



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:46 AM UTC

PDB ID : 9F9T / pdb_00009f9t
EMDB ID : EMD-50260
Title : CryoEM structure of native Trypanosoma cruzi apo proteasome 20S subunit
Authors : Rowland, P.
Deposited on : 2024-05-08
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

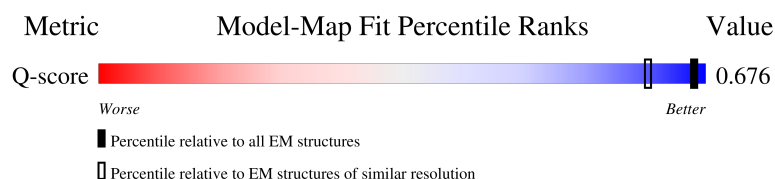
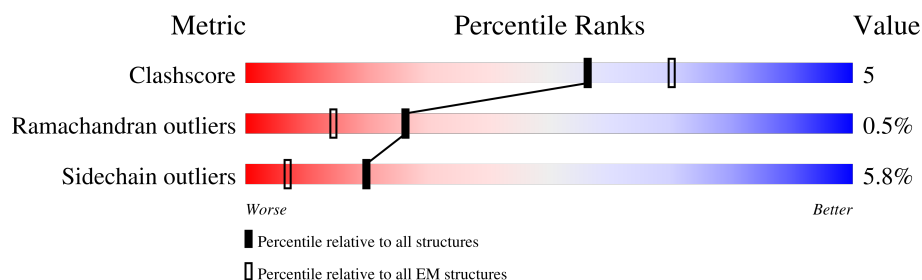
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.31 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	4306 (1.81 - 2.81)

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	250	
1	O	250	
2	B	288	
2	P	288	

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Mol	Chain	Length	Quality of chain
3	C	286	
3	Q	286	
4	D	247	
4	R	247	
5	E	245	
5	S	245	
6	F	265	
6	T	265	
7	G	237	
7	U	237	
8	H	284	
8	V	284	
9	I	292	
9	W	292	
10	J	205	
10	X	205	
11	K	206	
11	Y	206	
12	L	311	
12	Z	311	
13	M	246	
13	a	246	
14	N	218	
14	b	218	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 49724 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 Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1884	1190	328	353	13		
1	O	244	Total	C	N	O	S	0	0
			1884	1190	328	353	13		

- Molecule 2 is a protein called Proteasome 20S B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1737	1095	292	342	8		
2	P	228	Total	C	N	O	S	0	0
			1737	1095	292	342	8		

- Molecule 3 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	267	Total	C	N	O	S	0	0
			2098	1322	363	405	8		
3	Q	267	Total	C	N	O	S	0	0
			2098	1322	363	405	8		

- Molecule 4 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	234	Total	C	N	O	S	0	0
			1864	1173	329	355	7		
4	R	234	Total	C	N	O	S	0	0
			1864	1173	329	355	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	223	ARG	HIS	conflict	UNP A0A2V2WZ04

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Chain	Residue	Modelled	Actual	Comment	Reference
R	223	ARG	HIS	conflict	UNP A0A2V2WZ04

- Molecule 5 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	229	Total	C	N	O	S	0	0
			1778	1116	304	349	9		
5	S	229	Total	C	N	O	S	0	0
			1778	1116	304	349	9		

- Molecule 6 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	220	Total	C	N	O	S	0	0
			1716	1092	297	318	9		
6	T	220	Total	C	N	O	S	0	0
			1716	1092	297	318	9		

- Molecule 7 is a protein called Putative proteasome alpha 7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	227	Total	C	N	O	S	0	0
			1724	1078	297	336	13		
7	U	227	Total	C	N	O	S	0	0
			1724	1078	297	336	13		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	228	Total	C	N	O	S	0	0
			1723	1081	290	339	13		
8	V	228	Total	C	N	O	S	0	0
			1723	1081	290	339	13		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1663	1043	294	315	11		
9	W	219	Total	C	N	O	S	0	0
			1663	1043	294	315	11		

- Molecule 10 is a protein called Putative proteasome beta 3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1555	976	265	299	15		
10	X	204	Total	C	N	O	S	0	0
			1555	976	265	299	15		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1586	995	275	299	17		
11	Y	206	Total	C	N	O	S	0	0
			1586	995	275	299	17		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1569	989	273	298	9		
12	Z	200	Total	C	N	O	S	0	0
			1569	989	273	298	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	54	ILE	THR	conflict	UNP A0A2V2V5A7
Z	54	ILE	THR	conflict	UNP A0A2V2V5A7

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	209	Total	C	N	O	S	0	0
			1654	1047	280	315	12		
13	a	209	Total	C	N	O	S	0	0
			1654	1047	280	315	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	245	ASN	LYS	conflict	UNP A0A2V2VW62
a	245	ASN	LYS	conflict	UNP A0A2V2VW62

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1695	1075	290	313	17		
14	b	218	Total	C	N	O	S	0	0
			1695	1075	290	313	17		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	38	Total	O	0
			38	38	
15	B	37	Total	O	0
			37	37	
15	C	24	Total	O	0
			24	24	
15	D	17	Total	O	0
			17	17	
15	E	16	Total	O	0
			16	16	
15	F	37	Total	O	0
			37	37	
15	G	34	Total	O	0
			34	34	
15	H	67	Total	O	0
			67	67	
15	I	59	Total	O	0
			59	59	
15	J	47	Total	O	0
			47	47	
15	K	41	Total	O	0
			41	41	
15	L	37	Total	O	0
			37	37	
15	M	68	Total	O	0
			68	68	
15	N	93	Total	O	0
			93	93	
15	O	38	Total	O	0
			38	38	
15	P	37	Total	O	0
			37	37	
15	Q	23	Total	O	0
			23	23	

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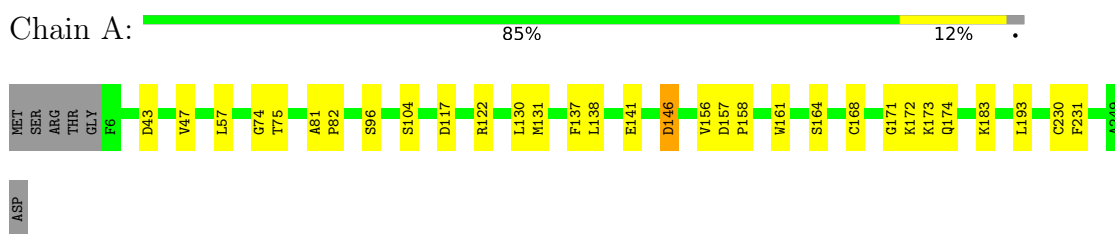
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Mol	Chain	Residues	Atoms		AltConf
15	R	16	Total 16	O 16	0
15	S	17	Total 17	O 17	0
15	T	37	Total 37	O 37	0
15	U	34	Total 34	O 34	0
15	V	67	Total 67	O 67	0
15	W	59	Total 59	O 59	0
15	X	48	Total 48	O 48	0
15	Y	42	Total 42	O 42	0
15	Z	38	Total 38	O 38	0
15	a	68	Total 68	O 68	0
15	b	93	Total 93	O 93	0

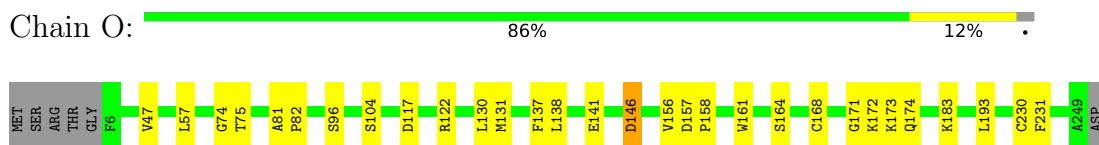
3 Residue-property plots

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.

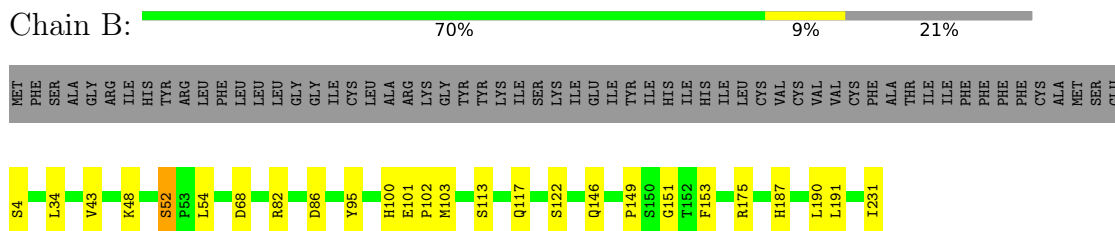
- Molecule 1: Proteasome subunit alpha type



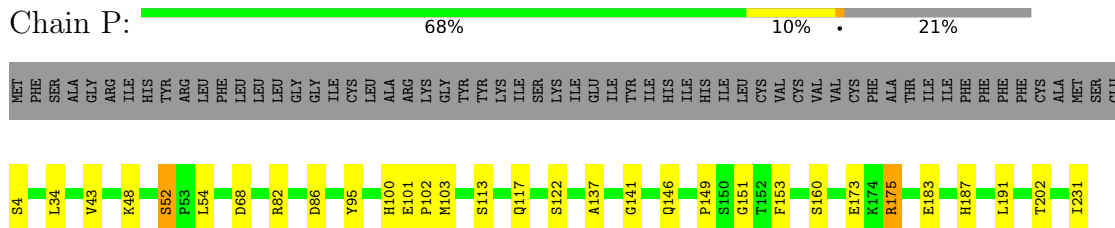
- Molecule 1: Proteasome subunit alpha type



- Molecule 2: Proteasome 20S B subunit

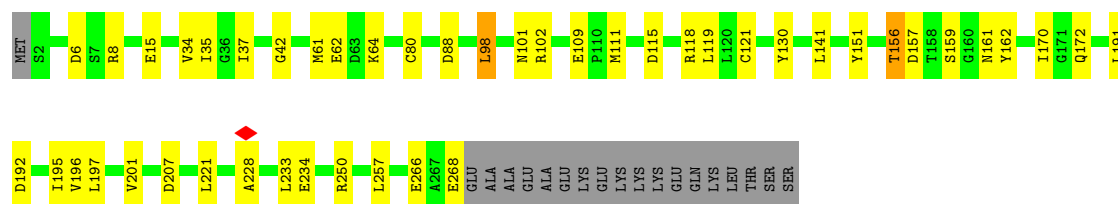


- Molecule 2: Proteasome 20S B subunit



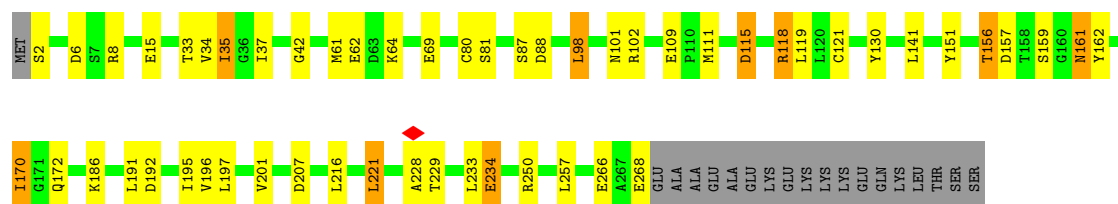
- Molecule 3: Proteasome subunit alpha type

Chain C:  77% 15% • 7%



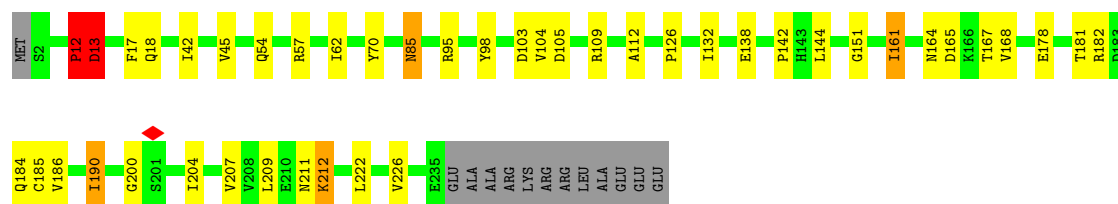
- Molecule 3: Proteasome subunit alpha type

Chain Q:  74% 16% • 7%



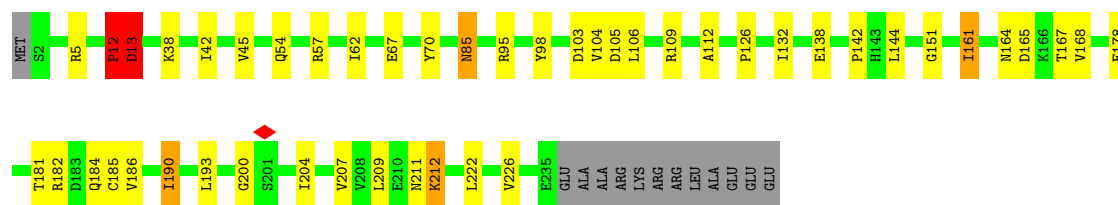
- Molecule 4: Proteasome subunit alpha type

Chain D:  77% 15% •• 5%



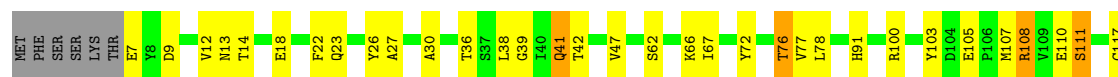
- Molecule 4: Proteasome subunit alpha type

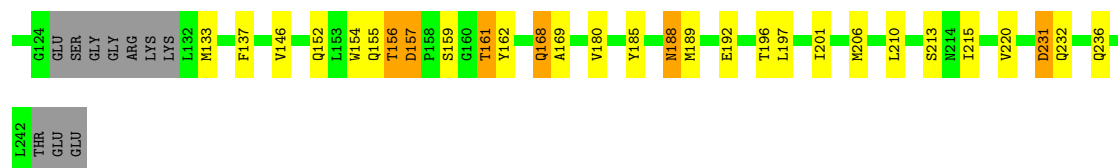
Chain R:  76% 17% •• 5%



- Molecule 5: Proteasome subunit alpha type

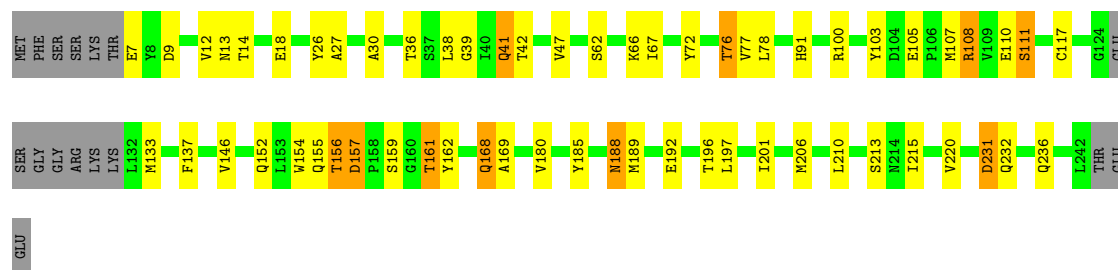
Chain E:  68% 21% • 7%





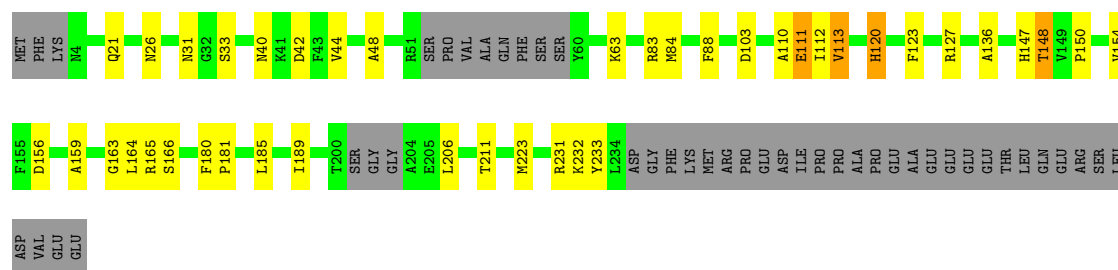
- Molecule 5: Proteasome subunit alpha type

Chain S: 69% 20% 7%



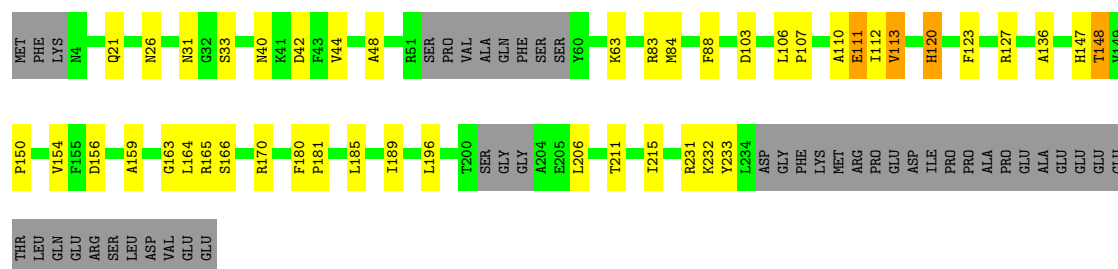
- Molecule 6: Proteasome subunit alpha type

Chain F: 68% 14% 17%



- Molecule 6: Proteasome subunit alpha type

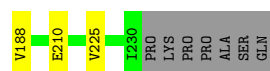
Chain T: 66% 15% 17%



- Molecule 7: Putative proteasome alpha 7 subunit

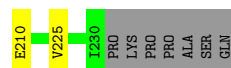
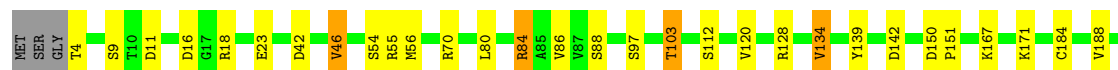
Chain G: 82% 12% 6%





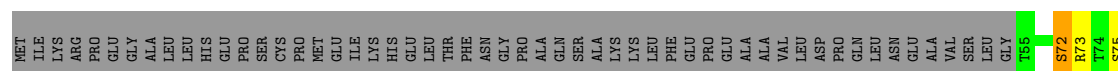
- Molecule 7: Putative proteasome alpha 7 subunit

Chain U: 82% 12% . .



