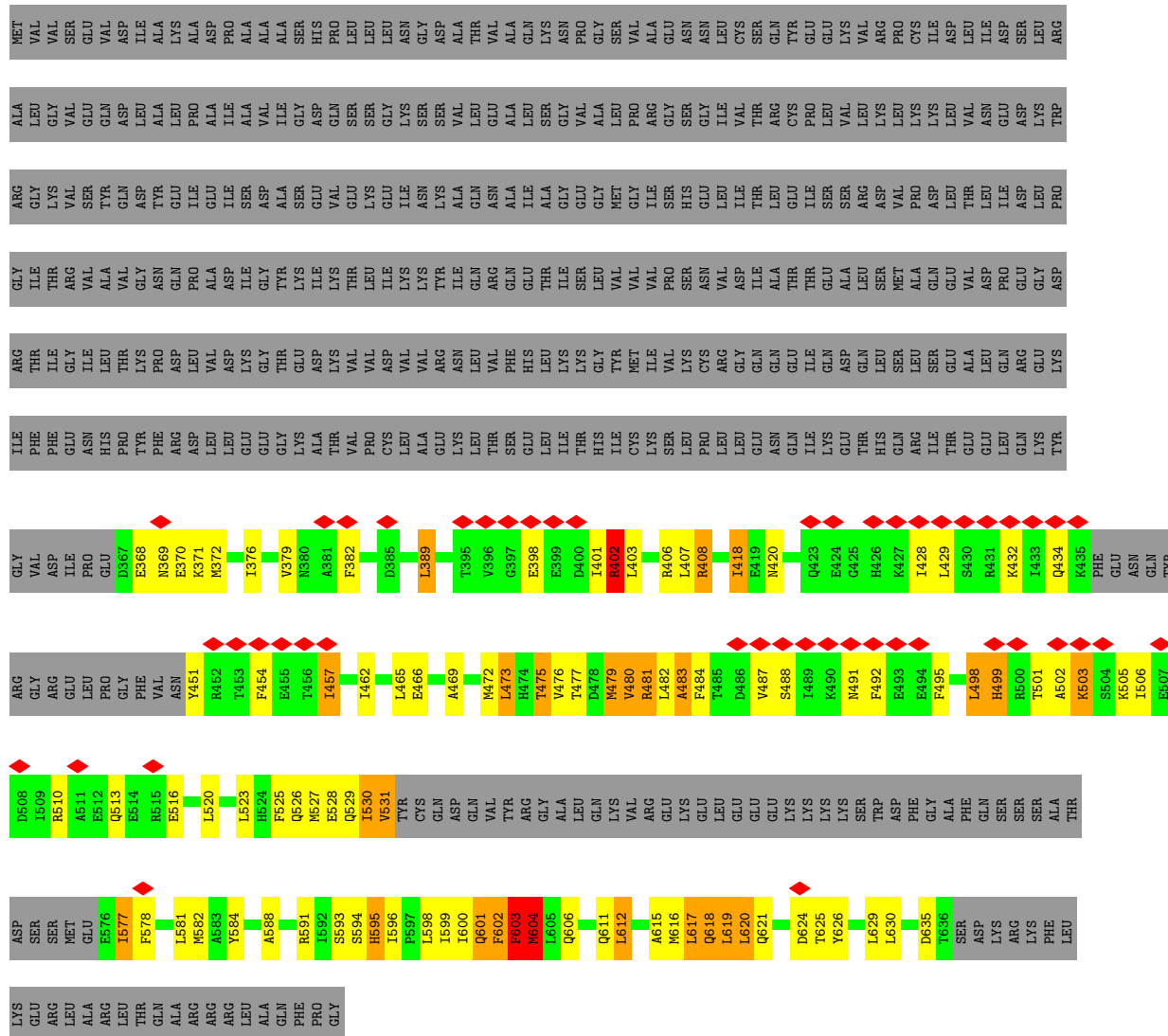


• Molecule 1: DYNAMIN-1

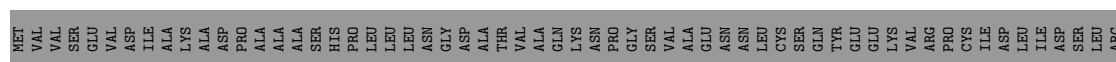


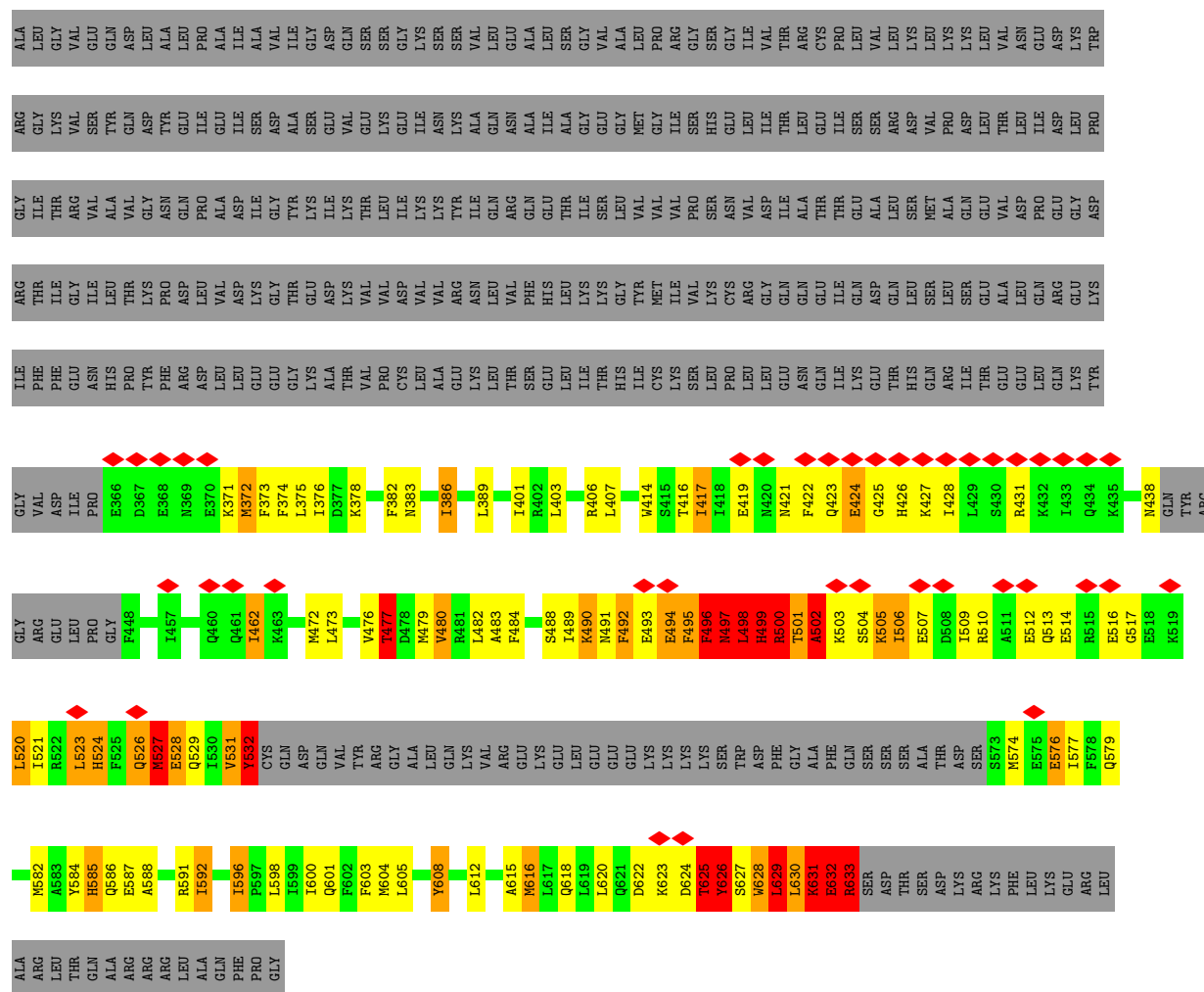


• Molecule 2: INTERFERON-INDUCED GTP-BINDING PROTEIN MX1

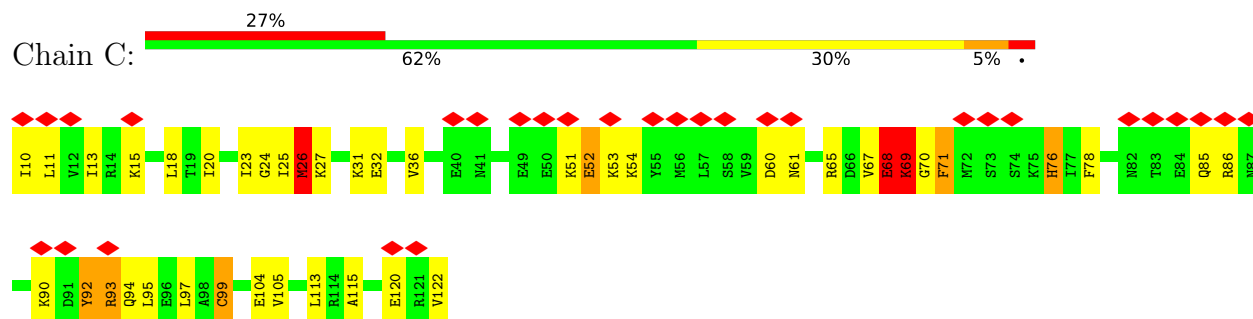


• Molecule 2: INTERFERON-INDUCED GTP-BINDING PROTEIN MX1

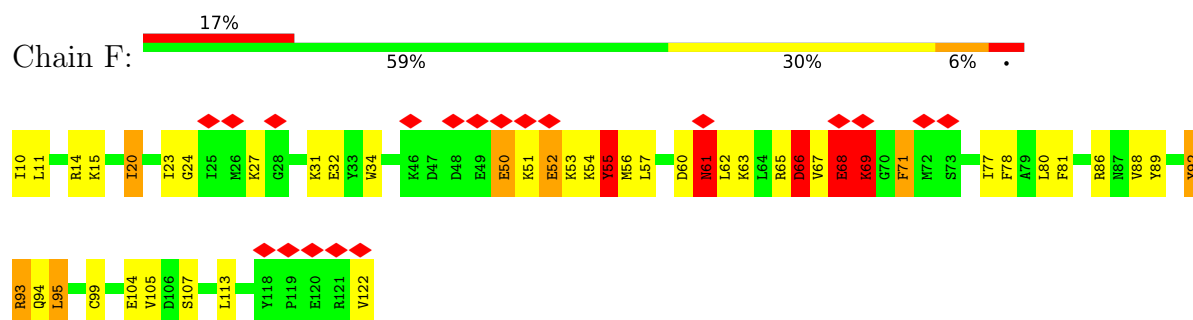




• Molecule 3: DYNAMIN-1



• 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 ($e^-/\text{\AA}^2$)	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	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 ⓘ

