



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:26 AM UTC

PDB ID : 8CXB / pdb_00008cxb
EMDB ID : EMD-24276
Title : Human PA28-20S (PA28-4a3b)
Authors : Zhao, J.; Makhija, S.; Huang, B.; Cheng, Y.
Deposited on : 2022-05-20
Resolution : 2.90 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:

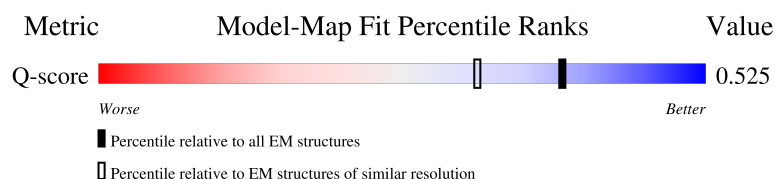
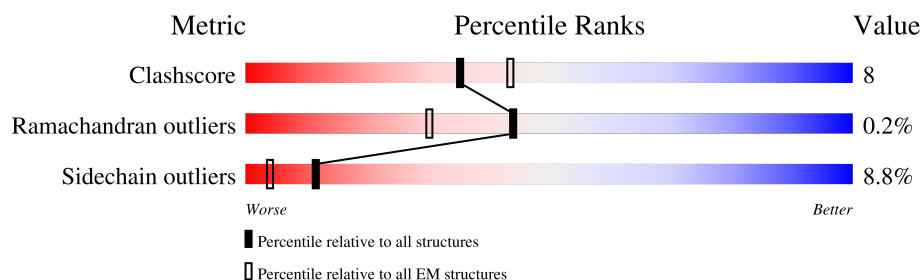
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.90 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.



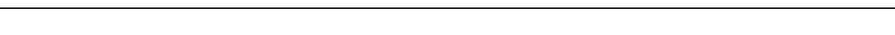
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	c	239	
1	e	239	
1	g	239	
2	d	249	

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Mol	Chain	Length	Quality of chain
2	f	249	
2	h	249	
2	i	249	
3	A	234	
3	O	234	
4	B	261	
4	P	261	
5	C	248	
5	Q	248	
6	D	241	
6	R	241	
7	E	263	
7	S	263	
8	F	255	
8	T	255	
9	G	246	
9	U	246	
10	H	277	
10	V	277	
11	I	205	
11	W	205	
12	J	201	
12	X	201	
13	K	263	
13	Y	263	

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Mol	Chain	Length	Quality of chain
14	L	241	 64% 21% • 12%
14	Z	241	 64% 21% • 12%
15	M	264	 57% 22% • 19%
15	a	264	 64% 14% • 19%
16	N	239	 70% 14% • 15%
16	b	239	 68% 15% • 15%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 57967 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 activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	214	Total	C	N	O	S	0	0
			1666	1080	281	301	4		
1	e	213	Total	C	N	O	S	0	0
			1661	1077	280	300	4		
1	g	214	Total	C	N	O	S	0	0
			1666	1080	281	301	4		

- Molecule 2 is a protein called Proteasome activator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	211	Total	C	N	O	S	0	0
			1634	1054	281	295	4		
2	f	204	Total	C	N	O	S	0	0
			1590	1025	274	287	4		
2	h	211	Total	C	N	O	S	0	0
			1636	1058	283	289	6		
2	i	211	Total	C	N	O	S	0	0
			1630	1053	282	289	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	229	Total	C	N	O	S	0	0
			1696	1101	294	295	6		
3	O	229	Total	C	N	O	S	0	0
			1678	1089	290	293	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	249	Total	C	N	O	S	0	0
			1793	1146	318	319	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	251	Total	C	N	O	S	0	0
			1843	1174	328	331	10		

- Molecule 5 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	235	Total	C	N	O	S	0	0
			1703	1082	314	302	5		
5	Q	236	Total	C	N	O	S	0	0
			1723	1095	320	303	5		

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	241	Total	C	N	O	S	0	0
			1751	1116	301	322	12		
6	R	235	Total	C	N	O	S	0	0
			1693	1076	292	314	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	239	Total	C	N	O	S	0	0
			1810	1144	331	324	11		
7	S	237	Total	C	N	O	S	0	0
			1759	1119	329	301	10		

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	240	Total	C	N	O	S	0	0
			1785	1145	313	316	11		
8	T	239	Total	C	N	O	S	0	0
			1784	1143	314	317	10		

- Molecule 9 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	239	Total	C	N	O	S	0	0
			1769	1133	305	319	12		
9	U	242	Total	C	N	O	S	0	0
			1789	1146	307	323	13		

- Molecule 10 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	222	Total	C	N	O	S	0	0
			1609	1023	276	299	11		
10	V	222	Total	C	N	O	S	0	0
			1612	1023	274	304	11		

- Molecule 11 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	204	Total	C	N	O	S	0	0
			1564	1003	264	278	19		
11	W	204	Total	C	N	O	S	0	0
			1559	1000	264	277	18		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	197	Total	C	N	O	S	0	0
			1544	998	265	272	9		
12	X	196	Total	C	N	O	S	0	0
			1535	990	264	273	8		

- Molecule 13 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	200	Total	C	N	O	S	0	0
			1525	968	273	275	9		
13	Y	200	Total	C	N	O	S	0	0
			1532	970	272	281	9		

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	213	Total	C	N	O	S	0	0
			1599	1022	279	288	10		
14	Z	213	Total	C	N	O	S	0	0
			1593	1022	281	280	10		

- Molecule 15 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	215	Total	C	N	O	S	0	0
			1643	1043	289	299	12		
15	a	215	Total	C	N	O	S	0	0
			1624	1034	288	290	12		

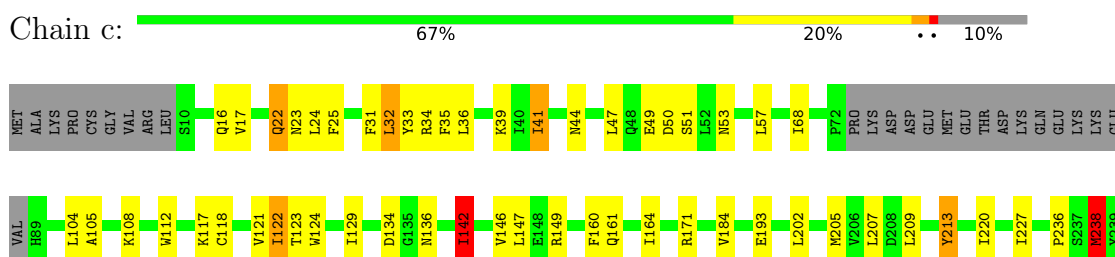
- Molecule 16 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	202	Total	C	N	O	S	0	0
			1491	939	258	282	12		
16	b	202	Total	C	N	O	S	0	0
			1478	934	258	274	12		

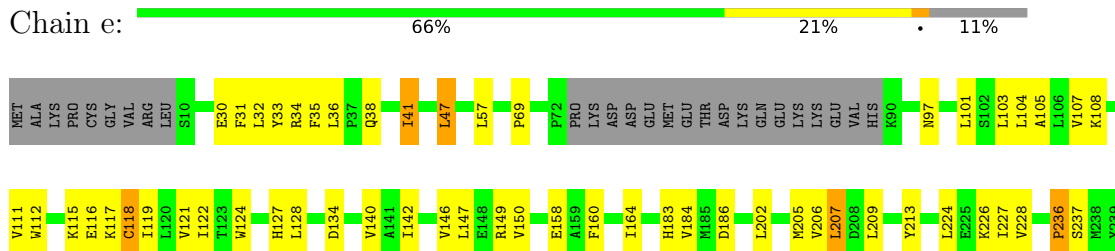
3 Residue-property plots

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.

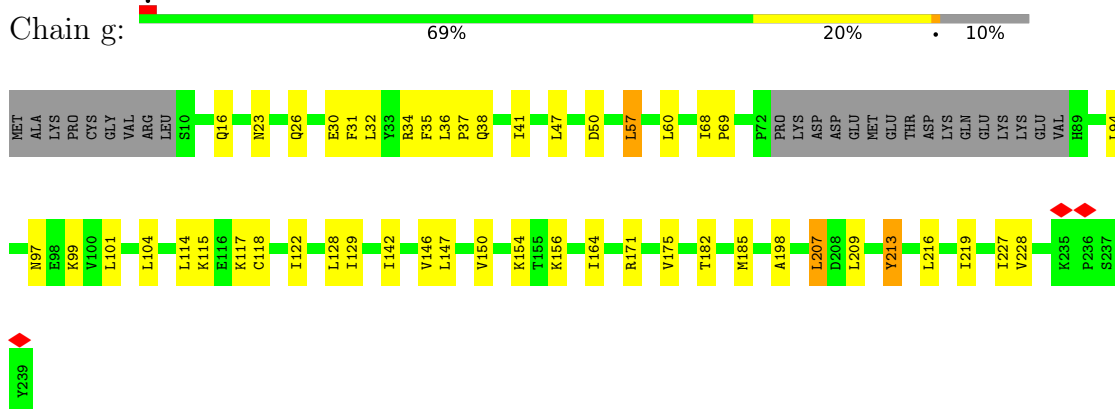
• Molecule 1: Proteasome activator complex subunit 2



• Molecule 1: Proteasome activator complex subunit 2

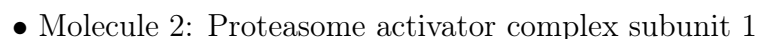


• Molecule 1: Proteasome activator complex subunit 2



• Molecule 2: Proteasome activator complex subunit 1

15%



18%



15%



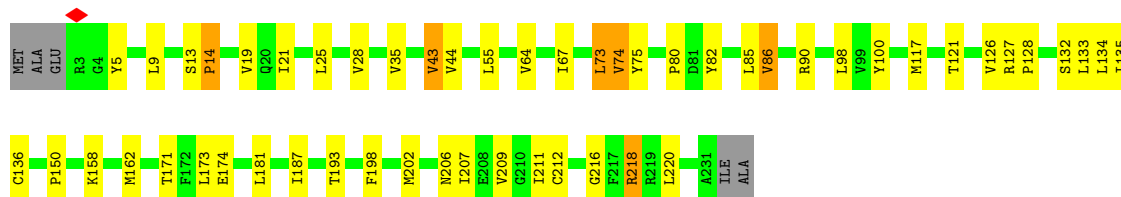
15%





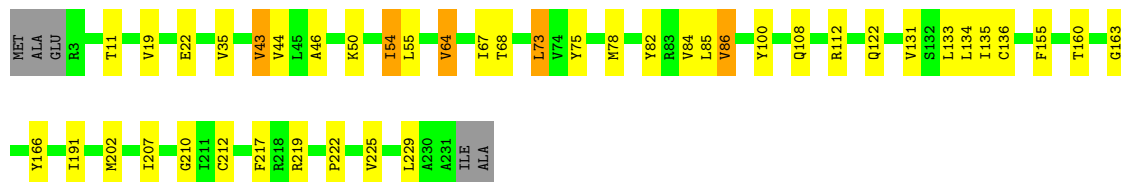
• Molecule 3: Proteasome subunit alpha type-2

Chain A: 75% 20% • •



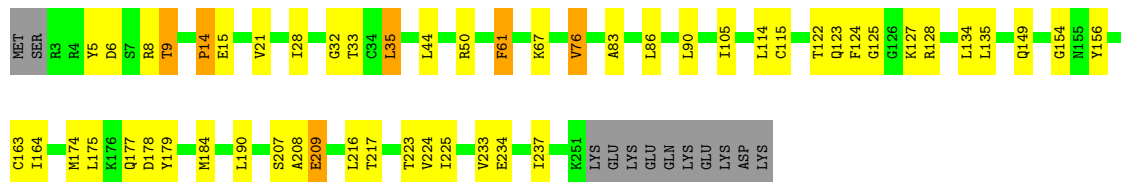
• Molecule 3: Proteasome subunit alpha type-2

Chain O: 79% 16% • •



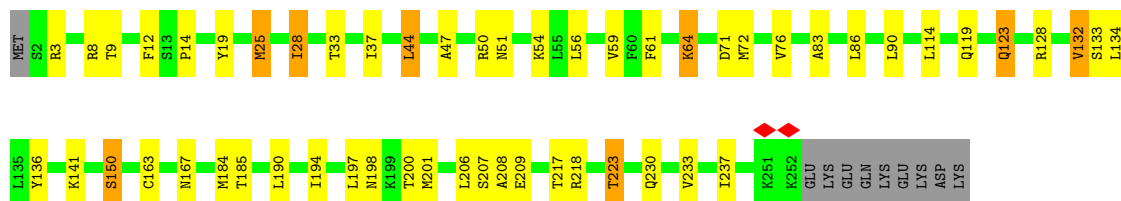
• Molecule 4: Proteasome subunit alpha type-4

Chain B: 75% 18% • 5%



• Molecule 4: Proteasome subunit alpha type-4

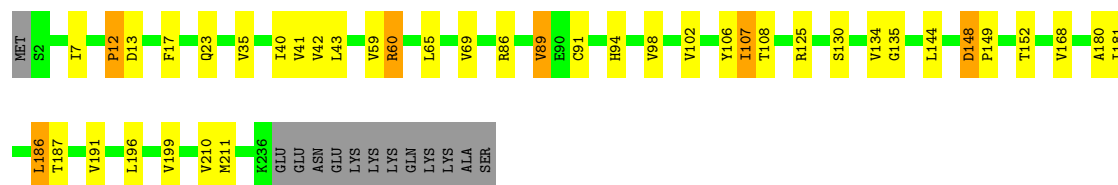
Chain P: 75% 18% • •



• Molecule 5: Proteasome subunit alpha type-7

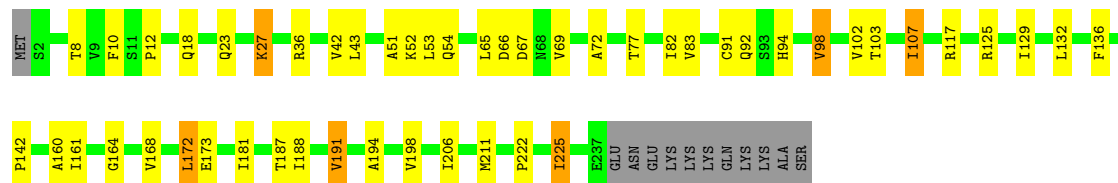
Chain C: 78% 14% • 5%





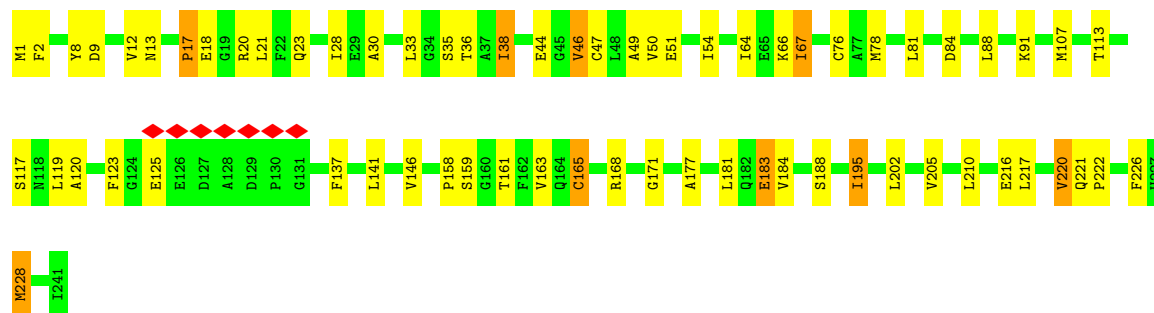
• Molecule 5: Proteasome subunit alpha type-7

Chain Q: 75% 18% 5%



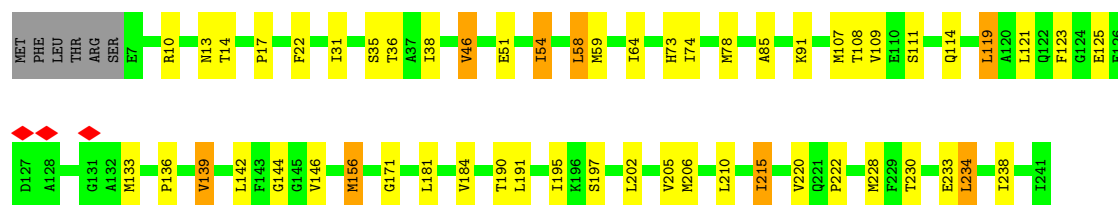
• Molecule 6: Proteasome subunit alpha type-5

Chain D: 73% 24% 3%



• Molecule 6: Proteasome subunit alpha type-5

Chain R: 75% 20% 5%



• Molecule 7: Proteasome subunit alpha type-1

Chain E: 71% 17% 9%

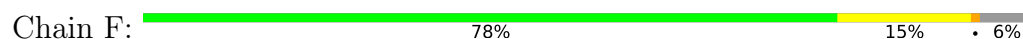




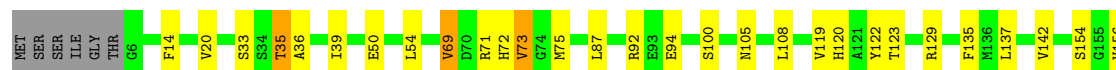
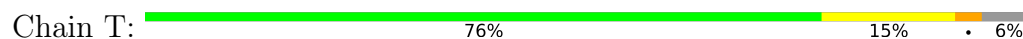
• Molecule 7: Proteasome subunit alpha type-1



• Molecule 8: Proteasome subunit alpha type-3



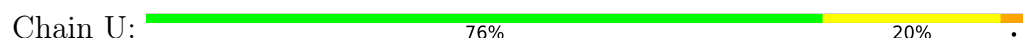
• Molecule 8: Proteasome subunit alpha type-3



• Molecule 9: Proteasome subunit alpha type-6



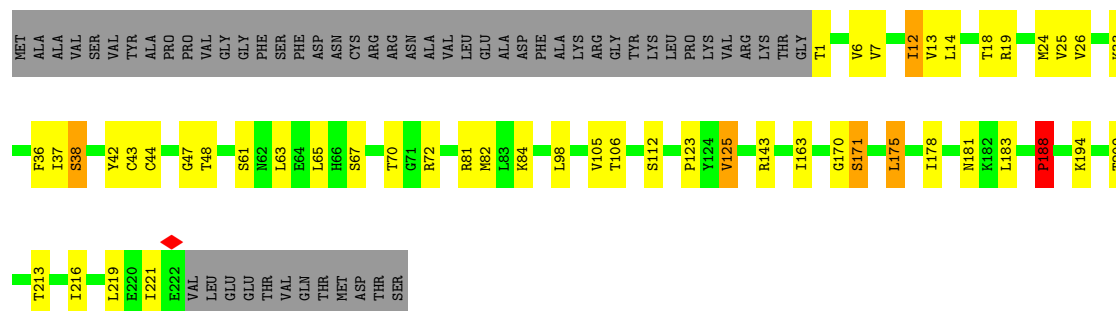
• Molecule 9: Proteasome subunit alpha type-6





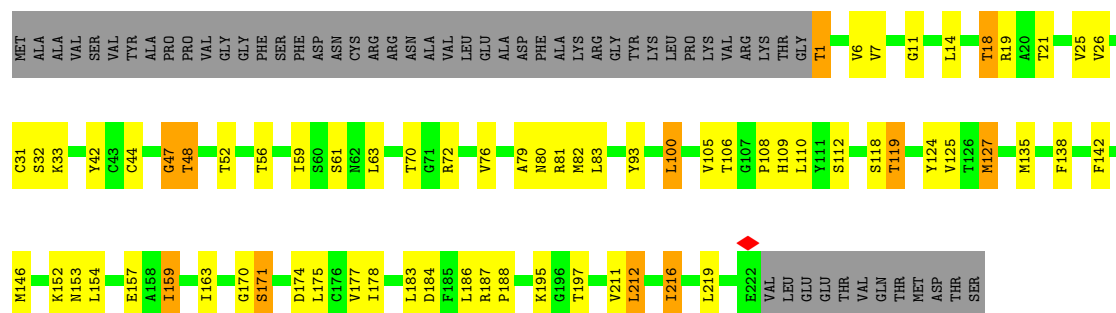
• Molecule 10: Proteasome subunit beta type-7

Chain H: 62% 16% 20%



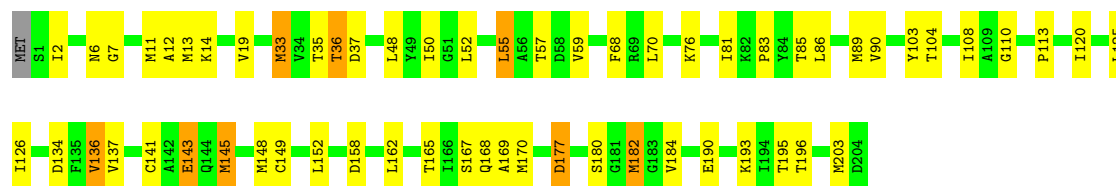
• Molecule 10: Proteasome subunit beta type-7

Chain V: 55% 21% 20%



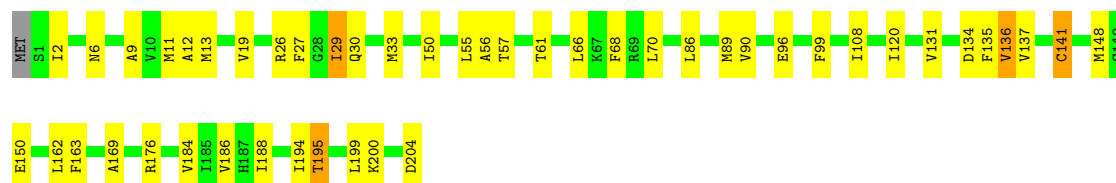
• Molecule 11: Proteasome subunit beta type-3

