



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2024 – 04:24 PM JST

PDB ID : 8YPK  
EMDB ID : EMD-39482  
Title : mouse proteasome 20S subunit in complex with compound 1  
Authors : Kashima, A.; Arai, Y.  
Deposited on : 2024-03-17  
Resolution : 2.70 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](mailto: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>.

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

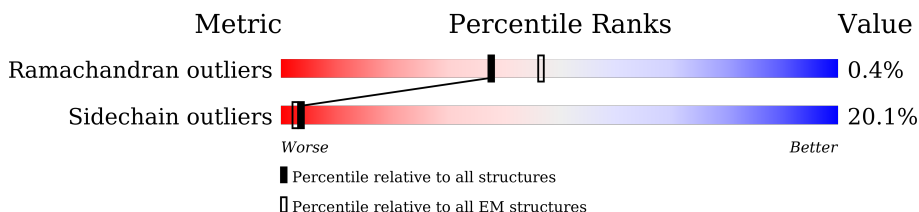
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 2.70 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.






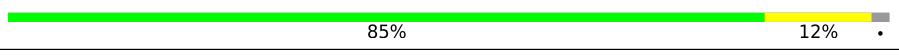
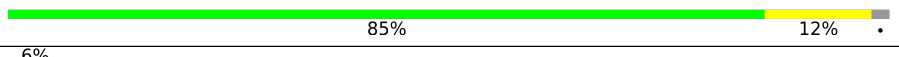



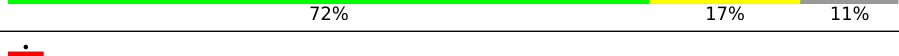
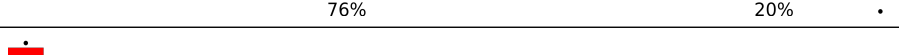
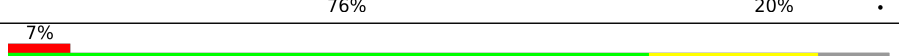
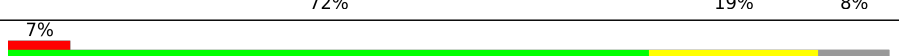

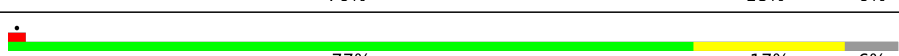
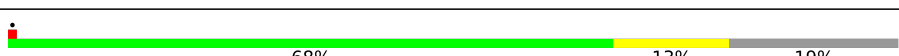
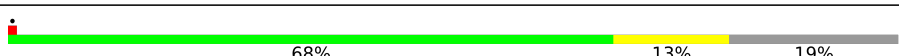



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	83% 16%
1	F	204	83% 16%
2	P	234	77% 20%
2	b	234	5% 77% 20%
3	I	248	6% 76% 18% 6%
3	N	248	6% 76% 18% 6%
4	K	246	9% 80% 15%
4	R	246	10% 80% 15%
5	T	201	88% 9%

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Mol	Chain	Length	Quality of chain
5	V	201	 88% 9%
6	S	240	 74% 15% 12%
6	X	240	 74% 15% 12%
7	C	204	 85% 12%
7	D	204	 85% 12%
8	J	255	 6% 78% 15% 8%
8	Q	255	 5% 78% 15% 8%
9	G	263	 72% 17% 11%
9	L	263	 5% 72% 17% 11%
10	H	241	 76% 20%
10	M	241	 76% 20%
11	O	261	 7% 72% 19% 8%
11	Z	261	 7% 72% 19% 8%
12	B	234	 76% 18% 6%
12	E	234	 77% 17% 6%
13	W	264	 68% 13% 19%
13	a	264	 68% 13% 19%
14	U	205	 86% 14%
14	Y	205	 86% 13%

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 47992 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	201	Total	C	N	O	S	0	0
			1512	948	258	294	12		
1	F	201	Total	C	N	O	S	0	0
			1512	948	258	294	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	227	Total	C	N	O	S	0	0
			1782	1138	304	334	6		
2	b	227	Total	C	N	O	S	0	0
			1782	1138	304	334	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	232	Total	C	N	O	S	0	0
			1819	1146	322	346	5		
3	I	232	Total	C	N	O	S	0	0
			1819	1146	322	346	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	236	Total	C	N	O	S	0	0
			1831	1163	304	351	13		
4	K	236	Total	C	N	O	S	0	0
			1831	1163	304	351	13		

- Molecule 5 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	196	Total	C	N	O	S	0	0
			1570	1006	267	288	9		
5	V	196	Total	C	N	O	S	0	0
			1570	1006	267	288	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
6	X	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	199	Total	C	N	O	S	0	0
			1544	976	269	290	9		
7	C	199	Total	C	N	O	S	0	0
			1544	976	269	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	235	Total	C	N	O	S	0	0
			1840	1168	315	346	11		
8	Q	235	Total	C	N	O	S	0	0
			1840	1168	315	346	11		

- Molecule 9 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	234	Total	C	N	O	S	0	0
			1836	1150	328	347	11		
9	G	234	Total	C	N	O	S	0	0
			1836	1150	328	347	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	231	1761	1106	292	352	11	0	0

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	239	1881	1191	321	359	10	0	0
11	Z	239	1881	1191	321	359	10	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	220	1656	1044	282	318	12	0	0
12	E	220	1656	1044	282	318	12	0	0

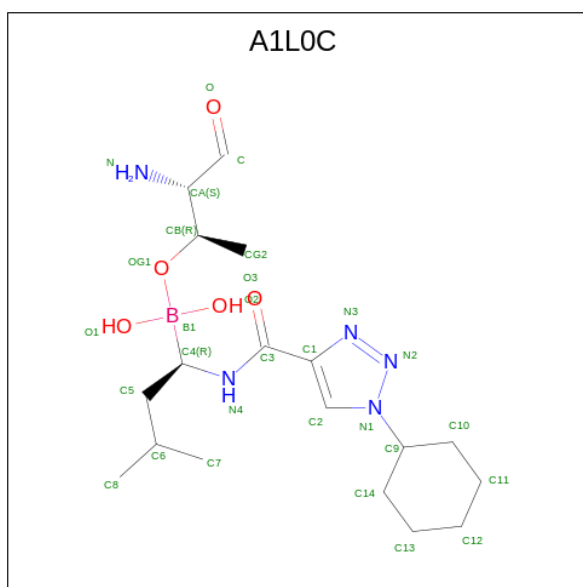
- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	W	214	1671	1054	289	316	12	0	0
13	a	214	1671	1054	289	316	12	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Y	204	1592	1013	265	295	19	0	0
14	U	204	1592	1013	265	295	19	0	0

- Molecule 15 is [(2 {R},3 {S})-3-azanyl-4-oxidanylidene-butan-2-yl]oxy-[(1 {R})-1-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]-3-methyl-butyl]- $\text{B}(\text{O})_3$ -oxidanyl-oxidanyl-boron (three-letter code: A1L0C) (formula:  $\text{C}_{18}\text{H}_{33}\text{BN}_5\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).

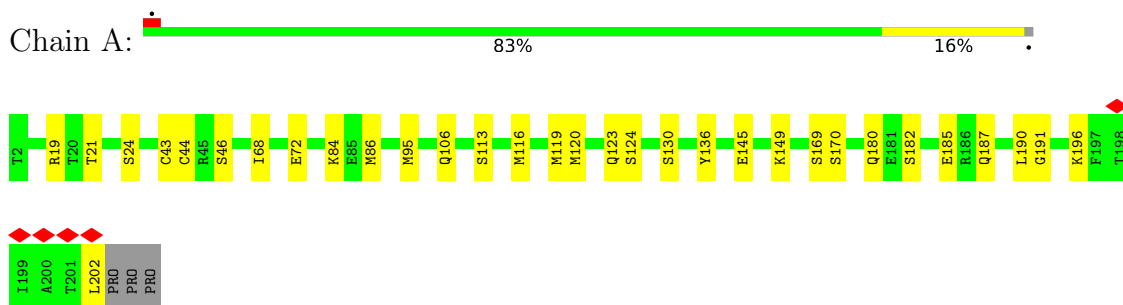


Mol	Chain	Residues	Atoms					AltConf
			Total	B	C	N	O	
15	A	1	Total	B	C	N	O	0
			29	1	18	5	5	
15	D	1	Total	B	C	N	O	0
			29	1	18	5	5	
15	C	1	Total	B	C	N	O	0
			29	1	18	5	5	
15	F	1	Total	B	C	N	O	0
			29	1	18	5	5	

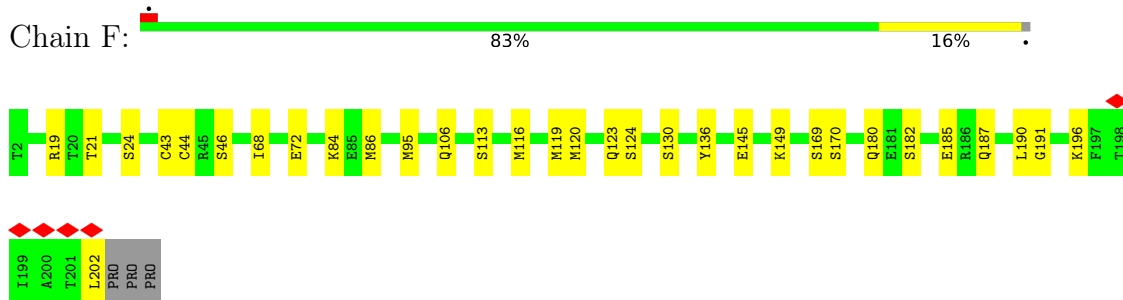
### 3 Residue-property plots [i](#)

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.

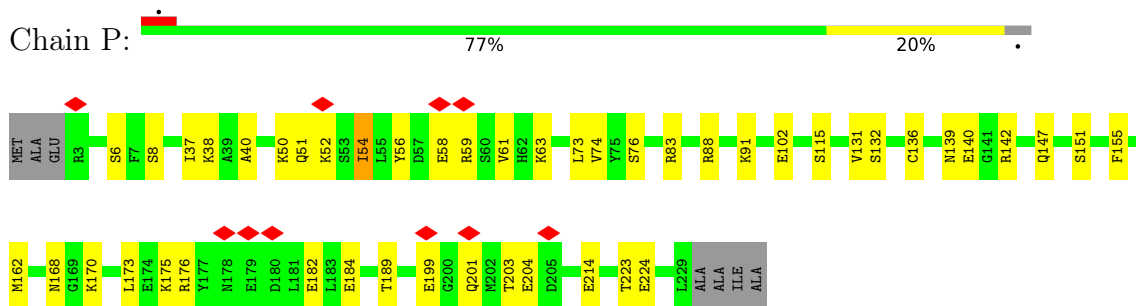
- Molecule 1: Proteasome subunit beta type-6



- Molecule 1: Proteasome subunit beta type-6



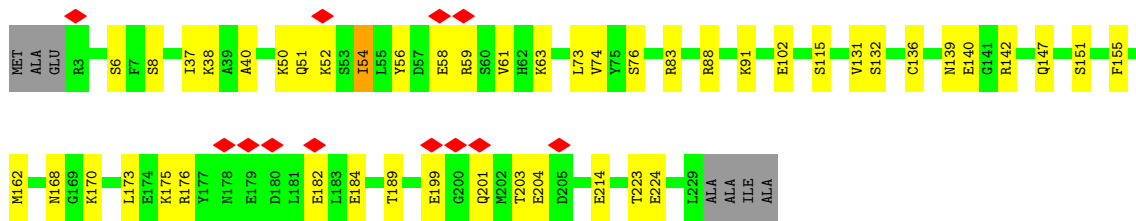
- Molecule 2: Proteasome subunit alpha type-2



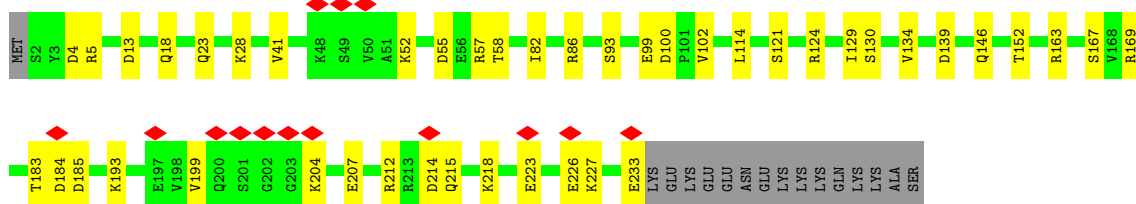
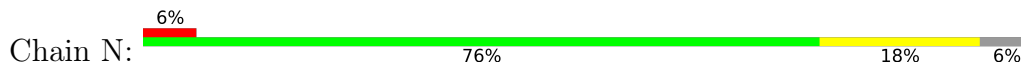
- Molecule 2: Proteasome subunit alpha type-2



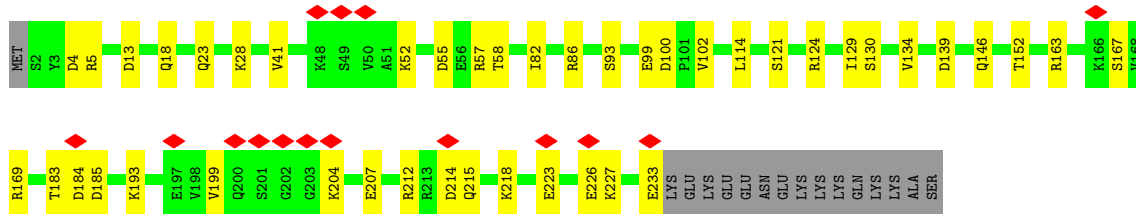
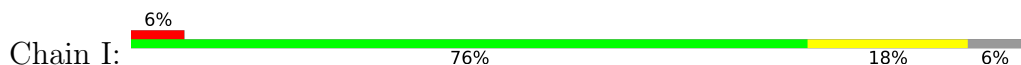




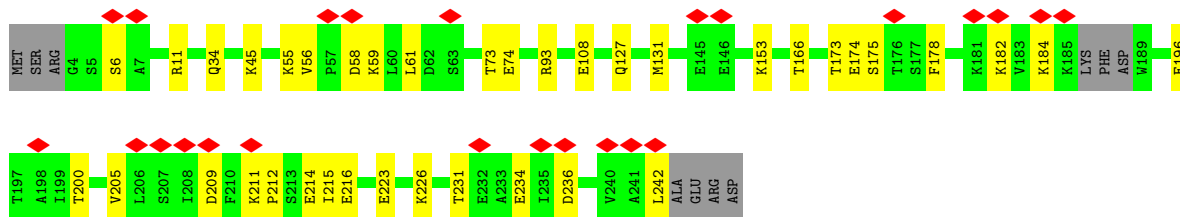
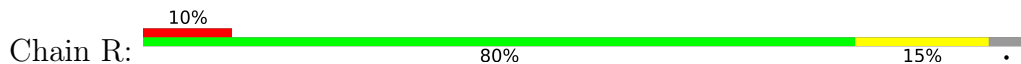
• Molecule 3: Proteasome subunit alpha type-7



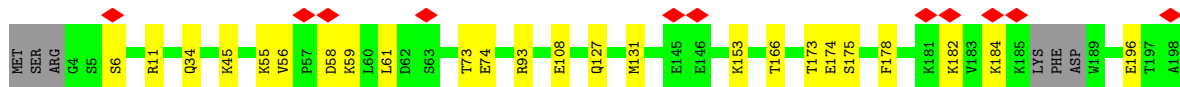
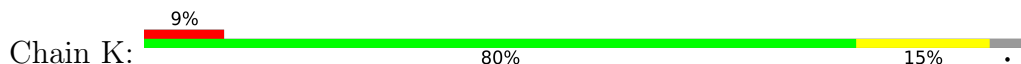
• Molecule 3: Proteasome subunit alpha type-7