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	1.04	11/2610 (0.4%)	1.84	74/3532 (2.1%)
1	D	1.09	12/2610 (0.5%)	1.85	92/3532 (2.6%)
2	B	1.18	4/1812 (0.2%)	1.88	59/2428 (2.4%)
2	E	1.77	36/1892 (1.9%)	3.35	178/2535 (7.0%)
3	C	1.02	8/966 (0.8%)	1.80	31/1298 (2.4%)
3	F	1.21	9/966 (0.9%)	2.02	39/1298 (3.0%)
All	All	1.25	80/10856 (0.7%)	2.20	473/14623 (3.2%)

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	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 (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	495	PHE	C-O	-23.71	0.95	1.23
3	F	61	ASN	CA-CB	-13.41	1.35	1.53
2	E	497	ASN	C-O	-13.14	0.97	1.23
2	E	500	ARG	CD-NE	-11.84	1.29	1.46
2	E	496	PHE	C-O	-11.05	1.04	1.23
1	D	115	ILE	N-CA	-11.02	1.32	1.46
1	A	61	SER	N-CA	-10.52	1.32	1.46
2	E	498	LEU	C-N	-9.82	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	245	LYS	CA-CB	-9.66	1.39	1.53
2	E	500	ARG	CA-C	-9.50	1.40	1.52
2	E	500	ARG	C-O	-9.36	1.12	1.24
2	E	499	HIS	CA-C	-9.32	1.40	1.52
2	E	496	PHE	CA-C	-9.14	1.40	1.52
2	E	496	PHE	N-CA	-9.11	1.35	1.46
2	E	495	PHE	N-CA	-8.91	1.35	1.46
2	B	603	PHE	CA-CB	-8.77	1.42	1.52
3	F	66	ASP	CA-CB	-8.67	1.41	1.52
2	E	628	TRP	C-O	-8.65	1.13	1.24
1	D	61	SER	CA-CB	8.29	1.66	1.53
2	E	629	LEU	C-O	-8.19	1.14	1.24
2	E	500	ARG	N-CA	-8.03	1.35	1.46
3	F	53	LYS	N-CA	-8.02	1.35	1.46
3	C	53	LYS	N-CA	-7.90	1.35	1.46
2	E	500	ARG	C-N	-7.80	1.22	1.33
2	E	499	HIS	C-N	-7.66	1.23	1.33
1	D	61	SER	CB-OG	-7.61	1.26	1.42
2	B	603	PHE	N-CA	-7.47	1.36	1.46
2	E	496	PHE	CA-CB	7.37	1.64	1.52
1	D	130	LEU	CA-CB	-7.28	1.41	1.53
3	C	26	MET	N-CA	-7.12	1.37	1.46
2	E	579	GLN	CA-CB	-7.05	1.42	1.53
2	E	501	THR	N-CA	-6.93	1.37	1.46
1	D	224	LEU	CA-CB	-6.85	1.42	1.53
1	A	130	LEU	CA-CB	-6.80	1.42	1.53
3	C	69	LYS	C-N	-6.61	1.25	1.32
2	E	503	LYS	C-N	-6.19	1.25	1.33
3	C	70	GLY	N-CA	-6.16	1.39	1.45
3	C	76	HIS	CA-CB	-6.15	1.44	1.53
1	A	60	GLY	C-N	-6.12	1.25	1.33
3	F	52	GLU	CA-C	-6.02	1.44	1.52
2	E	499	HIS	ND1-CE1	5.96	1.38	1.32
2	E	500	ARG	CB-CG	-5.96	1.34	1.52
1	D	72	GLN	CA-CB	-5.93	1.44	1.53
3	F	93	ARG	C-N	-5.93	1.26	1.33
3	F	94	GLN	N-CA	-5.85	1.38	1.45
1	D	91	PHE	N-CA	-5.82	1.38	1.46
1	A	130	LEU	N-CA	-5.77	1.38	1.45
1	A	72	GLN	CA-CB	-5.72	1.44	1.53
1	A	129	VAL	CA-C	-5.71	1.45	1.52
2	E	527	MET	C-O	-5.71	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	69	LYS	C-N	-5.70	1.25	1.33
3	C	52	GLU	CA-C	-5.68	1.45	1.52
2	E	501	THR	C-N	-5.67	1.25	1.33
1	A	129	VAL	CA-CB	5.60	1.64	1.55
2	E	386	ILE	CA-CB	-5.59	1.47	1.54
2	B	602	PHE	C-O	-5.59	1.17	1.24
3	C	94	GLN	N-CA	-5.57	1.39	1.45
3	C	93	ARG	C-N	-5.53	1.26	1.33
1	A	129	VAL	C-N	-5.49	1.26	1.33
3	F	55	TYR	CA-CB	-5.31	1.44	1.53
1	A	73	LEU	CA-CB	-5.29	1.45	1.53
3	F	52	GLU	N-CA	-5.25	1.39	1.46
2	E	497	ASN	N-CA	-5.25	1.36	1.46
2	E	576	GLU	CA-CB	-5.25	1.45	1.53
2	E	524	HIS	N-CA	-5.23	1.40	1.46
1	A	73	LEU	N-CA	-5.21	1.39	1.46
2	E	498	LEU	N-CA	-5.18	1.36	1.46
2	E	596	ILE	CA-C	5.16	1.56	1.52
1	D	234	VAL	N-CA	-5.11	1.40	1.46
2	E	507	GLU	C-N	-5.10	1.27	1.33
2	E	492	PHE	N-CA	-5.08	1.38	1.46
1	D	273	GLY	N-CA	-5.06	1.39	1.45
1	A	131	ASN	C-N	-5.05	1.26	1.33
2	B	523	LEU	C-O	-5.04	1.18	1.24
2	E	495	PHE	C-N	-5.03	1.27	1.33
1	D	270	ASP	C-N	-5.03	1.26	1.33
2	E	496	PHE	CG-CD2	-5.03	1.28	1.38
1	D	61	SER	CA-C	-5.01	1.46	1.52
2	E	503	LYS	C-O	-5.01	1.17	1.24
2	E	499	HIS	CE1-NE2	-5.01	1.27	1.32

