



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 07:25 AM JST

PDB ID : 7W3B
EMDB ID : EMD-32276
Title : Structure of USP14-bound human 26S proteasome in substrate-engaged state
ED5_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary 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:

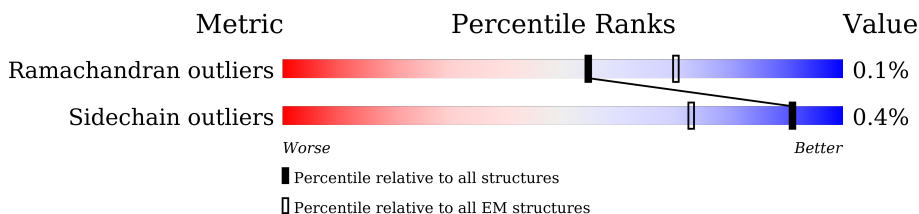
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.60 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 ≥ 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	433	
2	B	440	
3	C	398	
4	D	418	
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	


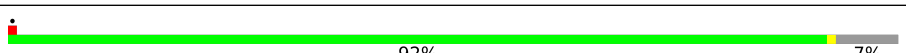
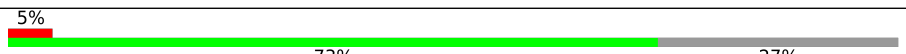
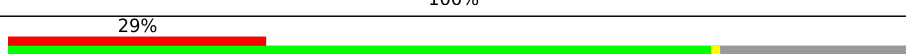
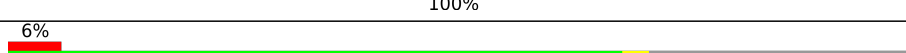
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	h	234	99%
9	I	261	95%
9	i	261	95%
10	J	248	96%
10	j	248	95%
11	K	241	98%
11	k	241	97%
12	L	269	88%
12	l	269	88%
13	M	255	95%
13	m	255	94%
14	N	239	85%
14	n	239	85%
15	O	277	79%
15	o	277	79%
16	P	205	100%
16	p	205	100%
17	Q	201	99%
17	q	201	99%
18	R	263	76%
18	r	263	76%
19	S	241	88%
19	s	241	88%
20	T	264	82%
20	t	264	81%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	U	953	 86% 13%
22	V	534	 83% 17%
23	W	456	 15% 96%
24	X	422	 5% 90% 10%
25	Y	389	 96%
26	Z	324	 88% 12%
27	a	376	 98%
28	b	377	 50% 49%
29	c	310	 92% 7%
30	d	350	 5% 73% 27%
31	f	908	 19% 97%
32	v	28	 11% 100%
33	x	494	 29% 79% 21%
34	y	76	 74% 100%
35	e	70	 6% 69% 29%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 109441 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 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	413	3229	2034	566	611	18	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	399	3122	1967	529	611	15	0	0

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	396	3105	1954	558	576	17	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	389	3097	1947	552	581	17	0	0

- Molecule 6 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	395	3098	1951	533	596	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1861	1166	327	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	238	Total	C	N	O	S	0	0
			1813	1139	302	361	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1549	977	270	293	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1650	1044	283	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	827	Total	C	N	O	S	0	0
			6459	4101	1097	1217	44		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	446	3635	2302	622	687	24	0	0

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	380	3009	1918	509	570	12	0	0

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	378	3115	1987	533	578	17	0	0

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	286	2281	1457	392	427	5	0	0

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	373	2995	1911	510	559	15	0	0

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	191	1458	910	261	279	8	0	0

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	287	2260	1430	389	422	19	0	0

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 32 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	v	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	392	Total	C	N	O	S	0	0
			3144	1985	523	616	20		

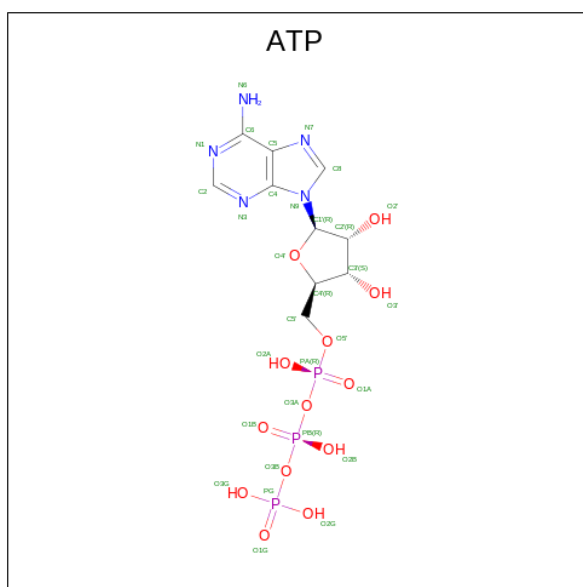
- Molecule 34 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	y	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 35 is a protein called 26S proteasome complex subunit DSS1.