• Molecule 4: Proteasome subunit alpha type-6

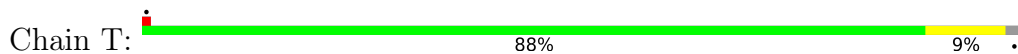


• Molecule 4: Proteasome subunit alpha type-6

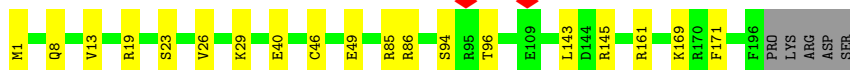




• Molecule 5: Proteasome subunit beta type-2



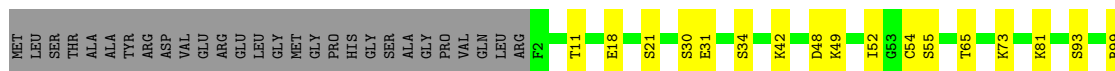
• Molecule 5: Proteasome subunit beta type-2



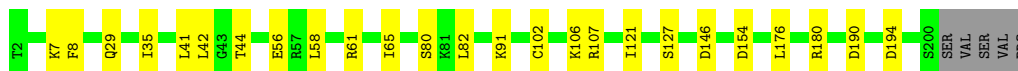
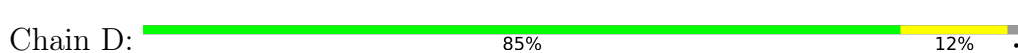
• Molecule 6: Proteasome subunit beta type-1



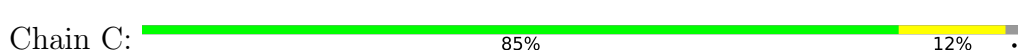
• Molecule 6: Proteasome subunit beta type-1

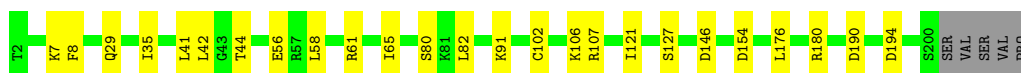


• Molecule 7: Proteasome subunit beta type-5

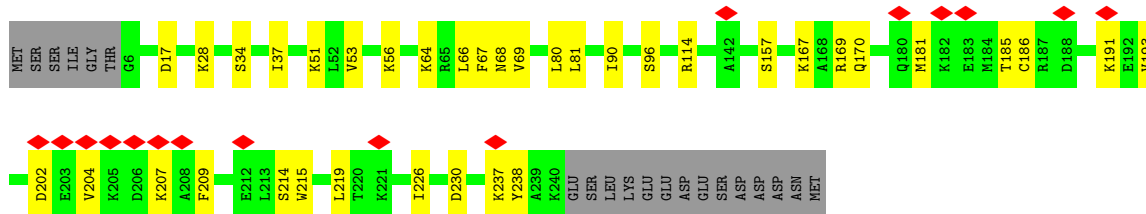
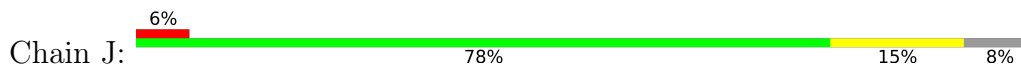


• Molecule 7: Proteasome subunit beta type-5

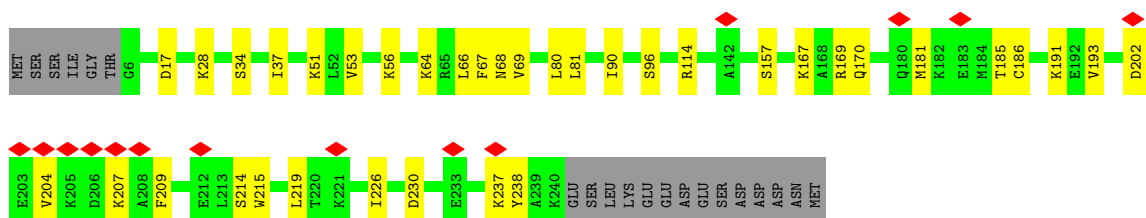
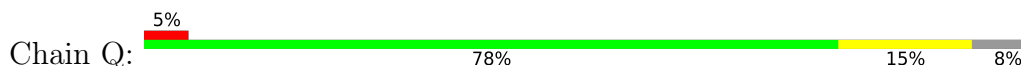




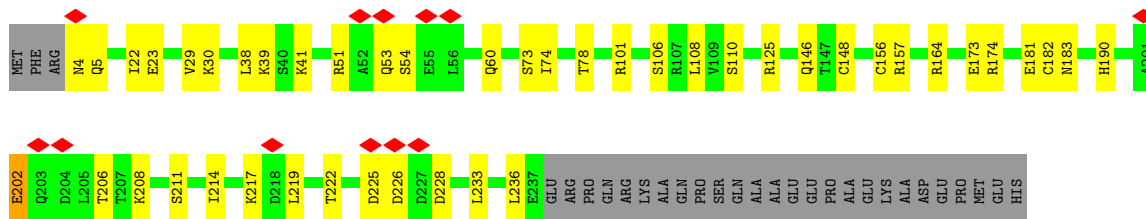
• Molecule 8: Proteasome subunit alpha type-3



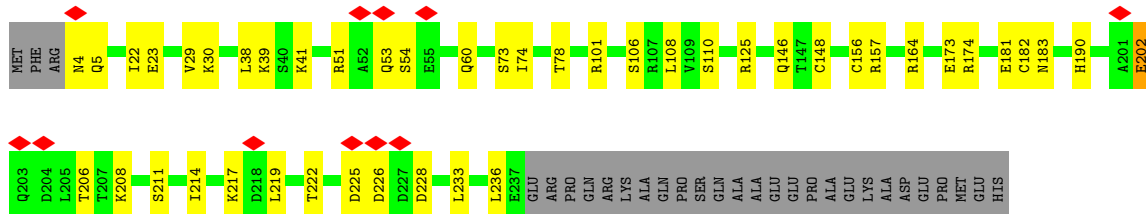
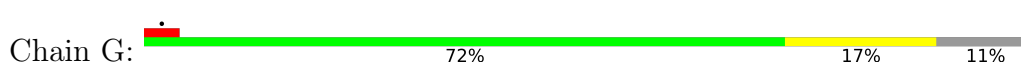
• Molecule 8: Proteasome subunit alpha type-3



• Molecule 9: Proteasome subunit alpha type-1

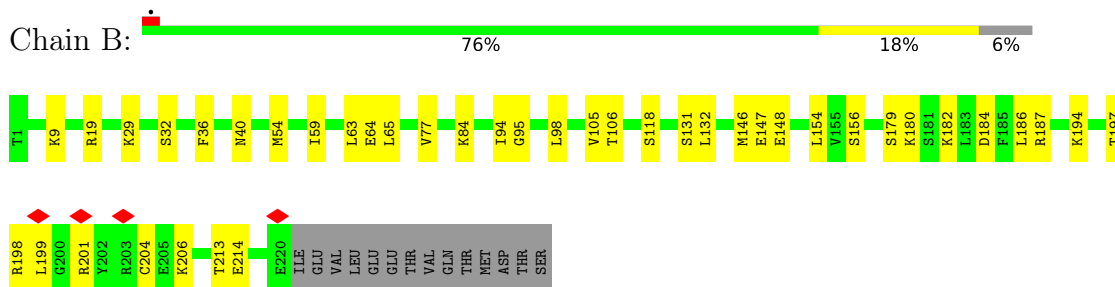


• Molecule 9: Proteasome subunit alpha type-1

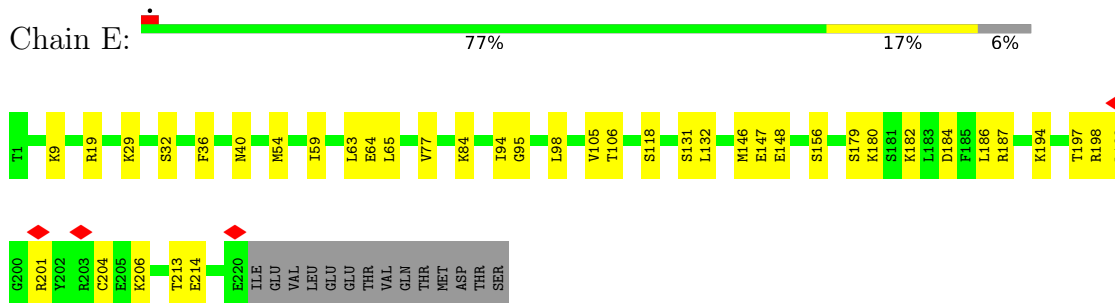


• Molecule 10: Proteasome subunit alpha type-5

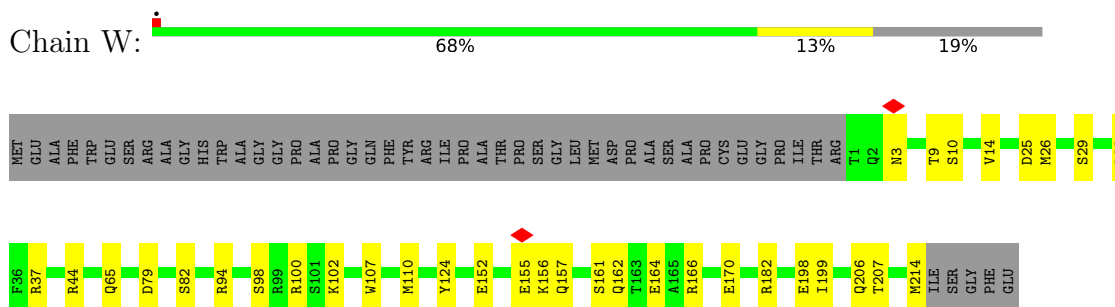




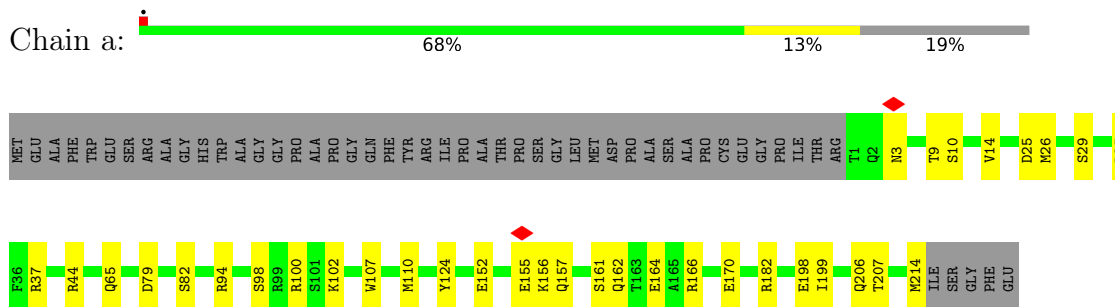
• Molecule 12: Proteasome subunit beta type-7



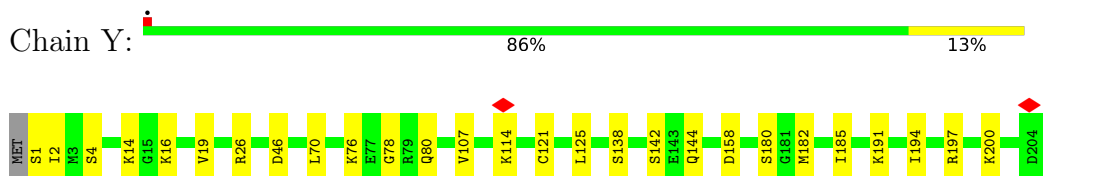
• Molecule 13: Proteasome subunit beta type-4




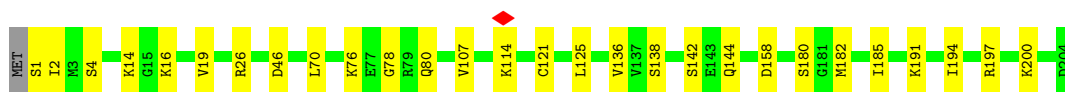
• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-3



## ● Molecule 14: Proteasome subunit beta type-3

Chain U:  86% 14%

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.692	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0343	Depositor
Map size ( $\text{\AA}$ )	292.16095, 292.16095, 292.16095	wwPDB
Map dimensions	254, 254, 254	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.15024, 1.15024, 1.15024	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1L0C

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/1539	0.46	0/2084
1	F	0.28	0/1539	0.46	0/2084
2	P	0.25	0/1821	0.43	0/2466
2	b	0.26	0/1821	0.43	0/2466
3	I	0.25	0/1846	0.44	0/2495
3	N	0.25	0/1846	0.44	0/2495
4	K	0.25	0/1863	0.44	0/2518
4	R	0.25	0/1863	0.44	0/2518
5	T	0.27	0/1602	0.45	0/2167
5	V	0.27	0/1602	0.45	0/2167
6	S	0.27	0/1674	0.45	0/2257
6	X	0.27	0/1674	0.45	0/2257
7	C	0.28	0/1575	0.41	0/2127
7	D	0.27	0/1575	0.41	0/2127
8	J	0.25	0/1875	0.41	0/2524
8	Q	0.25	0/1875	0.41	0/2524
9	G	0.25	0/1870	0.42	0/2528
9	L	0.25	0/1870	0.42	0/2528
10	H	0.24	0/1788	0.42	0/2415
10	M	0.25	0/1788	0.42	0/2415
11	O	0.27	0/1910	0.49	0/2573
11	Z	0.27	0/1910	0.49	0/2573
12	B	0.26	0/1683	0.45	0/2276
12	E	0.26	0/1683	0.45	0/2276
13	W	0.27	0/1704	0.45	0/2306
13	a	0.27	0/1704	0.45	0/2306
14	U	0.27	0/1621	0.46	0/2185
14	Y	0.27	0/1621	0.46	0/2185
All	All	0.26	0/48742	0.44	0/65842

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/204 (98%)	187 (94%)	11 (6%)	1 (0%)	29	54
1	F	199/204 (98%)	187 (94%)	11 (6%)	1 (0%)	29	54
2	P	225/234 (96%)	206 (92%)	16 (7%)	3 (1%)	12	30
2	b	225/234 (96%)	206 (92%)	16 (7%)	3 (1%)	12	30
3	I	230/248 (93%)	217 (94%)	13 (6%)	0	100	100
3	N	230/248 (93%)	217 (94%)	13 (6%)	0	100	100
4	K	232/246 (94%)	215 (93%)	16 (7%)	1 (0%)	34	60
4	R	232/246 (94%)	215 (93%)	16 (7%)	1 (0%)	34	60
5	T	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
5	V	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
6	S	210/240 (88%)	193 (92%)	15 (7%)	2 (1%)	15	37
6	X	210/240 (88%)	193 (92%)	15 (7%)	2 (1%)	15	37
7	C	197/204 (97%)	184 (93%)	13 (7%)	0	100	100
7	D	197/204 (97%)	184 (93%)	13 (7%)	0	100	100
8	J	233/255 (91%)	217 (93%)	16 (7%)	0	100	100
8	Q	233/255 (91%)	218 (94%)	15 (6%)	0	100	100
9	G	232/263 (88%)	215 (93%)	16 (7%)	1 (0%)	34	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	L	232/263 (88%)	215 (93%)	16 (7%)	1 (0%)	34	60
10	H	229/241 (95%)	215 (94%)	14 (6%)	0	100	100
10	M	229/241 (95%)	215 (94%)	14 (6%)	0	100	100
11	O	235/261 (90%)	224 (95%)	10 (4%)	1 (0%)	34	60
11	Z	235/261 (90%)	224 (95%)	10 (4%)	1 (0%)	34	60
12	B	218/234 (93%)	206 (94%)	11 (5%)	1 (0%)	29	54
12	E	218/234 (93%)	206 (94%)	11 (5%)	1 (0%)	29	54
13	W	212/264 (80%)	195 (92%)	16 (8%)	1 (0%)	29	54
13	a	212/264 (80%)	195 (92%)	16 (8%)	1 (0%)	29	54
14	U	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	15	37
14	Y	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	15	37
All	All	6096/6600 (92%)	5677 (93%)	393 (6%)	26 (0%)	38	60

