



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 8YYU / pdb_00008yyu
EMDB ID : EMD-39679
Title : A tetrameric STAT1-DNA complex
Authors : Sugiyama, A.; Minami, M.; Sugita, Y.; Ose, T.
Deposited on : 2024-04-04
Resolution : 3.84 Å(reported)
Based on initial model : 1BF5

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:

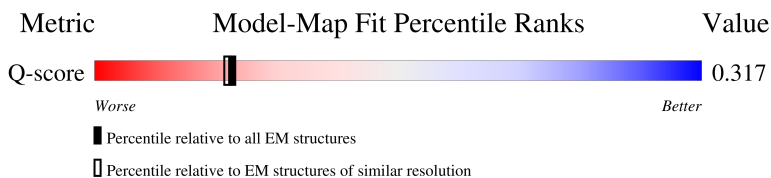
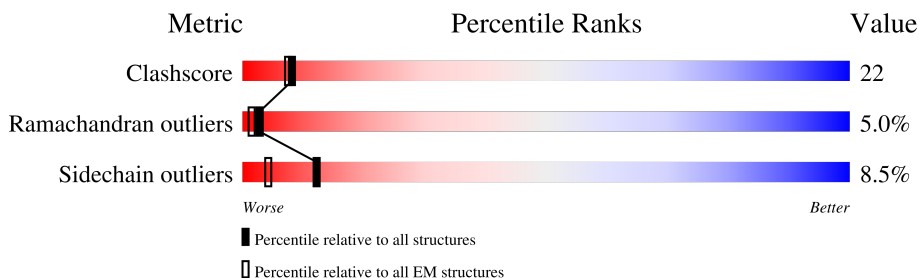
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.84 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	9033 (3.34 - 4.34)

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	776	18% 40% 24% 6% 29%
1	D	776	5% 34% 26% 9% 29%
2	C	18	72% 28%
2	E	18	83% 17%

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Mol	Chain	Length	Quality of chain
3	B	18	 89% 11%
3	F	18	 72% 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10498 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 Signal transducer and activator of transcription 1-alpha/beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	553	Total	C	N	O	P	S	0	0
			4511	2880	774	836	1	20		
1	D	553	Total	C	N	O	P	S	0	0
			4511	2880	774	836	1	20		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP P42224
A	-24	ASN	-	expression tag	UNP P42224
A	-23	HIS	-	expression tag	UNP P42224
A	-22	LYS	-	expression tag	UNP P42224
A	-21	HIS	-	expression tag	UNP P42224
A	-20	HIS	-	expression tag	UNP P42224
A	-19	HIS	-	expression tag	UNP P42224
A	-18	HIS	-	expression tag	UNP P42224
A	-17	HIS	-	expression tag	UNP P42224
A	-16	HIS	-	expression tag	UNP P42224
A	-15	HIS	-	expression tag	UNP P42224
A	-14	HIS	-	expression tag	UNP P42224
A	-13	HIS	-	expression tag	UNP P42224
A	-12	HIS	-	expression tag	UNP P42224
A	-11	SER	-	expression tag	UNP P42224
A	-10	SER	-	expression tag	UNP P42224
A	-9	GLY	-	expression tag	UNP P42224
A	-8	GLU	-	expression tag	UNP P42224
A	-7	ASN	-	expression tag	UNP P42224
A	-6	LEU	-	expression tag	UNP P42224
A	-5	TYR	-	expression tag	UNP P42224
A	-4	PHE	-	expression tag	UNP P42224
A	-3	GLN	-	expression tag	UNP P42224
A	-2	GLY	-	expression tag	UNP P42224
A	-1	HIS	-	expression tag	UNP P42224
A	0	MET	-	expression tag	UNP P42224

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-25	MET	-	initiating methionine	UNP P42224
D	-24	ASN	-	expression tag	UNP P42224
D	-23	HIS	-	expression tag	UNP P42224
D	-22	LYS	-	expression tag	UNP P42224
D	-21	HIS	-	expression tag	UNP P42224
D	-20	HIS	-	expression tag	UNP P42224
D	-19	HIS	-	expression tag	UNP P42224
D	-18	HIS	-	expression tag	UNP P42224
D	-17	HIS	-	expression tag	UNP P42224
D	-16	HIS	-	expression tag	UNP P42224
D	-15	HIS	-	expression tag	UNP P42224
D	-14	HIS	-	expression tag	UNP P42224
D	-13	HIS	-	expression tag	UNP P42224
D	-12	HIS	-	expression tag	UNP P42224
D	-11	SER	-	expression tag	UNP P42224
D	-10	SER	-	expression tag	UNP P42224
D	-9	GLY	-	expression tag	UNP P42224
D	-8	GLU	-	expression tag	UNP P42224
D	-7	ASN	-	expression tag	UNP P42224
D	-6	LEU	-	expression tag	UNP P42224
D	-5	TYR	-	expression tag	UNP P42224
D	-4	PHE	-	expression tag	UNP P42224
D	-3	GLN	-	expression tag	UNP P42224
D	-2	GLY	-	expression tag	UNP P42224
D	-1	HIS	-	expression tag	UNP P42224
D	0	MET	-	expression tag	UNP P42224

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*AP*GP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	18	Total	C	N	O	P	0	0
			366	175	65	108	18		
2	E	18	Total	C	N	O	P	0	0
			366	175	65	108	18		

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	18	Total	C	N	O	P	0	0
			372	177	69	108	18		

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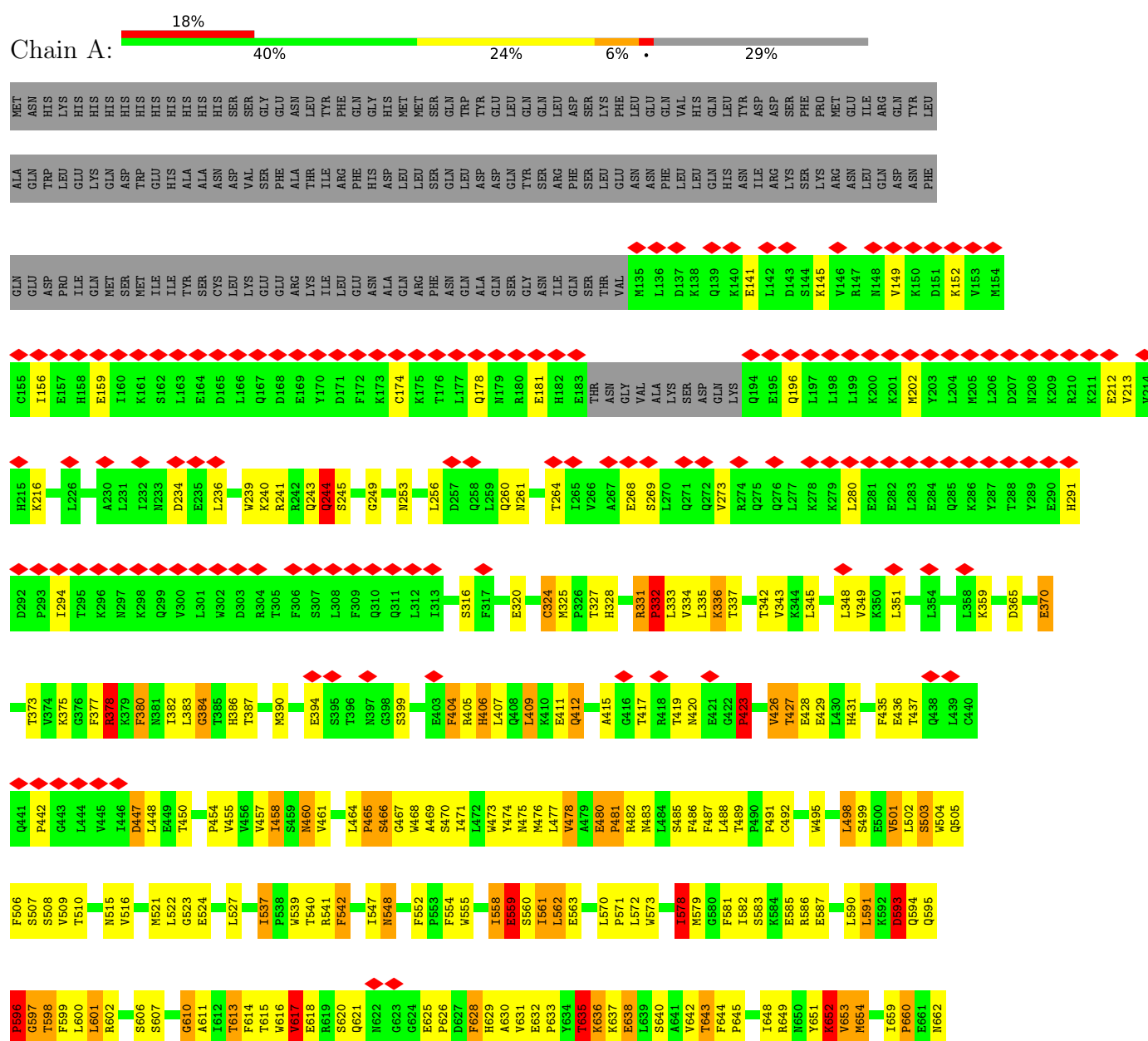
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	18	Total	C	N	O	P	0	0
			372	177	69	108	18		

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: Signal transducer and activator of transcription 1-alpha/beta



Chain C:  72% 28%



- Molecule 2: DNA (5'-D(P*AP*CP*AP*GP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*T
P*GP*C)-3')

Chain E:  83% 17%



- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*C
P*TP*G)-3')

Chain B:  89% 11%



- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*C
P*TP*G)-3')

Chain F:  72% 28%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	17869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.000	Depositor
Minimum map value	0.000	Depositor
Average map value	0.144	Depositor
Map value standard deviation	0.336	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	214.72, 214.72, 214.72	wwPDB
Map dimensions	122, 122, 122	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.76, 1.76, 1.76	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

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	0.68	1/4589 (0.0%)	1.53	64/6206 (1.0%)
1	D	0.86	4/4589 (0.1%)	1.83	131/6206 (2.1%)
2	C	0.54	0/409	1.42	8/628 (1.3%)
2	E	0.53	0/409	1.40	4/628 (0.6%)
3	B	0.54	0/417	1.38	3/642 (0.5%)
3	F	0.54	0/417	1.38	7/642 (1.1%)
All	All	0.74	5/10830 (0.0%)	1.64	217/14952 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	D	0	12
All	All	0	17

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	427	THR	CA-C	7.66	1.64	1.53
1	D	560	SER	CA-CB	-6.61	1.43	1.53
1	D	427	THR	C-O	5.88	1.32	1.23
1	D	562	LEU	N-CA	-5.79	1.39	1.46
1	A	458	ILE	CB-CG1	5.61	1.64	1.53