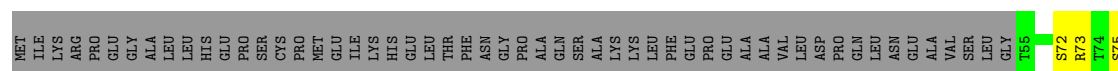
- Molecule 8: Proteasome subunit beta

Chain H: 68% 11% . 20%



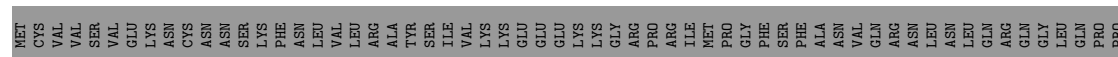
- Molecule 8: Proteasome subunit beta

Chain V: 68% 11% . 20%

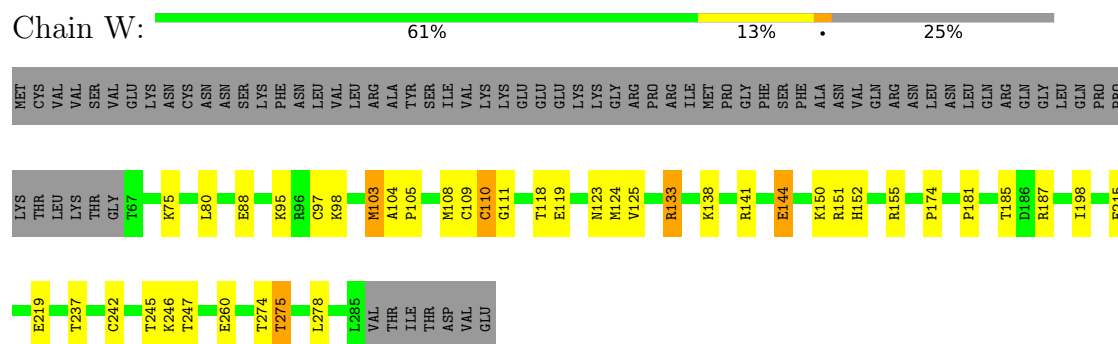


- Molecule 9: Proteasome subunit beta

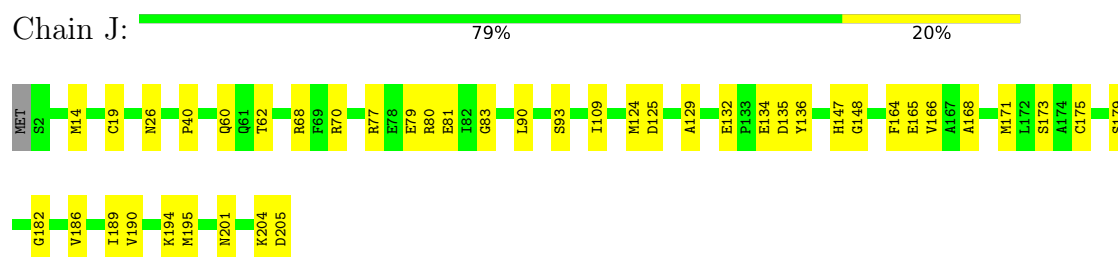
Chain I: 62% 12% . 25%



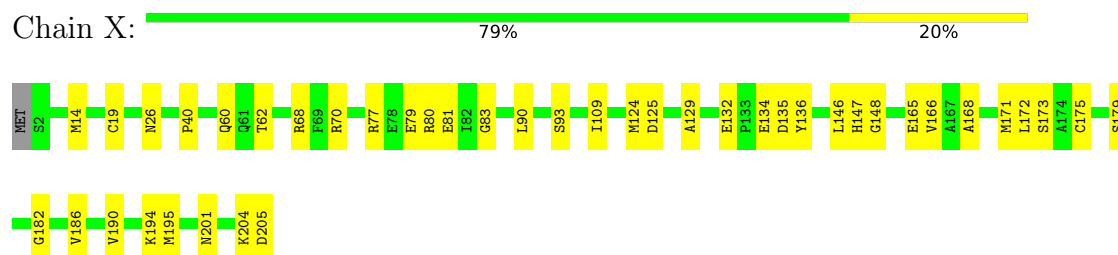
- Molecule 9: Proteasome subunit beta



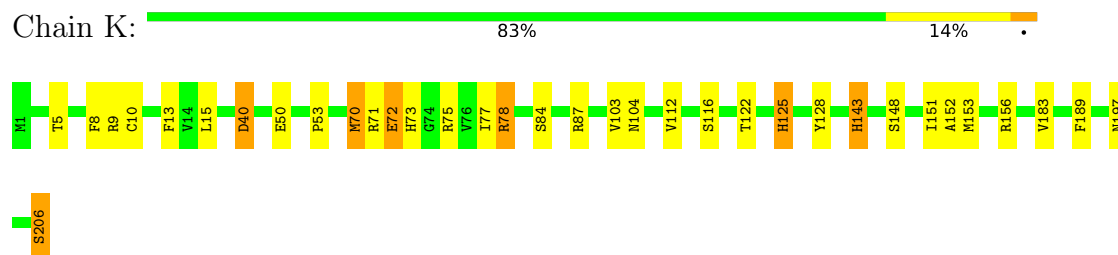
- Molecule 10: Putative proteasome beta 3 subunit



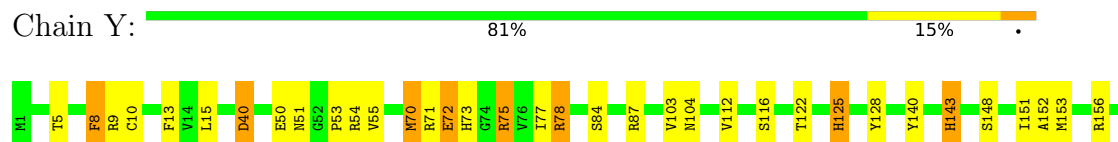
- Molecule 10: Putative proteasome beta 3 subunit



- Molecule 11: Proteasome subunit beta



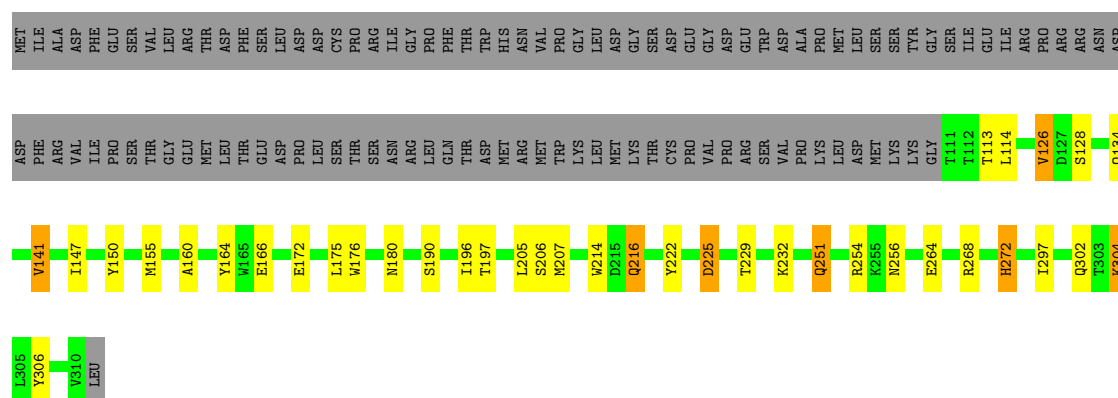
- Molecule 11: Proteasome subunit beta





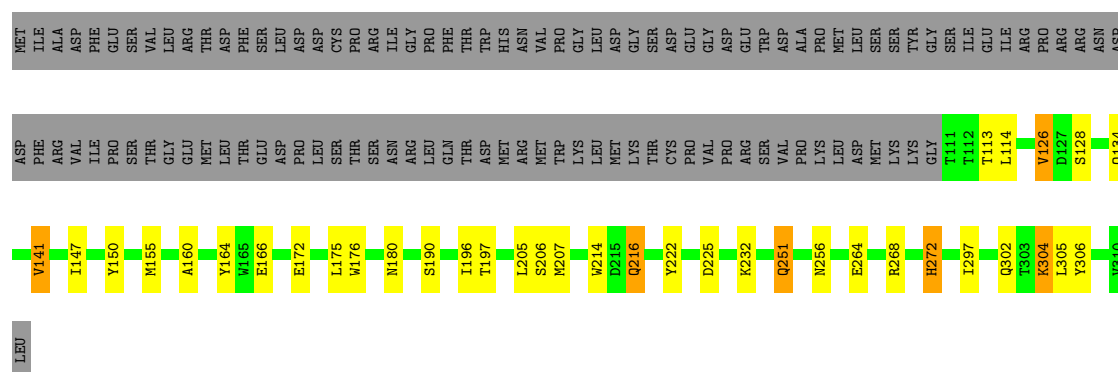
• Molecule 12: Proteasome subunit beta

Chain L: 52% 10% 36%



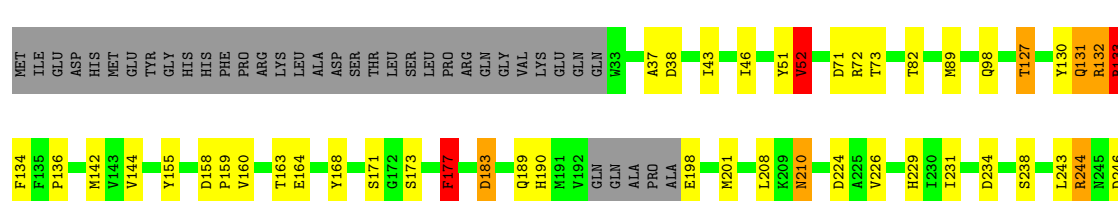
• Molecule 12: Proteasome subunit beta

Chain Z: 52% 10% 36%



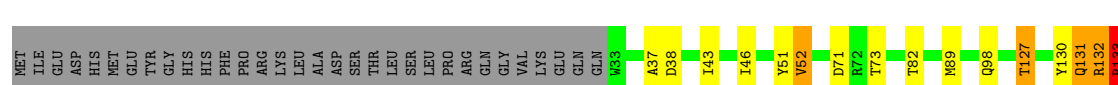
• Molecule 13: Proteasome subunit beta

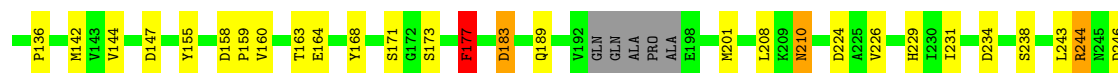
Chain M: 66% 15% 15%



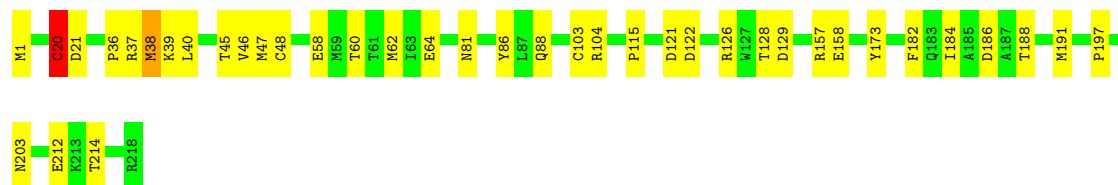
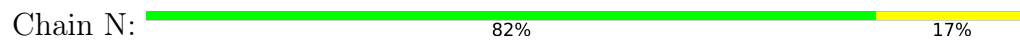
• Molecule 13: Proteasome subunit beta

Chain a: 67% 14% 15%

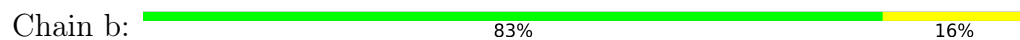




• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50663	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 ($e^-/\text{\AA}^2$)	1.43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.001	Depositor
Map size ($\text{\AA}$)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	0/1922	1.27	1/2605 (0.0%)
1	O	0.87	0/1922	1.27	1/2605 (0.0%)
2	B	0.85	1/1770 (0.1%)	1.30	4/2398 (0.2%)
2	P	0.85	1/1770 (0.1%)	1.30	4/2398 (0.2%)
3	C	0.73	0/2140	1.20	10/2901 (0.3%)
3	Q	0.73	0/2140	1.20	10/2901 (0.3%)
4	D	0.65	0/1894	1.22	8/2549 (0.3%)
4	R	0.65	0/1894	1.22	8/2549 (0.3%)
5	E	0.72	0/1805	1.29	8/2447 (0.3%)
5	S	0.72	0/1805	1.29	8/2447 (0.3%)
6	F	0.86	1/1751 (0.1%)	1.33	7/2367 (0.3%)
6	T	0.86	1/1751 (0.1%)	1.33	7/2367 (0.3%)
7	G	0.93	1/1755 (0.1%)	1.33	7/2379 (0.3%)
7	U	0.93	1/1755 (0.1%)	1.33	7/2379 (0.3%)
8	H	1.12	3/1757 (0.2%)	1.40	6/2380 (0.3%)
8	V	1.12	3/1757 (0.2%)	1.40	7/2380 (0.3%)
9	I	1.09	0/1690	1.40	7/2286 (0.3%)
9	W	1.09	0/1690	1.40	7/2286 (0.3%)
10	J	1.06	0/1580	1.47	10/2131 (0.5%)
10	X	1.06	0/1580	1.47	10/2131 (0.5%)
11	K	0.98	2/1612 (0.1%)	1.35	8/2177 (0.4%)
11	Y	0.98	2/1612 (0.1%)	1.35	8/2177 (0.4%)
12	L	1.05	1/1602 (0.1%)	1.36	10/2167 (0.5%)
12	Z	1.05	1/1602 (0.1%)	1.36	10/2167 (0.5%)
13	M	1.04	2/1689 (0.1%)	1.50	13/2280 (0.6%)
13	a	1.04	2/1689 (0.1%)	1.50	13/2280 (0.6%)
14	N	1.16	1/1733 (0.1%)	1.49	16/2344 (0.7%)
14	b	1.16	1/1733 (0.1%)	1.49	16/2344 (0.7%)
All	All	0.94	24/49400 (0.0%)	1.35	231/66822 (0.3%)

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
2	B	0	2
2	P	0	2
3	C	0	1
3	Q	0	1
4	D	0	1
4	R	0	1
5	E	0	1
5	S	0	1
6	F	0	1
6	T	0	2
7	G	0	2
7	U	0	2
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
11	K	0	2
11	Y	0	2
13	M	0	2
13	a	0	2
14	N	0	4
14	b	0	4
All	All	0	39

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	167	SER	CA-CB	-7.02	1.43	1.53
8	V	167	SER	CA-CB	-6.99	1.43	1.53
14	N	36	PRO	C-O	-6.52	1.18	1.24
14	b	36	PRO	C-O	-6.52	1.18	1.24
8	H	72	SER	CA-CB	-6.38	1.44	1.53
8	V	72	SER	CA-CB	-6.38	1.44	1.53
8	V	164	SER	CA-CB	-6.27	1.42	1.54
8	H	164	SER	CA-CB	-6.26	1.42	1.54
6	F	120	HIS	ND1-CE1	6.14	1.38	1.32
6	T	120	HIS	ND1-CE1	6.11	1.38	1.32
12	L	190	SER	CA-CB	-5.92	1.43	1.53
12	Z	190	SER	CA-CB	-5.92	1.43	1.53
13	M	98	GLN	C-O	-5.87	1.17	1.24
13	a	98	GLN	C-O	-5.86	1.17	1.24
13	M	52	VAL	C-O	-5.57	1.18	1.24
13	a	52	VAL	C-O	-5.57	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	148	SER	CA-CB	-5.28	1.45	1.53
11	Y	148	SER	CA-CB	-5.24	1.45	1.53
7	G	97	SER	CA-CB	-5.17	1.45	1.53
7	U	97	SER	CA-CB	-5.13	1.45	1.53
11	K	84	SER	CA-CB	-5.11	1.45	1.53
11	Y	84	SER	CA-CB	-5.06	1.45	1.53
2	B	86	ASP	CG-OD1	5.04	1.34	1.25
2	P	86	ASP	CG-OD1	5.03	1.34	1.25