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	40	ALA
2	b	40	ALA
11	O	59	VAL
11	Z	59	VAL
14	Y	78	GLY
14	U	78	GLY
2	P	199	GLU
6	S	191	ASP
2	b	199	GLU
14	Y	46	ASP
14	U	46	ASP
6	X	191	ASP
4	R	212	PRO
4	K	212	PRO
12	B	95	GLY
13	W	107	TRP
12	E	95	GLY
13	a	107	TRP
2	P	54	ILE
2	b	54	ILE
9	L	202	GLU
9	G	202	GLU

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Mol	Chain	Res	Type
6	S	102	PHE
6	X	102	PHE
1	A	191	GLY
1	F	191	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	A	158/161 (98%)	127 (80%)	31 (20%)	1	3
1	F	158/161 (98%)	127 (80%)	31 (20%)	1	3
2	P	188/191 (98%)	143 (76%)	45 (24%)	0	2
2	b	188/191 (98%)	143 (76%)	45 (24%)	0	2
3	I	195/211 (92%)	151 (77%)	44 (23%)	1	2
3	N	195/211 (92%)	151 (77%)	44 (23%)	1	2
4	K	201/210 (96%)	164 (82%)	37 (18%)	1	4
4	R	201/210 (96%)	164 (82%)	37 (18%)	1	4
5	T	166/171 (97%)	147 (89%)	19 (11%)	5	13
5	V	166/171 (97%)	147 (89%)	19 (11%)	5	13
6	S	177/198 (89%)	144 (81%)	33 (19%)	1	4
6	X	177/198 (89%)	144 (81%)	33 (19%)	1	4
7	C	155/160 (97%)	130 (84%)	25 (16%)	2	6
7	D	155/160 (97%)	130 (84%)	25 (16%)	2	6
8	J	192/211 (91%)	155 (81%)	37 (19%)	1	3
8	Q	192/211 (91%)	155 (81%)	37 (19%)	1	3
9	G	200/224 (89%)	155 (78%)	45 (22%)	1	2
9	L	200/224 (89%)	155 (78%)	45 (22%)	1	2
10	H	193/203 (95%)	144 (75%)	49 (25%)	0	1
10	M	193/203 (95%)	144 (75%)	49 (25%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	O	201/221 (91%)	151 (75%)	50 (25%)	0	1
11	Z	201/221 (91%)	151 (75%)	50 (25%)	0	1
12	B	181/195 (93%)	141 (78%)	40 (22%)	1	2
12	E	181/195 (93%)	142 (78%)	39 (22%)	1	3
13	W	176/212 (83%)	142 (81%)	34 (19%)	1	3
13	a	176/212 (83%)	142 (81%)	34 (19%)	1	3
14	U	174/175 (99%)	148 (85%)	26 (15%)	3	7
14	Y	174/175 (99%)	149 (86%)	25 (14%)	3	8
All	All	5114/5486 (93%)	4086 (80%)	1028 (20%)	3	3