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	PRO	N-CA-CB	-14.10	88.45	103.25
1	A	332	PRO	N-CA-CB	-11.94	90.71	103.25
1	D	427	THR	CA-CB-OG1	-10.97	93.14	109.60
1	D	331	ARG	NE-CZ-NH2	-10.90	109.39	119.20
1	D	428	GLU	CB-CG-CD	10.52	130.49	112.60
1	D	506	PHE	CA-CB-CG	-10.35	103.45	113.80
1	A	598	THR	CA-CB-OG1	-9.41	95.49	109.60
1	D	322	GLN	CB-CG-CD	9.20	128.24	112.60
1	A	561	ILE	CA-C-N	-9.04	108.69	120.44
1	A	561	ILE	C-N-CA	-9.04	108.69	120.44
1	A	427	THR	CA-CB-OG1	-9.01	96.08	109.60
1	D	459	SER	N-CA-CB	-8.84	97.58	110.40
1	D	598	THR	CA-CB-OG1	-8.80	96.40	109.60
1	D	561	ILE	CA-C-N	-8.75	109.06	120.44
1	D	561	ILE	C-N-CA	-8.75	109.06	120.44
1	D	489	THR	CA-CB-OG1	-8.68	96.58	109.60
1	D	642	VAL	N-CA-CB	-8.59	99.60	111.19
1	D	465	PRO	N-CD-CG	-8.51	90.44	103.20
1	D	427	THR	CA-C-N	8.46	138.58	123.34
1	D	427	THR	C-N-CA	8.46	138.58	123.34
1	D	427	THR	CA-C-O	8.46	137.92	121.35
1	D	668	TYR	N-CA-CB	8.34	125.22	110.37
1	A	542	PHE	CA-CB-CG	8.34	122.14	113.80
1	A	668	TYR	N-CA-CB	8.32	125.18	110.37
1	D	427	THR	N-CA-CB	-8.28	98.56	111.23
1	D	322	GLN	OE1-CD-NE2	-8.20	114.40	122.60
1	A	703	LYS	N-CA-CB	8.12	122.53	109.95
1	D	486	PHE	CB-CA-C	8.09	124.16	110.74
1	D	557	TRP	CB-CG-CD2	-8.06	115.51	126.80
1	D	426	VAL	N-CA-CB	-8.04	97.96	111.23
2	C	4	DG	C4-N9-C1'	-8.02	114.97	127.00
1	D	542	PHE	CB-CA-C	-7.98	98.04	110.81
1	D	506	PHE	CB-CA-C	-7.89	95.52	110.67
1	A	331	ARG	NE-CZ-NH2	-7.84	112.15	119.20
2	C	4	DG	C8-N9-C1'	7.76	138.64	127.00
1	D	558	ILE	CA-C-N	-7.74	110.38	120.44
1	D	558	ILE	C-N-CA	-7.74	110.38	120.44
1	D	488	LEU	N-CA-CB	-7.73	98.72	110.16
1	D	476	MET	CG-SD-CE	7.66	117.75	100.90
1	D	426	VAL	CA-C-N	7.65	133.28	123.03
1	D	426	VAL	C-N-CA	7.65	133.28	123.03
1	D	635	THR	CA-CB-OG1	-7.61	98.18	109.60
1	D	630	ALA	N-CA-CB	-7.53	98.59	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	LYS	CB-CA-C	-7.51	99.09	110.88
1	D	602	ARG	CB-CA-C	-7.47	93.76	109.38
1	D	711	GLU	CB-CG-CD	7.46	125.29	112.60
1	D	378	ARG	CA-C-N	-7.42	110.94	122.59
1	D	378	ARG	C-N-CA	-7.42	110.94	122.59
1	D	454	PRO	CB-CA-C	-7.38	102.19	111.56
1	D	326	PRO	N-CA-CB	-7.32	95.11	103.30
1	D	590	LEU	N-CA-CB	-7.26	100.54	111.15
1	D	609	GLU	N-CA-C	-7.25	104.47	113.38
1	D	538	PRO	CB-CA-C	-7.23	98.86	110.21
1	A	635	THR	CA-CB-OG1	-7.23	98.76	109.60
1	A	427	THR	CB-CA-C	7.20	124.74	110.42
1	D	365	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	617	VAL	N-CA-CB	-6.99	98.85	111.92
1	D	647	ILE	O-C-N	6.87	128.64	121.91
1	D	427	THR	CB-CA-C	6.83	121.89	111.85
1	D	365	ASP	CB-CA-C	6.82	122.28	111.51
1	A	465	PRO	N-CD-CG	-6.75	93.08	103.20
1	A	460	ASN	CA-CB-CG	-6.74	105.86	112.60
1	D	327	THR	OG1-CB-CG2	6.73	122.76	109.30
1	D	541	ARG	CB-CA-C	6.71	121.93	110.79
1	A	501	VAL	N-CA-CB	-6.69	102.61	110.64
1	D	427	THR	N-CA-C	6.64	119.44	108.49
1	D	380	PHE	CB-CA-C	-6.63	96.20	110.45
1	D	475	ASN	CB-CA-C	6.61	123.65	110.17
1	D	515	ASN	CA-CB-CG	-6.59	106.01	112.60
1	A	404	PHE	N-CA-CB	6.58	120.67	110.21
1	D	703	LYS	N-CA-CB	6.52	120.91	110.16
1	A	652	LYS	CB-CG-CD	6.48	126.20	111.30
1	D	562	LEU	N-CA-CB	-6.46	100.64	110.01
1	D	336	LYS	CB-CA-C	6.44	121.50	109.71
1	D	342	THR	CA-C-N	-6.43	113.66	122.92
1	D	342	THR	C-N-CA	-6.43	113.66	122.92
1	D	523	GLY	N-CA-C	-6.41	104.89	112.64
1	A	642	VAL	N-CA-CB	-6.39	100.87	111.36
1	D	677	PHE	CB-CA-C	-6.39	101.16	111.06
1	D	460	ASN	CA-CB-CG	-6.39	106.21	112.60
1	D	652	LYS	CB-CG-CD	6.38	125.96	111.30
1	D	334	VAL	N-CA-C	-6.37	98.44	107.75
1	A	365	ASP	CA-CB-CG	6.37	118.97	112.60
1	D	612	ILE	CA-C-O	-6.36	114.80	121.93
1	D	652	LYS	CB-CA-C	6.32	123.00	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ARG	CB-CA-C	6.31	120.90	110.81
1	A	404	PHE	CB-CA-C	-6.30	100.41	110.81
1	A	596	PRO	N-CA-CB	-6.29	96.65	103.25
1	D	560	SER	N-CA-C	6.25	118.09	111.28
1	D	492	CYS	CB-CA-C	6.24	121.97	110.24
1	A	337	THR	OG1-CB-CG2	-6.23	96.84	109.30
1	D	511	LYS	N-CA-CB	-6.21	101.96	111.66
1	A	324	CYS	CB-CA-C	-6.19	100.02	109.99
1	A	558	ILE	CA-C-N	-6.16	112.02	120.28
1	A	558	ILE	C-N-CA	-6.16	112.02	120.28
1	A	654	MET	CG-SD-CE	-6.12	87.44	100.90
1	D	475	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	A	562	LEU	N-CA-CB	-6.10	101.16	110.01
2	C	5	DT	O3'-P-O5'	-6.08	94.89	104.00
1	A	336	LYS	CB-CA-C	6.06	120.80	109.71
1	D	602	ARG	CD-NE-CZ	-6.03	115.95	124.40
1	D	319	VAL	CA-C-O	-6.02	113.76	120.74
3	F	5	DT	O3'-P-O5'	-6.01	94.98	104.00
1	D	472	LEU	O-C-N	5.99	128.50	122.03
2	E	15	DA	C4-N9-C1'	-5.97	118.09	127.05
1	D	378	ARG	N-CA-CB	-5.97	101.73	110.26
1	D	509	VAL	O-C-N	5.95	129.63	121.90
1	A	489	THR	CA-CB-OG1	-5.92	100.72	109.60
1	D	486	PHE	CA-CB-CG	5.89	119.69	113.80
3	B	15	DA	C4-N9-C1'	-5.86	118.26	127.05
1	D	477	LEU	N-CA-CB	-5.86	101.55	110.92
2	E	15	DA	C8-N9-C1'	5.81	135.77	127.05
1	A	590	LEU	CA-C-O	5.81	125.09	118.47
1	D	321	ARG	CA-CB-CG	-5.80	102.50	114.10
1	A	559	GLU	N-CA-CB	5.78	118.61	110.12
1	D	608	ARG	N-CA-C	-5.77	104.95	113.61
2	C	11	DG	C4-N9-C1'	-5.76	118.35	127.00
1	D	263	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	320	GLU	CB-CG-CD	5.73	122.34	112.60
1	D	587	GLU	N-CA-CB	-5.71	101.23	110.14
1	D	523	GLY	CA-C-O	-5.69	115.19	121.05
2	E	16	DT	O3'-P-O5'	-5.68	95.47	104.00
1	D	240	LYS	CB-CG-CD	5.68	124.37	111.30
1	D	592	LYS	N-CA-C	-5.68	103.61	110.88
1	A	492	CYS	CB-CA-C	5.66	122.65	111.22
1	D	596	PRO	N-CA-CB	-5.64	97.33	103.25
1	A	458	ILE	CA-C-O	5.64	127.09	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	537	ILE	N-CA-C	-5.63	101.75	107.89
1	A	380	PHE	CB-CA-C	-5.62	97.96	109.94
3	B	15	DA	C8-N9-C1'	5.59	135.43	127.05
1	A	365	ASP	CB-CA-C	5.58	120.33	111.51
1	D	404	PHE	CB-CA-C	-5.58	101.15	110.19
1	A	447	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	244	GLN	CB-CA-C	-5.58	99.33	110.42
1	A	540	THR	CA-CB-OG1	-5.57	101.25	109.60
2	C	11	DG	C8-N9-C1'	5.56	135.34	127.00
1	A	578	ILE	CB-CA-C	5.56	119.26	110.81
1	D	575	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	566	LYS	CB-CA-C	-5.53	98.88	110.17
1	A	427	THR	CA-C-O	5.53	128.42	120.51
1	A	590	LEU	N-CA-CB	-5.53	103.08	111.15
1	D	632	GLU	CA-C-N	5.53	125.80	119.83
1	D	632	GLU	C-N-CA	5.53	125.80	119.83
2	C	13	DA	C4'-C3'-O3'	-5.52	101.73	110.00
1	D	567	LYS	CA-C-N	-5.51	112.67	121.44
1	D	567	LYS	C-N-CA	-5.51	112.67	121.44
1	D	557	TRP	CB-CG-CD1	5.51	135.16	126.90
1	D	617	VAL	N-CA-CB	-5.48	101.80	111.93
1	D	497	GLN	N-CA-CB	-5.47	101.70	110.19
1	D	320	GLU	CB-CG-CD	5.46	121.88	112.60
1	D	557	TRP	CE2-CD2-CE3	5.45	124.25	118.80
2	E	5	DT	O3'-P-O5'	-5.44	95.84	104.00
1	D	601	LEU	N-CA-CB	-5.44	101.55	110.52
1	A	476	MET	CB-CA-C	5.43	118.61	110.08
1	D	512	ARG	CB-CA-C	-5.42	99.64	110.42
1	D	361	LYS	CB-CA-C	5.41	118.65	109.50
1	D	333	LEU	CA-C-O	5.41	124.44	118.65
1	A	602	ARG	CB-CA-C	-5.39	98.71	109.33
1	A	406	HIS	CB-CA-C	5.39	118.96	111.63
1	D	456	VAL	CA-C-N	-5.38	116.09	123.14
1	D	456	VAL	C-N-CA	-5.38	116.09	123.14
1	D	424	LEU	N-CA-CB	-5.37	101.76	110.14
1	A	486	PHE	N-CA-CB	-5.37	101.94	109.94
1	A	244	GLN	CB-CA-C	-5.36	99.75	110.42
2	C	5	DT	C4-C5-C7	-5.34	114.40	122.40
3	F	5	DT	C4-C5-C7	-5.34	114.39	122.40
1	A	378	ARG	N-CA-CB	-5.33	102.73	110.36
3	F	11	DG	C4-N9-C1'	-5.33	119.01	127.00
1	D	333	LEU	N-CA-CB	-5.31	100.51	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	11	DG	C8-N9-C1'	5.30	134.95	127.00
1	A	628	PHE	CA-CB-CG	5.28	119.08	113.80
3	F	10	DG	C4'-C3'-O3'	-5.27	102.09	110.00
3	F	13	DA	C4'-C3'-O3'	-5.27	102.09	110.00
1	A	651	TYR	N-CA-CB	5.27	117.76	110.17
3	B	5	DT	O3'-P-O5'	-5.26	96.11	104.00
3	F	8	DA	O3'-P-O5'	-5.24	96.14	104.00
1	A	552	PHE	CA-C-N	5.24	125.14	119.85
1	A	552	PHE	C-N-CA	5.24	125.14	119.85
1	D	251	PRO	CA-C-N	5.22	125.16	119.78
1	D	251	PRO	C-N-CA	5.22	125.16	119.78
1	D	517	ASP	O-C-N	5.21	129.42	122.43
1	D	654	MET	CG-SD-CE	-5.21	89.43	100.90
1	A	601	LEU	N-CA-CB	-5.19	101.95	110.42
1	A	331	ARG	NH1-CZ-NH2	5.19	126.05	119.30
1	A	709	VAL	N-CA-CB	-5.19	102.84	111.36
1	D	505	GLN	CB-CA-C	5.19	119.12	110.81
1	D	546	ASN	CA-CB-CG	-5.18	107.42	112.60
1	D	335	LEU	CB-CA-C	5.16	118.22	109.50
1	A	412	GLN	N-CA-CB	-5.16	102.91	110.49
1	A	638	GLU	N-CA-CB	5.15	117.79	110.16
1	D	404	PHE	N-CA-CB	5.15	118.81	110.42
1	D	490	PRO	N-CA-C	-5.15	104.42	110.70
1	D	552	PHE	CA-C-N	5.15	125.43	119.92
1	D	552	PHE	C-N-CA	5.15	125.43	119.92
1	D	651	TYR	N-CA-CB	5.15	117.58	110.17
1	D	663	PRO	O-C-N	5.15	129.59	122.64
1	D	378	ARG	CD-NE-CZ	5.13	131.58	124.40
1	D	676	ALA	O-C-N	5.13	127.57	122.08
1	D	461	VAL	CA-CB-CG2	-5.12	101.69	110.40
1	D	252	PRO	N-CA-CB	5.12	107.80	103.35
1	D	500	GLU	CB-CA-C	-5.11	99.63	110.31
1	D	455	VAL	N-CA-CB	-5.11	103.86	112.44
1	D	564	LEU	CA-C-N	5.10	127.45	120.46
1	D	564	LEU	C-N-CA	5.10	127.45	120.46
1	A	486	PHE	CB-CA-C	5.09	118.96	110.81
1	D	335	LEU	CD1-CG-CD2	-5.08	99.62	110.80
2	C	8	DC	O3'-P-O5'	-5.08	96.39	104.00
1	A	268	GLU	CB-CA-C	-5.07	102.38	110.79
1	A	334	VAL	O-C-N	5.07	128.50	123.18
1	D	605	GLU	N-CA-CB	5.07	118.34	110.44
1	D	325	MET	CB-CA-C	-5.06	100.19	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	PHE	CB-CA-C	-5.04	102.10	110.81
1	D	610	GLY	CA-C-N	5.03	129.73	121.58
1	D	610	GLY	C-N-CA	5.03	129.73	121.58
1	D	628	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	542	PHE	CB-CA-C	-5.02	102.77	110.81
1	A	559	GLU	N-CA-C	-5.02	105.81	111.28