Chain I: 70% 25% 5%

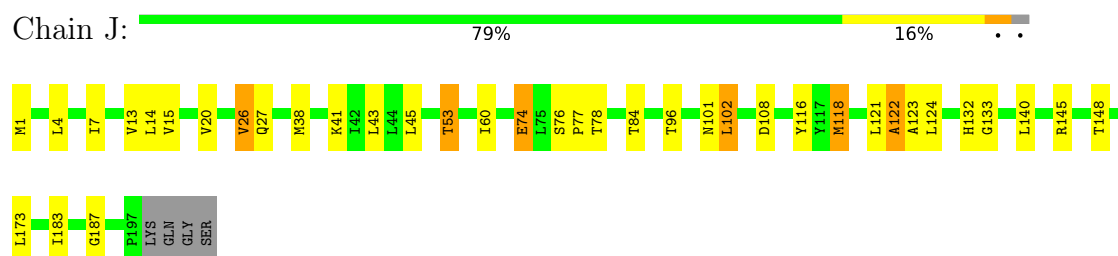


• Molecule 11: Proteasome subunit beta type-3

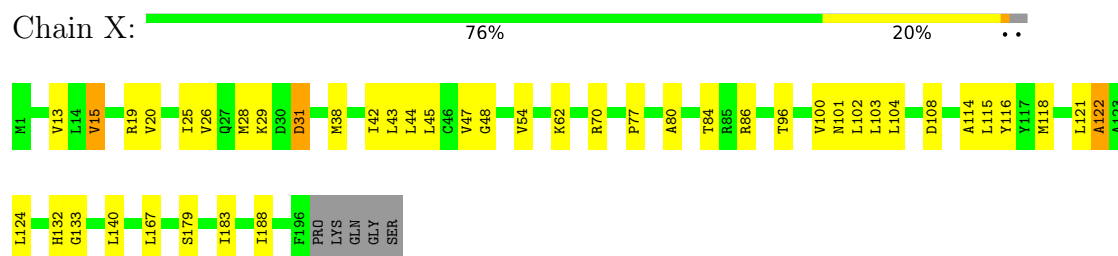
Chain W: 77% 21% 2%



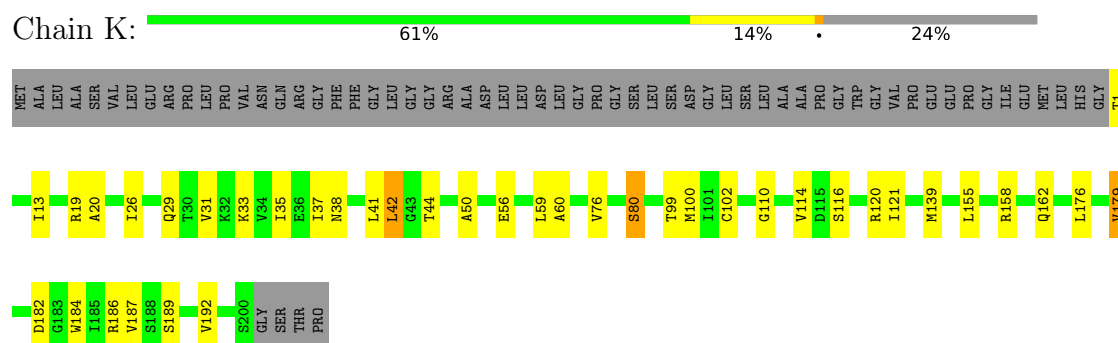
- Molecule 12: Proteasome subunit beta type-2



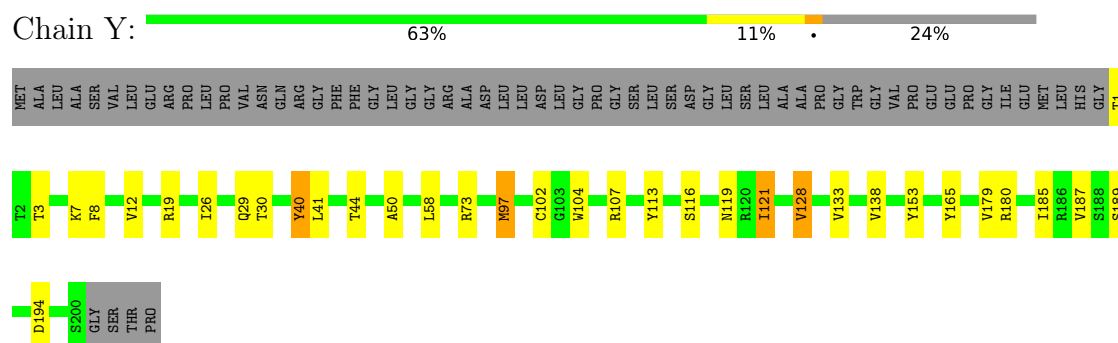
- Molecule 12: Proteasome subunit beta type-2



- Molecule 13: Proteasome subunit beta type-5

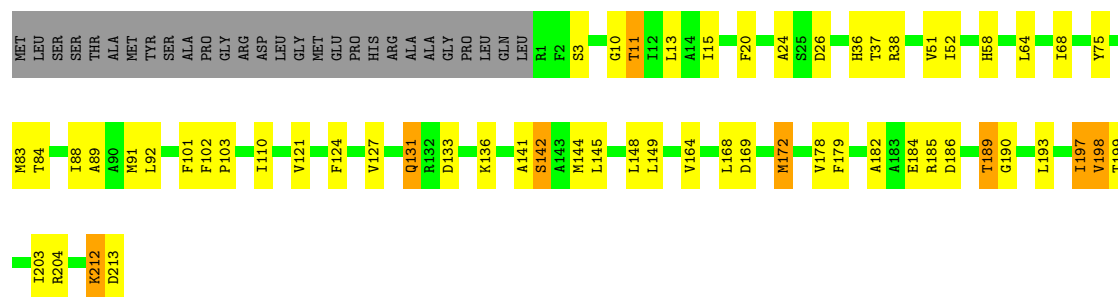


- Molecule 13: Proteasome subunit beta type-5



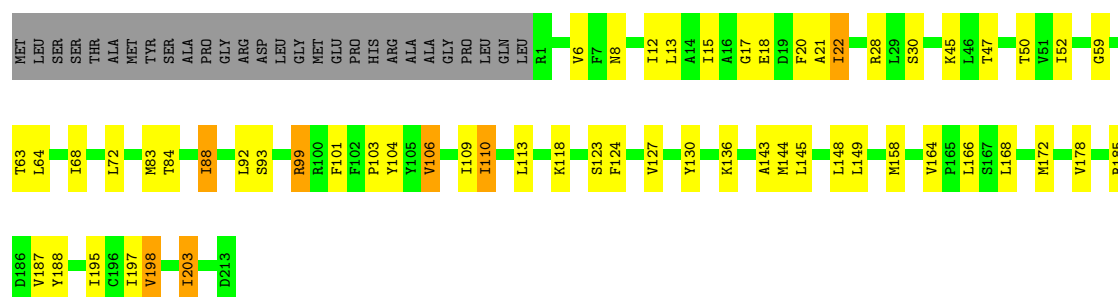
- Molecule 14: Proteasome subunit beta type-1





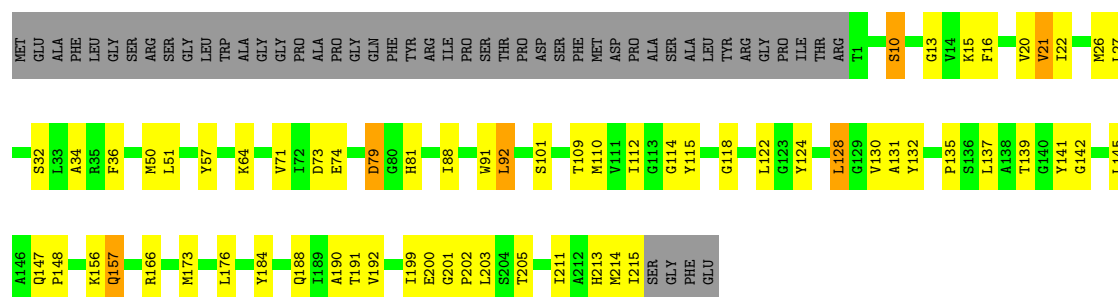
• Molecule 14: Proteasome subunit beta type-1

Chain Z: 64% 21% 12%



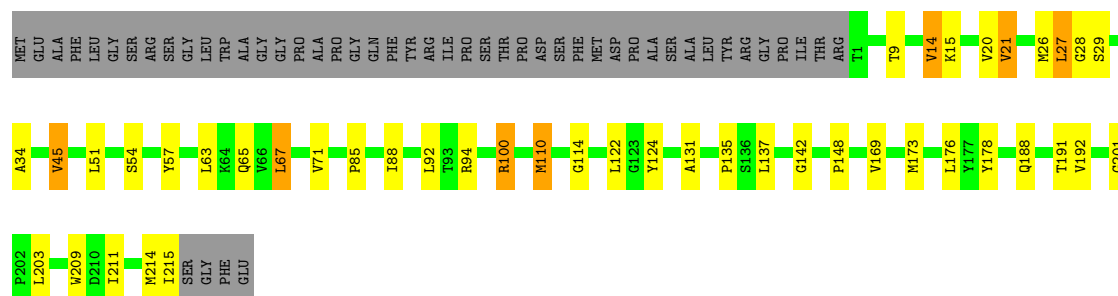
• Molecule 15: Proteasome subunit beta type-4

Chain M: 57% 22% 19%



• Molecule 15: Proteasome subunit beta type-4

Chain a: 64% 14% 19%



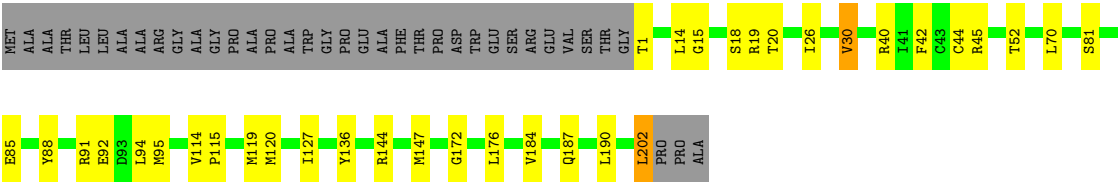
• Molecule 16: Proteasome subunit beta type-6

Chain N:

70%

14%

15%



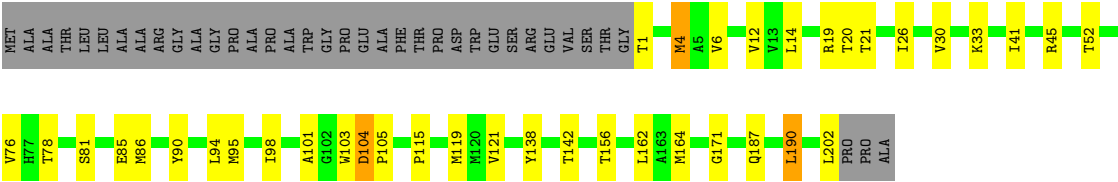
● Molecule 16: Proteasome subunit beta type-6

Chain b:

68%

15%

15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	26.106	Depositor
Minimum map value	-10.669	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	388.992, 388.992, 388.992	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	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	c	0.81	0/1700	1.43	6/2310 (0.3%)
1	e	0.81	0/1695	1.45	5/2303 (0.2%)
1	g	0.82	0/1700	1.42	4/2310 (0.2%)
2	d	0.80	0/1665	1.49	7/2258 (0.3%)
2	f	0.81	0/1620	1.47	3/2196 (0.1%)
2	h	0.79	0/1667	1.47	6/2258 (0.3%)
2	i	0.80	0/1661	1.45	6/2251 (0.3%)
3	A	0.95	0/1735	1.46	5/2362 (0.2%)
3	O	0.93	0/1717	1.39	0/2339
4	B	0.91	0/1821	1.50	9/2477 (0.4%)
4	P	0.90	0/1872	1.44	5/2541 (0.2%)
5	C	0.93	0/1729	1.50	4/2356 (0.2%)
5	Q	0.89	0/1749	1.46	3/2380 (0.1%)
6	D	0.97	0/1780	1.47	7/2417 (0.3%)
6	R	0.91	0/1720	1.41	3/2336 (0.1%)
7	E	0.95	1/1845 (0.1%)	1.43	4/2504 (0.2%)
7	S	0.94	0/1794	1.46	5/2437 (0.2%)
8	F	0.94	0/1820	1.42	3/2464 (0.1%)
8	T	0.93	0/1819	1.41	4/2463 (0.2%)
9	G	0.95	0/1802	1.49	8/2449 (0.3%)
9	U	0.91	1/1823 (0.1%)	1.43	3/2478 (0.1%)
10	H	0.97	1/1636 (0.1%)	1.51	5/2223 (0.2%)
10	V	0.97	0/1639	1.46	3/2228 (0.1%)
11	I	0.92	0/1593	1.47	5/2149 (0.2%)
11	W	0.94	0/1588	1.46	5/2144 (0.2%)
12	J	0.93	0/1577	1.41	2/2138 (0.1%)
12	X	0.94	0/1567	1.41	2/2124 (0.1%)
13	K	0.95	0/1556	1.44	2/2104 (0.1%)
13	Y	0.93	1/1563 (0.1%)	1.43	2/2115 (0.1%)
14	L	0.98	0/1629	1.48	7/2201 (0.3%)
14	Z	0.96	0/1623	1.46	5/2192 (0.2%)
15	M	0.94	0/1676	1.47	7/2272 (0.3%)
15	a	0.97	0/1657	1.44	3/2250 (0.1%)
16	N	0.99	0/1517	1.43	0/2056

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	b	0.98	0/1504	1.45	3/2038 (0.1%)
All	All	0.92	4/59059 (0.0%)	1.45	151/80123 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	127	PRO	C-O	-5.36	1.17	1.23
13	Y	189	SER	CA-CB	-5.36	1.48	1.53
10	H	38	SER	CA-CB	-5.09	1.47	1.54
9	U	133	PRO	C-O	-5.06	1.17	1.23

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	238	MET	N-CA-C	-11.12	98.40	113.30
5	C	12	PRO	N-CA-C	-10.69	94.46	111.14
6	D	17	PRO	N-CA-C	-9.82	95.83	111.14
4	B	14	PRO	N-CA-C	-9.70	96.02	111.14
14	L	103	PRO	N-CA-C	9.60	125.81	111.41
3	A	14	PRO	N-CA-C	-9.53	96.27	111.14
2	d	157	PHE	CB-CA-C	-8.51	96.67	110.79
12	X	25	ILE	N-CA-C	-8.22	105.12	113.10
10	H	188	PRO	CA-N-CD	-7.95	100.87	112.00
4	P	209	GLU	N-CA-C	-7.68	103.45	114.12
10	H	188	PRO	CB-CA-C	7.62	124.14	111.56
16	b	104	ASP	CB-CA-C	-7.54	97.46	108.84
7	E	149	PRO	N-CA-C	-7.43	103.21	113.53
10	H	188	PRO	N-CA-CB	-7.43	95.45	103.25
4	B	209	GLU	N-CA-C	-7.41	102.50	113.61
14	Z	101	PHE	CB-CA-C	7.39	124.87	110.67
2	d	150	VAL	N-CA-C	-7.39	103.26	110.72
9	G	129	ALA	N-CA-C	7.38	119.40	111.36
2	i	242	GLY	CA-C-O	-7.26	117.22	122.23
2	i	150	VAL	N-CA-C	-6.83	103.82	110.72
7	S	150	SER	N-CA-C	-6.78	101.13	110.35
12	J	53	THR	CB-CA-C	-6.78	100.24	110.88
4	B	125	GLY	N-CA-C	6.71	120.61	112.49
10	H	37	ILE	N-CA-C	-6.69	105.23	111.45
7	E	4	ASN	N-CA-C	-6.63	104.05	111.28
2	i	240	PRO	CB-CA-C	-6.63	102.51	113.06
3	A	216	GLY	CA-C-O	-6.57	117.58	122.37
9	U	211	LYS	N-CA-C	-6.51	102.64	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	150	VAL	N-CA-C	-6.47	104.18	110.72
14	L	101	PHE	CB-CA-C	6.44	121.80	110.85
12	X	133	GLY	CA-C-O	-6.44	117.79	122.23
2	h	150	VAL	N-CA-C	-6.42	104.23	110.72
6	D	195	ILE	N-CA-C	-6.37	104.31	110.42
2	h	152	VAL	N-CA-C	-6.37	104.13	110.62
2	h	146	ASN	N-CA-C	-6.36	105.48	113.23
4	P	61	PHE	N-CA-C	-6.32	104.30	111.07
15	a	178	TYR	CB-CA-C	-6.27	100.19	110.85
7	E	157	ARG	N-CA-C	-6.25	104.55	111.36
9	U	208	ILE	N-CA-C	6.24	117.02	110.72
7	S	149	PRO	N-CA-C	-6.22	104.89	113.53
1	c	136	ASN	N-CA-C	-6.21	104.29	112.24
7	S	157	ARG	N-CA-C	-6.21	104.59	111.36
13	Y	153	TYR	N-CA-C	-6.17	104.56	111.28
3	A	158	LYS	N-CA-C	-6.14	104.67	111.36
9	G	188	ASP	CA-C-N	-6.14	113.28	122.74
9	G	188	ASP	C-N-CA	-6.14	113.28	122.74
8	T	122	TYR	CB-CA-C	6.12	121.25	110.85
1	e	213	TYR	N-CA-C	-6.08	104.65	111.28
2	i	226	LEU	N-CA-C	-5.97	104.77	111.28
15	M	16	PHE	CA-CB-CG	5.97	119.77	113.80
10	V	93	TYR	CB-CA-C	5.94	120.95	110.85
10	V	159	ILE	N-CA-C	-5.90	104.60	110.62
12	J	133	GLY	CA-C-O	-5.89	118.07	122.37
6	R	195	ILE	N-CA-C	-5.87	104.63	110.62
7	E	150	SER	N-CA-C	-5.86	102.38	110.35
14	Z	88	ILE	N-CA-C	-5.81	104.69	110.62
4	P	14	PRO	N-CA-C	-5.78	105.49	113.53
2	f	146	ASN	N-CA-C	-5.76	104.87	112.24
15	M	157	GLN	CB-CA-C	-5.76	102.86	110.34
4	B	124	PHE	CB-CA-C	5.75	120.03	109.46
14	L	10	GLY	CA-C-O	-5.73	118.27	122.23
14	L	212	LYS	N-CA-C	-5.71	101.84	110.28
11	W	99	PHE	N-CA-C	-5.70	102.04	110.48
9	G	9	PHE	CB-CA-C	5.70	120.54	110.85
1	c	171	ARG	N-CA-C	-5.68	105.09	111.28
11	W	26	ARG	CB-CA-C	-5.68	100.49	109.80
3	A	14	PRO	CA-C-O	-5.67	114.87	121.34
4	B	5	TYR	N-CA-C	-5.65	105.70	112.59
1	g	238	MET	N-CA-C	-5.65	106.05	113.17
8	F	193	VAL	N-CA-C	-5.60	104.91	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	59	VAL	N-CA-C	-5.59	105.05	110.42
4	B	61	PHE	CA-CB-CG	5.56	119.36	113.80
8	T	92	ARG	N-CA-C	-5.55	105.22	111.28
11	W	27	PHE	CB-CA-C	-5.54	101.11	110.19
5	Q	117	ARG	N-CA-C	-5.52	105.26	111.28
2	d	226	LEU	N-CA-C	-5.51	105.27	111.28
4	B	190	LEU	N-CA-C	-5.50	105.29	111.28
14	L	172	MET	N-CA-C	-5.48	105.30	111.28
11	W	68	PHE	CA-CB-CG	5.48	119.28	113.80
1	g	171	ARG	N-CA-C	-5.48	105.31	111.28
8	F	143	ASN	CB-CA-C	-5.48	102.25	110.90
15	M	141	TYR	N-CA-C	-5.48	106.44	113.01
5	Q	53	LEU	N-CA-C	-5.45	106.63	113.72
14	Z	6	VAL	CA-C-O	-5.45	116.23	121.63
7	S	195	LEU	N-CA-C	-5.45	105.34	111.28
1	e	118	CYS	N-CA-C	-5.44	105.34	111.28
4	P	50	ARG	N-CA-C	-5.41	106.63	113.18
2	i	146	ASN	N-CA-C	-5.41	105.32	112.24
1	g	213	TYR	N-CA-C	-5.41	105.39	111.28
7	S	190	HIS	N-CA-C	-5.40	105.40	111.28
8	T	167	LYS	CB-CA-C	-5.39	101.84	110.79
16	b	78	THR	N-CA-C	-5.38	105.41	111.28
15	a	57	TYR	N-CA-C	-5.38	105.58	111.82
14	L	142	SER	N-CA-C	-5.38	105.42	111.28
6	R	17	PRO	N-CA-C	-5.37	106.86	113.84
2	d	103	PRO	N-CA-C	-5.34	102.80	111.03
2	d	37	ILE	N-CA-C	-5.33	105.18	110.62
6	D	125	GLU	N-CA-C	-5.32	106.09	112.58
9	G	210	PHE	N-CA-C	5.32	117.58	110.35
1	c	213	TYR	N-CA-C	-5.31	105.49	111.28
11	I	68	PHE	N-CA-C	-5.30	105.40	111.07
16	b	162	LEU	N-CA-C	-5.29	105.51	111.28
6	R	114	GLN	N-CA-C	-5.28	105.52	111.28
14	Z	45	LYS	CB-CA-C	-5.28	102.32	111.30
10	H	36	PHE	CA-CB-CG	5.28	119.08	113.80
11	I	68	PHE	CA-CB-CG	5.27	119.07	113.80
5	Q	12	PRO	N-CA-C	-5.27	102.83	111.15
5	C	130	SER	N-CA-C	-5.25	100.84	109.40
14	L	168	LEU	N-CA-C	-5.25	105.56	111.28
9	G	120	ASP	CB-CA-C	5.25	119.50	110.79
6	D	17	PRO	CA-C-O	-5.22	115.38	121.34
2	f	209	TYR	N-CA-C	-5.22	105.59	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	128	LEU	N-CA-C	-5.21	106.75	113.01
2	d	152	VAL	N-CA-C	-5.19	105.33	110.62
8	T	161	TRP	N-CA-C	-5.18	105.71	111.36
9	U	185	LYS	N-CA-C	-5.18	105.63	111.28
2	h	246	GLY	CA-C-O	-5.18	115.41	120.75
11	I	7	GLY	CA-C-O	-5.17	117.74	122.24
2	i	104	VAL	N-CA-C	-5.17	104.41	110.05
5	C	17	PHE	CB-CA-C	5.17	119.64	110.85
1	c	142	ILE	N-CA-C	-5.17	105.35	110.62
4	B	154	GLY	N-CA-C	-5.17	108.09	115.64
15	M	57	TYR	N-CA-C	-5.16	105.84	111.82
14	Z	103	PRO	N-CA-C	5.15	119.40	111.21
2	h	240	PRO	CB-CA-C	-5.15	104.87	113.06
1	c	160	PHE	N-CA-C	-5.15	105.67	111.28
4	P	71	ASP	CB-CA-C	-5.14	102.03	110.72
6	D	8	TYR	N-CA-C	-5.14	106.98	114.12
15	M	73	ASP	CB-CA-C	5.14	119.32	110.79
9	G	10	ASP	CA-C-O	-5.13	116.08	121.88
9	G	202	LEU	N-CA-C	-5.13	105.69	111.28
15	a	85	PRO	N-CA-C	-5.13	106.40	113.53
1	g	198	ALA	N-CA-C	-5.12	105.70	111.28
5	C	106	TYR	N-CA-C	-5.10	105.72	111.28
13	Y	8	PHE	CA-CB-CG	5.10	118.90	113.80
3	A	90	ARG	N-CA-C	-5.09	105.73	111.28
1	e	160	PHE	N-CA-C	-5.09	105.73	111.28
1	e	140	VAL	N-CA-C	-5.08	105.44	110.62
6	D	91	LYS	N-CA-C	-5.08	105.75	111.28
10	V	47	GLY	CA-C-O	-5.08	117.22	122.25
2	h	186	THR	CB-CA-C	-5.06	102.40	110.79
2	d	102	GLY	CA-C-O	-5.06	117.56	122.46
8	F	112	ALA	N-CA-C	-5.04	105.78	111.28
11	W	96	GLU	N-CA-C	-5.03	105.79	111.28
1	e	111	VAL	N-CA-C	-5.03	105.49	110.62
6	D	177	ALA	N-CA-C	-5.02	105.89	111.36
11	I	203	MET	N-CA-C	-5.02	106.93	113.16
15	M	64	LYS	CB-CA-C	-5.02	102.46	110.79
4	B	178	ASP	N-CA-C	5.01	116.82	111.36
13	K	33	LYS	CA-C-N	-5.00	116.38	122.93
13	K	33	LYS	C-N-CA	-5.00	116.38	122.93

There are no chirality outliers.