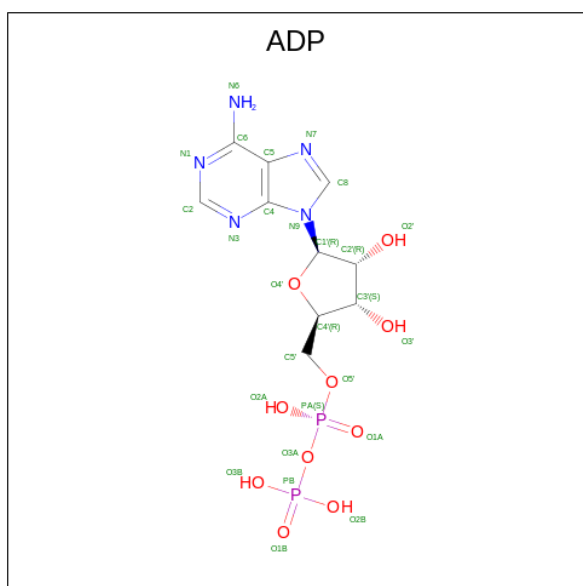
Mol	Chain	Residues	Atoms				AltConf	Trace
35	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	F	1	27	10	5	10	2	0

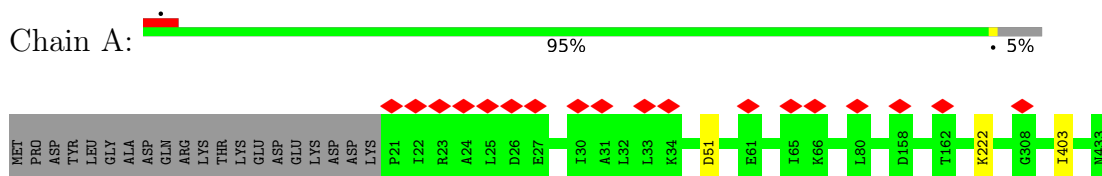
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
38	c	1	1	1	0

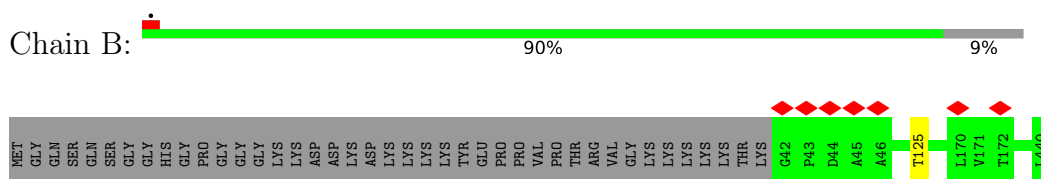
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

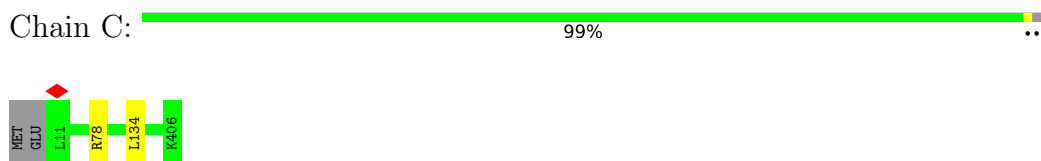
- Molecule 1: 26S protease regulatory subunit 7



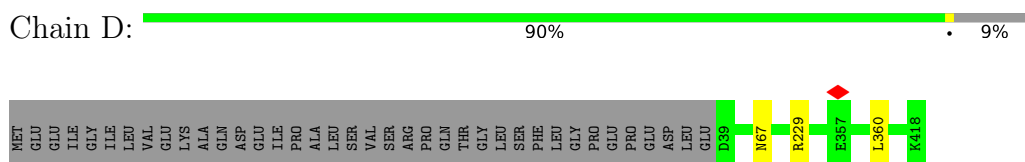
- Molecule 2: 26S protease regulatory subunit 4