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	ARG	Sidechain
1	A	542	PHE	Peptide
1	A	591	LEU	Peptide
1	A	593	ASP	Peptide
1	A	652	LYS	Peptide
1	D	338	GLY	Peptide
1	D	427	THR	Peptide
1	D	458	ILE	Mainchain
1	D	461	VAL	Peptide
1	D	485	SER	Peptide
1	D	486	PHE	Peptide
1	D	575	ASP	Peptide
1	D	591	LEU	Peptide
1	D	593	ASP	Peptide
1	D	600	LEU	Peptide
1	D	610	GLY	Peptide
1	D	652	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4511	0	4527	215	0
1	D	4511	0	4527	243	0
2	C	366	0	193	0	0
2	E	366	0	188	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	372	0	186	0	0
3	F	372	0	181	0	0
All	All	10498	0	9802	446	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 22.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:PRO:O	1:A:664:LEU:HD23	1.51	1.08
1:D:643:THR:OG1	1:D:645:PRO:HD2	1.61	1.00
1:D:664:LEU:O	1:D:673:LYS:NZ	1.95	0.99
1:D:668:TYR:HB3	1:D:669:PRO:HD3	1.41	0.99
1:A:664:LEU:O	1:A:673:LYS:NZ	1.95	0.98
1:A:599:PHE:HA	1:A:615:THR:O	1.63	0.98
1:A:643:THR:OG1	1:A:645:PRO:HD2	1.65	0.97
1:A:668:TYR:HB3	1:A:669:PRO:HD3	1.48	0.96
1:D:599:PHE:HA	1:D:615:THR:O	1.64	0.96
1:A:614:PHE:HE1	1:A:631:VAL:HG11	1.32	0.95
1:D:572:LEU:H	1:D:572:LEU:HD12	1.32	0.95
1:A:654:MET:HE1	1:D:654:MET:HE1	1.47	0.94
1:D:663:PRO:O	1:D:664:LEU:HD23	1.64	0.94
1:A:614:PHE:CE1	1:A:631:VAL:HG11	2.07	0.90
1:A:707:ILE:HG22	1:D:707:ILE:HG22	1.53	0.87
1:D:428:GLU:O	1:D:428:GLU:HG3	1.73	0.87
1:D:613:THR:CG2	1:D:614:PHE:N	2.39	0.86
1:D:428:GLU:O	1:D:428:GLU:CG	2.26	0.84
1:D:635:THR:OG1	1:D:636:LYS:N	2.10	0.83
1:A:654:MET:HE1	1:D:654:MET:CE	2.09	0.83
1:D:649:ARG:HD3	1:D:681:TYR:CZ	2.13	0.83
1:A:649:ARG:HD3	1:A:681:TYR:CZ	2.13	0.82
1:A:662:ASN:O	1:A:664:LEU:N	2.13	0.81
1:D:598:THR:HA	1:D:666:TYR:O	1.79	0.81
1:A:618:GLU:H	1:A:626:PRO:HG2	1.44	0.81
1:A:466:SER:O	1:A:469:ALA:HB3	1.80	0.81
1:D:428:GLU:OE1	1:D:487:PHE:CD1	2.34	0.81
1:D:632:GLU:OE1	1:D:633:PRO:HD2	1.82	0.80
1:D:618:GLU:H	1:D:626:PRO:HG2	1.45	0.80
1:D:481:PRO:O	1:D:483:ASN:N	2.15	0.79
1:D:245:SER:O	1:D:249:GLY:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:ARG:HB3	1:D:684:PRO:HD3	1.64	0.79
1:A:325:MET:HE3	1:A:328:HIS:CD2	2.18	0.79
1:A:245:SER:O	1:A:249:GLY:O	2.00	0.79
1:D:613:THR:HG23	1:D:614:PHE:N	1.99	0.78
1:A:481:PRO:O	1:A:483:ASN:N	2.16	0.78
1:A:606:SER:HB3	1:D:701:PTR:O1P	1.84	0.78
1:A:325:MET:HE3	1:A:328:HIS:HD2	1.50	0.77
1:A:582:ILE:HD11	1:A:586:ARG:HH11	1.50	0.77
1:A:598:THR:HA	1:A:666:TYR:O	1.85	0.77
1:D:615:THR:HG23	1:D:630:ALA:HB2	1.67	0.76
1:D:614:PHE:CE1	1:D:631:VAL:HG11	2.19	0.76
1:A:473:TRP:CZ2	1:A:539:TRP:HA	2.21	0.75
1:D:527:LEU:HD21	1:D:537:ILE:HG13	1.67	0.75
1:D:464:LEU:C	1:D:464:LEU:HD23	2.11	0.75
1:D:572:LEU:HD12	1:D:572:LEU:N	2.02	0.75
1:A:521:MET:HE3	1:A:581:PHE:HB3	1.68	0.75
1:A:428:GLU:HG3	1:A:428:GLU:O	1.85	0.75
1:D:626:PRO:HB2	1:D:628:PHE:H	1.52	0.75
1:A:464:LEU:C	1:A:464:LEU:HD23	2.12	0.75
1:A:598:THR:O	1:A:616:TRP:HA	1.87	0.74
1:D:613:THR:HG23	1:D:614:PHE:H	1.50	0.74
1:A:649:ARG:HB2	1:A:681:TYR:CE1	2.22	0.74
1:D:459:SER:OG	1:D:463:GLN:OE1	2.06	0.74
1:D:152:LYS:O	1:D:156:ILE:HG12	1.88	0.74
1:A:152:LYS:O	1:A:156:ILE:HG12	1.88	0.73
1:A:654:MET:CE	1:D:654:MET:HE1	2.17	0.73
1:D:521:MET:HE2	1:D:582:ILE:H	1.52	0.73
1:D:598:THR:O	1:D:616:TRP:HA	1.88	0.73
1:D:649:ARG:HB2	1:D:681:TYR:CE1	2.22	0.73
1:D:485:SER:O	1:D:486:PHE:C	2.32	0.72
1:A:652:LYS:O	1:A:653:VAL:HB	1.88	0.72
1:A:378:ARG:HH11	1:A:380:PHE:HZ	1.35	0.72
1:A:683:ARG:HB3	1:A:684:PRO:HD3	1.71	0.72
1:D:454:PRO:HG2	1:D:474:TYR:CE2	2.24	0.72
1:A:635:THR:OG1	1:A:636:LYS:N	2.23	0.72
1:A:706:LEU:O	1:A:707:ILE:HG13	1.90	0.72
1:A:587:GLU:HG3	1:A:600:LEU:CD1	2.20	0.71
1:A:620:SER:O	1:A:621:GLN:HB3	1.90	0.71
1:A:495:TRP:HB2	1:A:537:ILE:HD11	1.72	0.71
1:A:428:GLU:OE1	1:A:487:PHE:CD1	2.43	0.71
1:D:359:LYS:HG3	1:D:387:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:TYR:HB3	1:D:669:PRO:CD	2.18	0.71
1:D:325:MET:HE3	1:D:328:HIS:HD2	1.56	0.70
1:D:620:SER:O	1:D:621:GLN:HB3	1.90	0.70
1:A:701:PTR:O1P	1:D:604:SER:OG	2.08	0.70
1:D:515:ASN:C	1:D:515:ASN:OD1	2.33	0.69
1:A:411:GLU:HG2	1:A:412:GLN:N	2.07	0.69
1:D:662:ASN:O	1:D:664:LEU:N	2.23	0.69
1:A:515:ASN:C	1:A:515:ASN:OD1	2.36	0.69
1:D:593:ASP:OD2	1:D:594:GLN:HB2	1.92	0.69
1:A:501:VAL:O	1:A:504:TRP:N	2.25	0.69
1:A:668:TYR:HB3	1:A:669:PRO:CD	2.22	0.69
1:D:506:PHE:O	1:D:510:THR:OG1	2.08	0.68
1:D:350:LYS:HE2	1:D:398:GLY:HA3	1.75	0.68
1:D:637:LYS:O	1:D:640:SER:OG	2.05	0.68
1:A:426:VAL:HG23	1:A:427:THR:N	2.08	0.68
1:A:617:VAL:HG12	1:A:628:PHE:CD1	2.28	0.68
1:D:495:TRP:HB2	1:D:537:ILE:HD11	1.75	0.68
1:D:386:HIS:O	1:D:404:PHE:HE2	1.76	0.68
1:A:606:SER:CB	1:D:701:PTR:O1P	2.42	0.68
1:D:652:LYS:O	1:D:653:VAL:HB	1.93	0.67
1:D:454:PRO:HG2	1:D:474:TYR:CZ	2.29	0.67
1:A:626:PRO:HB2	1:A:628:PHE:H	1.58	0.67
1:D:501:VAL:O	1:D:504:TRP:N	2.27	0.67
1:D:648:ILE:O	1:D:649:ARG:C	2.34	0.67
1:A:614:PHE:HE1	1:A:631:VAL:CG1	2.05	0.67
1:D:485:SER:O	1:D:487:PHE:N	2.28	0.67
1:D:428:GLU:OE1	1:D:487:PHE:CG	2.47	0.66
1:A:454:PRO:HG2	1:A:474:TYR:CE2	2.31	0.66
1:A:359:LYS:HG3	1:A:387:THR:HG23	1.78	0.66
1:D:409:LEU:HD23	1:D:457:VAL:HG11	1.78	0.65
1:D:547:ILE:HD11	1:D:554:PHE:HA	1.77	0.65
1:D:332:PRO:HD3	1:D:468:TRP:CH2	2.31	0.65
1:A:386:HIS:O	1:A:404:PHE:HE2	1.80	0.65
1:D:521:MET:HE2	1:D:582:ILE:N	2.11	0.65
1:A:547:ILE:HD11	1:A:554:PHE:HA	1.79	0.65
1:A:663:PRO:O	1:A:664:LEU:CD2	2.37	0.64
1:D:672:ASP:CG	1:D:675:HIS:HB2	2.23	0.64
1:A:591:LEU:HB3	1:A:617:VAL:HG11	1.78	0.64
1:D:599:PHE:CA	1:D:615:THR:O	2.43	0.64
1:D:636:LYS:O	1:D:637:LYS:C	2.40	0.64
1:A:473:TRP:CE2	1:A:539:TRP:HE3	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:HD12	1:A:572:LEU:H	1.63	0.63
1:A:632:GLU:OE1	1:A:633:PRO:HD2	1.98	0.63
1:A:595:GLN:HG3	1:A:666:TYR:CE2	2.34	0.63
1:A:572:LEU:O	1:A:578:ILE:HG13	1.99	0.63
1:A:473:TRP:CZ2	1:A:539:TRP:CA	2.82	0.63
1:A:599:PHE:CA	1:A:615:THR:O	2.44	0.62
1:D:643:THR:OG1	1:D:645:PRO:CD	2.44	0.62
1:A:572:LEU:HD12	1:A:572:LEU:N	2.15	0.62
1:A:614:PHE:CE1	1:A:631:VAL:CG1	2.81	0.62
1:A:506:PHE:O	1:A:510:THR:OG1	2.13	0.62
1:A:636:LYS:O	1:A:637:LYS:C	2.39	0.62
1:D:591:LEU:HB3	1:D:617:VAL:HG11	1.81	0.62
1:A:593:ASP:OD2	1:A:594:GLN:HB2	1.99	0.62
1:D:547:ILE:O	1:D:548:ASN:C	2.42	0.62
1:A:336:LYS:HA	1:A:458:ILE:O	2.00	0.62
1:D:461:VAL:HG23	1:D:461:VAL:O	1.97	0.62
1:D:332:PRO:HD3	1:D:468:TRP:HH2	1.64	0.62
1:A:547:ILE:O	1:A:548:ASN:C	2.42	0.61
1:A:345:LEU:HD11	1:A:435:PHE:CE2	2.35	0.61
1:A:670:ASN:O	1:A:670:ASN:ND2	2.33	0.61
1:D:325:MET:HE3	1:D:328:HIS:CD2	2.36	0.61
1:D:572:LEU:H	1:D:572:LEU:CD1	2.11	0.61
1:A:618:GLU:N	1:A:626:PRO:HG2	2.16	0.60
1:D:613:THR:OG1	1:D:633:PRO:HA	2.02	0.60
1:D:672:ASP:OD2	1:D:675:HIS:HB2	2.02	0.60
1:A:587:GLU:HG3	1:A:600:LEU:HD12	1.83	0.60
1:A:632:GLU:OE1	1:A:633:PRO:CD	2.49	0.60
1:D:644:PHE:N	1:D:645:PRO:HD2	2.17	0.60
1:D:345:LEU:HD11	1:D:435:PHE:CE2	2.36	0.59
1:D:564:LEU:HG	1:D:569:LEU:HD12	1.83	0.59
1:A:644:PHE:N	1:A:645:PRO:HD2	2.18	0.59
1:D:663:PRO:O	1:D:664:LEU:CD2	2.45	0.59
1:D:670:ASN:O	1:D:670:ASN:ND2	2.36	0.59
1:A:454:PRO:HG2	1:A:474:TYR:CZ	2.36	0.59
1:A:638:GLU:OE1	1:A:638:GLU:N	2.36	0.59
1:D:495:TRP:CG	1:D:495:TRP:O	2.56	0.59
1:D:240:LYS:O	1:D:243:GLN:N	2.35	0.59
1:D:260:GLN:HG3	1:D:348:LEU:O	2.03	0.58
1:D:635:THR:O	1:D:639:LEU:HD13	2.03	0.58
1:D:598:THR:HG22	1:D:666:TYR:HB2	1.84	0.58
1:A:342:THR:HG22	1:A:405:ARG:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PRO:CD	1:D:468:TRP:CH2	2.86	0.58
1:D:616:TRP:CH2	1:D:629:HIS:HB3	2.38	0.58
1:A:473:TRP:CD2	1:A:539:TRP:HE3	2.20	0.58
1:A:652:LYS:O	1:A:653:VAL:CB	2.50	0.58
1:D:683:ARG:CB	1:D:684:PRO:HD3	2.32	0.58
1:A:704:THR:HG22	1:D:710:SER:OG	2.03	0.57
1:D:632:GLU:OE1	1:D:633:PRO:CD	2.51	0.57
1:A:428:GLU:OE1	1:A:487:PHE:CG	2.58	0.57
1:A:618:GLU:H	1:A:626:PRO:CG	2.16	0.57
1:D:583:SER:O	1:D:585:GLU:N	2.36	0.57
1:D:607:SER:HB3	1:D:609:GLU:H	1.68	0.57
1:A:672:ASP:OD2	1:A:675:HIS:HB2	2.04	0.57
1:D:644:PHE:N	1:D:645:PRO:CD	2.67	0.57
1:A:644:PHE:N	1:A:645:PRO:CD	2.67	0.57
1:A:649:ARG:HD3	1:A:681:TYR:CE2	2.39	0.57
1:D:521:MET:HE3	1:D:581:PHE:HB3	1.86	0.57
1:D:375:LYS:O	1:D:423:PRO:HB2	2.04	0.57
1:A:331:ARG:HG3	1:A:468:TRP:CZ3	2.40	0.57
1:A:607:SER:OG	1:A:611:ALA:HB3	2.04	0.57
1:D:613:THR:HG22	1:D:614:PHE:N	2.19	0.57
1:A:331:ARG:HA	1:A:468:TRP:CZ3	2.40	0.56
1:A:644:PHE:O	1:A:645:PRO:C	2.48	0.56
1:D:618:GLU:H	1:D:626:PRO:CG	2.16	0.56
1:A:668:TYR:CB	1:A:669:PRO:HD3	2.28	0.56
1:D:583:SER:C	1:D:585:GLU:H	2.13	0.56
1:D:617:VAL:HG12	1:D:628:PHE:CD1	2.41	0.56
1:D:618:GLU:C	1:D:626:PRO:HG3	2.31	0.56
1:A:429:GLU:HG3	1:A:431:HIS:NE2	2.21	0.56
1:A:614:PHE:CE1	1:A:631:VAL:HG21	2.41	0.56
1:A:648:ILE:O	1:A:649:ARG:C	2.49	0.55
1:D:347:LEU:HD23	1:D:400:LEU:HD23	1.88	0.55
1:A:260:GLN:HG3	1:A:348:LEU:O	2.05	0.55
1:A:505:GLN:O	1:A:508:SER:OG	2.21	0.55
1:A:370:GLU:HA	1:A:373:THR:OG1	2.06	0.55
1:D:668:TYR:CB	1:D:669:PRO:HD3	2.23	0.55
1:D:672:ASP:OD1	1:D:675:HIS:CB	2.54	0.55
1:A:464:LEU:HD23	1:A:464:LEU:O	2.06	0.55
1:D:638:GLU:N	1:D:638:GLU:OE1	2.39	0.55
1:A:598:THR:HG22	1:A:666:TYR:HB2	1.88	0.54
1:D:239:TRP:NE1	1:D:253:ASN:OD1	2.39	0.54
1:D:506:PHE:N	1:D:506:PHE:CD1	2.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:NE1	1:A:253:ASN:OD1	2.40	0.54
1:A:473:TRP:CH2	1:A:539:TRP:HA	2.42	0.54
1:D:485:SER:HB3	1:D:488:LEU:HD12	1.90	0.54
1:D:651:TYR:CD1	1:D:652:LYS:N	2.75	0.54
1:D:336:LYS:HA	1:D:458:ILE:O	2.07	0.54
1:A:559:GLU:OE1	1:A:559:GLU:O	2.26	0.54
1:D:349:VAL:HG12	1:D:351:LEU:HG	1.90	0.54
1:D:565:ILE:HA	1:D:569:LEU:HB2	1.87	0.54
1:A:325:MET:SD	1:A:336:LYS:HB3	2.47	0.54
1:A:460:ASN:OD1	1:A:461:VAL:N	2.40	0.54
1:D:495:TRP:O	1:D:495:TRP:CD1	2.60	0.54
1:D:467:GLY:O	1:D:468:TRP:C	2.48	0.54
1:D:594:GLN:CG	1:D:595:GLN:H	2.20	0.54
1:D:240:LYS:O	1:D:241:ARG:C	2.51	0.54
1:A:504:TRP:HA	1:A:507:SER:OG	2.08	0.53
1:A:613:THR:OG1	1:A:633:PRO:HB3	2.09	0.53
1:D:429:GLU:HG3	1:D:431:HIS:NE2	2.23	0.53
1:D:460:ASN:OD1	1:D:462:SER:N	2.29	0.53
1:D:332:PRO:CD	1:D:468:TRP:HH2	2.20	0.53
1:A:683:ARG:CB	1:A:684:PRO:HD3	2.38	0.53
1:D:370:GLU:HA	1:D:373:THR:OG1	2.09	0.53
1:D:386:HIS:O	1:D:404:PHE:CE2	2.58	0.53