There are no planarity outliers.

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	c	1666	0	1655	35	0
1	e	1661	0	1653	27	0
1	g	1666	0	1655	27	0
2	d	1634	0	1625	36	0
2	f	1590	0	1594	30	0
2	h	1636	0	1652	31	0
2	i	1630	0	1634	33	0
3	A	1696	0	1647	30	0
3	O	1678	0	1616	24	0
4	B	1793	0	1704	25	0
4	P	1843	0	1780	38	0
5	C	1703	0	1616	17	0
5	Q	1723	0	1659	30	0
6	D	1751	0	1707	35	0
6	R	1693	0	1629	29	0
7	E	1810	0	1759	31	0
7	S	1759	0	1711	32	0
8	F	1785	0	1717	17	0
8	T	1784	0	1718	26	0
9	G	1769	0	1730	26	0
9	U	1789	0	1743	32	0
10	H	1609	0	1609	23	0
10	V	1612	0	1602	51	0
11	I	1564	0	1587	30	0
11	W	1559	0	1575	26	0
12	J	1544	0	1537	19	0
12	X	1535	0	1527	25	0
13	K	1525	0	1490	20	0
13	Y	1532	0	1483	10	0
14	L	1599	0	1582	31	0
14	Z	1593	0	1595	34	0
15	M	1643	0	1611	40	0
15	a	1624	0	1585	27	0
16	N	1491	0	1458	21	0
16	b	1478	0	1448	24	0
All	All	57967	0	56893	903	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 8.