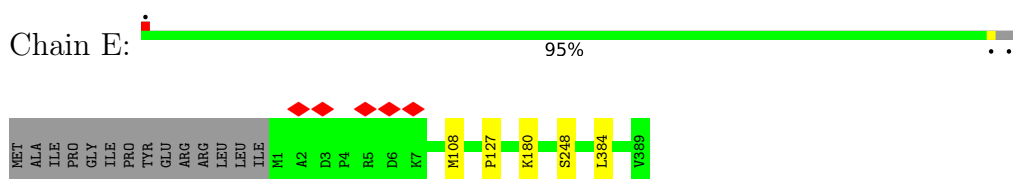
- Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8



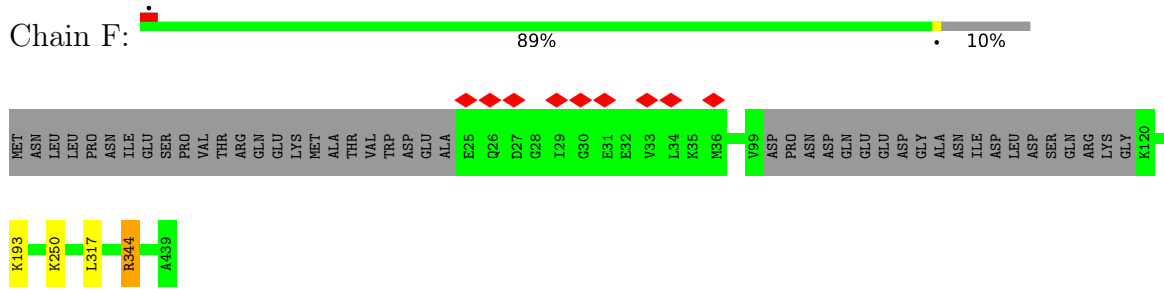
- Molecule 4: 26S protease regulatory subunit 6B



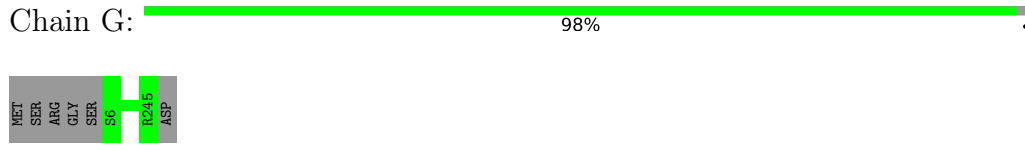
- Molecule 5: 26S proteasome regulatory subunit 10B



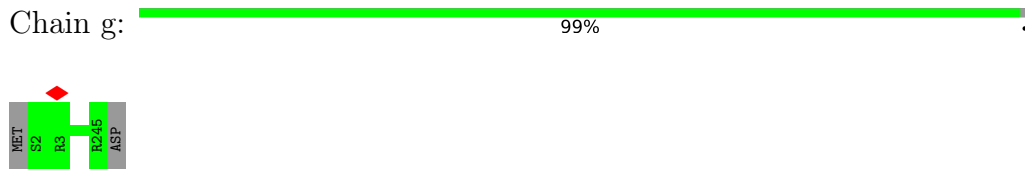
- Molecule 6: 26S protease regulatory subunit 6A



- Molecule 7: Proteasome subunit alpha type-6



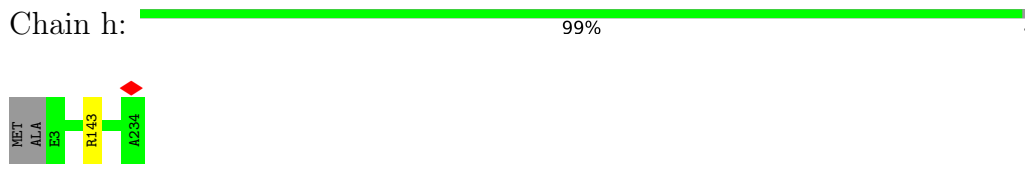
- Molecule 7: Proteasome subunit alpha type-6