All (473) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	497	ASN	O-C-N	-36.75	64.19	123.00
2	E	496	PHE	O-C-N	-34.54	68.35	121.89
2	E	495	PHE	O-C-N	-30.98	83.48	123.14
2	E	497	ASN	CA-C-N	29.82	175.38	121.70
2	E	497	ASN	C-N-CA	29.82	175.38	121.70
3	F	61	ASN	CA-CB-CG	25.91	138.51	112.60
2	E	495	PHE	CA-C-N	23.79	164.97	122.62
2	E	495	PHE	C-N-CA	23.79	164.97	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	496	PHE	CA-C-N	23.11	163.29	121.70
2	E	496	PHE	C-N-CA	23.11	163.29	121.70
2	E	494	GLU	CA-C-N	22.81	156.69	122.47
2	E	494	GLU	C-N-CA	22.81	156.69	122.47
2	E	498	LEU	CA-C-N	22.46	164.44	121.54
2	E	498	LEU	C-N-CA	22.46	164.44	121.54
2	E	496	PHE	N-CA-C	21.64	141.20	111.55
2	E	500	ARG	NE-CZ-NH2	21.32	138.39	119.20
2	E	500	ARG	CD-NE-CZ	19.83	152.17	124.40
2	E	498	LEU	O-C-N	-19.57	91.69	123.00
3	C	69	LYS	CA-C-N	18.07	137.22	121.86
3	C	69	LYS	C-N-CA	18.07	137.22	121.86
1	D	114	GLY	CA-C-N	16.81	152.23	121.97
1	D	114	GLY	C-N-CA	16.81	152.23	121.97
2	E	527	MET	O-C-N	-16.73	104.83	122.07
2	E	579	GLN	N-CA-CB	16.57	134.03	110.01
1	A	60	GLY	CA-C-N	15.78	151.67	121.54
1	A	60	GLY	C-N-CA	15.78	151.67	121.54
2	B	603	PHE	N-CA-CB	15.37	134.16	109.88
2	E	500	ARG	O-C-N	-15.05	102.57	122.59
2	E	499	HIS	CA-C-N	14.83	149.87	121.54
2	E	499	HIS	C-N-CA	14.83	149.87	121.54
2	B	603	PHE	CA-C-O	14.74	137.97	121.02
2	E	527	MET	CA-C-O	14.68	136.24	120.82
2	E	495	PHE	CB-CA-C	13.89	130.96	111.23
2	E	625	THR	O-C-N	-13.89	101.83	122.39
1	A	129	VAL	CA-CB-CG1	-13.73	87.06	110.40
2	E	497	ASN	CA-C-O	13.64	144.00	120.80
1	A	131	ASN	CA-C-N	13.15	145.41	122.67
1	A	131	ASN	C-N-CA	13.15	145.41	122.67
2	E	499	HIS	O-C-N	-13.11	105.16	122.59
2	B	602	PHE	O-C-N	-13.00	108.05	122.09
2	B	604	MET	N-CA-CB	12.99	132.44	110.49
2	E	500	ARG	CG-CD-NE	12.93	140.44	112.00
1	D	61	SER	CA-CB-OG	-12.82	85.46	111.10
2	E	496	PHE	CB-CA-C	-12.68	95.04	111.40
2	E	625	THR	CA-CB-CG2	12.39	131.57	110.50
2	E	500	ARG	CB-CG-CD	12.28	139.54	111.30
2	E	532	TYR	CA-C-O	12.28	141.67	120.80
1	D	90	LYS	CA-C-N	12.26	144.96	121.54
1	D	90	LYS	C-N-CA	12.26	144.96	121.54
2	E	628	TRP	O-C-N	-12.18	106.39	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	LEU	N-CA-CB	12.02	127.54	110.36
1	A	129	VAL	CA-C-N	11.90	142.64	120.97
1	A	129	VAL	C-N-CA	11.90	142.64	120.97
2	E	576	GLU	CA-CB-CG	11.76	137.61	114.10
2	E	501	THR	CA-CB-CG2	11.66	130.32	110.50
3	F	61	ASN	OD1-CG-ND2	-11.62	110.98	122.60
1	D	72	GLN	CB-CA-C	11.61	129.80	109.72
3	F	50	GLU	CA-CB-CG	11.56	137.22	114.10
2	E	497	ASN	CA-CB-CG	11.50	124.10	112.60
2	E	629	LEU	O-C-N	-11.50	109.67	122.09
1	A	72	GLN	CB-CA-C	11.43	129.50	109.72
2	B	617	LEU	CA-C-N	11.15	136.65	120.38
2	B	617	LEU	C-N-CA	11.15	136.65	120.38
1	A	130	LEU	N-CA-CB	11.06	126.18	110.36
2	E	498	LEU	N-CA-CB	11.05	129.28	110.50
2	E	497	ASN	N-CA-C	10.79	141.21	111.00
3	F	66	ASP	CA-CB-CG	10.75	123.35	112.60
2	E	630	LEU	N-CA-C	10.65	125.53	112.54
2	E	501	THR	N-CA-CB	10.58	128.37	110.49
3	F	61	ASN	CB-CG-ND2	-10.47	100.70	116.40
2	E	438	ASN	CA-C-O	-10.43	103.08	120.80
2	B	602	PHE	CA-C-N	10.35	139.67	122.07
2	B	602	PHE	C-N-CA	10.35	139.67	122.07
3	C	52	GLU	CA-C-N	10.30	141.21	121.54
3	C	52	GLU	C-N-CA	10.30	141.21	121.54
2	E	631	LYS	CA-CB-CG	10.24	134.59	114.10
2	B	601	GLN	CA-CB-CG	10.19	134.48	114.10
1	A	73	LEU	N-CA-CB	10.18	126.71	110.23
2	E	507	GLU	CA-C-N	10.12	134.21	120.54
2	E	507	GLU	C-N-CA	10.12	134.21	120.54
1	A	212	GLU	CA-CB-CG	10.04	134.18	114.10
1	D	61	SER	CA-C-O	-10.02	109.95	121.47
3	F	52	GLU	CA-C-N	9.97	140.59	121.54
3	F	52	GLU	C-N-CA	9.97	140.59	121.54
2	E	631	LYS	CG-CD-CE	9.97	134.22	111.30
1	D	212	GLU	CA-CB-CG	9.91	133.93	114.10
2	E	503	LYS	CA-C-N	9.76	133.35	120.28
2	E	503	LYS	C-N-CA	9.76	133.35	120.28
1	D	131	ASN	CA-C-N	9.73	139.50	122.67
1	D	131	ASN	C-N-CA	9.73	139.50	122.67
1	D	115	ILE	N-CA-CB	9.64	127.14	111.23
3	F	66	ASP	N-CA-CB	9.63	124.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	O-C-N	-9.58	110.89	122.96
2	E	516	GLU	CA-C-N	9.55	130.54	119.94
2	E	516	GLU	C-N-CA	9.55	130.54	119.94
1	D	72	GLN	CA-C-O	-9.50	110.03	120.38
1	A	67	ARG	NE-CZ-NH1	-9.47	112.03	121.50
1	A	129	VAL	CA-C-O	-9.41	111.30	121.28
2	E	631	LYS	CB-CG-CD	9.40	132.93	111.30
2	E	625	THR	CA-C-O	9.33	131.34	119.12
1	D	248	ILE	N-CA-C	9.24	120.06	110.36
1	D	90	LYS	O-C-N	-9.21	110.96	123.12
2	E	629	LEU	CA-C-O	-9.21	111.22	120.70
3	F	93	ARG	CA-C-N	9.18	138.10	121.85
3	F	93	ARG	C-N-CA	9.18	138.10	121.85
2	E	499	HIS	CB-CA-C	9.15	128.62	110.42
1	A	61	SER	N-CA-CB	9.13	125.92	110.49
2	E	498	LEU	CA-CB-CG	9.03	147.89	116.30
2	E	493	GLU	N-CA-CB	8.93	123.66	110.53
3	F	66	ASP	CA-C-O	-8.90	111.36	120.98
2	E	500	ARG	NH1-CZ-NH2	-8.84	107.80	119.30
3	C	92	TYR	N-CA-C	8.84	125.72	114.31
2	B	408	ARG	NE-CZ-NH1	-8.81	112.69	121.50
1	A	131	ASN	O-C-N	-8.79	112.00	122.46
1	A	60	GLY	O-C-N	-8.75	114.21	122.79
3	F	92	TYR	N-CA-C	8.72	125.56	114.31
2	E	576	GLU	N-CA-CB	8.71	123.39	110.33
2	B	621	GLN	CG-CD-NE2	8.70	129.46	116.40
2	E	626	TYR	N-CA-CB	8.68	125.16	110.49
1	A	72	GLN	CA-C-O	-8.54	111.07	120.38
2	E	527	MET	CG-SD-CE	-8.51	82.17	100.90
3	C	93	ARG	CA-C-N	8.44	136.79	121.85
3	C	93	ARG	C-N-CA	8.44	136.79	121.85
2	E	527	MET	CA-CB-CG	8.36	130.82	114.10
2	E	501	THR	O-C-N	-8.32	111.53	122.59
1	A	128	HIS	CB-CG-CD2	8.31	142.01	131.20
3	C	25	ILE	CA-C-N	8.30	137.39	121.54
3	C	25	ILE	C-N-CA	8.30	137.39	121.54
2	E	483	ALA	CA-C-N	8.28	131.72	120.38
2	E	483	ALA	C-N-CA	8.28	131.72	120.38
2	E	527	MET	CA-C-N	8.27	136.36	120.99
2	E	527	MET	C-N-CA	8.27	136.36	120.99
2	B	526	GLN	CA-C-N	8.25	131.67	120.54
2	B	526	GLN	C-N-CA	8.25	131.67	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	596	ILE	N-CA-CB	8.23	115.69	110.50
1	D	178	ASN	CA-C-N	8.20	135.50	122.21
1	D	178	ASN	C-N-CA	8.20	135.50	122.21
1	D	245	LYS	CB-CG-CD	-8.19	92.45	111.30
2	E	507	GLU	O-C-N	-8.19	111.25	122.30
1	A	130	LEU	CA-C-O	-8.16	112.40	121.87
2	E	500	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	D	67	ARG	NE-CZ-NH1	-8.10	113.40	121.50
2	E	527	MET	N-CA-CB	8.06	121.70	110.01
1	D	224	LEU	CB-CG-CD1	8.04	134.83	110.70
1	A	72	GLN	CA-C-N	8.01	133.94	122.09
1	A	72	GLN	C-N-CA	8.01	133.94	122.09
2	B	621	GLN	N-CA-C	7.96	119.59	111.07
2	B	620	LEU	N-CA-C	7.92	122.04	112.38
1	A	125	TYR	N-CA-CB	7.89	122.18	109.95
1	A	248	ILE	N-CA-C	7.88	118.63	110.36
3	F	51	LYS	CA-C-N	7.87	136.56	121.54
3	F	51	LYS	C-N-CA	7.87	136.56	121.54
3	C	51	LYS	CA-C-N	7.83	136.49	121.54
3	C	51	LYS	C-N-CA	7.83	136.49	121.54
1	A	124	VAL	CA-C-N	7.82	132.68	121.50
1	A	124	VAL	C-N-CA	7.82	132.68	121.50