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	177	PHE	CB-CA-C	-14.17	86.07	109.03
13	M	177	PHE	CB-CA-C	-14.16	86.09	109.03
10	X	136	TYR	N-CA-CB	-9.65	96.60	111.46
10	J	136	TYR	N-CA-CB	-9.63	96.64	111.46
13	a	127	THR	CA-CB-OG1	-9.27	95.69	109.60
13	M	127	THR	CA-CB-OG1	-9.24	95.74	109.60
7	G	142	ASP	CA-CB-CG	9.15	121.75	112.60
7	U	142	ASP	CA-CB-CG	9.13	121.73	112.60
11	Y	40	ASP	CA-CB-CG	9.03	121.63	112.60
11	K	40	ASP	CA-CB-CG	9.01	121.61	112.60
13	a	183	ASP	CA-CB-CG	8.47	121.07	112.60
13	M	183	ASP	CA-CB-CG	8.46	121.06	112.60
6	F	156	ASP	CA-CB-CG	8.46	121.06	112.60
6	T	156	ASP	CA-CB-CG	8.31	120.91	112.60
13	a	177	PHE	N-CA-CB	8.21	121.51	110.59
13	M	177	PHE	N-CA-CB	8.20	121.50	110.59
8	H	267	PRO	CB-CA-C	-7.88	100.66	110.98
13	M	177	PHE	CA-CB-CG	7.86	121.66	113.80
8	V	267	PRO	CB-CA-C	-7.85	100.70	110.98
14	b	103	CYS	CB-CA-C	-7.81	93.24	110.67
13	a	177	PHE	CA-CB-CG	7.80	121.60	113.80
14	N	103	CYS	CB-CA-C	-7.79	93.30	110.67
3	Q	156	THR	CA-CB-OG1	7.78	121.27	109.60
3	C	156	THR	CA-CB-OG1	7.76	121.25	109.60
5	S	91	HIS	CA-CB-CG	7.61	121.41	113.80
5	E	91	HIS	CA-CB-CG	7.57	121.37	113.80
10	J	60	GLN	CB-CA-C	-7.55	98.26	110.79
10	X	60	GLN	CB-CA-C	-7.54	98.28	110.79
6	T	147	HIS	CB-CA-C	7.34	122.22	110.19
6	F	147	HIS	CB-CA-C	7.33	122.22	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	134	VAL	N-CA-CB	-7.20	102.83	111.90
7	U	134	VAL	N-CA-CB	-7.20	102.83	111.90
3	C	115	ASP	CA-CB-CG	6.96	119.56	112.60
14	b	38	MET	CA-C-O	-6.95	112.93	120.92
3	C	234	GLU	CB-CA-C	-6.95	101.99	110.81
3	Q	234	GLU	CB-CA-C	-6.95	101.99	110.81
3	Q	115	ASP	CA-CB-CG	6.93	119.53	112.60
14	N	38	MET	CA-C-O	-6.92	112.96	120.92
4	D	98	TYR	CB-CA-C	-6.78	99.93	110.37
4	R	98	TYR	CB-CA-C	-6.78	99.93	110.37
2	B	68	ASP	CA-CB-CG	6.72	119.32	112.60
2	P	68	ASP	CA-CB-CG	6.70	119.30	112.60
5	S	105	GLU	CB-CG-CD	6.65	123.90	112.60
5	E	161	THR	N-CA-CB	6.63	119.72	109.97
5	S	161	THR	N-CA-CB	6.60	119.67	109.97
5	E	105	GLU	CB-CG-CD	6.58	123.79	112.60
4	D	165	ASP	CA-CB-CG	6.55	119.15	112.60
4	R	165	ASP	CA-CB-CG	6.53	119.13	112.60
14	N	86	TYR	N-CA-CB	-6.46	100.60	110.16
14	b	86	TYR	N-CA-CB	-6.43	100.65	110.16
9	I	144	GLU	CB-CG-CD	6.41	123.50	112.60
9	I	133	ARG	CB-CA-C	-6.40	99.97	110.85
9	W	133	ARG	CB-CA-C	-6.39	99.98	110.85
13	a	82	THR	CA-CB-OG1	6.37	119.15	109.60
13	a	246	ASP	CA-CB-CG	6.37	118.97	112.60
13	M	246	ASP	CA-CB-CG	6.36	118.96	112.60
13	M	82	THR	CA-CB-OG1	6.35	119.13	109.60
9	I	181	PRO	CB-CA-C	-6.34	102.85	112.11
9	W	181	PRO	CB-CA-C	-6.34	102.85	112.11
7	G	210	GLU	CB-CA-C	6.31	120.73	109.38
12	L	272	HIS	CA-CB-CG	-6.30	107.50	113.80
10	J	205	ASP	CA-CB-CG	6.29	118.89	112.60
9	W	144	GLU	CB-CG-CD	6.29	123.29	112.60
10	X	205	ASP	CA-CB-CG	6.29	118.89	112.60
7	U	210	GLU	CB-CA-C	6.27	120.67	109.38
12	Z	272	HIS	CA-CB-CG	-6.27	107.53	113.80
11	K	78	ARG	CB-CA-C	-6.25	98.03	109.54
11	Y	78	ARG	CB-CA-C	-6.23	98.07	109.54
14	b	203	ASN	CB-CA-C	-6.21	98.34	109.71
6	F	123	PHE	CA-CB-CG	6.19	119.99	113.80
14	N	203	ASN	CB-CA-C	-6.19	98.39	109.71
6	T	123	PHE	CA-CB-CG	6.18	119.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	100	ARG	CB-CA-C	-6.16	100.57	110.79
5	E	100	ARG	CB-CA-C	-6.15	100.59	110.79
3	Q	109	GLU	CB-CG-CD	6.13	123.03	112.60
3	Q	101	ASN	CA-CB-CG	-6.10	106.50	112.60
3	C	101	ASN	CA-CB-CG	-6.09	106.51	112.60
3	C	109	GLU	CB-CG-CD	6.07	122.91	112.60
6	F	150	PRO	N-CA-C	6.06	121.72	113.84
12	L	172	GLU	O-C-N	-6.06	115.25	122.15
12	Z	172	GLU	O-C-N	-6.06	115.24	122.15
6	T	150	PRO	N-CA-C	6.04	121.69	113.84
14	N	20	CYS	N-CA-C	6.02	117.05	108.74
14	b	20	CYS	N-CA-C	6.02	117.05	108.74
12	L	164	TYR	N-CA-CB	-6.00	101.36	110.07
8	V	98	CYS	CB-CA-C	-6.00	100.34	110.19
5	E	72	TYR	CB-CA-C	-6.00	98.82	110.46
4	D	126	PRO	CB-CA-C	-6.00	103.55	111.23
4	R	126	PRO	CB-CA-C	-6.00	103.55	111.23
8	H	98	CYS	CB-CA-C	-5.99	100.36	110.19
14	b	188	THR	CA-CB-OG1	5.99	118.59	109.60
5	S	72	TYR	CB-CA-C	-5.98	98.85	110.46
14	N	188	THR	CA-CB-OG1	5.98	118.57	109.60
6	T	148	THR	CA-CB-OG1	5.98	118.57	109.60
10	J	77	ARG	CB-CA-C	-5.96	101.27	110.81
12	Z	164	TYR	N-CA-CB	-5.96	101.33	110.16
6	F	148	THR	CA-CB-OG1	5.95	118.53	109.60
10	X	77	ARG	CB-CA-C	-5.94	101.30	110.81
4	D	142	PRO	N-CA-C	5.93	120.81	111.38
8	V	135	ASN	CB-CA-C	-5.92	100.97	110.79
11	Y	143	HIS	CA-CB-CG	5.91	119.71	113.80
8	H	135	ASN	CB-CA-C	-5.91	100.98	110.79
14	N	214	THR	CA-CB-OG1	-5.90	100.75	109.60
4	R	142	PRO	N-CA-C	5.90	120.76	111.38
13	M	38	ASP	CA-CB-CG	5.90	118.50	112.60
2	B	48	LYS	CB-CA-C	-5.89	103.67	112.09
11	K	143	HIS	CA-CB-CG	5.89	119.69	113.80
2	P	48	LYS	CB-CA-C	-5.88	103.68	112.09
14	b	214	THR	CA-CB-OG1	-5.88	100.78	109.60
8	H	266	PRO	N-CA-CB	-5.86	100.17	103.22
10	J	81	GLU	CB-CG-CD	5.85	122.54	112.60
13	a	38	ASP	CA-CB-CG	5.83	118.43	112.60
14	b	36	PRO	N-CA-CB	-5.83	99.66	102.92
14	N	36	PRO	N-CA-CB	-5.82	99.66	102.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	81	GLU	CB-CG-CD	5.81	122.47	112.60
4	R	98	TYR	N-CA-CB	5.80	121.79	110.88
8	V	266	PRO	N-CA-CB	-5.79	100.21	103.22
4	D	98	TYR	N-CA-CB	5.78	121.75	110.88
7	U	103	THR	CA-CB-OG1	5.73	118.19	109.60
7	G	103	THR	CA-CB-OG1	5.72	118.18	109.60
6	T	103	ASP	CA-CB-CG	5.72	118.32	112.60
6	F	103	ASP	CA-CB-CG	5.72	118.32	112.60
10	J	83	GLY	CA-C-N	5.72	126.43	120.03
10	J	83	GLY	C-N-CA	5.72	126.43	120.03
12	Z	147	ILE	N-CA-C	-5.68	105.19	110.53
5	E	103	TYR	CB-CA-C	-5.66	100.94	110.44
12	Z	150	TYR	N-CA-CB	-5.66	102.07	111.06
14	N	122	ASP	CA-C-N	-5.65	114.25	122.28
14	N	122	ASP	C-N-CA	-5.65	114.25	122.28
10	X	83	GLY	CA-C-N	5.65	126.36	120.03
10	X	83	GLY	C-N-CA	5.65	126.36	120.03
14	b	122	ASP	CA-C-N	-5.64	114.26	122.28
14	b	122	ASP	C-N-CA	-5.64	114.26	122.28
12	L	147	ILE	N-CA-C	-5.64	105.23	110.53
12	L	150	TYR	N-CA-CB	-5.63	102.10	111.06
5	S	103	TYR	CB-CA-C	-5.63	100.98	110.44
7	G	46	VAL	CB-CA-C	-5.61	102.19	110.82
7	U	46	VAL	CB-CA-C	-5.61	102.19	110.82
10	X	135	ASP	CA-CB-CG	5.59	118.19	112.60
10	J	135	ASP	CA-CB-CG	5.58	118.18	112.60
5	E	161	THR	CA-CB-OG1	-5.58	101.24	109.60
12	Z	197	THR	CA-CB-OG1	5.55	117.93	109.60
9	I	275	THR	CB-CA-C	5.55	116.18	109.85
12	L	197	THR	CA-CB-OG1	5.55	117.92	109.60
9	W	275	THR	CB-CA-C	5.53	116.15	109.85
4	R	12	PRO	N-CA-C	5.46	123.72	112.47
3	C	98	LEU	N-CA-CB	-5.46	102.08	110.16
14	N	186	ASP	CA-CB-CG	5.45	118.05	112.60
5	S	161	THR	CA-CB-OG1	-5.45	101.42	109.60
14	b	186	ASP	CA-CB-CG	5.44	118.04	112.60
4	D	12	PRO	N-CA-C	5.44	123.68	112.47
7	U	80	LEU	O-C-N	-5.43	115.65	120.48
9	I	198	ILE	N-CA-C	5.42	115.62	110.42
12	L	264	GLU	CB-CG-CD	5.42	121.81	112.60
3	Q	98	LEU	N-CA-CB	-5.42	102.15	110.16
12	Z	264	GLU	CB-CG-CD	5.41	121.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	198	ILE	N-CA-C	5.40	115.60	110.42
1	O	117	ASP	CB-CA-C	-5.39	101.83	110.79
12	L	166	GLU	CB-CG-CD	5.38	121.74	112.60
6	F	150	PRO	CB-CA-C	-5.37	104.23	111.85
7	G	80	LEU	O-C-N	-5.37	115.71	120.48
6	T	150	PRO	CB-CA-C	-5.37	104.23	111.85
12	Z	166	GLU	CB-CG-CD	5.36	121.72	112.60
1	A	117	ASP	CB-CA-C	-5.36	101.89	110.79
14	b	64	GLU	N-CA-CB	5.36	117.99	110.12
14	N	64	GLU	N-CA-CB	5.34	117.97	110.12
11	K	73	HIS	CA-CB-CG	-5.33	108.47	113.80
8	H	209	PHE	CB-CA-C	5.33	119.24	110.88
8	V	209	PHE	CB-CA-C	5.33	119.24	110.88
14	N	173	TYR	N-CA-CB	5.30	118.47	110.30
13	M	131	GLN	CB-CA-C	-5.30	98.31	110.18
14	b	81	ASN	CA-CB-CG	-5.29	107.31	112.60
14	b	173	TYR	N-CA-CB	5.28	118.44	110.30
11	K	128	TYR	N-CA-CB	-5.28	102.09	110.06
11	Y	128	TYR	N-CA-CB	-5.28	102.09	110.06
3	C	161	ASN	CB-CA-C	-5.26	100.61	109.50
13	a	131	GLN	CB-CA-C	-5.26	98.39	110.18
3	Q	161	ASN	CB-CA-C	-5.25	100.62	109.50
9	I	123	ASN	CA-CB-CG	-5.25	107.35	112.60
13	M	155	TYR	N-CA-CB	-5.25	101.76	110.47
9	W	123	ASN	CA-CB-CG	-5.25	107.35	112.60
11	Y	73	HIS	CA-CB-CG	-5.25	108.56	113.80
3	C	6	ASP	CA-CB-CG	5.24	117.84	112.60
10	J	182	GLY	CA-C-O	-5.23	116.34	121.05
3	Q	6	ASP	CA-CB-CG	5.23	117.83	112.60
14	N	81	ASN	CA-CB-CG	-5.22	107.38	112.60
13	a	155	TYR	N-CA-CB	-5.21	101.82	110.47
12	L	196	ILE	N-CA-C	-5.20	105.78	110.82
12	Z	196	ILE	N-CA-C	-5.19	105.78	110.82
13	M	210	ASN	CA-CB-CG	-5.18	107.42	112.60
13	a	136	PRO	N-CA-C	5.17	120.32	111.68
2	B	149	PRO	CB-CA-C	-5.17	103.63	112.26
9	I	174	PRO	CB-CA-C	-5.16	104.63	111.23
13	M	136	PRO	N-CA-C	5.16	120.30	111.68
10	X	182	GLY	CA-C-O	-5.16	116.41	121.05
11	Y	125	HIS	CA-CB-CG	-5.16	108.64	113.80
11	K	125	HIS	CA-CB-CG	-5.16	108.64	113.80
3	C	80	CYS	N-CA-C	5.15	116.12	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	149	PRO	CB-CA-C	-5.15	103.66	112.26
7	U	97	SER	CA-C-O	-5.15	115.09	120.55
3	Q	109	GLU	O-C-N	-5.15	118.25	121.85
13	a	210	ASN	CA-CB-CG	-5.15	107.45	112.60
7	G	97	SER	CA-C-O	-5.14	115.10	120.55
3	Q	80	CYS	N-CA-C	5.14	116.10	108.60
9	W	174	PRO	CB-CA-C	-5.13	104.66	111.23
11	K	8	PHE	CA-CB-CG	5.13	118.93	113.80
14	N	115	PRO	N-CA-C	5.12	118.53	110.80
8	V	89	THR	CB-CA-C	5.12	118.60	109.38
12	L	126	VAL	N-CA-CB	-5.11	106.44	112.32
11	Y	8	PHE	CA-CB-CG	5.09	118.89	113.80
12	Z	126	VAL	N-CA-CB	-5.09	106.47	112.32
14	b	115	PRO	N-CA-C	5.09	118.48	110.80
2	B	100	HIS	CB-CA-C	-5.09	104.51	111.73
8	H	89	THR	CB-CA-C	5.09	118.53	109.38
2	P	100	HIS	CB-CA-C	-5.09	104.51	111.73
3	C	109	GLU	O-C-N	-5.07	118.30	121.85
11	Y	5	THR	CA-CB-OG1	-5.07	102.00	109.60
11	K	5	THR	CA-CB-OG1	-5.07	102.00	109.60
4	D	85	ASN	CB-CA-C	-5.06	102.88	110.92
4	R	13	ASP	CA-CB-CG	5.06	117.66	112.60
14	b	48	CYS	N-CA-CB	-5.05	103.22	111.66
4	R	85	ASN	CB-CA-C	-5.05	102.89	110.92
14	N	48	CYS	N-CA-CB	-5.04	103.25	111.66
5	E	231	ASP	CA-CB-CG	5.03	117.63	112.60
5	S	231	ASP	CA-CB-CG	5.03	117.62	112.60
10	X	26	ASN	CB-CA-C	-5.02	101.11	109.75
8	V	218	TYR	N-CA-CB	5.02	118.72	110.39
13	a	147	ASP	CA-CB-CG	5.02	117.62	112.60
4	D	13	ASP	CA-CB-CG	5.01	117.61	112.60
10	J	26	ASN	CB-CA-C	-5.01	101.14	109.75
13	M	72	ARG	CB-CA-C	-5.00	103.38	111.28

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	175	ARG	Sidechain
2	B	82	ARG	Sidechain
3	C	130	TYR	Peptide
4	D	95	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	E	108	ARG	Sidechain
6	F	83	ARG	Sidechain
7	G	128	ARG	Sidechain
7	G	70	ARG	Sidechain
9	I	187	ARG	Sidechain
10	J	68	ARG	Sidechain
10	J	70	ARG	Sidechain
11	K	156	ARG	Sidechain
11	K	78	ARG	Sidechain
13	M	132	ARG	Sidechain
13	M	244	ARG	Sidechain
14	N	1	MET	Peptide
14	N	104	ARG	Sidechain
14	N	157	ARG	Sidechain
14	N	20	CYS	Mainchain
2	P	175	ARG	Sidechain
2	P	82	ARG	Sidechain
3	Q	130	TYR	Peptide
4	R	95	ARG	Sidechain
5	S	108	ARG	Sidechain
6	T	170	ARG	Sidechain
6	T	83	ARG	Sidechain
7	U	128	ARG	Sidechain
7	U	70	ARG	Sidechain
9	W	187	ARG	Sidechain
10	X	68	ARG	Sidechain
10	X	70	ARG	Sidechain
11	Y	156	ARG	Sidechain
11	Y	78	ARG	Sidechain
13	a	132	ARG	Sidechain
13	a	244	ARG	Sidechain
14	b	1	MET	Peptide
14	b	104	ARG	Sidechain
14	b	157	ARG	Sidechain
14	b	20	CYS	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	1884	0	1874	16	0
1	O	1884	0	1874	15	0
2	B	1737	0	1716	11	0
2	P	1737	0	1716	12	0
3	C	2098	0	2068	22	0
3	Q	2098	0	2068	23	0
4	D	1864	0	1861	20	0
4	R	1864	0	1861	21	0
5	E	1778	0	1770	27	0
5	S	1778	0	1770	26	0
6	F	1716	0	1698	17	0
6	T	1716	0	1698	20	0
7	G	1724	0	1691	14	0
7	U	1724	0	1691	12	0
8	H	1723	0	1694	14	0
8	V	1723	0	1694	14	0
9	I	1663	0	1698	16	0
9	W	1663	0	1698	18	0
10	J	1555	0	1549	18	0
10	X	1555	0	1549	20	0
11	K	1586	0	1573	15	0
11	Y	1586	0	1573	20	0
12	L	1569	0	1515	20	0
12	Z	1569	0	1515	19	0
13	M	1654	0	1603	24	0
13	a	1654	0	1603	23	0
14	N	1695	0	1654	17	0
14	b	1695	0	1654	17	0
15	A	38	0	0	1	0
15	B	37	0	0	1	0
15	C	24	0	0	0	0
15	D	17	0	0	1	0
15	E	16	0	0	0	0
15	F	37	0	0	1	0
15	G	34	0	0	2	0
15	H	67	0	0	2	0
15	I	59	0	0	0	0
15	J	47	0	0	1	0
15	K	41	0	0	1	0
15	L	37	0	0	1	0
15	M	68	0	0	3	0
15	N	93	0	0	1	0
15	O	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	37	0	0	1	0
15	Q	23	0	0	0	0
15	R	16	0	0	1	0
15	S	17	0	0	0	0
15	T	37	0	0	1	0
15	U	34	0	0	2	0
15	V	67	0	0	3	0
15	W	59	0	0	0	0
15	X	48	0	0	1	0
15	Y	42	0	0	1	0
15	Z	38	0	0	1	0
15	a	68	0	0	3	0
15	b	93	0	0	1	0
All	All	49724	0	47928	470	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 5.