All (903) 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)
2:h:122:LYS:HG3	2:i:210:ARG:HD3	1.52	0.92
10:V:42:TYR:CE1	10:V:183:LEU:HD11	2.09	0.88
10:V:216:ILE:HD12	10:V:216:ILE:N	1.90	0.86
9:U:103:TYR:O	10:V:81:ARG:HD3	1.74	0.86
5:Q:27:LYS:NZ	5:Q:27:LYS:HB3	1.91	0.85
6:D:117:SER:HB3	7:E:82:ARG:HH12	1.40	0.84
14:L:148:LEU:HD23	14:L:178:VAL:HG12	1.56	0.84
4:P:76:VAL:HG11	4:P:83:ALA:HB2	1.60	0.84
14:Z:148:LEU:HD23	14:Z:178:VAL:HG12	1.60	0.83
2:f:157:PHE:HA	2:f:160:MET:HE2	1.59	0.83
10:H:123:PRO:HG3	15:a:211:ILE:HG23	1.60	0.82
1:g:36:LEU:HD23	1:g:213:TYR:HD1	1.44	0.82
1:c:32:LEU:HA	1:c:36:LEU:HD12	1.62	0.81
11:W:148:MET:HG2	11:W:169:ALA:HA	1.61	0.81
16:b:4:MET:HG2	16:b:156:THR:HG23	1.63	0.80
2:d:21:LEU:HD11	2:d:134:TRP:HA	1.64	0.79
3:O:202:MET:HE3	3:O:207:ILE:HG21	1.64	0.79
11:I:148:MET:HG2	11:I:169:ALA:HA	1.65	0.78
6:D:35:SER:HB2	6:D:51:GLU:HG3	1.66	0.78
7:S:81:ALA:HB2	7:S:130:VAL:HG11	1.67	0.77
4:P:76:VAL:HG22	4:P:134:LEU:HD22	1.65	0.77
6:R:85:ALA:HB2	6:R:139:VAL:HG11	1.67	0.76
15:M:20:VAL:HG11	15:M:122:LEU:HD13	1.67	0.75
1:c:36:LEU:HD23	1:c:213:TYR:HD1	1.51	0.75
11:I:2:ILE:HG13	11:I:55:LEU:HD11	1.66	0.75
13:K:42:LEU:HD21	13:K:179:VAL:HG22	1.70	0.73
7:S:50:LYS:HB3	7:S:59:HIS:HB3	1.70	0.73
6:R:146:VAL:HG11	6:R:222:PRO:HA	1.71	0.73
5:Q:27:LYS:HB3	5:Q:27:LYS:HZ1	1.52	0.73
2:h:66:PRO:HG3	2:h:192:PRO:HB2	1.71	0.73
5:C:135:GLY:HA2	5:C:211:MET:HE1	1.71	0.73
9:G:72:ILE:HG21	9:G:114:LEU:HD21	1.68	0.73
10:V:163:ILE:HG23	10:V:170:GLY:HA2	1.71	0.73
2:d:66:PRO:HG3	2:d:192:PRO:HB2	1.71	0.72
4:P:3:ARG:HB3	4:P:8:ARG:HH22	1.55	0.71
1:c:104:LEU:HD23	1:c:202:LEU:HD21	1.72	0.71
11:W:66:LEU:HD11	11:W:90:VAL:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:19:ARG:HG3	16:b:26:ILE:HG23	1.73	0.70
10:H:13:VAL:HG12	10:H:175:LEU:HD12	1.72	0.70
11:W:50:ILE:HG13	11:W:108:ILE:HG12	1.73	0.70
7:S:120:THR:HG23	8:T:129:ARG:HH21	1.57	0.69
14:Z:198:VAL:HB	14:Z:203:ILE:HD13	1.75	0.69
3:A:211:ILE:HD11	3:A:218:ARG:HE	1.58	0.68
6:D:13:ASN:HA	7:E:126:ARG:HB3	1.75	0.68
10:V:42:TYR:CD1	10:V:183:LEU:HD11	2.28	0.68
16:b:12:VAL:HG11	16:b:101:ALA:HB1	1.75	0.68
15:a:27:LEU:HD11	15:a:34:ALA:HB1	1.75	0.68
11:I:50:ILE:HG13	11:I:108:ILE:HG12	1.75	0.68
10:V:7:VAL:HG23	10:V:7:VAL:O	1.93	0.68
3:O:191:ILE:HG23	3:O:202:MET:HE1	1.76	0.68
15:a:14:VAL:HG13	15:a:21:VAL:HG13	1.76	0.68
7:S:72:ILE:HG22	7:S:134:ILE:HG12	1.76	0.67
14:Z:68:ILE:HD11	14:Z:92:LEU:HD13	1.76	0.67
10:V:18:THR:HG22	10:V:31:CYS:N	2.09	0.67
10:H:216:ILE:HG12	11:I:195:THR:HG23	1.77	0.67
12:X:101:ASN:HB3	12:X:132:HIS:CE1	2.29	0.67
15:a:20:VAL:HG11	15:a:122:LEU:HD13	1.78	0.66
1:g:146:VAL:HG21	1:g:227:ILE:HD11	1.76	0.66
1:c:33:TYR:HB2	1:c:34:ARG:HH21	1.61	0.66
7:E:81:ALA:HB2	7:E:130:VAL:HG21	1.77	0.66
14:L:144:MET:HE1	14:L:185:ARG:HB2	1.78	0.66
11:W:12:ALA:HB3	11:W:136:VAL:HG23	1.77	0.66
4:P:33:THR:HG21	4:P:200:THR:HG21	1.77	0.66
10:H:42:TYR:HB2	10:H:178:ILE:HD11	1.77	0.66
14:Z:63:THR:HG22	15:a:94:ARG:HH22	1.61	0.66
4:P:76:VAL:HG11	4:P:83:ALA:CB	2.25	0.66
16:b:45:ARG:HB3	16:b:52:THR:HB	1.78	0.65
2:h:33:PHE:HB2	2:h:34:PRO:HD3	1.77	0.65
1:g:32:LEU:HA	1:g:36:LEU:HD12	1.76	0.65
4:B:123:GLN:HG3	5:C:125:ARG:HG2	1.77	0.65
9:U:138:MET:HE3	9:U:140:LEU:HD11	1.78	0.65
6:D:44:GLU:O	6:D:222:PRO:HD3	1.97	0.65
10:H:24:MET:HE3	14:Z:187:VAL:HG21	1.78	0.64
11:W:29:ILE:HG22	11:W:30:GLN:H	1.62	0.64
14:L:68:ILE:HD11	14:L:92:LEU:HD13	1.78	0.64
9:U:141:ILE:HG22	9:U:151:VAL:HG22	1.78	0.64
2:i:44:LEU:HA	2:i:49:LEU:HD23	1.78	0.64
10:V:170:GLY:O	10:V:171:SER:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:91:CYS:HA	5:C:102:VAL:HG21	1.80	0.64
8:T:108:LEU:HD11	8:T:137:LEU:HB3	1.78	0.64
8:T:159:GLY:HA3	9:U:65:THR:HG21	1.79	0.64
4:B:216:LEU:HD12	4:B:225:ILE:HG12	1.79	0.63
4:B:35:LEU:HD11	4:B:175:LEU:HD11	1.80	0.63
10:V:42:TYR:CE1	10:V:183:LEU:CD1	2.80	0.63
16:b:115:PRO:HD2	16:b:119:MET:O	1.99	0.62
1:g:128:LEU:HD13	1:g:228:VAL:HA	1.81	0.62
11:I:143:GLU:HG3	14:Z:144:MET:HG2	1.82	0.62
1:c:146:VAL:HG21	1:c:227:ILE:HD11	1.82	0.62
8:F:158:TYR:HB3	9:G:61:LEU:HD21	1.80	0.62
1:g:104:LEU:HD22	1:g:164:ILE:HG23	1.81	0.62
5:Q:27:LYS:NZ	5:Q:27:LYS:CB	2.58	0.62
2:h:156:VAL:HG12	2:h:160:MET:HE3	1.82	0.62
2:d:159:LEU:HD22	6:D:1:MET:HB2	1.81	0.61
7:E:47:VAL:HG12	7:E:212:ILE:HG12	1.81	0.61
2:d:44:LEU:HA	2:d:49:LEU:HD11	1.81	0.61
6:R:230:THR:HG22	6:R:233:GLU:HG3	1.83	0.61
2:d:117:LEU:HD22	2:d:212:ILE:HG23	1.82	0.61
10:H:19:ARG:HB2	10:H:170:GLY:O	2.00	0.61
15:a:63:LEU:HD12	15:a:110:MET:HE1	1.83	0.61
5:Q:42:VAL:HG11	5:Q:191:VAL:HG11	1.83	0.61
2:d:58:LYS:HE3	2:d:202:HIS:HB3	1.83	0.61
13:Y:97:MET:H	13:Y:116:SER:HB3	1.65	0.61
14:L:198:VAL:HB	14:L:203:ILE:HD13	1.83	0.61
8:T:39:ILE:HD12	8:T:193:VAL:HG22	1.81	0.60
1:e:112:TRP:HZ2	2:f:213:ARG:HE	1.47	0.60
12:X:44:LEU:HD12	12:X:104:LEU:HD12	1.83	0.60
7:E:109:VAL:HA	7:E:112:ILE:HD12	1.83	0.60
2:f:66:PRO:HG3	2:f:192:PRO:HB2	1.84	0.60
11:I:11:MET:HE2	11:I:170:MET:HG2	1.83	0.60
6:R:10:ARG:HB2	6:R:14:THR:HG21	1.84	0.60
6:D:67:ILE:HG22	6:D:226:PHE:HZ	1.67	0.60
10:V:112:SER:HB2	10:V:127:MET:HE2	1.84	0.60
4:B:67:LYS:HG3	4:B:225:ILE:HD12	1.83	0.60
12:X:38:MET:HB2	12:X:42:ILE:HG13	1.83	0.60
14:Z:52:ILE:HG13	14:Z:110:ILE:HG12	1.84	0.60
1:e:47:LEU:HD21	1:e:207:LEU:HD23	1.84	0.59
9:U:103:TYR:O	10:V:81:ARG:CD	2.47	0.59
10:H:70:THR:HG23	10:H:72:ARG:H	1.67	0.59
11:I:35:THR:HG22	11:I:37:ASP:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:188:VAL:HG21	7:E:232:PHE:CD1	2.38	0.59
2:i:132:THR:HG23	2:i:157:PHE:HE1	1.67	0.59
1:e:69:PRO:HG3	1:e:183:HIS:HA	1.84	0.59
2:f:117:LEU:HD22	2:f:212:ILE:HG23	1.84	0.59
9:U:38:THR:HA	9:U:169:GLY:HA3	1.85	0.59
3:A:198:PHE:HZ	3:A:206:ASN:HB3	1.68	0.59
4:B:76:VAL:HG11	4:B:83:ALA:CB	2.33	0.59
2:d:157:PHE:HA	2:d:160:MET:HE2	1.83	0.59
8:T:75:MET:HE2	8:T:137:LEU:HD11	1.85	0.59
7:S:50:LYS:CB	7:S:59:HIS:HB3	2.33	0.58
10:V:159:ILE:O	10:V:163:ILE:HG13	2.03	0.58
12:J:102:LEU:HB2	12:J:118:MET:HG3	1.86	0.58
9:U:72:ILE:HG21	9:U:114:LEU:HD21	1.85	0.58
15:M:51:LEU:HD12	15:M:112:ILE:HG13	1.85	0.58
12:X:43:LEU:HB2	12:X:183:ILE:HD11	1.85	0.58
2:h:57:LEU:HD21	2:h:110:ILE:HD11	1.85	0.58
10:V:80:ASN:HD21	10:V:119:THR:HG21	1.67	0.58
13:K:158:ARG:HE	13:K:162:GLN:HE21	1.51	0.58
10:V:216:ILE:HD12	10:V:216:ILE:H	1.66	0.58
8:F:30:VAL:HG21	8:F:134:SER:HB3	1.84	0.58
14:Z:18:GLU:O	14:Z:118:LYS:HA	2.03	0.58
12:J:20:VAL:HG13	12:J:27:GLN:HG3	1.86	0.58
15:M:213:HIS:HE1	16:b:190:LEU:HD11	1.69	0.58
10:V:32:SER:HB2	10:V:187:ARG:NH1	2.18	0.58
2:f:63:ILE:HD11	2:f:192:PRO:HA	1.86	0.58
15:a:114:GLY:HA2	15:a:192:VAL:HG11	1.86	0.58
3:O:75:TYR:HB3	3:O:82:TYR:CD1	2.39	0.57
6:R:74:ILE:HG12	6:R:109:VAL:HG22	1.86	0.57
6:D:117:SER:CB	7:E:82:ARG:HH12	2.15	0.57
7:S:38:LEU:HD11	7:S:179:PHE:CD2	2.39	0.57
1:c:24:LEU:HD21	1:c:123:THR:HB	1.85	0.57
1:c:31:PHE:HD1	1:c:35:PHE:HB3	1.69	0.57
5:C:181:ILE:HA	5:C:187:THR:HG22	1.85	0.57
11:I:182:MET:HE1	13:Y:165:TYR:O	2.04	0.57
9:U:38:THR:H	9:U:53:GLN:HE21	1.53	0.57
14:Z:144:MET:HE1	14:Z:185:ARG:HB2	1.85	0.57
10:V:216:ILE:N	10:V:216:ILE:CD1	2.63	0.57
3:A:127:ARG:HG2	9:G:127:GLN:HG3	1.87	0.57
3:O:64:VAL:HG12	3:O:217:PHE:HZ	1.68	0.57
1:c:236:PRO:HD2	6:D:28:ILE:HG21	1.85	0.57
13:K:192:VAL:HG11	11:W:204:ASP:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:219:LEU:HD11	11:W:194:ILE:HG13	1.85	0.57
15:M:142:GLY:HA2	15:M:176:LEU:HD21	1.86	0.56
6:D:46:VAL:HG13	6:D:220:VAL:HG13	1.87	0.56
5:Q:8:THR:HG22	5:Q:18:GLN:HB2	1.88	0.56
2:h:65:VAL:HA	2:h:198:ARG:HH22	1.69	0.56
7:S:88:MET:HE3	7:S:112:ILE:HD11	1.88	0.56
7:S:121:GLN:HG3	8:T:129:ARG:HG3	1.86	0.56
5:C:196:LEU:HA	5:C:199:VAL:HG12	1.88	0.56
3:O:202:MET:HE2	3:O:229:LEU:HD21	1.86	0.56
4:P:86:LEU:HD22	4:P:114:LEU:HD11	1.86	0.56
5:Q:187:THR:O	5:Q:191:VAL:HG12	2.04	0.56
7:S:176:MET:HA	7:S:179:PHE:CD2	2.40	0.56
16:b:14:LEU:HD21	16:b:101:ALA:HB3	1.88	0.56
10:V:32:SER:HA	10:V:187:ARG:HH12	1.71	0.56
7:E:14:SER:HB2	7:E:18:ARG:O	2.05	0.56
16:b:76:VAL:HG23	16:b:104:ASP:OD1	2.06	0.56
1:g:30:GLU:HG2	1:g:34:ARG:HD2	1.88	0.56
4:B:86:LEU:HD22	4:B:114:LEU:HD11	1.87	0.55
4:P:33:THR:HG23	4:P:163:CYS:SG	2.47	0.55
10:V:59:ILE:HD12	10:V:82:MET:HB3	1.87	0.55
5:C:42:VAL:HG13	5:C:210:VAL:HG12	1.88	0.55
15:M:190:ALA:HB2	15:M:199:ILE:HG23	1.88	0.55
11:W:184:VAL:HB	11:W:199:LEU:HD12	1.89	0.55
11:W:188:ILE:HB	11:W:195:THR:HG23	1.88	0.55
5:Q:91:CYS:HA	5:Q:102:VAL:HG21	1.88	0.55
14:Z:21:ALA:HB3	14:Z:198:VAL:HG13	1.87	0.55
3:A:198:PHE:CZ	3:A:206:ASN:HB3	2.40	0.55
4:B:14:PRO:O	4:B:15:GLU:HB2	2.05	0.55
13:Y:7:LYS:HG2	13:Y:12:VAL:HG22	1.87	0.55
15:a:26:MET:HE3	15:a:188:GLN:HB3	1.87	0.55
2:i:132:THR:HG23	2:i:157:PHE:CE1	2.42	0.55
4:B:90:LEU:HD11	4:B:114:LEU:HD22	1.89	0.55
15:M:124:TYR:O	15:M:131:ALA:HA	2.06	0.55
2:f:44:LEU:HA	2:f:49:LEU:HD11	1.89	0.55
11:I:13:MET:HB3	11:I:162:LEU:HD11	1.89	0.55
15:a:15:LYS:HE2	15:a:135:PRO:HA	1.88	0.55
2:i:121:ILE:HD12	2:i:174:ILE:HD11	1.89	0.55
2:i:156:VAL:HG12	2:i:160:MET:HE3	1.89	0.54
8:F:107:PRO:HG2	16:N:70:LEU:HD21	1.89	0.54
16:N:19:ARG:HG3	16:N:26:ILE:HG23	1.88	0.54
13:K:42:LEU:HD22	13:K:184:TRP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:100:TYR:HE1	11:W:89:MET:HE2	1.71	0.54
4:P:90:LEU:HD11	4:P:114:LEU:HD22	1.89	0.54
7:E:26:MET:HA	7:E:149:PRO:HG2	1.89	0.54
3:O:85:LEU:HD13	3:O:133:LEU:HD11	1.90	0.54
12:X:116:TYR:HB3	12:X:124:LEU:HD11	1.88	0.54
1:e:118:CYS:O	1:e:122:ILE:HG23	2.08	0.54
1:c:31:PHE:CZ	1:c:117:LYS:HB3	2.42	0.54
7:E:26:MET:O	7:E:29:VAL:HG12	2.08	0.54
14:L:52:ILE:HG13	14:L:110:ILE:HG12	1.88	0.54
15:M:91:TRP:HE3	15:M:92:LEU:HD22	1.73	0.54
1:c:31:PHE:CE1	1:c:36:LEU:HG	2.43	0.53
11:I:141:CYS:O	11:I:145:MET:HG2	2.08	0.53
16:N:115:PRO:HD2	16:N:119:MET:O	2.08	0.53
12:X:43:LEU:HG	12:X:188:ILE:HD13	1.90	0.53
11:I:11:MET:SD	11:I:149:CYS:SG	3.06	0.53
1:c:32:LEU:HD11	1:c:220:ILE:HG21	1.89	0.53
10:H:19:ARG:HG3	10:H:26:VAL:HG13	1.89	0.53
3:A:127:ARG:HH21	9:G:126:THR:HG23	1.74	0.53
3:A:25:LEU:HD23	3:A:150:PRO:HD2	1.90	0.53
6:D:195:ILE:HD12	6:D:217:LEU:HD21	1.91	0.53
3:O:43:VAL:HG13	3:O:212:CYS:HB3	1.89	0.53
5:Q:43:LEU:HD13	5:Q:72:ALA:HB2	1.89	0.53
7:S:26:MET:O	7:S:29:VAL:HG12	2.09	0.53
10:V:7:VAL:O	10:V:7:VAL:CG2	2.57	0.53
16:N:144:ARG:HG2	16:N:147:MET:HG3	1.90	0.53
2:d:108:GLU:HA	2:d:111:VAL:HG22	1.91	0.53
8:F:20:VAL:HG23	9:G:83:MET:HE1	1.91	0.53
8:F:34:SER:HB3	8:F:65:ARG:HH22	1.74	0.53
8:T:69:VAL:HG11	8:T:75:MET:HE3	1.91	0.53
15:a:45:VAL:HG12	15:a:71:VAL:HG11	1.90	0.53
2:f:66:PRO:HG2	2:f:193:HIS:HA	1.91	0.52
8:T:120:HIS:O	8:T:123:THR:HG22	2.09	0.52
6:D:76:CYS:SG	6:D:141:LEU:HB3	2.48	0.52
10:H:209:THR:HG21	11:I:167:SER:OG	2.09	0.52
4:P:136:TYR:HE1	4:P:150:SER:HB3	1.73	0.52
8:F:14:PHE:H	9:G:24:GLN:HE22	1.55	0.52
9:G:175:SER:HA	9:G:205:VAL:HG11	1.91	0.52
11:I:55:LEU:HD13	11:I:103:TYR:HB2	1.91	0.52
14:L:145:LEU:HD21	14:L:182:ALA:HB2	1.91	0.52
16:N:114:VAL:HA	16:N:119:MET:O	2.09	0.52
1:g:69:PRO:HD3	1:g:182:THR:OG1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:19:ARG:HH11	12:X:179:SER:HB3	1.75	0.52
6:D:50:VAL:HG11	6:D:66:LYS:HB2	1.92	0.52
14:Z:47:THR:HG22	14:Z:50:THR:HB	1.90	0.52
12:J:116:TYR:HB3	12:J:124:LEU:HD11	1.92	0.52
7:S:11:THR:HA	8:T:129:ARG:HB3	1.91	0.52
1:g:31:PHE:CZ	1:g:117:LYS:HB3	2.44	0.52
1:g:118:CYS:O	1:g:122:ILE:HG23	2.09	0.52
1:c:142:ILE:HG23	2:i:142:ILE:HD12	1.91	0.52
7:E:40:SER:HB3	7:E:187:LEU:HD22	1.92	0.52
10:V:19:ARG:HG3	10:V:26:VAL:HG13	1.92	0.52
2:f:128:LEU:HD21	2:f:163:LEU:HB2	1.91	0.52
16:N:30:VAL:HG21	15:a:211:ILE:HG22	1.91	0.52
9:U:125:TYR:HA	9:U:131:MET:HG3	1.92	0.52
1:c:112:TRP:CZ2	1:c:161:GLN:HG2	2.45	0.51
15:M:213:HIS:CE1	16:b:190:LEU:HD11	2.45	0.51
1:c:25:PHE:HD1	1:c:124:TRP:CD1	2.28	0.51
10:H:163:ILE:HG23	10:H:170:GLY:HA2	1.91	0.51
5:Q:65:LEU:HB2	5:Q:69:VAL:HG13	1.91	0.51
6:D:50:VAL:HG12	6:D:216:GLU:HB3	1.91	0.51
6:D:36:THR:HA	6:D:171:GLY:HA3	1.92	0.51
12:J:15:VAL:HB	12:J:45:LEU:HD21	1.93	0.51
12:J:118:MET:HA	12:J:123:ALA:O	2.10	0.51
1:c:105:ALA:HA	1:c:108:LYS:HE3	1.92	0.51
6:R:215:ILE:HD11	6:R:238:ILE:HD11	1.92	0.51
1:e:104:LEU:HD23	1:e:202:LEU:HD21	1.92	0.51
7:E:193:ARG:HG3	7:E:236:LEU:HD11	1.91	0.51
14:L:24:ALA:HB1	14:L:193:LEU:HD11	1.93	0.51
2:f:57:LEU:HD21	2:f:110:ILE:HD11	1.92	0.51
6:D:17:PRO:O	6:D:18:GLU:HB2	2.11	0.51
2:i:121:ILE:HG12	2:i:219:ILE:HD11	1.93	0.51
5:C:12:PRO:O	5:C:13:ASP:HB2	2.10	0.51
12:J:1:MET:HE3	12:J:173:LEU:HD13	1.93	0.51
4:B:76:VAL:HG11	4:B:83:ALA:HB2	1.93	0.51
4:B:90:LEU:HG	4:B:114:LEU:HD13	1.92	0.51
6:D:159:SER:HB2	6:D:161:THR:HG23	1.92	0.51
1:c:147:LEU:HD22	6:D:2:PHE:HE2	1.76	0.51
11:I:36:THR:HG22	11:I:182:MET:HB3	1.93	0.51
15:M:211:ILE:HA	15:M:214:MET:HE3	1.91	0.51
9:U:191:PHE:HE1	9:U:219:VAL:HG21	1.74	0.51
10:V:110:LEU:HD21	10:V:125:VAL:HG22	1.93	0.51
2:f:159:LEU:HD22	2:f:229:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:151:ILE:HD13	8:F:157:SER:HB2	1.93	0.50
15:M:71:VAL:O	15:M:74:GLU:HG2	2.11	0.50
4:P:28:ILE:HD12	4:P:133:SER:HB3	1.92	0.50
4:B:32:GLY:HA2	4:B:50:ARG:HH11	1.76	0.50
2:d:150:VAL:O	2:d:154:GLU:HG2	2.11	0.50
15:a:142:GLY:HA2	15:a:176:LEU:HD21	1.93	0.50
2:d:160:MET:HG2	2:d:226:LEU:HD11	1.93	0.50
11:I:48:LEU:HD12	11:I:110:GLY:HA3	1.93	0.50
11:I:143:GLU:HG2	14:Z:143:ALA:HB3	1.94	0.50
13:K:76:VAL:HG21	13:K:110:GLY:HA3	1.93	0.50
5:Q:164:GLY:O	5:Q:168:VAL:HG12	2.11	0.50
7:S:109:VAL:HA	7:S:112:ILE:HD12	1.92	0.50
4:B:149:GLN:HE21	4:B:164:ILE:HG22	1.76	0.50
8:F:27:MET:O	8:F:30:VAL:HG12	2.11	0.50
4:P:76:VAL:HG21	4:P:83:ALA:HB1	1.94	0.50
2:h:142:ILE:HD12	2:i:152:VAL:HG13	1.93	0.50
14:L:75:TYR:CD1	14:L:83:MET:HG2	2.47	0.50
13:Y:19:ARG:HG3	13:Y:26:ILE:HG23	1.93	0.50
1:g:31:PHE:HD1	1:g:35:PHE:HB3	1.76	0.50
1:c:184:VAL:HA	2:i:104:VAL:HG22	1.94	0.50
9:G:51:VAL:HG12	9:G:217:VAL:HB	1.94	0.50
10:V:124:TYR:CE2	10:V:135:MET:HE1	2.47	0.50
12:X:100:VAL:HG22	12:X:102:LEU:HG	1.94	0.49
16:b:115:PRO:HG2	16:b:119:MET:HG3	1.94	0.49
3:A:43:VAL:HG13	3:A:212:CYS:HB3	1.94	0.49
7:E:36:VAL:HG13	7:E:172:LEU:HD11	1.95	0.49
15:M:27:LEU:HD11	15:M:34:ALA:HB1	1.93	0.49
16:N:81:SER:O	16:N:85:GLU:HG2	2.12	0.49
7:S:40:SER:HB3	7:S:187:LEU:HD22	1.94	0.49
7:S:116:THR:O	7:S:119:PRO:HD2	2.12	0.49
1:g:31:PHE:CE1	1:g:36:LEU:HG	2.47	0.49
4:B:135:LEU:HG	4:B:164:ILE:HD13	1.94	0.49
7:E:184:LEU:HD11	7:E:214:ILE:HD13	1.94	0.49
10:H:7:VAL:HG12	10:H:12:ILE:HD11	1.95	0.49
3:O:54:ILE:HG22	9:U:180:GLU:HG3	1.92	0.49
4:P:208:ALA:HB2	4:P:237:ILE:HG13	1.94	0.49
10:V:124:TYR:HE2	10:V:135:MET:HE1	1.76	0.49
11:W:135:PHE:HZ	11:W:150:GLU:HG2	1.77	0.49
12:X:38:MET:HE2	12:X:44:LEU:HB3	1.92	0.49
2:h:131:VAL:HG21	2:h:230:ILE:HD11	1.93	0.49
7:E:119:PRO:HG2	7:E:128:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:50:ALA:HB2	14:L:127:VAL:HG13	1.95	0.49
8:T:69:VAL:HG23	8:T:73:VAL:HG13	1.94	0.49
1:c:49:GLU:HG3	1:c:51:SER:H	1.78	0.49
6:R:13:ASN:HB3	7:S:126:ARG:HB3	1.95	0.49
4:B:122:THR:HG22	5:C:125:ARG:HE	1.77	0.49
2:f:160:MET:HG2	2:f:226:LEU:HD11	1.95	0.49
8:F:69:VAL:HG23	8:F:73:VAL:HG13	1.93	0.49
3:O:122:GLN:HG3	4:P:128:ARG:HG2	1.94	0.49
4:P:230:GLN:HA	4:P:233:VAL:HG22	1.94	0.49
9:U:69:LEU:HD23	9:U:79:VAL:HB	1.94	0.49
2:f:156:VAL:HG21	2:f:237:LEU:HD21	1.95	0.49
12:J:77:PRO:HD2	12:J:108:ASP:HB2	1.95	0.49
11:W:6:ASN:HD22	11:W:56:ALA:H	1.61	0.49
1:e:31:PHE:CZ	1:e:36:LEU:HG	2.47	0.49
10:H:219:LEU:H	11:I:193:LYS:HA	1.77	0.49
14:L:13:LEU:HD11	14:L:149:LEU:HD11	1.95	0.49
5:Q:181:ILE:HA	5:Q:187:THR:HG22	1.94	0.49
1:c:41:ILE:HA	1:c:44:ASN:ND2	2.28	0.48
14:L:3:SER:O	15:M:128:LEU:HD21	2.12	0.48
8:T:14:PHE:HE2	9:U:133:PRO:O	1.95	0.48
10:V:32:SER:CA	10:V:187:ARG:HH12	2.26	0.48
14:Z:63:THR:HG22	15:a:94:ARG:NH2	2.26	0.48
1:g:146:VAL:HG13	1:g:219:ILE:HD12	1.95	0.48
3:A:21:ILE:HD11	3:A:121:THR:HG23	1.95	0.48
16:N:119:MET:HE3	16:N:119:MET:HB3	1.60	0.48
8:T:72:HIS:CE1	8:T:105:ASN:HB3	2.49	0.48
7:S:26:MET:HA	7:S:149:PRO:HG2	1.94	0.48
2:d:63:ILE:HD11	2:d:192:PRO:HA	1.95	0.48
3:A:98:LEU:HD21	10:H:61:SER:HB3	1.96	0.48
5:Q:51:ALA:O	5:Q:52:LYS:HB3	2.12	0.48
4:B:234:GLU:O	4:B:237:ILE:HG12	2.14	0.48
5:C:23:GLN:HG2	5:C:149:PRO:HD2	1.96	0.48
6:D:88:LEU:HD23	6:D:119:LEU:HD23	1.95	0.48
3:O:67:ILE:HG12	3:O:73:LEU:HG	1.94	0.48
10:V:42:TYR:HB2	10:V:178:ILE:HD11	1.95	0.48
13:Y:50:ALA:HB2	14:Z:127:VAL:HG13	1.94	0.48
1:c:118:CYS:O	1:c:122:ILE:HG23	2.14	0.48
3:A:100:TYR:HE1	11:I:89:MET:HE2	1.78	0.48
5:Q:66:ASP:HB3	5:Q:69:VAL:HG12	1.96	0.48
6:R:35:SER:HB2	6:R:51:GLU:HG3	1.94	0.48
9:U:52:THR:HG23	9:U:216:GLU:HG3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:117:LEU:HD22	2:h:212:ILE:HG23	1.96	0.48
12:J:26:VAL:O	12:J:27:GLN:C	2.57	0.48
3:A:127:ARG:HH21	9:G:126:THR:CG2	2.25	0.48
8:F:12:SER:HA	9:G:132:ARG:HB3	1.95	0.48
4:B:8:ARG:O	4:B:9:THR:HG22	2.14	0.48
14:L:197:ILE:HG23	14:L:204:ARG:HB3	1.95	0.48
4:P:132:VAL:HB	4:P:134:LEU:HD21	1.95	0.48
2:d:124:VAL:HG13	2:d:167:LEU:HD13	1.94	0.48
16:b:86:MET:HE2	16:b:86:MET:HB3	1.81	0.48
2:i:135:LEU:HB3	2:i:157:PHE:CE2	2.49	0.48
1:c:22:GLN:HG2	1:c:23:ASN:N	2.28	0.47
1:c:31:PHE:CE1	1:c:117:LYS:HB3	2.49	0.47
13:K:186:ARG:HH22	13:K:189:SER:HB2	1.79	0.47
13:Y:180:ARG:HH21	13:Y:185:ILE:HG21	1.79	0.47
14:L:51:VAL:HG23	14:L:203:ILE:HD12	1.96	0.47
2:h:123:ASP:O	2:h:127:GLN:HG2	2.14	0.47
1:c:112:TRP:HZ2	1:c:161:GLN:HG2	1.79	0.47
1:c:149:ARG:HA	1:c:149:ARG:HD2	1.60	0.47
9:G:32:ILE:HA	9:G:82:GLY:HA2	1.97	0.47
14:L:64:LEU:HD21	14:L:92:LEU:HD11	1.96	0.47
14:L:212:LYS:O	14:L:213:ASP:C	2.58	0.47
14:Z:17:GLY:HA3	14:Z:20:PHE:CE2	2.49	0.47
2:h:246:GLY:O	2:h:247:MET:HB2	2.14	0.47
9:G:10:ASP:O	9:G:11:ARG:HB2	2.15	0.47
11:I:170:MET:HE3	11:I:170:MET:HB3	1.79	0.47
1:e:104:LEU:HD22	1:e:164:ILE:HG23	1.96	0.47
2:f:21:LEU:HD21	2:f:133:THR:HG23	1.96	0.47
14:Z:123:SER:HB3	14:Z:136:LYS:HG2	1.95	0.47
14:Z:145:LEU:HD22	14:Z:178:VAL:HB	1.95	0.47
2:i:233:ASN:O	2:i:237:LEU:HG	2.15	0.47
7:E:35:THR:HG21	7:E:73:SER:CB	2.44	0.47
14:L:102:PHE:HE2	15:M:101:SER:HA	1.79	0.47
8:T:158:TYR:HB3	9:U:61:LEU:HD21	1.97	0.47
12:X:80:ALA:O	12:X:84:THR:HG23	2.15	0.47
1:e:119:ILE:O	1:e:122:ILE:HG12	2.14	0.47
3:A:211:ILE:HG13	3:A:218:ARG:HG3	1.96	0.47
7:E:237:GLU:H	7:E:237:GLU:HG3	1.31	0.47
14:L:89:ALA:HA	14:L:124:PHE:HZ	1.79	0.47
4:P:72:MET:HE2	4:P:72:MET:HB3	1.65	0.47
6:R:234:LEU:HD12	6:R:234:LEU:HA	1.75	0.47
3:A:74:VAL:HG12	3:A:134:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:92:GLN:HB3	12:X:62:LYS:HG3	1.95	0.47
14:Z:72:LEU:HD23	14:Z:83:MET:SD	2.55	0.47
1:e:33:TYR:HB2	1:e:34:ARG:HH21	1.80	0.47
9:G:56:VAL:HG12	9:G:66:VAL:HG11	1.97	0.47
12:J:43:LEU:HB2	12:J:183:ILE:HD11	1.97	0.47
15:a:63:LEU:HD13	15:a:92:LEU:HD11	1.96	0.47
2:d:154:GLU:O	2:d:157:PHE:HB2	2.14	0.46
1:e:115:LYS:HE3	1:e:158:GLU:HG2	1.97	0.46
2:f:226:LEU:HD12	2:f:226:LEU:HA	1.73	0.46
7:E:62:LYS:HE2	7:E:74:ILE:O	2.15	0.46
5:Q:36:ARG:HG2	5:Q:142:PRO:HB2	1.96	0.46
7:S:101:ARG:HH12	7:S:107:ARG:NH1	2.12	0.46
13:Y:113:TYR:HB3	13:Y:121:ILE:HG13	1.97	0.46
3:A:35:VAL:HG21	3:A:193:THR:HB	1.97	0.46
15:M:173:MET:HE2	15:M:173:MET:HB2	1.77	0.46
10:V:142:PHE:CD2	10:V:142:PHE:C	2.93	0.46
14:L:75:TYR:CG	14:L:83:MET:HG2	2.50	0.46
2:d:226:LEU:HD12	2:d:226:LEU:HA	1.73	0.46
5:C:180:ALA:O	5:C:186:LEU:HB3	2.15	0.46
9:G:80:MET:HB3	9:G:80:MET:HE2	1.43	0.46
14:L:91:MET:HE2	14:L:91:MET:HB3	1.77	0.46
15:M:10:SER:HA	15:M:139:THR:O	2.15	0.46
7:S:39:LYS:HD3	7:S:142:PRO:HB2	1.97	0.46
7:S:220:GLU:O	7:S:221:PHE:C	2.59	0.46
4:B:35:LEU:HD12	4:B:163:CYS:HB2	1.96	0.46
7:E:184:LEU:HD12	7:E:214:ILE:HG21	1.96	0.46
15:M:27:LEU:HB2	15:M:184:TYR:HB2	1.98	0.46
14:Z:59:GLY:O	14:Z:63:THR:HG23	2.15	0.46
2:i:114:LEU:HG	2:i:212:ILE:HD11	1.97	0.46
12:J:101:ASN:HB3	12:J:132:HIS:CE1	2.51	0.46
16:N:14:LEU:HD23	16:N:44:CYS:SG	2.56	0.46
16:N:127:ILE:HD11	16:N:136:TYR:CD1	2.50	0.46
1:g:114:LEU:HD23	1:g:209:LEU:HD22	1.97	0.46
1:c:117:LYS:HA	1:c:117:LYS:HD3	1.76	0.46
2:f:108:GLU:HA	2:f:111:VAL:HG22	1.98	0.46
14:Z:17:GLY:HA3	14:Z:20:PHE:CZ	2.51	0.46
7:E:230:SER:N	7:E:231:PRO:HD2	2.31	0.46
16:N:120:MET:HE2	16:N:120:MET:HB3	1.65	0.46
4:P:136:TYR:CE1	4:P:150:SER:HB3	2.50	0.46
6:R:206:MET:HE2	6:R:206:MET:HB3	1.71	0.46
2:i:49:LEU:HD12	2:i:49:LEU:HA	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:112:TRP:CD1	2:d:210:ARG:HD3	2.51	0.46
2:f:44:LEU:HA	2:f:49:LEU:HD21	1.96	0.46
12:J:60:ILE:HG21	12:J:84:THR:HG22	1.98	0.46
14:L:26:ASP:CG	14:L:190:GLY:H	2.24	0.46
3:O:67:ILE:HG22	3:O:68:THR:HG23	1.98	0.46
6:D:38:ILE:HG13	6:D:181:LEU:HD11	1.98	0.46
8:F:159:GLY:N	9:G:65:THR:HG21	2.31	0.46
10:H:112:SER:HB3	10:H:125:VAL:HG21	1.96	0.46
13:K:158:ARG:HE	13:K:162:GLN:NE2	2.14	0.46
14:L:186:ASP:HB3	14:L:189:THR:HG23	1.98	0.46
2:d:33:PHE:CE2	2:d:226:LEU:HB3	2.51	0.45
4:B:115:CYS:SG	4:B:156:TYR:HB3	2.55	0.45
6:D:202:LEU:HA	6:D:205:VAL:HG22	1.98	0.45
3:O:108:GLN:HE21	3:O:112:ARG:HH12	1.63	0.45
14:Z:123:SER:CB	14:Z:136:LYS:HG2	2.46	0.45
6:D:12:VAL:O	6:D:13:ASN:HB2	2.16	0.45
7:E:35:THR:HG21	7:E:73:SER:HB2	1.98	0.45
3:O:122:GLN:HG3	4:P:128:ARG:CG	2.45	0.45
4:P:119:GLN:OE1	5:Q:82:ILE:HG13	2.15	0.45
12:X:103:LEU:HG	12:X:115:LEU:HD11	1.99	0.45
14:Z:64:LEU:HD21	14:Z:92:LEU:HD11	1.97	0.45
16:b:76:VAL:H	16:b:104:ASP:CG	2.24	0.45
2:i:33:PHE:CD1	2:i:223:TYR:HD1	2.35	0.45
7:E:237:GLU:HB2	7:E:238:GLU:H	1.38	0.45
8:T:187:ARG:O	8:T:190:VAL:HG22	2.16	0.45