1:A:473:TRP:CD2	1:A:539:TRP:CE3	2.97	0.53
1:D:618:GLU:N	1:D:626:PRO:HG2	2.19	0.53
1:D:645:PRO:O	1:D:648:ILE:HB	2.09	0.53
1:A:595:GLN:HG3	1:A:666:TYR:HE2	1.74	0.53
1:D:467:GLY:O	1:D:470:SER:N	2.42	0.53
1:D:652:LYS:O	1:D:653:VAL:CB	2.56	0.53
1:A:384:GLY:HA3	1:A:406:HIS:O	2.09	0.53
1:D:555:TRP:O	1:D:559:GLU:N	2.41	0.53
1:D:570:LEU:HD22	1:D:574:ASN:HD21	1.74	0.52
1:D:554:PHE:CG	1:D:554:PHE:O	2.62	0.52
1:D:460:ASN:OD1	1:D:461:VAL:N	2.43	0.52
1:D:595:GLN:O	1:D:597:GLY:N	2.43	0.52
1:A:600:LEU:N	1:A:615:THR:O	2.41	0.52
1:D:345:LEU:HD11	1:D:435:PHE:CD2	2.44	0.52
1:D:480:GLU:O	1:D:481:PRO:C	2.53	0.52
1:D:668:TYR:CB	1:D:669:PRO:CD	2.86	0.52
1:A:316:SER:HG	1:A:348:LEU:H	1.58	0.52
1:A:583:SER:C	1:A:585:GLU:H	2.17	0.52
1:A:509:VAL:HG12	1:A:510:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ARG:HG3	1:D:468:TRP:CZ3	2.44	0.52
1:A:626:PRO:C	1:A:628:PHE:H	2.18	0.51
1:A:240:LYS:O	1:A:243:GLN:N	2.42	0.51
1:A:644:PHE:HB3	1:A:645:PRO:HD3	1.91	0.51
1:A:212:GLU:O	1:A:216:LYS:HB2	2.11	0.51
1:D:578:ILE:HA	1:D:601:LEU:HB2	1.91	0.51
1:A:359:LYS:CG	1:A:387:THR:HG23	2.40	0.51
1:A:583:SER:O	1:A:585:GLU:N	2.38	0.51
1:D:316:SER:OG	1:D:348:LEU:N	2.40	0.51
1:D:522:LEU:O	1:D:523:GLY:C	2.50	0.51
1:D:626:PRO:C	1:D:628:PHE:H	2.16	0.51
1:D:512:ARG:HD2	1:D:573:TRP:O	2.10	0.51
1:D:359:LYS:CG	1:D:387:THR:HG23	2.38	0.51
1:D:644:PHE:O	1:D:645:PRO:C	2.52	0.51
1:D:419:THR:HG22	1:D:419:THR:O	2.10	0.51
1:D:479:ALA:HB3	1:D:481:PRO:HD2	1.93	0.51
1:D:506:PHE:HD1	1:D:506:PHE:H	1.59	0.51
1:D:564:LEU:HG	1:D:569:LEU:CD1	2.41	0.51
1:D:586:ARG:O	1:D:586:ARG:HG2	2.11	0.51
1:D:594:GLN:HG2	1:D:595:GLN:H	1.76	0.51
1:D:480:GLU:O	1:D:482:ARG:N	2.44	0.51
1:D:582:ILE:HD11	1:D:586:ARG:HH11	1.76	0.51
1:D:313:ILE:HG12	1:D:349:VAL:HG21	1.93	0.51
1:D:673:LYS:C	1:D:675:HIS:H	2.17	0.51
1:A:411:GLU:HG2	1:A:412:GLN:H	1.76	0.50
1:D:212:GLU:O	1:D:216:LYS:HB2	2.11	0.50
1:D:504:TRP:HA	1:D:507:SER:OG	2.10	0.50
1:D:552:PHE:CD1	1:D:608:ARG:HG2	2.46	0.50
1:A:495:TRP:O	1:A:495:TRP:CG	2.63	0.50
1:A:522:LEU:O	1:A:523:GLY:C	2.54	0.50
1:D:142:LEU:HD23	1:D:262:TRP:CZ3	2.47	0.50
1:D:428:GLU:OE1	1:D:487:PHE:HB3	2.11	0.50
1:D:649:ARG:HD3	1:D:681:TYR:CE2	2.45	0.50
1:A:349:VAL:HG12	1:A:351:LEU:HG	1.93	0.50
1:A:613:THR:OG1	1:A:633:PRO:CB	2.60	0.50
1:A:244:GLN:OE1	1:A:475:ASN:ND2	2.40	0.49
1:A:595:GLN:O	1:A:597:GLY:N	2.44	0.49
1:A:483:ASN:OD1	1:A:483:ASN:C	2.56	0.49
1:A:240:LYS:O	1:A:241:ARG:C	2.56	0.49
1:A:332:PRO:O	1:A:333:LEU:HG	2.11	0.49
1:A:554:PHE:CG	1:A:554:PHE:O	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:THR:OG1	1:A:645:PRO:CD	2.51	0.49
1:A:672:ASP:OD1	1:A:675:HIS:HB3	2.12	0.49
1:D:261:ASN:HA	1:D:264:THR:HG22	1.95	0.49
1:D:377:PHE:O	1:D:417:THR:HG21	2.12	0.49
1:D:501:VAL:HG12	1:D:502:LEU:N	2.26	0.49
1:A:331:ARG:HG3	1:A:468:TRP:CE3	2.48	0.49
1:D:468:TRP:HA	1:D:468:TRP:CE3	2.46	0.49
1:A:617:VAL:CG1	1:A:628:PHE:CD1	2.94	0.49
1:A:659:ILE:HG23	1:A:660:PRO:HD2	1.94	0.49
1:D:359:LYS:HA	1:D:389:VAL:HA	1.95	0.49
1:D:631:VAL:O	1:D:632:GLU:C	2.55	0.49
1:A:261:ASN:HA	1:A:264:THR:HG22	1.94	0.49
1:A:419:THR:HG22	1:A:419:THR:O	2.11	0.49
1:D:495:TRP:HB2	1:D:527:LEU:HD11	1.95	0.49
1:A:618:GLU:C	1:A:626:PRO:HG3	2.38	0.48
1:A:672:ASP:CG	1:A:675:HIS:HB2	2.38	0.48
1:D:680:TYR:O	1:D:681:TYR:C	2.56	0.48
1:D:384:GLY:HA3	1:D:406:HIS:O	2.13	0.48
1:D:464:LEU:HD23	1:D:464:LEU:O	2.14	0.48
1:D:518:GLN:HG2	1:D:581:PHE:HB2	1.95	0.48
1:D:649:ARG:HD3	1:D:681:TYR:CE1	2.49	0.48
1:A:630:ALA:O	1:D:702:ILE:HB	2.13	0.48
1:A:672:ASP:OD1	1:A:675:HIS:CB	2.62	0.48
1:A:617:VAL:CG1	1:A:628:PHE:HD1	2.27	0.48
1:A:677:PHE:HA	1:A:680:TYR:HD2	1.78	0.48
1:D:342:THR:HG22	1:D:405:ARG:HG2	1.96	0.48
1:D:483:ASN:C	1:D:483:ASN:OD1	2.56	0.48
1:A:335:LEU:HB2	1:A:457:VAL:HG22	1.96	0.47
1:A:375:LYS:O	1:A:423:PRO:HB2	2.14	0.47
1:A:426:VAL:HG23	1:A:427:THR:H	1.78	0.47
1:A:673:LYS:C	1:A:675:HIS:H	2.22	0.47
1:D:378:ARG:NH1	1:D:380:PHE:HZ	2.11	0.47
1:D:498:LEU:O	1:D:499:SER:C	2.56	0.47
1:D:572:LEU:HB2	1:D:578:ILE:HD11	1.96	0.47
1:D:598:THR:CG2	1:D:666:TYR:HB2	2.43	0.47
1:D:599:PHE:CG	1:D:664:LEU:HD13	2.50	0.47
1:A:498:LEU:O	1:A:499:SER:C	2.58	0.47
1:A:498:LEU:HD22	1:A:502:LEU:HG	1.96	0.47
1:D:663:PRO:O	1:D:663:PRO:HG2	2.15	0.47
1:A:598:THR:O	1:A:617:VAL:HG22	2.14	0.47
1:A:594:GLN:CG	1:A:595:GLN:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PRO:HD2	1:D:468:TRP:CZ3	2.50	0.47
1:D:555:TRP:C	1:D:557:TRP:H	2.23	0.47
1:A:625:GLU:OE1	1:A:625:GLU:N	2.48	0.47
1:A:616:TRP:CH2	1:A:629:HIS:HB3	2.49	0.46
1:A:707:ILE:HG23	1:A:709:VAL:HG23	1.97	0.46
1:D:383:LEU:O	1:D:384:GLY:O	2.34	0.46
1:D:261:ASN:O	1:D:264:THR:HG22	2.15	0.46
1:A:331:ARG:N	1:A:332:PRO:HD3	2.31	0.46
1:A:637:LYS:O	1:A:640:SER:OG	2.19	0.46
1:D:618:GLU:O	1:D:626:PRO:HG3	2.15	0.46
1:D:626:PRO:C	1:D:628:PHE:N	2.73	0.46
1:A:600:LEU:C	1:A:601:LEU:HD23	2.41	0.46
1:D:141:GLU:O	1:D:145:LYS:HG3	2.15	0.46
1:D:159:GLU:HB3	1:D:213:VAL:HG22	1.97	0.46
1:D:428:GLU:O	1:D:428:GLU:HG2	2.13	0.46
1:D:503:SER:OG	1:D:504:TRP:N	2.44	0.46
1:A:404:PHE:CB	1:A:407:LEU:HD11	2.46	0.46
1:A:480:GLU:O	1:A:481:PRO:C	2.57	0.46
1:D:672:ASP:O	1:D:673:LYS:C	2.59	0.46
1:A:600:LEU:O	1:A:614:PHE:HA	2.16	0.45
1:D:644:PHE:HB3	1:D:645:PRO:HD3	1.97	0.45
1:A:515:ASN:OD1	1:A:516:VAL:N	2.49	0.45
1:A:419:THR:O	1:A:420:ASN:C	2.60	0.45
1:A:467:GLY:O	1:A:470:SER:N	2.49	0.45
1:D:524:GLU:CD	1:D:524:GLU:C	2.85	0.45
1:D:580:GLY:HA2	1:D:603:PHE:CD2	2.52	0.45
1:D:648:ILE:HG22	1:D:673:LYS:HD3	1.98	0.45
1:A:261:ASN:O	1:A:264:THR:HG22	2.17	0.45
1:D:370:GLU:HA	1:D:373:THR:HG1	1.82	0.45
1:D:625:GLU:OE1	1:D:625:GLU:N	2.48	0.45
1:A:495:TRP:O	1:A:499:SER:HB3	2.17	0.45
1:A:672:ASP:O	1:A:673:LYS:C	2.59	0.45
1:D:332:PRO:HD2	1:D:468:TRP:CH2	2.52	0.45
1:D:339:VAL:HG12	1:D:340:GLN:O	2.17	0.44
1:D:673:LYS:O	1:D:675:HIS:N	2.49	0.44
1:D:145:LYS:O	1:D:149:VAL:HG23	2.17	0.44
1:D:280:LEU:O	1:D:294:ILE:HD12	2.18	0.44
1:D:419:THR:O	1:D:420:ASN:C	2.59	0.44
1:D:515:ASN:OD1	1:D:516:VAL:N	2.50	0.44
1:D:672:ASP:OD1	1:D:672:ASP:N	2.51	0.44
1:A:377:PHE:O	1:A:417:THR:HG21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:LEU:HD23	1:D:457:VAL:CG1	2.47	0.44
1:A:316:SER:OG	1:A:348:LEU:N	2.45	0.44
1:A:495:TRP:HB2	1:A:527:LEU:HD11	2.00	0.44
1:A:524:GLU:C	1:A:524:GLU:CD	2.86	0.44
1:D:672:ASP:OD1	1:D:675:HIS:HB2	2.16	0.44
1:A:331:ARG:HA	1:A:468:TRP:CH2	2.53	0.44
1:D:325:MET:CE	1:D:328:HIS:CD2	3.01	0.44
1:D:546:ASN:HB3	1:D:550:LYS:O	2.18	0.44
1:D:635:THR:O	1:D:639:LEU:CD1	2.65	0.44
1:D:500:GLU:O	1:D:500:GLU:CG	2.66	0.44
1:D:659:ILE:HG23	1:D:660:PRO:HD2	2.00	0.44
1:A:145:LYS:O	1:A:149:VAL:HG23	2.18	0.43
1:A:572:LEU:H	1:A:572:LEU:CD1	2.31	0.43
1:A:626:PRO:C	1:A:628:PHE:N	2.75	0.43
1:D:335:LEU:O	1:D:458:ILE:HG12	2.18	0.43
1:D:424:LEU:N	1:D:424:LEU:HD22	2.33	0.43
1:D:566:LYS:O	1:D:566:LYS:HG2	2.19	0.43
1:D:644:PHE:O	1:D:647:ILE:HB	2.19	0.43
1:D:672:ASP:OD1	1:D:675:HIS:HB3	2.18	0.43
1:A:466:SER:O	1:A:469:ALA:CB	2.59	0.43
1:A:707:ILE:HG22	1:D:707:ILE:CG2	2.36	0.43
1:D:598:THR:O	1:D:617:VAL:HG22	2.18	0.43
1:A:280:LEU:O	1:A:294:ILE:HD12	2.19	0.43
1:A:495:TRP:CB	1:A:537:ILE:HD11	2.45	0.43
1:A:701:PTR:P	1:D:604:SER:OG	2.77	0.43
1:A:471:ILE:HD13	1:A:471:ILE:HA	1.83	0.43
1:D:333:LEU:HD22	1:D:455:VAL:HG23	2.00	0.43
1:A:159:GLU:HB3	1:A:213:VAL:HG22	2.00	0.43
1:A:707:ILE:CG2	1:D:707:ILE:HG22	2.37	0.42
1:D:466:SER:O	1:D:467:GLY:C	2.62	0.42
1:D:614:PHE:CE1	1:D:631:VAL:CG1	2.95	0.42
1:A:670:ASN:C	1:A:671:ILE:HG13	2.43	0.42
1:D:350:LYS:CE	1:D:398:GLY:HA3	2.47	0.42
1:D:558:ILE:O	1:D:559:GLU:C	2.56	0.42
1:D:600:LEU:N	1:D:615:THR:O	2.51	0.42
1:A:617:VAL:HG12	1:A:628:PHE:HD1	1.79	0.42
1:D:648:ILE:HD13	1:D:677:PHE:CE2	2.54	0.42
1:D:332:PRO:CD	1:D:468:TRP:CZ3	3.02	0.42
1:A:437:THR:HG23	1:A:448:LEU:HB2	2.02	0.42
1:D:594:GLN:HG2	1:D:595:GLN:N	2.35	0.42
1:A:618:GLU:O	1:A:626:PRO:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ARG:HA	1:D:468:TRP:CZ3	2.54	0.42
1:D:481:PRO:O	1:D:482:ARG:C	2.63	0.42
1:A:174:CYS:O	1:A:178:GLN:HG2	2.20	0.42
1:A:503:SER:OG	1:A:504:TRP:N	2.50	0.42
1:A:558:ILE:O	1:A:559:GLU:C	2.57	0.42
1:A:668:TYR:CB	1:A:669:PRO:CD	2.89	0.42
1:D:543:CYS:O	1:D:543:CYS:SG	2.78	0.42
1:D:634:TYR:HB3	1:D:639:LEU:HD11	2.02	0.42
1:A:586:ARG:O	1:A:586:ARG:HG2	2.20	0.41
1:A:600:LEU:O	1:A:601:LEU:HD23	2.20	0.41
1:A:598:THR:OG1	1:A:617:VAL:CG2	2.69	0.41
1:A:378:ARG:NH2	1:A:457:VAL:O	2.49	0.41
1:A:477:LEU:O	1:A:478:VAL:HG23	2.21	0.41
1:D:269:SER:O	1:D:273:VAL:HG23	2.19	0.41
1:D:347:LEU:CD2	1:D:400:LEU:HD23	2.49	0.41
1:A:316:SER:OG	1:A:348:LEU:HB2	2.20	0.41
1:D:428:GLU:OE1	1:D:487:PHE:CB	2.68	0.41
1:D:521:MET:HE3	1:D:581:PHE:CA	2.51	0.41
1:A:480:GLU:N	1:A:481:PRO:HD2	2.35	0.41
1:A:141:GLU:O	1:A:145:LYS:HG3	2.20	0.41
1:A:485:SER:O	1:A:488:LEU:HB2	2.21	0.41
1:A:680:TYR:O	1:A:681:TYR:C	2.64	0.41
1:D:224:THR:HG21	1:D:270:LEU:HD21	2.01	0.41
1:A:239:TRP:CZ2	1:A:256:LEU:HD21	2.56	0.41
1:A:269:SER:O	1:A:273:VAL:HG23	2.21	0.41
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.92	0.41
1:A:324:CYS:SG	1:A:325:MET:N	2.94	0.41
1:A:560:SER:OG	1:A:561:ILE:N	2.54	0.41
1:A:649:ARG:HD3	1:A:681:TYR:CE1	2.54	0.41
1:A:591:LEU:O	1:A:628:PHE:HE1	2.05	0.40
1:A:598:THR:CG2	1:A:666:TYR:HB2	2.50	0.40
1:A:668:TYR:CD1	1:A:668:TYR:C	2.98	0.40
1:D:382:ILE:HD12	1:D:382:ILE:H	1.86	0.40
1:D:596:PRO:HA	1:D:617:VAL:O	2.21	0.40
1:A:560:SER:OG	1:A:610:GLY:HA3	2.21	0.40
1:A:677:PHE:HA	1:A:680:TYR:CD2	2.57	0.40
1:D:174:CYS:O	1:D:178:GLN:HG2	2.20	0.40
1:D:393:GLU:O	1:D:394:GLU:HB3	2.21	0.40
1:D:562:LEU:O	1:D:563:GLU:C	2.61	0.40
1:D:649:ARG:HB2	1:D:681:TYR:HE1	1.83	0.40
1:A:555:TRP:O	1:A:559:GLU:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LEU:N	1:A:571:PRO:CD	2.84	0.40
1:A:573:TRP:O	1:A:573:TRP:CG	2.73	0.40
1:A:662:ASN:O	1:A:662:ASN:CG	2.65	0.40
1:D:248:ILE:HG21	1:D:248:ILE:HD13	1.77	0.40
1:D:262:TRP:O	1:D:263:PHE:C	2.64	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	546/776 (70%)	443 (81%)	77 (14%)	26 (5%)	2	19
1	D	546/776 (70%)	433 (79%)	84 (15%)	29 (5%)	1	17
All	All	1092/1552 (70%)	876 (80%)	161 (15%)	55 (5%)	3	18

