



Full wwPDB EM Validation Report ⓘ

Sep 2, 2024 – 12:32 pm BST

PDB ID : 8RVL
EMDB ID : EMD-19523
Title : Proteasomal late precursor complex from pre1-1
Authors : Mark, E.; Ramos, P.C.; Kayser, F.; Hoekendorff, J.; Dohmen, R.J.; Wendler, P.
Deposited on : 2024-02-01
Resolution : 2.14 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.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

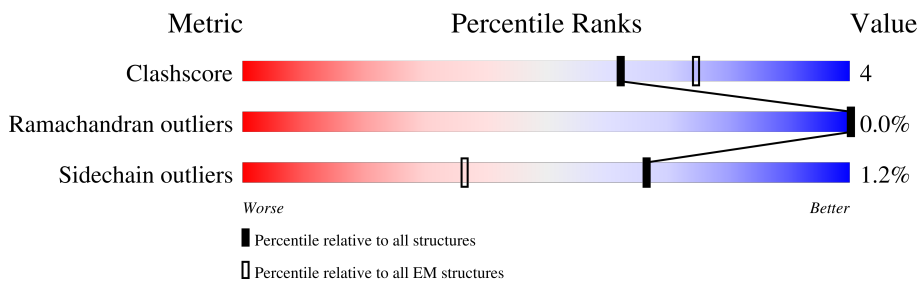
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




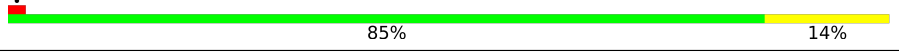

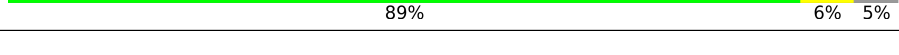
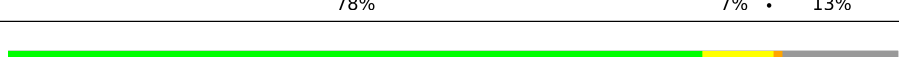
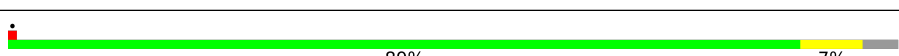












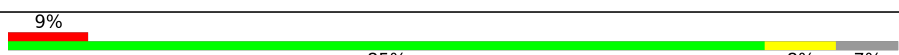
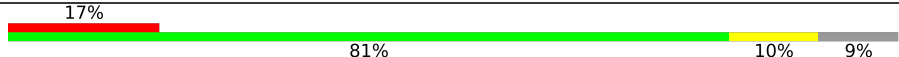





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2	266	
1	N	266	
2	A	252	
2	O	252	
3	D	254	
3	R	254	
4	E	260	
4	S	260	

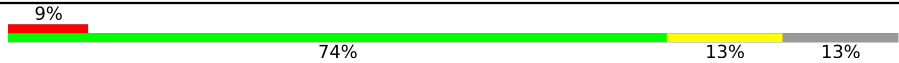
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Mol	Chain	Length	Quality of chain
5	F	234	 85% 15%
5	T	234	 85% 14%
6	H	215	 88% 7% 5%
6	V	215	 89% 6% 5%
7	1	241	 78% 7% 13%
7	M	241	 78% 8% 13%
8	3	148	 89% 7%
8	6	148	 89% 7%
9	4	276	 74% 12% 13% 13%
9	7	276	 74% 12% 13% 14%
10	5	267	 85% 13%
10	8	267	 83% 14%
11	B	250	 86% 13%
11	P	250	 86% 13%
12	C	258	 79% 12% 8% 6%
12	Q	258	 79% 13% 8% 6%
13	G	288	 76% 7% 16% 7%
13	U	288	 76% 8% 16% 7%
14	I	261	 73% 7% 20%
14	W	261	 73% 7% 20%
15	J	205	 80% 12% 6% 9%
15	X	205	 85% 8% 7% 9%
16	K	212	 81% 10% 9% 17%
16	Y	212	 82% 9% 9% 17%
17	L	287	 75% 12% 13% 9%

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Mol	Chain	Length	Quality of chain
17	Z	287	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '9%', a large green segment labeled '74%', a yellow segment labeled '13%', and a grey segment at the end labeled '13%'.</p>

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 62379 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 beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	224	Total	C	N	O	S	0	0
			1753	1108	300	338	7		
1	N	224	Total	C	N	O	S	0	0
			1753	1108	300	338	7		

- Molecule 2 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	240	Total	C	N	O	S	0	0
			1892	1204	318	362	8		
2	O	240	Total	C	N	O	S	0	0
			1892	1204	318	362	8		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	240	Total	C	N	O	S	0	0
			1877	1174	328	370	5		
3	R	240	Total	C	N	O	S	0	0
			1877	1174	328	370	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	247	Total	C	N	O	S	0	0
			1914	1198	322	386	8		
4	S	247	Total	C	N	O	S	0	0
			1914	1198	322	386	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		
5	T	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		

- Molecule 6 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	205	Total	C	N	O	S	0	0
			1575	996	261	311	7		
6	V	205	Total	C	N	O	S	0	0
			1575	996	261	311	7		

- Molecule 7 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	210	Total	C	N	O	S	0	0
			1663	1058	286	315	4		
7	M	210	Total	C	N	O	S	0	0
			1663	1058	286	315	4		

- Molecule 8 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	142	Total	C	N	O	S	0	0
			1133	698	200	228	7		
8	6	142	Total	C	N	O	S	0	0
			1133	698	200	228	7		

- Molecule 9 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	239	Total	C	N	O	S	0	0
			1865	1215	290	347	13		
9	7	239	Total	C	N	O	S	0	0
			1865	1215	290	347	13		

- Molecule 10 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	262	Total	C	N	O	S	0	0
			2128	1377	341	402	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	8	261	Total	C	N	O	S	0	0
			2120	1372	338	402	8		

- Molecule 11 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	248	Total	C	N	O	S	0	0
			1900	1210	313	373	4		
11	P	248	Total	C	N	O	S	0	0
			1900	1210	313	373	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	237	Total	C	N	O	S	0	0
			1862	1179	313	367	3		
12	Q	237	Total	C	N	O	S	0	0
			1862	1179	313	367	3		

- Molecule 13 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	242	Total	C	N	O	S	0	0
			1876	1195	326	351	4		
13	U	242	Total	C	N	O	S	0	0
			1876	1195	326	351	4		

- Molecule 14 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	209	Total	C	N	O	S	0	0
			1582	996	275	305	6		
14	W	209	Total	C	N	O	S	0	0
			1582	996	275	305	6		

- Molecule 15 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	192	Total	C	N	O	S	0	0
			1490	960	240	282	8		
15	X	191	Total	C	N	O	S	0	0
			1485	957	239	281	8		

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	K	193	1552	987	263	297	5	0	0
16	Y	193	1552	987	263	297	5	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	engineered mutation	UNP P22141
K	199	ASP	-	expression tag	UNP P22141
K	200	TYR	-	expression tag	UNP P22141
K	201	LYS	-	expression tag	UNP P22141
K	202	ASP	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	ASP	-	expression tag	UNP P22141
K	205	ASP	-	expression tag	UNP P22141
K	206	LYS	-	expression tag	UNP P22141
K	207	HIS	-	expression tag	UNP P22141
K	208	HIS	-	expression tag	UNP P22141
K	209	HIS	-	expression tag	UNP P22141
K	210	HIS	-	expression tag	UNP P22141
K	211	HIS	-	expression tag	UNP P22141
K	212	HIS	-	expression tag	UNP P22141
Y	142	PHE	SER	engineered mutation	UNP P22141
Y	199	ASP	-	expression tag	UNP P22141
Y	200	TYR	-	expression tag	UNP P22141
Y	201	LYS	-	expression tag	UNP P22141
Y	202	ASP	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	ASP	-	expression tag	UNP P22141
Y	205	ASP	-	expression tag	UNP P22141
Y	206	LYS	-	expression tag	UNP P22141
Y	207	HIS	-	expression tag	UNP P22141
Y	208	HIS	-	expression tag	UNP P22141
Y	209	HIS	-	expression tag	UNP P22141
Y	210	HIS	-	expression tag	UNP P22141
Y	211	HIS	-	expression tag	UNP P22141
Y	212	HIS	-	expression tag	UNP P22141

- Molecule 17 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	250	Total	C	N	O	S	0	0
			1937	1229	332	367	9		
17	Z	250	Total	C	N	O	S	0	0
			1937	1229	332	367	9		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	2	88	Total	O	0
			88	88	
18	A	101	Total	O	0
			101	101	
18	D	70	Total	O	0
			70	70	
18	E	100	Total	O	0
			100	100	
18	F	84	Total	O	0
			84	84	
18	H	81	Total	O	0
			81	81	
18	N	86	Total	O	0
			86	86	
18	O	102	Total	O	0
			102	102	
18	R	71	Total	O	0
			71	71	
18	S	97	Total	O	0
			97	97	
18	T	82	Total	O	0
			82	82	
18	V	75	Total	O	0
			75	75	
18	1	96	Total	O	0
			96	96	
18	3	63	Total	O	0
			63	63	
18	4	56	Total	O	0
			56	56	
18	5	94	Total	O	0
			94	94	
18	6	59	Total	O	0
			59	59	
18	7	54	Total	O	0
			54	54	

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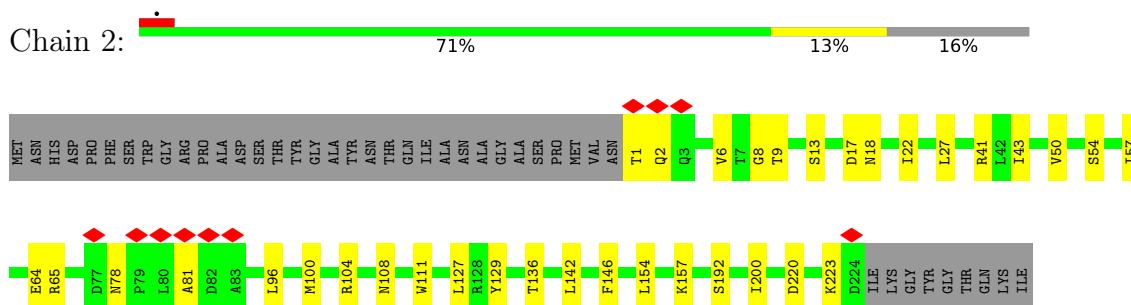
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Mol	Chain	Residues	Atoms		AltConf
18	8	98	Total 98	O 98	0
18	B	90	Total 90	O 90	0
18	C	88	Total 88	O 88	0
18	G	93	Total 93	O 93	0
18	I	66	Total 66	O 66	0
18	J	80	Total 80	O 80	0
18	K	69	Total 69	O 69	0
18	L	79	Total 79	O 79	0
18	M	98	Total 98	O 98	0
18	P	89	Total 89	O 89	0
18	Q	84	Total 84	O 84	0
18	U	94	Total 94	O 94	0
18	W	74	Total 74	O 74	0
18	X	86	Total 86	O 86	0
18	Y	65	Total 65	O 65	0
18	Z	78	Total 78	O 78	0

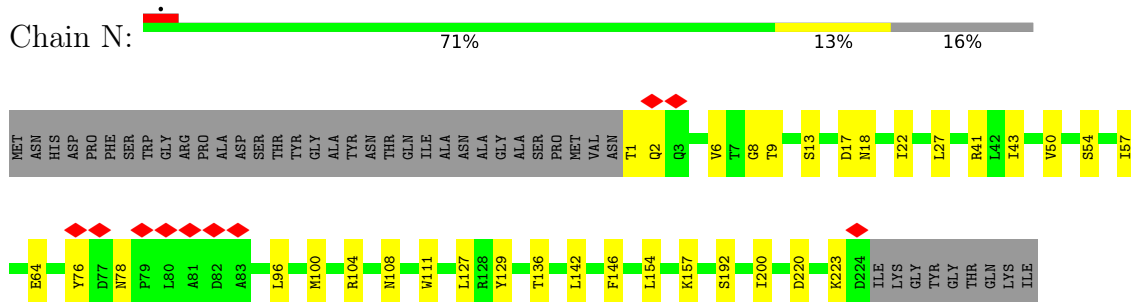
3 Residue-property plots [i](#)

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.

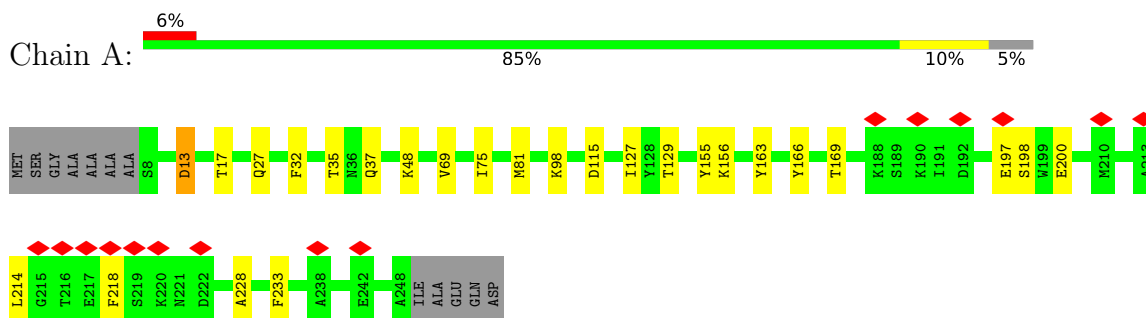
- Molecule 1: Proteasome subunit beta type-7



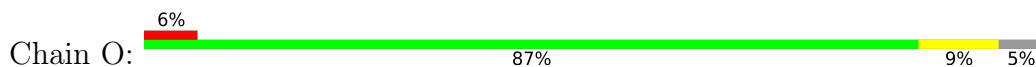
- Molecule 1: Proteasome subunit beta type-7

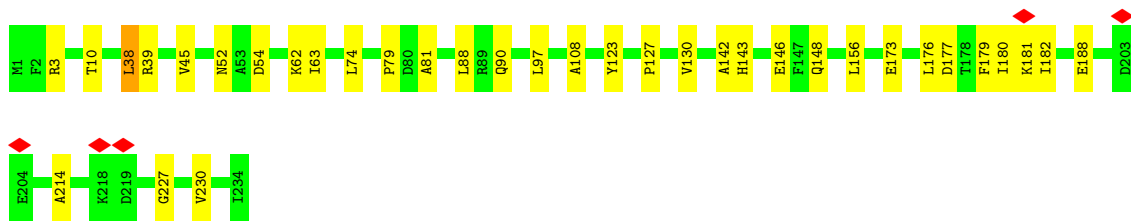


- Molecule 2: Proteasome subunit alpha type-1

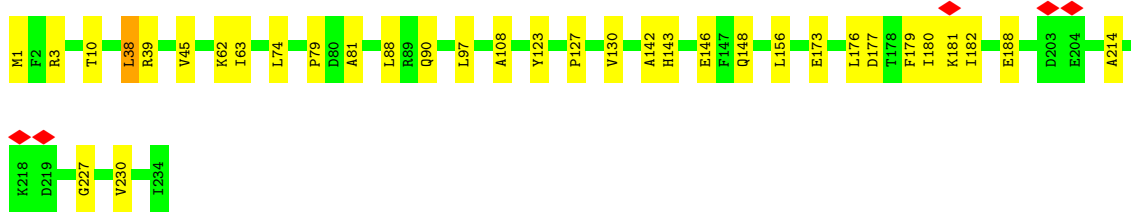
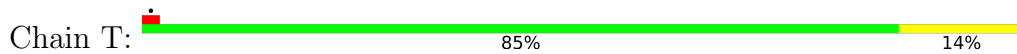


- Molecule 2: Proteasome subunit alpha type-1

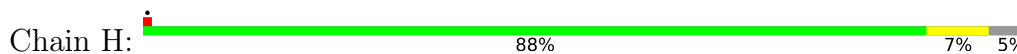




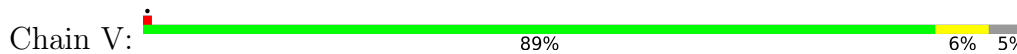
• Molecule 5: Proteasome subunit alpha type-6