2:d:220:ARG:HE	2:d:220:ARG:HB3	1.37	0.45
1:e:147:LEU:HA	1:e:150:VAL:HG22	1.98	0.45
11:I:86:LEU:O	11:I:90:VAL:HG23	2.17	0.45
13:K:19:ARG:HG3	13:K:26:ILE:HG23	1.97	0.45
14:L:13:LEU:HD21	14:L:15:ILE:HG13	1.98	0.45
15:M:156:LYS:HG3	15:M:157:GLN:HG3	1.99	0.45
7:S:106:SER:O	7:S:109:VAL:HG22	2.16	0.45
8:T:71:ARG:H	8:T:71:ARG:HG2	1.43	0.45
14:Z:124:PHE:CE2	14:Z:130:TYR:HB3	2.51	0.45
14:L:58:HIS:HB3	15:M:130:VAL:HG13	1.98	0.45
11:W:33:MET:HE3	11:W:33:MET:HB3	1.79	0.45
12:X:29:LYS:HG2	12:X:31:ASP:H	1.82	0.45
1:e:146:VAL:HG21	1:e:227:ILE:HD11	1.98	0.45
3:A:202:MET:HE2	3:A:202:MET:HB3	1.72	0.45
6:D:49:ALA:HB2	6:D:217:LEU:HD12	1.98	0.45
6:D:183:GLU:HG2	6:D:184:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:90:LEU:HG	4:P:114:LEU:HD13	1.99	0.45
8:T:228:PRO:HB2	8:T:231:ILE:HG13	1.98	0.45
2:f:25:THR:HG21	2:f:134:TRP:CD2	2.51	0.45
14:L:11:THR:HG23	14:L:179:PHE:HE2	1.81	0.45
15:M:110:MET:HB2	15:M:110:MET:HE3	1.75	0.45
4:P:37:ILE:HB	4:P:44:LEU:HD23	1.97	0.45
5:Q:132:LEU:HG	5:Q:161:ILE:HD13	1.97	0.45
6:R:36:THR:HA	6:R:171:GLY:HA3	1.99	0.45
10:V:152:LYS:HD3	10:V:177:VAL:HG21	1.98	0.45
2:h:29:LEU:HD21	2:h:230:ILE:HG21	1.98	0.45
1:c:47:LEU:HD11	1:c:207:LEU:HA	1.98	0.45
4:B:179:TYR:CE2	4:B:184:MET:HG3	2.51	0.45
13:K:13:ILE:CG2	13:K:176:LEU:HD11	2.46	0.45
13:K:35:ILE:HD12	13:K:56:GLU:HG3	1.98	0.45
15:M:27:LEU:HD12	15:M:36:PHE:O	2.17	0.45
15:M:132:TYR:CE1	15:M:137:LEU:HD21	2.52	0.45
3:O:78:MET:HE2	3:O:78:MET:HB3	1.64	0.45
3:O:82:TYR:O	3:O:86:VAL:HG13	2.17	0.45
9:U:205:VAL:HG23	9:U:206:LEU:HG	1.99	0.45
1:c:50:ASP:HA	1:c:53:ASN:HB2	1.99	0.45
12:J:140:LEU:HD23	12:J:140:LEU:HA	1.73	0.45
14:L:184:GLU:HG3	10:V:195:LYS:HD2	1.99	0.45
7:S:199:LEU:HD12	7:S:200:PRO:HD2	1.98	0.45
9:U:215:ILE:H	9:U:215:ILE:HG13	1.71	0.45
14:Z:172:MET:HE1	14:Z:197:ILE:HG12	1.98	0.45
11:I:90:VAL:HG21	11:I:108:ILE:HD11	1.99	0.45
13:K:20:ALA:HB2	13:K:31:VAL:HG21	1.98	0.45
5:Q:107:ILE:HD12	5:Q:107:ILE:HA	1.67	0.45
2:i:117:LEU:HD22	2:i:212:ILE:HG23	1.99	0.45
1:e:105:ALA:HA	1:e:108:LYS:HE3	1.99	0.44
13:K:80:SER:HB2	13:K:120:ARG:HH21	1.82	0.44
14:L:131:GLN:H	14:L:131:GLN:HG2	1.68	0.44
9:U:32:ILE:HA	9:U:82:GLY:HA2	1.98	0.44
12:X:114:ALA:HB1	12:X:116:TYR:CE2	2.52	0.44
9:G:21:ARG:O	9:G:22:LEU:C	2.59	0.44
2:i:57:LEU:HG	2:i:107:ASN:HD21	1.82	0.44
2:i:163:LEU:O	2:i:167:LEU:HG	2.17	0.44
1:g:23:ASN:O	1:g:26:GLN:HG2	2.17	0.44
1:c:41:ILE:CG2	2:i:13:LYS:HB3	2.48	0.44
2:d:102:GLY:O	2:d:103:PRO:C	2.60	0.44
2:f:118:LYS:N	2:f:119:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:132:THR:HG23	2:f:157:PHE:CZ	2.52	0.44
9:G:231:THR:O	9:G:235:ILE:HG13	2.17	0.44
10:H:47:GLY:O	10:H:48:THR:C	2.60	0.44
15:M:145:LEU:O	15:M:148:PRO:HD2	2.17	0.44
8:T:35:THR:HA	8:T:166:GLY:HA3	1.98	0.44
10:V:14:LEU:HB3	10:V:44:CYS:SG	2.57	0.44
1:g:30:GLU:HA	1:g:34:ARG:NH1	2.33	0.44
2:d:233:ASN:O	2:d:237:LEU:HG	2.18	0.44
6:D:120:ALA:O	6:D:123:PHE:HD2	2.01	0.44
10:H:63:LEU:HD23	10:H:63:LEU:HA	1.75	0.44
15:M:132:TYR:HE1	15:M:137:LEU:HD21	1.81	0.44
15:M:166:ARG:HH22	15:M:200:GLU:HG2	1.82	0.44
4:P:233:VAL:O	4:P:237:ILE:HG12	2.16	0.44
11:W:55:LEU:HD12	11:W:55:LEU:HA	1.88	0.44
14:Z:84:THR:O	14:Z:88:ILE:HG13	2.17	0.44
2:h:18:ARG:HH21	2:h:137:LEU:HB3	1.82	0.44
2:h:156:VAL:CG1	2:h:160:MET:HE3	2.47	0.44
1:g:47:LEU:HD11	1:g:207:LEU:HA	1.99	0.44
1:c:129:ILE:HD11	2:d:229:ILE:HD11	2.00	0.44
11:I:152:LEU:HB3	11:I:165:THR:HG23	1.99	0.44
6:R:73:HIS:CD2	6:R:74:ILE:HG13	2.52	0.44
7:S:59:HIS:O	7:S:60:GLN:HB3	2.17	0.44
11:W:135:PHE:CZ	11:W:150:GLU:HG2	2.53	0.44
11:W:148:MET:HE2	11:W:148:MET:HB2	1.79	0.44
15:a:27:LEU:HG	15:a:28:GLY:N	2.32	0.44
2:h:181:ARG:O	2:h:185:VAL:HG22	2.17	0.44
2:h:217:MET:HE2	2:h:217:MET:HB3	1.81	0.44
1:g:117:LYS:HA	1:g:117:LYS:HD3	1.78	0.44
2:d:166:LYS:HB3	2:d:166:LYS:HE2	1.84	0.44
4:B:127:LYS:H	4:B:127:LYS:HG2	1.34	0.44
6:D:137:PHE:O	6:D:158:PRO:HB3	2.18	0.44
4:P:54:LYS:H	4:P:54:LYS:HD3	1.83	0.44
5:Q:173:GLU:HA	6:R:58:LEU:HD21	2.00	0.44
6:R:107:MET:HE2	6:R:111:SER:HB3	1.99	0.44
10:V:52:THR:O	10:V:56:THR:HG23	2.18	0.44
15:a:124:TYR:O	15:a:131:ALA:HA	2.17	0.44
2:i:66:PRO:HG3	2:i:193:HIS:HA	2.00	0.44
2:d:55:SER:O	2:d:58:LYS:HB2	2.18	0.44
2:f:135:LEU:HD12	2:f:135:LEU:HA	1.84	0.44
3:A:136:CYS:O	3:A:136:CYS:SG	2.75	0.44
16:N:42:PHE:CZ	16:N:184:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:207:SER:O	4:P:208:ALA:HB3	2.18	0.44
12:X:38:MET:HB2	12:X:42:ILE:CG1	2.47	0.44
16:b:138:TYR:O	16:b:142:THR:HG22	2.17	0.44
1:g:57:LEU:HA	1:g:60:LEU:HD12	2.00	0.44
10:H:14:LEU:HB3	10:H:44:CYS:SG	2.58	0.44
11:I:12:ALA:HB3	11:I:136:VAL:HG23	1.99	0.44
13:K:42:LEU:HD21	13:K:179:VAL:CG2	2.43	0.44
5:Q:168:VAL:O	5:Q:172:LEU:HG	2.18	0.44
10:V:211:VAL:CG1	11:W:163:PHE:HZ	2.30	0.44
14:Z:104:TYR:HB3	14:Z:106:VAL:HG12	1.99	0.44
2:h:114:LEU:HG	2:h:212:ILE:HD11	2.00	0.44
1:e:38:GLN:O	1:e:41:ILE:HG13	2.17	0.44
2:f:124:VAL:HG13	2:f:167:LEU:HD13	2.00	0.44
9:G:111:VAL:HG21	9:G:142:GLY:HA3	2.00	0.44
3:O:222:PRO:O	3:O:225:VAL:HG12	2.17	0.44
5:Q:42:VAL:CG1	5:Q:191:VAL:HG11	2.47	0.44
8:T:36:ALA:HB3	8:T:165:ILE:HG13	1.99	0.44
13:Y:19:ARG:HH21	13:Y:29:GLN:HE21	1.65	0.44
2:h:128:LEU:HD21	2:h:163:LEU:HB2	2.00	0.44
1:c:104:LEU:HD22	1:c:164:ILE:HG23	2.00	0.43
5:C:107:ILE:HD12	5:C:107:ILE:HA	1.65	0.43
10:H:81:ARG:HD3	10:H:84:LYS:HD3	1.99	0.43
9:U:232:GLU:O	9:U:235:ILE:HG12	2.18	0.43
2:i:135:LEU:HD12	2:i:135:LEU:HA	1.79	0.43
10:H:175:LEU:HD13	10:H:175:LEU:HA	1.84	0.43
5:Q:222:PRO:O	5:Q:225:ILE:HG12	2.18	0.43
6:R:46:VAL:HG21	6:R:144:GLY:HA3	1.99	0.43
2:d:31:SER:C	2:d:34:PRO:HD2	2.44	0.43
3:A:67:ILE:HG12	3:A:73:LEU:HG	1.99	0.43
3:A:75:TYR:HB3	3:A:82:TYR:CD1	2.52	0.43
9:G:138:MET:HB3	9:G:154:CYS:SG	2.58	0.43
9:U:118:ILE:HG13	9:U:138:MET:HE1	1.99	0.43
12:X:47:VAL:HG22	12:X:48:GLY:H	1.82	0.43
2:h:28:LEU:HD12	2:h:32:TYR:HB3	1.99	0.43
2:h:229:ILE:HD11	1:g:129:ILE:HD11	1.99	0.43
1:g:60:LEU:HA	1:g:99:LYS:HD2	2.01	0.43
1:e:149:ARG:HD2	1:e:149:ARG:HA	1.72	0.43
3:A:117:MET:HE2	3:A:150:PRO:HA	2.00	0.43
5:C:94:HIS:CE1	5:C:98:VAL:HG21	2.53	0.43
6:D:228:MET:HE3	6:D:228:MET:HB3	1.78	0.43
8:F:50:GLU:HB2	8:F:197:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:14:LYS:HE3	11:I:120:ILE:HG12	1.99	0.43
13:K:38:ASN:HD22	13:K:38:ASN:HA	1.68	0.43
15:M:211:ILE:HG13	16:b:30:VAL:HG11	2.00	0.43
6:R:184:VAL:HG11	6:R:197:SER:HB2	2.00	0.43
9:U:191:PHE:CE1	9:U:219:VAL:HG21	2.53	0.43
10:V:79:ALA:HB3	10:V:100:LEU:HD21	2.00	0.43
14:Z:12:ILE:HD12	14:Z:109:ILE:HG12	2.00	0.43
2:h:147:ASN:O	2:h:148:PHE:C	2.60	0.43
7:E:116:THR:O	7:E:119:PRO:HD2	2.19	0.43
16:N:88:TYR:O	16:N:91:ARG:HG2	2.17	0.43
2:i:238:LYS:HD2	2:i:238:LYS:HA	1.91	0.43
4:B:207:SER:C	4:B:209:GLU:H	2.26	0.43
4:B:208:ALA:HB2	4:B:237:ILE:HD13	2.00	0.43
12:J:74:GLU:H	12:J:74:GLU:HG2	1.54	0.43
12:J:121:LEU:O	12:J:122:ALA:HB3	2.19	0.43
13:K:37:ILE:HD13	13:K:59:LEU:HD23	1.99	0.43
13:Y:40:TYR:CD1	13:Y:73:ARG:HD2	2.53	0.43
1:e:128:LEU:HD13	1:e:228:VAL:HA	2.00	0.43
1:e:236:PRO:HB2	1:e:237:SER:H	1.32	0.43
6:D:146:VAL:HG11	6:D:222:PRO:HA	2.01	0.43
15:M:91:TRP:CE3	15:M:92:LEU:HD22	2.52	0.43
4:P:194:ILE:HG23	4:P:206:LEU:HD12	1.99	0.43
6:R:156:MET:HB3	6:R:156:MET:HE3	1.74	0.43
8:T:50:GLU:HB2	8:T:197:ILE:HG23	2.01	0.43
9:U:50:ILE:HG23	9:U:141:ILE:HG21	2.00	0.43
2:d:33:PHE:HE2	2:d:226:LEU:HB3	1.83	0.43
2:d:54:LEU:HD11	2:d:209:TYR:CD2	2.54	0.43
7:E:88:MET:HE3	7:E:112:ILE:HD11	2.00	0.43
11:I:177:ASP:OD1	11:I:180:SER:HB2	2.18	0.43
12:J:1:MET:HE2	12:J:1:MET:HB3	1.83	0.43
7:S:38:LEU:HB3	7:S:45:VAL:HG22	2.00	0.43
7:S:47:VAL:HG12	7:S:195:LEU:HD22	2.00	0.43
7:S:50:LYS:HB3	7:S:59:HIS:CB	2.45	0.43
9:U:80:MET:HB3	9:U:87:SER:HB2	2.01	0.43
11:W:120:ILE:HD12	11:W:136:VAL:HG22	2.01	0.43
2:h:121:ILE:HD13	2:h:219:ILE:HD11	2.00	0.43
1:e:127:HIS:CE1	2:f:224:ALA:HB1	2.54	0.43
3:A:73:LEU:HD11	3:A:86:VAL:HG22	2.01	0.43
3:A:171:THR:O	3:A:174:GLU:HG2	2.19	0.43
9:G:27:TYR:O	9:G:30:LYS:HB2	2.18	0.43
10:H:1:THR:HG23	10:H:33:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:121:VAL:HB	14:L:133:ASP:O	2.19	0.43
15:M:13:GLY:HA2	15:M:21:VAL:O	2.18	0.43
4:P:198:ASN:HA	4:P:206:LEU:HD21	2.00	0.43
5:Q:94:HIS:CE1	5:Q:98:VAL:HG21	2.53	0.43
6:R:59:MET:HE2	6:R:59:MET:HB2	1.79	0.43
6:R:228:MET:HE3	6:R:228:MET:HB3	1.79	0.43
2:i:118:LYS:HG2	2:i:174:ILE:HD13	1.99	0.43
2:d:128:LEU:HA	2:d:128:LEU:HD13	1.77	0.43
2:f:123:ASP:O	2:f:127:GLN:HG2	2.19	0.43
2:f:134:TRP:O	2:f:138:GLN:HG2	2.19	0.43
7:E:31:GLN:HE21	7:E:31:GLN:HB3	1.57	0.43
8:F:27:MET:HB3	8:F:27:MET:HE2	1.66	0.43
8:T:223:ARG:HE	8:T:223:ARG:HB3	1.57	0.43
10:V:11:GLY:HA2	10:V:108:PRO:HB3	2.01	0.43
11:W:13:MET:HB3	11:W:162:LEU:HD11	2.00	0.43
12:X:28:MET:HE2	12:X:28:MET:HB3	1.83	0.43
1:c:147:LEU:HD22	6:D:2:PHE:CE2	2.54	0.42
1:e:47:LEU:HG	1:e:206:VAL:HG13	2.01	0.42
6:D:1:MET:HE2	6:D:1:MET:HB3	1.88	0.42
15:M:214:MET:HE3	15:M:214:MET:HB2	1.90	0.42
2:d:118:LYS:N	2:d:119:PRO:HD2	2.34	0.42
12:J:77:PRO:CD	12:J:108:ASP:HB2	2.49	0.42
12:X:140:LEU:HD23	12:X:140:LEU:HA	1.92	0.42
15:a:173:MET:HE2	15:a:173:MET:HB2	1.86	0.42
15:a:201:GLY:O	15:a:203:LEU:HG	2.19	0.42
1:g:97:ASN:O	1:g:101:LEU:HG	2.19	0.42
1:e:30:GLU:HA	1:e:34:ARG:CZ	2.49	0.42
5:C:43:LEU:HD12	5:C:43:LEU:HA	1.87	0.42
5:C:60:ARG:HA	5:C:60:ARG:HD3	1.78	0.42
7:E:184:LEU:CD1	7:E:214:ILE:HG21	2.50	0.42
10:H:81:ARG:HA	10:H:84:LYS:HG2	2.01	0.42
13:K:44:THR:HG21	13:K:100:MET:HE3	2.02	0.42
15:M:15:LYS:HG2	15:M:135:PRO:O	2.19	0.42
15:M:22:ILE:HG23	15:M:50:MET:HE3	2.01	0.42
15:M:50:MET:HE2	15:M:192:VAL:HG12	2.02	0.42
1:c:205:MET:O	1:c:209:LEU:HG	2.20	0.42
3:A:162:MET:HE3	3:A:162:MET:HB2	1.94	0.42
7:E:36:VAL:HB	7:E:47:VAL:HG23	2.01	0.42
11:I:33:MET:HE2	11:I:33:MET:HB2	1.57	0.42
11:I:76:LYS:HA	11:I:76:LYS:HD3	1.85	0.42
11:I:168:GLN:HE22	14:Z:158:MET:HG2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:202:LEU:HD23	16:N:202:LEU:HA	1.86	0.42
3:O:163:GLY:O	3:O:166:TYR:HB3	2.20	0.42
7:S:117:GLN:O	7:S:120:THR:HG22	2.20	0.42
15:a:67:LEU:HD12	15:a:67:LEU:HA	1.85	0.42
1:e:226:LYS:HD3	1:e:226:LYS:HA	1.94	0.42
2:f:225:VAL:O	2:f:229:ILE:HG12	2.19	0.42
12:J:4:LEU:HD22	12:J:45:LEU:HB3	2.01	0.42
5:Q:136:PHE:HE2	5:Q:211:MET:O	2.03	0.42
6:R:123:PHE:HA	6:R:133:MET:O	2.19	0.42
8:T:20:VAL:HG23	9:U:83:MET:HE1	2.01	0.42
9:U:80:MET:HB3	9:U:80:MET:HE2	1.65	0.42
14:Z:8:ASN:HA	14:Z:30:SER:O	2.20	0.42
1:g:216:LEU:HD23	1:g:216:LEU:HA	1.85	0.42
3:A:173:LEU:HD23	3:A:173:LEU:HA	1.86	0.42
5:C:134:VAL:HG12	5:C:144:LEU:HD13	2.02	0.42
6:D:165:CYS:SG	6:D:168:ARG:HB2	2.60	0.42
12:J:41:LYS:HG2	12:J:187:GLY:HA2	2.01	0.42
10:V:32:SER:HA	10:V:187:ARG:NH1	2.35	0.42
10:V:63:LEU:HA	10:V:63:LEU:HD23	1.76	0.42
2:i:226:LEU:HD12	2:i:226:LEU:HA	1.74	0.42
2:d:139:ILE:HD11	2:d:157:PHE:CE2	2.55	0.42
1:e:32:LEU:HA	1:e:36:LEU:HD12	2.01	0.42
2:f:198:ARG:H	2:f:198:ARG:HG2	1.70	0.42
4:B:207:SER:O	4:B:208:ALA:HB3	2.19	0.42
13:K:13:ILE:HG22	13:K:176:LEU:HD11	2.01	0.42
3:O:210:GLY:HA2	3:O:219:ARG:HA	2.01	0.42
6:R:78:MET:HE2	6:R:78:MET:HB3	1.94	0.42
10:V:76:VAL:HG21	10:V:109:HIS:HB2	2.02	0.42
11:W:86:LEU:O	11:W:90:VAL:HG23	2.20	0.42
13:Y:3:THR:OG1	13:Y:128:VAL:HG13	2.19	0.42
16:b:119:MET:HE3	16:b:119:MET:HB2	1.77	0.42
9:G:22:LEU:O	9:G:25:VAL:HG12	2.20	0.42
11:I:83:PRO:HD3	11:I:113:PRO:HD3	2.02	0.42
14:L:172:MET:HE3	14:L:172:MET:HB3	1.89	0.42
4:P:167:ASN:HB2	4:P:200:THR:OG1	2.20	0.42
5:Q:160:ALA:CB	5:Q:168:VAL:HG13	2.49	0.42
5:Q:168:VAL:HG23	5:Q:194:ALA:HB1	2.00	0.42
11:W:29:ILE:HG22	11:W:30:GLN:N	2.33	0.42
16:b:45:ARG:HB3	16:b:52:THR:CB	2.48	0.42
2:f:128:LEU:HD13	2:f:226:LEU:HD21	2.01	0.42
16:N:45:ARG:HB3	16:N:52:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:14:THR:HG23	6:R:22:PHE:HD2	1.85	0.42
9:U:22:LEU:HD23	9:U:22:LEU:HA	1.76	0.42
1:c:238:MET:HB2	1:c:238:MET:HE2	1.76	0.42
1:e:124:TRP:HZ2	1:e:228:VAL:HG22	1.84	0.42
7:E:143:HIS:HB3	7:E:145:PHE:CE2	2.55	0.42
7:S:62:LYS:HE2	7:S:62:LYS:HB3	1.89	0.42
9:U:113:MET:HG3	10:V:70:THR:HG22	2.01	0.42
10:V:153:ASN:O	10:V:157:GLU:HG2	2.20	0.42
14:Z:99:ARG:HH12	15:a:100:ARG:HH22	1.67	0.42
11:I:6:ASN:HD22	11:I:6:ASN:HA	1.73	0.41
15:M:114:GLY:HA2	15:M:192:VAL:HG11	2.02	0.41
15:M:211:ILE:HG21	10:V:124:TYR:HE1	1.85	0.41
4:P:25:MET:HE3	4:P:25:MET:HB3	1.67	0.41
7:S:196:ARG:HD2	7:S:239:ARG:HB3	2.01	0.41
8:T:87:LEU:HD13	8:T:135:PHE:CE1	2.55	0.41
9:U:211:LYS:HB3	9:U:212:PRO:HD2	2.01	0.41
14:Z:166:LEU:HD12	14:Z:166:LEU:HA	1.82	0.41
14:Z:172:MET:HE2	14:Z:172:MET:HB2	1.67	0.41
15:a:92:LEU:HD12	15:a:92:LEU:HA	1.77	0.41
2:d:20:ASP:HB3	2:d:24:LYS:HE3	2.02	0.41
14:L:20:PHE:HB2	14:L:197:ILE:HD11	2.02	0.41
4:P:197:LEU:HA	4:P:200:THR:HG22	2.02	0.41
10:V:1:THR:HB	10:V:33:LYS:HE2	2.01	0.41
10:V:146:MET:HE3	10:V:146:MET:HB2	1.87	0.41
11:W:29:ILE:O	11:W:30:GLN:C	2.62	0.41
2:h:191:GLN:HE21	2:h:191:GLN:HB2	1.67	0.41
1:g:16:GLN:HE21	1:g:16:GLN:HB3	1.69	0.41
6:D:30:ALA:O	6:D:33:LEU:HB2	2.20	0.41
13:K:37:ILE:HG23	13:K:60:ALA:HB2	2.01	0.41
4:P:218:ARG:HD3	4:P:223:THR:HG22	2.02	0.41
9:U:115:CYS:SG	9:U:154:CYS:HB3	2.61	0.41
10:V:211:VAL:HG12	11:W:199:LEU:HD23	2.03	0.41
15:a:67:LEU:HD21	15:a:88:ILE:HG23	2.01	0.41
7:E:122:ARG:NH1	8:F:122:TYR:HE1	2.18	0.41
13:K:139:MET:HA	13:K:155:LEU:HD11	2.01	0.41
15:M:115:TYR:CZ	15:M:118:GLY:HA2	2.55	0.41
16:N:176:LEU:HB2	16:N:187:GLN:HG2	2.03	0.41
3:O:35:VAL:HG13	3:O:46:ALA:HB3	2.00	0.41
4:P:12:PHE:CE1	5:Q:125:ARG:HD2	2.55	0.41
7:S:50:LYS:HD3	7:S:211:SER:HB2	2.03	0.41
10:V:70:THR:HB	10:V:72:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:15:VAL:HB	12:X:45:LEU:HD21	2.02	0.41
16:b:164:MET:HB2	16:b:164:MET:HE2	1.84	0.41
2:h:103:PRO:HD3	2:i:66:PRO:HG2	2.02	0.41
2:i:21:LEU:HD22	2:i:21:LEU:HA	1.88	0.41
2:d:123:ASP:O	2:d:127:GLN:HG2	2.20	0.41
1:e:31:PHE:HD1	1:e:35:PHE:HB3	1.85	0.41
6:D:20:ARG:O	6:D:21:LEU:C	2.62	0.41
8:F:47:PHE:HZ	8:F:138:GLY:N	2.18	0.41
4:P:54:LYS:HE2	4:P:54:LYS:HB2	1.89	0.41
4:P:184:MET:HE3	4:P:184:MET:HB3	1.98	0.41
7:S:239:ARG:HE	7:S:239:ARG:HB2	1.39	0.41
8:T:158:TYR:HB3	9:U:61:LEU:CD2	2.50	0.41
10:V:59:ILE:HG13	10:V:83:LEU:HG	2.01	0.41
12:X:70:ARG:HE	12:X:70:ARG:HB3	1.59	0.41
12:X:121:LEU:O	12:X:122:ALA:HB3	2.21	0.41
16:b:19:ARG:CZ	16:b:171:GLY:HA3	2.51	0.41
16:b:90:TYR:HB2	16:b:94:LEU:HD23	2.03	0.41
2:h:21:LEU:HD22	2:h:21:LEU:HA	1.85	0.41
2:h:49:LEU:HD12	2:h:49:LEU:HA	1.77	0.41
2:i:123:ASP:O	2:i:127:GLN:HG2	2.20	0.41
2:i:191:GLN:HE21	2:i:191:GLN:HB2	1.58	0.41
3:A:13:SER:O	3:A:14:PRO:C	2.61	0.41
4:P:19:TYR:HD1	4:P:19:TYR:HA	1.59	0.41
4:P:51:ASN:HB3	4:P:56:LEU:HD13	2.02	0.41
7:S:225:ASP:O	7:S:229:VAL:HG13	2.20	0.41
11:W:9:ALA:HB2	11:W:141:CYS:SG	2.61	0.41
2:h:155:LYS:HE3	2:h:155:LYS:HB3	1.88	0.41
1:g:147:LEU:HA	1:g:150:VAL:HG22	2.02	0.41
2:d:36:LYS:HD2	2:d:36:LYS:HA	1.79	0.41
5:C:86:ARG:O	5:C:89:VAL:HG12	2.21	0.41
3:O:55:LEU:HD22	9:U:165:ALA:HB3	2.03	0.41
16:b:1:THR:HG23	16:b:33:LYS:HD3	2.03	0.41
1:g:115:LYS:HE3	1:g:154:LYS:HE2	2.02	0.41
1:e:97:ASN:O	1:e:101:LEU:HG	2.20	0.41
3:A:181:LEU:HA	3:A:181:LEU:HD23	1.84	0.41
3:A:218:ARG:HH21	3:A:220:LEU:HD23	1.84	0.41
4:B:174:MET:HE3	4:B:174:MET:HB2	1.67	0.41
8:F:11:ALA:O	9:G:132:ARG:HD3	2.21	0.41
14:L:84:THR:O	14:L:88:ILE:HG13	2.20	0.41
15:M:79:ASP:HB2	15:M:81:HIS:HD2	1.86	0.41
15:M:201:GLY:O	15:M:203:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:45:VAL:HG13	7:S:187:LEU:HD23	2.03	0.41
9:U:206:LEU:HD12	9:U:210:PHE:HZ	1.85	0.41
10:V:80:ASN:ND2	10:V:119:THR:HG21	2.34	0.41
16:b:103:TRP:CH2	16:b:105:PRO:HA	2.56	0.41
2:h:194:VAL:HG22	1:g:175:VAL:HG12	2.03	0.41
2:d:163:LEU:O	2:d:167:LEU:HG	2.20	0.41
8:F:167:LYS:HB2	8:F:167:LYS:HE2	1.72	0.41
15:M:215:ILE:HD12	15:M:215:ILE:HA	1.90	0.41
16:N:115:PRO:CG	16:N:119:MET:HB2	2.50	0.41
16:N:172:GLY:HA2	15:a:209:TRP:CH2	2.56	0.41
3:O:134:LEU:HD21	3:O:160:THR:HG21	2.01	0.41
4:P:119:GLN:HE22	4:P:123:GLN:HB2	1.85	0.41
4:P:201:MET:HE2	4:P:201:MET:HB3	1.84	0.41
5:Q:188:ILE:O	5:Q:191:VAL:HG13	2.21	0.41
6:R:54:ILE:HD13	6:R:64:ILE:HD13	2.03	0.41
6:R:202:LEU:HA	6:R:205:VAL:HG22	2.03	0.41
8:T:181:MET:H	8:T:181:MET:HG3	1.68	0.41
10:V:138:PHE:CE1	10:V:154:LEU:HG	2.56	0.41
10:V:212:LEU:HD23	11:W:200:LYS:HB2	2.02	0.41
14:Z:22:ILE:HD11	14:Z:168:LEU:HD12	2.02	0.41
15:a:63:LEU:HD23	15:a:63:LEU:HA	1.92	0.41
16:b:41:ILE:HG12	16:b:76:VAL:HG22	2.02	0.41
2:h:109:LYS:O	2:h:112:VAL:HG12	2.21	0.41
2:i:28:LEU:HD12	2:i:32:TYR:HD2	1.86	0.41
2:i:109:LYS:H	2:i:109:LYS:HG2	1.72	0.41
1:c:39:LYS:HA	1:c:39:LYS:HD2	1.94	0.41
1:e:117:LYS:HD3	1:e:117:LYS:HA	1.81	0.41
2:f:36:LYS:HD2	2:f:36:LYS:HA	1.91	0.41
2:f:118:LYS:HE2	2:f:118:LYS:HB3	1.78	0.41
2:f:121:ILE:HD13	2:f:219:ILE:HD11	2.02	0.41
3:A:28:VAL:HG11	3:A:132:SER:HB3	2.03	0.41
3:A:85:LEU:HD13	3:A:133:LEU:HD11	2.02	0.41
6:D:21:LEU:HD12	6:D:21:LEU:HA	1.91	0.41
6:D:84:ASP:HB2	6:D:137:PHE:HD2	1.86	0.41
9:G:118:ILE:HD13	9:G:118:ILE:HA	1.86	0.41
15:M:26:MET:SD	15:M:188:GLN:HG3	2.61	0.41
10:V:18:THR:HG22	10:V:31:CYS:H	1.83	0.41
2:i:173:GLN:O	2:i:176:LYS:HG2	2.21	0.41
9:G:105:TYR:HE1	10:H:82:MET:HE3	1.87	0.40
15:M:201:GLY:O	15:M:202:PRO:C	2.64	0.40
15:M:214:MET:O	15:M:215:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:47:ALA:HB1	4:P:64:LYS:HD3	2.03	0.40
5:Q:52:LYS:HB3	5:Q:52:LYS:HE3	1.92	0.40
6:R:191:LEU:HD12	6:R:191:LEU:HA	1.89	0.40
10:V:32:SER:CB	10:V:187:ARG:NH1	2.84	0.40
16:b:81:SER:O	16:b:85:GLU:HG2	2.21	0.40
2:d:55:SER:HA	2:d:58:LYS:HD3	2.03	0.40
2:d:131:VAL:HG21	2:d:230:ILE:HD11	2.03	0.40
4:B:233:VAL:O	4:B:237:ILE:HG23	2.21	0.40
5:Q:10:PHE:HE2	6:R:136:PRO:O	2.04	0.40
6:R:38:ILE:HG23	6:R:181:LEU:HD11	2.02	0.40
11:W:61:THR:HG23	12:X:86:ARG:HH12	1.86	0.40
14:Z:28:ARG:HD2	14:Z:188:TYR:O	2.21	0.40
15:a:114:GLY:CA	15:a:192:VAL:HG11	2.51	0.40
2:h:238:LYS:HD2	2:h:238:LYS:HA	1.95	0.40
2:i:25:THR:HG21	2:i:134:TRP:CD2	2.56	0.40
10:H:67:SER:HA	10:H:70:THR:HG22	2.02	0.40
16:N:15:GLY:HA3	16:N:176:LEU:HD23	2.02	0.40
3:O:136:CYS:O	3:O:136:CYS:SG	2.78	0.40
8:T:33:SER:O	8:T:167:LYS:HG3	2.22	0.40
8:T:87:LEU:HD21	8:T:119:VAL:HG22	2.02	0.40
10:V:47:GLY:O	10:V:48:THR:C	2.64	0.40
15:a:20:VAL:CG1	15:a:122:LEU:HD13	2.50	0.40
16:b:202:LEU:HD12	16:b:202:LEU:HA	1.81	0.40
1:g:36:LEU:HB2	1:g:37:PRO:HD3	2.03	0.40
1:e:205:MET:O	1:e:209:LEU:HG	2.21	0.40
3:A:9:LEU:HD22	3:A:128:PRO:HD3	2.03	0.40
6:D:9:ASP:O	6:D:23:GLN:HG2	2.21	0.40
7:E:170:THR:O	7:E:174:ARG:HG2	2.22	0.40
9:G:141:ILE:HD12	9:G:220:VAL:HG22	2.03	0.40
14:L:141:ALA:O	14:L:142:SER:C	2.64	0.40
16:N:91:ARG:HG3	16:N:92:GLU:N	2.36	0.40
3:O:19:VAL:HA	3:O:22:GLU:HG2	2.04	0.40
6:R:119:LEU:HA	6:R:119:LEU:HD23	1.72	0.40
12:X:77:PRO:HD2	12:X:108:ASP:HB2	2.03	0.40
12:X:121:LEU:HD23	12:X:121:LEU:HA	1.94	0.40
12:X:167:LEU:HD23	12:X:167:LEU:HA	1.88	0.40
2:d:22:CYS:O	2:d:25:THR:HG22	2.21	0.40
2:d:249:TYR:OH	7:E:18:ARG:HA	2.21	0.40
3:A:55:LEU:HD12	9:G:176:THR:HG23	2.03	0.40
5:C:148:ASP:OD1	5:C:152:THR:HG22	2.22	0.40
12:J:7:ILE:HD12	12:J:14:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:95:MET:HE3	16:N:95:MET:HB3	1.97	0.40
6:R:142:LEU:HD23	6:R:142:LEU:HA	1.99	0.40
15:a:9:THR:O	15:a:54:SER:HB2	2.21	0.40
2:h:248:ILE:H	2:h:248:ILE:HG12	1.48	0.40
2:i:57:LEU:HD21	2:i:110:ILE:HD11	2.02	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	c	210/239 (88%)	209 (100%)	1 (0%)	0	100	100
1	e	209/239 (87%)	206 (99%)	2 (1%)	1 (0%)	24	54
1	g	210/239 (88%)	210 (100%)	0	0	100	100
2	d	207/249 (83%)	204 (99%)	3 (1%)	0	100	100
2	f	200/249 (80%)	197 (98%)	3 (2%)	0	100	100
2	h	207/249 (83%)	204 (99%)	2 (1%)	1 (0%)	24	54
2	i	207/249 (83%)	205 (99%)	2 (1%)	0	100	100
3	A	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
3	O	227/234 (97%)	226 (100%)	1 (0%)	0	100	100
4	B	247/261 (95%)	241 (98%)	6 (2%)	0	100	100
4	P	249/261 (95%)	245 (98%)	3 (1%)	1 (0%)	30	59
5	C	233/248 (94%)	230 (99%)	3 (1%)	0	100	100
5	Q	234/248 (94%)	232 (99%)	2 (1%)	0	100	100
6	D	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
6	R	233/241 (97%)	232 (100%)	1 (0%)	0	100	100
7	E	237/263 (90%)	233 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S	235/263 (89%)	230 (98%)	5 (2%)	0	100	100
8	F	238/255 (93%)	238 (100%)	0	0	100	100
8	T	237/255 (93%)	236 (100%)	1 (0%)	0	100	100
9	G	237/246 (96%)	232 (98%)	4 (2%)	1 (0%)	30	59
9	U	240/246 (98%)	239 (100%)	1 (0%)	0	100	100
10	H	220/277 (79%)	215 (98%)	3 (1%)	2 (1%)	14	41
10	V	220/277 (79%)	217 (99%)	1 (0%)	2 (1%)	14	41
11	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	W	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	24	54
12	J	195/201 (97%)	191 (98%)	3 (2%)	1 (0%)	24	54
12	X	194/201 (96%)	189 (97%)	4 (2%)	1 (0%)	24	54
13	K	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
13	Y	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
14	L	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
14	Z	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
15	M	213/264 (81%)	209 (98%)	3 (1%)	1 (0%)	24	54
15	a	213/264 (81%)	205 (96%)	7 (3%)	1 (0%)	24	54
16	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
16	b	200/239 (84%)	197 (98%)	3 (2%)	0	100	100
All	All	7640/8589 (89%)	7527 (98%)	100 (1%)	13 (0%)	44	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	e	236	PRO
10	H	171	SER
10	H	188	PRO
10	V	171	SER
2	h	247	MET
15	M	10	SER
12	X	122	ALA
9	G	11	ARG
12	J	122	ALA
11	W	29	ILE
15	a	214	MET