All (470) 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)
13:a:210:ASN:HB2	15:a:303:HOH:O	1.60	0.99
13:M:210:ASN:HB2	15:M:303:HOH:O	1.61	0.97
3:C:121:CYS:SG	3:C:156:THR:HG23	2.15	0.87
3:Q:121:CYS:SG	3:Q:156:THR:HG23	2.15	0.86
14:N:47:MET:HE2	14:N:60:THR:HG22	1.61	0.83
14:b:47:MET:HE2	14:b:60:THR:HG22	1.61	0.82
9:I:103:MET:HE1	9:I:125:VAL:HG12	1.62	0.81
9:W:103:MET:HE1	9:W:125:VAL:HG12	1.62	0.80
9:I:150:LYS:HE2	9:I:185:THR:HG23	1.67	0.76
13:a:43:ILE:HG13	13:a:142:MET:CE	2.17	0.75
9:W:150:LYS:HE2	9:W:185:THR:HG23	1.67	0.74
13:M:43:ILE:HG13	13:M:142:MET:CE	2.17	0.73
13:M:226:VAL:CG2	13:M:243:LEU:HD11	2.21	0.71
12:L:114:LEU:HD12	12:L:114:LEU:C	2.16	0.70
13:a:210:ASN:CB	15:a:303:HOH:O	2.30	0.70
8:H:73:ARG:HB2	15:H:305:HOH:O	1.92	0.70
13:a:226:VAL:CG2	13:a:243:LEU:HD11	2.21	0.69
12:Z:114:LEU:HD12	12:Z:114:LEU:C	2.16	0.69
8:V:73:ARG:HB2	15:V:305:HOH:O	1.92	0.68
11:K:50:GLU:HA	11:K:50:GLU:OE1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:197:LEU:O	3:Q:201:VAL:HG23	1.93	0.68
3:C:197:LEU:O	3:C:201:VAL:HG23	1.93	0.68
8:V:117:LEU:HD22	8:V:128:VAL:HG21	1.75	0.67
14:N:88:GLN:HG3	14:N:126:ARG:HG2	1.77	0.67
8:H:117:LEU:HD22	8:H:128:VAL:HG21	1.75	0.67
14:b:88:GLN:HG3	14:b:126:ARG:HG2	1.77	0.66
11:Y:50:GLU:OE1	11:Y:50:GLU:HA	1.94	0.66
1:O:122:ARG:NH1	1:O:131:MET:HE3	2.11	0.66
12:Z:268:ARG:HE	12:Z:272:HIS:HE1	1.44	0.66
1:A:122:ARG:NH1	1:A:131:MET:HE3	2.11	0.66
12:L:268:ARG:HE	12:L:272:HIS:HE1	1.44	0.66
13:a:226:VAL:HG22	13:a:243:LEU:HD11	1.78	0.66
13:M:226:VAL:HG22	13:M:243:LEU:HD11	1.78	0.65
8:H:258:TYR:OH	8:V:194:ASP:OD1	2.14	0.64
4:R:12:PRO:O	4:R:13:ASP:CG	2.41	0.63
4:D:12:PRO:O	4:D:13:ASP:CG	2.41	0.63
12:Z:113:THR:HG22	12:Z:126:VAL:HG12	1.80	0.63
3:C:121:CYS:SG	3:C:156:THR:CG2	2.87	0.62
3:Q:121:CYS:SG	3:Q:156:THR:CG2	2.87	0.62
12:L:113:THR:HG22	12:L:126:VAL:HG12	1.80	0.62
5:S:213:SER:HA	5:S:232:GLN:HE21	1.65	0.62
5:E:213:SER:HA	5:E:232:GLN:HE21	1.65	0.62
2:B:4:SER:HB3	15:B:334:HOH:O	2.00	0.62
4:R:62:ILE:HG21	4:R:207:VAL:HG21	1.82	0.62
5:S:206:MET:HE1	5:S:215:ILE:CG2	2.30	0.62
14:N:47:MET:HE2	14:N:60:THR:CG2	2.31	0.61
1:O:230:CYS:HB3	15:O:327:HOH:O	2.00	0.61
12:Z:114:LEU:HD12	12:Z:114:LEU:O	2.01	0.61
11:Y:9:ARG:HG2	11:Y:9:ARG:HH21	1.65	0.61
11:K:9:ARG:HG2	11:K:9:ARG:HH21	1.65	0.61
8:H:194:ASP:OD1	8:V:258:TYR:OH	2.13	0.61
5:E:206:MET:HE1	5:E:215:ILE:CG2	2.31	0.60
2:P:4:SER:HB3	15:P:333:HOH:O	1.99	0.60
14:b:47:MET:HE2	14:b:60:THR:CG2	2.31	0.60
14:N:20:CYS:SG	14:N:38:MET:HE3	2.42	0.60
7:G:86:VAL:HG11	7:G:134:VAL:HG21	1.83	0.60
4:D:62:ILE:HG21	4:D:207:VAL:HG21	1.82	0.60
12:L:114:LEU:HD12	12:L:114:LEU:O	2.01	0.60
13:M:210:ASN:CB	15:M:303:HOH:O	2.30	0.60
9:W:150:LYS:HE2	9:W:185:THR:CG2	2.32	0.60
1:A:230:CYS:HB3	15:A:330:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:130:TYR:O	13:M:133:ARG:HB2	2.02	0.60
14:b:20:CYS:SG	14:b:38:MET:HE3	2.42	0.60
1:A:157:ASP:HB2	1:A:158:PRO:CD	2.32	0.60
7:U:86:VAL:HG11	7:U:134:VAL:HG21	1.83	0.59
1:O:157:ASP:HB2	1:O:158:PRO:CD	2.32	0.59
14:N:128:THR:O	14:N:129:ASP:HB2	2.02	0.59
2:P:101:GLU:HB2	2:P:102:PRO:HD2	1.85	0.59
13:a:130:TYR:O	13:a:133:ARG:HB2	2.02	0.59
13:a:46:ILE:HD12	13:a:208:LEU:HG	1.84	0.59
3:C:111:MET:HE1	3:C:119:LEU:HD12	1.85	0.59
13:M:46:ILE:HD12	13:M:208:LEU:HG	1.84	0.59
13:a:210:ASN:CG	15:a:303:HOH:O	2.46	0.59
14:b:21:ASP:OD1	14:b:21:ASP:C	2.46	0.59
9:I:150:LYS:HE2	9:I:185:THR:CG2	2.32	0.59
1:O:47:VAL:HB	1:O:138:LEU:HD21	1.85	0.58
1:A:47:VAL:HB	1:A:138:LEU:HD21	1.85	0.58
2:B:101:GLU:HB2	2:B:102:PRO:HD2	1.85	0.58
13:M:210:ASN:CG	15:M:303:HOH:O	2.47	0.58
1:O:172:LYS:O	1:O:173:LYS:HB2	2.02	0.58
14:b:128:THR:O	14:b:129:ASP:HB2	2.02	0.58
12:L:256:ASN:OD1	12:L:256:ASN:C	2.46	0.58
1:A:172:LYS:O	1:A:173:LYS:HB2	2.02	0.58
3:C:157:ASP:OD1	3:C:159:SER:OG	2.21	0.58
5:E:157:ASP:OD1	5:E:157:ASP:C	2.46	0.58
12:Z:256:ASN:OD1	12:Z:256:ASN:C	2.46	0.57
11:K:104:ASN:HB3	11:K:143:HIS:CE1	2.39	0.57
3:C:61:MET:HG3	10:J:79:GLU:OE2	2.04	0.57
3:Q:111:MET:HE1	3:Q:119:LEU:HD12	1.85	0.57
14:N:21:ASP:OD1	14:N:21:ASP:C	2.46	0.57
5:S:157:ASP:OD1	5:S:157:ASP:C	2.46	0.57
13:M:229:HIS:ND1	13:M:238:SER:OG	2.36	0.57
8:V:219:SER:O	8:V:252:MET:HE2	2.05	0.57
3:Q:157:ASP:OD1	3:Q:159:SER:OG	2.21	0.56
13:a:158:ASP:HB2	13:a:159:PRO:CD	2.35	0.56
11:Y:104:ASN:HB3	11:Y:143:HIS:CE1	2.39	0.56
3:Q:61:MET:HG3	10:X:79:GLU:OE2	2.05	0.56
8:H:219:SER:O	8:H:252:MET:HE2	2.05	0.56
6:T:163:GLY:O	6:T:166:SER:OG	2.23	0.56
10:X:62:THR:OG1	11:Y:87:ARG:NH1	2.36	0.56
13:a:229:HIS:ND1	13:a:238:SER:OG	2.36	0.55
2:P:187:HIS:ND1	2:P:231:ILE:HG22	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:52:VAL:HG21	13:M:144:VAL:HG13	1.88	0.55
2:B:187:HIS:ND1	2:B:231:ILE:HG22	2.21	0.55
6:F:206:LEU:HD22	6:F:211:THR:OG1	2.07	0.54
13:M:158:ASP:HB2	13:M:159:PRO:CD	2.36	0.54
13:a:52:VAL:HG21	13:a:144:VAL:HG13	1.88	0.54
3:C:98:LEU:HD21	3:C:102:ARG:CZ	2.37	0.54
11:Y:9:ARG:HG2	11:Y:9:ARG:NH2	2.23	0.54
6:T:206:LEU:HD22	6:T:211:THR:OG1	2.08	0.54
5:E:110:GLU:HG3	5:E:154:TRP:CH2	2.43	0.54
11:K:9:ARG:HG2	11:K:9:ARG:NH2	2.23	0.54
8:V:92:ALA:O	8:V:93:GLU:C	2.50	0.54
9:W:108:MET:HG3	9:W:242:CYS:SG	2.48	0.54
6:T:159:ALA:O	7:U:56:MET:HE3	2.09	0.53
1:A:122:ARG:HH11	1:A:131:MET:HE3	1.73	0.53
3:C:233:LEU:HD23	10:J:186:VAL:HG11	1.90	0.53
3:Q:98:LEU:HD21	3:Q:102:ARG:CZ	2.37	0.53
9:I:108:MET:HG3	9:I:242:CYS:SG	2.48	0.53
6:F:159:ALA:O	7:G:56:MET:HE3	2.08	0.53
10:J:90:LEU:O	10:J:93:SER:OG	2.21	0.53
9:W:133:ARG:NH1	9:W:133:ARG:HG3	2.23	0.53
4:D:132:ILE:HG23	4:D:144:LEU:HD11	1.90	0.53
9:I:133:ARG:HG3	9:I:133:ARG:NH1	2.23	0.53
8:H:251:CYS:HB2	8:H:253:GLU:OE1	2.09	0.53
8:V:251:CYS:HB2	8:V:253:GLU:OE1	2.09	0.53
3:Q:233:LEU:HD23	10:X:186:VAL:HG11	1.91	0.53
1:O:122:ARG:HH11	1:O:131:MET:HE3	1.74	0.52
4:R:132:ILE:HG23	4:R:144:LEU:HD11	1.90	0.52
5:S:110:GLU:HG3	5:S:154:TRP:CH2	2.43	0.52
9:W:155:ARG:HH11	9:W:155:ARG:HG3	1.74	0.52
13:a:71:ASP:OD1	13:a:73:THR:HG23	2.10	0.52
2:P:34:LEU:C	2:P:34:LEU:HD12	2.34	0.52
2:B:34:LEU:C	2:B:34:LEU:HD12	2.34	0.52
2:B:52:SER:OG	2:B:54:LEU:HB2	2.10	0.52
2:P:52:SER:OG	2:P:54:LEU:HB2	2.10	0.52
14:b:21:ASP:O	14:b:37:ARG:HD3	2.10	0.52
10:J:62:THR:OG1	11:K:87:ARG:NH1	2.36	0.52
11:K:71:ARG:O	11:K:72:GLU:HB2	2.10	0.52
6:F:163:GLY:O	6:F:166:SER:OG	2.23	0.52
9:I:103:MET:HE1	9:I:125:VAL:CG1	2.37	0.52
12:L:304:LYS:HE2	15:L:425:HOH:O	2.10	0.51
14:N:21:ASP:O	14:N:37:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD12	5:E:78:LEU:C	2.36	0.51
10:X:90:LEU:O	10:X:93:SER:OG	2.21	0.51
13:M:71:ASP:OD1	13:M:73:THR:HG23	2.10	0.51
8:H:92:ALA:O	8:H:93:GLU:C	2.50	0.50
13:M:168:TYR:OH	13:M:183:ASP:OD1	2.18	0.50
4:D:42:ILE:HG13	4:D:185:CYS:HB3	1.93	0.50
5:S:78:LEU:C	5:S:78:LEU:HD12	2.36	0.50
5:E:157:ASP:OD1	5:E:159:SER:OG	2.28	0.50
4:R:42:ILE:HG13	4:R:185:CYS:HB3	1.94	0.50
9:W:124:MET:HE1	9:W:152:HIS:ND1	2.27	0.50
10:J:148:GLY:HA3	13:a:177:PHE:HB3	1.93	0.50
13:a:132:ARG:O	13:a:133:ARG:C	2.55	0.50
9:I:124:MET:HE1	9:I:152:HIS:ND1	2.26	0.50
5:E:38:LEU:HD12	5:E:38:LEU:C	2.37	0.50
13:M:177:PHE:HB3	10:X:148:GLY:HA3	1.93	0.50
12:Z:304:LYS:HE2	15:Z:428:HOH:O	2.11	0.50
10:J:109:ILE:CD1	10:J:124:MET:HE3	2.42	0.50
6:F:48:ALA:HB1	6:F:63:LYS:HD3	1.93	0.50
13:M:51:TYR:HA	13:M:231:ILE:O	2.12	0.50
13:M:132:ARG:O	13:M:133:ARG:C	2.55	0.50
6:T:26:ASN:HB2	15:T:305:HOH:O	2.11	0.50
9:W:103:MET:HE1	9:W:125:VAL:CG1	2.37	0.50
9:I:155:ARG:HG3	9:I:155:ARG:HH11	1.74	0.49
11:Y:71:ARG:O	11:Y:72:GLU:HB2	2.10	0.49
14:b:182:PHE:O	14:b:197:PRO:HA	2.12	0.49
4:R:109:ARG:NH1	12:Z:180:ASN:OD1	2.45	0.49
10:X:109:ILE:CD1	10:X:124:MET:HE3	2.42	0.49
5:E:168:GLN:HG3	5:E:169:ALA:N	2.28	0.49
2:P:113:SER:OG	2:P:151:GLY:O	2.30	0.49
2:B:113:SER:OG	2:B:151:GLY:O	2.30	0.49
6:F:31:ASN:HA	6:F:164:LEU:HD13	1.95	0.49
13:M:43:ILE:HG13	13:M:142:MET:HE1	1.95	0.49
5:E:39:GLY:HA2	5:E:47:VAL:O	2.13	0.49
5:S:38:LEU:C	5:S:38:LEU:HD12	2.37	0.49
13:a:51:TYR:HA	13:a:231:ILE:O	2.12	0.49
6:F:26:ASN:HB2	15:F:305:HOH:O	2.11	0.49
5:S:41:GLN:O	5:S:185:TYR:OH	2.31	0.49
6:T:48:ALA:HB1	6:T:63:LYS:HD3	1.93	0.49
5:S:180:VAL:HG12	5:S:180:VAL:O	2.13	0.49
10:J:204:LYS:HG2	12:Z:306:TYR:CG	2.48	0.49
6:T:185:LEU:O	6:T:189:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:139:TYR:C	7:U:139:TYR:CD2	2.90	0.48
5:E:197:LEU:O	5:E:201:ILE:HG13	2.13	0.48
3:C:118:ARG:HD2	3:C:162:TYR:OH	2.13	0.48
3:C:191:LEU:O	3:C:195:ILE:HG13	2.13	0.48
4:D:42:ILE:CG1	4:D:185:CYS:HB3	2.44	0.48
14:N:40:LEU:HD23	14:N:46:VAL:HG23	1.95	0.48
14:N:182:PHE:O	14:N:197:PRO:HA	2.12	0.48
13:M:158:ASP:HB2	13:M:159:PRO:HD3	1.95	0.48
12:L:306:TYR:CG	10:X:204:LYS:HG2	2.48	0.48
7:U:184:CYS:O	7:U:188:VAL:HG23	2.14	0.48
12:L:251:GLN:NE2	11:Y:153:MET:HE3	2.28	0.48
1:O:75:THR:CG2	1:O:137:PHE:CE1	2.97	0.48
5:S:39:GLY:HA2	5:S:47:VAL:O	2.12	0.48
5:S:197:LEU:O	5:S:201:ILE:HG13	2.13	0.48
6:T:31:ASN:HA	6:T:164:LEU:HD13	1.95	0.48
10:J:40:PRO:HD2	15:J:319:HOH:O	2.13	0.48
1:A:75:THR:CG2	1:A:137:PHE:CE1	2.97	0.48
4:D:109:ARG:NH1	12:L:180:ASN:OD1	2.46	0.48
5:S:168:GLN:HG3	5:S:169:ALA:N	2.27	0.48
14:b:40:LEU:HD23	14:b:46:VAL:HG23	1.95	0.48
5:E:180:VAL:HG12	5:E:180:VAL:O	2.13	0.48
6:F:113:VAL:HG11	6:F:148:THR:HG21	1.96	0.48
10:X:40:PRO:HD2	15:X:320:HOH:O	2.13	0.48
1:A:141:GLU:OE1	9:I:138:LYS:NZ	2.46	0.48
3:C:35:ILE:HD11	3:C:37:ILE:HD11	1.95	0.48
6:F:185:LEU:O	6:F:189:ILE:HG13	2.13	0.48
7:G:184:CYS:O	7:G:188:VAL:HG23	2.14	0.48
3:Q:118:ARG:HD2	3:Q:162:TYR:OH	2.14	0.48
11:K:153:MET:HE3	12:Z:251:GLN:NE2	2.28	0.47
3:Q:35:ILE:HD11	3:Q:37:ILE:HD11	1.95	0.47
4:R:42:ILE:CG1	4:R:185:CYS:HB3	2.44	0.47
9:I:278:LEU:HD11	10:J:201:ASN:OD1	2.14	0.47
5:S:206:MET:HE1	5:S:215:ILE:HG23	1.96	0.47
9:W:278:LEU:HD11	10:X:201:ASN:OD1	2.14	0.47
10:X:62:THR:HG1	11:Y:87:ARG:HH12	1.59	0.47
3:Q:191:LEU:O	3:Q:195:ILE:HG13	2.13	0.47
10:J:125:ASP:OD2	10:J:129:ALA:HB3	2.14	0.47
7:G:139:TYR:CD2	7:G:139:TYR:C	2.90	0.47
3:C:62:GLU:HB3	10:J:80:ARG:HB3	1.97	0.47
6:F:88:PHE:CE2	6:F:112:ILE:HD12	2.50	0.47
7:G:139:TYR:C	7:G:139:TYR:HD2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:206:SER:C	12:L:207:MET:HG3	2.39	0.47
4:R:62:ILE:HG21	4:R:207:VAL:CG2	2.45	0.47
12:Z:206:SER:C	12:Z:207:MET:HG3	2.39	0.47
13:a:158:ASP:HB2	13:a:159:PRO:HD3	1.95	0.47
7:G:4:THR:HB	15:G:331:HOH:O	2.14	0.47
4:R:182:ARG:O	4:R:186:VAL:HG23	2.15	0.47
4:R:211:ASN:O	4:R:212:LYS:HB2	2.14	0.47
6:T:110:ALA:HB1	6:T:154:VAL:HG11	1.97	0.47
10:X:125:ASP:OD2	10:X:129:ALA:HB3	2.14	0.47
4:D:182:ARG:O	4:D:186:VAL:HG23	2.15	0.47
5:E:41:GLN:O	5:E:185:TYR:OH	2.31	0.47
6:F:40:ASN:C	6:F:40:ASN:OD1	2.57	0.47
6:T:113:VAL:HG11	6:T:148:THR:HG21	1.96	0.47
14:b:158:GLU:HG3	15:b:366:HOH:O	2.15	0.47
3:C:34:VAL:HB	3:C:170:ILE:HG12	1.97	0.46
5:E:117:CYS:SG	5:E:162:TYR:HB3	2.55	0.46
9:I:275:THR:HG21	10:J:168:ALA:HB1	1.96	0.46
3:Q:34:VAL:HB	3:Q:170:ILE:HG12	1.97	0.46
5:S:117:CYS:SG	5:S:162:TYR:HB3	2.55	0.46
6:T:180:PHE:N	6:T:181:PRO:CD	2.79	0.46
7:U:139:TYR:C	7:U:139:TYR:HD2	2.23	0.46
3:C:221:LEU:HD13	3:C:221:LEU:C	2.40	0.46
2:P:95:TYR:CD2	2:P:103:MET:HA	2.51	0.46
3:Q:62:GLU:HB3	10:X:80:ARG:HB3	1.97	0.46
7:U:18:ARG:NH1	7:U:23:GLU:OE1	2.41	0.46
4:D:62:ILE:HG21	4:D:207:VAL:CG2	2.45	0.46