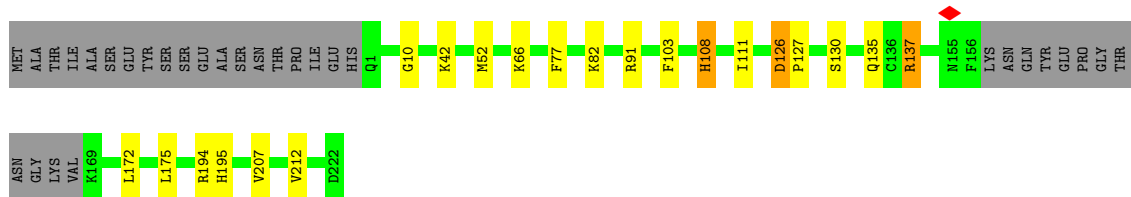
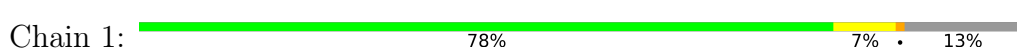
• Molecule 6: Proteasome subunit beta type-1



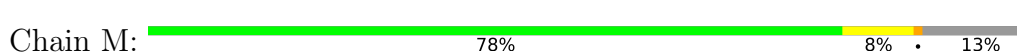
• Molecule 6: Proteasome subunit beta type-1

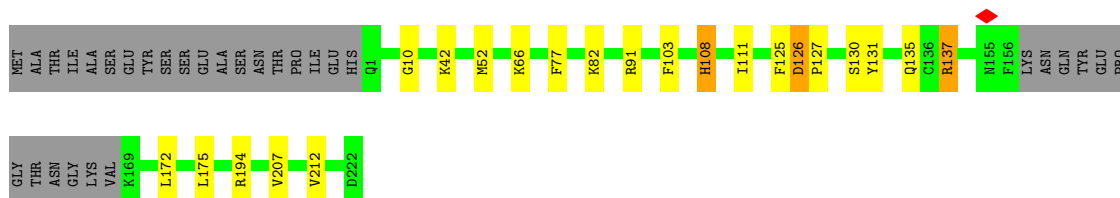


• Molecule 7: Proteasome subunit beta type-6

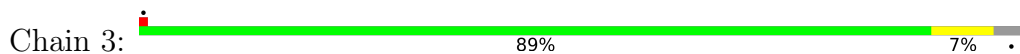


• Molecule 7: Proteasome subunit beta type-6

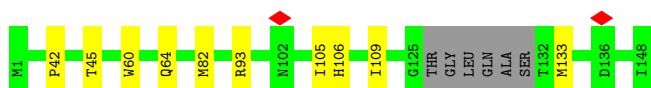
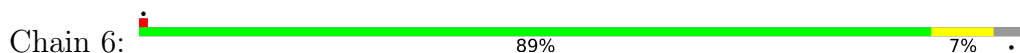




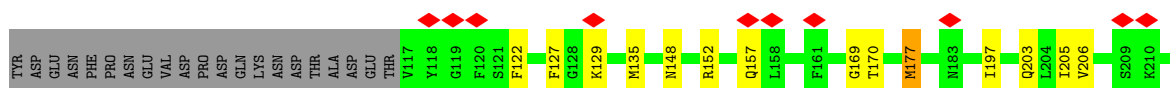
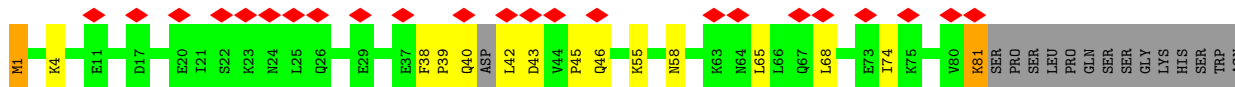
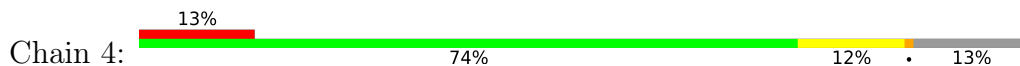
• Molecule 8: Proteasome maturation factor UMP1



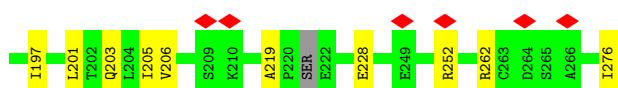
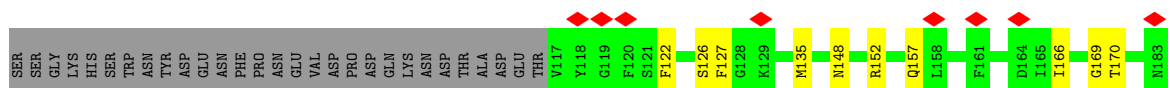
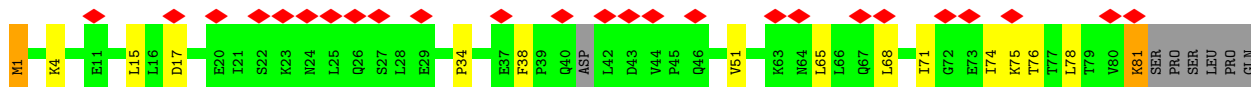
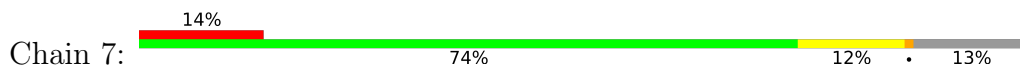
• Molecule 8: Proteasome maturation factor UMP1



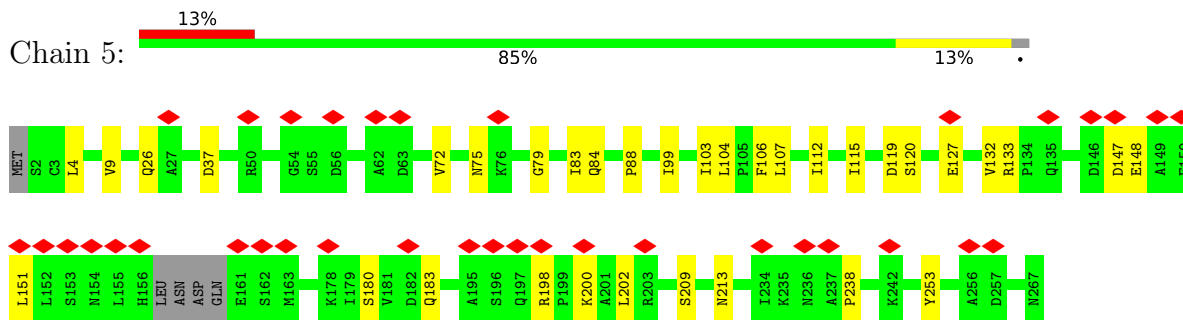
• Molecule 9: Proteasome chaperone 1



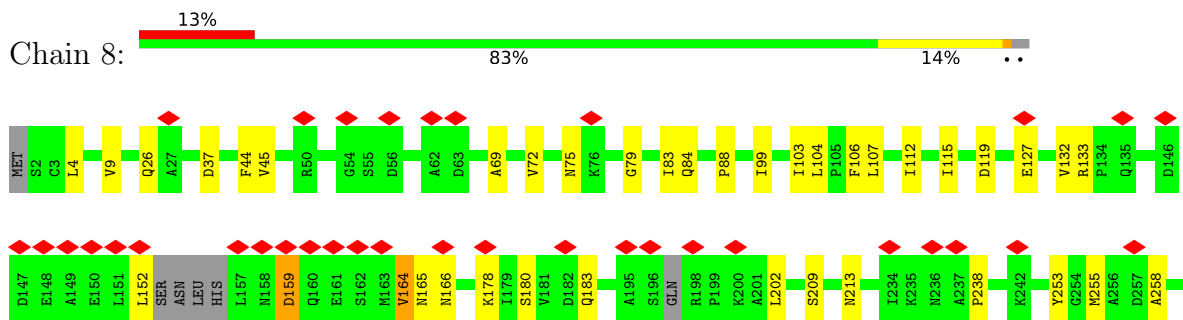
• Molecule 9: Proteasome chaperone 1



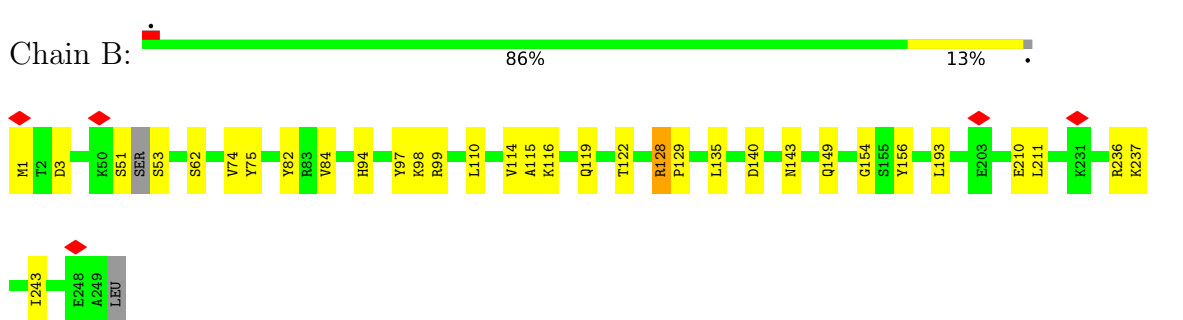
• Molecule 10: Proteasome assembly chaperone 2



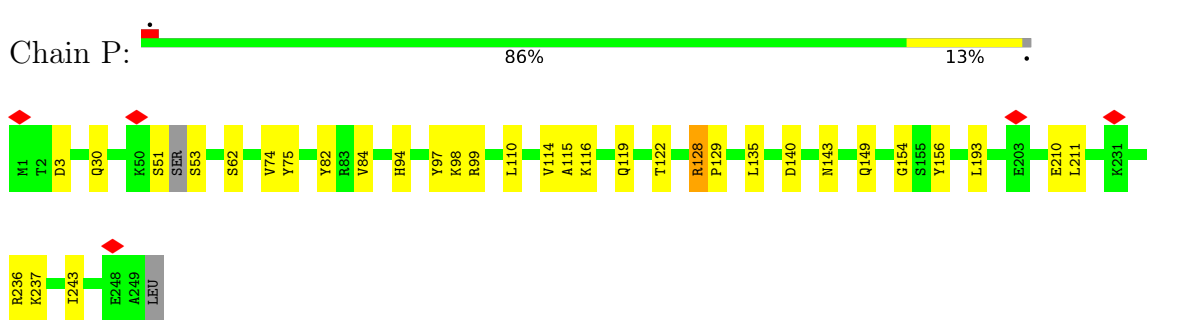
• Molecule 10: Proteasome assembly chaperone 2



• Molecule 11: Proteasome subunit alpha type-2



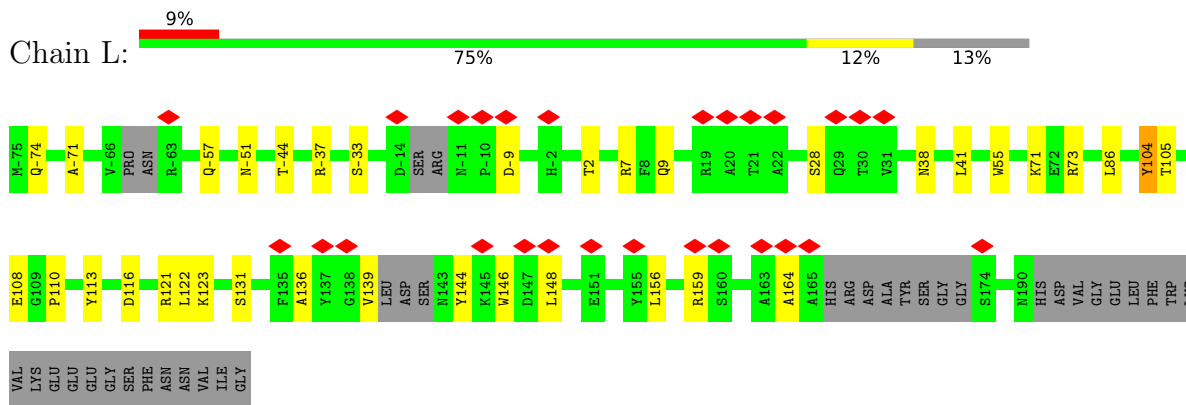
• Molecule 11: Proteasome subunit alpha type-2



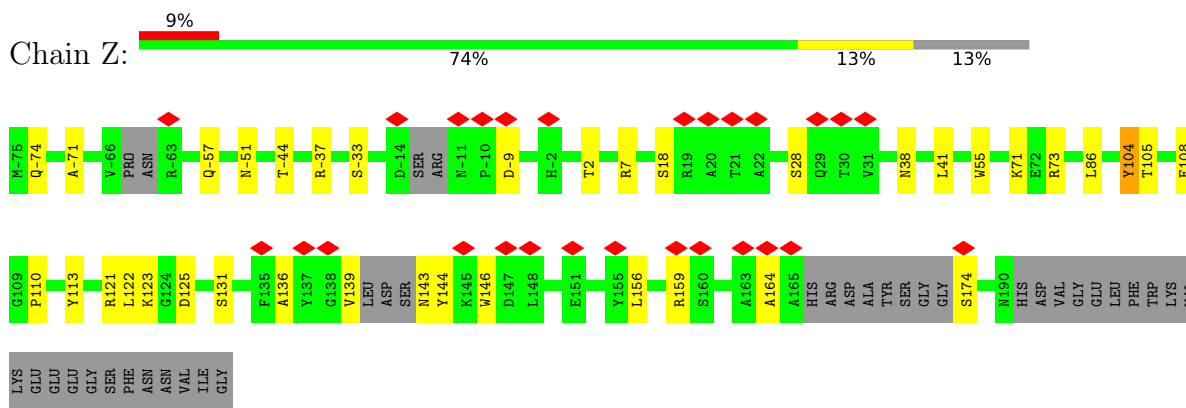
• Molecule 12: Proteasome subunit alpha type-3