2	E	629	LEU	CA-C-N	7.79	133.72	120.72
2	E	629	LEU	C-N-CA	7.79	133.72	120.72
2	B	603	PHE	O-C-N	-7.76	111.92	122.48
1	D	91	PHE	N-CA-CB	7.76	123.60	110.49
2	E	503	LYS	O-C-N	-7.71	112.34	122.59
2	E	598	LEU	CA-C-N	7.70	130.53	120.60
2	E	598	LEU	C-N-CA	7.70	130.53	120.60
2	E	500	ARG	N-CA-CB	7.70	123.50	110.49
1	D	67	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	A	282	ASN	CA-C-N	7.60	130.47	120.28
1	A	282	ASN	C-N-CA	7.60	130.47	120.28
2	E	495	PHE	CA-CB-CG	7.53	121.33	113.80
3	C	26	MET	N-CA-CB	7.50	123.17	110.49
1	D	270	ASP	CA-C-N	7.48	135.83	121.54
1	D	270	ASP	C-N-CA	7.48	135.83	121.54
2	E	488	SER	CA-C-N	7.48	130.25	120.60
2	E	488	SER	C-N-CA	7.48	130.25	120.60
1	D	114	GLY	O-C-N	-7.45	114.82	123.17
2	E	492	PHE	N-CA-CB	7.45	122.08	111.65
3	F	61	ASN	CB-CG-OD1	7.42	135.64	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	483	ALA	CA-C-N	7.41	130.20	120.28
2	B	483	ALA	C-N-CA	7.41	130.20	120.28
3	F	67	VAL	CA-C-N	7.39	135.66	121.54
3	F	67	VAL	C-N-CA	7.39	135.66	121.54
2	B	529	GLN	O-C-N	-7.39	112.27	122.46
3	F	55	TYR	N-CA-CB	7.38	122.96	110.49
1	D	91	PHE	O-C-N	-7.36	112.80	122.59
2	E	496	PHE	CA-CB-CG	-7.34	106.46	113.80
2	E	496	PHE	CZ-CE2-CD2	-7.31	106.84	120.00
2	E	386	ILE	CB-CG1-CD1	-7.31	98.45	113.80
3	F	53	LYS	N-CA-CB	7.29	122.81	110.49
1	A	285	LEU	CA-C-N	7.27	130.35	120.54
1	A	285	LEU	C-N-CA	7.27	130.35	120.54
3	F	69	LYS	CA-C-N	7.26	135.65	121.41
3	F	69	LYS	C-N-CA	7.26	135.65	121.41
1	D	224	LEU	N-CA-CB	7.26	120.86	109.82
2	E	502	ALA	CA-C-N	7.20	135.30	121.54
2	E	502	ALA	C-N-CA	7.20	135.30	121.54
2	E	505	LYS	CD-CE-NZ	7.15	134.79	111.90
2	E	492	PHE	O-C-N	-7.15	113.13	121.99
2	E	417	ILE	CB-CG1-CD1	7.14	128.80	113.80
1	A	72	GLN	CG-CD-NE2	-7.08	105.78	116.40
3	C	53	LYS	N-CA-CB	7.07	122.44	110.49
2	E	421	ASN	CA-C-N	7.07	129.63	120.44
2	E	421	ASN	C-N-CA	7.07	129.63	120.44
1	A	272	MET	CA-C-N	7.04	133.33	121.57
1	A	272	MET	C-N-CA	7.04	133.33	121.57
1	D	285	LEU	CA-C-N	7.03	130.01	120.38
1	D	285	LEU	C-N-CA	7.03	130.01	120.38
3	C	76	HIS	CA-CB-CG	7.02	120.82	113.80
2	E	498	LEU	CB-CG-CD2	7.01	131.72	110.70
2	E	495	PHE	CD1-CG-CD2	-6.97	108.14	118.60
2	B	488	SER	CA-C-N	6.96	129.33	120.56
2	B	488	SER	C-N-CA	6.96	129.33	120.56
2	E	625	THR	OG1-CB-CG2	6.96	123.21	109.30
2	E	512	GLU	CA-C-N	6.89	130.07	120.29
2	E	512	GLU	C-N-CA	6.89	130.07	120.29
3	C	76	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	A	129	VAL	N-CA-C	6.85	119.91	108.81
2	B	601	GLN	N-CA-CB	6.85	119.91	109.98
2	E	492	PHE	CA-CB-CG	6.84	120.64	113.80
2	B	480	VAL	CA-C-N	6.84	129.75	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	VAL	C-N-CA	6.84	129.75	120.38
2	E	497	ASN	CB-CA-C	-6.81	97.16	110.10
3	F	93	ARG	O-C-N	-6.81	113.54	122.59
3	C	76	HIS	N-CA-CB	6.79	121.75	110.47
3	F	52	GLU	N-CA-C	6.79	125.27	110.80
2	B	530	ILE	N-CA-C	6.77	117.83	108.89
2	E	633	ARG	N-CA-C	6.77	129.96	111.00
2	E	502	ALA	O-C-N	-6.76	113.60	122.59
1	D	277	LEU	CA-C-N	6.70	129.59	120.54
1	D	277	LEU	C-N-CA	6.70	129.59	120.54
3	C	93	ARG	O-C-N	-6.68	113.71	122.59
2	B	621	GLN	CG-CD-OE1	-6.67	107.46	120.80
2	E	628	TRP	CZ3-CH2-CZ2	-6.67	112.83	121.50
3	C	67	VAL	CA-C-N	6.66	134.25	121.54
3	C	67	VAL	C-N-CA	6.66	134.25	121.54
2	E	500	ARG	CA-C-N	6.64	134.22	121.54
2	E	500	ARG	C-N-CA	6.64	134.22	121.54
1	D	67	ARG	CD-NE-CZ	6.62	133.68	124.40
2	E	601	GLN	CA-C-N	6.62	129.05	120.44
2	E	601	GLN	C-N-CA	6.62	129.05	120.44
1	D	286	THR	CA-C-N	6.60	129.42	120.38
1	D	286	THR	C-N-CA	6.60	129.42	120.38
3	C	25	ILE	O-C-N	-6.58	115.46	121.91
2	E	510	ARG	CA-C-N	6.57	129.93	120.79
2	E	510	ARG	C-N-CA	6.57	129.93	120.79
2	E	633	ARG	NE-CZ-NH2	6.55	125.09	119.20
1	D	130	LEU	CA-C-O	-6.54	114.28	121.87
2	E	497	ASN	N-CA-CB	6.54	121.62	110.50
1	D	266	ARG	N-CA-C	6.52	119.21	111.71
3	F	50	GLU	CB-CG-CD	6.51	123.67	112.60
2	E	503	LYS	CA-CB-CG	6.51	127.12	114.10
2	E	504	SER	CA-C-N	6.51	129.00	120.28
2	E	504	SER	C-N-CA	6.51	129.00	120.28
1	D	71	LEU	CA-C-N	6.50	131.97	123.00
1	D	71	LEU	C-N-CA	6.50	131.97	123.00
1	A	72	GLN	OE1-CD-NE2	6.49	129.09	122.60
2	E	495	PHE	CA-C-O	-6.48	111.72	120.47
1	A	129	VAL	O-C-N	-6.46	115.63	123.00
2	E	627	SER	CA-CB-OG	6.45	124.00	111.10
2	E	417	ILE	CA-CB-CG1	6.42	121.31	110.40
2	E	501	THR	CA-C-N	6.39	133.75	121.54
2	E	501	THR	C-N-CA	6.39	133.75	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	528	GLU	O-C-N	-6.35	113.98	122.43
1	D	219	VAL	CB-CA-C	-6.35	103.84	111.97
1	A	140	MET	CA-CB-CG	6.33	126.77	114.10
2	E	386	ILE	N-CA-CB	6.28	118.32	110.47
1	A	269	ALA	N-CA-C	6.27	119.78	111.75
1	D	282	ASN	CA-C-N	6.26	128.67	120.28
1	D	282	ASN	C-N-CA	6.26	128.67	120.28
1	A	178	ASN	CA-C-N	6.26	132.61	122.29
1	A	178	ASN	C-N-CA	6.26	132.61	122.29
2	E	506	ILE	O-C-N	-6.25	115.81	121.87
1	D	272	MET	O-C-N	-6.23	114.41	122.94
1	A	60	GLY	N-CA-C	6.21	120.24	112.79
1	D	296	LEU	CA-C-N	6.19	128.48	120.44
1	D	296	LEU	C-N-CA	6.19	128.48	120.44
3	C	52	GLU	N-CA-CB	6.17	120.92	110.49
1	D	270	ASP	O-C-N	-6.17	113.95	122.46
3	F	61	ASN	CB-CA-C	6.17	124.20	110.76
2	E	386	ILE	CA-CB-CG2	6.16	120.98	110.50
1	D	72	GLN	CG-CD-NE2	-6.15	107.18	116.40
1	A	266	ARG	N-CA-C	6.09	118.71	111.71
3	F	69	LYS	O-C-N	-6.08	114.50	122.59
1	A	273	GLY	CA-C-N	6.08	131.16	121.62
1	A	273	GLY	C-N-CA	6.08	131.16	121.62
2	B	611	GLN	CA-C-N	6.07	128.41	120.28
2	B	611	GLN	C-N-CA	6.07	128.41	120.28
1	D	269	ALA	N-CA-C	6.07	119.52	111.75
2	B	606	GLN	CA-C-N	6.07	128.41	120.28
2	B	606	GLN	C-N-CA	6.07	128.41	120.28
2	E	626	TYR	CA-C-O	6.06	129.18	120.51
2	E	419	GLU	CA-C-N	6.05	128.70	120.54
2	E	419	GLU	C-N-CA	6.05	128.70	120.54
1	D	259	PHE	N-CA-C	6.04	119.48	111.75
3	F	77	ILE	N-CA-C	6.04	118.07	108.89
2	E	496	PHE	CA-C-O	-6.04	110.76	121.38
1	A	70	VAL	CA-C-N	6.03	131.05	122.72
1	A	70	VAL	C-N-CA	6.03	131.05	122.72
3	C	69	LYS	O-C-N	-6.02	114.58	122.59
1	D	201	ILE	CA-CB-CG1	-6.02	100.16	110.40
3	C	52	GLU	N-CA-C	5.96	123.51	110.80
1	A	120	ILE	N-CA-C	-5.96	99.83	108.71
2	B	368	GLU	CA-C-N	5.96	128.85	120.28
2	B	368	GLU	C-N-CA	5.96	128.85	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	68	GLU	CA-C-N	5.95	132.91	121.54
3	F	68	GLU	C-N-CA	5.95	132.91	121.54
1	A	293	LEU	N-CA-C	5.94	121.77	113.57
2	E	489	ILE	CA-C-N	5.94	128.51	120.38
2	E	489	ILE	C-N-CA	5.94	128.51	120.38
1	A	219	VAL	CB-CA-C	-5.92	104.39	111.97
1	D	224	LEU	CB-CA-C	5.92	120.34	110.92
2	E	505	LYS	CG-CD-CE	5.92	124.92	111.30
1	D	245	LYS	N-CA-CB	5.91	121.05	112.13
1	D	131	ASN	O-C-N	-5.89	115.45	122.46
2	E	477	THR	N-CA-CB	5.86	119.37	110.28
2	E	492	PHE	N-CA-C	5.85	117.92	110.61