All (1028) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	21	THR
1	A	24	SER
1	A	43	CYS
1	A	44	CYS
1	A	46	SER
1	A	68	ILE
1	A	72	GLU
1	A	84	LYS
1	A	86	MET
1	A	95	MET
1	A	106	GLN
1	A	113	SER
1	A	116	MET
1	A	119	MET
1	A	120	MET
1	A	123	GLN
1	A	124	SER
1	A	130	SER
1	A	136	TYR
1	A	145	GLU
1	A	149	LYS
1	A	169	SER
1	A	170	SER
1	A	180	GLN
1	A	182	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	185	GLU
1	A	187	GLN
1	A	190	LEU
1	A	196	LYS
1	A	202	LEU
2	P	6	SER
2	P	8	SER
2	P	37	ILE
2	P	38	LYS
2	P	50	LYS
2	P	51	GLN
2	P	52	LYS
2	P	54	ILE
2	P	56	TYR
2	P	58	GLU
2	P	59	ARG
2	P	61	VAL
2	P	63	LYS
2	P	73	LEU
2	P	74	VAL
2	P	76	SER
2	P	83	ARG
2	P	88	ARG
2	P	91	LYS
2	P	102	GLU
2	P	115	SER
2	P	131	VAL
2	P	132	SER
2	P	136	CYS
2	P	139	ASN
2	P	140	GLU
2	P	142	ARG
2	P	147	GLN
2	P	151	SER
2	P	155	PHE
2	P	162	MET
2	P	168	ASN
2	P	170	LYS
2	P	173	LEU
2	P	175	LYS
2	P	176	ARG
2	P	182	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	184	GLU
2	P	189	THR
2	P	201	GLN
2	P	203	THR
2	P	204	GLU
2	P	214	GLU
2	P	223	THR
2	P	224	GLU
3	N	4	ASP
3	N	5	ARG
3	N	13	ASP
3	N	18	GLN
3	N	23	GLN
3	N	28	LYS
3	N	41	VAL
3	N	52	LYS
3	N	55	ASP
3	N	57	ARG
3	N	58	THR
3	N	82	ILE
3	N	86	ARG
3	N	93	SER
3	N	99	GLU
3	N	100	ASP
3	N	102	VAL
3	N	114	LEU
3	N	121	SER
3	N	124	ARG
3	N	129	ILE
3	N	130	SER
3	N	134	VAL
3	N	139	ASP
3	N	146	GLN
3	N	152	THR
3	N	163	ARG
3	N	167	SER
3	N	169	ARG
3	N	183	THR
3	N	184	ASP
3	N	185	ASP
3	N	193	LYS
3	N	199	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	204	LYS
3	N	207	GLU
3	N	212	ARG
3	N	214	ASP
3	N	215	GLN
3	N	218	LYS
3	N	223	GLU
3	N	226	GLU
3	N	227	LYS
3	N	233	GLU
4	R	6	SER
4	R	11	ARG
4	R	34	GLN
4	R	45	LYS
4	R	55	LYS
4	R	56	VAL
4	R	58	ASP
4	R	59	LYS
4	R	61	LEU
4	R	73	THR
4	R	74	GLU
4	R	93	ARG
4	R	108	GLU
4	R	127	GLN
4	R	131	MET
4	R	153	LYS
4	R	166	THR
4	R	173	THR
4	R	174	GLU
4	R	175	SER
4	R	178	PHE
4	R	182	LYS
4	R	184	LYS
4	R	196	GLU
4	R	200	THR
4	R	205	VAL
4	R	209	ASP
4	R	211	LYS
4	R	214	GLU
4	R	215	ILE
4	R	216	GLU
4	R	223	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	R	226	LYS
4	R	231	THR
4	R	234	GLU
4	R	236	ASP
4	R	242	LEU
5	T	1	MET
5	T	8	GLN
5	T	13	VAL
5	T	19	ARG
5	T	23	SER
5	T	26	VAL
5	T	29	LYS
5	T	40	GLU
5	T	46	CYS
5	T	49	GLU
5	T	85	ARG
5	T	86	ARG
5	T	94	SER
5	T	96	THR
5	T	143	LEU
5	T	145	ARG
5	T	161	ARG
5	T	169	LYS
5	T	171	PHE
6	S	11	THR
6	S	18	GLU
6	S	21	SER
6	S	30	SER
6	S	31	GLU
6	S	34	SER
6	S	42	LYS
6	S	48	ASP
6	S	49	LYS
6	S	52	ILE
6	S	54	CYS
6	S	55	SER
6	S	65	THR
6	S	73	LYS
6	S	81	LYS
6	S	93	SER
6	S	99	ARG
6	S	115	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	S	118	LYS
6	S	123	SER
6	S	125	ASP
6	S	127	VAL
6	S	133	ASP
6	S	136	LYS
6	S	146	GLN
6	S	148	LEU
6	S	159	GLN
6	S	162	GLU
6	S	166	LEU
6	S	170	ARG
6	S	195	ILE
6	S	208	VAL
6	S	211	ARG
7	D	7	LYS
7	D	8	PHE
7	D	29	GLN
7	D	35	ILE
7	D	41	LEU
7	D	42	LEU
7	D	44	THR
7	D	56	GLU
7	D	58	LEU
7	D	61	ARG
7	D	65	ILE
7	D	80	SER
7	D	82	LEU
7	D	91	LYS
7	D	102	CYS
7	D	106	LYS
7	D	107	ARG
7	D	121	ILE
7	D	127	SER
7	D	146	ASP
7	D	154	ASP
7	D	176	LEU
7	D	180	ARG
7	D	190	ASP
7	D	194	ASP
8	J	17	ASP
8	J	28	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	J	34	SER
8	J	37	ILE
8	J	51	LYS
8	J	53	VAL
8	J	56	LYS
8	J	64	LYS
8	J	66	LEU
8	J	67	PHE
8	J	68	ASN
8	J	69	VAL
8	J	80	LEU
8	J	81	LEU
8	J	90	ILE
8	J	96	SER
8	J	114	ARG
8	J	157	SER
8	J	167	LYS
8	J	169	ARG
8	J	170	GLN
8	J	181	MET
8	J	185	THR
8	J	186	CYS
8	J	191	LYS
8	J	193	VAL
8	J	202	ASP
8	J	204	VAL
8	J	207	LYS
8	J	209	PHE
8	J	214	SER
8	J	215	TRP
8	J	219	LEU
8	J	226	ILE
8	J	230	ASP
8	J	237	LYS
8	J	238	TYR
4	K	6	SER
4	K	11	ARG
4	K	34	GLN
4	K	45	LYS
4	K	55	LYS
4	K	56	VAL
4	K	58	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	K	59	LYS
4	K	61	LEU
4	K	73	THR
4	K	74	GLU
4	K	93	ARG
4	K	108	GLU
4	K	127	GLN
4	K	131	MET
4	K	153	LYS
4	K	166	THR
4	K	173	THR
4	K	174	GLU
4	K	175	SER
4	K	178	PHE
4	K	182	LYS
4	K	184	LYS
4	K	196	GLU
4	K	200	THR
4	K	205	VAL
4	K	209	ASP
4	K	211	LYS
4	K	214	GLU
4	K	215	ILE
4	K	216	GLU
4	K	223	GLU
4	K	226	LYS
4	K	231	THR
4	K	234	GLU
4	K	236	ASP
4	K	242	LEU
5	V	1	MET
5	V	8	GLN
5	V	13	VAL
5	V	19	ARG
5	V	23	SER
5	V	26	VAL
5	V	29	LYS
5	V	40	GLU
5	V	46	CYS
5	V	49	GLU
5	V	85	ARG
5	V	86	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	V	94	SER
5	V	96	THR
5	V	143	LEU
5	V	145	ARG
5	V	161	ARG
5	V	169	LYS
5	V	171	PHE
2	b	6	SER
2	b	8	SER
2	b	37	ILE
2	b	38	LYS
2	b	50	LYS
2	b	51	GLN
2	b	52	LYS
2	b	54	ILE
2	b	56	TYR
2	b	58	GLU
2	b	59	ARG
2	b	61	VAL
2	b	63	LYS
2	b	73	LEU
2	b	74	VAL
2	b	76	SER
2	b	83	ARG
2	b	88	ARG
2	b	91	LYS
2	b	102	GLU
2	b	115	SER
2	b	131	VAL
2	b	132	SER
2	b	136	CYS
2	b	139	ASN
2	b	140	GLU
2	b	142	ARG
2	b	147	GLN
2	b	151	SER
2	b	155	PHE
2	b	162	MET
2	b	168	ASN
2	b	170	LYS
2	b	173	LEU
2	b	175	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	b	176	ARG
2	b	182	GLU
2	b	184	GLU
2	b	189	THR
2	b	201	GLN
2	b	203	THR
2	b	204	GLU
2	b	214	GLU
2	b	223	THR
2	b	224	GLU
9	L	4	ASN
9	L	5	GLN
9	L	22	ILE
9	L	23	GLU
9	L	29	VAL
9	L	30	LYS
9	L	38	LEU
9	L	39	LYS
9	L	41	LYS
9	L	51	ARG
9	L	53	GLN
9	L	54	SER
9	L	60	GLN
9	L	73	SER
9	L	74	ILE
9	L	78	THR
9	L	101	ARG
9	L	106	SER
9	L	108	LEU
9	L	110	SER
9	L	125	ARG
9	L	146	GLN
9	L	148	CYS
9	L	156	CYS
9	L	157	ARG
9	L	164	ARG
9	L	173	GLU
9	L	174	ARG
9	L	181	GLU
9	L	182	CYS
9	L	183	ASN
9	L	190	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	L	202	GLU
9	L	206	THR
9	L	208	LYS
9	L	211	SER
9	L	214	ILE
9	L	217	LYS
9	L	219	LEU
9	L	222	THR
9	L	225	ASP
9	L	226	ASP
9	L	228	ASP
9	L	233	LEU
9	L	236	LEU
10	H	10	ARG
10	H	40	ILE
10	H	43	SER
10	H	47	CYS
10	H	50	VAL
10	H	54	ILE
10	H	62	SER
10	H	64	ILE
10	H	65	GLU
10	H	69	GLU
10	H	78	MET
10	H	84	ASP
10	H	89	ILE
10	H	90	ASP
10	H	91	LYS
10	H	95	GLU
10	H	97	GLN
10	H	111	SER
10	H	114	GLN
10	H	117	SER
10	H	119	LEU
10	H	129	ASP
10	H	133	MET
10	H	139	VAL
10	H	147	ASP
10	H	148	GLU
10	H	149	LYS
10	H	152	GLN
10	H	159	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	H	163	VAL
10	H	164	GLN
10	H	165	CYS
10	H	170	ILE
10	H	172	SER
10	H	174	SER
10	H	183	GLU
10	H	190	THR
10	H	192	LYS
10	H	197	SER
10	H	198	SER
10	H	207	GLU
10	H	208	GLU
10	H	209	LYS
10	H	217	LEU
10	H	228	MET
10	H	236	GLU
10	H	237	VAL
10	H	238	ILE
10	H	239	LYS
7	C	7	LYS
7	C	8	PHE
7	C	29	GLN
7	C	35	ILE
7	C	41	LEU
7	C	42	LEU
7	C	44	THR
7	C	56	GLU
7	C	58	LEU
7	C	61	ARG
7	C	65	ILE
7	C	80	SER
7	C	82	LEU
7	C	91	LYS
7	C	102	CYS
7	C	106	LYS
7	C	107	ARG
7	C	121	ILE
7	C	127	SER
7	C	146	ASP
7	C	154	ASP
7	C	176	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	C	180	ARG
7	C	190	ASP
7	C	194	ASP
11	O	3	ARG
11	O	7	SER
11	O	11	ILE
11	O	17	ARG
11	O	26	GLU
11	O	35	LEU
11	O	38	LEU
11	O	41	ASP
11	O	48	GLU
11	O	50	ARG
11	O	52	ILE
11	O	58	GLU
11	O	59	VAL
11	O	61	PHE
11	O	63	GLU
11	O	64	LYS
11	O	70	GLU
11	O	71	ASP
11	O	72	MET
11	O	80	THR
11	O	81	SER
11	O	95	GLN
11	O	119	GLN
11	O	127	LYS
11	O	132	VAL
11	O	133	SER
11	O	136	TYR
11	O	150	SER
11	O	155	ASN
11	O	160	LYS
11	O	174	MET
11	O	176	LYS
11	O	180	LYS
11	O	183	GLU
11	O	184	MET
11	O	186	LEU
11	O	187	LYS
11	O	192	LEU
11	O	195	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	O	200	THR
11	O	206	LEU
11	O	222	LYS
11	O	226	ARG
11	O	228	LEU
11	O	230	GLN
11	O	234	GLU
11	O	237	ILE
11	O	239	LYS
11	O	241	GLU
11	O	243	GLU
3	I	4	ASP
3	I	5	ARG
3	I	13	ASP
3	I	18	GLN
3	I	23	GLN
3	I	28	LYS
3	I	41	VAL
3	I	52	LYS
3	I	55	ASP
3	I	57	ARG
3	I	58	THR
3	I	82	ILE
3	I	86	ARG
3	I	93	SER
3	I	99	GLU
3	I	100	ASP
3	I	102	VAL
3	I	114	LEU
3	I	121	SER
3	I	124	ARG
3	I	129	ILE
3	I	130	SER
3	I	134	VAL
3	I	139	ASP
3	I	146	GLN
3	I	152	THR
3	I	163	ARG
3	I	167	SER
3	I	169	ARG
3	I	183	THR
3	I	184	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	I	185	ASP
3	I	193	LYS
3	I	199	VAL
3	I	204	LYS
3	I	207	GLU
3	I	212	ARG
3	I	214	ASP
3	I	215	GLN
3	I	218	LYS
3	I	223	GLU
3	I	226	GLU
3	I	227	LYS
3	I	233	GLU
12	B	9	LYS
12	B	19	ARG
12	B	29	LYS
12	B	32	SER
12	B	36	PHE
12	B	40	ASN
12	B	54	MET
12	B	59	ILE
12	B	63	LEU
12	B	64	GLU
12	B	65	LEU
12	B	77	VAL
12	B	84	LYS
12	B	94	ILE
12	B	98	LEU
12	B	105	VAL
12	B	106	THR
12	B	118	SER
12	B	131	SER
12	B	132	LEU
12	B	146	MET
12	B	147	GLU
12	B	148	GLU
12	B	154	LEU
12	B	156	SER
12	B	179	SER
12	B	180	LYS
12	B	182	LYS
12	B	184	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	B	186	LEU
12	B	187	ARG
12	B	194	LYS
12	B	197	THR
12	B	198	ARG
12	B	199	LEU
12	B	201	ARG
12	B	204	CYS
12	B	206	LYS
12	B	213	THR
12	B	214	GLU
10	M	10	ARG
10	M	40	ILE
10	M	43	SER
10	M	47	CYS
10	M	50	VAL
10	M	54	ILE
10	M	62	SER
10	M	64	ILE
10	M	65	GLU
10	M	69	GLU
10	M	78	MET
10	M	84	ASP
10	M	89	ILE
10	M	90	ASP
10	M	91	LYS
10	M	95	GLU
10	M	97	GLN
10	M	111	SER
10	M	114	GLN
10	M	117	SER
10	M	119	LEU
10	M	129	ASP
10	M	133	MET
10	M	139	VAL
10	M	147	ASP
10	M	148	GLU
10	M	149	LYS
10	M	152	GLN
10	M	159	SER
10	M	163	VAL
10	M	164	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	M	165	CYS
10	M	170	ILE
10	M	172	SER
10	M	174	SER
10	M	183	GLU
10	M	190	THR
10	M	192	LYS
10	M	197	SER
10	M	198	SER
10	M	207	GLU
10	M	208	GLU
10	M	209	LYS
10	M	217	LEU
10	M	228	MET
10	M	236	GLU
10	M	237	VAL
10	M	238	ILE
10	M	239	LYS
13	W	3	ASN
13	W	9	THR
13	W	10	SER
13	W	14	VAL
13	W	25	ASP
13	W	26	MET
13	W	29	SER
13	W	35	ARG
13	W	37	ARG
13	W	44	ARG
13	W	65	GLN
13	W	79	ASP
13	W	82	SER
13	W	94	ARG
13	W	98	SER
13	W	100	ARG
13	W	102	LYS
13	W	110	MET
13	W	124	TYR
13	W	152	GLU
13	W	155	GLU
13	W	156	LYS
13	W	157	GLN
13	W	161	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	W	162	GLN
13	W	164	GLU
13	W	166	ARG
13	W	170	GLU
13	W	182	ARG
13	W	198	GLU
13	W	199	ILE
13	W	206	GLN
13	W	207	THR
13	W	214	MET
12	E	9	LYS
12	E	19	ARG
12	E	29	LYS
12	E	32	SER
12	E	36	PHE
12	E	40	ASN
12	E	54	MET
12	E	59	ILE
12	E	63	LEU
12	E	64	GLU
12	E	65	LEU
12	E	77	VAL
12	E	84	LYS
12	E	94	ILE
12	E	98	LEU
12	E	105	VAL
12	E	106	THR
12	E	118	SER
12	E	131	SER
12	E	132	LEU
12	E	146	MET
12	E	147	GLU
12	E	148	GLU
12	E	156	SER
12	E	179	SER
12	E	180	LYS
12	E	182	LYS
12	E	184	ASP
12	E	186	LEU
12	E	187	ARG
12	E	194	LYS
12	E	197	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	E	198	ARG
12	E	199	LEU
12	E	201	ARG
12	E	204	CYS
12	E	206	LYS
12	E	213	THR
12	E	214	GLU
9	G	4	ASN
9	G	5	GLN
9	G	22	ILE
9	G	23	GLU
9	G	29	VAL
9	G	30	LYS
9	G	38	LEU
9	G	39	LYS
9	G	41	LYS
9	G	51	ARG
9	G	53	GLN
9	G	54	SER
9	G	60	GLN
9	G	73	SER
9	G	74	ILE
9	G	78	THR
9	G	101	ARG
9	G	106	SER
9	G	108	LEU
9	G	110	SER
9	G	125	ARG
9	G	146	GLN
9	G	148	CYS
9	G	156	CYS
9	G	157	ARG
9	G	164	ARG
9	G	173	GLU
9	G	174	ARG
9	G	181	GLU
9	G	182	CYS
9	G	183	ASN
9	G	190	HIS
9	G	202	GLU
9	G	206	THR
9	G	208	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	G	211	SER
9	G	214	ILE
9	G	217	LYS
9	G	219	LEU
9	G	222	THR
9	G	225	ASP
9	G	226	ASP
9	G	228	ASP
9	G	233	LEU
9	G	236	LEU
8	Q	17	ASP
8	Q	28	LYS
8	Q	34	SER
8	Q	37	ILE
8	Q	51	LYS
8	Q	53	VAL
8	Q	56	LYS
8	Q	64	LYS
8	Q	66	LEU
8	Q	67	PHE
8	Q	68	ASN
8	Q	69	VAL
8	Q	80	LEU
8	Q	81	LEU
8	Q	90	ILE
8	Q	96	SER
8	Q	114	ARG
8	Q	157	SER
8	Q	167	LYS
8	Q	169	ARG
8	Q	170	GLN
8	Q	181	MET
8	Q	185	THR
8	Q	186	CYS
8	Q	191	LYS
8	Q	193	VAL
8	Q	202	ASP
8	Q	204	VAL
8	Q	207	LYS
8	Q	209	PHE
8	Q	214	SER
8	Q	215	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	Q	219	LEU
8	Q	226	ILE
8	Q	230	ASP
8	Q	237	LYS
8	Q	238	TYR
13	a	3	ASN
13	a	9	THR
13	a	10	SER
13	a	14	VAL
13	a	25	ASP
13	a	26	MET
13	a	29	SER
13	a	35	ARG
13	a	37	ARG
13	a	44	ARG
13	a	65	GLN
13	a	79	ASP
13	a	82	SER
13	a	94	ARG
13	a	98	SER
13	a	100	ARG
13	a	102	LYS
13	a	110	MET
13	a	124	TYR
13	a	152	GLU
13	a	155	GLU
13	a	156	LYS
13	a	157	GLN
13	a	161	SER
13	a	162	GLN
13	a	164	GLU
13	a	166	ARG
13	a	170	GLU
13	a	182	ARG
13	a	198	GLU
13	a	199	ILE
13	a	206	GLN
13	a	207	THR
13	a	214	MET
1	F	19	ARG
1	F	21	THR
1	F	24	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	43	CYS
1	F	44	CYS
1	F	46	SER
1	F	68	ILE
1	F	72	GLU
1	F	84	LYS
1	F	86	MET
1	F	95	MET
1	F	106	GLN
1	F	113	SER
1	F	116	MET
1	F	119	MET
1	F	120	MET
1	F	123	GLN
1	F	124	SER
1	F	130	SER
1	F	136	TYR
1	F	145	GLU
1	F	149	LYS
1	F	169	SER
1	F	170	SER
1	F	180	GLN
1	F	182	SER
1	F	185	GLU
1	F	187	GLN
1	F	190	LEU
1	F	196	LYS
1	F	202	LEU
11	Z	3	ARG
11	Z	7	SER
11	Z	11	ILE
11	Z	17	ARG
11	Z	26	GLU
11	Z	35	LEU
11	Z	38	LEU
11	Z	41	ASP
11	Z	48	GLU
11	Z	50	ARG
11	Z	52	ILE
11	Z	58	GLU
11	Z	59	VAL
11	Z	61	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	Z	63	GLU
11	Z	64	LYS
11	Z	70	GLU
11	Z	71	ASP
11	Z	72	MET
11	Z	80	THR
11	Z	81	SER
11	Z	95	GLN
11	Z	119	GLN
11	Z	127	LYS
11	Z	132	VAL
11	Z	133	SER
11	Z	136	TYR
11	Z	150	SER
11	Z	155	ASN
11	Z	160	LYS
11	Z	174	MET
11	Z	176	LYS
11	Z	180	LYS
11	Z	183	GLU
11	Z	184	MET
11	Z	186	LEU
11	Z	187	LYS
11	Z	192	LEU
11	Z	195	LYS
11	Z	200	THR
11	Z	206	LEU
11	Z	222	LYS
11	Z	226	ARG
11	Z	228	LEU
11	Z	230	GLN
11	Z	234	GLU
11	Z	237	ILE
11	Z	239	LYS
11	Z	241	GLU
11	Z	243	GLU
14	Y	1	SER
14	Y	2	ILE
14	Y	4	SER
14	Y	14	LYS
14	Y	16	LYS
14	Y	19	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	Y	26	ARG
14	Y	70	LEU
14	Y	76	LYS
14	Y	80	GLN
14	Y	107	VAL
14	Y	114	LYS
14	Y	121	CYS
14	Y	125	LEU
14	Y	138	SER
14	Y	142	SER
14	Y	144	GLN
14	Y	158	ASP
14	Y	180	SER
14	Y	182	MET
14	Y	185	ILE
14	Y	191	LYS
14	Y	194	ILE
14	Y	197	ARG
14	Y	200	LYS
14	U	1	SER
14	U	2	ILE
14	U	4	SER
14	U	14	LYS
14	U	16	LYS
14	U	19	VAL
14	U	26	ARG
14	U	70	LEU
14	U	76	LYS
14	U	80	GLN
14	U	107	VAL
14	U	114	LYS
14	U	121	CYS
14	U	125	LEU
14	U	136	VAL
14	U	138	SER
14	U	142	SER
14	U	144	GLN
14	U	158	ASP
14	U	180	SER
14	U	182	MET
14	U	185	ILE
14	U	191	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	U	194	ILE
14	U	197	ARG
14	U	200	LYS
6	X	11	THR
6	X	18	GLU
6	X	21	SER
6	X	30	SER
6	X	31	GLU
6	X	34	SER
6	X	42	LYS
6	X	48	ASP
6	X	49	LYS
6	X	52	ILE
6	X	54	CYS
6	X	55	SER
6	X	65	THR
6	X	73	LYS
6	X	81	LYS
6	X	93	SER
6	X	99	ARG
6	X	115	GLU
6	X	118	LYS
6	X	123	SER
6	X	125	ASP
6	X	127	VAL
6	X	133	ASP
6	X	136	LYS
6	X	146	GLN
6	X	148	LEU
6	X	159	GLN
6	X	162	GLU
6	X	166	LEU
6	X	170	ARG
6	X	195	ILE
6	X	208	VAL
6	X	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	77	HIS
1	A	180	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	187	GLN
2	P	111	GLN
2	P	188	HIS
3	N	23	GLN
3	N	92	GLN
3	N	146	GLN
3	N	159	ASN
4	R	34	GLN
4	R	127	GLN
4	R	150	GLN
4	R	224	ASN
5	T	55	GLN
5	T	71	ASN
5	T	132	HIS
6	S	8	ASN
6	S	131	GLN
6	S	146	GLN
6	S	159	GLN
6	S	163	HIS
7	D	89	GLN
7	D	162	GLN
7	D	175	ASN
7	D	178	HIS
8	J	22	GLN
8	J	170	GLN
4	K	34	GLN
4	K	127	GLN
4	K	150	GLN
4	K	224	ASN
5	V	55	GLN
5	V	71	ASN
5	V	132	HIS
2	b	111	GLN
2	b	139	ASN
2	b	188	HIS
9	L	5	GLN
9	L	53	GLN
9	L	60	GLN
9	L	146	GLN
9	L	183	ASN
9	L	203	GLN
10	H	152	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	H	227	HIS
7	C	38	ASN
7	C	89	GLN
7	C	162	GLN
7	C	175	ASN
7	C	178	HIS
11	O	40	ASN
11	O	95	GLN
11	O	230	GLN
3	I	23	GLN
3	I	92	GLN
3	I	146	GLN
3	I	159	ASN
12	B	40	ASN
10	M	152	GLN
10	M	227	HIS
13	W	104	ASN
13	W	147	GLN
13	W	188	GLN
13	W	206	GLN
12	E	40	ASN
9	G	5	GLN
9	G	53	GLN
9	G	60	GLN
9	G	146	GLN
9	G	183	ASN
9	G	203	GLN
8	Q	22	GLN
8	Q	170	GLN
13	a	81	HIS
13	a	104	ASN
13	a	147	GLN
13	a	188	GLN
13	a	206	GLN
1	F	77	HIS
1	F	180	GLN
1	F	187	GLN
11	Z	40	ASN
11	Z	95	GLN
11	Z	230	GLN
14	Y	6	ASN
14	Y	64	GLN