• Molecule 17: Proteasome subunit beta type-5



• Molecule 17: Proteasome subunit beta type-5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	233748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.189	Depositor
Minimum map value	-1.440	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.282	Depositor
Map size (\AA)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.834, 0.834, 0.834	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	2	0.25	0/1783	0.50	0/2420
1	N	0.24	0/1783	0.50	0/2420
2	A	0.25	0/1930	0.47	0/2614
2	O	0.25	0/1930	0.47	0/2614
3	D	0.24	0/1906	0.48	0/2580
3	R	0.24	0/1906	0.48	0/2580
4	E	0.24	0/1941	0.46	0/2614
4	S	0.24	0/1941	0.46	0/2614
5	F	0.24	0/1830	0.49	0/2473
5	T	0.24	0/1830	0.49	0/2473
6	H	0.24	0/1604	0.46	0/2171
6	V	0.24	0/1604	0.46	0/2171
7	1	0.24	0/1698	0.48	0/2289
7	M	0.24	0/1698	0.48	0/2289
8	3	0.23	0/1151	0.47	0/1556
8	6	0.23	0/1151	0.47	0/1556
9	4	0.24	0/1907	0.43	0/2583
9	7	0.24	0/1907	0.43	0/2583
10	5	0.25	0/2180	0.42	0/2962
10	8	0.25	0/2170	0.42	0/2947
11	B	0.25	0/1936	0.46	0/2620
11	P	0.25	0/1936	0.46	0/2620
12	C	0.24	0/1890	0.47	0/2555
12	Q	0.24	0/1890	0.47	0/2555
13	G	0.25	0/1915	0.45	0/2584
13	U	0.25	0/1915	0.45	0/2584
14	I	0.24	0/1611	0.47	0/2185
14	W	0.24	0/1611	0.47	0/2185
15	J	0.25	0/1519	0.47	0/2049
15	X	0.25	0/1513	0.46	0/2039
16	K	0.24	0/1579	0.47	0/2128
16	Y	0.24	0/1579	0.47	0/2128
17	L	0.24	0/1975	0.45	0/2672
17	Z	0.24	0/1975	0.45	0/2672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.24	0/60694	0.46	0/82085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1753	0	1754	18	0
1	N	1753	0	1754	16	0
2	A	1892	0	1886	17	0
2	O	1892	0	1886	16	0
3	D	1877	0	1895	26	0
3	R	1877	0	1895	23	0
4	E	1914	0	1892	12	0
4	S	1914	0	1892	13	0
5	F	1802	0	1809	24	0
5	T	1802	0	1809	24	0
6	H	1575	0	1555	8	0
6	V	1575	0	1555	6	0
7	1	1663	0	1620	14	0
7	M	1663	0	1620	14	0
8	3	1133	0	1113	8	0
8	6	1133	0	1113	8	0
9	4	1865	0	1899	23	0
9	7	1865	0	1899	24	0
10	5	2128	0	2085	21	0
10	8	2120	0	2076	24	0
11	B	1900	0	1912	22	0
11	P	1900	0	1912	23	0
12	C	1862	0	1866	23	0
12	Q	1862	0	1866	22	0
13	G	1876	0	1875	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	U	1876	0	1875	16	0
14	I	1582	0	1563	10	0
14	W	1582	0	1563	11	0
15	J	1490	0	1490	15	0
15	X	1485	0	1484	10	0
16	K	1552	0	1556	13	0
16	Y	1552	0	1556	13	0
17	L	1937	0	1904	22	0
17	Z	1937	0	1904	24	0
18	1	96	0	0	0	0
18	2	88	0	0	1	0
18	3	63	0	0	0	0
18	4	56	0	0	1	0
18	5	94	0	0	1	0
18	6	59	0	0	0	0
18	7	54	0	0	1	0
18	8	98	0	0	1	0
18	A	101	0	0	0	0
18	B	90	0	0	2	0
18	C	88	0	0	1	0
18	D	70	0	0	0	0
18	E	100	0	0	2	0
18	F	84	0	0	1	0
18	G	93	0	0	1	0
18	H	81	0	0	1	0
18	I	66	0	0	0	0
18	J	80	0	0	0	0
18	K	69	0	0	0	0
18	L	79	0	0	0	0
18	M	98	0	0	0	0
18	N	86	0	0	0	0
18	O	102	0	0	0	0
18	P	89	0	0	2	0
18	Q	84	0	0	1	0
18	R	71	0	0	0	0
18	S	97	0	0	2	0
18	T	82	0	0	1	0
18	U	94	0	0	1	0
18	V	75	0	0	0	0
18	W	74	0	0	0	0
18	X	86	0	0	2	0
18	Y	65	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Z	78	0	0	1	0
All	All	62379	0	59333	492	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 4.