1	D	174	VAL	O-C-N	-5.83	116.55	123.03
1	D	120	ILE	N-CA-C	-5.82	100.03	108.36
2	B	624	ASP	CA-C-N	5.82	132.92	121.58
2	B	624	ASP	C-N-CA	5.82	132.92	121.58
1	A	277	LEU	CA-C-N	5.81	128.39	120.54
1	A	277	LEU	C-N-CA	5.81	128.39	120.54
2	B	618	GLN	CA-C-N	5.81	128.06	120.28
2	B	618	GLN	C-N-CA	5.81	128.06	120.28
2	E	626	TYR	CE1-CZ-CE2	-5.81	108.69	120.30
2	B	499	HIS	CA-C-N	5.79	128.04	120.28
2	B	499	HIS	C-N-CA	5.79	128.04	120.28
2	E	480	VAL	CA-C-N	5.78	128.30	120.38
2	E	480	VAL	C-N-CA	5.78	128.30	120.38
2	E	579	GLN	CA-C-O	5.77	126.88	120.82
2	E	383	ASN	CA-C-N	5.76	128.00	120.28
2	E	383	ASN	C-N-CA	5.76	128.00	120.28
2	E	628	TRP	CG-CD2-CE3	5.76	139.66	133.90
2	B	603	PHE	CA-C-N	5.74	132.50	121.54
2	B	603	PHE	C-N-CA	5.74	132.50	121.54
2	E	633	ARG	CG-CD-NE	5.72	124.59	112.00
2	E	628	TRP	CA-C-O	5.72	128.69	120.51
1	A	128	HIS	CB-CG-ND1	-5.71	114.14	122.70
2	B	594	SER	N-CA-C	5.71	118.71	111.69
1	A	226	PRO	N-CA-C	5.68	119.78	111.03
2	E	632	GLU	CA-C-O	-5.68	112.15	118.69
1	A	90	LYS	CA-C-N	5.68	128.90	120.95
1	A	90	LYS	C-N-CA	5.68	128.90	120.95
2	E	488	SER	CA-CB-OG	-5.67	99.75	111.10
1	D	115	ILE	CA-CB-CG1	-5.67	100.76	110.40
3	C	60	ASP	N-CA-C	5.66	118.40	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	499	HIS	CA-CB-CG	5.65	119.45	113.80
1	D	273	GLY	CA-C-N	5.63	130.47	121.62
1	D	273	GLY	C-N-CA	5.63	130.47	121.62
2	E	491	ASN	CA-C-N	5.63	132.80	122.54
2	E	491	ASN	C-N-CA	5.63	132.80	122.54
2	E	622	ASP	N-CA-C	5.63	118.57	107.98
1	A	736	LYS	CA-C-N	5.63	128.14	120.54
1	A	736	LYS	C-N-CA	5.63	128.14	120.54
3	C	68	GLU	CA-C-N	5.62	132.27	121.54
3	C	68	GLU	C-N-CA	5.62	132.27	121.54
1	A	223	LYS	N-CA-CB	5.61	119.97	110.49
1	A	130	LEU	CB-CA-C	5.60	121.16	109.68
1	D	252	LEU	CA-C-N	5.57	127.75	120.28
1	D	252	LEU	C-N-CA	5.57	127.75	120.28
1	A	296	LEU	CA-C-N	5.57	127.68	120.44
1	A	296	LEU	C-N-CA	5.57	127.68	120.44
1	A	223	LYS	CB-CG-CD	5.56	124.08	111.30
3	F	20	ILE	N-CA-CB	5.54	118.13	111.31
3	F	60	ASP	N-CA-C	5.53	118.20	109.96
2	E	592	ILE	CA-C-N	5.52	127.68	120.28
2	E	592	ILE	C-N-CA	5.52	127.68	120.28
3	C	76	HIS	CB-CA-C	5.51	119.77	110.79
2	B	420	ASN	CA-C-N	5.49	127.64	120.28
2	B	420	ASN	C-N-CA	5.49	127.64	120.28
1	D	33	GLN	CA-C-N	5.49	130.33	123.14
1	D	33	GLN	C-N-CA	5.49	130.33	123.14
1	D	233	GLY	CA-C-N	5.48	130.12	122.23
1	D	233	GLY	C-N-CA	5.48	130.12	122.23
1	D	736	LYS	CA-C-N	5.47	127.93	120.54
1	D	736	LYS	C-N-CA	5.47	127.93	120.54
2	E	506	ILE	CA-C-N	5.47	133.62	121.80
2	E	506	ILE	C-N-CA	5.47	133.62	121.80
2	E	633	ARG	CD-NE-CZ	5.46	132.05	124.40
1	D	273	GLY	O-C-N	-5.46	117.39	122.47
2	B	527	MET	O-C-N	-5.44	116.43	122.09
1	D	201	ILE	CA-CB-CG2	5.44	119.75	110.50
1	D	289	ILE	CA-C-N	5.44	127.56	120.28
1	D	289	ILE	C-N-CA	5.44	127.56	120.28
2	E	499	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
1	D	201	ILE	CG1-CB-CG2	-5.41	94.48	110.70
1	A	67	ARG	CD-NE-CZ	5.39	131.94	124.40
2	E	462	ILE	CA-C-N	5.38	128.24	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	462	ILE	C-N-CA	5.38	128.24	120.38
2	E	529	GLN	CA-C-N	5.38	130.25	123.10
2	E	529	GLN	C-N-CA	5.38	130.25	123.10
2	E	494	GLU	O-C-N	-5.37	112.94	121.53
1	D	72	GLN	CA-C-N	5.34	130.61	122.65
1	D	72	GLN	C-N-CA	5.34	130.61	122.65
1	A	133	THR	O-C-N	-5.33	117.03	123.27
3	C	85	GLN	N-CA-C	5.33	116.37	108.60
1	D	293	LEU	N-CA-C	5.32	121.56	109.81
2	E	624	ASP	CA-C-N	5.32	132.57	121.94
2	E	624	ASP	C-N-CA	5.32	132.57	121.94
2	B	402	ARG	NE-CZ-NH1	-5.31	116.19	121.50
2	E	372	MET	CB-CA-C	-5.31	101.65	110.68
2	E	416	THR	CA-C-N	5.30	127.24	120.56
2	E	416	THR	C-N-CA	5.30	127.24	120.56
2	E	424	GLU	CA-C-N	5.30	125.83	120.00
2	E	424	GLU	C-N-CA	5.30	125.83	120.00
1	A	44	LYS	N-CA-C	5.30	120.11	111.37
1	A	225	LEU	CA-C-N	5.28	125.54	119.83
1	A	225	LEU	C-N-CA	5.28	125.54	119.83
2	E	579	GLN	CA-CB-CG	5.28	124.66	114.10
2	B	619	LEU	CA-C-N	5.27	129.03	120.60
2	B	619	LEU	C-N-CA	5.27	129.03	120.60
3	F	67	VAL	N-CA-C	5.26	114.84	107.37
1	A	33	GLN	CA-C-N	5.26	130.03	123.14
1	A	33	GLN	C-N-CA	5.26	130.03	123.14
2	B	617	LEU	O-C-N	-5.26	114.76	122.43
2	B	603	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	61	SER	N-CA-CB	-5.25	102.31	110.29
1	D	72	GLN	OE1-CD-NE2	5.25	127.85	122.60
1	D	272	MET	CA-C-N	5.24	136.58	121.60
1	D	272	MET	C-N-CA	5.24	136.58	121.60
2	B	618	GLN	CG-CD-NE2	-5.23	108.55	116.40
3	C	113	LEU	CA-C-N	5.22	127.80	120.28
3	C	113	LEU	C-N-CA	5.22	127.80	120.28
2	B	618	GLN	O-C-N	-5.21	116.26	122.20
3	F	56	MET	CA-C-N	5.21	130.42	122.65
3	F	56	MET	C-N-CA	5.21	130.42	122.65
1	D	194	ASP	CA-C-N	5.21	125.01	119.28
1	D	194	ASP	C-N-CA	5.21	125.01	119.28
1	D	113	LYS	CA-C-O	-5.21	112.23	119.16
1	D	21	SER	CA-C-N	5.21	127.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	SER	C-N-CA	5.21	127.26	120.28
1	D	124	VAL	CA-C-N	5.21	129.80	122.09
1	D	124	VAL	C-N-CA	5.21	129.80	122.09
2	B	577	ILE	CA-C-N	5.20	127.51	120.38
2	B	577	ILE	C-N-CA	5.20	127.51	120.38
2	E	513	GLN	CA-C-N	5.20	127.24	120.28
2	E	513	GLN	C-N-CA	5.20	127.24	120.28
1	D	43	GLY	CA-C-O	5.19	124.77	119.01
3	F	113	LEU	CA-C-N	5.18	127.74	120.28
3	F	113	LEU	C-N-CA	5.18	127.74	120.28
3	F	78	PHE	O-C-N	-5.17	117.15	123.10
2	E	532	TYR	CB-CG-CD2	-5.16	113.07	120.80
3	F	52	GLU	N-CA-CB	5.14	119.17	110.49
1	D	225	LEU	N-CA-CB	-5.13	103.96	111.20
2	B	516	GLU	CA-C-N	5.13	131.46	121.41
2	B	516	GLU	C-N-CA	5.13	131.46	121.41
2	B	526	GLN	O-C-N	-5.12	116.69	122.12
2	B	635	ASP	N-CA-C	5.12	116.58	110.44
1	A	303	GLN	CA-C-N	5.12	127.45	120.54
1	A	303	GLN	C-N-CA	5.12	127.45	120.54
2	E	492	PHE	CA-C-N	-5.11	113.07	121.92
2	E	492	PHE	C-N-CA	-5.11	113.07	121.92
2	E	523	LEU	CA-C-N	5.11	127.09	120.44
2	E	523	LEU	C-N-CA	5.11	127.09	120.44
1	A	277	LEU	N-CA-C	-5.10	105.61	111.07
2	E	386	ILE	CA-CB-CG1	-5.10	101.73	110.40
1	A	307	ILE	CA-C-N	5.05	127.05	120.28
1	A	307	ILE	C-N-CA	5.05	127.05	120.28
2	E	531	VAL	CA-C-N	5.05	130.79	121.70
2	E	531	VAL	C-N-CA	5.05	130.79	121.70
3	F	50	GLU	N-CA-C	5.05	118.41	111.54
1	D	106	ASP	CA-C-N	5.04	128.39	120.82
1	D	106	ASP	C-N-CA	5.04	128.39	120.82
1	D	88	GLY	N-CA-C	5.04	122.28	115.32
2	E	423	GLN	CA-C-N	5.04	126.99	120.44
2	E	423	GLN	C-N-CA	5.04	126.99	120.44
2	B	491	ASN	N-CA-C	5.04	118.58	112.23
1	D	284	GLN	CA-C-N	5.04	126.99	120.44
1	D	284	GLN	C-N-CA	5.04	126.99	120.44
2	E	628	TRP	CD2-CE2-CZ2	-5.04	117.36	122.40
2	B	475	THR	N-CA-CB	5.02	117.59	110.16
2	E	526	GLN	CA-C-N	5.02	126.96	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	526	GLN	C-N-CA	5.02	126.96	120.44
1	D	113	LYS	N-CA-C	5.02	121.34	113.72
3	C	67	VAL	N-CA-CB	5.01	117.31	111.90