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	VAL
1	A	480	GLU
1	A	482	ARG
1	A	548	ASN
1	A	596	PRO
1	A	668	TYR
1	A	683	ARG
1	D	426	VAL
1	D	480	GLU
1	D	482	ARG
1	D	548	ASN
1	D	596	PRO
1	D	668	TYR

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Mol	Chain	Res	Type
1	D	683	ARG
1	A	181	GLU
1	A	202	MET
1	A	244	GLN
1	A	384	GLY
1	A	423	PRO
1	A	481	PRO
1	A	610	GLY
1	A	653	VAL
1	A	667	LEU
1	D	181	GLU
1	D	202	MET
1	D	244	GLN
1	D	332	PRO
1	D	384	GLY
1	D	423	PRO
1	D	481	PRO
1	D	610	GLY
1	D	653	VAL
1	A	332	PRO
1	A	399	SER
1	A	415	ALA
1	A	597	GLY
1	D	399	SER
1	D	465	PRO
1	D	597	GLY
1	D	667	LEU
1	A	394	GLU
1	A	465	PRO
1	A	593	ASP
1	D	240	LYS
1	D	394	GLU
1	D	415	ALA
1	D	681	TYR
1	A	442	PRO
1	A	669	PRO
1	D	442	PRO
1	D	491	PRO
1	D	593	ASP
1	D	502	LEU
1	D	669	PRO
1	A	491	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	506/719 (70%)	470 (93%)	36 (7%)	13	40
1	D	506/719 (70%)	456 (90%)	50 (10%)	7	28
All	All	1012/1438 (70%)	926 (92%)	86 (8%)	12	33

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	234	ASP
1	A	236	LEU
1	A	291	HIS
1	A	327	THR
1	A	332	PRO
1	A	343	VAL
1	A	370	GLU
1	A	382	ILE
1	A	383	LEU
1	A	390	MET
1	A	409	LEU
1	A	423	PRO
1	A	436	GLU
1	A	447	ASP
1	A	450	THR
1	A	455	VAL
1	A	466	SER
1	A	478	VAL
1	A	498	LEU
1	A	503	SER
1	A	537	ILE
1	A	559	GLU
1	A	562	LEU
1	A	563	GLU
1	A	578	ILE
1	A	579	MET

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Mol	Chain	Res	Type
1	A	596	PRO
1	A	613	THR
1	A	617	VAL
1	A	635	THR
1	A	643	THR
1	A	660	PRO
1	A	671	ILE
1	A	707	ILE
1	A	708	SER
1	D	196	GLN
1	D	234	ASP
1	D	240	LYS
1	D	291	HIS
1	D	326	PRO
1	D	327	THR
1	D	330	GLN
1	D	331	ARG
1	D	332	PRO
1	D	343	VAL
1	D	382	ILE
1	D	383	LEU
1	D	390	MET
1	D	404	PHE
1	D	409	LEU
1	D	423	PRO
1	D	436	GLU
1	D	445	VAL
1	D	447	ASP
1	D	450	THR
1	D	455	VAL
1	D	471	ILE
1	D	478	VAL
1	D	498	LEU
1	D	501	VAL
1	D	502	LEU
1	D	503	SER
1	D	512	ARG
1	D	536	LEU
1	D	537	ILE
1	D	559	GLU
1	D	562	LEU
1	D	563	GLU

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Mol	Chain	Res	Type
1	D	575	ASP
1	D	578	ILE
1	D	579	MET
1	D	596	PRO
1	D	606	SER
1	D	609	GLU
1	D	613	THR
1	D	617	VAL
1	D	635	THR
1	D	643	THR
1	D	647	ILE
1	D	649	ARG
1	D	660	PRO
1	D	667	LEU
1	D	671	ILE
1	D	707	ILE
1	D	708	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	271	GLN
1	A	297	ASN
1	A	381	ASN
1	A	391	ASN
1	A	670	ASN
1	D	196	GLN
1	D	243	GLN
1	D	271	GLN
1	D	297	ASN
1	D	330	GLN
1	D	391	ASN
1	D	475	ASN
1	D	574	ASN
1	D	662	ASN
1	D	670	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PTR	A	701	1	15,16,17	0.75	0	17,22,24	1.53	2 (11%)
1	PTR	D	701	1	15,16,17	0.61	0	17,22,24	1.71	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	701	1	-	0/10/11/13	0/1/1/1
1	PTR	D	701	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	701	PTR	O2P-P-OH	6.20	123.64	105.32
1	A	701	PTR	O2P-P-OH	3.62	116.03	105.32
1	D	701	PTR	O3P-P-OH	-2.40	98.23	105.32
1	A	701	PTR	OH-CZ-CE1	2.40	126.40	119.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	701	PTR	2	0
1	D	701	PTR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

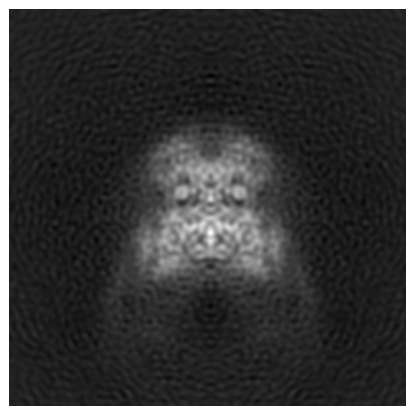
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39679. These allow visual inspection of the internal detail of the map and identification of artifacts.