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Mol	Chain	Res	Type
14	Y	144	GLN
14	Y	161	HIS
14	U	6	ASN
14	U	64	GLN
14	U	144	GLN
14	U	161	HIS
6	X	8	ASN
6	X	131	GLN
6	X	146	GLN
6	X	159	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	A1L0C	F	301	1	21,30,30	0.67	1 (4%)	21,42,42	1.54	2 (9%)
15	A1L0C	C	301	7	21,30,30	0.68	0	21,42,42	1.57	2 (9%)
15	A1L0C	A	301	1	21,30,30	0.67	1 (4%)	21,42,42	1.54	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	A1L0C	D	301	7	21,30,30	0.67	0	21,42,42	1.57	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1L0C	F	301	1	-	4/10/41/41	0/2/2/2
15	A1L0C	C	301	7	-	2/10/41/41	0/2/2/2
15	A1L0C	A	301	1	-	4/10/41/41	0/2/2/2
15	A1L0C	D	301	7	-	2/10/41/41	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	301	A1L0C	N3-N2	-2.04	1.30	1.34
15	A	301	A1L0C	N3-N2	-2.02	1.30	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	301	A1L0C	C2-N1-C9	6.23	131.00	125.48
15	D	301	A1L0C	C2-N1-C9	6.18	130.96	125.48
15	A	301	A1L0C	C2-N1-C9	5.99	130.79	125.48
15	F	301	A1L0C	C2-N1-C9	5.98	130.78	125.48
15	F	301	A1L0C	O-C-CA	-2.64	117.85	124.78
15	A	301	A1L0C	O-C-CA	-2.63	117.87	124.78
15	D	301	A1L0C	O-C-CA	-2.56	118.06	124.78
15	C	301	A1L0C	O-C-CA	-2.55	118.10	124.78

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	301	A1L0C	O3-C3-N4-C4
15	A	301	A1L0C	O-C-CA-CB
15	D	301	A1L0C	O-C-CA-CB
15	C	301	A1L0C	O-C-CA-CB
15	F	301	A1L0C	O3-C3-N4-C4

*Continued on next page...*



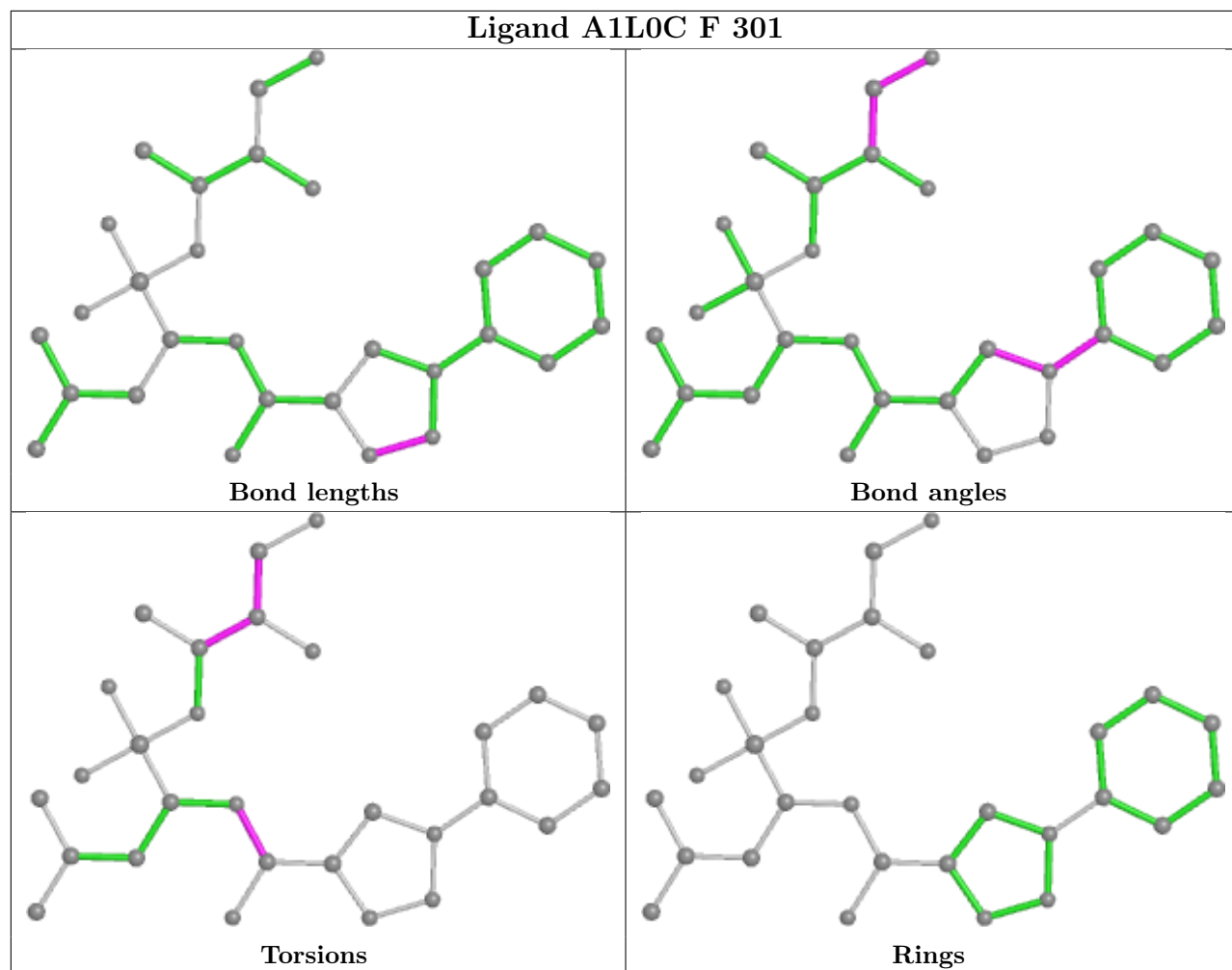
*Continued from previous page...*

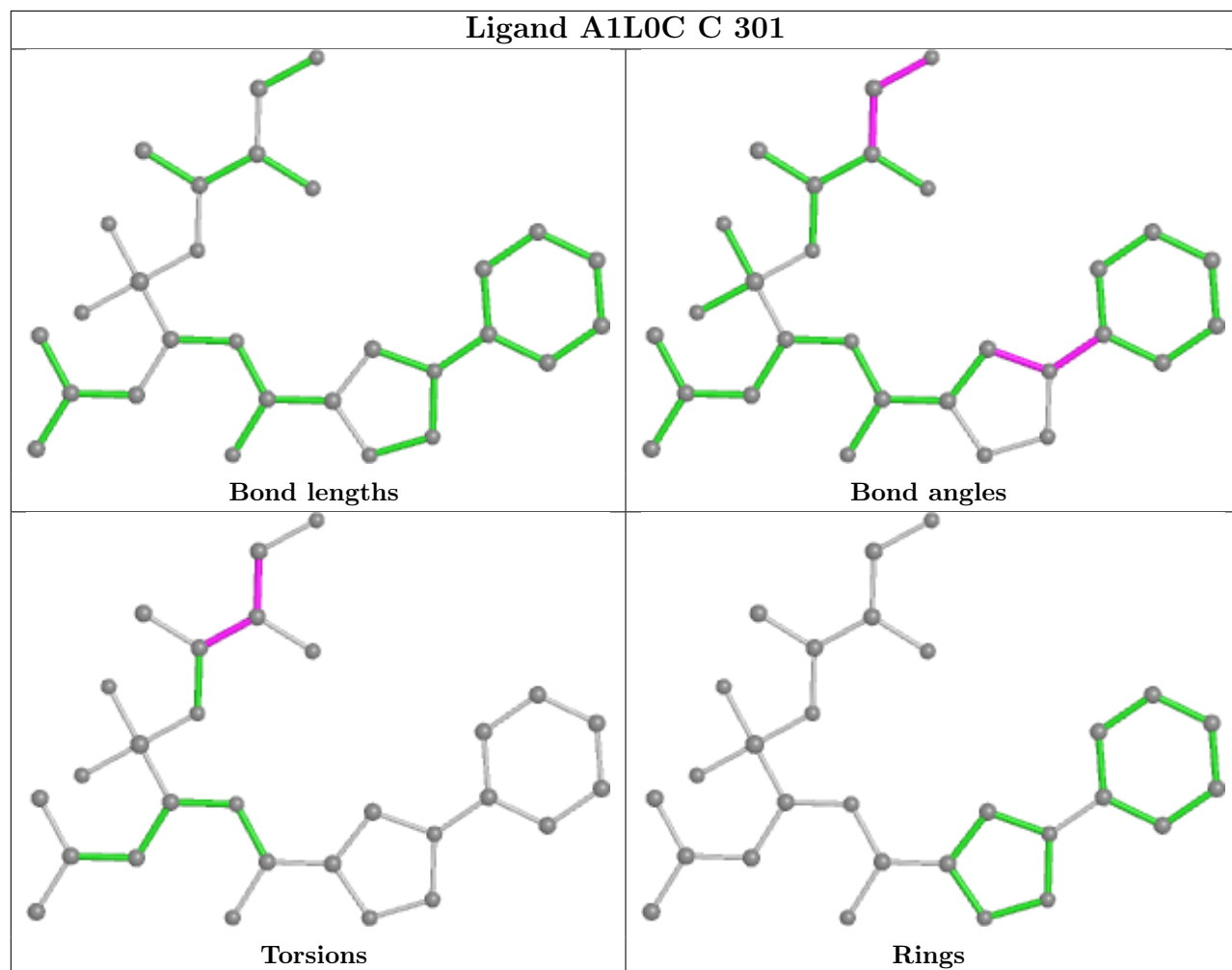
Mol	Chain	Res	Type	Atoms
15	F	301	A1L0C	O-C-CA-CB
15	A	301	A1L0C	C-CA-CB-CG2
15	D	301	A1L0C	C-CA-CB-CG2
15	C	301	A1L0C	C-CA-CB-CG2
15	F	301	A1L0C	C-CA-CB-CG2
15	A	301	A1L0C	C1-C3-N4-C4
15	F	301	A1L0C	C1-C3-N4-C4

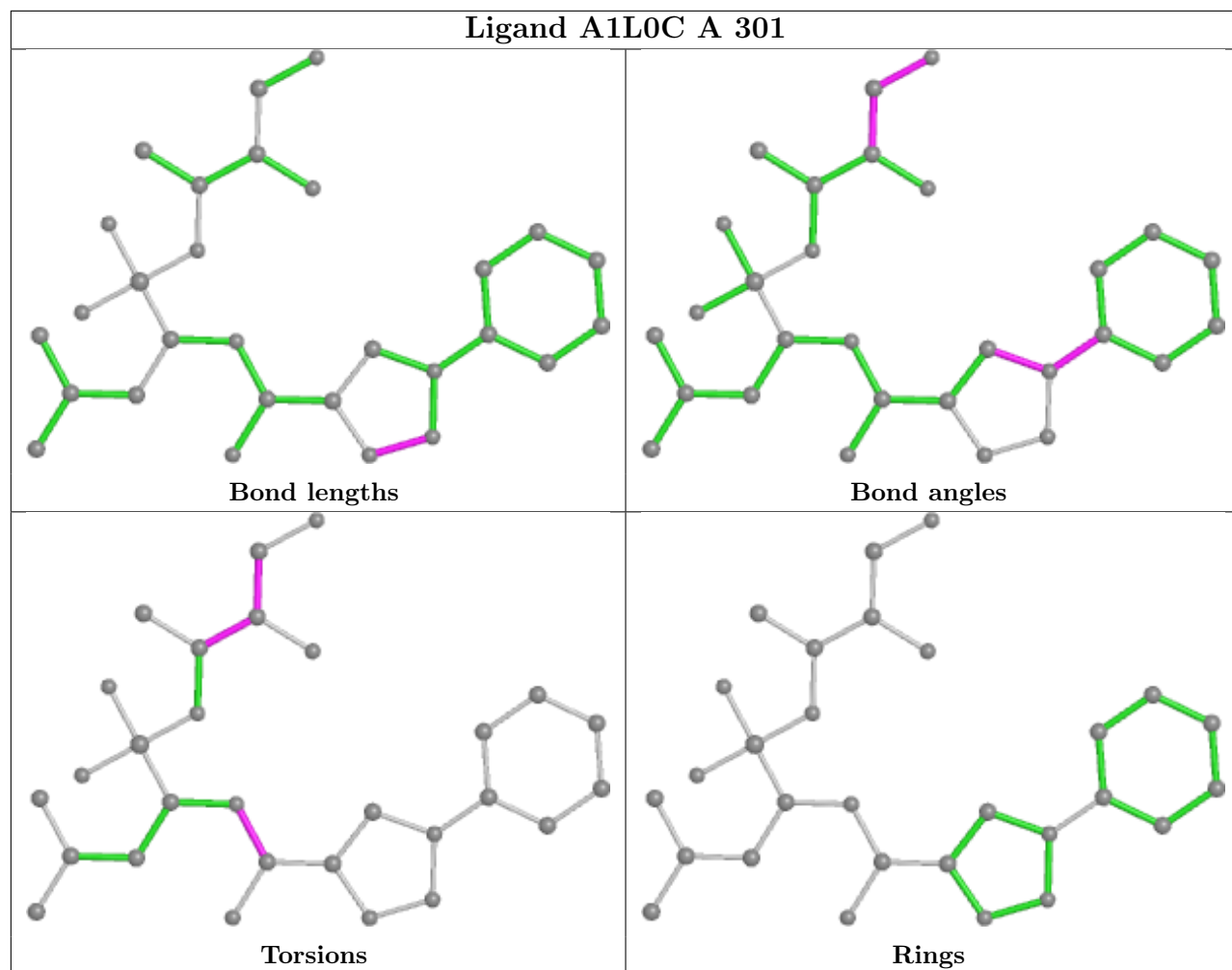
There are no ring outliers.

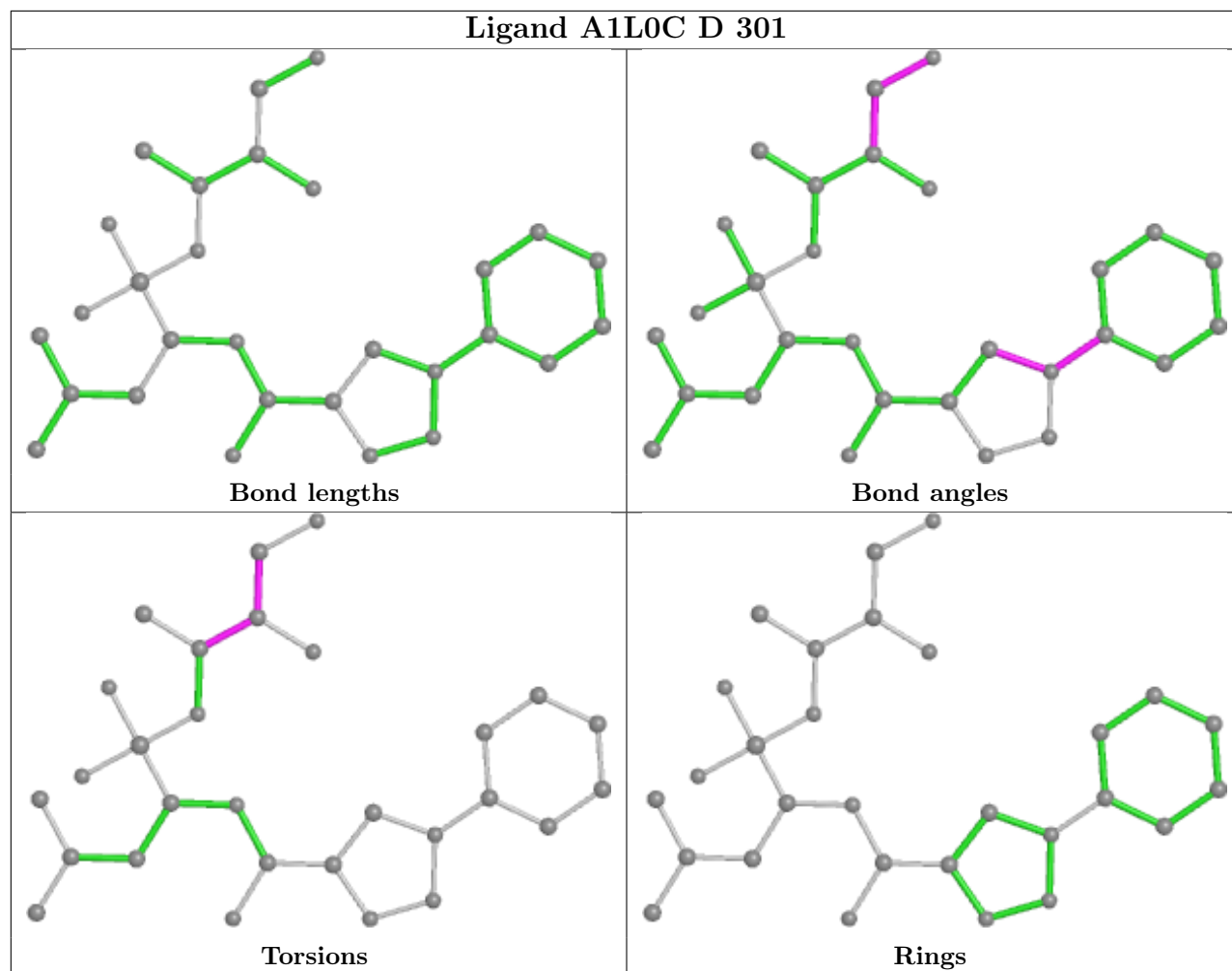
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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.