All (492) 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)
14:W:163:ILE:HG23	14:W:170:GLY:HA2	1.66	0.77
14:I:163:ILE:HG23	14:I:170:GLY:HA2	1.66	0.77
3:D:73:LEU:HD11	3:D:133:THR:HB	1.71	0.72
3:R:73:LEU:HD11	3:R:133:THR:HB	1.71	0.72
13:G:219:CYS:HG	13:G:228:HIS:HD1	1.38	0.70
3:D:81:ASP:HB3	3:D:129:PHE:HD1	1.57	0.70
17:Z:139:VAL:HG12	17:Z:144:TYR:HB2	1.74	0.70
2:A:129:THR:O	11:B:128:ARG:NH1	2.26	0.69
2:O:129:THR:O	11:P:128:ARG:NH1	2.26	0.69
17:L:139:VAL:HG12	17:L:144:TYR:HB2	1.73	0.69
12:Q:150:THR:HG1	12:Q:160:TRP:HE1	1.40	0.69
3:R:81:ASP:HB3	3:R:129:PHE:HD1	1.57	0.68
3:D:58:ARG:HG3	3:D:59:ILE:HG13	1.76	0.67
15:J:107:PRO:HG2	15:J:124:PHE:HB2	1.77	0.67
4:E:205:LYS:HB2	4:E:212:LEU:HD22	1.77	0.67
15:X:107:PRO:HG2	15:X:124:PHE:HB2	1.76	0.67
12:C:150:THR:HG1	12:C:160:TRP:HE1	1.42	0.66
3:D:58:ARG:NH2	12:C:146:TYR:O	2.28	0.66
9:4:152:ARG:NH2	10:5:37:ASP:OD1	2.28	0.66
4:S:31:ILE:HD13	4:S:141:ALA:HB2	1.78	0.66
9:4:74:ILE:HB	9:4:122:PHE:HB3	1.78	0.66
3:R:73:LEU:HD13	3:R:135:ILE:HG12	1.77	0.66
5:T:39:ARG:NH1	5:T:142:ALA:O	2.29	0.66
9:7:152:ARG:NH2	10:8:37:ASP:OD1	2.28	0.65
3:R:37:LYS:HE2	3:R:160:SER:HA	1.79	0.65
6:V:152:VAL:HG13	6:V:175:MET:HE1	1.78	0.65
3:D:73:LEU:HD13	3:D:135:ILE:HG12	1.78	0.65
4:E:31:ILE:HD13	4:E:141:ALA:HB2	1.78	0.65
3:R:188:VAL:HG21	3:R:216:LYS:HE2	1.78	0.65
3:D:188:VAL:HG21	3:D:216:LYS:HE2	1.78	0.65
7:1:135:GLN:HG3	17:Z:28:SER:HA	1.78	0.65
8:6:105:ILE:HG21	11:P:84:VAL:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:39:ARG:NH1	5:F:142:ALA:O	2.29	0.64
4:S:205:LYS:HB2	4:S:212:LEU:HD22	1.77	0.64
8:3:105:ILE:HG21	11:B:84:VAL:HG13	1.79	0.64
3:D:37:LYS:HE2	3:D:160:SER:HA	1.78	0.64
13:U:219:CYS:HG	13:U:228:HIS:HD1	1.45	0.64
17:L:73:ARG:HH21	17:L:105:THR:HA	1.63	0.64
16:K:179:VAL:H	16:K:196:GLN:HE21	1.46	0.63
12:Q:64:GLU:HG3	12:Q:65:LYS:HG2	1.78	0.63
3:D:97:ARG:HH21	3:D:103:PRO:HB3	1.63	0.63
3:R:97:ARG:HH21	3:R:103:PRO:HB3	1.63	0.63
3:R:101:GLU:OE1	17:Z:121:ARG:NH2	2.31	0.62
6:H:152:VAL:HG13	6:H:175:MET:HE1	1.80	0.62
17:Z:73:ARG:HH21	17:Z:105:THR:HA	1.63	0.62
17:Z:18:SER:HG	17:Z:174:SER:HG	1.47	0.62
9:7:74:ILE:HB	9:7:122:PHE:HB3	1.81	0.61
15:X:39:LYS:NZ	16:Y:127:GLU:OE1	2.33	0.61
16:K:29:LYS:HE2	17:L:122:LEU:HD11	1.81	0.61
12:Q:4:ARG:HG3	12:Q:5:ARG:HH21	1.66	0.61
1:N:2:GLN:H	1:N:111:TRP:HE1	1.48	0.61
17:Z:2:THR:OG1	17:Z:131:SER:O	2.19	0.61
13:G:51:GLU:OE2	13:G:204:HIS:ND1	2.33	0.61
2:A:13:ASP:OD1	2:A:13:ASP:N	2.32	0.60
6:H:34:LEU:HD13	6:H:176:VAL:HG23	1.83	0.60
16:Y:23:ARG:NH2	18:Y:303:HOH:O	2.33	0.60
1:2:43:ILE:HG12	1:2:64:GLU:HG2	1.84	0.60
6:V:34:LEU:HD13	6:V:176:VAL:HG23	1.83	0.60
11:P:51:SER:O	11:P:53:SER:N	2.34	0.60
1:N:43:ILE:HG12	1:N:64:GLU:HG2	1.84	0.60
17:L:2:THR:OG1	17:L:131:SER:O	2.19	0.60
16:K:149:ARG:NH2	16:K:156:GLU:OE1	2.32	0.59
11:B:51:SER:O	11:B:53:SER:N	2.35	0.59
3:R:205:THR:OG1	3:R:209:ASN:OD1	2.17	0.59
10:8:132:VAL:HG23	10:8:133:ARG:HG3	1.84	0.59
8:3:133:MET:SD	12:C:102:TYR:OH	2.61	0.59
12:Q:206:LEU:HD11	12:Q:211:LEU:HD21	1.85	0.59
3:D:101:GLU:OE1	17:L:121:ARG:NH2	2.31	0.59
8:6:133:MET:SD	12:Q:102:TYR:OH	2.61	0.59
11:P:62:SER:OG	11:P:210:GLU:OE2	2.19	0.59
12:C:191:GLU:HG2	12:C:242:THR:HG22	1.85	0.58
16:K:21:VAL:HG12	16:K:29:LYS:HE3	1.85	0.58
17:L:28:SER:HA	7:M:135:GLN:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:236:ARG:NH2	18:B:304:HOH:O	2.35	0.58
12:C:64:GLU:HG3	12:C:65:LYS:HG2	1.83	0.58
15:J:125:ASP:OD1	15:J:129:CYS:N	2.35	0.58
1:2:2:GLN:H	1:2:111:TRP:HE1	1.51	0.58
10:5:132:VAL:HG23	10:5:133:ARG:HG3	1.85	0.58
12:C:206:LEU:HD11	12:C:211:LEU:HD21	1.85	0.58
11:P:236:ARG:NH2	18:P:303:HOH:O	2.35	0.58
3:D:205:THR:OG1	3:D:209:ASN:OD1	2.17	0.58
4:E:32:LYS:NZ	18:E:306:HOH:O	2.36	0.57
12:Q:191:GLU:HG2	12:Q:242:THR:HG22	1.85	0.57
9:7:170:THR:OG1	9:7:228:GLU:OE1	2.20	0.57
16:Y:149:ARG:NH2	16:Y:156:GLU:OE1	2.32	0.57
1:2:41:ARG:HH22	1:2:54:SER:HA	1.69	0.57
9:4:262:ARG:NH1	18:4:305:HOH:O	2.38	0.57
7:M:126:ASP:OD1	7:M:130:SER:N	2.38	0.57
15:X:21:VAL:HG23	15:X:190:ILE:HB	1.87	0.57
1:N:41:ARG:HH22	1:N:54:SER:HA	1.69	0.56
9:4:1:MET:HG3	11:B:3:ASP:HB3	1.87	0.56
7:1:172:LEU:HD12	7:1:175:LEU:HD12	1.88	0.56
3:R:34:VAL:HG22	3:R:163:THR:HG22	1.88	0.56
5:T:3:ARG:HB2	10:8:253:TYR:HA	1.88	0.56
7:M:172:LEU:HD12	7:M:175:LEU:HD12	1.88	0.56
5:F:3:ARG:HB2	10:5:253:TYR:HA	1.88	0.56
10:5:107:LEU:HD23	10:5:112:ILE:HD12	1.87	0.56
2:O:37:GLN:NE2	13:U:19:GLY:O	2.39	0.55
11:B:62:SER:OG	11:B:210:GLU:OE2	2.19	0.55
2:O:198:SER:OG	2:O:200:GLU:OE1	2.25	0.55
16:Y:184:VAL:HG22	16:Y:189:ILE:HG12	1.89	0.55
3:D:34:VAL:HG22	3:D:163:THR:HG22	1.88	0.55
5:T:156:LEU:HG	13:U:59:LEU:HD23	1.89	0.55
10:8:107:LEU:HD23	10:8:112:ILE:HD12	1.88	0.55
15:J:6:SER:O	15:J:28:ARG:NH1	2.39	0.55
1:2:220:ASP:OD1	1:2:223:LYS:NZ	2.40	0.55
5:T:88:LEU:HD11	5:T:108:ALA:HB1	1.88	0.55
10:5:4:LEU:HD11	10:5:83:ILE:HG13	1.89	0.55
15:J:29:LEU:HB3	15:J:182:GLY:HA3	1.88	0.54
1:N:220:ASP:OD1	1:N:223:LYS:NZ	2.40	0.54
7:1:126:ASP:OD1	7:1:130:SER:N	2.37	0.54
10:8:166:ASN:HB3	10:8:178:LYS:HG2	1.88	0.54
3:D:181:ARG:NH2	4:E:59:LEU:O	2.40	0.54
9:7:122:PHE:HE2	9:7:135:MET:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:262:ARG:NH1	18:7:308:HOH:O	2.40	0.54
5:F:88:LEU:HD11	5:F:108:ALA:HB1	1.88	0.54
5:F:156:LEU:HG	13:G:59:LEU:HD23	1.90	0.54
3:R:181:ARG:NH2	4:S:59:LEU:O	2.40	0.54
2:A:198:SER:OG	2:A:200:GLU:OE1	2.25	0.54
10:8:4:LEU:HD11	10:8:83:ILE:HG13	1.88	0.54
12:Q:141:ASP:OD1	12:Q:147:GLN:NE2	2.40	0.54
16:K:184:VAL:HG22	16:K:189:ILE:HG12	1.89	0.54
14:W:18:THR:OG1	14:W:171:SER:OG	2.27	0.53
2:A:127:ILE:HD11	8:3:109:ILE:HB	1.91	0.53
5:F:39:ARG:HH11	5:F:143:HIS:HA	1.72	0.53
2:O:127:ILE:HG12	8:6:106:HIS:CD2	2.44	0.53
5:T:39:ARG:HH11	5:T:143:HIS:HA	1.73	0.53
15:X:125:ASP:OD1	15:X:129:CYS:N	2.35	0.53
9:4:170:THR:HG22	9:4:219:ALA:HB3	1.90	0.53
12:Q:181:LYS:H	12:Q:184:MET:HE3	1.73	0.53
1:2:127:LEU:HG	1:2:142:LEU:HD12	1.90	0.53
12:C:141:ASP:OD1	12:C:147:GLN:NE2	2.41	0.53
12:Q:83:ASP:HB3	12:Q:131:PHE:HD1	1.73	0.53
13:U:87:HIS:O	13:U:91:ARG:HG2	2.09	0.53
2:A:127:ILE:HG12	8:3:106:HIS:CD2	2.43	0.53
3:R:181:ARG:NH2	4:S:57:PRO:O	2.41	0.53
2:O:127:ILE:HD11	8:6:109:ILE:HB	1.91	0.53
2:A:37:GLN:NE2	13:G:19:GLY:O	2.42	0.53
13:U:214:LEU:HD21	13:U:216:ILE:HD11	1.90	0.53
13:G:87:HIS:O	13:G:91:ARG:HG2	2.08	0.52
3:D:181:ARG:NH2	4:E:57:PRO:O	2.42	0.52
15:J:21:VAL:HG23	15:J:190:ILE:HB	1.90	0.52
7:1:108:HIS:NE2	17:Z:-9:ASP:O	2.43	0.52
9:7:205:ILE:HG22	9:7:206:VAL:HG13	1.92	0.52
15:J:58:THR:O	16:K:85:ARG:NH2	2.42	0.52
9:4:65:LEU:HD13	9:4:252:ARG:HE	1.75	0.52
9:4:122:PHE:HE2	9:4:135:MET:HB2	1.75	0.52
9:7:68:LEU:HD23	9:7:127:PHE:HB3	1.92	0.52
15:X:58:THR:O	16:Y:85:ARG:NH2	2.43	0.52
1:N:127:LEU:HG	1:N:142:LEU:HD12	1.90	0.52
1:N:129:TYR:O	1:N:136:THR:HA	2.09	0.52
2:O:115:ASP:HB3	2:O:155:TYR:CZ	2.44	0.52
9:4:170:THR:OG1	9:4:228:GLU:OE1	2.21	0.52
11:B:193:LEU:HD21	11:B:211:LEU:HD11	1.92	0.52
2:A:115:ASP:HB3	2:A:155:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:12:SER:HB3	3:R:16:HIS:H	1.74	0.52
3:D:12:SER:HB3	3:D:16:HIS:H	1.75	0.52
13:G:220:SER:HB3	13:G:223:GLU:HB2	1.91	0.52
12:C:26:LEU:HD23	12:C:153:PRO:HD2	1.93	0.51
12:C:83:ASP:HB3	12:C:131:PHE:HD1	1.73	0.51
9:4:46:GLN:O	9:4:129:LYS:NZ	2.37	0.51
13:G:214:LEU:HD21	13:G:216:ILE:HD11	1.92	0.51
18:S:303:HOH:O	7:1:82:LYS:NZ	2.42	0.51
11:B:211:LEU:HD12	11:B:243:ILE:HG12	1.92	0.51
7:M:108:HIS:CE1	7:M:127:PRO:HD3	2.46	0.51
1:2:50:VAL:HG23	1:2:200:ILE:HD11	1.92	0.51
1:2:129:TYR:O	1:2:136:THR:HA	2.09	0.51
4:E:70:ILE:HG21	4:E:112:LEU:HD21	1.93	0.51
7:1:108:HIS:CE1	7:1:127:PRO:HD3	2.45	0.51
13:U:220:SER:HB3	13:U:223:GLU:HB2	1.92	0.51
11:P:30:GLN:NE2	18:P:306:HOH:O	2.37	0.51
13:G:245:LYS:NZ	18:G:309:HOH:O	2.44	0.51
11:P:97:TYR:OH	15:X:78:GLU:OE2	2.17	0.51
18:E:303:HOH:O	7:M:82:LYS:NZ	2.42	0.51
1:N:50:VAL:HG23	1:N:200:ILE:HD11	1.92	0.51
11:P:193:LEU:HD21	11:P:211:LEU:HD11	1.92	0.51
9:4:205:ILE:HG22	9:4:206:VAL:HG13	1.93	0.51
12:C:216:ILE:HG12	12:C:227:GLN:HG2	1.93	0.51
11:P:74:VAL:HG12	11:P:135:LEU:HB2	1.93	0.51
12:Q:216:ILE:HG12	12:Q:227:GLN:HG2	1.93	0.50
5:F:180:ILE:HG23	5:F:181:LYS:HG3	1.92	0.50
12:C:136:ILE:HG12	12:C:150:THR:HG22	1.93	0.50
16:Y:179:VAL:H	16:Y:196:GLN:HE21	1.58	0.50
12:Q:26:LEU:HD23	12:Q:153:PRO:HD2	1.92	0.50
5:F:146:GLU:OE2	5:F:148:GLN:NE2	2.44	0.50
9:4:81:LYS:H	9:4:81:LYS:HD3	1.77	0.50
3:D:94:GLN:HG3	16:K:66:LEU:HB2	1.94	0.50
1:N:8:GLY:HA3	1:N:41:ARG:CZ	2.42	0.50
5:T:180:ILE:HG23	5:T:181:LYS:HG3	1.92	0.50
10:8:9:VAL:HG11	10:8:88:PRO:HB3	1.92	0.50
7:1:108:HIS:HE1	7:1:127:PRO:HD3	1.76	0.50
17:L:55:TRP:CE3	17:L:86:LEU:HD21	2.47	0.50
3:R:94:GLN:HG3	16:Y:66:LEU:HB2	1.94	0.50
5:T:146:GLU:OE2	5:T:148:GLN:NE2	2.44	0.50
12:Q:136:ILE:HG12	12:Q:150:THR:HG22	1.93	0.50
4:S:70:ILE:HG21	4:S:112:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:8:255:MET:HB2	10:8:258:ALA:HB2	1.93	0.49
10:8:159:ASP:OD1	10:8:159:ASP:N	2.43	0.49
4:E:85:ALA:HB2	4:E:140:VAL:HG21	1.94	0.49
1:N:17:ASP:OD1	1:N:18:ASN:N	2.46	0.49
10:5:148:GLU:HG3	10:5:151:LEU:HB3	1.95	0.49
9:7:1:MET:HG3	11:P:3:ASP:HB3	1.94	0.49
10:8:4:LEU:HB2	10:8:112:ILE:HD13	1.94	0.49
7:M:108:HIS:HE1	7:M:127:PRO:HD3	1.76	0.49
17:Z:55:TRP:CE3	17:Z:86:LEU:HD21	2.47	0.49
1:2:8:GLY:HA3	1:2:41:ARG:CZ	2.42	0.49
14:I:160:GLN:HE21	14:I:164:TRP:HE1	1.59	0.49
17:L:-9:ASP:O	7:M:108:HIS:NE2	2.45	0.49
11:P:75:TYR:HB3	11:P:82:TYR:CD1	2.48	0.49
1:2:17:ASP:OD1	1:2:18:ASN:N	2.46	0.49
12:C:181:LYS:H	12:C:184:MET:HE3	1.78	0.49
1:N:41:ARG:HH12	1:N:54:SER:HA	1.77	0.49
4:E:52:LYS:HE3	4:E:218:GLN:HB2	1.94	0.49
12:C:4:ARG:HG3	12:C:5:ARG:HH21	1.77	0.49
15:J:27:LEU:HD21	15:J:41:GLU:HG2	1.95	0.49
17:Z:73:ARG:NH2	17:Z:104:TYR:O	2.46	0.49
3:D:58:ARG:NH1	12:C:144:TYR:O	2.46	0.49
17:L:73:ARG:NH2	17:L:104:TYR:O	2.46	0.49
9:4:40:GLN:O	9:4:42:LEU:N	2.46	0.48
12:C:113:ARG:NH2	16:K:71:GLU:OE2	2.38	0.48
5:F:97:LEU:HD12	7:M:66:LYS:HE2	1.95	0.48
5:T:97:LEU:HD12	7:1:66:LYS:HE2	1.95	0.48
10:5:99:ILE:HD12	10:5:103:ILE:HB	1.95	0.48
10:8:180:SER:HB3	10:8:183:GLN:HG3	1.95	0.48
8:6:60:TRP:O	8:6:64:GLN:HG2	2.13	0.48
11:B:74:VAL:HG12	11:B:135:LEU:HB2	1.93	0.48
11:B:75:TYR:HB3	11:B:82:TYR:CD1	2.48	0.48
1:2:41:ARG:HH12	1:2:54:SER:HA	1.78	0.48
11:B:97:TYR:OH	15:J:78:GLU:OE2	2.17	0.48
11:P:116:LYS:HG3	12:Q:86:ILE:HD11	1.96	0.48
4:S:5:ARG:NH1	9:7:15:LEU:O	2.47	0.48
16:K:130:TYR:OH	16:K:145:ASP:OD1	2.25	0.48
13:U:51:GLU:OE2	13:U:204:HIS:ND1	2.37	0.48
10:5:180:SER:HB3	10:5:183:GLN:HG3	1.96	0.48
10:8:99:ILE:HD12	10:8:103:ILE:HB	1.94	0.48
3:D:7:ALA:HB3	3:D:10:ILE:HG12	1.95	0.48
11:B:116:LYS:HG3	12:C:86:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:211:LEU:HD12	11:P:243:ILE:HG12	1.94	0.48
5:F:177:ASP:O	5:F:181:LYS:NZ	2.43	0.48
10:5:4:LEU:HB2	10:5:112:ILE:HD13	1.96	0.48
3:R:50:SER:HA	3:R:209:ASN:HD21	1.79	0.47
9:7:65:LEU:HD13	9:7:252:ARG:HE	1.78	0.47
14:I:104:ASP:HB2	14:I:105:PRO:HD2	1.96	0.47
9:4:68:LEU:HD23	9:4:127:PHE:HB3	1.95	0.47
10:5:115:ILE:HG22	10:5:202:LEU:HD11	1.94	0.47
3:R:62:SER:OG	3:R:211:GLU:OE2	2.32	0.47
4:S:85:ALA:HB2	4:S:140:VAL:HG21	1.95	0.47
8:3:60:TRP:O	8:3:64:GLN:HG2	2.13	0.47
17:Z:7:ARG:HG3	17:Z:110:PRO:HB2	1.96	0.47
3:D:62:SER:OG	3:D:211:GLU:OE2	2.33	0.47
4:S:52:LYS:HE3	4:S:218:GLN:HB2	1.96	0.47
7:1:10:GLY:HA3	7:1:42:LYS:HZ3	1.79	0.47
6:V:42:TRP:HZ3	6:V:185:ARG:HH21	1.62	0.47
17:L:7:ARG:HG3	17:L:110:PRO:HB2	1.96	0.47
2:A:156:LYS:HB3	2:A:166:TYR:HE1	1.80	0.47
3:R:2:SER:HA	9:7:17:ASP:HB3	1.97	0.47
14:W:104:ASP:HB2	14:W:105:PRO:HD2	1.96	0.47
16:Y:29:LYS:HE2	17:Z:122:LEU:HD11	1.96	0.47
3:D:50:SER:HA	3:D:209:ASN:HD21	1.79	0.47
10:5:9:VAL:HG11	10:5:88:PRO:HB3	1.97	0.47
10:5:213:ASN:HB2	13:G:6:THR:HG22	1.96	0.47
1:2:13:SER:HB3	1:2:22:ILE:HG13	1.96	0.47
6:H:42:TRP:HZ3	6:H:185:ARG:HH21	1.62	0.46
14:W:18:THR:HG1	14:W:171:SER:HG	1.57	0.46
1:2:27:LEU:HB2	1:2:192:SER:HB2	1.97	0.46
1:N:1:THR:HG21	1:N:108:ASN:OD1	2.15	0.46
2:O:156:LYS:HB3	2:O:166:TYR:HE1	1.80	0.46
5:T:63:ILE:HG21	5:T:214:ALA:HB2	1.97	0.46
16:K:50:ALA:O	16:K:52:ASP:N	2.48	0.46
1:N:27:LEU:HB2	1:N:192:SER:HB2	1.97	0.46
3:R:67:ILE:HG21	3:R:109:LEU:HD21	1.98	0.46
5:F:62:LYS:HE3	9:4:276:ILE:HG22	1.97	0.46
1:N:13:SER:HB3	1:N:22:ILE:HG13	1.96	0.46
10:8:213:ASN:HB2	13:U:6:THR:HG22	1.96	0.46
3:D:54:LEU:HD13	12:C:162:ALA:HB3	1.98	0.46
2:O:228:ALA:HB2	2:O:233:PHE:HD1	1.81	0.46
3:R:7:ALA:HB3	3:R:10:ILE:HG12	1.97	0.46
5:T:74:LEU:HD22	5:T:81:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:50:ALA:O	16:Y:52:ASP:N	2.48	0.46
17:Z:-57:GLN:O	17:Z:-51:ASN:ND2	2.43	0.46
5:F:74:LEU:HD22	5:F:81:ALA:HB1	1.98	0.46
10:8:119:ASP:O	10:8:209:SER:HA	2.15	0.46
2:A:228:ALA:HB2	2:A:233:PHE:HD1	1.81	0.46
5:T:62:LYS:HE3	9:7:276:ILE:HG22	1.97	0.46
10:5:72:VAL:HG11	10:5:106:PHE:CZ	2.50	0.46
17:L:136:ALA:HB2	17:L:164:ALA:HB2	1.97	0.46
17:Z:136:ALA:HB2	17:Z:164:ALA:HB2	1.98	0.46
1:2:65:ARG:NH1	18:2:312:HOH:O	2.49	0.46
3:D:216:LYS:HB2	3:D:220:ASP:HB3	1.97	0.45
9:7:38:PHE:CG	9:7:157:GLN:HG3	2.50	0.45
10:5:119:ASP:O	10:5:209:SER:HA	2.16	0.45
5:F:63:ILE:HG21	5:F:214:ALA:HB2	1.98	0.45
8:6:42:PRO:HG2	8:6:45:THR:HG23	1.97	0.45
11:B:210:GLU:HG3	11:B:237:LYS:HE3	1.99	0.45
9:7:169:GLY:HA3	9:7:197:ILE:HG13	1.97	0.45
8:3:42:PRO:HG2	8:3:45:THR:HG23	1.97	0.45
3:D:67:ILE:HG21	3:D:109:LEU:HD21	1.98	0.45
17:Z:38:ASN:OD1	17:Z:41:LEU:N	2.50	0.45
3:R:216:LYS:HB2	3:R:220:ASP:HB3	1.97	0.45
14:I:112:SER:HB3	14:I:125:LEU:HD13	1.99	0.45
3:R:54:LEU:HD13	12:Q:162:ALA:HB3	1.98	0.45
17:L:38:ASN:OD1	17:L:41:LEU:N	2.50	0.45
11:P:122:THR:HG22	11:P:129:PRO:HB3	1.99	0.45
5:F:39:ARG:NH1	18:F:312:HOH:O	2.50	0.45
4:S:74:ILE:HG21	4:S:112:LEU:HD22	1.99	0.45
10:8:115:ILE:HG22	10:8:202:LEU:HD11	1.98	0.45
7:M:10:GLY:HA3	7:M:42:LYS:HZ3	1.82	0.45
11:P:149:GLN:O	11:P:156:TYR:HA	2.17	0.45
12:Q:52:VAL:HG11	12:Q:59:GLN:HE22	1.82	0.45
11:B:119:GLN:NE2	12:C:83:ASP:OD1	2.44	0.44
13:U:51:GLU:HB2	13:U:200:ILE:HG23	1.99	0.44
14:W:112:SER:HB3	14:W:125:LEU:HD13	1.99	0.44
10:5:84:GLN:HG3	18:5:345:HOH:O	2.17	0.44
11:B:149:GLN:O	11:B:156:TYR:HA	2.18	0.44
12:Q:190:ILE:HG23	12:Q:213:PHE:CZ	2.53	0.44
5:F:81:ALA:HB2	5:F:130:VAL:HG21	2.00	0.44
11:B:122:THR:HG22	11:B:129:PRO:HB3	1.98	0.44
14:I:-23:ASP:O	15:J:101:GLY:HA3	2.18	0.44
11:P:210:GLU:HG3	11:P:237:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:32:PHE:O	2:A:35:THR:OG1	2.23	0.44
2:A:156:LYS:O	2:A:163:TYR:HA	2.17	0.44
10:8:75:ASN:O	10:8:79:GLY:N	2.51	0.44
11:P:119:GLN:NE2	12:Q:83:ASP:OD1	2.44	0.44
3:D:141:ARG:HH12	17:L:108:GLU:HG2	1.82	0.44
16:K:149:ARG:HB2	16:K:152:MET:HG3	2.00	0.44
2:A:214:LEU:HD12	2:A:218:PHE:HZ	1.83	0.44
11:B:115:ALA:HB1	11:B:154:GLY:O	2.18	0.44
12:C:65:LYS:NZ	18:C:304:HOH:O	2.39	0.44
3:R:141:ARG:HH12	17:Z:108:GLU:HG2	1.82	0.44
12:C:190:ILE:HG23	12:C:213:PHE:CZ	2.53	0.44
14:W:148:LYS:HE3	14:W:177:VAL:HG11	1.99	0.44
2:O:156:LYS:O	2:O:163:TYR:HA	2.18	0.43
5:T:177:ASP:O	5:T:181:LYS:NZ	2.43	0.43
12:Q:65:LYS:NZ	18:Q:305:HOH:O	2.39	0.43
2:A:75:ILE:HD11	2:A:81:MET:HE1	2.00	0.43
4:E:74:ILE:HG21	4:E:112:LEU:HD22	1.99	0.43
6:H:171:GLY:O	6:H:193:TYR:OH	2.29	0.43
13:G:219:CYS:SG	13:G:228:HIS:ND1	2.74	0.43
15:J:63:LEU:HD11	15:J:105:VAL:HG21	2.00	0.43
13:U:229:LYS:NZ	18:U:307:HOH:O	2.47	0.43
11:P:94:HIS:HA	11:P:98:LYS:HB3	2.00	0.43
2:A:17:THR:HG22	2:A:27:GLN:HB2	2.00	0.43
5:T:39:ARG:NH1	18:T:311:HOH:O	2.52	0.43
10:5:119:ASP:OD1	10:5:120:SER:N	2.52	0.43
10:8:104:LEU:HD23	10:8:107:LEU:HD12	2.00	0.43
15:J:143:SER:OG	15:J:178:ASP:OD2	2.35	0.43
11:P:115:ALA:HB1	11:P:154:GLY:O	2.18	0.43
13:G:151:LEU:HD13	13:G:157:TYR:HB3	2.01	0.43
11:B:94:HIS:HA	11:B:98:LYS:HB3	2.00	0.43
14:I:148:LYS:HE3	14:I:177:VAL:HG11	1.99	0.43
3:D:80:ALA:HB1	12:C:120:GLN:HG3	2.01	0.43
1:N:154:LEU:HA	1:N:157:LYS:HE2	2.00	0.43
10:5:104:LEU:HD23	10:5:107:LEU:HD12	2.00	0.43
10:8:44:PHE:HB3	10:8:69:ALA:HB2	2.01	0.43
16:K:37:GLN:HA	16:K:43:LEU:HD12	2.01	0.43
14:W:-23:ASP:O	15:X:101:GLY:HA3	2.18	0.43
15:X:177:ARG:NH2	18:X:311:HOH:O	2.52	0.43
2:O:17:THR:HG22	2:O:27:GLN:HB2	2.00	0.43
2:O:214:LEU:HD12	2:O:218:PHE:HZ	1.84	0.43
9:4:169:GLY:HA3	9:4:197:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:71:ILE:HD11	9:7:126:SER:HB3	2.00	0.43
11:P:110:LEU:O	11:P:114:VAL:HG23	2.19	0.43
4:E:121:LEU:HD22	5:F:79:PRO:HB3	2.00	0.43
4:E:169:ALA:HB1	4:E:183:LEU:HD22	2.01	0.43
6:V:59:VAL:HG11	6:V:82:PHE:CE2	2.54	0.43
6:V:101:GLY:O	6:V:108:GLY:HA2	2.19	0.43
11:B:1:MET:N	18:B:307:HOH:O	2.40	0.43
12:C:91:ALA:HB2	12:C:115:LEU:HD11	2.01	0.43
16:Y:149:ARG:HB2	16:Y:152:MET:HG3	2.00	0.43
4:S:169:ALA:HB1	4:S:183:LEU:HD22	2.01	0.42
8:3:82:MET:SD	17:L:-71:ALA:HB2	2.59	0.42
9:4:39:PRO:HD3	9:4:74:ILE:HA	2.01	0.42
14:I:4:VAL:HG22	14:I:159:ILE:HD11	2.01	0.42
17:L:-57:GLN:O	17:L:-51:ASN:ND2	2.43	0.42
14:W:4:VAL:HG22	14:W:159:ILE:HD11	2.01	0.42
7:1:207:VAL:HG22	7:1:212:VAL:HG22	2.01	0.42
15:J:185:ALA:HB3	15:J:200:LEU:HB2	2.01	0.42
4:S:121:LEU:HD22	5:T:79:PRO:HB3	2.00	0.42
11:B:110:LEU:O	11:B:114:VAL:HG23	2.19	0.42
13:U:193:VAL:HG13	13:U:216:ILE:HG21	2.01	0.42
1:2:1:THR:HG21	1:2:108:ASN:OD1	2.19	0.42
2:A:48:LYS:NZ	2:A:197:GLU:OE2	2.43	0.42
6:H:59:VAL:HG11	6:H:82:PHE:CE2	2.54	0.42
5:T:10:THR:HG21	5:T:127:PRO:HD3	2.02	0.42
9:7:148:ASN:O	9:7:152:ARG:HG3	2.19	0.42
15:J:177:ARG:H	15:J:177:ARG:HG3	1.70	0.42
7:M:108:HIS:HB3	7:M:137:ARG:HH22	1.83	0.42
17:Z:7:ARG:NH2	17:Z:125:ASP:OD1	2.52	0.42
1:2:154:LEU:HA	1:2:157:LYS:HE2	2.00	0.42
5:F:173:GLU:HA	13:G:58:LEU:HD21	2.01	0.42
5:T:81:ALA:HB2	5:T:130:VAL:HG21	2.00	0.42
10:5:75:ASN:O	10:5:79:GLY:N	2.53	0.42
10:8:26:GLN:NE2	10:8:238:PRO:HG2	2.34	0.42
10:8:72:VAL:HG11	10:8:106:PHE:CZ	2.53	0.42
15:X:63:LEU:HD11	15:X:105:VAL:HG21	2.00	0.42
17:Z:7:ARG:O	17:Z:144:TYR:OH	2.30	0.42
4:S:65:GLU:OE2	17:Z:71:LYS:NZ	2.52	0.42
9:4:55:LYS:HD2	9:4:58:ASN:HD21	1.85	0.42
8:6:82:MET:SD	17:Z:-71:ALA:HB2	2.59	0.42
7:M:207:VAL:HG22	7:M:212:VAL:HG22	2.01	0.42
13:U:151:LEU:HD13	13:U:157:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:90:GLN:HG2	17:Z:-44:THR:HA	2.01	0.42
9:4:148:ASN:O	9:4:152:ARG:HG3	2.20	0.42
15:X:175:ALA:O	18:X:301:HOH:O	2.22	0.42
16:Y:37:GLN:HA	16:Y:43:LEU:HD12	2.01	0.42
3:D:14:ASP:OD1	3:D:14:ASP:N	2.53	0.42
4:E:65:GLU:OE2	17:L:71:LYS:NZ	2.51	0.42
5:T:176:LEU:HA	5:T:179:PHE:CE2	2.54	0.42
9:4:152:ARG:HG2	9:4:203:GLN:CD	2.40	0.42
9:7:34:PRO:HB3	9:7:78:LEU:HB2	2.01	0.42
5:F:176:LEU:HA	5:F:179:PHE:CE2	2.54	0.42
5:F:227:GLY:O	5:F:230:VAL:HG22	2.20	0.42
5:T:123:TYR:CD2	9:7:4:LYS:HG2	2.55	0.42
8:3:93:ARG:NE	11:B:3:ASP:O	2.48	0.42
10:5:147:ASP:OD1	10:5:147:ASP:N	2.52	0.42
2:A:98:LYS:HD3	6:H:68:SER:HB3	2.02	0.42
9:4:38:PHE:CG	9:4:157:GLN:HG3	2.54	0.42
9:7:152:ARG:HG2	9:7:203:GLN:CD	2.40	0.42
9:7:170:THR:HG22	9:7:219:ALA:HB3	2.02	0.42
12:Q:113:ARG:NH2	16:Y:71:GLU:OE2	2.38	0.42
14:W:174:ASP:OD2	14:W:188:ARG:NH1	2.53	0.42
1:2:96:LEU:O	1:2:100:MET:HG2	2.20	0.41
8:6:93:ARG:NE	11:P:3:ASP:O	2.50	0.41
10:8:159:ASP:OD2	10:8:165:ASN:ND2	2.53	0.41
17:L:156:LEU:HD13	17:L:159:ARG:HH21	1.85	0.41
12:Q:91:ALA:HB2	12:Q:115:LEU:HD11	2.01	0.41
5:F:10:THR:HG21	5:F:127:PRO:HD3	2.02	0.41
5:F:123:TYR:CD2	9:4:4:LYS:HG2	2.55	0.41
13:G:193:VAL:HG13	13:G:216:ILE:HG21	2.01	0.41
17:L:-37:ARG:HH11	17:L:-33:SER:HB2	1.86	0.41
11:P:140:ASP:OD2	11:P:143:ASN:ND2	2.39	0.41
14:W:191:LEU:HD23	14:W:191:LEU:HA	1.91	0.41
5:F:38:LEU:HD12	5:F:45:VAL:HB	2.01	0.41
5:F:90:GLN:HG2	17:L:-44:THR:HA	2.01	0.41
5:T:1:MET:HB3	5:T:1:MET:HE2	1.99	0.41
10:5:127:GLU:OE1	10:5:127:GLU:N	2.47	0.41
9:7:75:LYS:NZ	9:7:76:THR:O	2.53	0.41
16:K:181:VAL:HG21	16:K:196:GLN:HA	2.02	0.41
2:O:75:ILE:HD11	2:O:81:MET:HE1	2.02	0.41
3:R:80:ALA:HB1	12:Q:120:GLN:HG3	2.01	0.41
5:T:227:GLY:O	5:T:230:VAL:HG22	2.21	0.41
7:1:108:HIS:HB3	7:1:137:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:81:LYS:HD3	9:7:81:LYS:H	1.85	0.41
1:2:78:ASN:HB3	1:2:81:ALA:HB2	2.02	0.41
11:B:140:ASP:OD1	11:B:143:ASN:HB2	2.21	0.41
14:I:174:ASP:OD2	14:I:188:ARG:NH1	2.54	0.41
17:Z:113:TYR:CE1	17:Z:123:LYS:HB2	2.56	0.41
1:N:96:LEU:O	1:N:100:MET:HG2	2.20	0.41
9:4:177:MET:HE2	9:4:217:LEU:HD11	2.02	0.41
2:A:69:VAL:HA	13:G:158:TRP:CZ3	2.56	0.41
1:N:6:VAL:HG12	1:N:57:ILE:HG13	2.03	0.41
15:J:112:ILE:HD13	15:J:119:PRO:HA	2.03	0.41
17:L:9:GLN:NE2	17:L:148:LEU:O	2.44	0.41
5:F:52:ASN:ND2	5:F:54:ASP:O	2.54	0.41
2:O:115:ASP:OD1	2:O:115:ASP:N	2.51	0.41
5:T:38:LEU:HD12	5:T:45:VAL:HB	2.02	0.41
5:T:173:GLU:HA	13:U:58:LEU:HD21	2.02	0.41
9:4:43:ASP:OD1	9:4:45:PRO:HD2	2.21	0.41
9:7:51:VAL:HG22	9:7:166:ILE:HB	2.03	0.41
13:U:219:CYS:SG	13:U:228:HIS:ND1	2.75	0.41
16:Y:23:ARG:HA	16:Y:23:ARG:CZ	2.51	0.41
17:Z:143:ASN:N	18:Z:310:HOH:O	2.54	0.41
2:O:98:LYS:HD3	6:V:68:SER:HB3	2.02	0.41
7:1:52:MET:HG3	7:1:111:ILE:HG22	2.03	0.41
9:7:201:LEU:HB2	10:8:45:VAL:HG21	2.03	0.41
17:L:116:ASP:N	17:L:116:ASP:OD1	2.54	0.41
3:D:29:ARG:HH12	12:C:18:ARG:HD3	1.87	0.40
10:8:127:GLU:OE1	10:8:127:GLU:N	2.47	0.40
7:M:194:ARG:HD3	7:M:194:ARG:HA	1.93	0.40
14:W:103:VAL:HG11	14:W:180:ILE:HA	2.03	0.40
17:Z:-37:ARG:HH11	17:Z:-33:SER:HB2	1.86	0.40
17:L:113:TYR:CE1	17:L:123:LYS:HB2	2.55	0.40
17:Z:156:LEU:HD13	17:Z:159:ARG:HH21	1.85	0.40
6:H:101:GLY:O	6:H:108:GLY:HA2	2.21	0.40
2:O:69:VAL:HA	13:U:158:TRP:CZ3	2.56	0.40
4:S:32:LYS:NZ	18:S:307:HOH:O	2.36	0.40
7:1:194:ARG:HA	7:1:194:ARG:HD3	1.91	0.40
10:8:84:GLN:HG3	18:8:357:HOH:O	2.21	0.40
15:J:88:THR:HG23	15:J:124:PHE:CZ	2.57	0.40
13:U:116:LEU:HD23	13:U:116:LEU:HA	1.94	0.40
6:H:166:ASP:O	18:H:201:HOH:O	2.22	0.40
2:O:200:GLU:OE1	2:O:200:GLU:N	2.48	0.40
3:R:29:ARG:HH12	12:Q:18:ARG:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:103:VAL:HG11	14:I:180:ILE:HA	2.03	0.40
7:M:52:MET:HG3	7:M:111:ILE:HG22	2.04	0.40
1:2:6:VAL:HG12	1:2:57:ILE:HG13	2.02	0.40
5:F:182:ILE:HG21	5:F:188:GLU:HB3	2.04	0.40
5:T:182:ILE:HG21	5:T:188:GLU:HB3	2.04	0.40
7:1:195:HIS:CE1	14:I:24:PRO:HB2	2.57	0.40
10:5:26:GLN:NE2	10:5:238:PRO:HG2	2.36	0.40
7:M:125:PHE:CD2	7:M:131:TYR:HB3	2.57	0.40
11:P:140:ASP:OD1	11:P:143:ASN:HB2	2.21	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	2	222/266 (84%)	214 (96%)	8 (4%)	0	100	100
1	N	222/266 (84%)	211 (95%)	11 (5%)	0	100	100
2	A	238/252 (94%)	237 (100%)	1 (0%)	0	100	100
2	O	238/252 (94%)	237 (100%)	1 (0%)	0	100	100
3	D	238/254 (94%)	235 (99%)	3 (1%)	0	100	100
3	R	238/254 (94%)	236 (99%)	2 (1%)	0	100	100
4	E	245/260 (94%)	245 (100%)	0	0	100	100
4	S	245/260 (94%)	244 (100%)	1 (0%)	0	100	100
5	F	232/234 (99%)	227 (98%)	5 (2%)	0	100	100
5	T	232/234 (99%)	227 (98%)	5 (2%)	0	100	100
6	H	203/215 (94%)	200 (98%)	3 (2%)	0	100	100
6	V	203/215 (94%)	200 (98%)	3 (2%)	0	100	100
7	1	206/241 (86%)	201 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	206/241 (86%)	201 (98%)	5 (2%)	0	100	100
8	3	138/148 (93%)	137 (99%)	1 (1%)	0	100	100
8	6	138/148 (93%)	137 (99%)	1 (1%)	0	100	100
9	4	231/276 (84%)	227 (98%)	4 (2%)	0	100	100
9	7	231/276 (84%)	224 (97%)	7 (3%)	0	100	100
10	5	258/267 (97%)	254 (98%)	4 (2%)	0	100	100
10	8	255/267 (96%)	245 (96%)	9 (4%)	1 (0%)	30	26
11	B	244/250 (98%)	241 (99%)	3 (1%)	0	100	100
11	P	244/250 (98%)	241 (99%)	3 (1%)	0	100	100
12	C	231/258 (90%)	228 (99%)	3 (1%)	0	100	100
12	Q	231/258 (90%)	228 (99%)	3 (1%)	0	100	100
13	G	238/288 (83%)	235 (99%)	3 (1%)	0	100	100
13	U	238/288 (83%)	236 (99%)	2 (1%)	0	100	100
14	I	205/261 (78%)	202 (98%)	3 (2%)	0	100	100
14	W	205/261 (78%)	203 (99%)	2 (1%)	0	100	100
15	J	188/205 (92%)	180 (96%)	8 (4%)	0	100	100
15	X	185/205 (90%)	179 (97%)	6 (3%)	0	100	100
16	K	189/212 (89%)	184 (97%)	4 (2%)	1 (0%)	25	20
16	Y	189/212 (89%)	183 (97%)	5 (3%)	1 (0%)	25	20
17	L	240/287 (84%)	232 (97%)	8 (3%)	0	100	100
17	Z	240/287 (84%)	232 (97%)	8 (3%)	0	100	100
All	All	7486/8348 (90%)	7343 (98%)	140 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	8	164	VAL
16	K	51	GLY
16	Y	51	GLY