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
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

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Mol	Chain	Res	Type	Group
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	Mainchain,Peptide
1	D	114	GLY	Mainchain
1	D	197	GLY	Mainchain
1	D	43	GLY	Mainchain
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	Mainchain,Peptide
2	E	495	PHE	Mainchain,Sidechain,Peptide
2	E	496	PHE	Mainchain,Sidechain,Peptide
2	E	497	ASN	Mainchain
2	E	498	LEU	Peptide
2	E	499	HIS	Mainchain,Sidechain
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	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
2	E	629	LEU	Mainchain,Peptide
2	E	632	GLU	Mainchain
2	E	633	ARG	Sidechain
3	F	24	GLY	Mainchain
3	F	55	TYR	Mainchain,Sidechain
3	F	61	ASN	Mainchain,Sidechain
3	F	68	GLU	Mainchain
3	F	69	LYS	Mainchain

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	2573	0	2632	78	0
1	D	2573	0	2633	138	0
2	B	1781	0	1771	56	0
2	E	1858	0	1828	105	0
3	C	946	0	939	20	0
3	F	946	0	939	24	0
All	All	10677	0	10742	363	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 17.

All (363) 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:CG	2:E:632:GLU:CG	1.97	1.37
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:HG13	2:B:370:GLU:CD	1.60	1.25
1:D:726:ASP:CB	2:E:633:ARG:N	1.98	1.24
1:D:726:ASP:CG	2:E:632:GLU:HG2	1.60	1.23
1:A:311:VAL:HG13	2:B:370:GLU:OE1	1.40	1.16
1:D:726:ASP:CG	2:E:632:GLU:HG3	1.62	1.15
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:309:LYS:HE2	2:E:374:PHE:CG	1.94	1.02
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:311:VAL:CG1	2:B:370:GLU:CD	2.40	0.93
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: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
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
2:E:524:HIS:HA	2:E:527:MET:HE3	1.62	0.80
1:D:726:ASP:OD2	2:E:632:GLU:CG	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:513:GLN:HB2	2:B:604:MET:HE1	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:726:ASP:C	2:E:633:ARG:H	1.91	0.73
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
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
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
1:D:310:GLU:HB3	2:E:632:GLU:CD	2.21	0.65
1:D:726:ASP:CB	2:E:632:GLU:C	2.67	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:GLY:HA3	1:D:176:PRO:HG3	1.79	0.64
2:B:510:ARG:HA	2:B:604:MET:HE2	1.78	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
1:D:726:ASP:CG	2:E:633:ARG:N	2.54	0.64
2:B:502:ALA:HB1	2:B:616:MET:HE1	1.80	0.63
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
2:B:407:LEU:HD12	2:B:479:MET:HE3	1.83	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: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:D:310:GLU:CB	2:E:632:GLU:CD	2.74	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: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
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
1:D:727:GLU:C	2:E:633:ARG:HG2	2.23	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
3:C:10:ILE:HG13	3:C:11:LEU:N	2.16	0.58
1:A:48:LEU:HD22	1:A:134:LEU:HD13	1.87	0.57
1:A:115:ILE:HD12	1:A:159:MET:HE1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:MET:HE1	1:A:282:ASN:HD22	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
2:E:502:ALA:HB1	2:E:616:MET:HE1	1.87	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: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
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:726:ASP:OD1	2:E:632:GLU:CD	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:574:MET:HE3	2:E:574:MET:HA	1.93	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
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
3:F:54:LYS:O	3:F:55:TYR:HB3	2.12	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:A:299:LYS:HD3	1:A:299:LYS:C	2.38	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:426:HIS:HA	2:E:582:MET:HE2	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:D:299:LYS:HD3	1:D:299:LYS:C	2.39	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: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:117:PRO:HB3	1:D:159:MET:HE2	1.98	0.46
1:D:205:THR:HG22	1:D:234:VAL:CG2	2.45	0.46
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
1:D:310:GLU:O	2:E:630:LEU:C	2.58	0.46
2:E:403:LEU:CD2	2:E:605:LEU:HD13	2.45	0.46
2:E:472:MET:HE3	2:E:600:ILE:HD12	1.98	0.46
1:A:271:ARG:O	1:A:272:MET:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:140:MET:HE2	1:D:160:LEU:HD21	1.97	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:271:ARG:O	1:D:272:MET:HE2	2.16	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:D:727:GLU:N	2:E:633:ARG:HG2	1.65	0.44
2:B:472:MET:HE3	2:B:600:ILE:HD12	1.99	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
1:A:731:MET:HA	1:A:731:MET:HE2	1.99	0.43
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
3:F:31:LYS:HG2	3:F:32:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:382:PHE:CD2	2:B:487:VAL:HG12	2.55	0.42
2:B:513:GLN:HB2	2:B:604:MET:CE	2.44	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:490:LYS:O	2:E:490:LYS:NZ	2.48	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%)	14	51
2	B	205/662 (31%)	197 (96%)	7 (3%)	1 (0%)	24	63
2	E	213/662 (32%)	198 (93%)	10 (5%)	5 (2%)	5	28
3	C	111/113 (98%)	94 (85%)	13 (12%)	4 (4%)	2	20
3	F	111/113 (98%)	95 (86%)	13 (12%)	3 (3%)	4	25
All	All	1292/2256 (57%)	1213 (94%)	63 (5%)	16 (1%)	13	44

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 ⓘ

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%)	264 (92%)	24 (8%)	10	30
1	D	288/309 (93%)	265 (92%)	23 (8%)	11	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	196/588 (33%)	176 (90%)	20 (10%)	7	23
2	E	204/588 (35%)	188 (92%)	16 (8%)	11	32
3	C	102/102 (100%)	95 (93%)	7 (7%)	14	36
3	F	102/102 (100%)	93 (91%)	9 (9%)	9	28
All	All	1180/1998 (59%)	1081 (92%)	99 (8%)	12	30

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
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	89	LYS
1	A	125	TYR
1	A	128	HIS
1	A	129	VAL
1	A	130	LEU
1	A	134	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	301	GLN
1	A	305	LEU
1	A	309	LYS
1	A	727	GLU
2	B	389	LEU
2	B	418	ILE
2	B	432	LYS
2	B	434	GLN
2	B	457	ILE
2	B	473	LEU
2	B	475	THR
2	B	479	MET

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Mol	Chain	Res	Type
2	B	481	ARG
2	B	482	LEU
2	B	498	LEU
2	B	503	LYS
2	B	530	ILE
2	B	531	VAL
2	B	577	ILE
2	B	601	GLN
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	69	LYS
3	C	71	PHE
3	C	76	HIS
3	C	86	ARG
3	C	95	LEU
1	D	25	GLN
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	89	LYS
1	D	130	LEU
1	D	134	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	301	GLN
1	D	305	LEU
1	D	309	LYS
1	D	727	GLU

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Mol	Chain	Res	Type
2	E	386	ILE
2	E	417	ILE
2	E	477	THR
2	E	482	LEU
2	E	490	LYS
2	E	496	PHE
2	E	497	ASN
2	E	498	LEU
2	E	500	ARG
2	E	520	LEU
2	E	527	MET
2	E	576	GLU
2	E	577	ILE
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	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 (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	75	ASN
1	A	148	GLN
1	A	168	ASN
1	A	198	GLN
1	A	236	ASN
1	A	282	ASN
1	A	284	GLN
1	A	301	GLN
1	A	746	ASN
2	B	434	GLN
2	B	526	GLN
2	B	595	HIS

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Mol	Chain	Res	Type
2	B	601	GLN
3	C	94	GLN
1	D	33	GLN
1	D	40	GLN
1	D	75	ASN
1	D	85	HIS
1	D	168	ASN
1	D	183	ASN
1	D	239	GLN
1	D	284	GLN
1	D	301	GLN
1	D	744	ASN
1	D	746	ASN
2	E	391	GLN
2	E	497	ASN
2	E	499	HIS
2	E	513	GLN
2	E	618	GLN
3	F	21	ASN
3	F	94	GLN

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](#)

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.

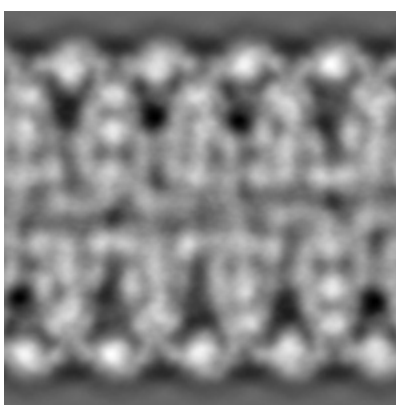
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

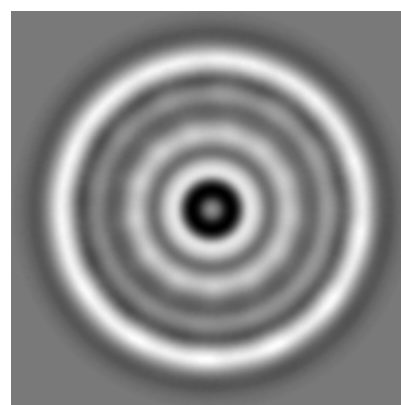
6.1.1 Primary map



X



Y

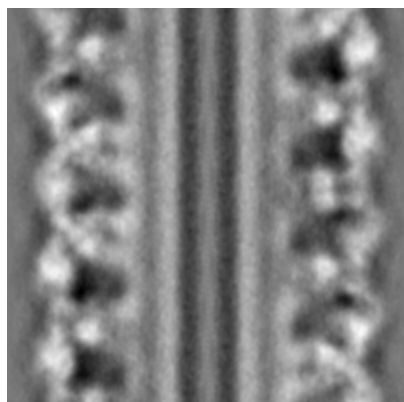


Z

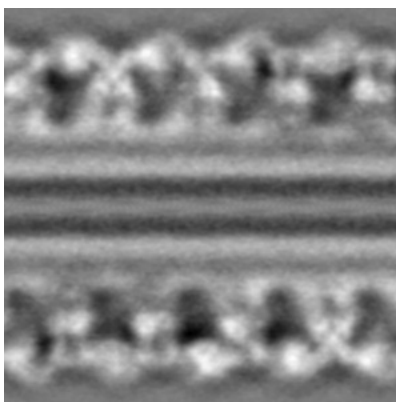
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100

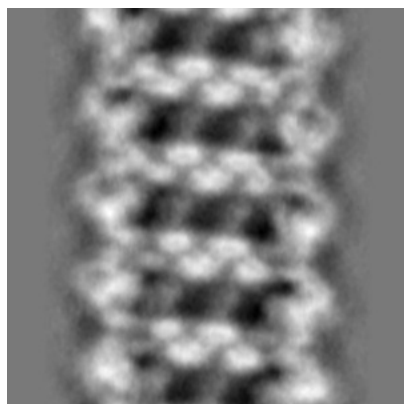


Z Index: 100

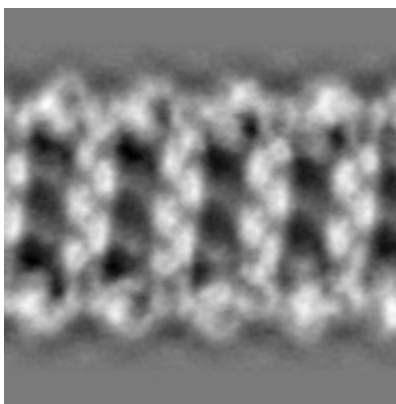
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

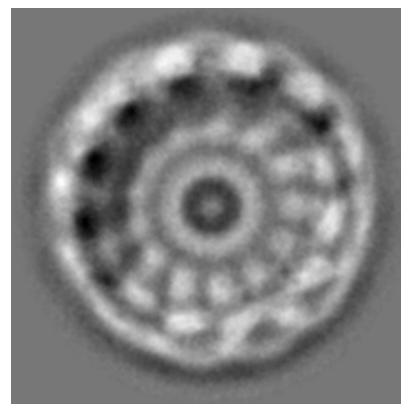
6.3.1 Primary map



X Index: 42



Y Index: 43

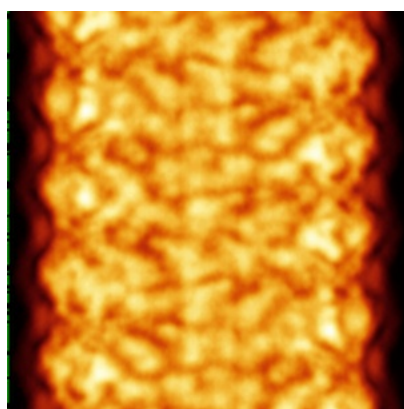


Z Index: 47

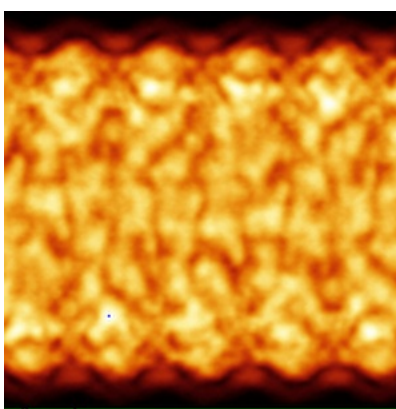
The images above show the largest variance slices of the map in three orthogonal directions.