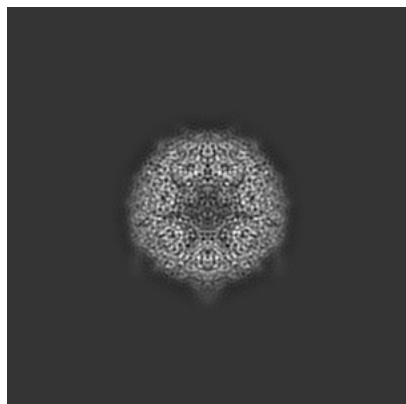
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39482. These allow visual inspection of the internal detail of the map and identification of artifacts.

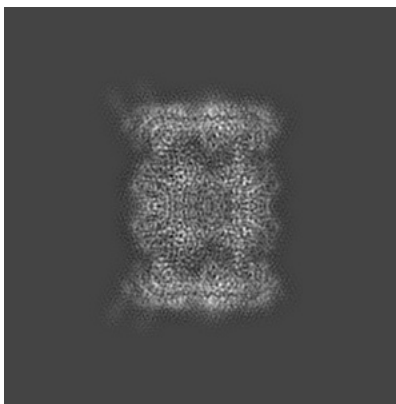
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

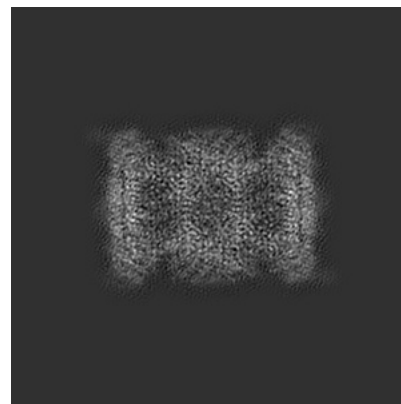
#### 6.1.1 Primary map



X

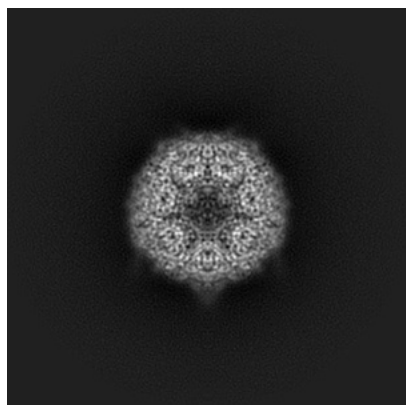


Y

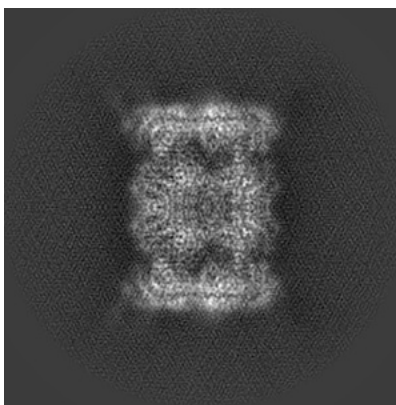


Z

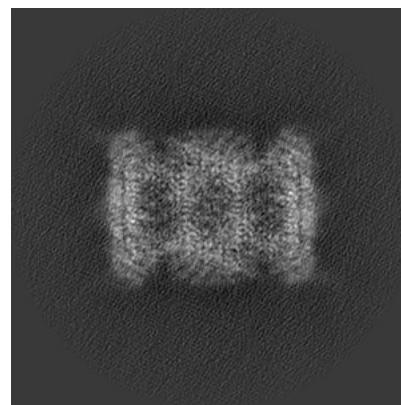
#### 6.1.2 Raw map



X



Y

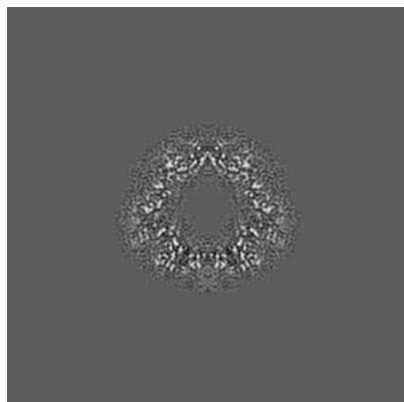


Z

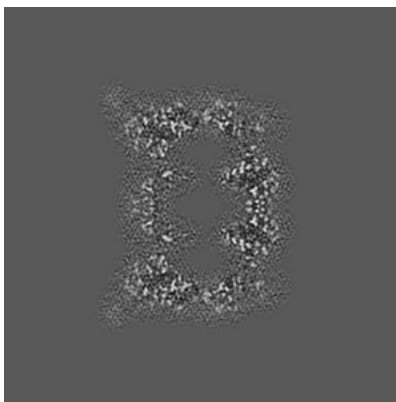
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

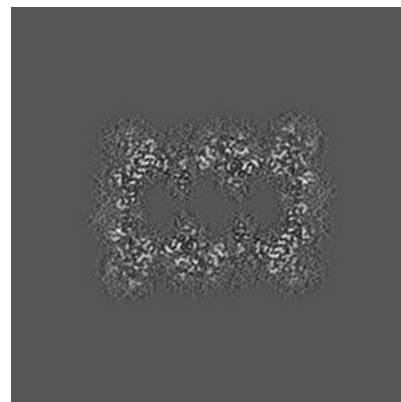
### 6.2.1 Primary map



X Index: 127

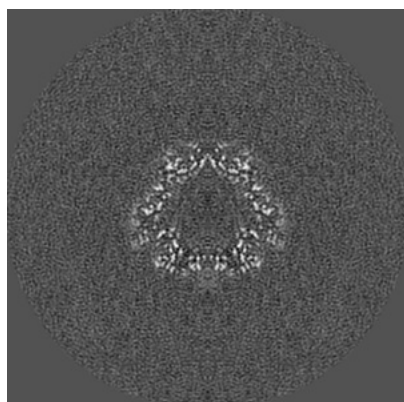


Y Index: 127

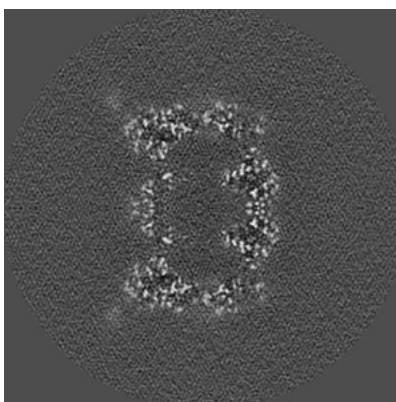


Z Index: 127

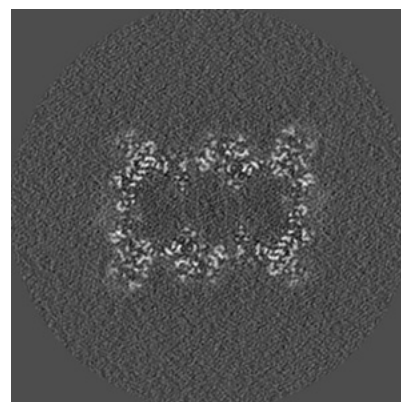
### 6.2.2 Raw map



X Index: 127



Y Index: 127

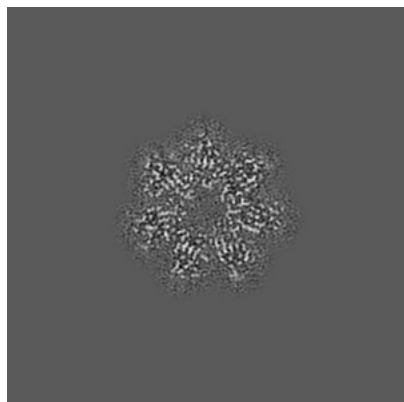


Z Index: 127

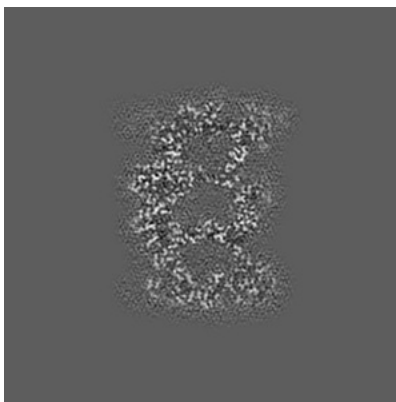
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