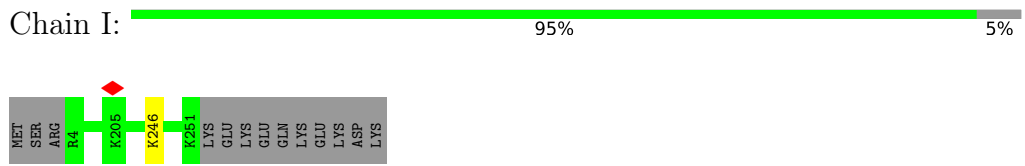
- Molecule 8: Proteasome subunit alpha type-2



- Molecule 8: Proteasome subunit alpha type-2

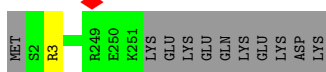


- Molecule 9: Proteasome subunit alpha type-4



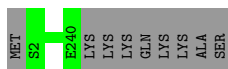
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  95%



- Molecule 10: Proteasome subunit alpha type-7

Chain J:  96%



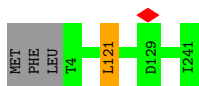
- Molecule 10: Proteasome subunit alpha type-7

Chain j:  95%



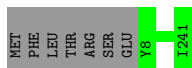
- Molecule 11: Proteasome subunit alpha type-5

Chain K:  98%




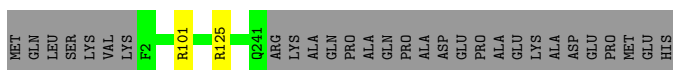
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  97%




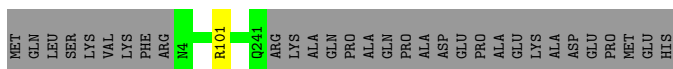
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L:  88% 11%

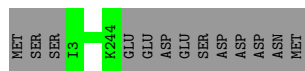


- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

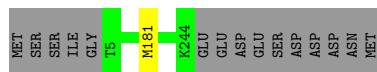
Chain l:  88% 12%



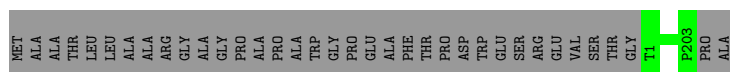
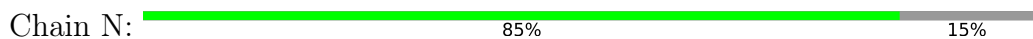
- Molecule 13: Proteasome subunit alpha type-3



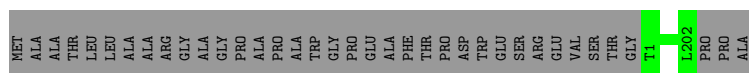
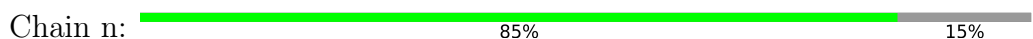
- Molecule 13: Proteasome subunit alpha type-3



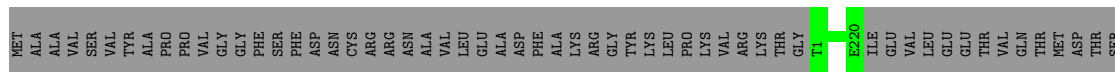
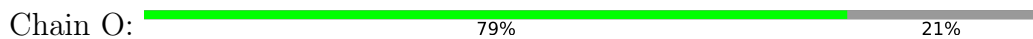
- Molecule 14: Proteasome subunit beta type-6



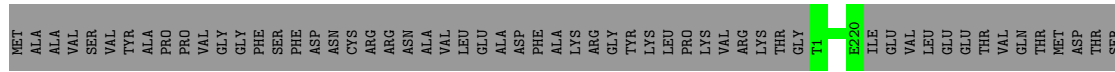
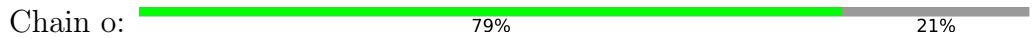
- Molecule 14: Proteasome subunit beta type-6



- Molecule 15: Proteasome subunit beta type-7



- Molecule 15: Proteasome subunit beta type-7



- Molecule 16: Proteasome subunit beta type-3



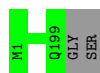
- Molecule 16: Proteasome subunit beta type-3

Chain p:  100%



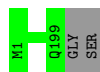
- Molecule 17: Proteasome subunit beta type-2