4:D:70:TYR:CD2	4:D:209:LEU:HD13	2.51	0.46
14:N:158:GLU:HG3	15:N:367:HOH:O	2.15	0.46
4:R:186:VAL:O	4:R:190:ILE:HG12	2.16	0.46
6:T:44:VAL:HG11	6:T:136:ALA:HB1	1.98	0.46
9:W:275:THR:HG21	10:X:168:ALA:HB1	1.96	0.46
3:C:195:ILE:HG21	3:C:257:LEU:HD13	1.97	0.46
5:E:206:MET:HE1	5:E:215:ILE:HG23	1.97	0.46
3:Q:34:VAL:HG12	3:Q:141:LEU:HD12	1.98	0.46
7:U:4:THR:HB	15:U:331:HOH:O	2.15	0.46
13:M:163:THR:OG1	13:M:164:GLU:N	2.49	0.46
6:T:88:PHE:CE2	6:T:112:ILE:HD12	2.50	0.46
5:E:27:ALA:O	5:E:30:ALA:HB3	2.15	0.46
9:I:133:ARG:HG3	9:I:133:ARG:HH11	1.81	0.46
12:L:114:LEU:C	12:L:114:LEU:CD1	2.87	0.46
11:Y:189:PHE:N	11:Y:206:SER:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:TYR:CD2	2:B:103:MET:HA	2.50	0.46
5:E:66:LYS:O	5:E:77:VAL:HA	2.16	0.46
6:F:120:HIS:HB3	6:F:127:ARG:O	2.16	0.46
6:F:180:PHE:N	6:F:181:PRO:CD	2.78	0.46
3:Q:221:LEU:HD13	3:Q:221:LEU:C	2.40	0.46
5:S:27:ALA:O	5:S:30:ALA:HB3	2.15	0.46
7:G:150:ASP:HB2	7:G:151:PRO:CD	2.46	0.46
1:O:146:ASP:OD1	1:O:146:ASP:N	2.49	0.46
1:A:81:ALA:N	1:A:82:PRO:HD2	2.31	0.46
4:D:211:ASN:O	4:D:212:LYS:HB2	2.15	0.46
4:R:70:TYR:CD2	4:R:209:LEU:HD13	2.51	0.46
5:S:66:LYS:O	5:S:77:VAL:HA	2.16	0.46
13:a:163:THR:OG1	13:a:164:GLU:N	2.49	0.46
3:C:34:VAL:HG12	3:C:141:LEU:HD12	1.98	0.45
5:S:157:ASP:OD1	5:S:159:SER:OG	2.27	0.45
12:Z:114:LEU:C	12:Z:114:LEU:CD1	2.87	0.45
6:F:110:ALA:HB1	6:F:154:VAL:HG11	1.97	0.45
13:M:133:ARG:HD2	13:M:133:ARG:HA	1.73	0.45
1:A:146:ASP:OD1	1:A:146:ASP:N	2.49	0.45
3:C:42:GLY:HA2	3:C:151:TYR:CE1	2.51	0.45
11:K:189:PHE:N	11:K:206:SER:O	2.39	0.45
11:Y:125:HIS:CG	15:Y:304:HOH:O	2.69	0.45
11:Y:152:ALA:O	11:Y:153:MET:C	2.59	0.45
4:D:164:ASN:O	4:D:168:VAL:HG23	2.17	0.45
9:I:141:ARG:HB2	9:I:144:GLU:HG3	1.99	0.45
1:O:141:GLU:OE1	9:W:138:LYS:NZ	2.46	0.45
6:T:40:ASN:C	6:T:40:ASN:OD1	2.57	0.45
8:V:88:LEU:HD13	8:V:231:ILE:HG22	1.99	0.45
9:W:133:ARG:HG3	9:W:133:ARG:HH11	1.81	0.45
9:W:141:ARG:HB2	9:W:144:GLU:HG3	1.99	0.45
1:A:43:ASP:OD1	1:A:43:ASP:N	2.49	0.45
1:O:81:ALA:N	1:O:82:PRO:HD2	2.31	0.45
3:Q:42:GLY:HA2	3:Q:151:TYR:CE1	2.51	0.45
3:Q:195:ILE:HG21	3:Q:257:LEU:HD13	1.97	0.45
4:D:186:VAL:O	4:D:190:ILE:HG12	2.16	0.45
4:R:112:ALA:HB1	4:R:151:GLY:O	2.17	0.45
6:T:120:HIS:HB3	6:T:127:ARG:O	2.16	0.45
5:E:155:GLN:HG2	5:E:156:THR:N	2.31	0.45
13:a:43:ILE:HG13	13:a:142:MET:HE1	1.95	0.45
10:J:109:ILE:HD12	10:J:124:MET:HE3	1.99	0.45
11:Y:70:MET:HE2	11:Y:70:MET:HB3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:125:HIS:CG	15:K:304:HOH:O	2.69	0.45
7:U:150:ASP:HB2	7:U:151:PRO:CD	2.47	0.45
10:X:109:ILE:HD12	10:X:124:MET:HE3	1.99	0.45
6:F:44:VAL:HG11	6:F:136:ALA:HB1	1.98	0.44
4:R:12:PRO:HA	5:S:26:TYR:CD1	2.52	0.44
1:A:168:CYS:O	1:A:168:CYS:SG	2.76	0.44
4:D:12:PRO:HA	5:E:26:TYR:CD1	2.52	0.44
7:G:84:ARG:HB3	15:G:304:HOH:O	2.16	0.44
5:S:67:ILE:HA	5:S:76:THR:O	2.17	0.44
4:D:112:ALA:HB1	4:D:151:GLY:O	2.17	0.44
12:L:214:TRP:CD1	12:L:214:TRP:C	2.96	0.44
5:S:108:ARG:HB2	5:S:111:SER:OG	2.17	0.44
5:E:67:ILE:HA	5:E:76:THR:O	2.17	0.44
5:E:108:ARG:HB2	5:E:111:SER:OG	2.17	0.44
8:H:280:ARG:NH2	14:b:191:MET:HE1	2.33	0.44
4:R:164:ASN:O	4:R:168:VAL:HG23	2.16	0.44
7:U:84:ARG:HB3	15:U:305:HOH:O	2.16	0.44
12:Z:222:TYR:CE2	12:Z:232:LYS:HB2	2.53	0.44
10:J:14:MET:SD	10:J:166:VAL:HG12	2.58	0.44
12:L:128:SER:O	12:L:141:VAL:HG23	2.17	0.44
10:X:14:MET:SD	10:X:166:VAL:HG12	2.58	0.44
14:N:191:MET:HE1	8:V:280:ARG:NH2	2.33	0.44
5:S:133:MET:HE1	5:S:137:PHE:HE2	1.83	0.44
5:S:188:ASN:HD22	5:S:188:ASN:HA	1.57	0.44
7:U:18:ARG:HH11	7:U:23:GLU:CD	2.26	0.44
14:b:62:MET:SD	14:b:62:MET:C	3.00	0.44
8:H:88:LEU:HD13	8:H:231:ILE:HG22	1.99	0.43
12:Z:128:SER:O	12:Z:141:VAL:HG23	2.17	0.43
10:J:165:GLU:O	10:J:166:VAL:C	2.61	0.43
14:N:62:MET:C	14:N:62:MET:SD	3.00	0.43
4:D:161:ILE:HG22	15:D:311:HOH:O	2.18	0.43
1:O:168:CYS:O	1:O:168:CYS:SG	2.76	0.43
1:A:74:GLY:HA3	1:A:231:PHE:CD2	2.54	0.43
4:R:161:ILE:HG22	15:R:311:HOH:O	2.16	0.43
11:Y:151:ILE:HD12	11:Y:151:ILE:HG23	1.65	0.43
12:Z:214:TRP:CD1	12:Z:214:TRP:C	2.96	0.43
10:X:146:LEU:HA	10:X:146:LEU:HD23	1.76	0.43
1:A:156:VAL:HA	1:A:161:TRP:O	2.19	0.43
7:G:9:SER:HB3	7:G:11:ASP:OD2	2.19	0.43
11:K:10:CYS:HB2	11:K:13:PHE:CE1	2.54	0.43
14:N:121:ASP:OD1	14:N:121:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:269:SER:HB2	15:V:337:HOH:O	2.19	0.43
11:Y:10:CYS:HB2	11:Y:13:PHE:CE1	2.53	0.43
3:C:192:ASP:O	3:C:196:VAL:HG23	2.19	0.43
1:O:172:LYS:O	1:O:173:LYS:CB	2.67	0.43
12:Z:216:GLN:H	12:Z:216:GLN:HG2	1.68	0.43
1:O:74:GLY:HA3	1:O:231:PHE:CD2	2.54	0.43
2:B:117:GLN:NE2	3:C:88:ASP:OD1	2.50	0.42
4:D:222:LEU:O	4:D:226:VAL:HG23	2.19	0.42
12:L:205:LEU:HD13	12:L:207:MET:SD	2.59	0.42
1:O:156:VAL:HA	1:O:161:TRP:O	2.19	0.42
4:R:132:ILE:CG2	4:R:144:LEU:HD11	2.49	0.42
6:T:113:VAL:CG1	6:T:148:THR:HG21	2.49	0.42
14:b:121:ASP:OD1	14:b:121:ASP:C	2.61	0.42
12:Z:160:ALA:CB	13:a:160:VAL:HG23	2.49	0.42
3:C:64:LYS:HB2	3:C:250:ARG:HH21	1.84	0.42
7:G:18:ARG:NH1	7:G:23:GLU:OE1	2.40	0.42
8:H:218:TYR:OH	15:H:301:HOH:O	2.21	0.42
12:L:222:TYR:CE2	12:L:232:LYS:HB2	2.53	0.42
12:Z:175:LEU:O	12:Z:176:TRP:C	2.62	0.42
13:a:168:TYR:OH	13:a:183:ASP:OD1	2.18	0.42
3:C:221:LEU:C	3:C:221:LEU:CD1	2.93	0.42
7:G:18:ARG:HH11	7:G:23:GLU:CD	2.25	0.42
8:H:280:ARG:HH22	14:b:191:MET:HE1	1.84	0.42
12:Z:205:LEU:HD13	12:Z:207:MET:SD	2.59	0.42
5:E:133:MET:HE1	5:E:137:PHE:HE2	1.83	0.42
6:F:113:VAL:CG1	6:F:148:THR:HG21	2.49	0.42
11:K:151:ILE:HG23	11:K:151:ILE:HD12	1.66	0.42
11:K:152:ALA:O	11:K:153:MET:C	2.59	0.42
12:L:160:ALA:CB	13:M:160:VAL:HG23	2.49	0.42
4:R:193:LEU:HD23	4:R:193:LEU:HA	1.93	0.42
5:E:188:ASN:HD22	5:E:188:ASN:HA	1.57	0.42
14:N:191:MET:HE1	8:V:280:ARG:HH22	1.84	0.42
1:A:172:LYS:O	1:A:173:LYS:CB	2.67	0.42
3:Q:192:ASP:O	3:Q:196:VAL:HG23	2.19	0.42
4:R:222:LEU:O	4:R:226:VAL:HG23	2.19	0.42
2:B:191:LEU:HD12	2:B:191:LEU:HA	1.89	0.42
10:J:171:MET:SD	10:J:175:CYS:SG	3.18	0.42
3:Q:64:LYS:HB2	3:Q:250:ARG:HH21	1.84	0.42
3:Q:221:LEU:C	3:Q:221:LEU:CD1	2.93	0.42
7:U:9:SER:HB3	7:U:11:ASP:OD2	2.19	0.42
9:W:245:THR:O	9:W:246:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:ILE:CG2	4:D:144:LEU:HD11	2.49	0.42
8:V:120:TYR:CZ	8:V:124:THR:HG21	2.55	0.42
9:W:104:ALA:HB1	9:W:105:PRO:HD2	2.02	0.42
10:X:165:GLU:O	10:X:166:VAL:C	2.60	0.42
11:K:50:GLU:HB2	11:K:53:PRO:HD2	2.02	0.42
5:S:155:GLN:HG2	5:S:156:THR:N	2.31	0.42
10:J:19:CYS:HA	10:J:190:VAL:O	2.20	0.41
6:T:110:ALA:O	6:T:111:GLU:C	2.61	0.41
5:E:13:ASN:O	5:E:14:THR:C	2.62	0.41
14:N:45:THR:HG22	14:N:46:VAL:N	2.35	0.41
5:S:107:MET:HE2	5:S:111:SER:HB2	2.02	0.41
5:S:210:LEU:C	5:S:210:LEU:HD23	2.45	0.41
2:B:190:LEU:HD23	2:B:190:LEU:HA	1.85	0.41
5:E:146:VAL:HG23	5:E:220:VAL:HG12	2.02	0.41
5:E:210:LEU:HD23	5:E:210:LEU:C	2.45	0.41
9:I:80:LEU:HB3	9:I:110:CYS:SG	2.60	0.41
4:R:45:VAL:O	4:R:204:ILE:HA	2.20	0.41
8:H:120:TYR:CZ	8:H:124:THR:HG21	2.55	0.41
2:P:146:GLN:O	2:P:153:PHE:HA	2.20	0.41
8:V:218:TYR:OH	15:V:301:HOH:O	2.21	0.41
9:W:111:GLY:HA3	9:W:118:THR:HG21	2.03	0.41
10:X:19:CYS:HA	10:X:190:VAL:O	2.20	0.41
10:X:171:MET:SD	10:X:175:CYS:SG	3.18	0.41
11:Y:51:ASN:O	11:Y:55:VAL:HG23	2.20	0.41
11:Y:75:ARG:HD2	11:Y:75:ARG:HA	1.97	0.41
5:S:13:ASN:O	5:S:14:THR:C	2.62	0.41
11:Y:50:GLU:HB2	11:Y:53:PRO:HD2	2.02	0.41
6:F:232:LYS:HE3	6:F:233:TYR:CZ	2.56	0.41
13:a:37:ALA:O	13:a:89:MET:HB2	2.21	0.41
14:b:45:THR:HG22	14:b:46:VAL:N	2.36	0.41
1:A:171:GLY:O	1:A:174:GLN:HB3	2.21	0.41
9:I:104:ALA:HB1	9:I:105:PRO:HD2	2.02	0.41
6:T:196:LEU:O	6:T:196:LEU:HG	2.21	0.41
13:a:133:ARG:HA	13:a:133:ARG:HD2	1.73	0.41
4:D:45:VAL:O	4:D:204:ILE:HA	2.21	0.41
5:E:22:PHE:O	5:E:23:GLN:C	2.64	0.41
5:E:107:MET:HE2	5:E:111:SER:HB2	2.02	0.41
8:H:142:TYR:CE2	14:N:58:GLU:HG3	2.56	0.41
13:M:132:ARG:C	13:M:134:PHE:N	2.79	0.41
13:M:190:HIS:CD2	10:X:172:LEU:HB3	2.56	0.41
2:P:117:GLN:HB2	3:Q:87:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:189:ILE:HD11	6:T:215:ILE:HD11	2.03	0.41
8:V:142:TYR:CE2	14:b:58:GLU:HG3	2.56	0.41
9:W:80:LEU:HB3	9:W:110:CYS:SG	2.61	0.41
9:W:151:ARG:HH11	9:W:151:ARG:HD3	1.72	0.41
11:Y:8:PHE:HB3	11:Y:140:TYR:HB3	2.03	0.41
13:a:132:ARG:HE	13:a:132:ARG:HB3	1.80	0.41
3:C:266:GLU:C	3:C:268:GLU:H	2.29	0.41
2:P:191:LEU:HD12	2:P:191:LEU:HA	1.89	0.41
4:R:106:LEU:HD13	4:R:109:ARG:HH11	1.86	0.41
4:R:200:GLY:O	4:R:226:VAL:HG21	2.21	0.41
2:B:146:GLN:O	2:B:153:PHE:HA	2.20	0.40
8:H:72:SER:HB3	8:H:227:LEU:HB2	2.03	0.40
12:L:216:GLN:H	12:L:216:GLN:HG2	1.68	0.40
12:L:225:ASP:OD2	12:L:229:THR:HB	2.21	0.40
13:M:37:ALA:O	13:M:89:MET:HB2	2.21	0.40
1:O:171:GLY:O	1:O:174:GLN:HB3	2.20	0.40
7:G:42:ASP:OD1	7:G:42:ASP:N	2.54	0.40
9:I:111:GLY:HA3	9:I:118:THR:HG21	2.03	0.40
11:K:70:MET:C	11:K:72:GLU:H	2.30	0.40
11:K:104:ASN:HB3	11:K:143:HIS:ND1	2.36	0.40
14:N:184:ILE:HG21	14:N:184:ILE:HD13	1.88	0.40
3:Q:266:GLU:C	3:Q:268:GLU:H	2.29	0.40
6:T:232:LYS:HE3	6:T:233:TYR:CZ	2.55	0.40
12:Z:305:LEU:O	12:Z:306:TYR:C	2.64	0.40
4:D:17:PHE:O	4:D:18:GLN:C	2.63	0.40
7:G:139:TYR:CD2	7:G:139:TYR:O	2.74	0.40
10:J:164:PHE:CD1	10:J:189:ILE:HD11	2.57	0.40
12:L:175:LEU:O	12:L:176:TRP:C	2.62	0.40
12:L:254:ARG:NH2	12:L:256:ASN:OD1	2.55	0.40
11:Y:104:ASN:HB3	11:Y:143:HIS:ND1	2.36	0.40
14:b:36:PRO:HG2	14:b:36:PRO:O	2.22	0.40
4:D:200:GLY:O	4:D:226:VAL:HG21	2.21	0.40
6:F:110:ALA:O	6:F:111:GLU:C	2.61	0.40
7:G:182:ILE:O	7:G:182:ILE:HG23	2.21	0.40
2:P:117:GLN:NE2	3:Q:88:ASP:OD1	2.50	0.40
2:P:137:ALA:HA	2:P:141:GLY:O	2.21	0.40
5:S:146:VAL:HG23	5:S:220:VAL:HG12	2.02	0.40
6:T:106:LEU:O	6:T:107:PRO:C	2.62	0.40
7:U:139:TYR:CD2	7:U:139:TYR:O	2.74	0.40
11:Y:54:ARG:HH21	11:Y:54:ARG:HD2	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/250 (97%)	231 (96%)	11 (4%)	0	100	100
1	O	242/250 (97%)	232 (96%)	10 (4%)	0	100	100
2	B	226/288 (78%)	220 (97%)	5 (2%)	1 (0%)	30	37
2	P	226/288 (78%)	220 (97%)	5 (2%)	1 (0%)	30	37
3	C	265/286 (93%)	246 (93%)	14 (5%)	5 (2%)	6	5
3	Q	265/286 (93%)	246 (93%)	14 (5%)	5 (2%)	6	5
4	D	232/247 (94%)	214 (92%)	13 (6%)	5 (2%)	5	4
4	R	232/247 (94%)	214 (92%)	13 (6%)	5 (2%)	5	4
5	E	225/245 (92%)	210 (93%)	15 (7%)	0	100	100
5	S	225/245 (92%)	210 (93%)	15 (7%)	0	100	100
6	F	214/265 (81%)	202 (94%)	12 (6%)	0	100	100
6	T	214/265 (81%)	202 (94%)	12 (6%)	0	100	100
7	G	225/237 (95%)	216 (96%)	8 (4%)	1 (0%)	30	37
7	U	225/237 (95%)	216 (96%)	8 (4%)	1 (0%)	30	37
8	H	226/284 (80%)	219 (97%)	7 (3%)	0	100	100
8	V	226/284 (80%)	219 (97%)	7 (3%)	0	100	100
9	I	217/292 (74%)	209 (96%)	7 (3%)	1 (0%)	24	30
9	W	217/292 (74%)	209 (96%)	7 (3%)	1 (0%)	24	30
10	J	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	24	30
10	X	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	24	30
11	K	204/206 (99%)	198 (97%)	5 (2%)	1 (0%)	24	30
11	Y	204/206 (99%)	198 (97%)	5 (2%)	1 (0%)	24	30
12	L	198/311 (64%)	188 (95%)	10 (5%)	0	100	100
12	Z	198/311 (64%)	188 (95%)	10 (5%)	0	100	100
13	M	205/246 (83%)	199 (97%)	4 (2%)	2 (1%)	12	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	205/246 (83%)	199 (97%)	4 (2%)	2 (1%)	12	14
14	N	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
14	b	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	6194/7160 (86%)	5915 (96%)	245 (4%)	34 (0%)	26	30