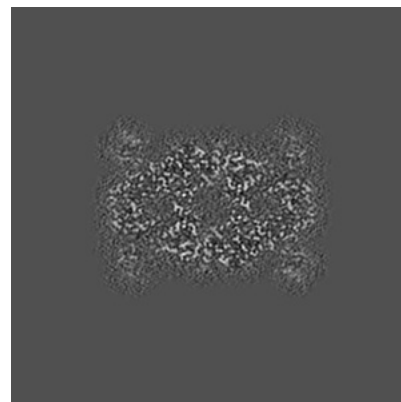
### 6.3.1 Primary map



X Index: 143

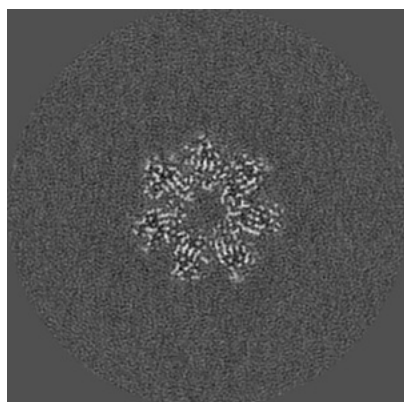


Y Index: 110

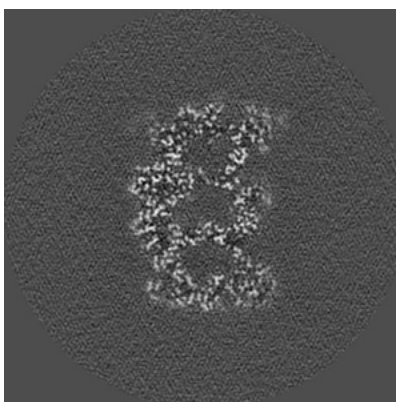


Z Index: 146

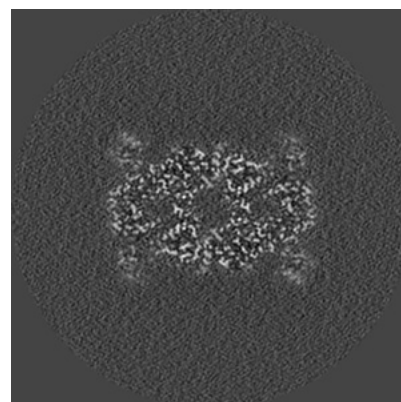
### 6.3.2 Raw map



X Index: 143



Y Index: 110



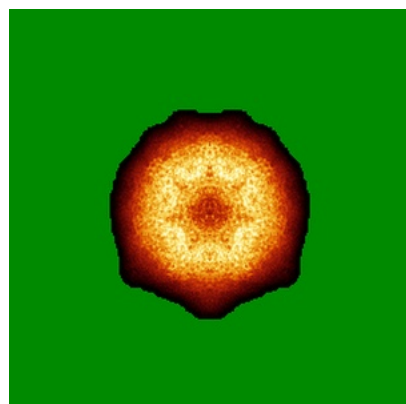
Z Index: 146

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

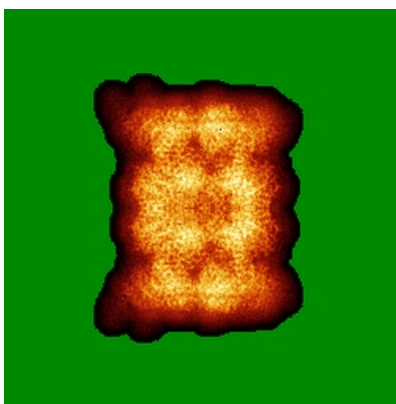


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

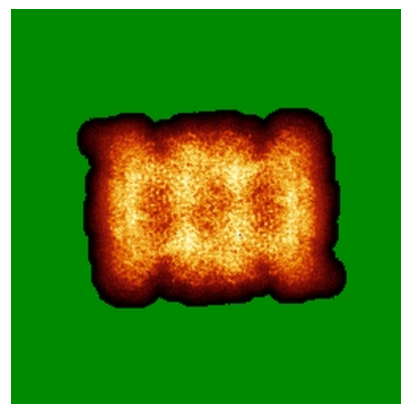
### 6.4.1 Primary map



X

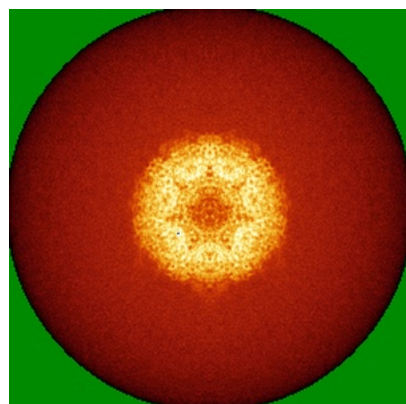


Y

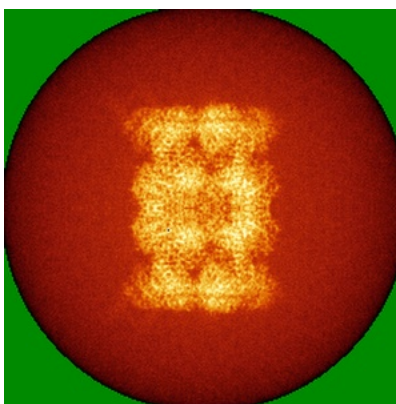


Z

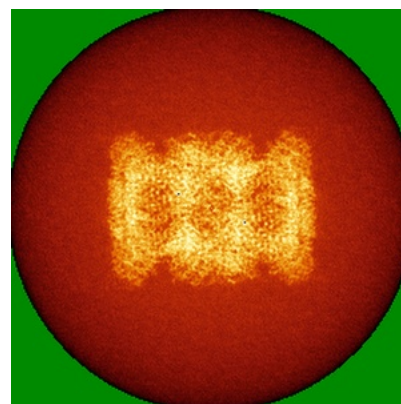
### 6.4.2 Raw map



X



Y

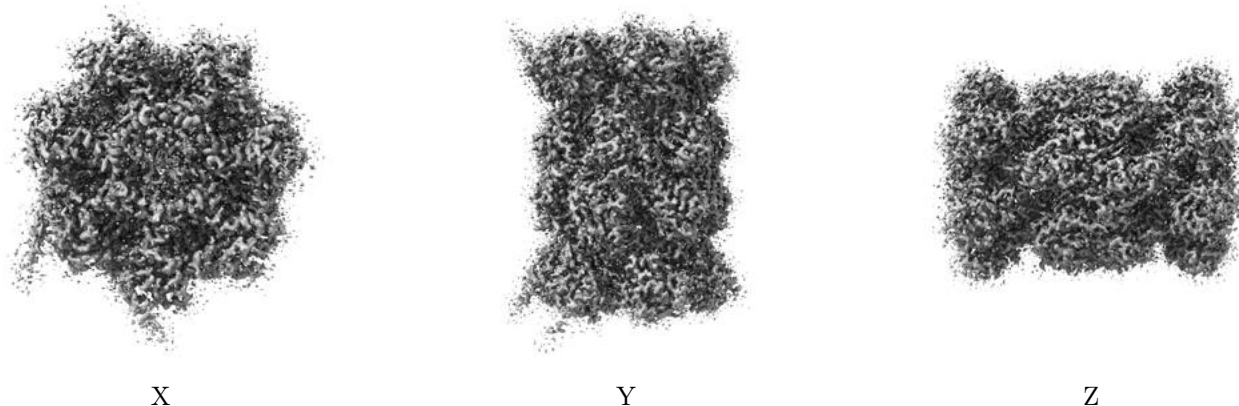


Z

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

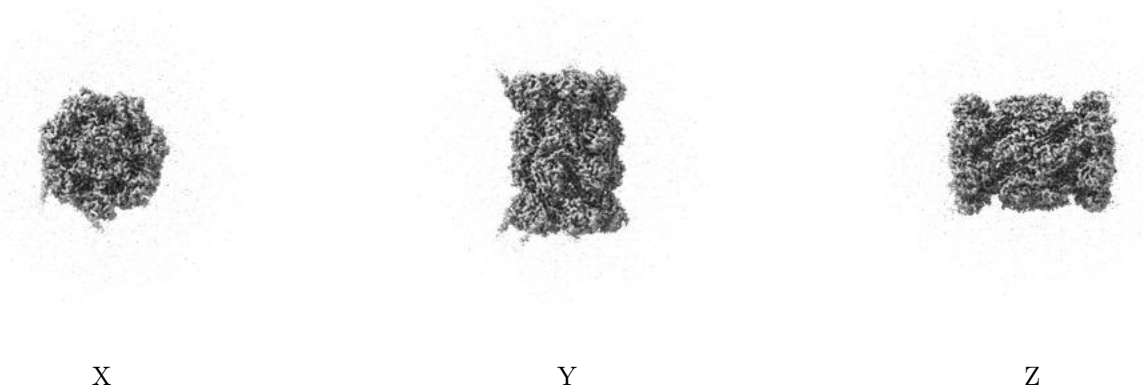
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0343. 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.

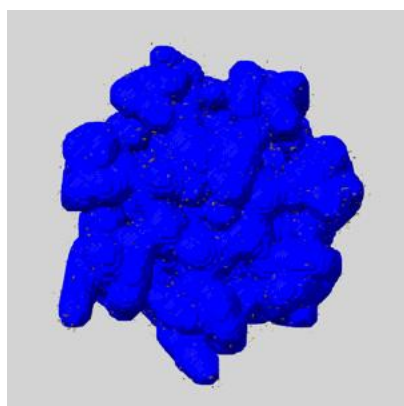
## 6.6 Mask visualisation [i](#)

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

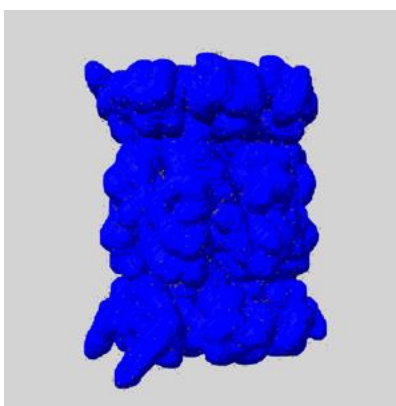
A mask typically either:

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

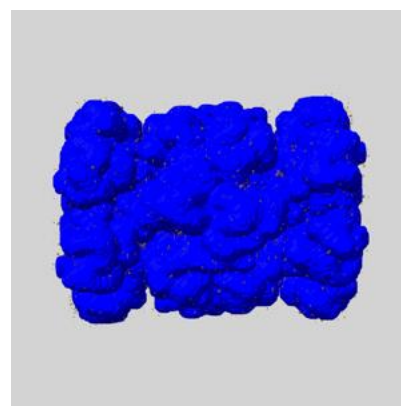
### 6.6.1 emd\_39482\_msk\_1.map [i](#)



X



Y

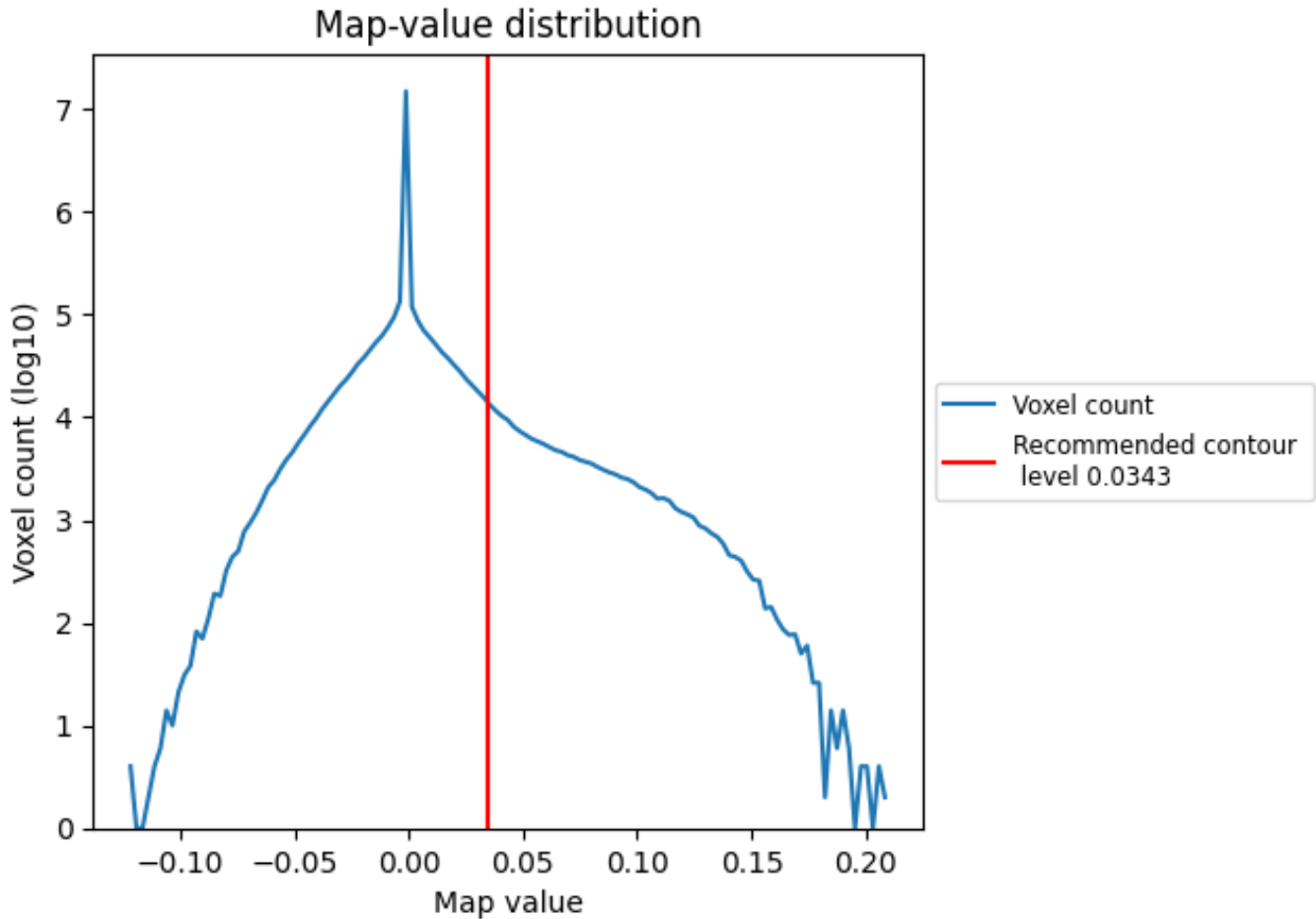


Z

## 7 Map analysis [i](#)

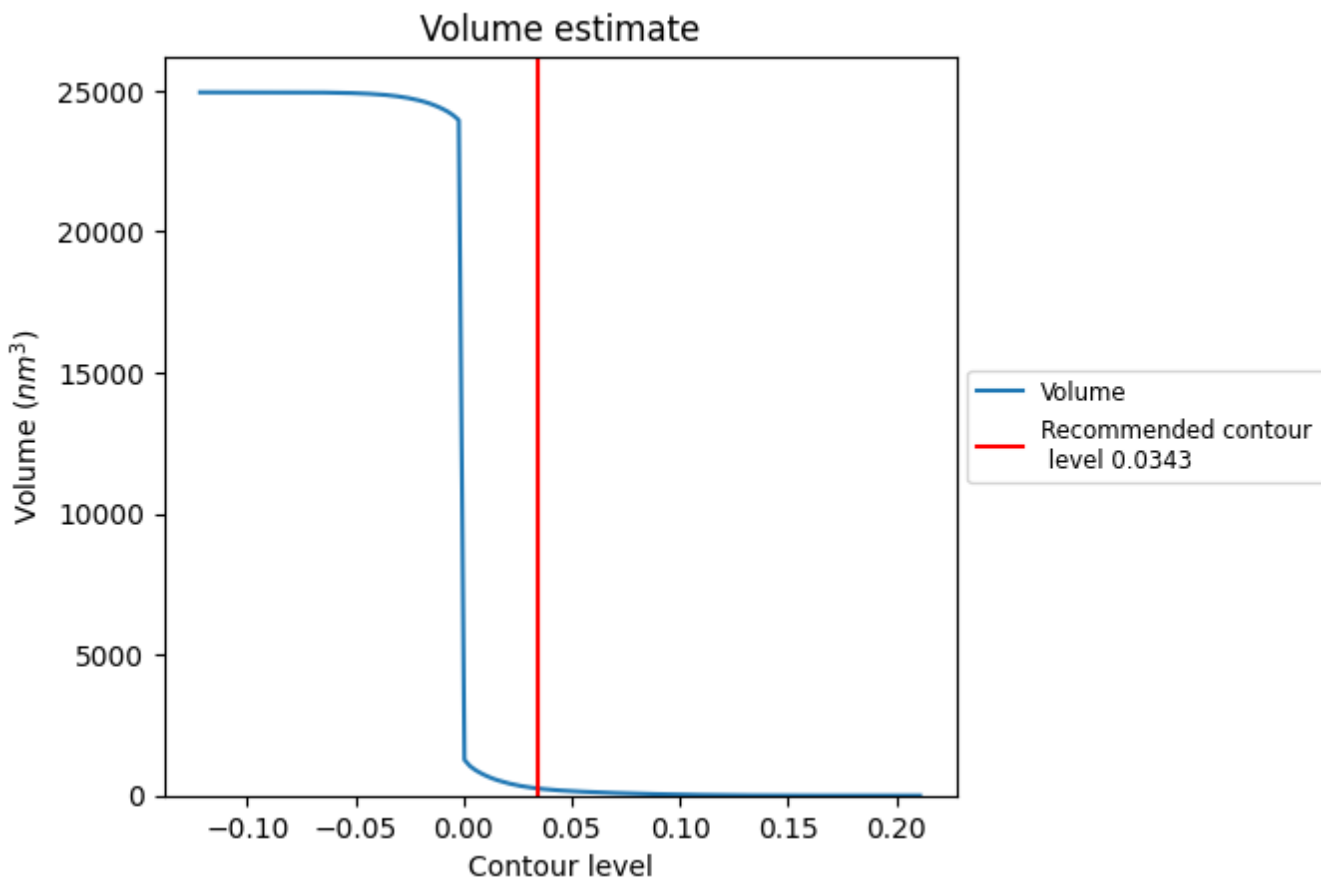
This section contains the results of statistical analysis of the map.

### 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.

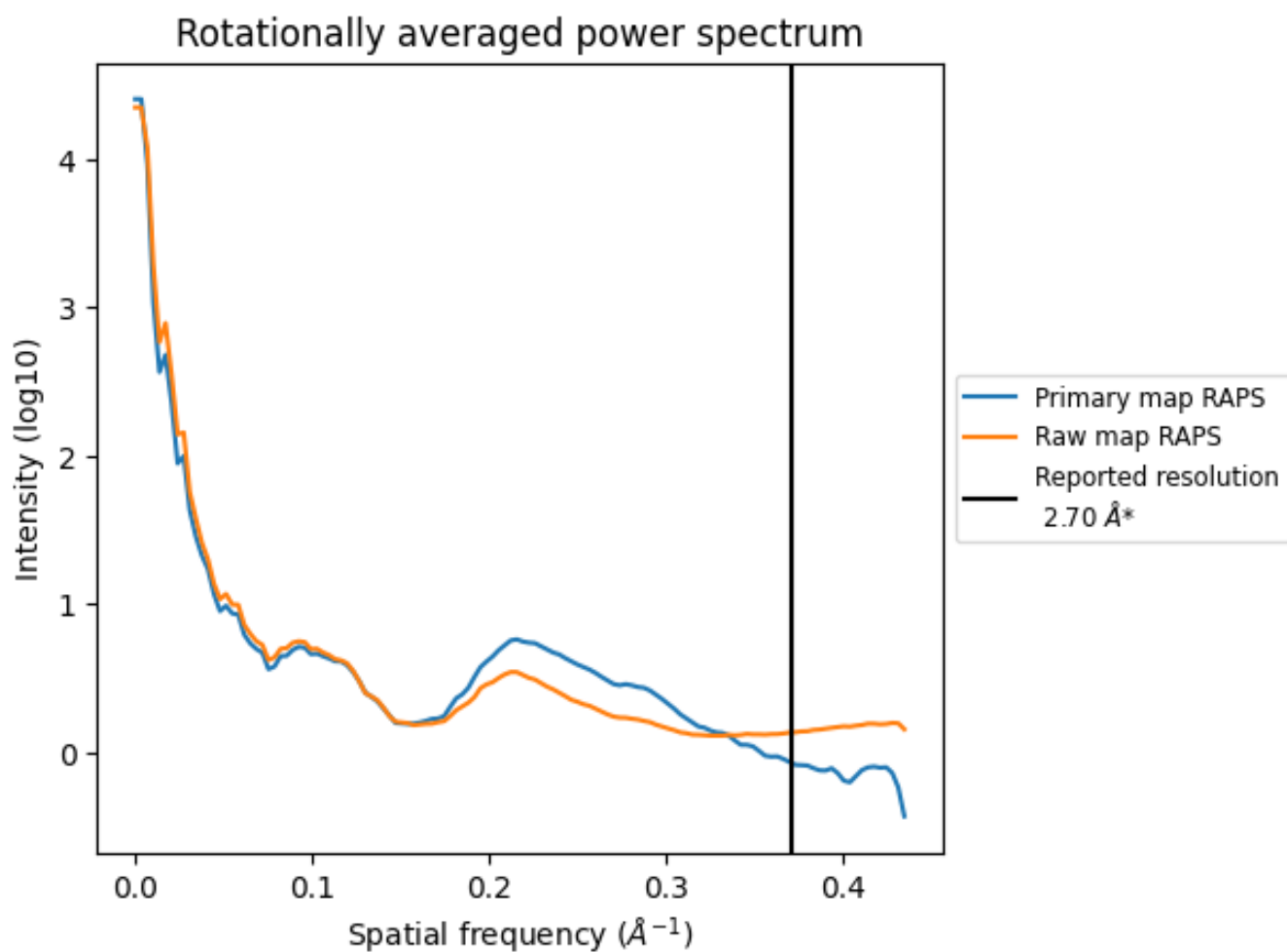
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 254 nm<sup>3</sup>; this corresponds to an approximate mass of 229 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