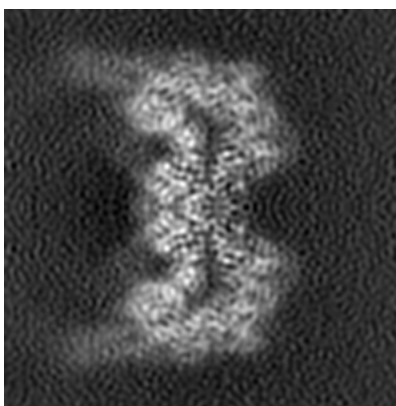
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

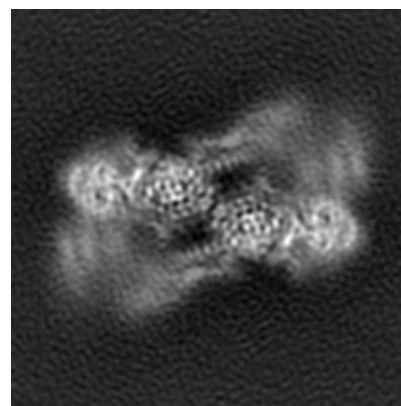
6.1.1 Primary map



X

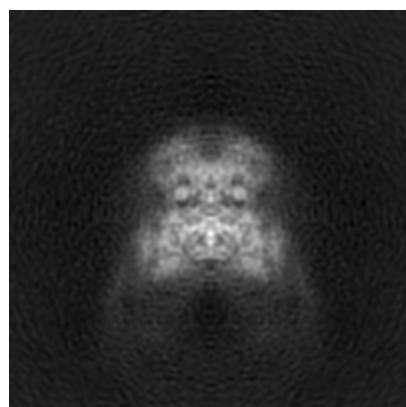


Y

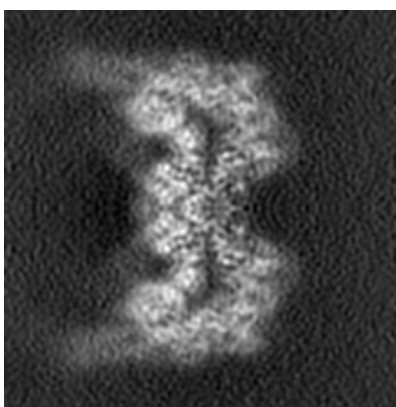


Z

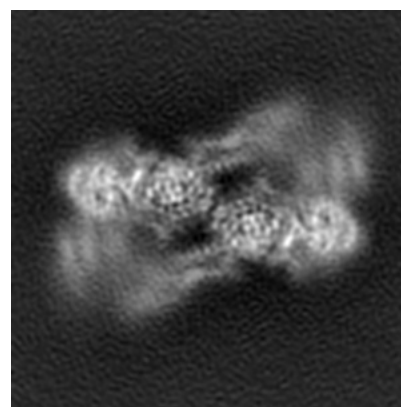
6.1.2 Raw map



X



Y

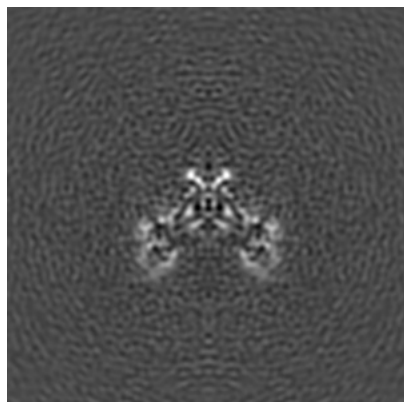


Z

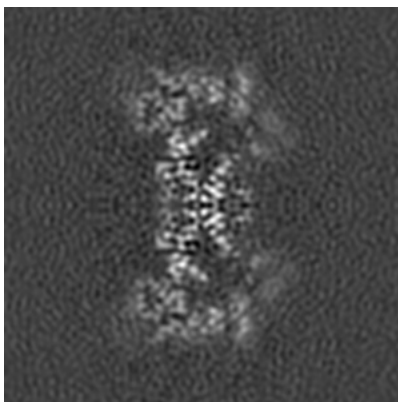
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

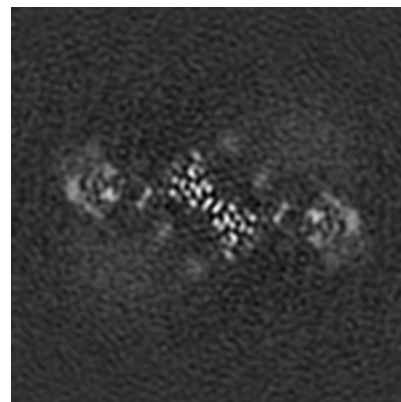
6.2.1 Primary map



X Index: 61

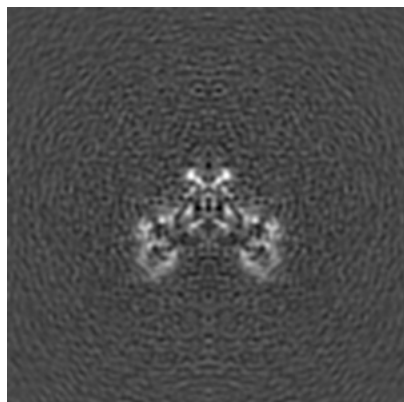


Y Index: 61

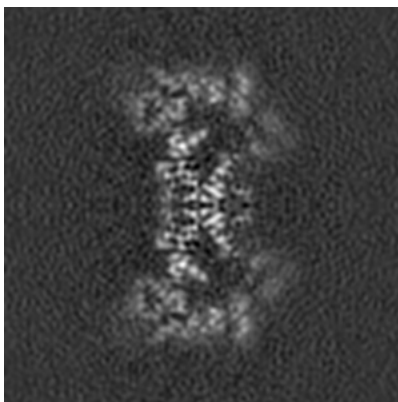


Z Index: 61

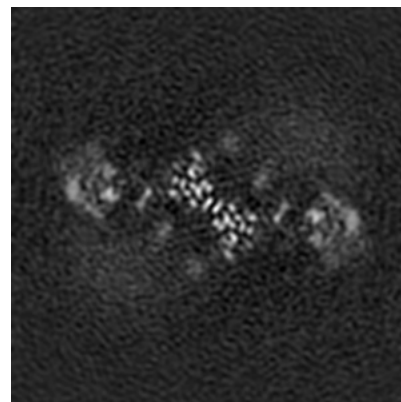
6.2.2 Raw map



X Index: 61



Y Index: 61

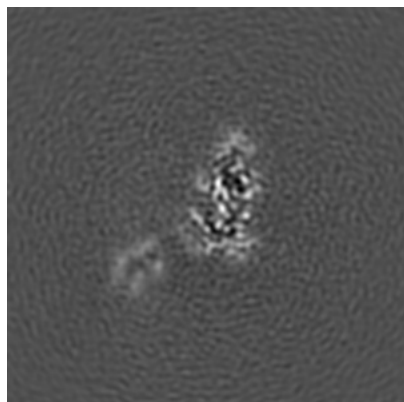


Z Index: 61

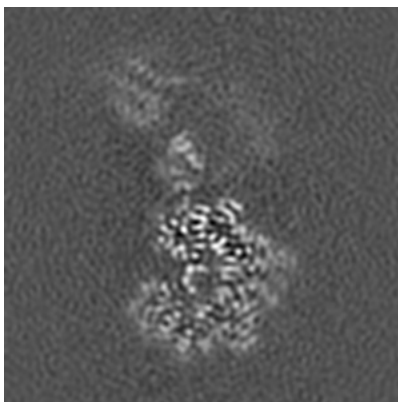
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

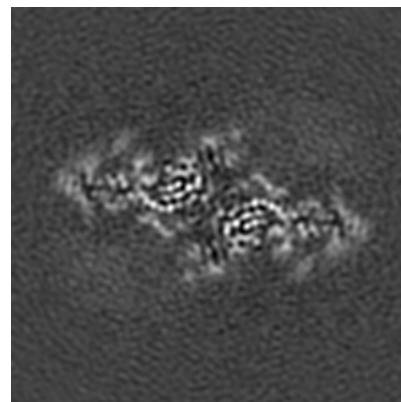
6.3.1 Primary map



X Index: 49

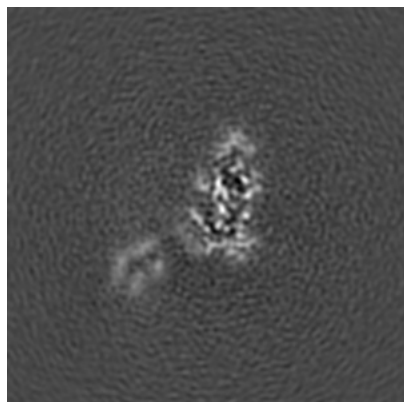


Y Index: 66

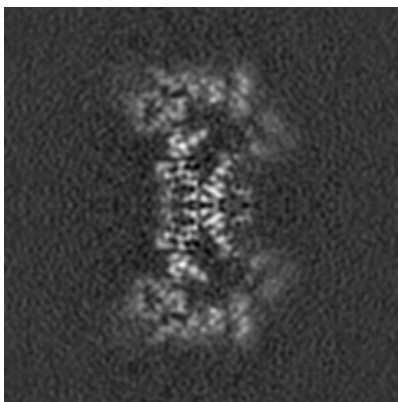


Z Index: 54

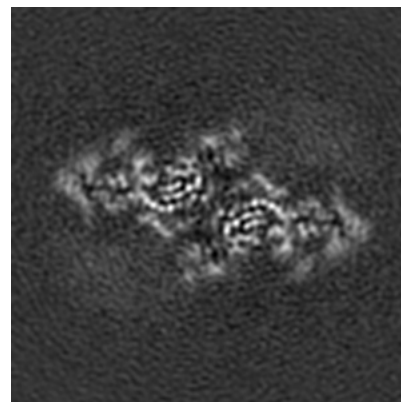
6.3.2 Raw map



X Index: 49



Y Index: 61

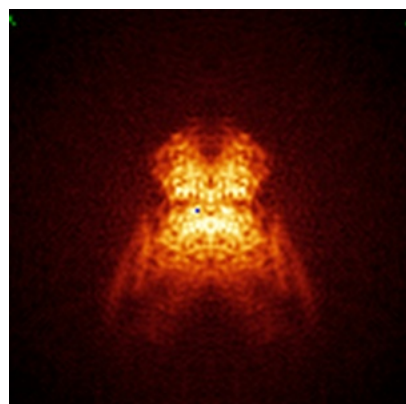


Z Index: 54

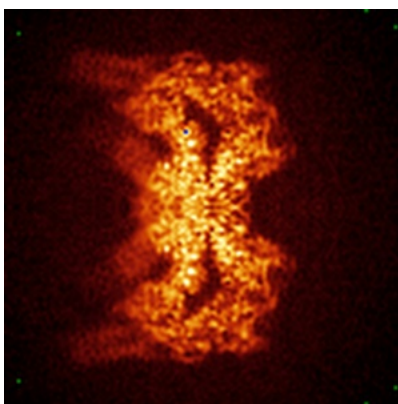
The images above show the largest variance slices of the map in three orthogonal directions.