Chain Q:  99%





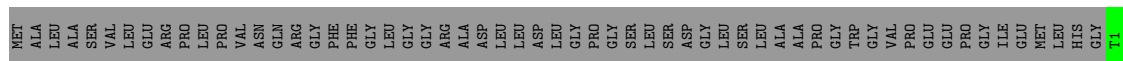
- Molecule 17: Proteasome subunit beta type-2

Chain q:  99%



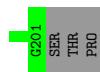
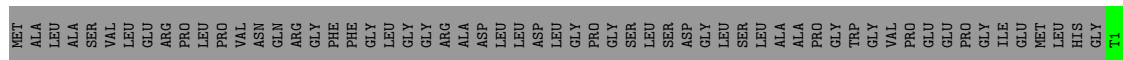
- Molecule 18: Proteasome subunit beta type-5

Chain R:  76%  24%





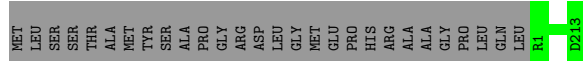
- Molecule 18: Proteasome subunit beta type-5

Chain r:  76%  24%





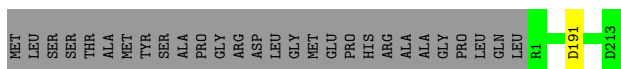
- Molecule 19: Proteasome subunit beta type-1

Chain S:  88%  12%

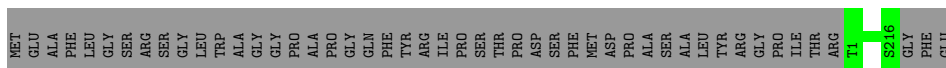
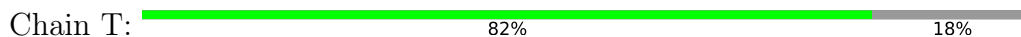


- Molecule 19: Proteasome subunit beta type-1

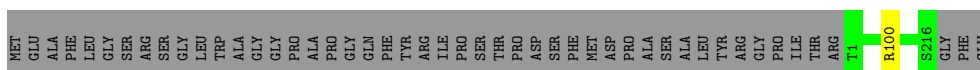
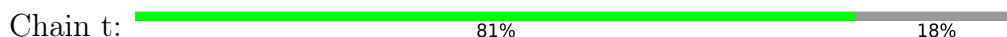
Chain s:  88%  12%



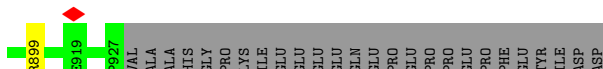
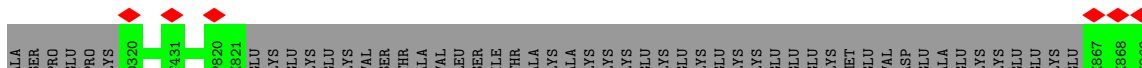
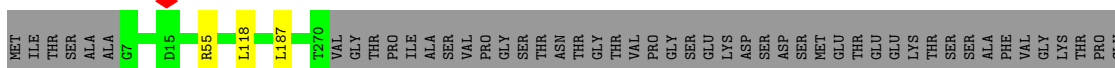
- Molecule 20: Proteasome subunit beta type-4



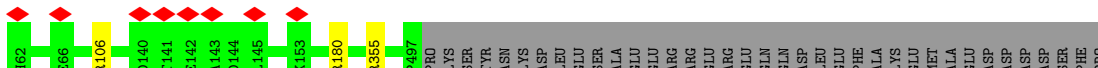
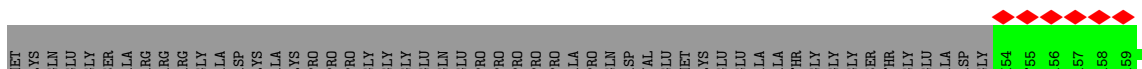
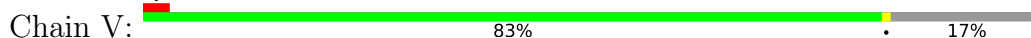
- Molecule 20: Proteasome subunit beta type-4



- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

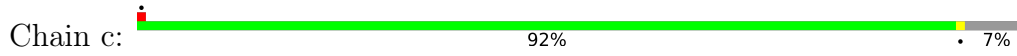


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



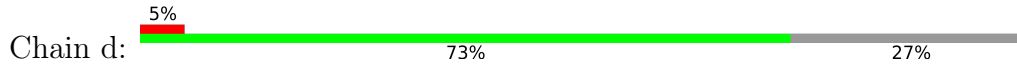
GLY
LYS
LYS
ASP
LYS
LYS
GLU
GLU
LYS
LYS

- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



MET
ASP
ARG
LEU
LEU
ARG
LEU
GLY
GLY
MET
PRO
PRO
GLY
LEU
GLY
GLN
GLY
PRO
PRO
THR
THR
ASP
ALA
ALA
PRO
A24
G81
R104
R161
L212
A271
K310

- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



MET
PHE
ILE
LYS
GLY
ARG
ALA
PRO
ARG
ASN
ALA
PRO
PRO
GLY
GLY
ARG
SER
SER
ALA
ALA
THR
ARG
GLY
GLY
LEU
THR
SER
GLN
VAL
VAL
ALA
LEU
PRO
PRO
ALA
ALA
THR
LEU
GLY
SER
THR
SER
ARG
ARG
PRO
HIS
PHE
ARG
ARG
ALA
SER
VAL
CYS
ARG
ARG
CYS
ARG
LYS
LYS
GLY
GLY
LEU
LEU
ALA
ALA

SER
ARG
LYS
MET
ALA
ALA
VAL
VAL
ASN
GLY
ALA
ALA
GLY
PHE
SER
SER
SER
GLY
PRO
ALA
ALA
THR
SER
GLY
ALA
VAL
VAL
LEU
GLN
PRO
ALA
ALA
THR
GLY
M1
L16
S17
E52
E57
Q128
A160
L190
K201
K204
K211
V216
L217
G218
F219
A226

S227
Q228
Q229
Q230
K231
V237

- Molecule 31: 26S proteasome non-ATPase regulatory subunit 2



M1
E2
E3
G4
G5
R6
D7
K8
A9
P10
V11
Q12
P13
Q14
Q15
S16
P17
A18
A19
A20
P21
G22
G23
T24
D25
E26
K27
P28
S29
G30
K31
E32
R33
R34
D35
A36
G37
D38
K39
D40
K41
E42
Q43
E44
L45
S46
E47
E48
D49
K50
Q51
L52
Q53
D54
E55
L59
V60
E61
R62

L63
G64
E65
K66
D67
T68
S69
L70
A74
L75
E76
E77
L78
R79
R80
Q81
I82
S85
K97
F98
L99
R100
P101
H102
Y103
G104
K105
E108
A123
D124
I125
S147
Q148
E149
E150
L151
A152
S153
H154
G155
H156
E157
D174
D175
V192
E203
L207
L208
M209
E210

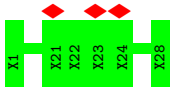
A247
L248
R273
V278
E279
D280
I281
F282
T283
L307
S308
E309
D310
V311
E312
E313
Y314
E315
S347
N355
N356
R357
F358
G359
G360
S361
G362
S363
L390
D393
D394
G395
N396
K397
K398
L399
A411
D430
Y434
S435
S436
C459
D460
A464
D468

L471
H472
H473
E495
D496
L502
K509
A572
E576
L580
V583
R673
S700
N705
R746
L796
W822
E835
E836
L837
R838
P839
L840
P841
W842
S843
W844
R845
W846
A849
W850
T870
L874
E886
F887
L888
P889
VAL
THR
PRO
ILE
LEU

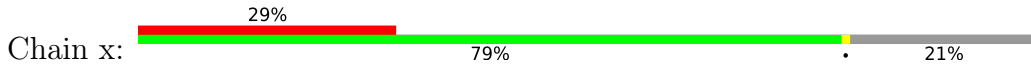
GLU
GLY
PHE
VAL
ILE
LEU
ARG
LYS
ASN
PRO
ASN
TYR
ASP
LEU