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	192/224 (86%)	189 (98%)	3 (2%)	58	63
1	N	192/224 (86%)	187 (97%)	5 (3%)	41	41
2	A	204/210 (97%)	202 (99%)	2 (1%)	73	77
2	O	204/210 (97%)	202 (99%)	2 (1%)	73	77
3	D	212/226 (94%)	211 (100%)	1 (0%)	86	90
3	R	212/226 (94%)	211 (100%)	1 (0%)	86	90
4	E	205/215 (95%)	205 (100%)	0	100	100
4	S	205/215 (95%)	205 (100%)	0	100	100
5	F	193/193 (100%)	192 (100%)	1 (0%)	86	90
5	T	193/193 (100%)	192 (100%)	1 (0%)	86	90
6	H	169/178 (95%)	167 (99%)	2 (1%)	67	72
6	V	169/178 (95%)	167 (99%)	2 (1%)	67	72
7	1	175/201 (87%)	169 (97%)	6 (3%)	32	30
7	M	175/201 (87%)	169 (97%)	6 (3%)	32	30
8	3	132/136 (97%)	132 (100%)	0	100	100
8	6	132/136 (97%)	132 (100%)	0	100	100
9	4	216/251 (86%)	213 (99%)	3 (1%)	62	67
9	7	216/251 (86%)	214 (99%)	2 (1%)	75	80
10	5	239/244 (98%)	237 (99%)	2 (1%)	79	83
10	8	238/244 (98%)	235 (99%)	3 (1%)	65	70
11	B	207/209 (99%)	205 (99%)	2 (1%)	73	77
11	P	207/209 (99%)	205 (99%)	2 (1%)	73	77
12	C	199/216 (92%)	196 (98%)	3 (2%)	60	65
12	Q	199/216 (92%)	197 (99%)	2 (1%)	73	77
13	G	199/239 (83%)	195 (98%)	4 (2%)	50	53
13	U	199/239 (83%)	195 (98%)	4 (2%)	50	53
14	I	167/214 (78%)	167 (100%)	0	100	100
14	W	167/214 (78%)	167 (100%)	0	100	100
15	J	161/173 (93%)	156 (97%)	5 (3%)	35	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	X	161/173 (93%)	159 (99%)	2 (1%)	67	72
16	K	172/189 (91%)	170 (99%)	2 (1%)	67	72
16	Y	172/189 (91%)	169 (98%)	3 (2%)	56	60
17	L	204/235 (87%)	201 (98%)	3 (2%)	60	65
17	Z	204/235 (87%)	201 (98%)	3 (2%)	60	65
All	All	6491/7106 (91%)	6414 (99%)	77 (1%)	66	72