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Mol	Chain	Res	Type
10	V	188	PRO
4	P	59	VAL

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	c	172/212 (81%)	159 (92%)	13 (8%)	12	36
1	e	172/212 (81%)	159 (92%)	13 (8%)	12	36
1	g	172/212 (81%)	162 (94%)	10 (6%)	18	49
2	d	168/224 (75%)	157 (94%)	11 (6%)	15	44
2	f	166/224 (74%)	149 (90%)	17 (10%)	7	23
2	h	170/224 (76%)	156 (92%)	14 (8%)	10	32
2	i	168/224 (75%)	147 (88%)	21 (12%)	4	15
3	A	158/191 (83%)	143 (90%)	15 (10%)	8	26
3	O	155/191 (81%)	143 (92%)	12 (8%)	12	35
4	B	159/221 (72%)	143 (90%)	16 (10%)	7	24
4	P	171/221 (77%)	158 (92%)	13 (8%)	12	36
5	C	152/211 (72%)	137 (90%)	15 (10%)	7	24
5	Q	157/211 (74%)	142 (90%)	15 (10%)	8	26
6	D	173/203 (85%)	155 (90%)	18 (10%)	7	23
6	R	164/203 (81%)	148 (90%)	16 (10%)	7	25
7	E	181/224 (81%)	169 (93%)	12 (7%)	15	43
7	S	169/224 (75%)	156 (92%)	13 (8%)	12	35
8	F	167/212 (79%)	149 (89%)	18 (11%)	6	21
8	T	168/212 (79%)	154 (92%)	14 (8%)	10	32
9	G	175/210 (83%)	156 (89%)	19 (11%)	6	20
9	U	177/210 (84%)	160 (90%)	17 (10%)	8	26
10	H	165/228 (72%)	145 (88%)	20 (12%)	5	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	V	166/228 (73%)	146 (88%)	20 (12%)	5	16
11	I	164/174 (94%)	141 (86%)	23 (14%)	3	11
11	W	162/174 (93%)	149 (92%)	13 (8%)	11	34
12	J	156/171 (91%)	144 (92%)	12 (8%)	12	35
12	X	156/171 (91%)	148 (95%)	8 (5%)	21	53
13	K	146/202 (72%)	133 (91%)	13 (9%)	9	28
13	Y	147/202 (73%)	129 (88%)	18 (12%)	5	16
14	L	161/199 (81%)	149 (92%)	12 (8%)	12	37
14	Z	160/199 (80%)	147 (92%)	13 (8%)	11	33
15	M	166/215 (77%)	157 (95%)	9 (5%)	20	51
15	a	160/215 (74%)	145 (91%)	15 (9%)	8	26
16	N	149/181 (82%)	141 (95%)	8 (5%)	20	51
16	b	145/181 (80%)	136 (94%)	9 (6%)	16	46
All	All	5717/7216 (79%)	5212 (91%)	505 (9%)	11	29

All (505) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	16	GLN
1	c	17	VAL
1	c	22	GLN
1	c	32	LEU
1	c	41	ILE
1	c	57	LEU
1	c	68	ILE
1	c	121	VAL
1	c	122	ILE
1	c	134	ASP
1	c	142	ILE
1	c	193	GLU
1	c	238	MET
2	d	21	LEU
2	d	25	THR
2	d	46	GLU
2	d	63	ILE
2	d	65	VAL
2	d	104	VAL

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Mol	Chain	Res	Type
2	d	114	LEU
2	d	128	LEU
2	d	136	GLN
2	d	226	LEU
2	d	248	ILE
1	e	41	ILE
1	e	47	LEU
1	e	57	LEU
1	e	103	LEU
1	e	107	VAL
1	e	116	GLU
1	e	121	VAL
1	e	134	ASP
1	e	142	ILE
1	e	184	VAL
1	e	186	ASP
1	e	207	LEU
1	e	224	LEU
2	f	11	GLN
2	f	21	LEU
2	f	29	LEU
2	f	39	GLU
2	f	46	GLU
2	f	63	ILE
2	f	65	VAL
2	f	110	ILE
2	f	121	ILE
2	f	128	LEU
2	f	132	THR
2	f	136	GLN
2	f	137	LEU
2	f	144	ASP
2	f	168	GLU
2	f	226	LEU
2	f	241	ARG
3	A	5	TYR
3	A	19	VAL
3	A	43	VAL
3	A	44	VAL
3	A	64	VAL
3	A	73	LEU
3	A	74	VAL

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Mol	Chain	Res	Type
3	A	80	PRO
3	A	86	VAL
3	A	126	VAL
3	A	135	ILE
3	A	187	ILE
3	A	207	ILE
3	A	209	VAL
3	A	218	ARG
4	B	6	ASP
4	B	9	THR
4	B	21	VAL
4	B	28	ILE
4	B	33	THR
4	B	35	LEU
4	B	44	LEU
4	B	61	PHE
4	B	76	VAL
4	B	105	ILE
4	B	128	ARG
4	B	134	LEU
4	B	177	GLN
4	B	217	THR
4	B	223	THR
4	B	224	VAL
5	C	7	ILE
5	C	35	VAL
5	C	40	ILE
5	C	41	VAL
5	C	59	VAL
5	C	60	ARG
5	C	65	LEU
5	C	69	VAL
5	C	89	VAL
5	C	107	ILE
5	C	108	THR
5	C	148	ASP
5	C	168	VAL
5	C	186	LEU
5	C	191	VAL
6	D	38	ILE
6	D	46	VAL
6	D	47	CYS

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Mol	Chain	Res	Type
6	D	54	ILE
6	D	64	ILE
6	D	67	ILE
6	D	78	MET
6	D	81	LEU
6	D	107	MET
6	D	113	THR
6	D	163	VAL
6	D	165	CYS
6	D	183	GLU
6	D	188	SER
6	D	210	LEU
6	D	220	VAL
6	D	221	GLN
6	D	228	MET
7	E	14	SER
7	E	63	ILE
7	E	109	VAL
7	E	122	ARG
7	E	132	LEU
7	E	139	ASP
7	E	147	THR
7	E	150	SER
7	E	173	GLU
7	E	184	LEU
7	E	222	THR
7	E	237	GLU
8	F	9	LEU
8	F	35	THR
8	F	37	ILE
8	F	53	VAL
8	F	54	LEU
8	F	66	LEU
8	F	69	VAL
8	F	71	ARG
8	F	80	LEU
8	F	96	SER
8	F	142	VAL
8	F	151	ILE
8	F	174	THR
8	F	178	LYS
8	F	179	LEU