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

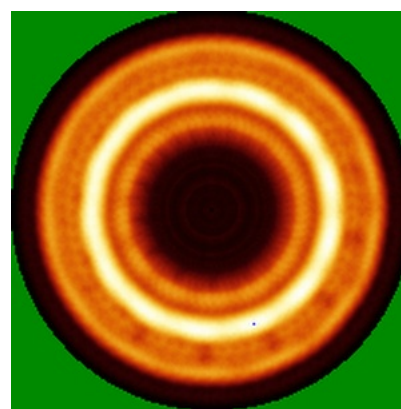
6.4.1 Primary map



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.

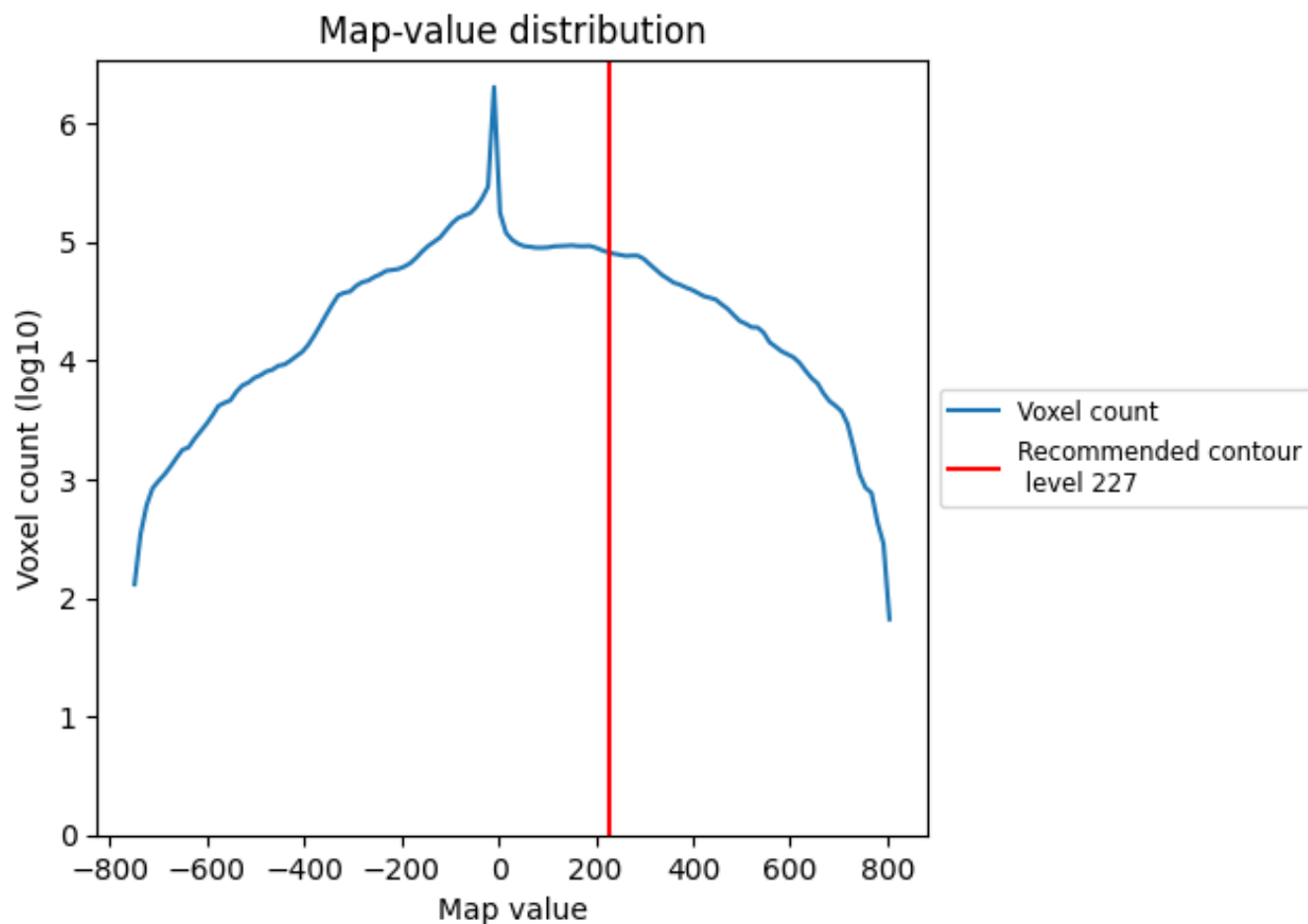
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

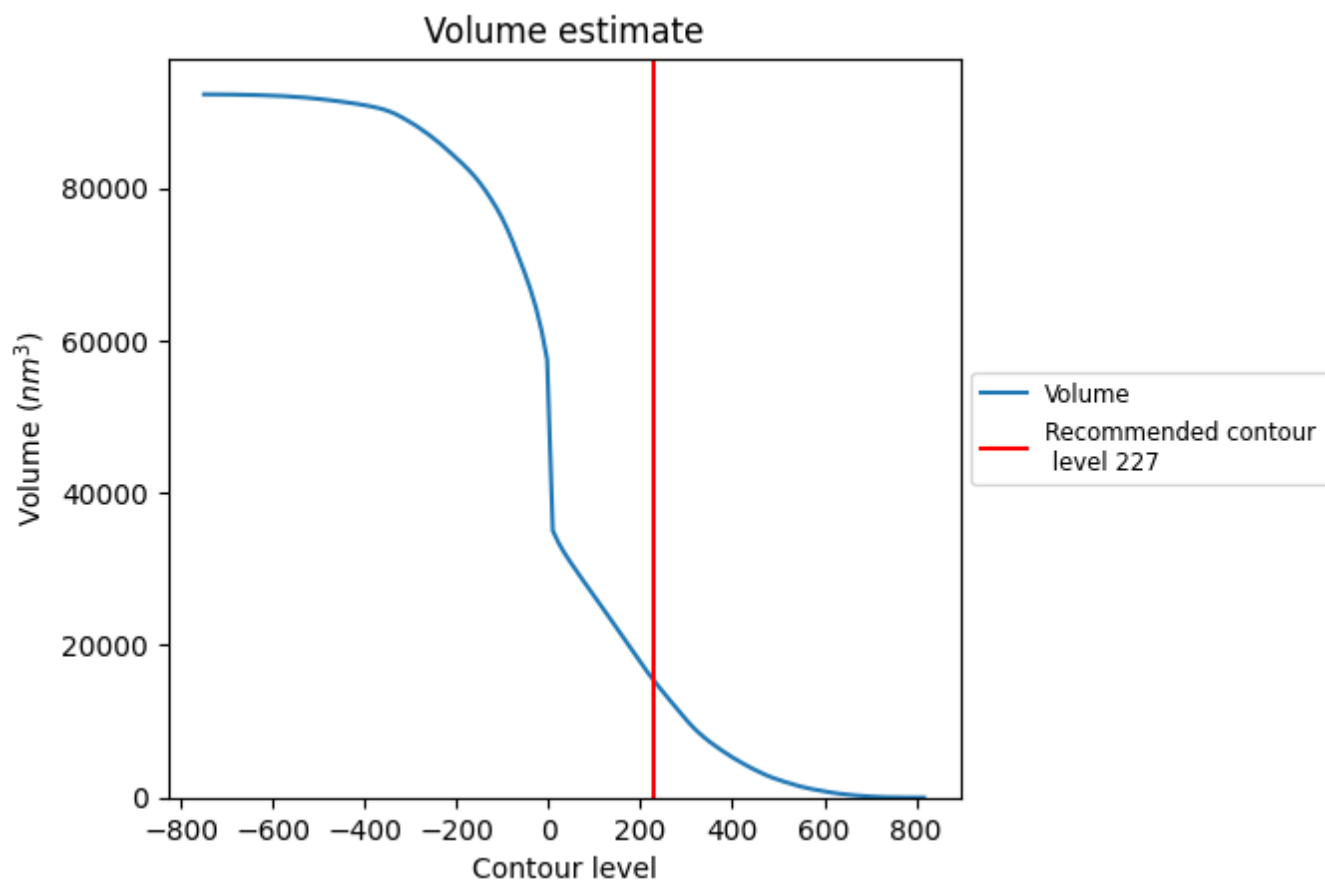
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

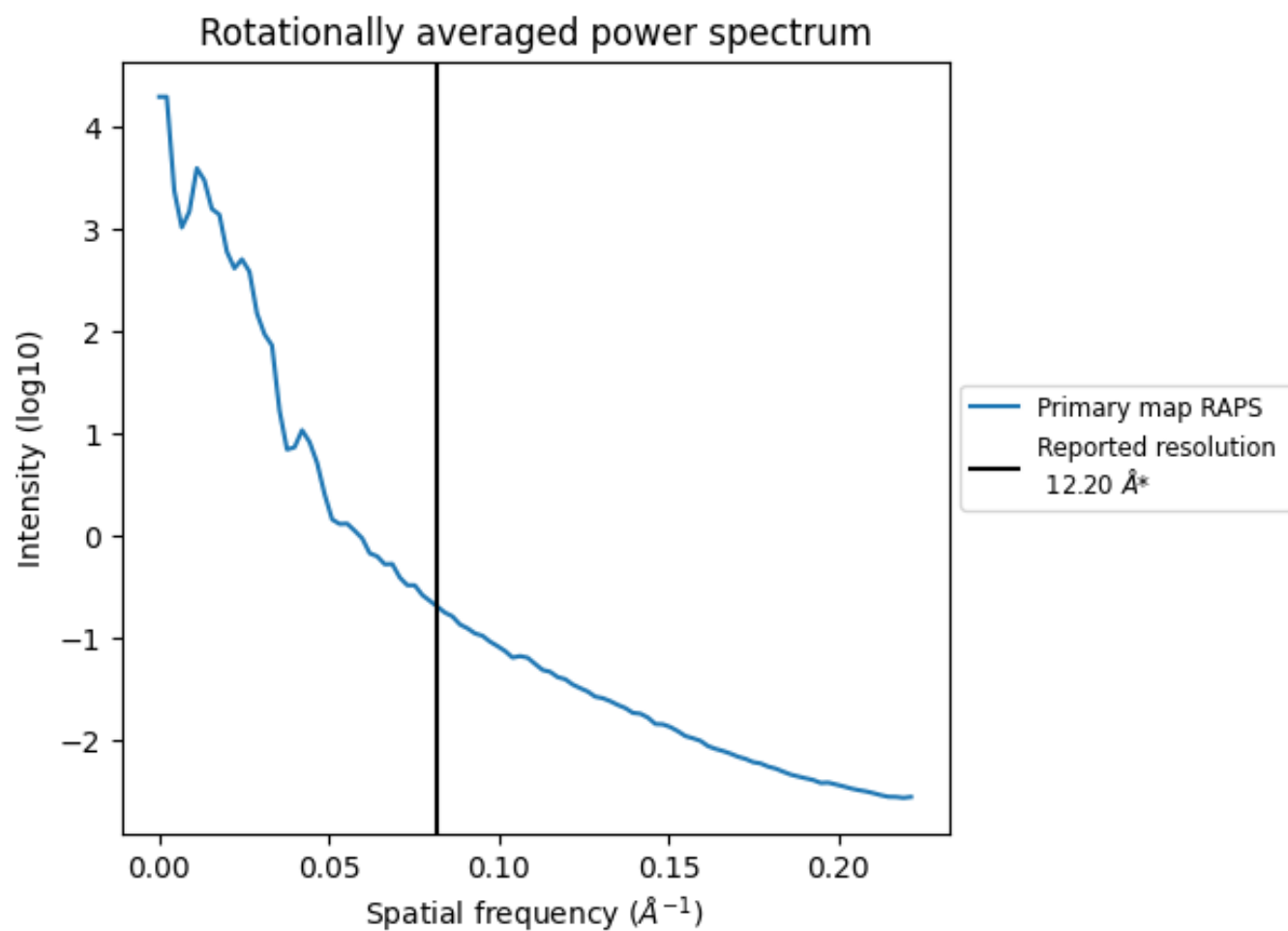
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15548 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.082 Å⁻¹