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	9	THR
1	2	104	ARG
1	2	146	PHE
2	A	13	ASP
2	A	169	THR
3	D	6	ARG
5	F	38	LEU
6	H	-7	LYS
6	H	31	THR
1	N	9	THR
1	N	76	TYR
1	N	78	ASN
1	N	104	ARG
1	N	146	PHE
2	O	13	ASP
2	O	169	THR
3	R	6	ARG
5	T	38	LEU
6	V	-7	LYS
6	V	31	THR
7	1	77	PHE
7	1	91	ARG
7	1	103	PHE
7	1	108	HIS
7	1	126	ASP
7	1	137	ARG
9	4	1	MET
9	4	81	LYS
9	4	177	MET
10	5	198	ARG

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Mol	Chain	Res	Type
10	5	200	LYS
9	7	1	MET
9	7	81	LYS
10	8	152	LEU
10	8	159	ASP
10	8	164	VAL
11	B	99	ARG
11	B	128	ARG
12	C	5	ARG
12	C	201	THR
12	C	213	PHE
13	G	55	THR
13	G	134	VAL
13	G	218	TRP
13	G	219	CYS
15	J	27	LEU
15	J	29	LEU
15	J	39	LYS
15	J	177	ARG
15	J	201	LYS
16	K	78	GLN
16	K	95	ARG
17	L	-74	GLN
17	L	104	TYR
17	L	146	TRP
7	M	77	PHE
7	M	91	ARG
7	M	103	PHE
7	M	108	HIS
7	M	126	ASP
7	M	137	ARG
11	P	99	ARG
11	P	128	ARG
12	Q	201	THR
12	Q	213	PHE
13	U	134	VAL
13	U	205	GLU
13	U	218	TRP
13	U	219	CYS
15	X	27	LEU
15	X	180	LEU
16	Y	23	ARG

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Mol	Chain	Res	Type
16	Y	78	GLN
16	Y	95	ARG
17	Z	-74	GLN
17	Z	104	TYR
17	Z	146	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
7	1	108	HIS
10	5	93	ASN
7	M	108	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.

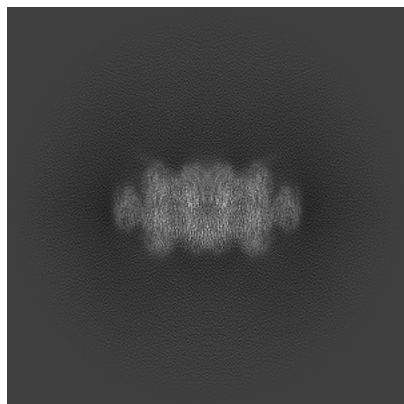
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19523. These allow visual inspection of the internal detail of the map and identification of artifacts.

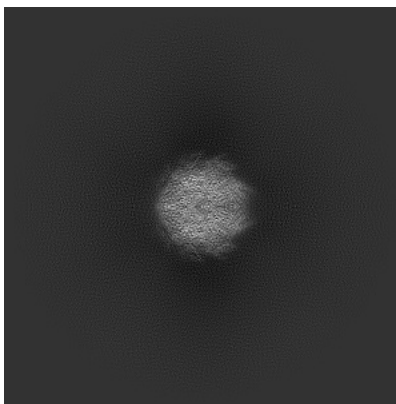
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

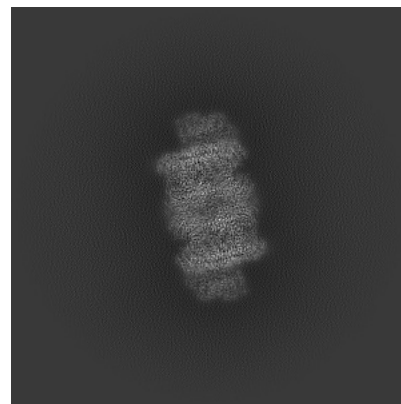
6.1.1 Primary map



X

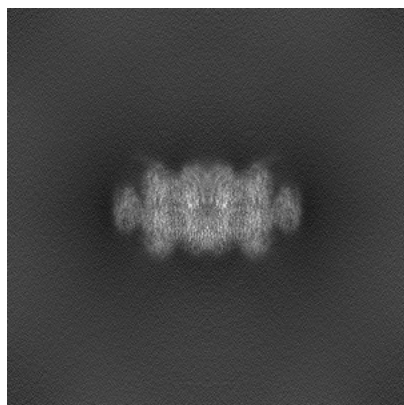


Y

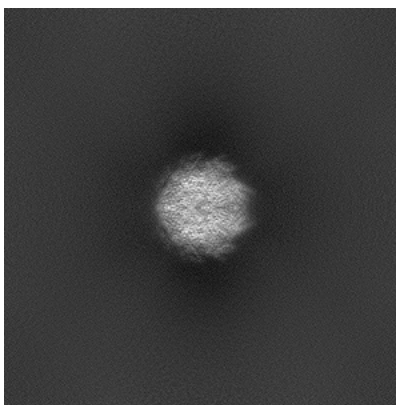


Z

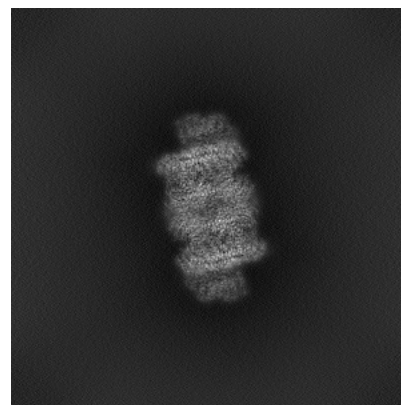
6.1.2 Raw map



X



Y

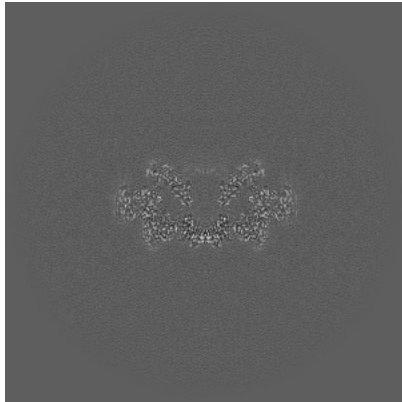


Z

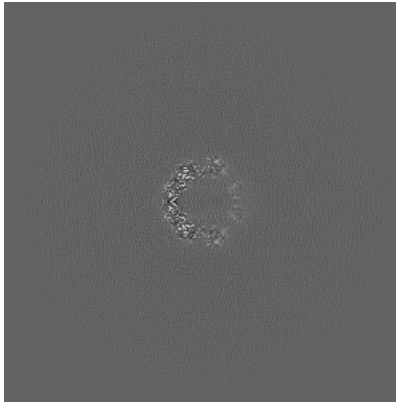
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

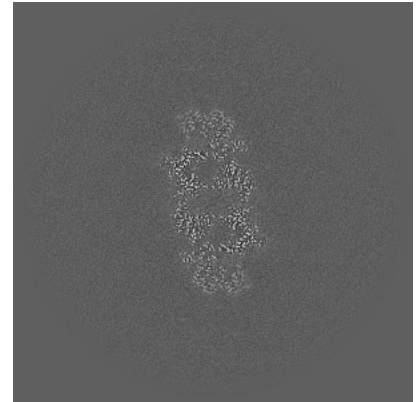
6.2.1 Primary map



X Index: 300

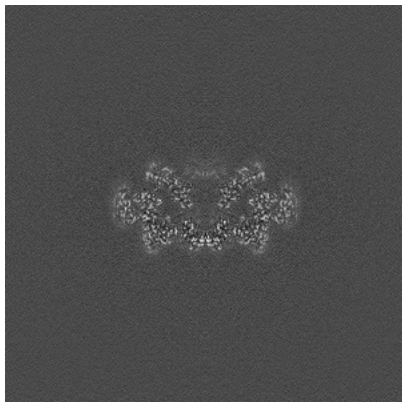


Y Index: 300

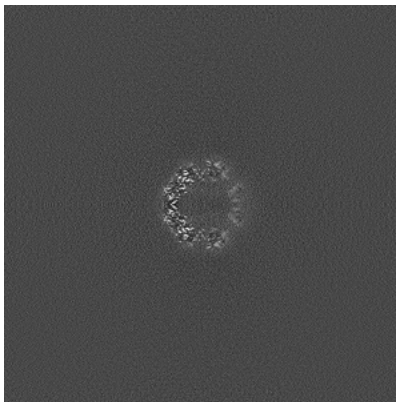


Z Index: 300

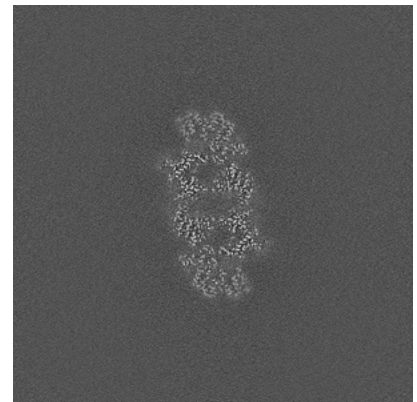
6.2.2 Raw map



X Index: 300



Y Index: 300

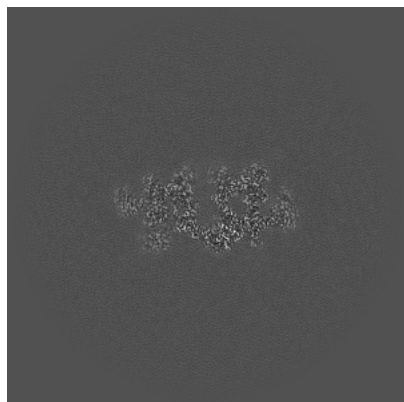


Z Index: 300

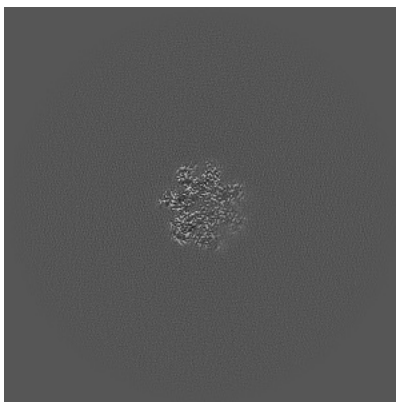
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

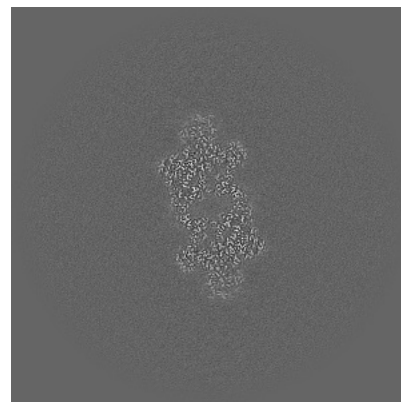
6.3.1 Primary map



X Index: 286

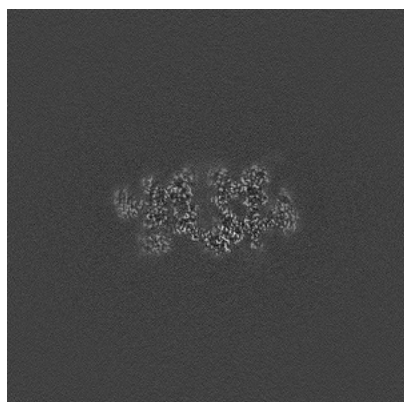


Y Index: 274

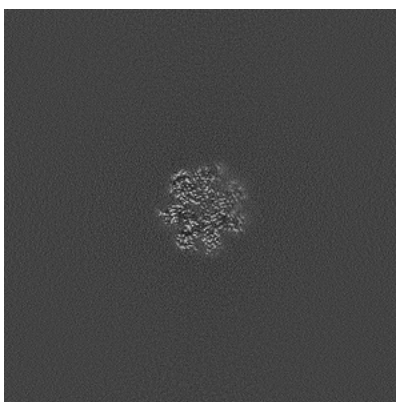


Z Index: 282

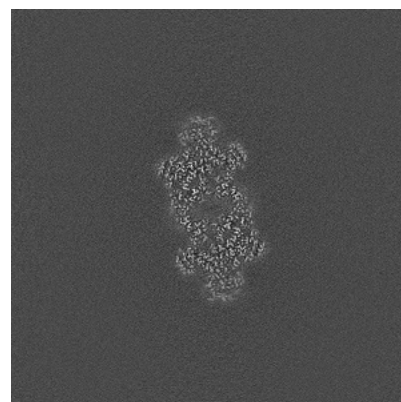
6.3.2 Raw map



X Index: 286



Y Index: 326

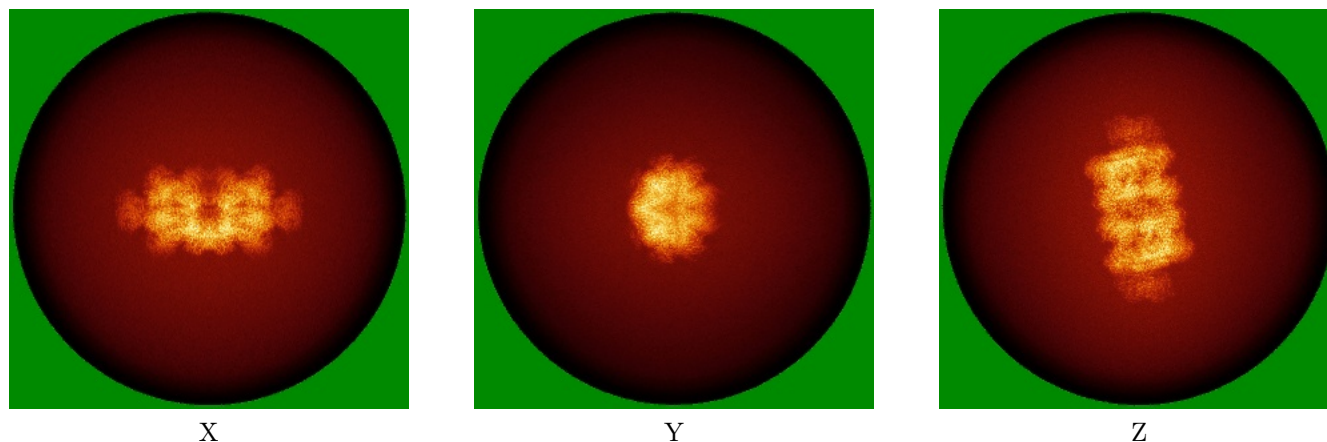


Z Index: 282

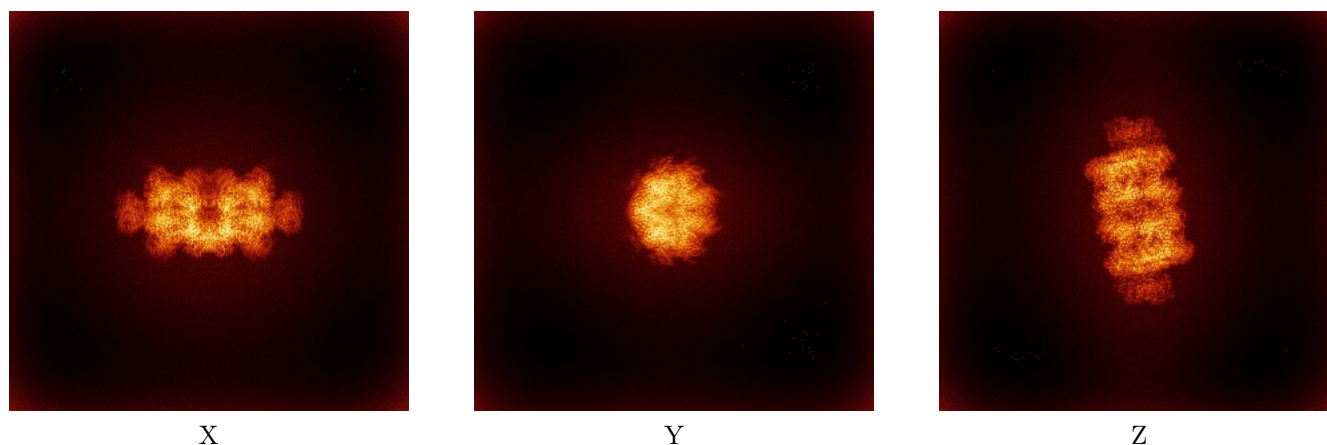
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