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Mol	Chain	Res	Type
8	F	186	CYS
8	F	190	VAL
8	F	192	GLU
9	G	13	ILE
9	G	17	SER
9	G	42	VAL
9	G	49	VAL
9	G	61	LEU
9	G	66	VAL
9	G	79	VAL
9	G	80	MET
9	G	112	ASP
9	G	115	CYS
9	G	124	VAL
9	G	126	THR
9	G	131	MET
9	G	137	CYS
9	G	166	THR
9	G	170	VAL
9	G	173	THR
9	G	215	ILE
9	G	217	VAL
10	H	6	VAL
10	H	12	ILE
10	H	18	THR
10	H	25	VAL
10	H	38	SER
10	H	43	CYS
10	H	65	LEU
10	H	98	LEU
10	H	105	VAL
10	H	106	THR
10	H	125	VAL
10	H	143	ARG
10	H	171	SER
10	H	175	LEU
10	H	181	ASN
10	H	183	LEU
10	H	188	PRO
10	H	194	LYS
10	H	213	THR
10	H	221	ILE

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Mol	Chain	Res	Type
11	I	19	VAL
11	I	33	MET
11	I	36	THR
11	I	52	LEU
11	I	55	LEU
11	I	57	THR
11	I	70	LEU
11	I	81	ILE
11	I	85	THR
11	I	104	THR
11	I	125	LEU
11	I	126	ILE
11	I	134	ASP
11	I	136	VAL
11	I	137	VAL
11	I	143	GLU
11	I	145	MET
11	I	158	ASP
11	I	177	ASP
11	I	182	MET
11	I	184	VAL
11	I	190	GLU
11	I	196	THR
12	J	13	VAL
12	J	26	VAL
12	J	38	MET
12	J	53	THR
12	J	74	GLU
12	J	76	SER
12	J	78	THR
12	J	96	THR
12	J	102	LEU
12	J	118	MET
12	J	145	ARG
12	J	148	THR
13	K	1	THR
13	K	29	GLN
13	K	41	LEU
13	K	42	LEU
13	K	80	SER
13	K	99	THR
13	K	102	CYS

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Mol	Chain	Res	Type
13	K	114	VAL
13	K	116	SER
13	K	121	ILE
13	K	179	VAL
13	K	182	ASP
13	K	187	VAL
14	L	11	THR
14	L	36	HIS
14	L	37	THR
14	L	38	ARG
14	L	131	GLN
14	L	136	LYS
14	L	164	VAL
14	L	169	ASP
14	L	189	THR
14	L	197	ILE
14	L	198	VAL
14	L	199	THR
15	M	21	VAL
15	M	32	SER
15	M	79	ASP
15	M	88	ILE
15	M	92	LEU
15	M	109	THR
15	M	147	GLN
15	M	191	THR
15	M	205	THR
16	N	1	THR
16	N	18	SER
16	N	20	THR
16	N	30	VAL
16	N	40	ARG
16	N	94	LEU
16	N	190	LEU
16	N	202	LEU
3	O	11	THR
3	O	43	VAL
3	O	44	VAL
3	O	50	LYS
3	O	54	ILE
3	O	64	VAL
3	O	73	LEU

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Mol	Chain	Res	Type
3	O	84	VAL
3	O	86	VAL
3	O	131	VAL
3	O	135	ILE
3	O	155	PHE
4	P	9	THR
4	P	25	MET
4	P	28	ILE
4	P	44	LEU
4	P	64	LYS
4	P	123	GLN
4	P	132	VAL
4	P	141	LYS
4	P	150	SER
4	P	185	THR
4	P	190	LEU
4	P	217	THR
4	P	223	THR
5	Q	23	GLN
5	Q	27	LYS
5	Q	54	GLN
5	Q	67	ASP
5	Q	77	THR
5	Q	83	VAL
5	Q	98	VAL
5	Q	103	THR
5	Q	107	ILE
5	Q	129	ILE
5	Q	172	LEU
5	Q	191	VAL
5	Q	198	VAL
5	Q	206	ILE
5	Q	225	ILE
6	R	31	ILE
6	R	46	VAL
6	R	54	ILE
6	R	58	LEU
6	R	91	LYS
6	R	108	THR
6	R	119	LEU
6	R	121	LEU
6	R	125	GLU

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Mol	Chain	Res	Type
6	R	139	VAL
6	R	156	MET
6	R	190	THR
6	R	210	LEU
6	R	215	ILE
6	R	220	VAL
6	R	234	LEU
7	S	5	GLN
7	S	35	THR
7	S	39	LYS
7	S	49	LEU
7	S	60	GLN
7	S	64	LEU
7	S	120	THR
7	S	130	VAL
7	S	133	LEU
7	S	144	ILE
7	S	150	SER
7	S	222	THR
7	S	228	ASP
8	T	35	THR
8	T	54	LEU
8	T	69	VAL
8	T	73	VAL
8	T	94	GLU
8	T	100	SER
8	T	142	VAL
8	T	154	SER
8	T	156	VAL
8	T	165	ILE
8	T	181	MET
8	T	182	LYS
8	T	216	VAL
8	T	231	ILE
9	U	49	VAL
9	U	50	ILE
9	U	66	VAL
9	U	73	THR
9	U	78	CYS
9	U	80	MET
9	U	81	THR
9	U	84	THR

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Mol	Chain	Res	Type
9	U	90	GLN
9	U	112	ASP
9	U	124	VAL
9	U	131	MET
9	U	170	VAL
9	U	173	THR
9	U	200	THR
9	U	215	ILE
9	U	216	GLU
10	V	1	THR
10	V	6	VAL
10	V	18	THR
10	V	21	THR
10	V	25	VAL
10	V	48	THR
10	V	61	SER
10	V	100	LEU
10	V	105	VAL
10	V	106	THR
10	V	118	SER
10	V	119	THR
10	V	127	MET
10	V	174	ASP
10	V	175	LEU
10	V	184	ASP
10	V	186	LEU
10	V	197	THR
10	V	212	LEU
10	V	216	ILE
11	W	2	ILE
11	W	11	MET
11	W	19	VAL
11	W	57	THR
11	W	70	LEU
11	W	131	VAL
11	W	134	ASP
11	W	136	VAL
11	W	137	VAL
11	W	141	CYS
11	W	176	ARG
11	W	186	VAL
11	W	195	THR

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Mol	Chain	Res	Type
12	X	13	VAL
12	X	15	VAL
12	X	20	VAL
12	X	26	VAL
12	X	31	ASP
12	X	54	VAL
12	X	96	THR
12	X	118	MET
13	Y	1	THR
13	Y	30	THR
13	Y	40	TYR
13	Y	41	LEU
13	Y	44	THR
13	Y	58	LEU
13	Y	97	MET
13	Y	102	CYS
13	Y	104	TRP
13	Y	107	ARG
13	Y	119	ASN
13	Y	121	ILE
13	Y	128	VAL
13	Y	133	VAL
13	Y	138	VAL
13	Y	179	VAL
13	Y	187	VAL
13	Y	194	ASP
14	Z	13	LEU
14	Z	15	ILE
14	Z	22	ILE
14	Z	93	SER
14	Z	99	ARG
14	Z	106	VAL
14	Z	110	ILE
14	Z	113	LEU
14	Z	149	LEU
14	Z	164	VAL
14	Z	195	ILE
14	Z	198	VAL
14	Z	203	ILE
15	a	14	VAL
15	a	21	VAL
15	a	27	LEU

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Mol	Chain	Res	Type
15	a	29	SER
15	a	45	VAL
15	a	51	LEU
15	a	65	GLN
15	a	67	LEU
15	a	100	ARG
15	a	110	MET
15	a	137	LEU
15	a	148	PRO
15	a	169	VAL
15	a	191	THR
15	a	215	ILE
16	b	4	MET
16	b	6	VAL
16	b	20	THR
16	b	21	THR
16	b	95	MET
16	b	98	ILE
16	b	121	VAL
16	b	187	GLN
16	b	190	LEU
2	h	21	LEU
2	h	49	LEU
2	h	50	ASN
2	h	61	LEU
2	h	63	ILE
2	h	65	VAL
2	h	121	ILE
2	h	128	LEU
2	h	144	ASP
2	h	159	LEU
2	h	185	VAL
2	h	191	GLN
2	h	229	ILE
2	h	248	ILE
2	i	21	LEU
2	i	28	LEU
2	i	50	ASN
2	i	61	LEU
2	i	63	ILE
2	i	65	VAL
2	i	106	CYS

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Mol	Chain	Res	Type
2	i	109	LYS
2	i	121	ILE
2	i	128	LEU
2	i	132	THR
2	i	136	GLN
2	i	144	ASP
2	i	155	LYS
2	i	157	PHE
2	i	159	LEU
2	i	185	VAL
2	i	191	GLN
2	i	199	GLN
2	i	213	ARG
2	i	248	ILE
1	g	38	GLN
1	g	41	ILE
1	g	50	ASP
1	g	57	LEU
1	g	68	ILE
1	g	94	LEU
1	g	142	ILE
1	g	156	LYS
1	g	185	MET
1	g	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	38	GLN
1	c	45	GLN
1	c	126	GLN
1	c	151	ASN
2	d	138	GLN
2	d	147	ASN
2	d	193	HIS
1	e	183	HIS
1	e	218	HIS
2	f	115	GLN
2	f	138	GLN
2	f	147	ASN
2	f	171	HIS
3	A	122	GLN

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Mol	Chain	Res	Type
4	B	102	GLN
4	B	149	GLN
4	B	230	GLN
5	C	85	ASN
6	D	99	HIS
6	D	227	HIS
7	E	31	GLN
7	E	65	HIS
7	E	68	ASN
7	E	183	ASN
8	F	120	HIS
9	G	24	GLN
9	G	53	GLN
9	G	75	ASN
9	G	128	ASN
9	G	193	GLN
10	H	80	ASN
11	I	17	ASN
12	J	63	ASN
12	J	82	ASN
12	J	87	ASN
12	J	132	HIS
12	J	168	GLN
13	K	162	GLN
13	K	175	ASN
14	L	77	HIS
14	L	79	ASN
14	L	80	ASN
15	M	81	HIS
15	M	147	GLN
15	M	157	GLN
15	M	188	GLN
15	M	213	HIS
16	N	66	HIS
16	N	106	GLN
16	N	110	GLN
3	O	108	GLN
3	O	168	ASN
4	P	102	GLN
4	P	109	GLN
4	P	123	GLN
4	P	142	HIS

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Mol	Chain	Res	Type
4	P	149	GLN
4	P	230	GLN
5	Q	15	HIS
5	Q	54	GLN
5	Q	94	HIS
6	R	152	GLN
6	R	182	GLN
6	R	227	HIS
7	S	16	GLN
7	S	68	ASN
7	S	90	GLN
8	T	110	HIS
9	U	24	GLN
9	U	147	GLN
9	U	224	ASN
10	V	80	ASN
11	W	6	ASN
11	W	80	GLN
12	X	63	ASN
12	X	71	ASN
12	X	82	ASN
12	X	87	ASN
12	X	132	HIS
13	Y	29	GLN
13	Y	119	ASN
14	Z	80	ASN
14	Z	108	ASN
14	Z	152	GLN
14	Z	157	ASN
14	Z	163	HIS
15	a	3	ASN
15	a	81	HIS
16	b	123	GLN
16	b	193	GLN
2	h	27	ASN
2	h	138	GLN
2	h	147	ASN
2	h	191	GLN
2	h	199	GLN
2	i	11	GLN
2	i	27	ASN
2	i	105	ASN

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Mol	Chain	Res	Type
2	i	107	ASN
2	i	147	ASN
2	i	171	HIS
2	i	173	GLN
2	i	191	GLN
2	i	199	GLN
2	i	202	HIS
1	g	16	GLN
1	g	38	GLN
1	g	126	GLN
1	g	127	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

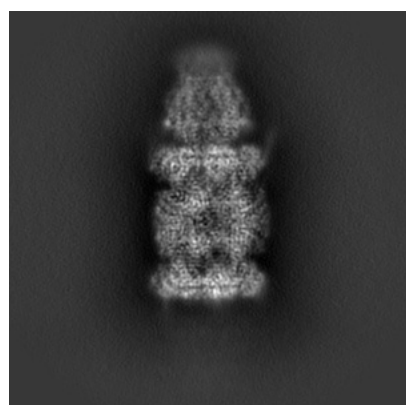
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24276. These allow visual inspection of the internal detail of the map and identification of artifacts.

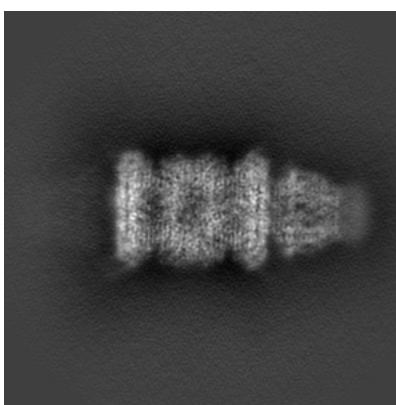
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

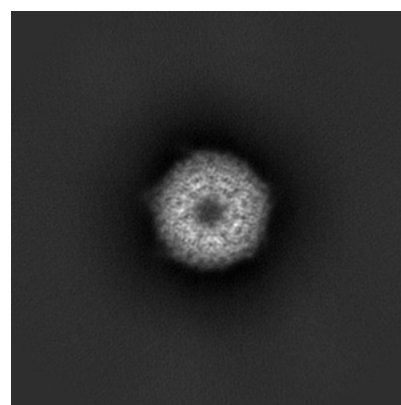
6.1.1 Primary map



X



Y

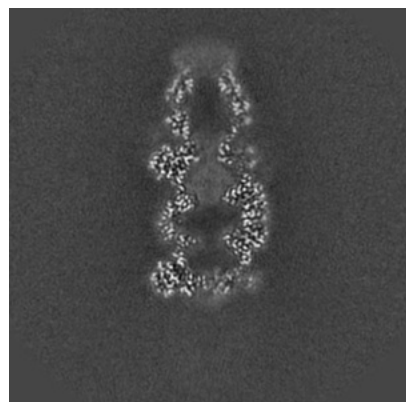


Z

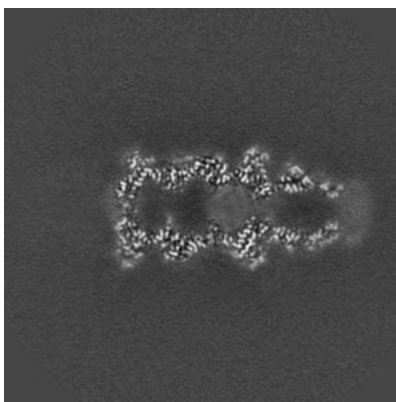
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

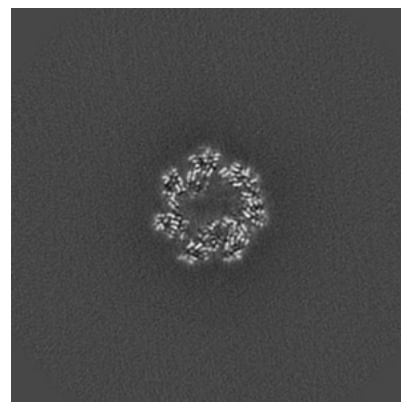
6.2.1 Primary map



X Index: 160



Y Index: 160

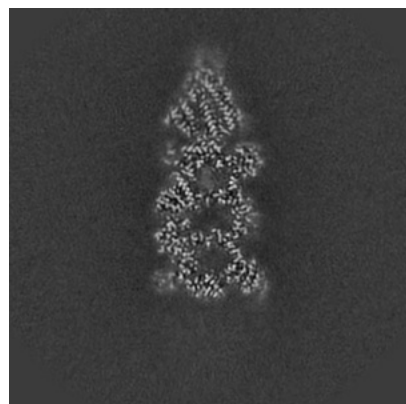


Z Index: 160

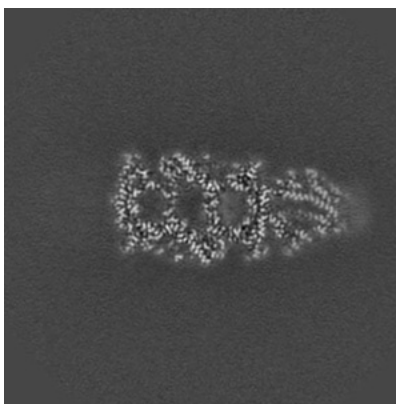
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

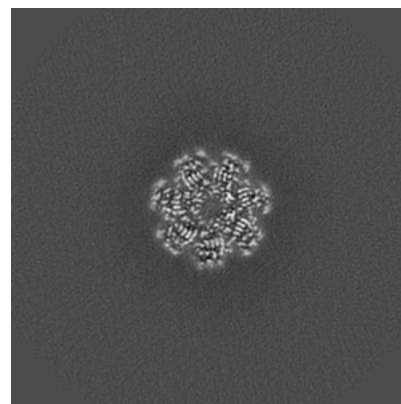
6.3.1 Primary map



X Index: 176



Y Index: 145

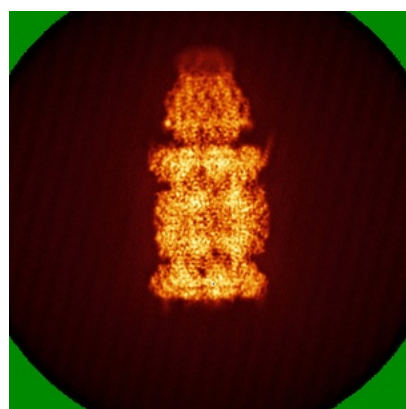


Z Index: 197

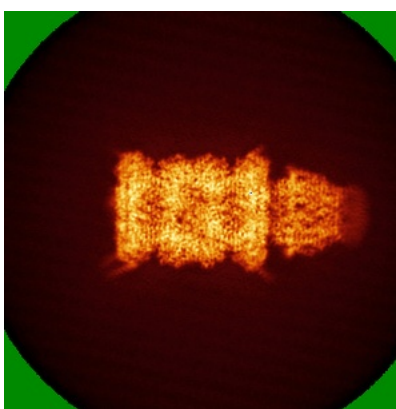
The images above show the largest variance slices of the map in three orthogonal directions.

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

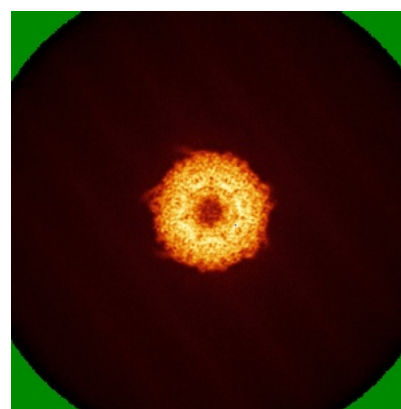
6.4.1 Primary map



X



Y

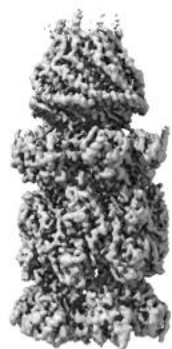


Z

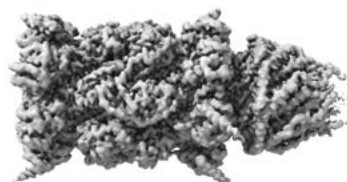
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

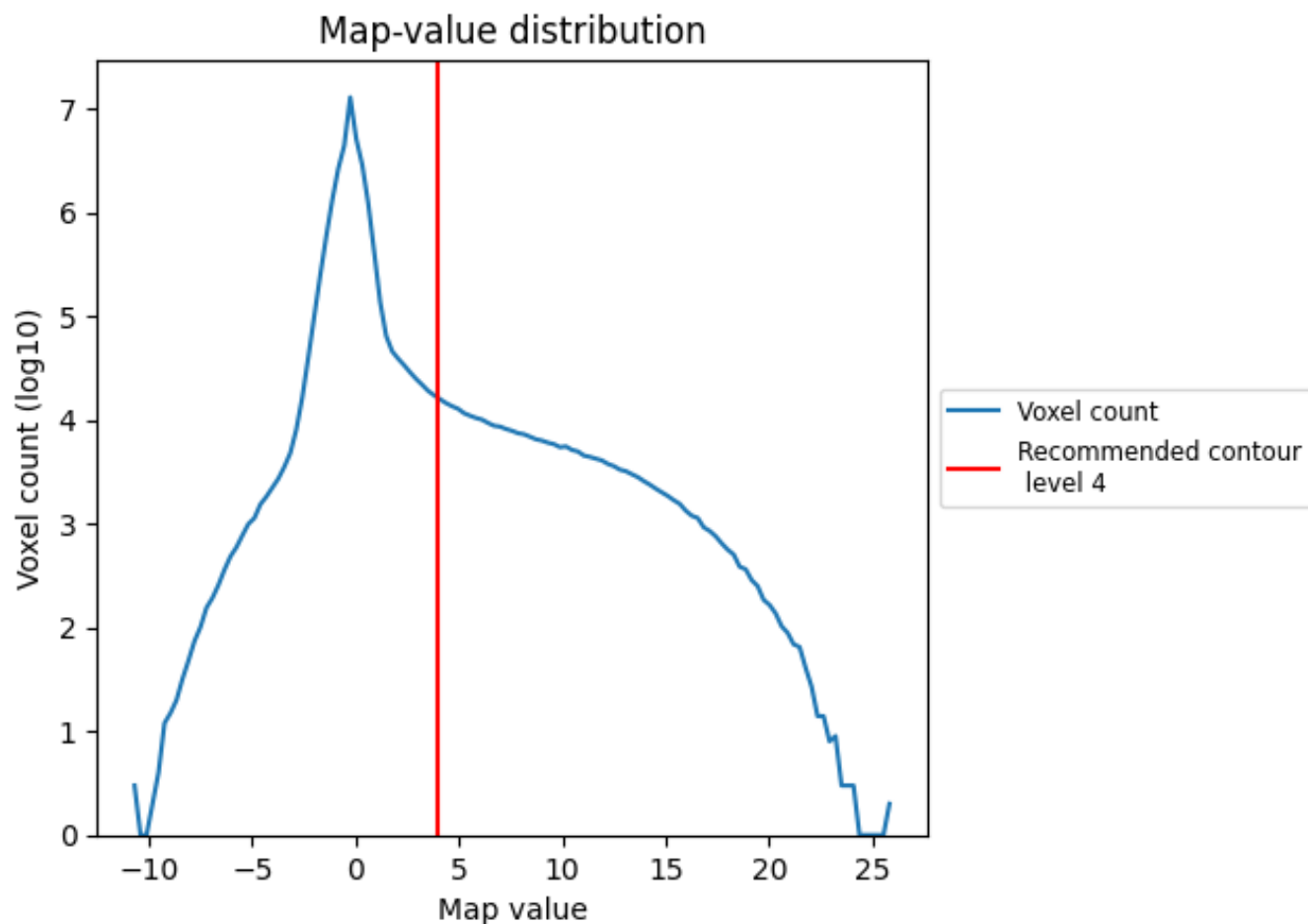
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