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	13	ASP
11	K	72	GLU
13	M	133	ARG
4	R	13	ASP
11	Y	72	GLU
13	a	133	ARG
3	C	15	GLU
3	C	207	ASP
4	D	54	GLN
9	I	237	THR
10	J	147	HIS
3	Q	15	GLU
3	Q	207	ASP
4	R	54	GLN
9	W	237	THR
10	X	147	HIS
3	C	8	ARG
3	C	172	GLN
3	C	228	ALA
13	M	224	ASP
3	Q	8	ARG
3	Q	172	GLN
3	Q	228	ALA
7	U	54	SER
13	a	224	ASP
4	D	57	ARG
7	G	54	SER
4	R	57	ARG
2	B	122	SER
4	D	212	LYS
2	P	122	SER
4	R	212	LYS
4	D	12	PRO

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Mol	Chain	Res	Type
4	R	12	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	199/204 (98%)	191 (96%)	8 (4%)	28	41
1	O	199/204 (98%)	191 (96%)	8 (4%)	28	41
2	B	111/239 (46%)	109 (98%)	2 (2%)	51	69
2	P	187/239 (78%)	180 (96%)	7 (4%)	30	44
3	Q	223/239 (93%)	209 (94%)	14 (6%)	16	22
4	D	144/211 (68%)	133 (92%)	11 (8%)	12	16
4	R	201/211 (95%)	187 (93%)	14 (7%)	14	18
5	E	193/207 (93%)	172 (89%)	21 (11%)	6	7
5	S	193/207 (93%)	172 (89%)	21 (11%)	6	7
6	F	178/217 (82%)	169 (95%)	9 (5%)	21	31
6	T	178/217 (82%)	170 (96%)	8 (4%)	24	36
7	G	188/196 (96%)	176 (94%)	12 (6%)	16	22
7	U	188/196 (96%)	176 (94%)	12 (6%)	16	22
8	H	187/234 (80%)	175 (94%)	12 (6%)	16	22
8	V	187/234 (80%)	175 (94%)	12 (6%)	16	22
9	I	179/246 (73%)	165 (92%)	14 (8%)	11	15
9	W	179/246 (73%)	165 (92%)	14 (8%)	11	15
10	J	166/167 (99%)	160 (96%)	6 (4%)	31	45
10	X	166/167 (99%)	160 (96%)	6 (4%)	31	45
11	K	168/168 (100%)	156 (93%)	12 (7%)	13	18
11	Y	168/168 (100%)	156 (93%)	12 (7%)	13	18
12	L	163/265 (62%)	154 (94%)	9 (6%)	19	27
12	Z	163/265 (62%)	154 (94%)	9 (6%)	19	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	176/208 (85%)	164 (93%)	12 (7%)	14	19
13	a	176/208 (85%)	166 (94%)	10 (6%)	18	26
14	N	177/177 (100%)	175 (99%)	2 (1%)	65	80
14	b	177/177 (100%)	175 (99%)	2 (1%)	65	80
All	All	4814/5717 (84%)	4535 (94%)	279 (6%)	20	25

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	96	SER
1	A	104	SER
1	A	130	LEU
1	A	146	ASP
1	A	164	SER
1	A	183	LYS
1	A	193	LEU
2	B	43	VAL
2	B	52	SER
4	D	85	ASN
4	D	103	ASP
4	D	104	VAL
4	D	105	ASP
4	D	138	GLU
4	D	161	ILE
4	D	167	THR
4	D	178	GLU
4	D	181	THR
4	D	184	GLN
4	D	190	ILE
5	E	7	GLU
5	E	9	ASP
5	E	12	VAL
5	E	18	GLU
5	E	36	THR
5	E	41	GLN
5	E	42	THR
5	E	62	SER
5	E	76	THR
5	E	111	SER
5	E	152	GLN

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Mol	Chain	Res	Type
5	E	156	THR
5	E	157	ASP
5	E	161	THR
5	E	168	GLN
5	E	188	ASN
5	E	189	MET
5	E	192	GLU
5	E	196	THR
5	E	231	ASP
5	E	236	GLN
6	F	21	GLN
6	F	33	SER
6	F	42	ASP
6	F	84	MET
6	F	111	GLU
6	F	113	VAL
6	F	165	ARG
6	F	223	MET
6	F	231	ARG
7	G	16	ASP
7	G	42	ASP
7	G	46	VAL
7	G	55	ARG
7	G	84	ARG
7	G	88	SER
7	G	103	THR
7	G	112	SER
7	G	120	VAL
7	G	167	LYS
7	G	171	LYS
7	G	225	VAL
8	H	75	SER
8	H	78	THR
8	H	128	VAL
8	H	139	LYS
8	H	149	SER
8	H	164	SER
8	H	199	THR
8	H	218	TYR
8	H	235	GLN
8	H	260	ASP
8	H	275	THR

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Mol	Chain	Res	Type
8	H	280	ARG
9	I	75	LYS
9	I	88	GLU
9	I	95	LYS
9	I	97	CYS
9	I	98	LYS
9	I	103	MET
9	I	109	CYS
9	I	110	CYS
9	I	119	GLU
9	I	215	GLU
9	I	219	GLU
9	I	247	THR
9	I	260	GLU
9	I	274	THR
10	J	132	GLU
10	J	134	GLU
10	J	173	SER
10	J	179	SER
10	J	194	LYS
10	J	195	MET
11	K	15	LEU
11	K	40	ASP
11	K	70	MET
11	K	75	ARG
11	K	77	ILE
11	K	103	VAL
11	K	112	VAL
11	K	116	SER
11	K	122	THR
11	K	183	VAL
11	K	197	ASN
11	K	206	SER
12	L	134	GLN
12	L	141	VAL
12	L	155	MET
12	L	216	GLN
12	L	225	ASP
12	L	251	GLN
12	L	297	ILE
12	L	302	GLN
12	L	304	LYS

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Mol	Chain	Res	Type
13	M	52	VAL
13	M	127	THR
13	M	131	GLN
13	M	133	ARG
13	M	171	SER
13	M	173	SER
13	M	177	PHE
13	M	189	GLN
13	M	198	GLU
13	M	201	MET
13	M	234	ASP
13	M	244	ARG
14	N	39	LYS
14	N	212	GLU
1	O	57	LEU
1	O	96	SER
1	O	104	SER
1	O	130	LEU
1	O	146	ASP
1	O	164	SER
1	O	183	LYS
1	O	193	LEU
2	P	43	VAL
2	P	52	SER
2	P	160	SER
2	P	173	GLU
2	P	175	ARG
2	P	183	GLU
2	P	202	THR
3	Q	2	SER
3	Q	33	THR
3	Q	35	ILE
3	Q	69	GLU
3	Q	81	SER
3	Q	115	ASP
3	Q	118	ARG
3	Q	161	ASN
3	Q	170	ILE
3	Q	186	LYS
3	Q	216	LEU
3	Q	221	LEU
3	Q	229	THR

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Mol	Chain	Res	Type
3	Q	234	GLU
4	R	5	ARG
4	R	38	LYS
4	R	67	GLU
4	R	85	ASN
4	R	103	ASP
4	R	104	VAL
4	R	105	ASP
4	R	138	GLU
4	R	161	ILE
4	R	167	THR
4	R	178	GLU
4	R	181	THR
4	R	184	GLN
4	R	190	ILE
5	S	7	GLU
5	S	9	ASP
5	S	12	VAL
5	S	18	GLU
5	S	36	THR
5	S	41	GLN
5	S	42	THR
5	S	62	SER
5	S	76	THR
5	S	111	SER
5	S	152	GLN
5	S	156	THR
5	S	157	ASP
5	S	161	THR
5	S	168	GLN
5	S	188	ASN
5	S	189	MET
5	S	192	GLU
5	S	196	THR
5	S	231	ASP
5	S	236	GLN
6	T	21	GLN
6	T	33	SER
6	T	42	ASP
6	T	84	MET
6	T	111	GLU
6	T	113	VAL

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Mol	Chain	Res	Type
6	T	165	ARG
6	T	231	ARG
7	U	16	ASP
7	U	42	ASP
7	U	46	VAL
7	U	55	ARG
7	U	84	ARG
7	U	88	SER
7	U	103	THR
7	U	112	SER
7	U	120	VAL
7	U	167	LYS
7	U	171	LYS
7	U	225	VAL
8	V	75	SER
8	V	78	THR
8	V	128	VAL
8	V	139	LYS
8	V	149	SER
8	V	164	SER
8	V	199	THR
8	V	218	TYR
8	V	235	GLN
8	V	260	ASP
8	V	275	THR
8	V	280	ARG
9	W	75	LYS
9	W	88	GLU
9	W	95	LYS
9	W	97	CYS
9	W	98	LYS
9	W	103	MET
9	W	109	CYS
9	W	110	CYS
9	W	119	GLU
9	W	215	GLU
9	W	219	GLU
9	W	247	THR
9	W	260	GLU
9	W	274	THR
10	X	132	GLU
10	X	134	GLU

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Mol	Chain	Res	Type
10	X	173	SER
10	X	179	SER
10	X	194	LYS
10	X	195	MET
11	Y	15	LEU
11	Y	40	ASP
11	Y	70	MET
11	Y	75	ARG
11	Y	77	ILE
11	Y	103	VAL
11	Y	112	VAL
11	Y	116	SER
11	Y	122	THR
11	Y	183	VAL
11	Y	197	ASN
11	Y	206	SER
12	Z	134	GLN
12	Z	141	VAL
12	Z	155	MET
12	Z	216	GLN
12	Z	225	ASP
12	Z	251	GLN
12	Z	297	ILE
12	Z	302	GLN
12	Z	304	LYS
13	a	127	THR
13	a	131	GLN
13	a	133	ARG
13	a	171	SER
13	a	173	SER
13	a	177	PHE
13	a	189	GLN
13	a	201	MET
13	a	234	ASP
13	a	244	ARG
14	b	39	LYS
14	b	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS

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Mol	Chain	Res	Type
2	B	100	HIS
4	D	68	HIS
4	D	97	ASN
4	D	137	ASN
4	D	164	ASN
4	D	179	ASN
5	E	65	ASN
5	E	91	HIS
5	E	152	GLN
5	E	155	GLN
5	E	168	GLN
5	E	188	ASN
5	E	232	GLN
6	F	26	ASN
6	F	104	ASN
6	F	207	ASN
7	G	178	ASN
7	G	196	HIS
7	G	219	ASN
7	G	223	GLN
7	G	224	HIS
8	H	112	GLN
8	H	196	ASN
8	H	211	GLN
8	H	278	GLN
11	K	11	ASN
11	K	73	HIS
11	K	186	ASN
12	L	117	HIS
12	L	251	GLN
12	L	272	HIS
13	M	81	HIS
13	M	98	GLN
13	M	245	ASN
14	N	70	GLN
14	N	81	ASN
14	N	93	HIS
1	O	229	HIS
3	Q	94	ASN
3	Q	101	ASN
3	Q	103	HIS
4	R	68	HIS

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Mol	Chain	Res	Type
4	R	97	ASN
4	R	137	ASN
4	R	164	ASN
4	R	179	ASN
5	S	65	ASN
5	S	91	HIS
5	S	152	GLN
5	S	155	GLN
5	S	168	GLN
5	S	188	ASN
5	S	232	GLN
6	T	26	ASN
6	T	104	ASN
6	T	207	ASN
7	U	178	ASN
7	U	219	ASN
7	U	223	GLN
7	U	224	HIS
8	V	112	GLN
8	V	196	ASN
8	V	211	GLN
8	V	278	GLN
11	Y	11	ASN
11	Y	73	HIS
11	Y	136	GLN
11	Y	186	ASN
12	Z	117	HIS
12	Z	251	GLN
12	Z	272	HIS
12	Z	296	GLN
13	a	81	HIS
13	a	98	GLN
13	a	245	ASN
14	b	70	GLN
14	b	81	ASN
14	b	93	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

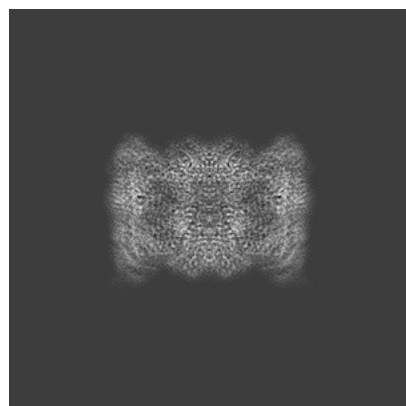
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50260. These allow visual inspection of the internal detail of the map and identification of artifacts.

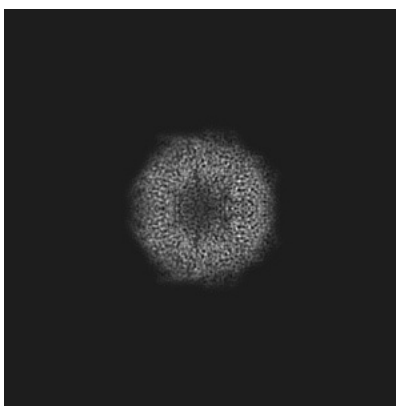
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

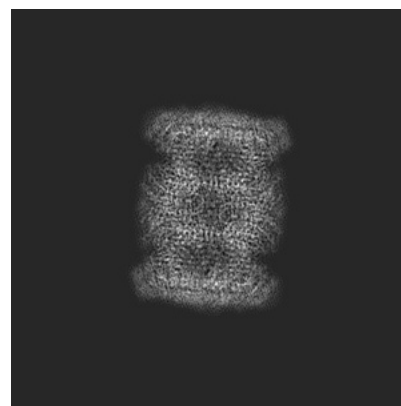
6.1.1 Primary map



X

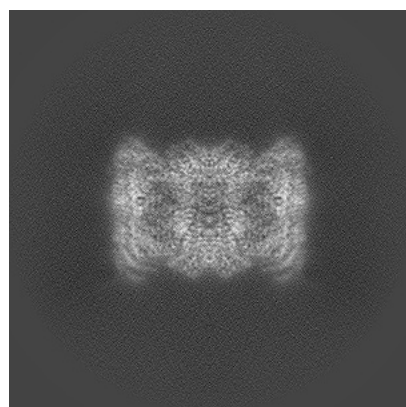


Y

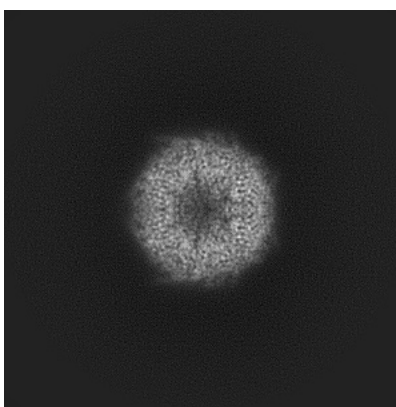


Z

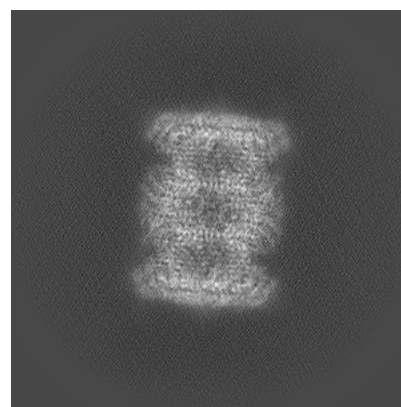
6.1.2 Raw map



X



Y

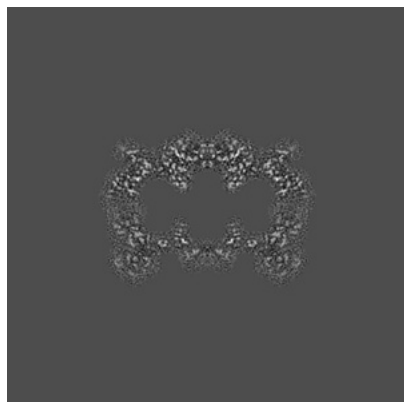


Z

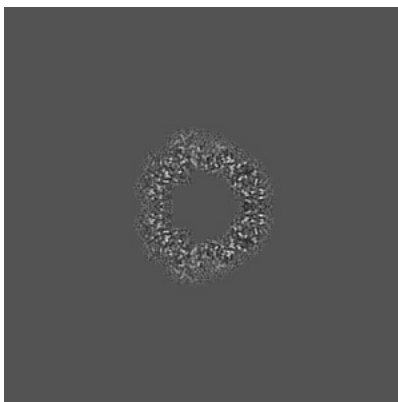
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