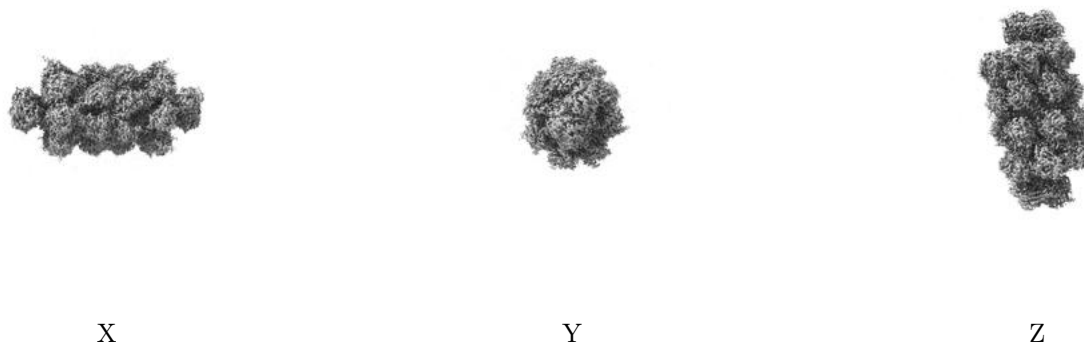
6.4.2 Raw map



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.

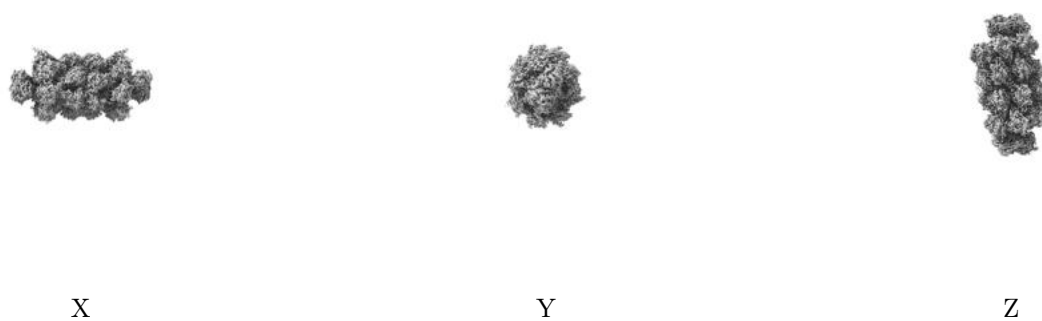
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.282. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

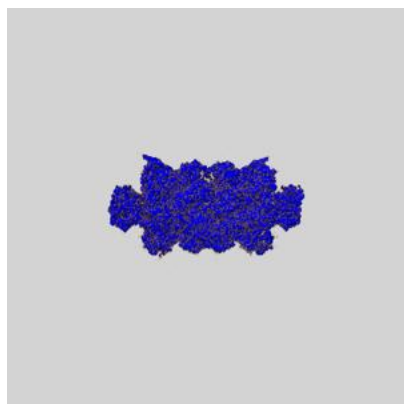
6.6 Mask visualisation [i](#)

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

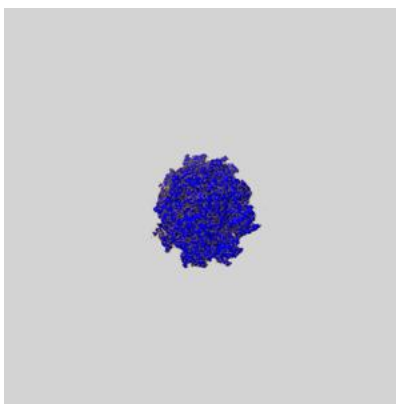
A mask typically either:

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

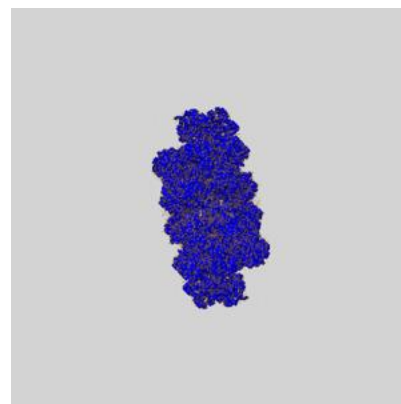
6.6.1 emd_19523_msk_1.map [i](#)



X



Y

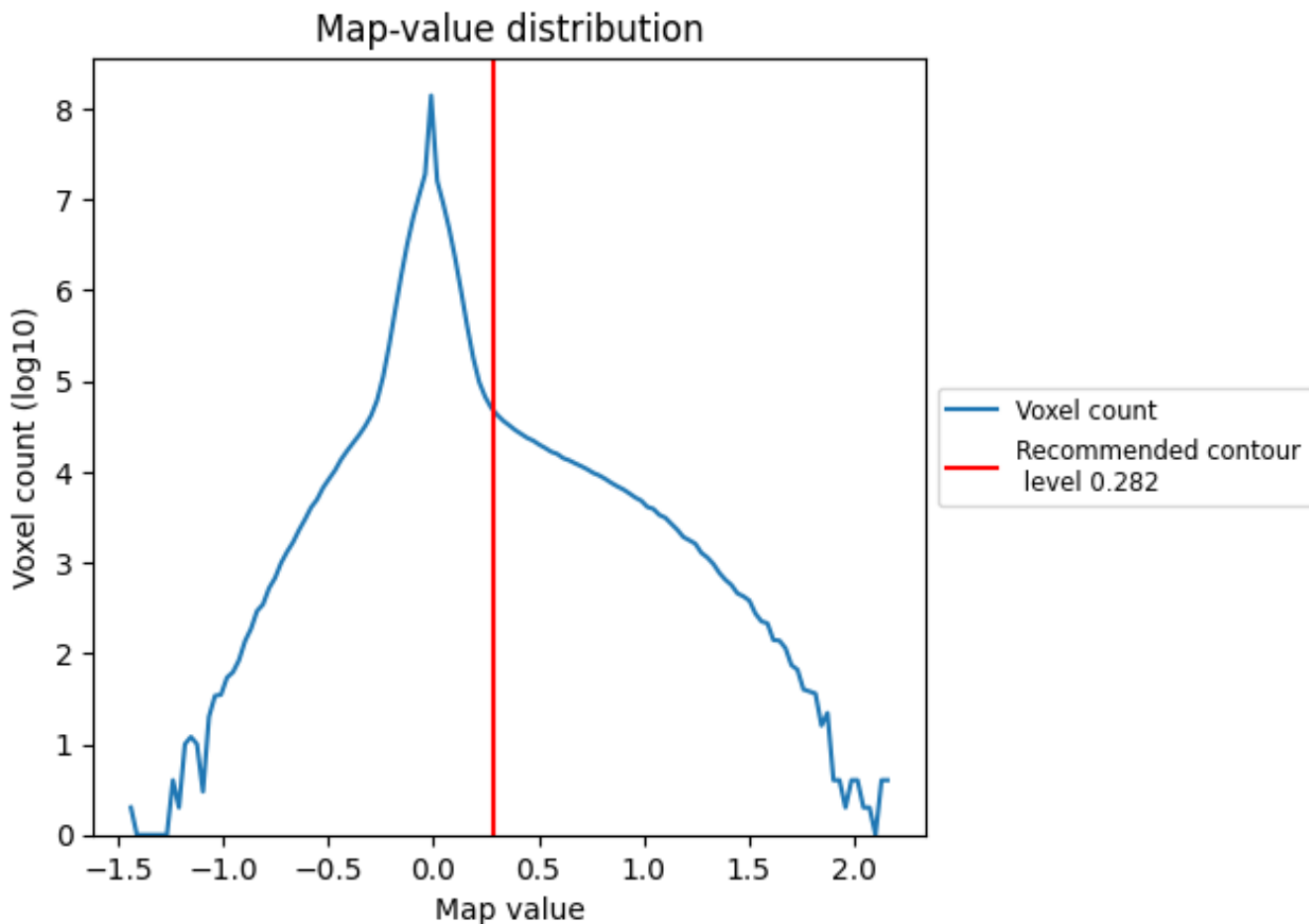


Z

7 Map analysis [i](#)

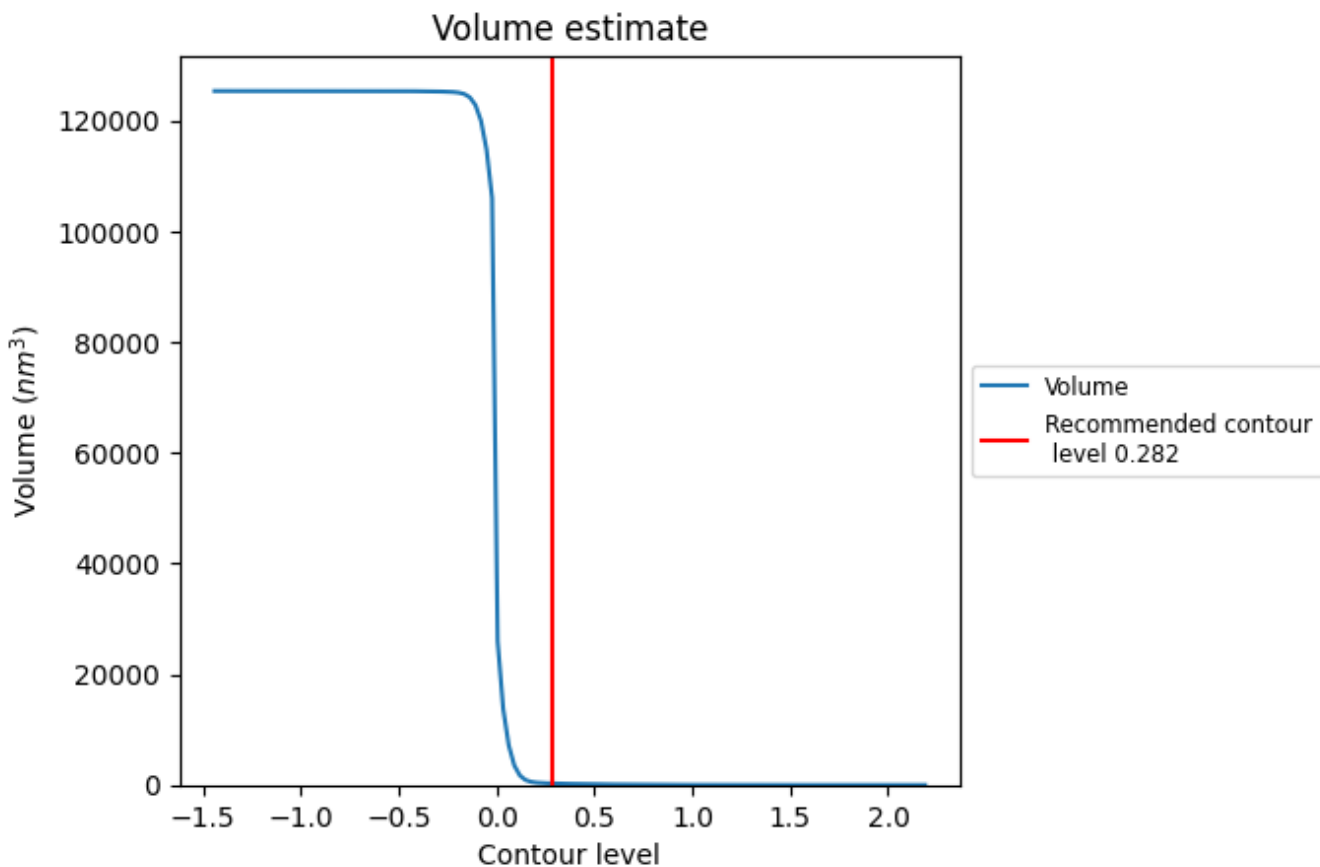
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

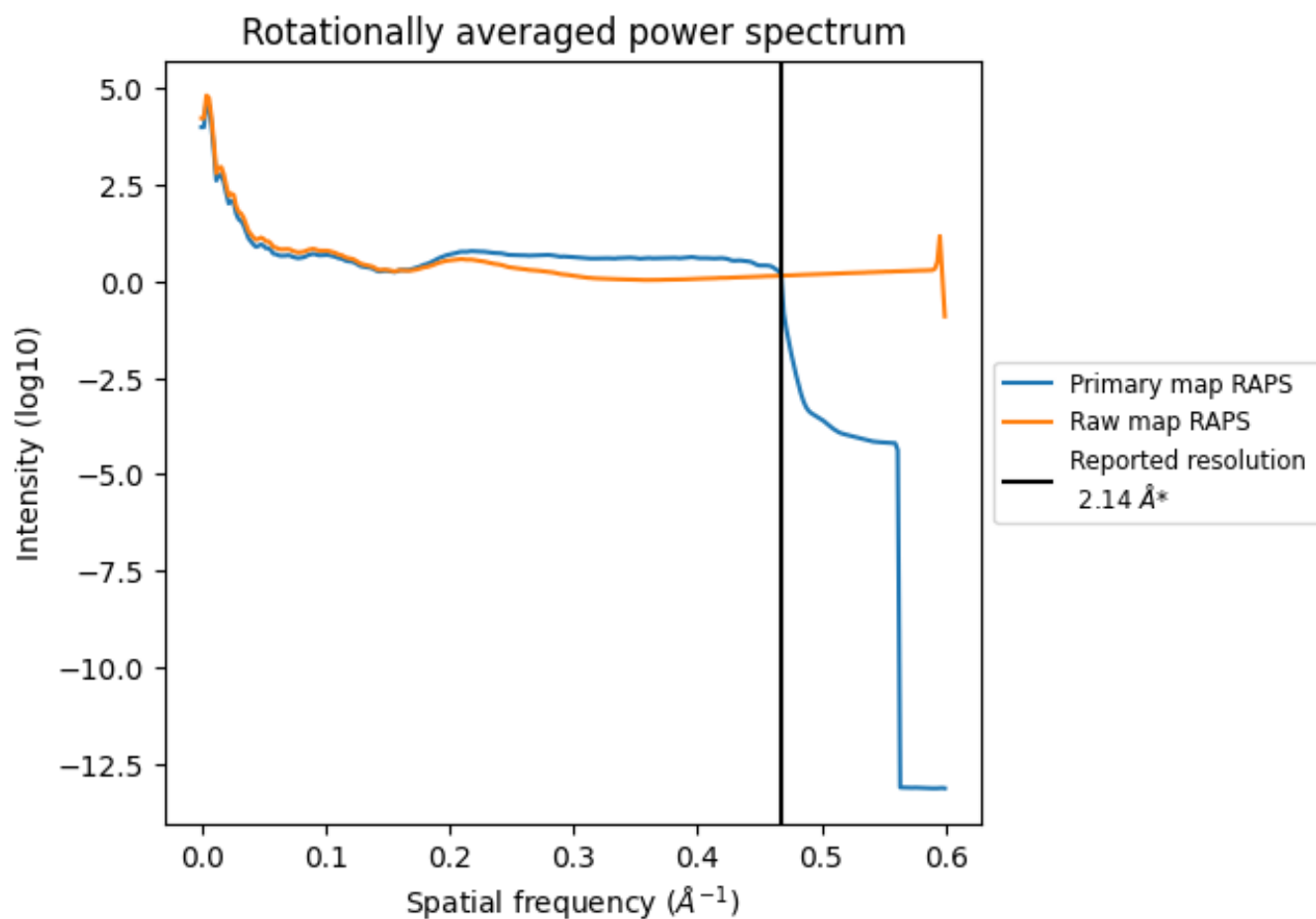
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm^3 ; this corresponds to an approximate mass of 251 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