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

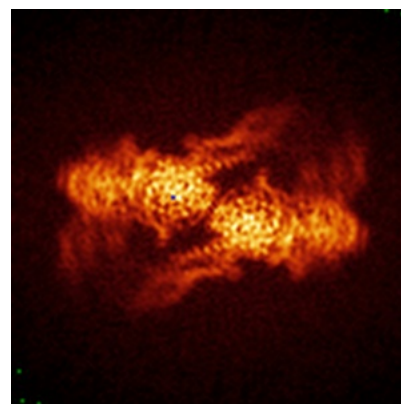
6.4.1 Primary map



X

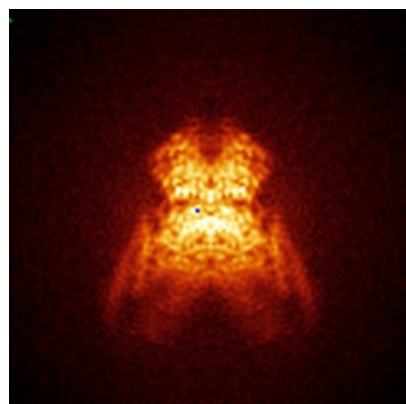


Y

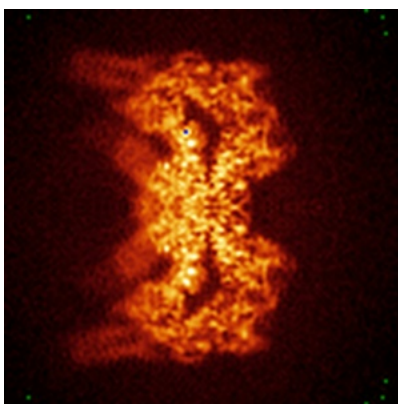


Z

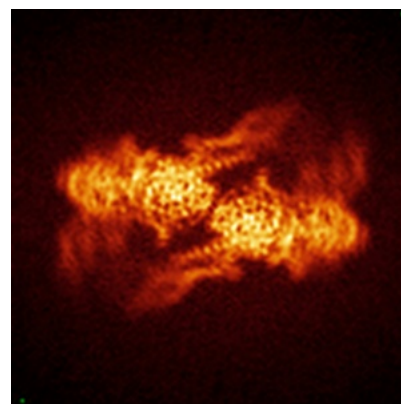
6.4.2 Raw map



X



Y



Z

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

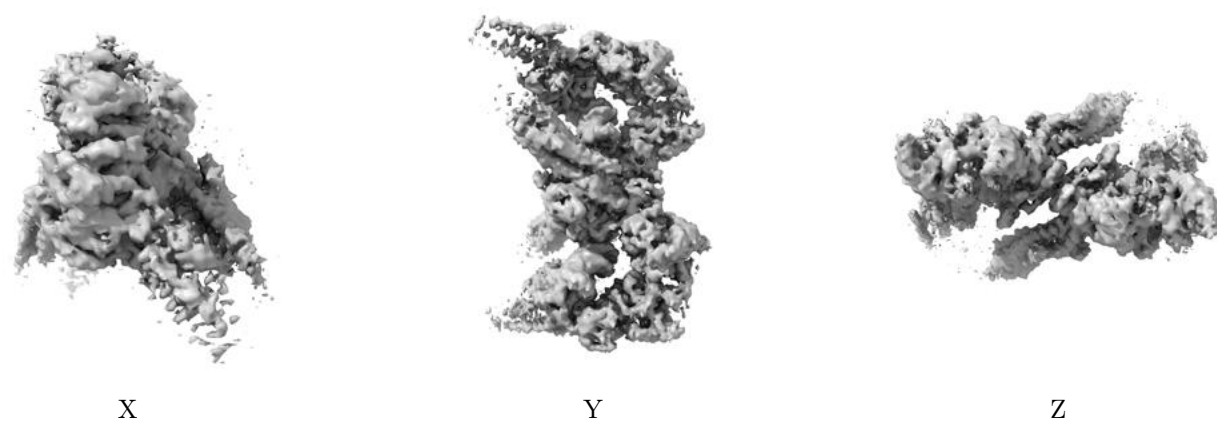
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

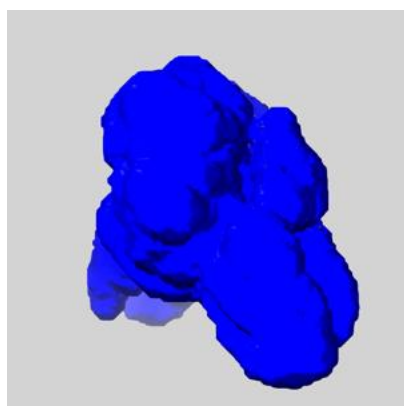
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

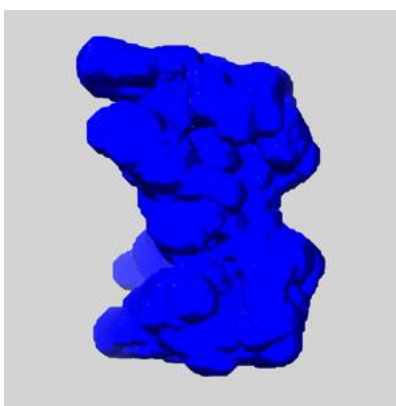
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

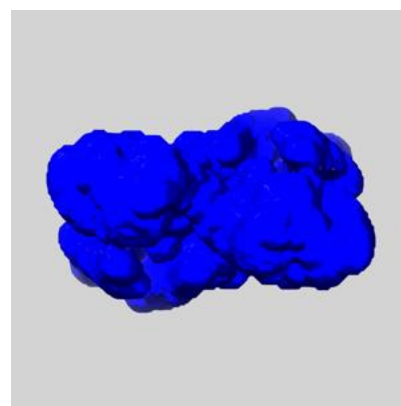
6.6.1 emd_39679_msk_1.map [i](#)



X



Y

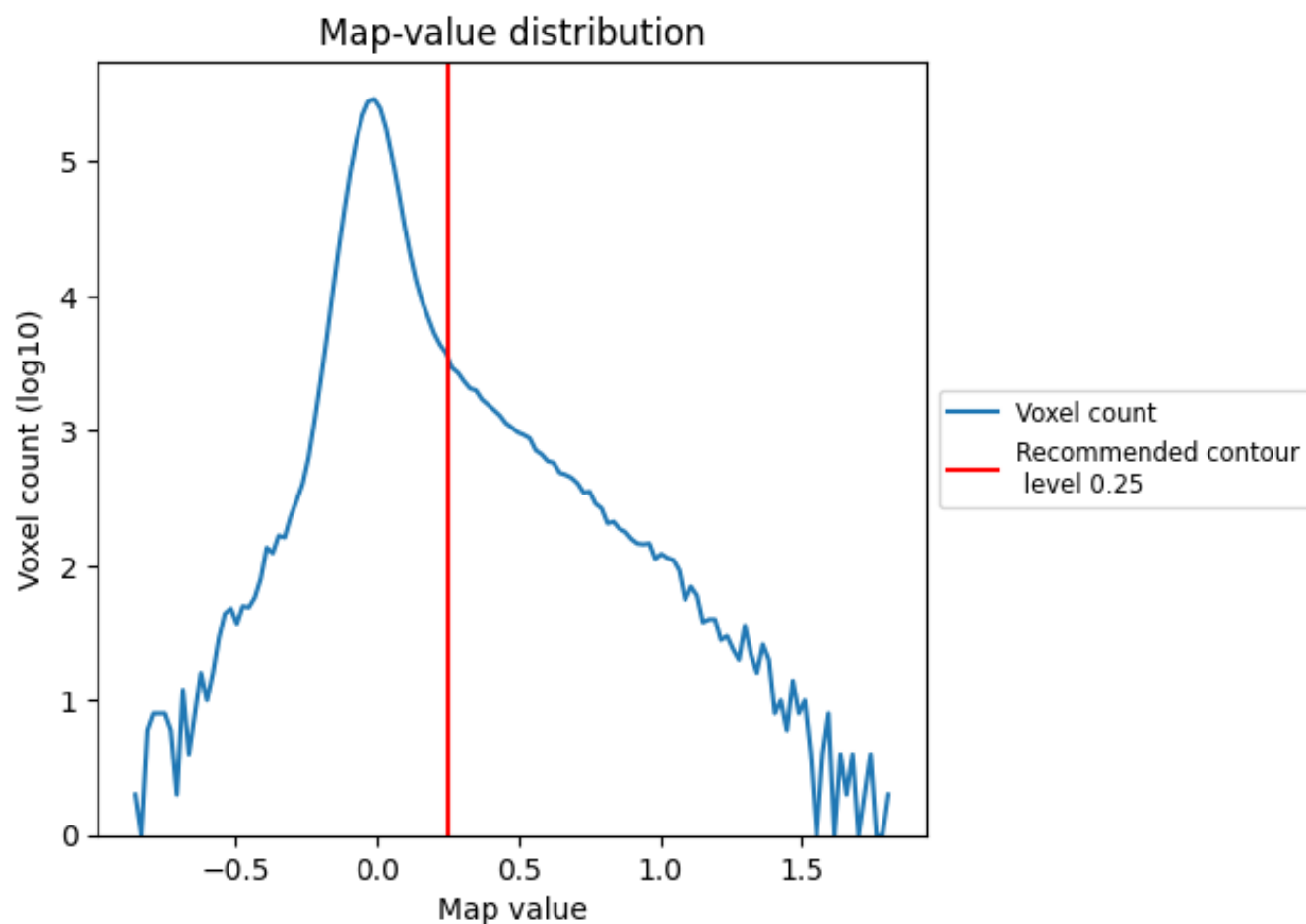


Z

7 Map analysis [i](#)

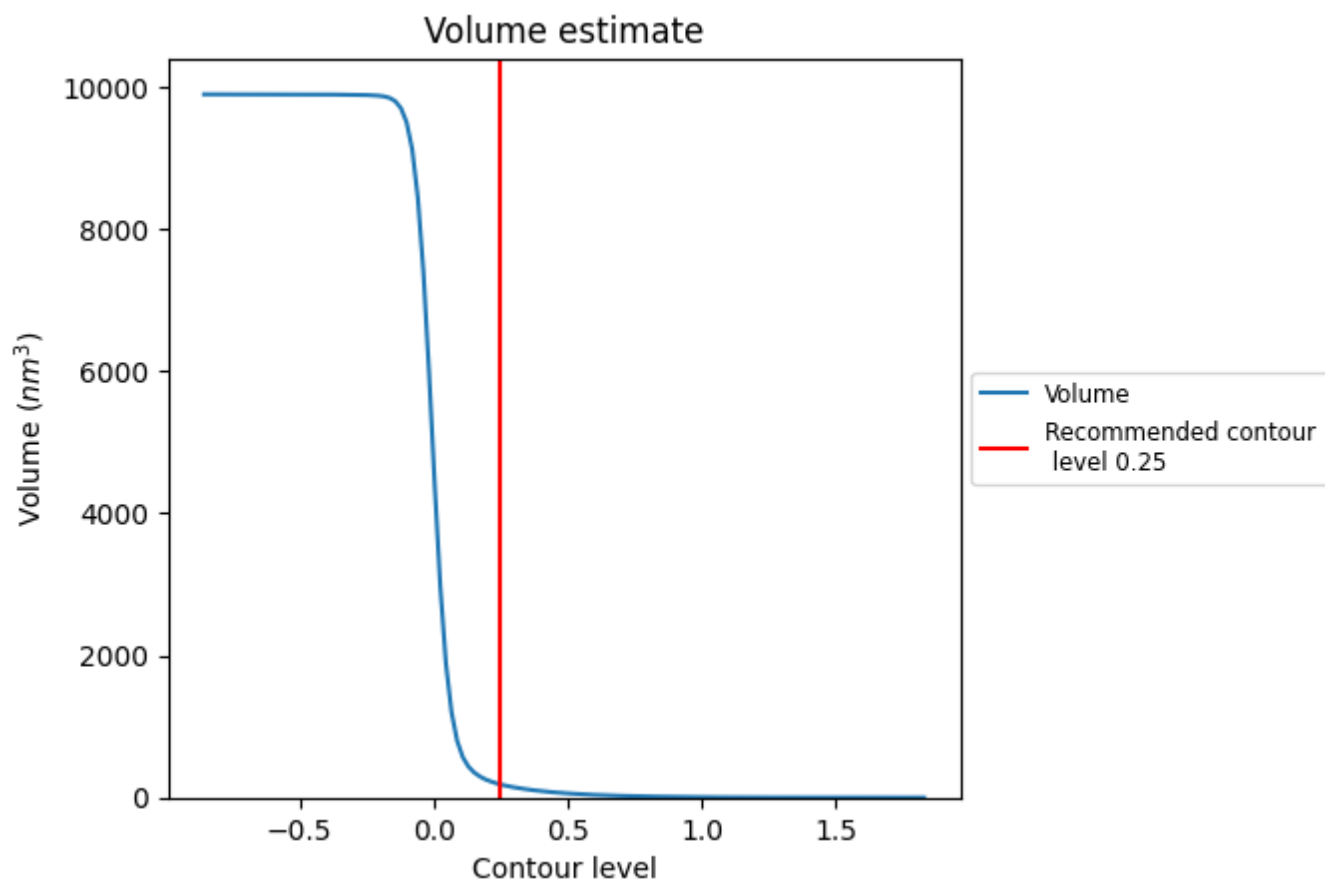
This section contains the results of statistical analysis of the map.

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.