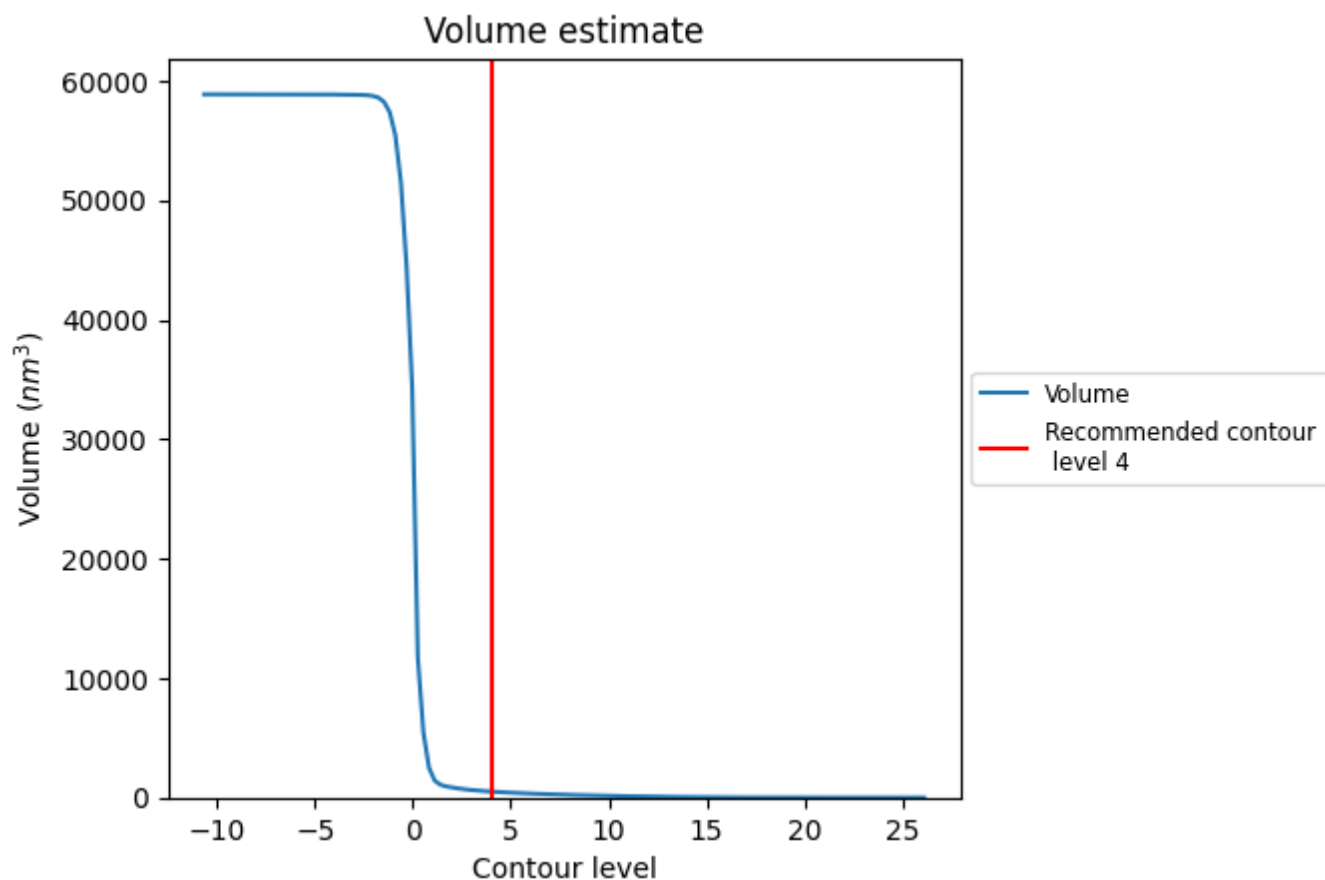
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

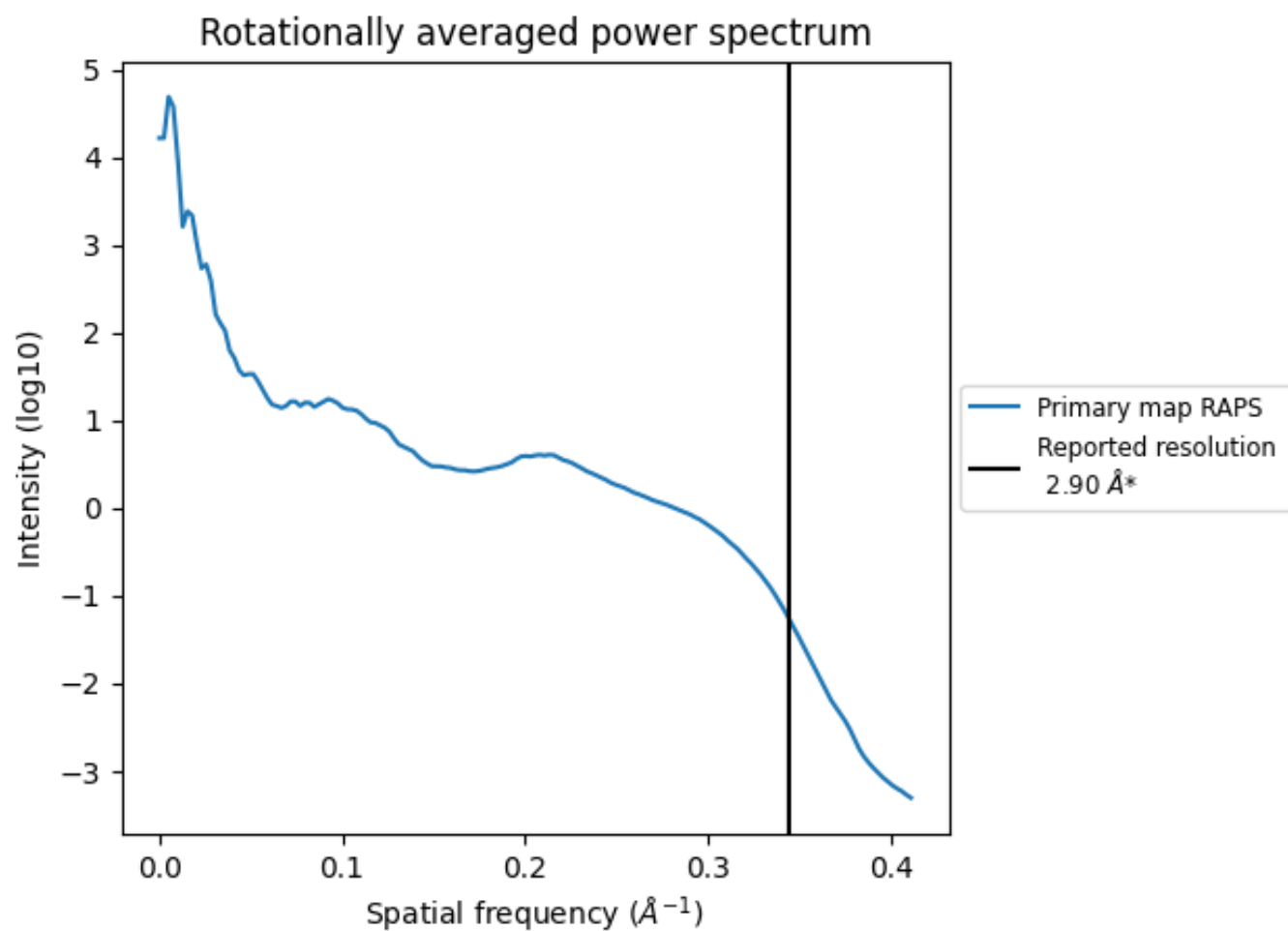
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 499 nm³; this corresponds to an approximate mass of 451 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 ⓘ

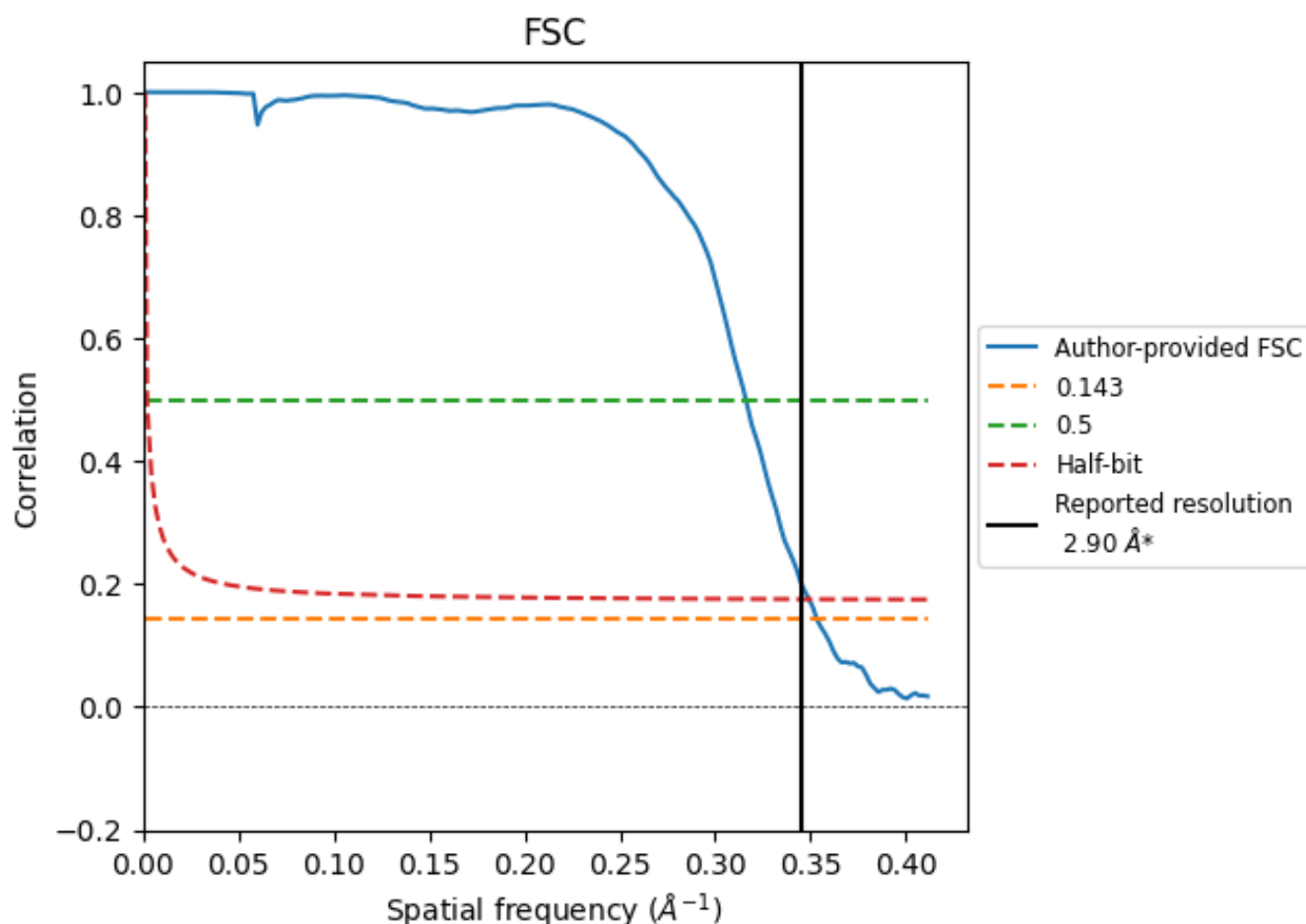


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

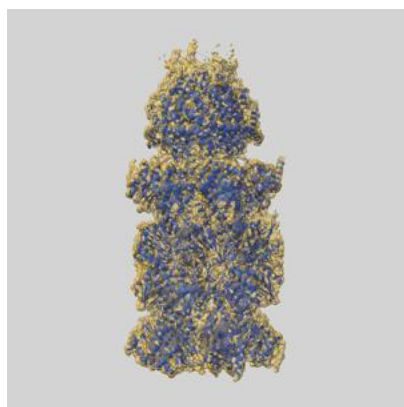
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.83	3.16	2.86
Unmasked-calculated*	-	-	-

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

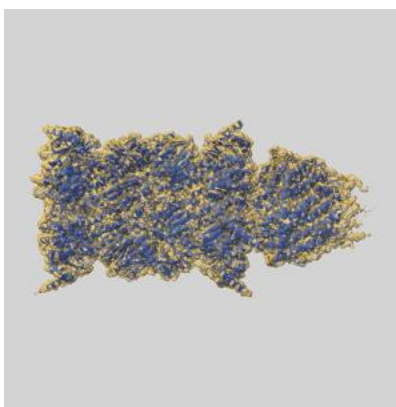
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24276 and PDB model 8CXB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

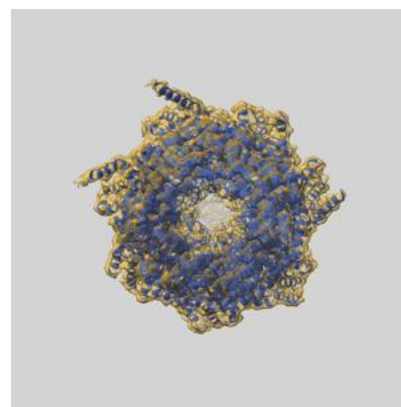
9.1 Map-model overlay [i](#)



X



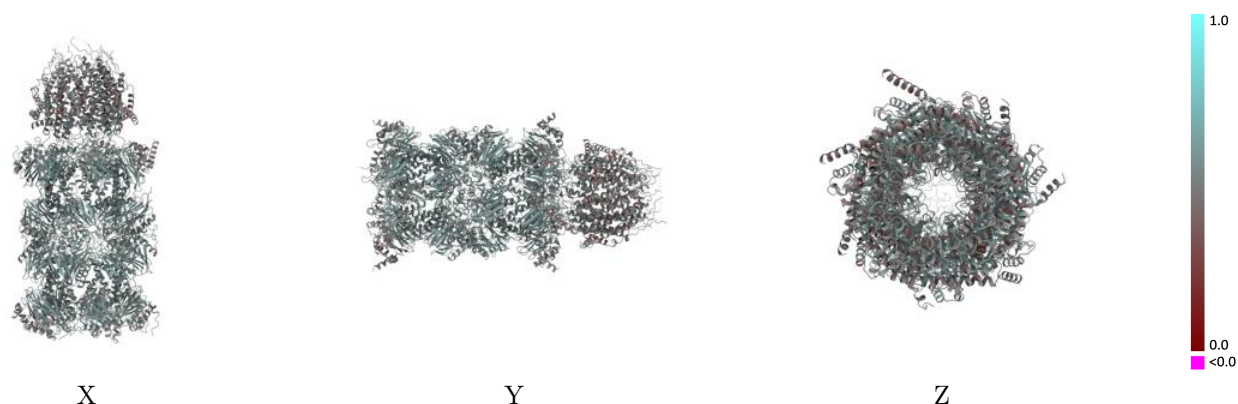
Y



Z

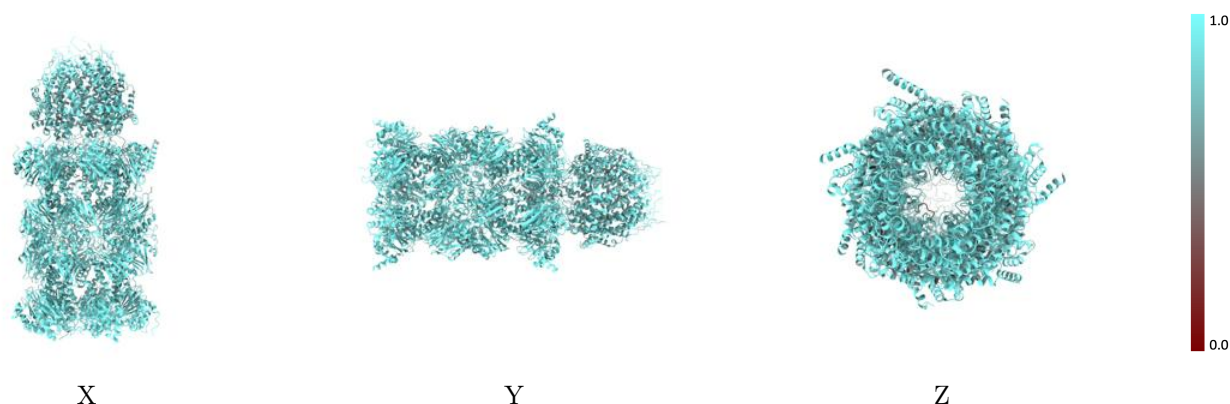
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



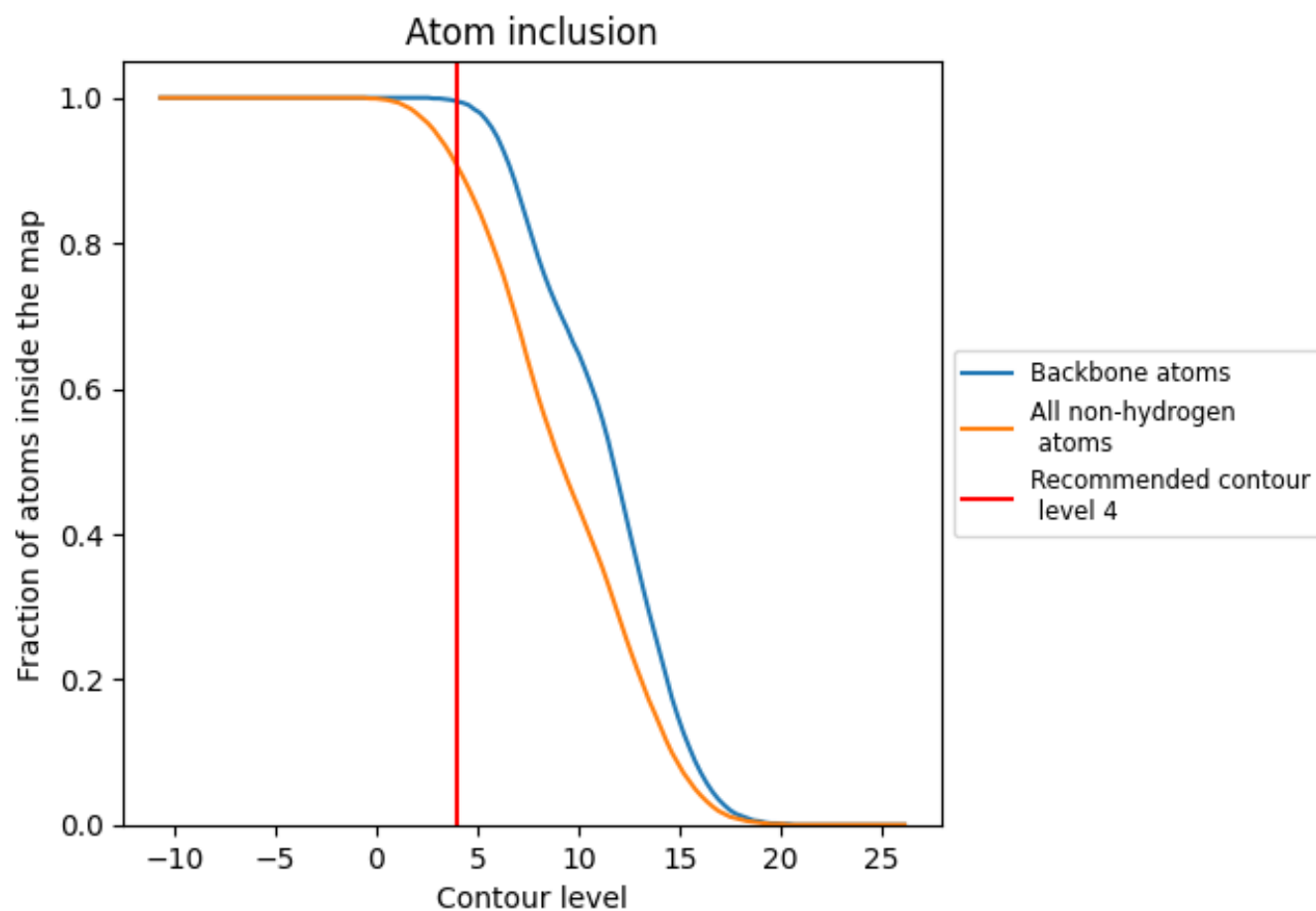
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 91% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.5250
A	 0.9160	 0.5310
B	 0.9080	 0.5290
C	 0.9230	 0.5300
D	 0.8930	 0.5260
E	 0.9130	 0.5370
F	 0.9210	 0.5430
G	 0.9270	 0.5340
H	 0.9300	 0.5470
I	 0.9090	 0.5460
J	 0.9140	 0.5500
K	 0.9390	 0.5490
L	 0.9200	 0.5490
M	 0.9270	 0.5420
N	 0.9270	 0.5540
O	 0.9360	 0.5390
P	 0.9140	 0.5240
Q	 0.9220	 0.5140
R	 0.9060	 0.5210
S	 0.9340	 0.5280
T	 0.9360	 0.5290
U	 0.9310	 0.5330
V	 0.9240	 0.5430
W	 0.9300	 0.5550
X	 0.9180	 0.5500
Y	 0.9300	 0.5410
Z	 0.9330	 0.5530
a	 0.9390	 0.5550
b	 0.9310	 0.5530
c	 0.8330	 0.4640
d	 0.8420	 0.4700
e	 0.8520	 0.4670
f	 0.8420	 0.4710
g	 0.8260	 0.4660
h	 0.8370	 0.4650
i	 0.8470	 0.4680