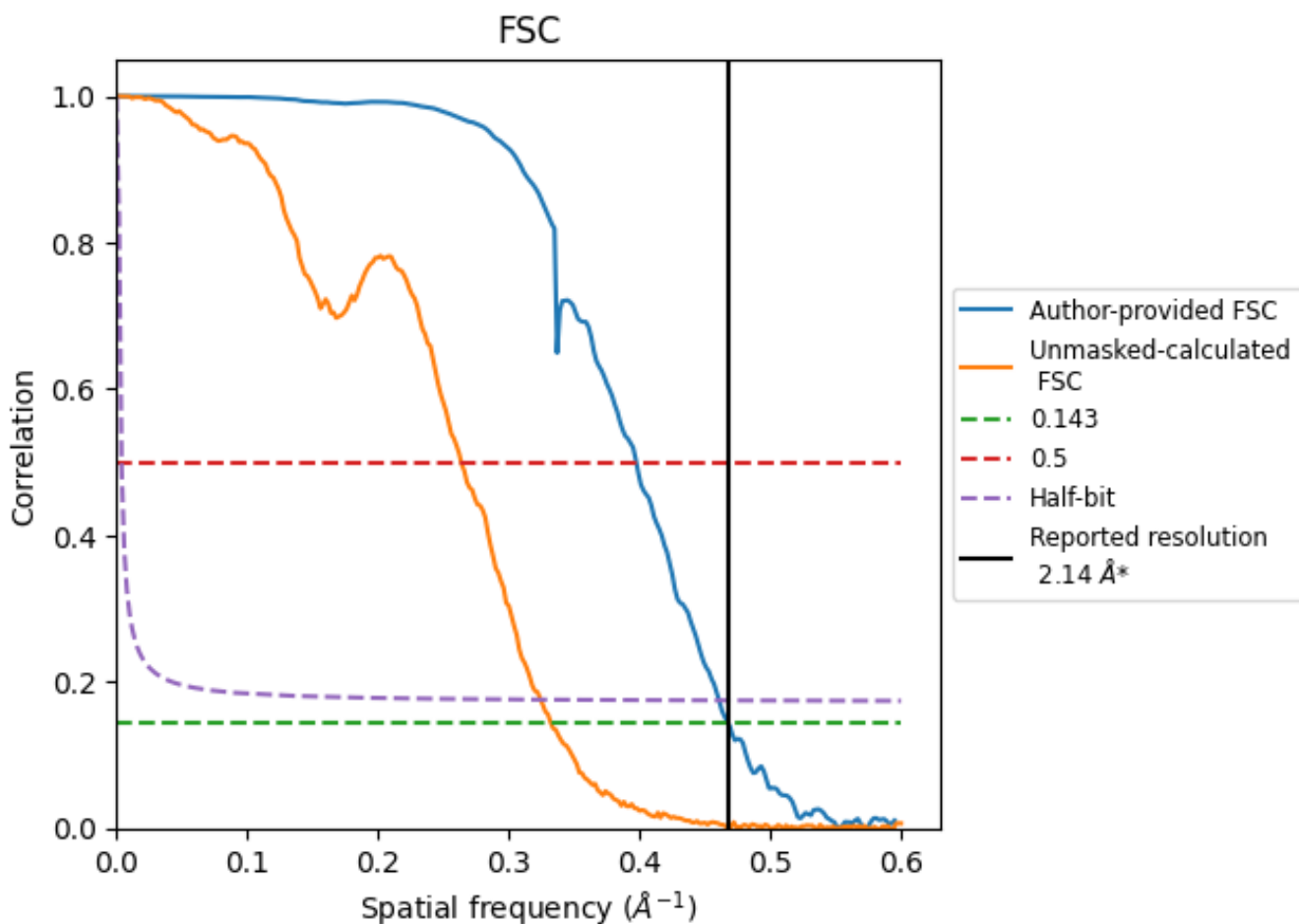


*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

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 0.467\AA^{-1}

8.2 Resolution estimates [i](#)

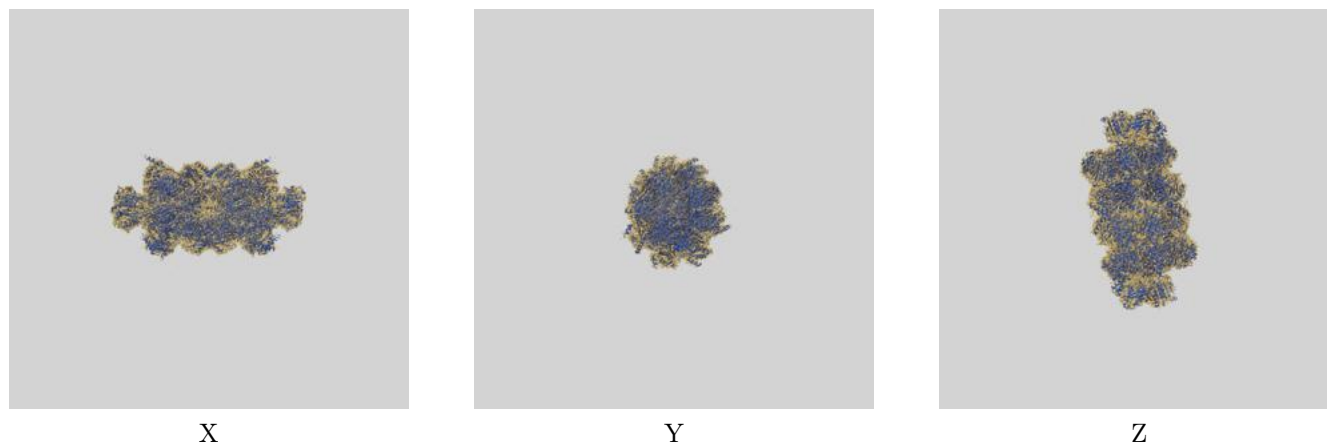
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.52	2.17
Unmasked-calculated*	3.01	3.80	3.08

*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 3.01 differs from the reported value 2.14 by more than 10 %

9 Map-model fit [i](#)

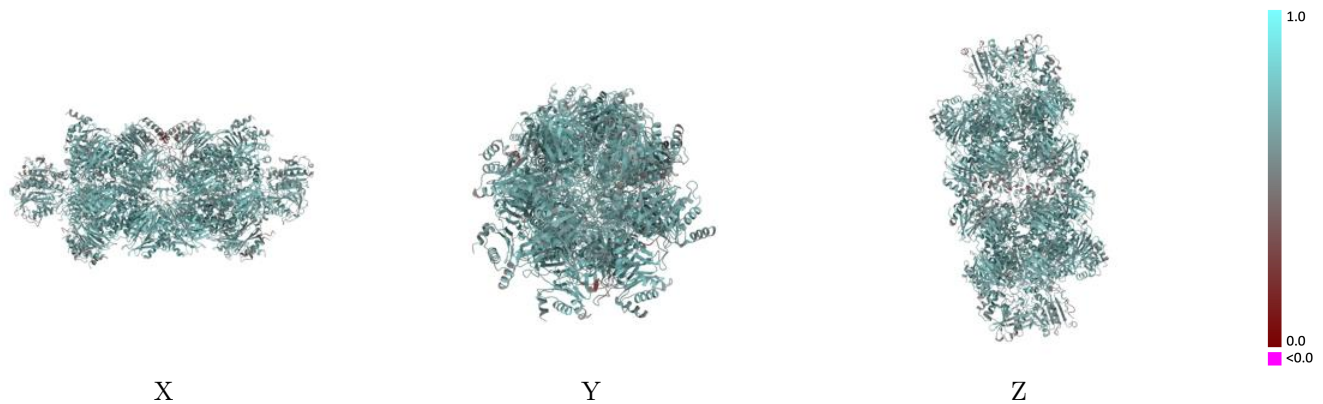
This section contains information regarding the fit between EMDB map EMD-19523 and PDB model 8RVL. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



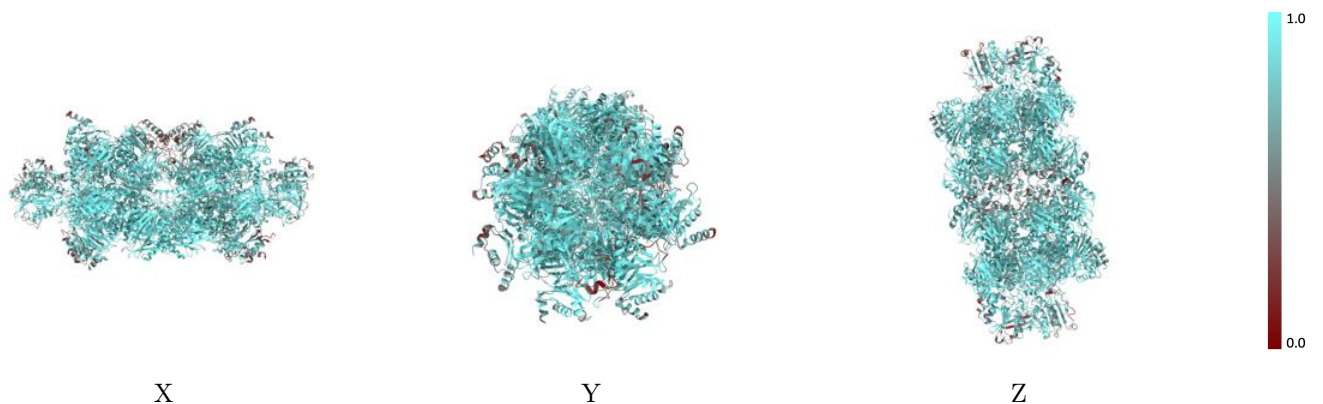
The images above show the 3D surface view of the map at the recommended contour level 0.282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



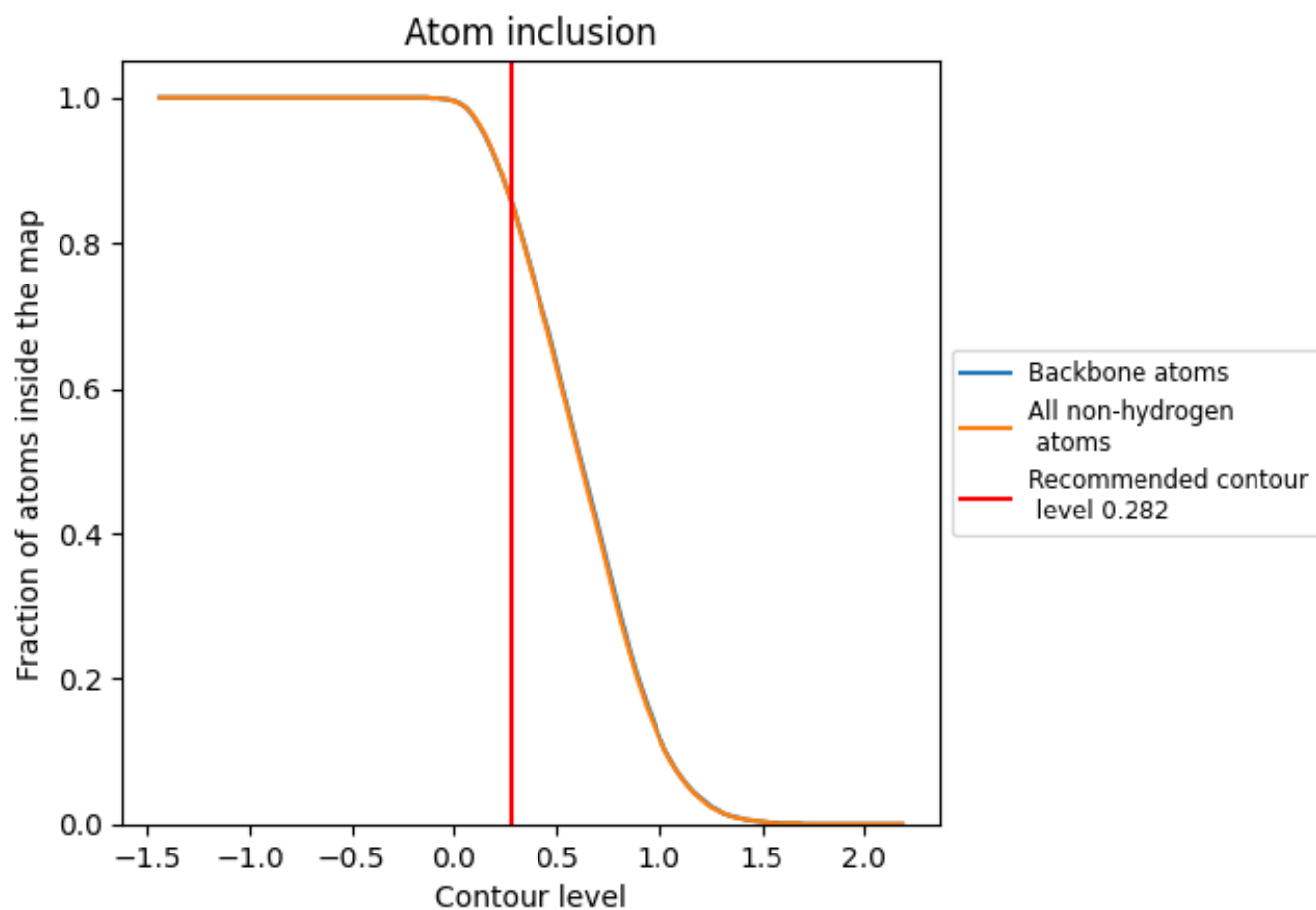
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.282).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.6580
1	 0.9210	 0.6870
2	 0.9170	 0.6870
3	 0.9240	 0.7010
4	 0.7270	 0.5930
5	 0.7360	 0.5930
6	 0.9240	 0.7000
7	 0.7340	 0.5950
8	 0.7420	 0.5900
A	 0.8520	 0.6670
B	 0.9090	 0.6810
C	 0.8560	 0.6630
D	 0.8520	 0.6580
E	 0.8980	 0.6740
F	 0.9210	 0.6820
G	 0.8110	 0.6450
H	 0.9490	 0.7100
I	 0.9600	 0.7090
J	 0.8460	 0.6560
K	 0.7370	 0.6020
L	 0.7870	 0.6250
M	 0.9220	 0.6880
N	 0.9170	 0.6850
O	 0.8520	 0.6650
P	 0.9070	 0.6800
Q	 0.8560	 0.6600
R	 0.8520	 0.6580
S	 0.8970	 0.6740
T	 0.9210	 0.6830
U	 0.8140	 0.6450
V	 0.9490	 0.7100
W	 0.9600	 0.7100
X	 0.8500	 0.6600
Y	 0.7360	 0.6040
Z	 0.7850	 0.6260