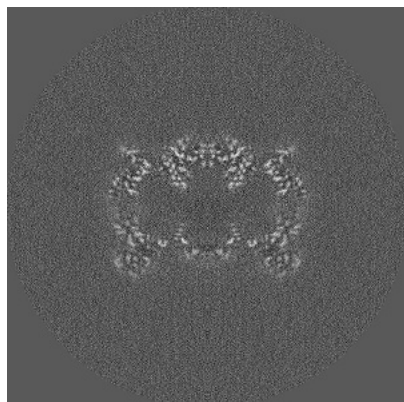


Y Index: 240

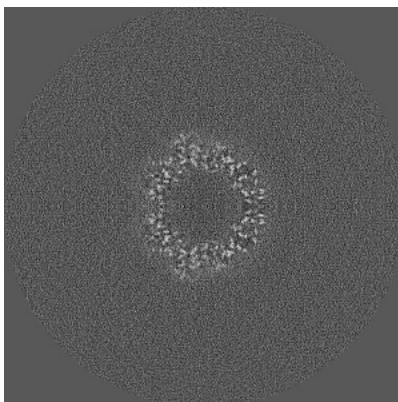


Z Index: 240

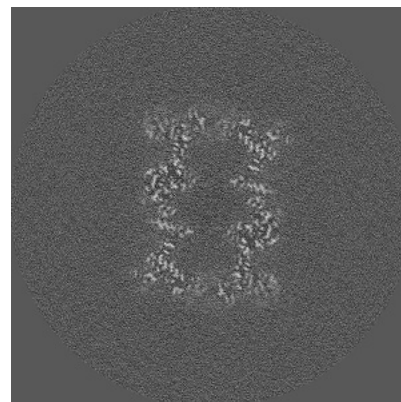
6.2.2 Raw map



X Index: 240



Y Index: 240

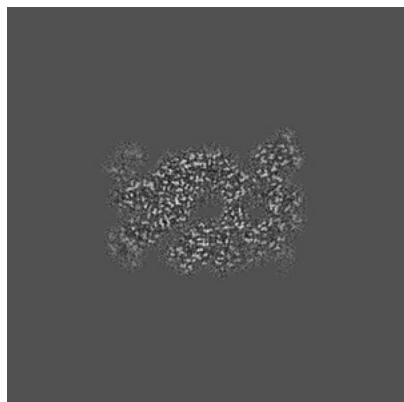


Z Index: 240

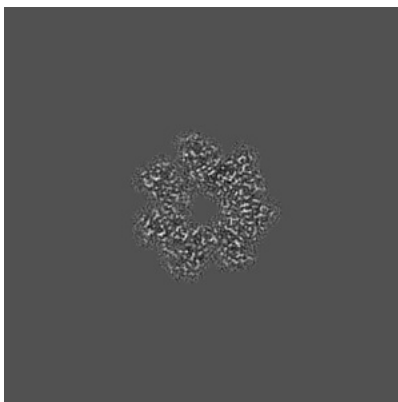
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

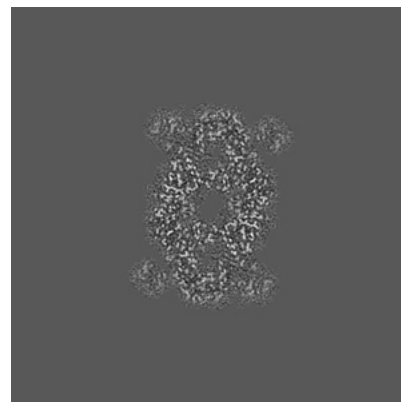
6.3.1 Primary map



X Index: 281

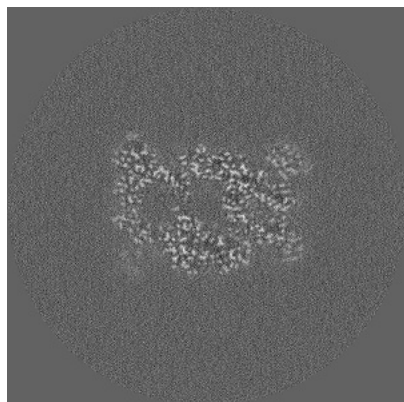


Y Index: 212

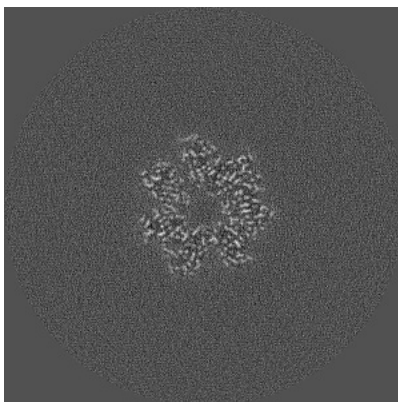


Z Index: 275

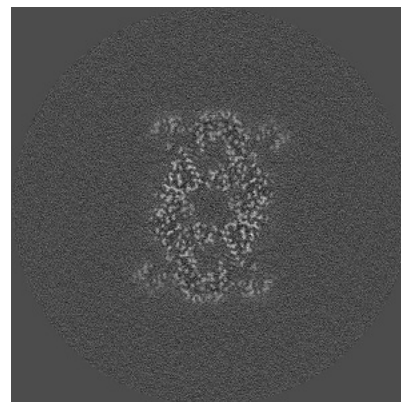
6.3.2 Raw map



X Index: 207



Y Index: 212

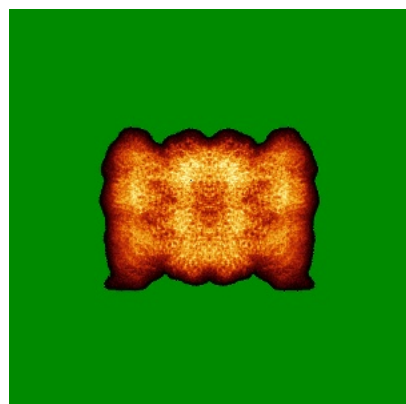


Z Index: 275

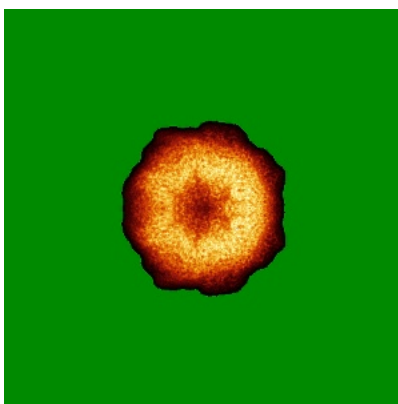
The images above show the largest variance slices of the map in three orthogonal directions.

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

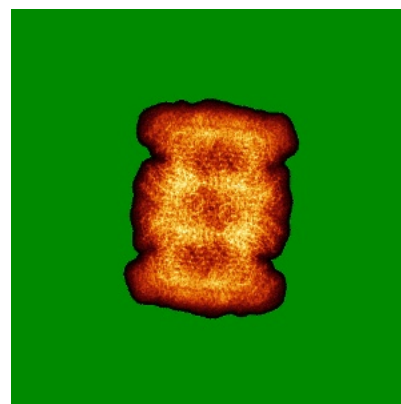
6.4.1 Primary map



X

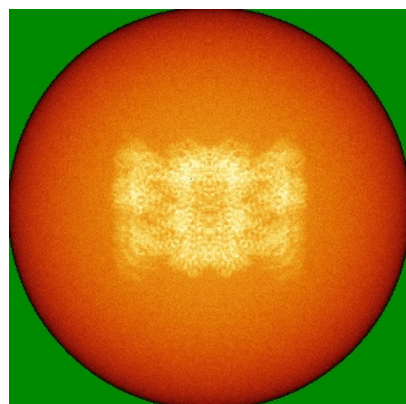


Y

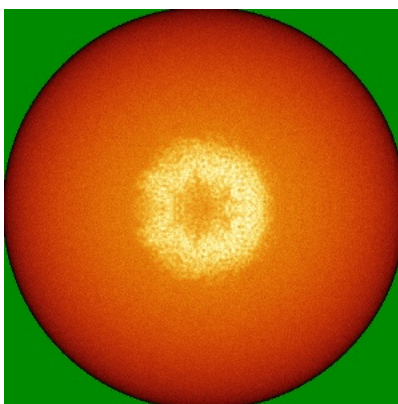


Z

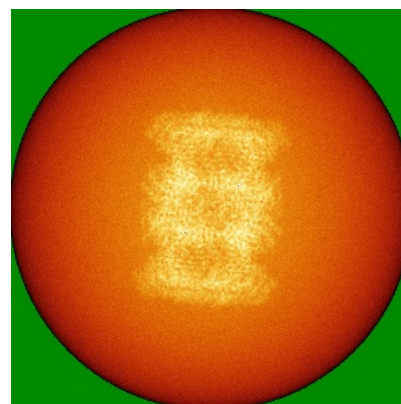
6.4.2 Raw map



X



Y

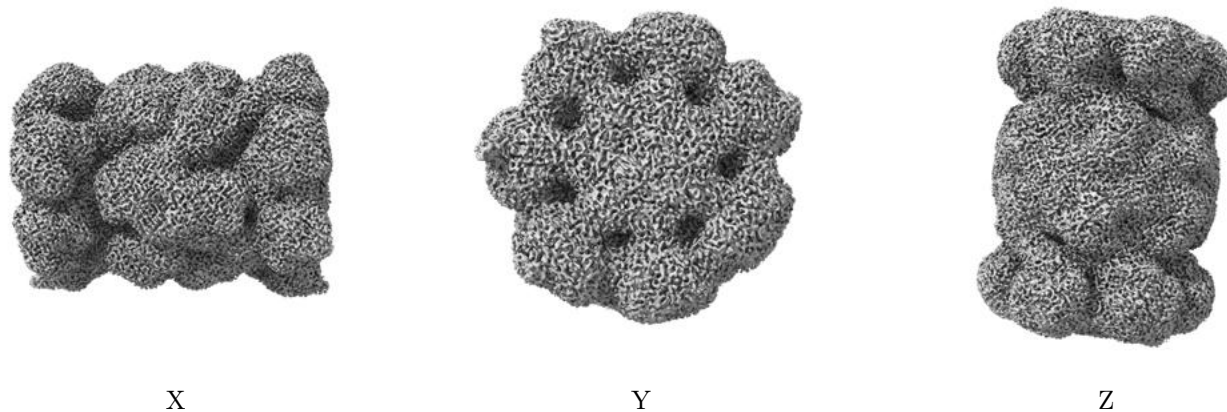


Z

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.

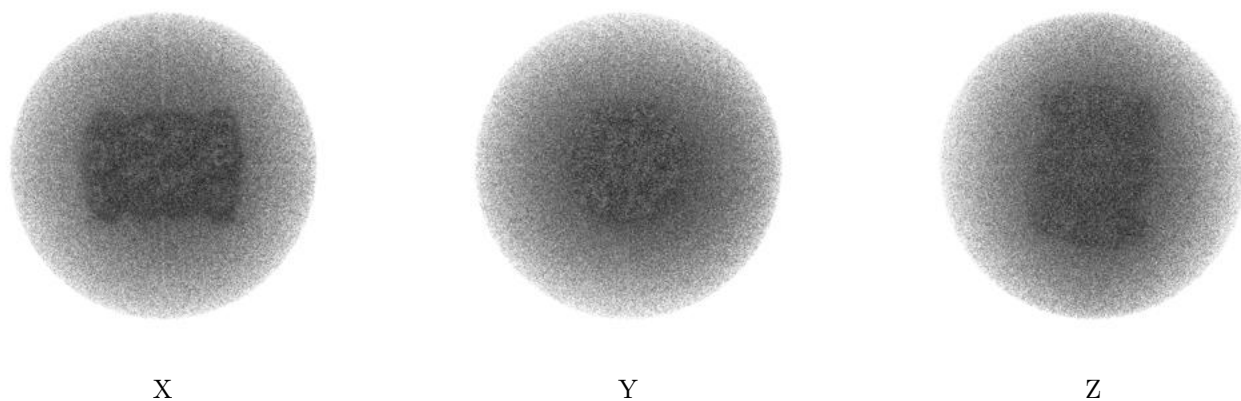
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. 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.

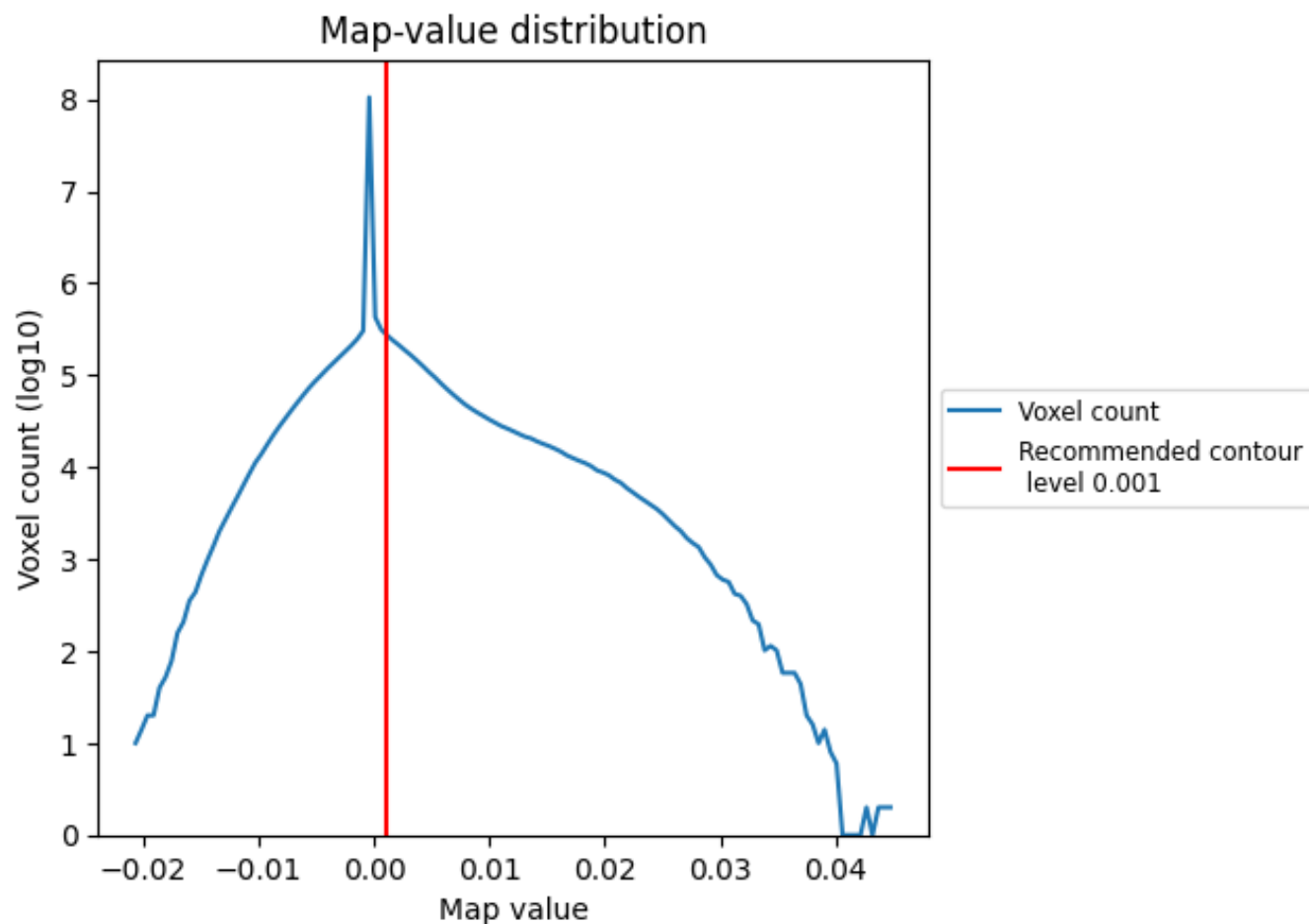
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

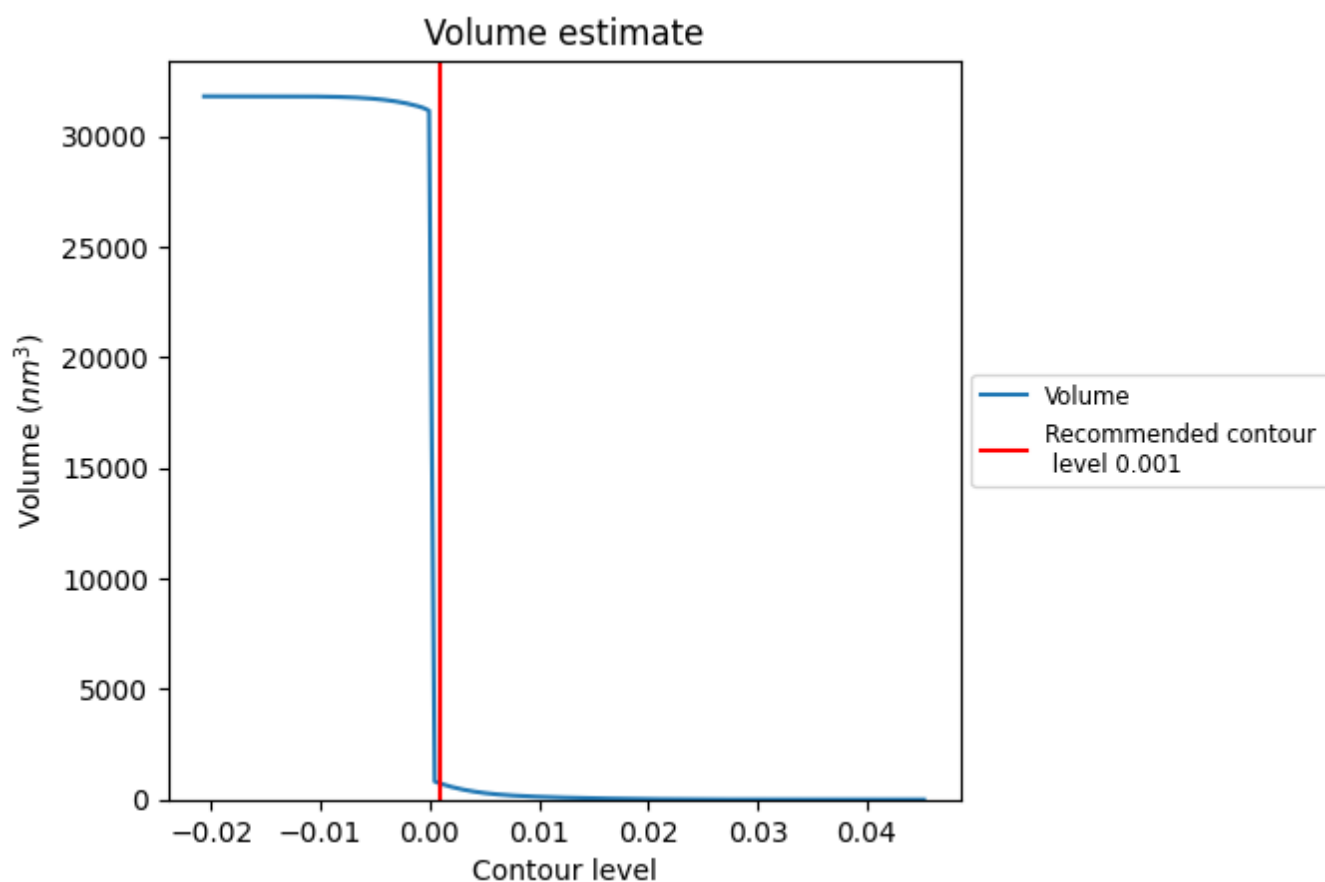
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