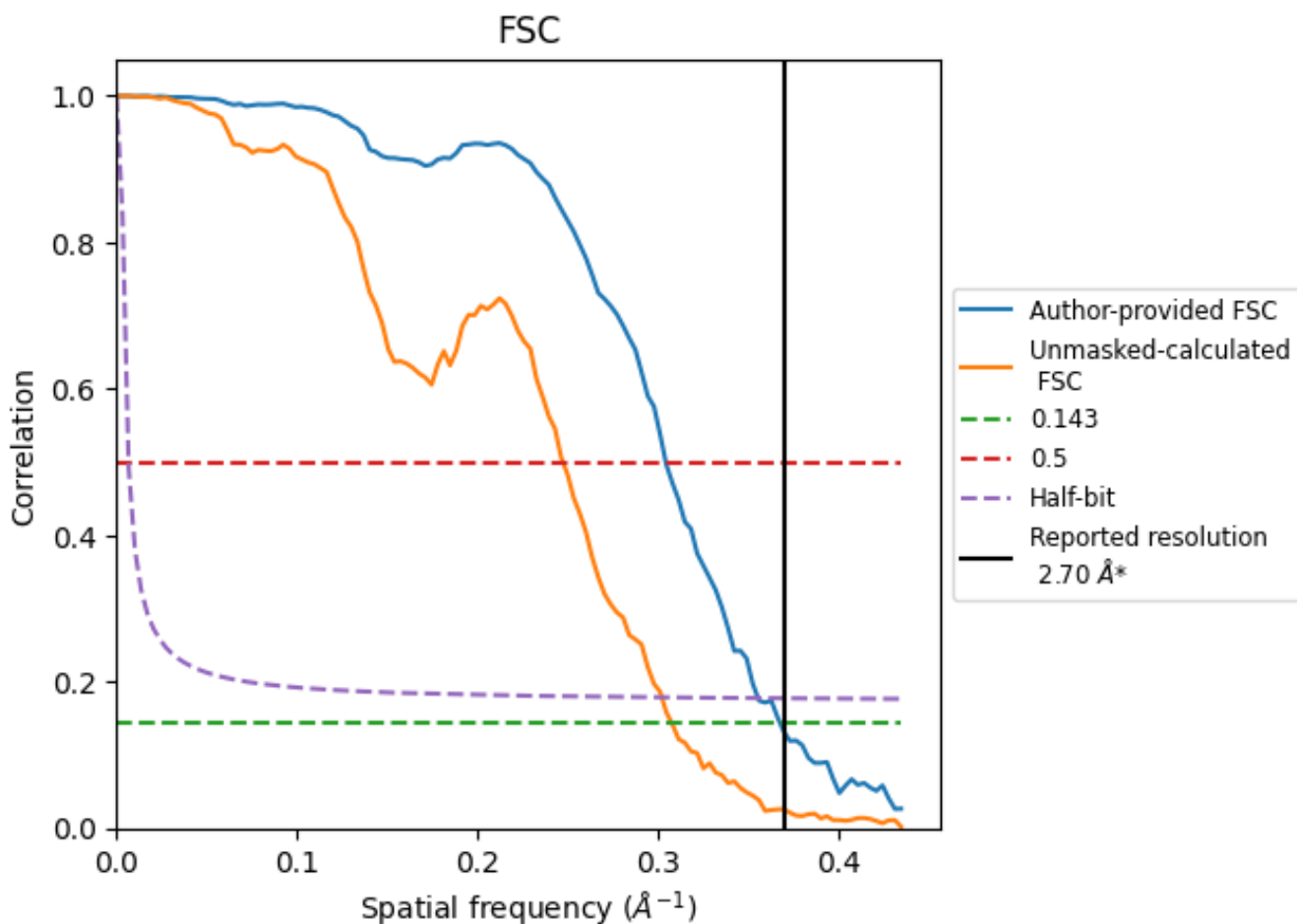


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.29	2.81
Unmasked-calculated*	3.25	4.04	3.31

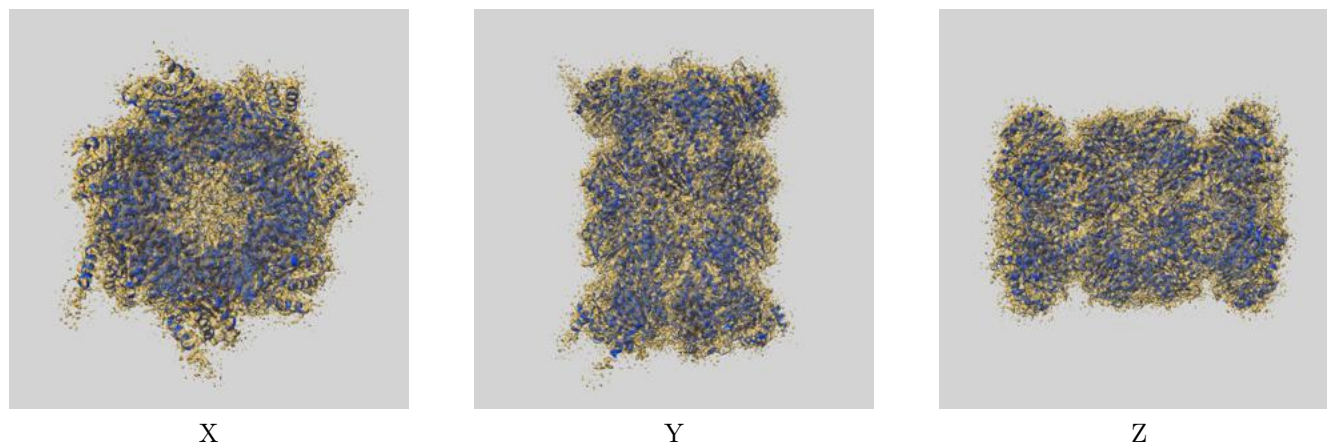
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.7 by more than 10 %



## 9 Map-model fit [i](#)

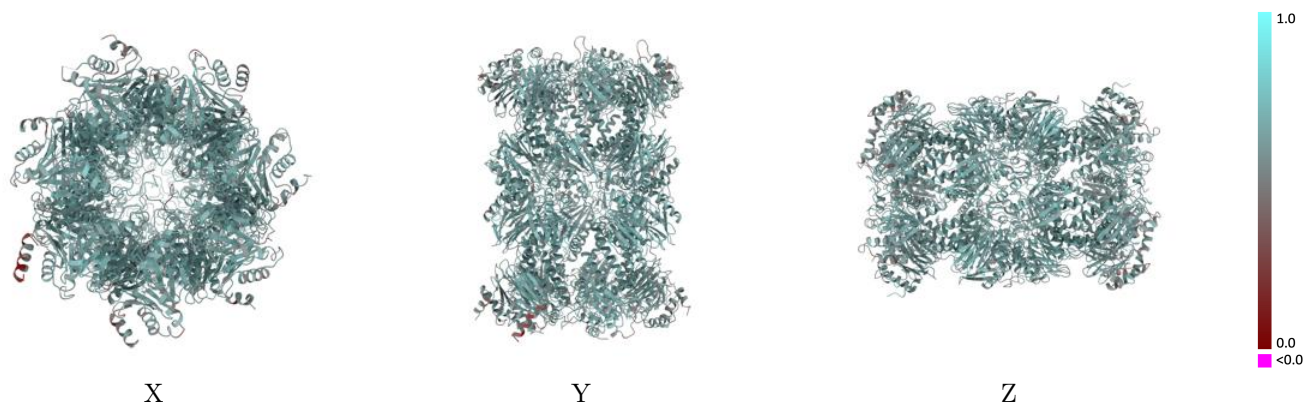
This section contains information regarding the fit between EMDB map EMD-39482 and PDB model 8YPK. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



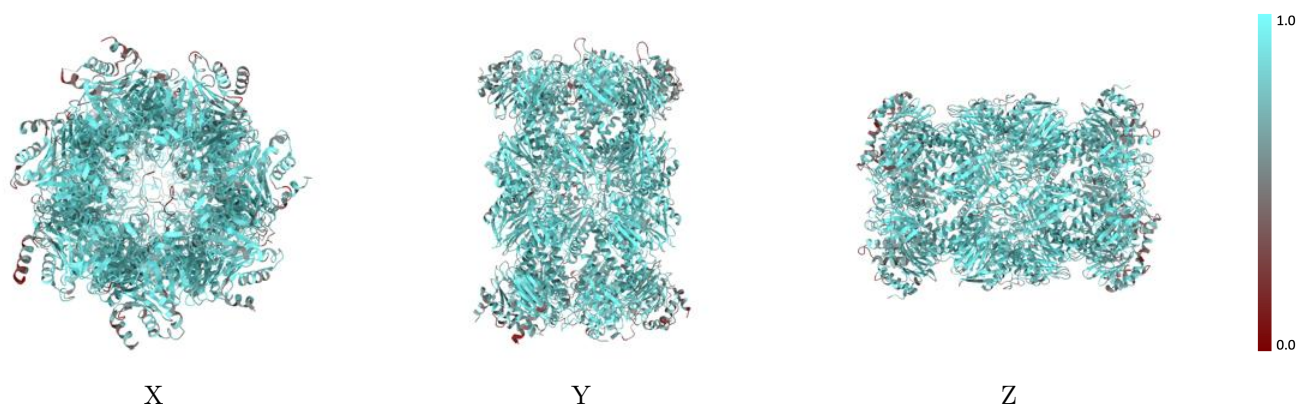
The images above show the 3D surface view of the map at the recommended contour level 0.0343 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



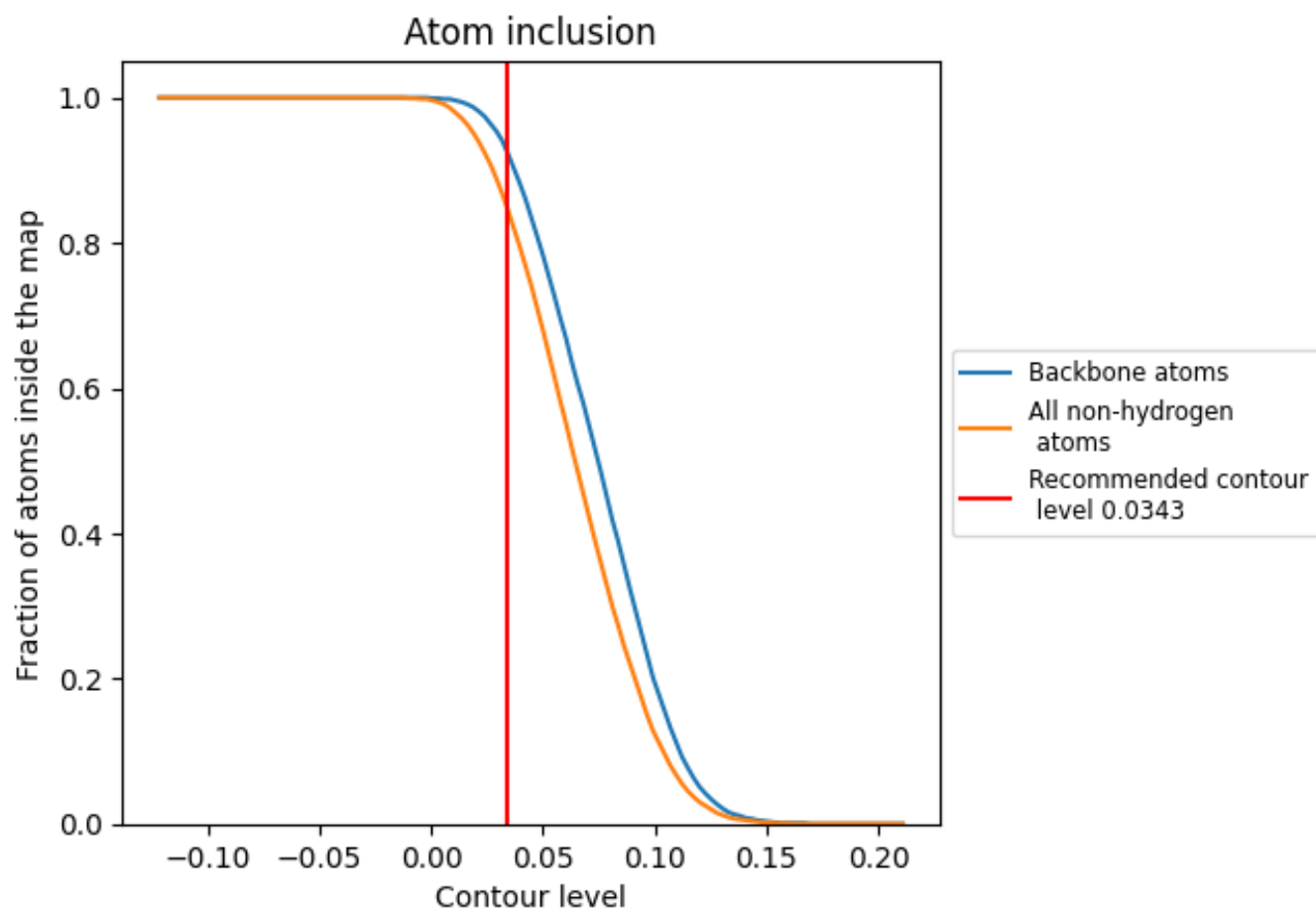
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0343).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.0343) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.6210
A	 0.8910	 0.6400
B	 0.8720	 0.6390
C	 0.9050	 0.6460
D	 0.9020	 0.6460
E	 0.8710	 0.6390
F	 0.8910	 0.6400
G	 0.8200	 0.6090
H	 0.8050	 0.6050
I	 0.8080	 0.5970
J	 0.7800	 0.5980
K	 0.7760	 0.6020
L	 0.8210	 0.6110
M	 0.8070	 0.6050
N	 0.8100	 0.5990
O	 0.8000	 0.5930
P	 0.8220	 0.6100
Q	 0.7840	 0.5990
R	 0.7730	 0.6010
S	 0.8770	 0.6350
T	 0.9100	 0.6490
U	 0.9080	 0.6500
V	 0.9090	 0.6480
W	 0.9010	 0.6440
X	 0.8750	 0.6340
Y	 0.9090	 0.6490
Z	 0.8000	 0.5910
a	 0.8980	 0.6440
b	 0.8240	 0.6100