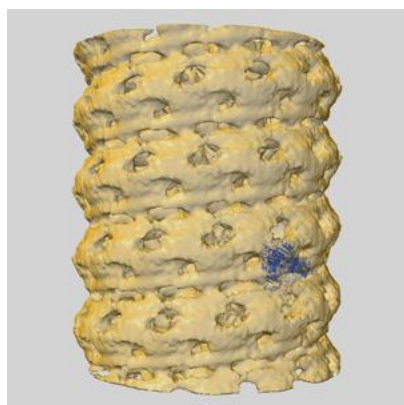
8 Fourier-Shell correlation

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

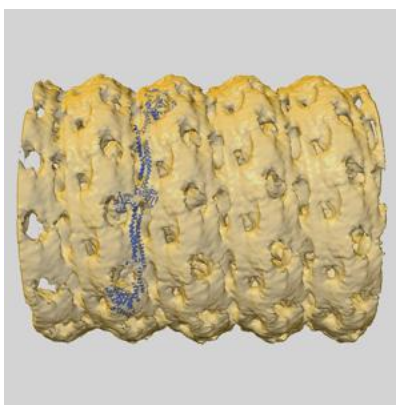
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1949 and PDB model 3ZYS. Per-residue inclusion information can be found in section [3](#) on page [6](#).

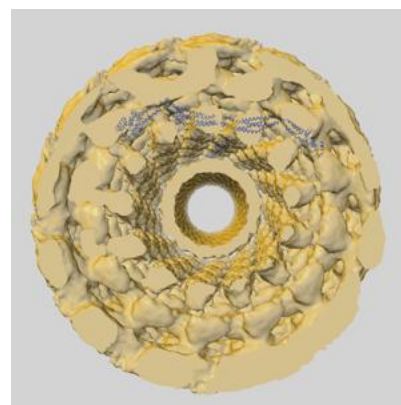
9.1 Map-model overlay [i](#)



X



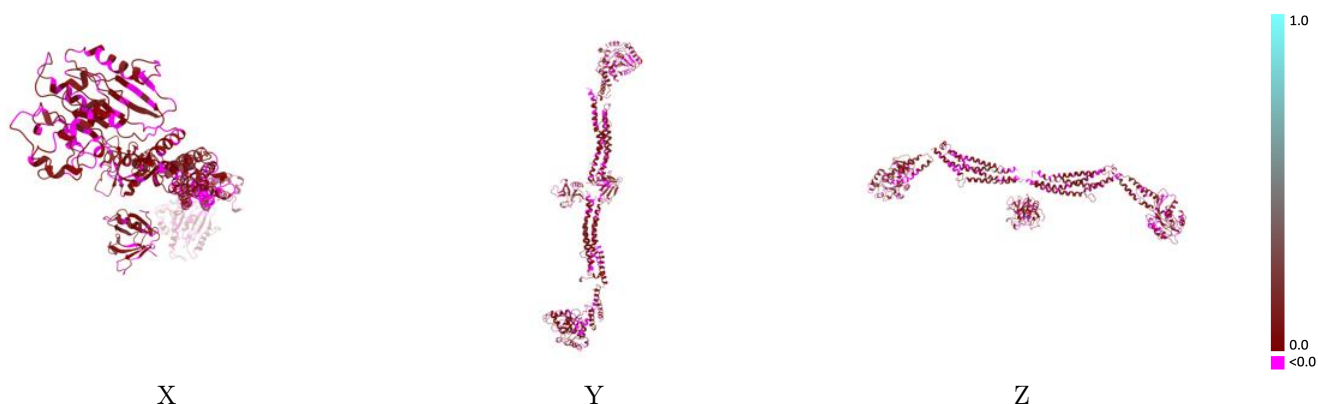
Y



Z

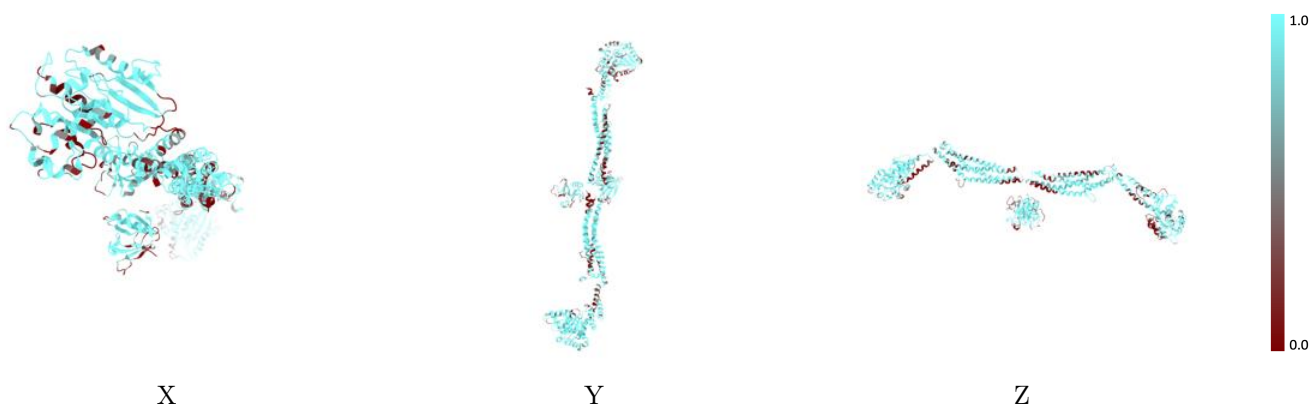
The images above show the 3D surface view of the map at the recommended contour level 227.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



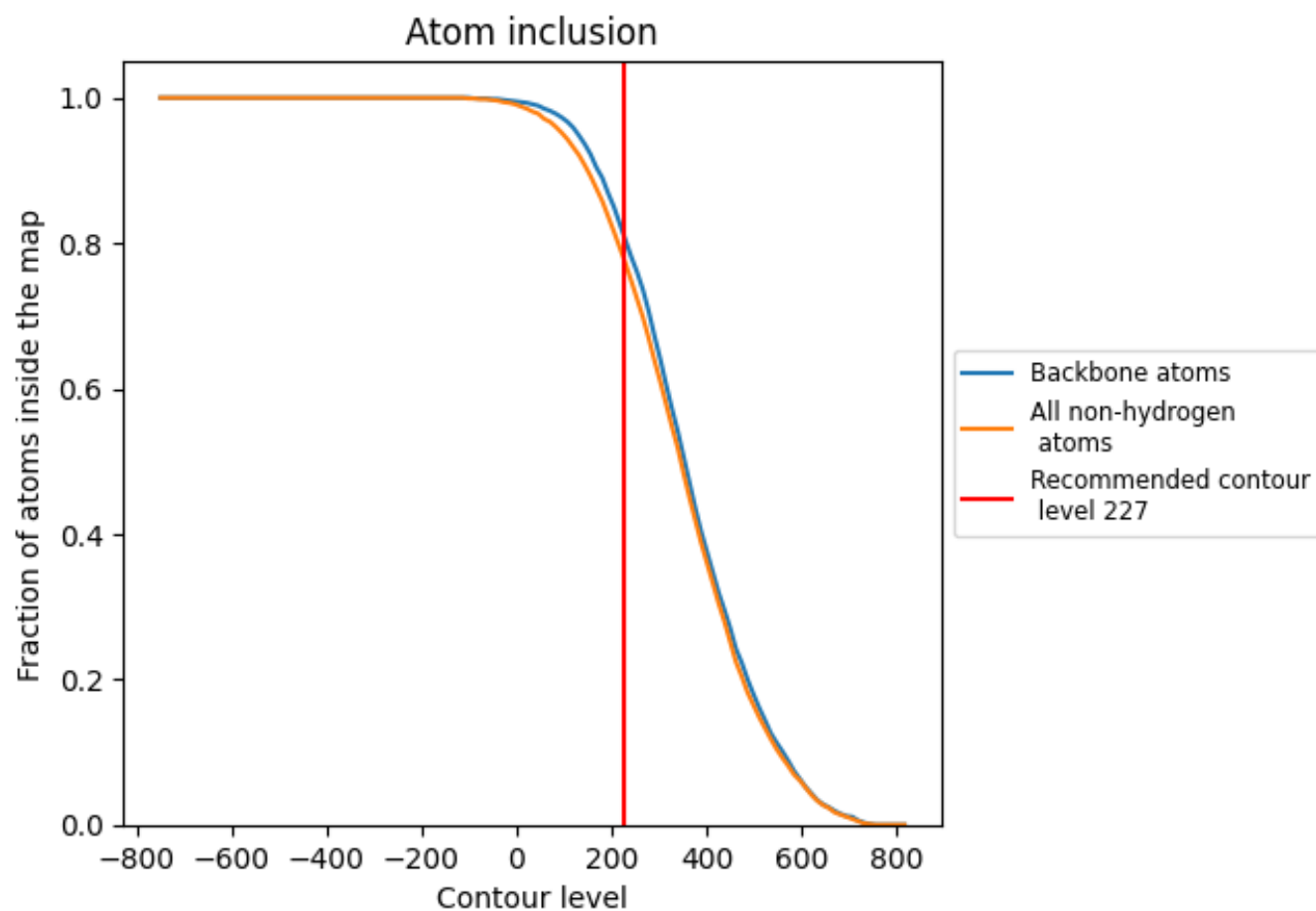
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 ⓘ

The table lists the average atom inclusion at the recommended contour level (227) 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

1.0

0.0

<0.0