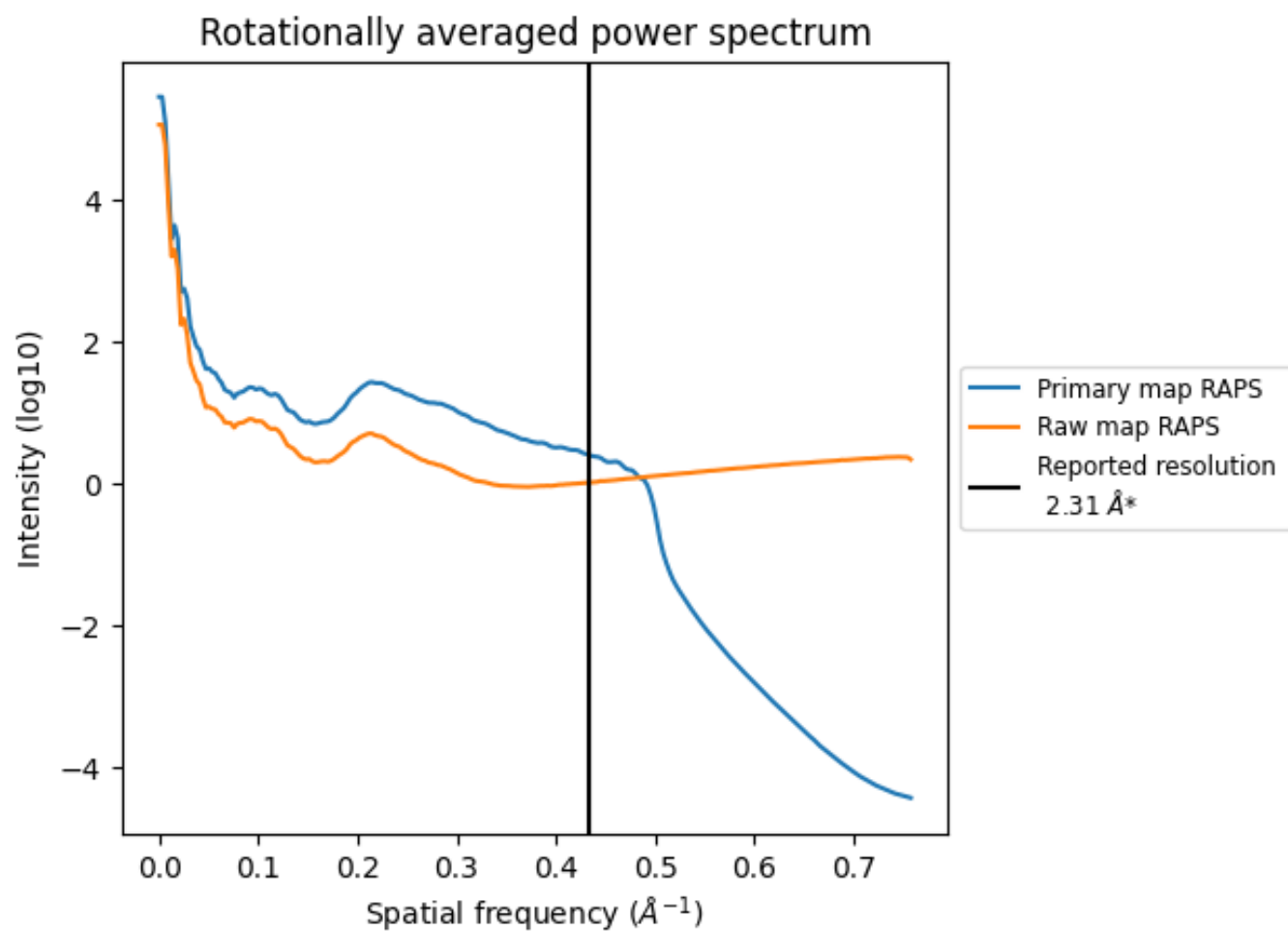
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 721 nm^3 ; this corresponds to an approximate mass of 651 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 ⓘ

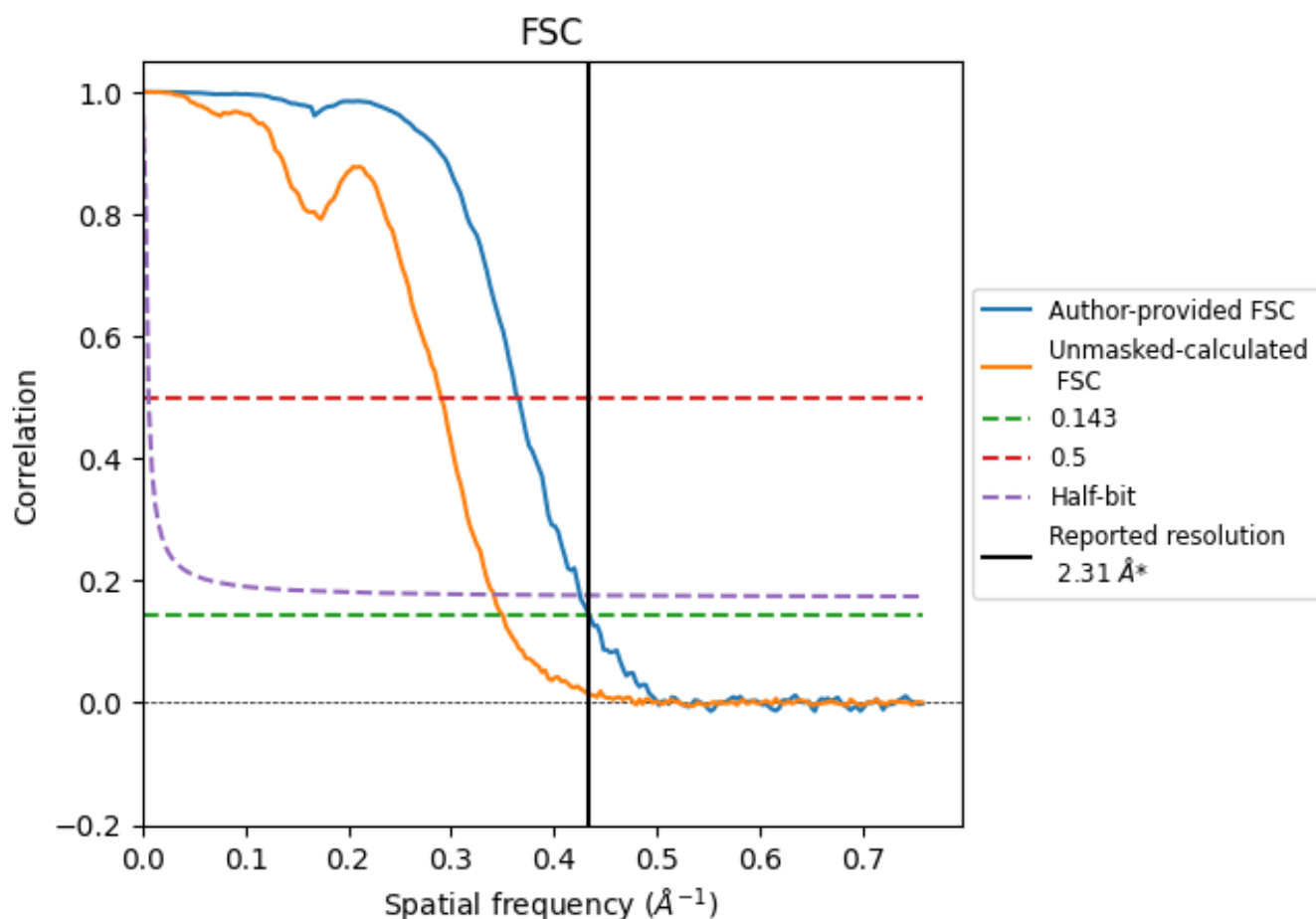


*Reported resolution corresponds to spatial frequency of 0.433 $\text{\AA}^{-1}$

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 0.433 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

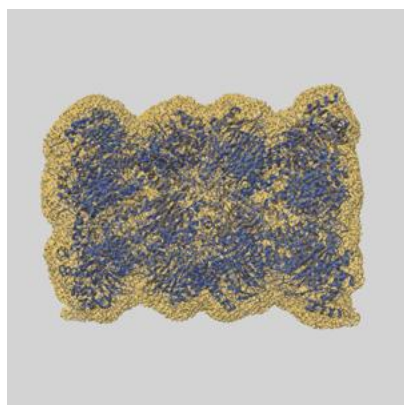
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.74	2.35
Unmasked-calculated*	2.86	3.44	2.93

*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 2.86 differs from the reported value 2.31 by more than 10 %

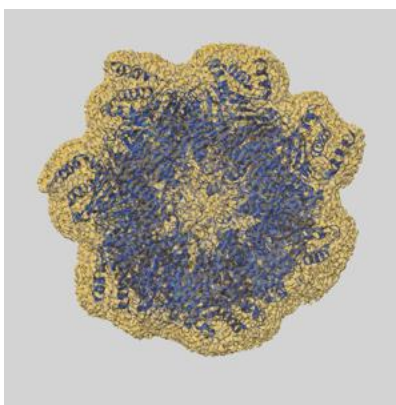
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50260 and PDB model 9F9T. Per-residue inclusion information can be found in section [3](#) on page [9](#).

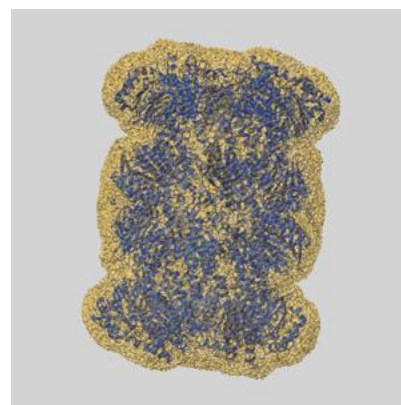
9.1 Map-model overlay [i](#)



X



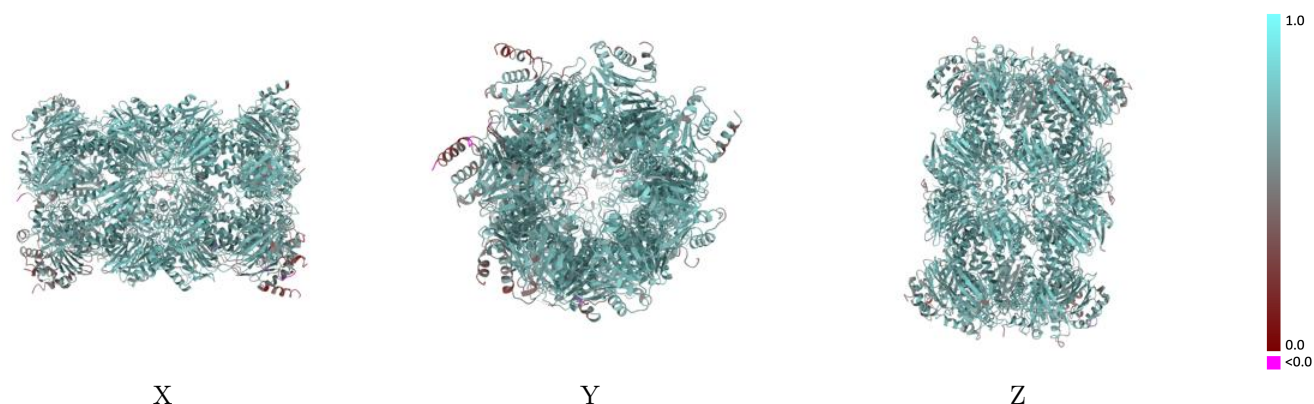
Y



Z

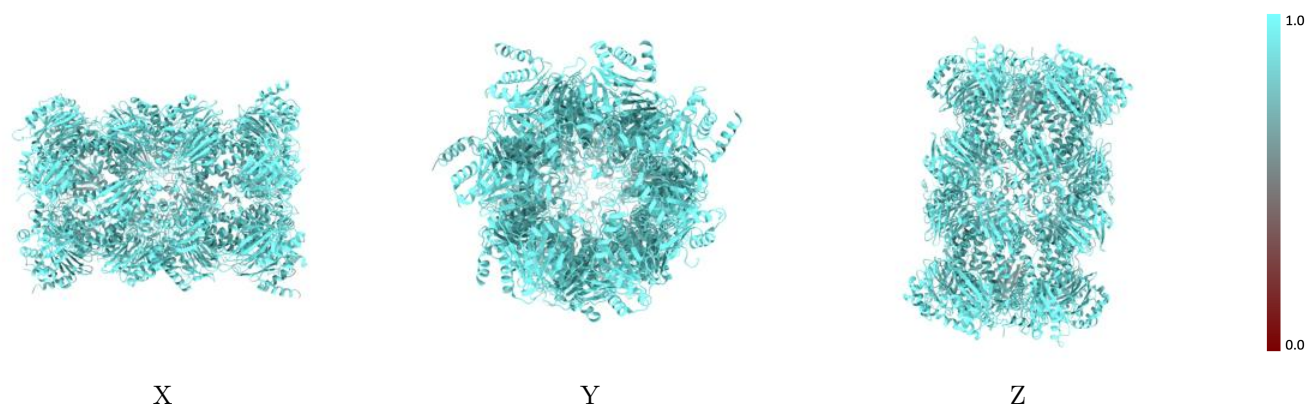
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



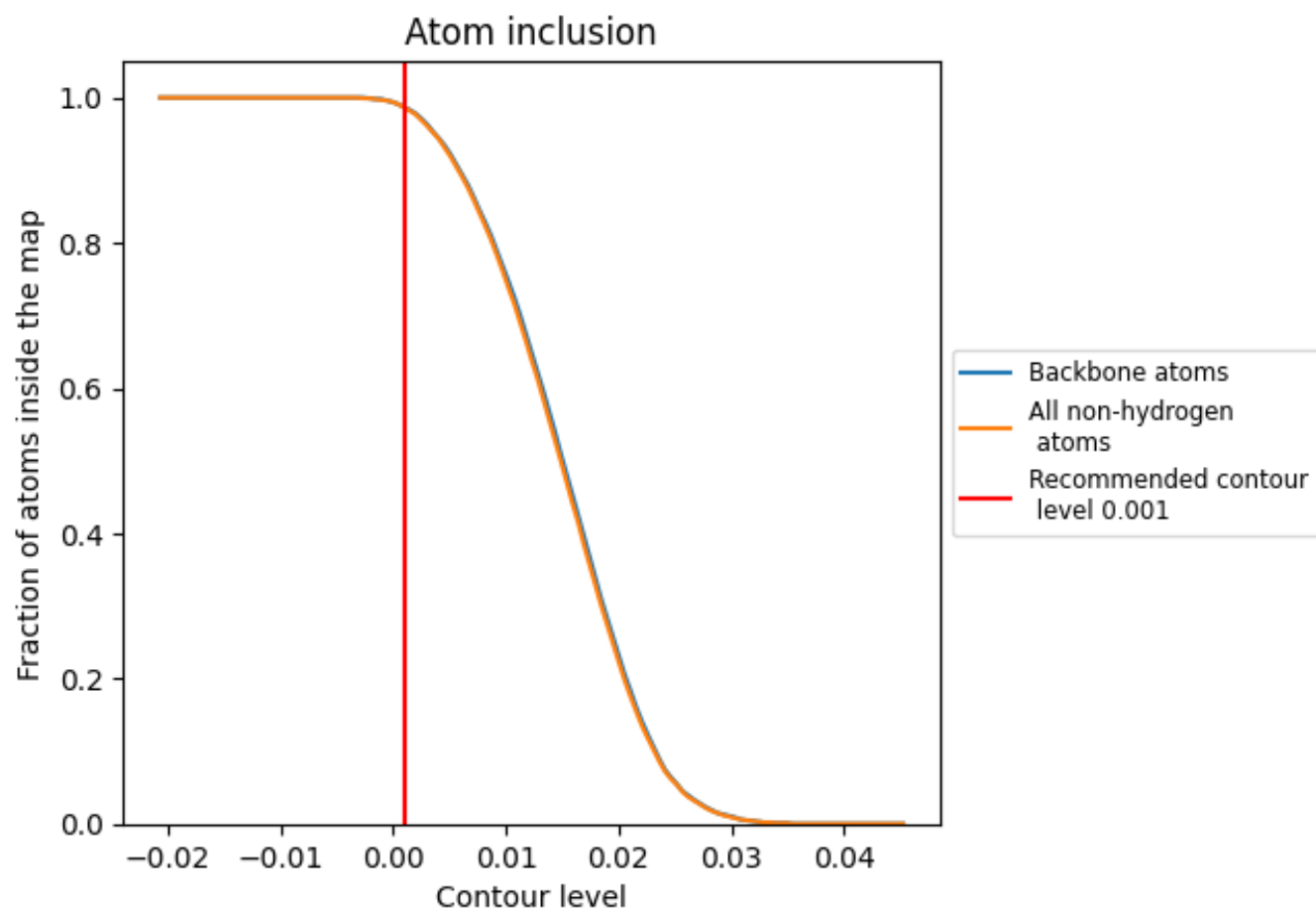
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.001).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9860	 0.6760
A	 0.9860	 0.6820
B	 0.9870	 0.6810
C	 0.9740	 0.6140
D	 0.9590	 0.5810
E	 0.9810	 0.6010
F	 0.9880	 0.6710
G	 0.9890	 0.6760
H	 0.9950	 0.7290
I	 0.9950	 0.7010
J	 0.9930	 0.7170
K	 0.9900	 0.6880
L	 0.9970	 0.7110
M	 0.9950	 0.7210
N	 0.9930	 0.7320
O	 0.9860	 0.6800
P	 0.9870	 0.6810
Q	 0.9750	 0.6140
R	 0.9590	 0.5820
S	 0.9820	 0.6010
T	 0.9880	 0.6710
U	 0.9890	 0.6740
V	 0.9950	 0.7280
W	 0.9950	 0.7030
X	 0.9930	 0.7150
Y	 0.9900	 0.6880
Z	 0.9970	 0.7120
a	 0.9950	 0.7190
b	 0.9930	 0.7300