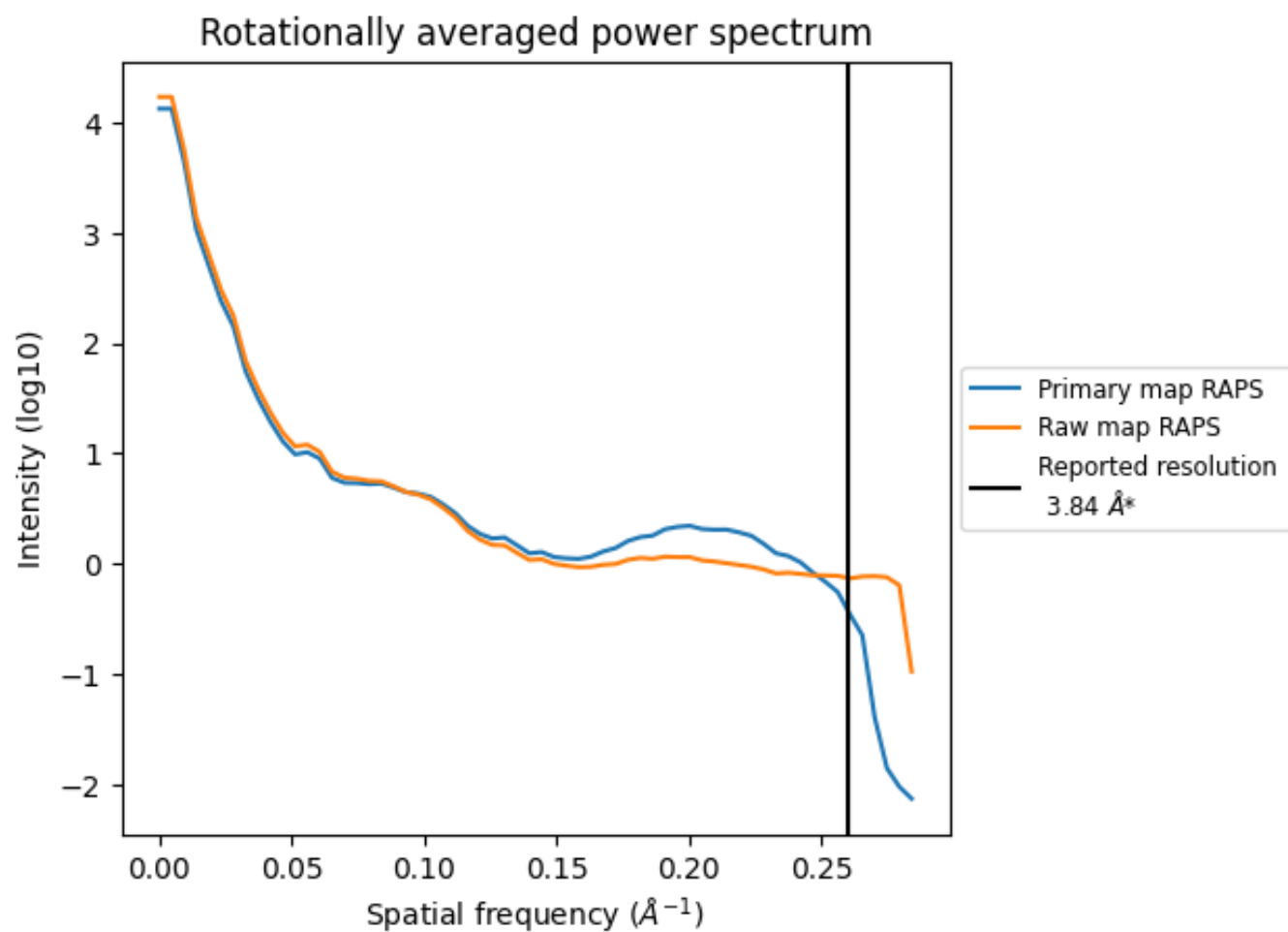
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

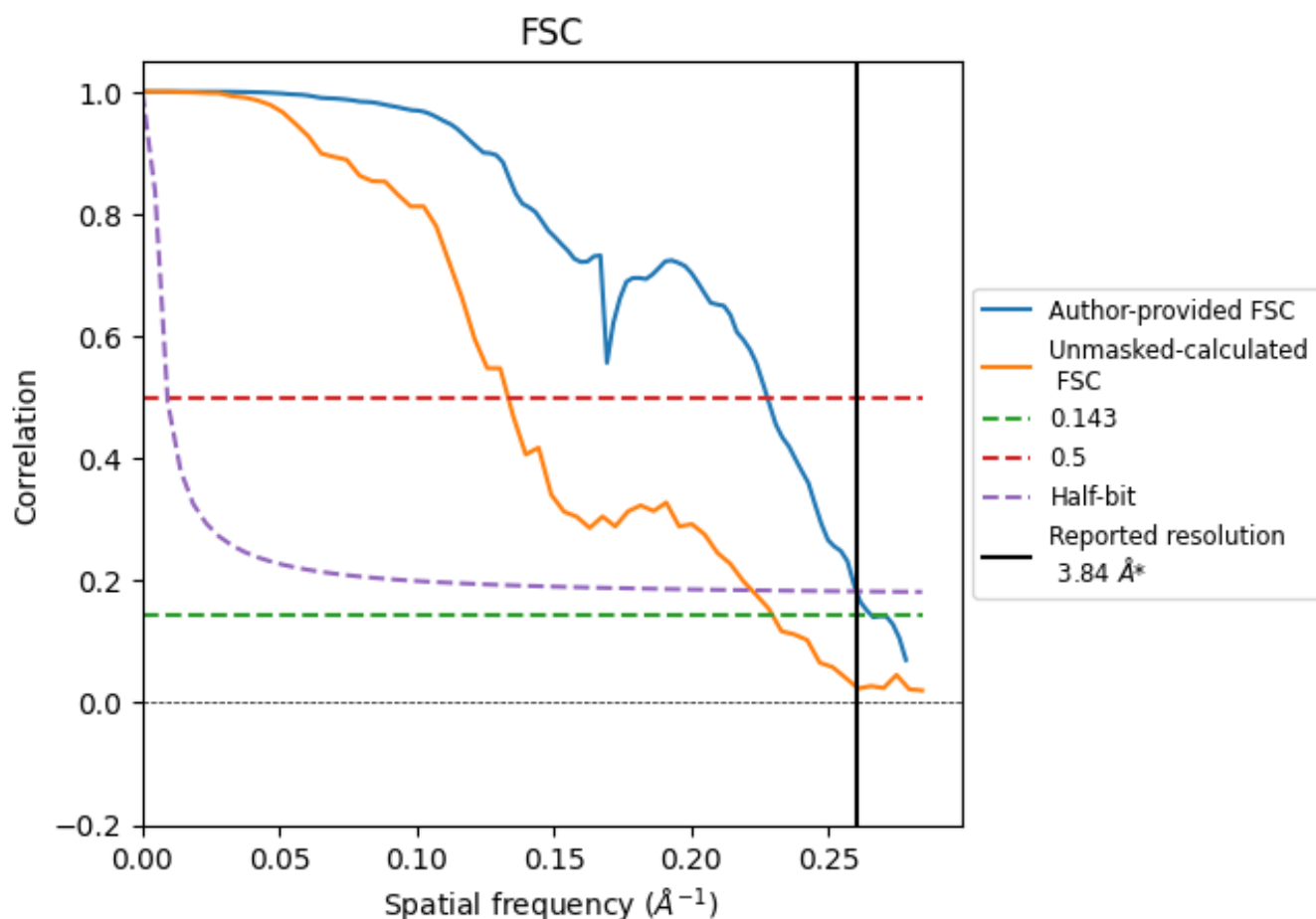


*Reported resolution corresponds to spatial frequency of 0.260 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.260 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.77	4.39	3.84
Unmasked-calculated*	4.36	7.51	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.36 differs from the reported value 3.84 by more than 10 %

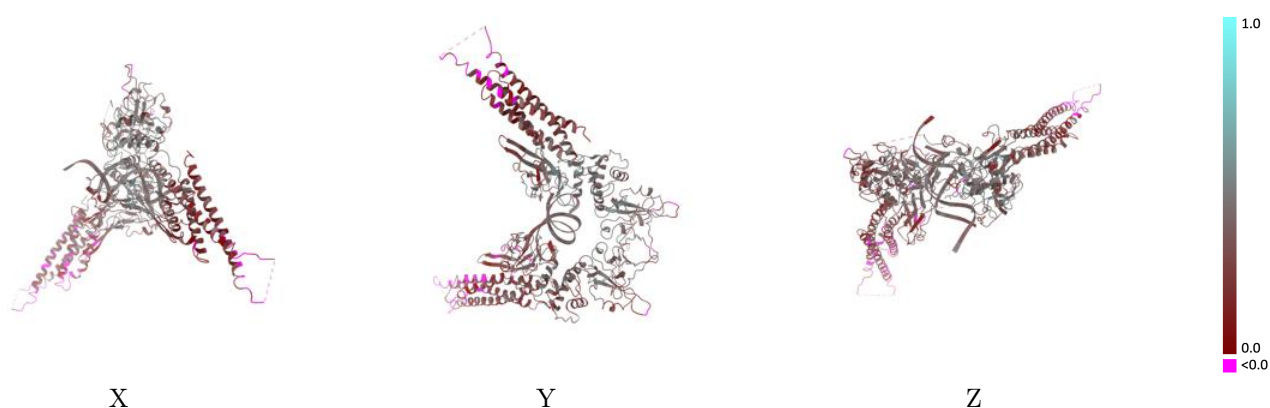
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-39679 and PDB model 8YYU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

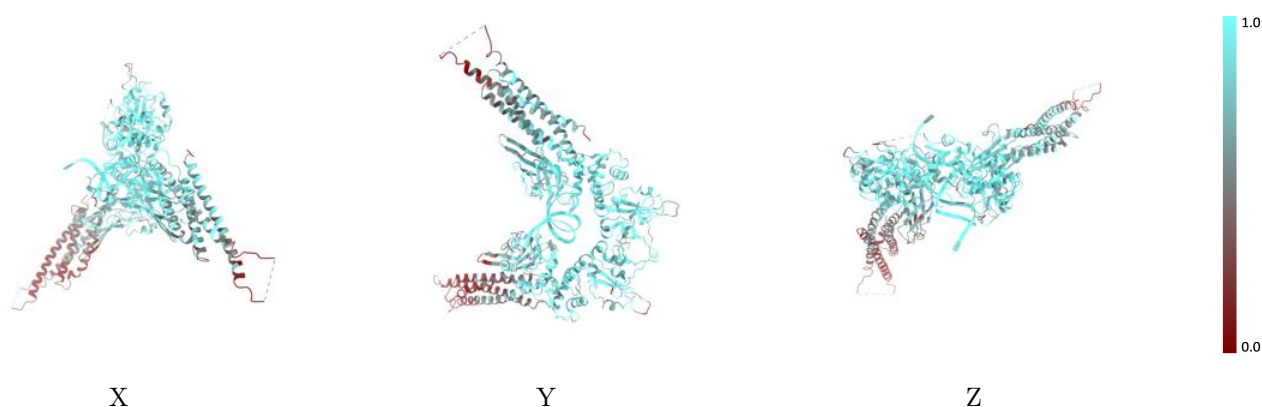
This section was not generated.

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



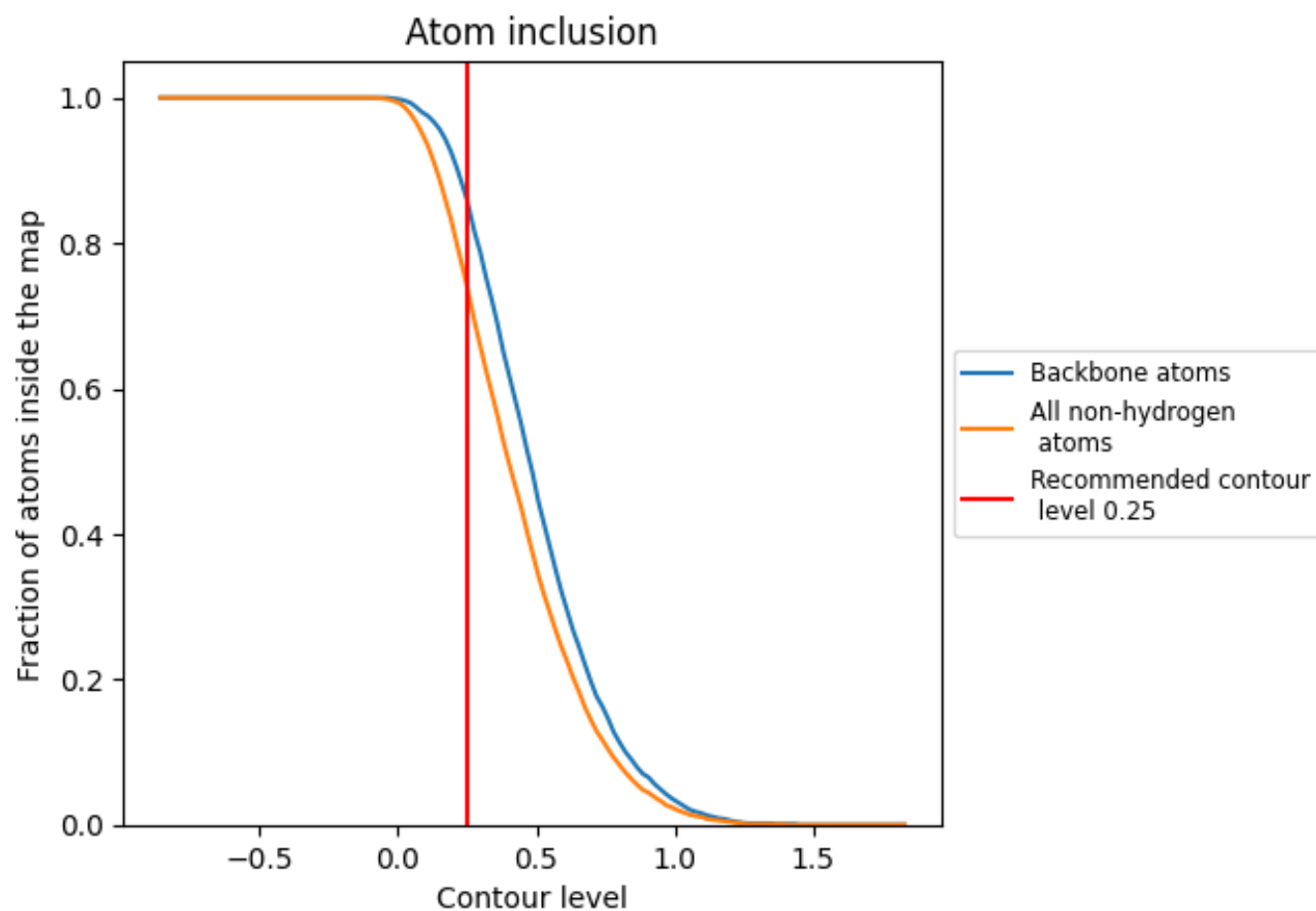
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.3170
A	0.6260	0.2670
B	0.9540	0.3670
C	0.9540	0.3900
D	0.7840	0.3470
E	0.9590	0.3650
F	0.9540	0.3840

1.0

0.0

<0.0