- Molecule 32: Substrate

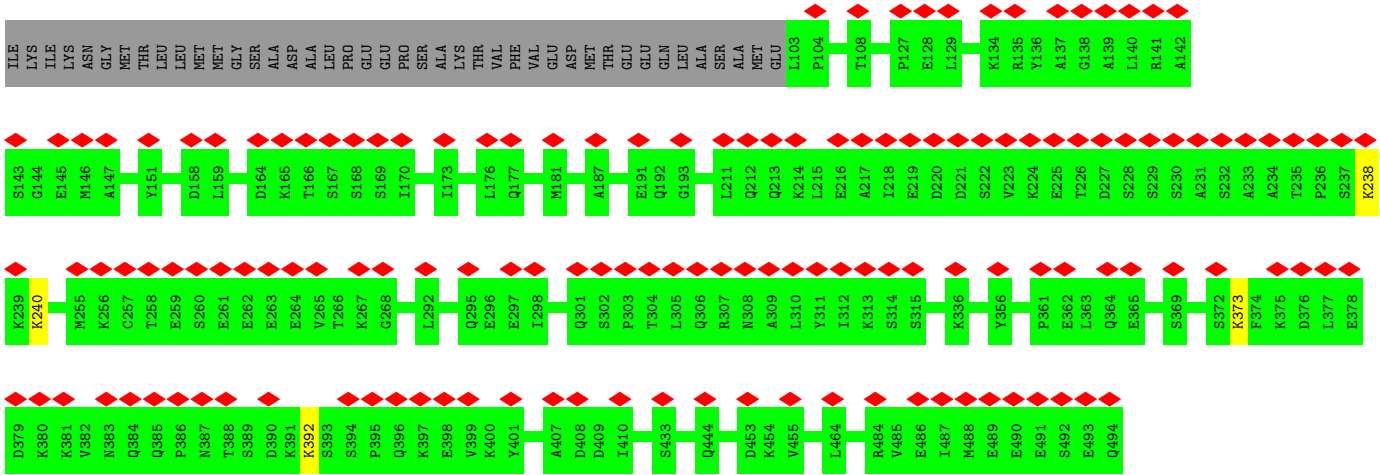




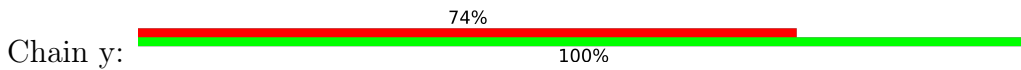
- Molecule 33: Ubiquitin carboxyl-terminal hydrolase 14



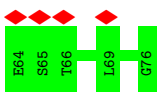
MET PRO LEU TYR SER ASN VAL THR VAL LYS TRP GLY LYS LEU LYS PHE ASP GLU ASP THR SER ASP MET PRO PRO THR MET VAL PHE VAL ASP ALA GLN LEU PHE ALA ALA ARG LYS VAL MET VAL LYS GLY THR LYS ASP ASP TRP GLY ASN



- Molecule 34: Ubiquitin



M1 Q2 I3 F4 V5 R6 T7 L8 T9 G10 K11 T12 I13 T14 L15 E16 V17 E18 P19 S20 D21 T22 I23 E24 N25 V26 K27 A28 K29 I30 Q31 D32 K33 E34 G35 I36 P37 F38 R42 L43 I44 F45 A46 C47 L50 E51 D52 G53 R54 T55 L56 S57 D58 Y59 M60 I61 O62 K63



- Molecule 35: 26S proteasome complex subunit DSS1



MET SER LEU LYS VAL PRO ASP LEU LEU GLU D16 A28 G29 L30 D31 D35 G64 Y65 MET GLU THR SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.020	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.685, 0.685, 0.685	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: ATP, ADP, ZN

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	0.26	0/3283	0.57	1/4433 (0.0%)
2	B	0.26	0/3168	0.56	0/4276
3	C	0.26	0/3146	0.57	1/4226 (0.0%)
4	D	0.26	0/3090	0.55	1/4168 (0.0%)
5	E	0.26	0/3145	0.61	1/4233 (0.0%)
6	F	0.26	0/3137	0.57	1/4223 (0.0%)
7	G	0.28	0/1901	0.52	0/2572
7	g	0.27	0/1913	0.51	0/2589
8	H	0.28	0/1840	0.52	0/2495
8	h	0.27	0/1844	0.50	0/2497
9	I	0.26	0/1963	0.52	0/2650
9	i	0.27	0/1985	0.53	0/2677
10	J	0.27	0/1887	0.56	0/2553
10	j	0.26	0/1887	0.56	0/2549
11	K	0.27	0/1841	0.53	1/2486 (0.0%)
11	k	0.26	0/1809	0.50	0/2444
12	L	0.26	0/1911	0.53	0/2584
12	l	0.26	0/1896	0.53	0/2565
13	M	0.27	0/1925	0.51	0/2592
13	m	0.27	0/1916	0.53	0/2580
14	N	0.26	0/1548	0.52	0/2097
14	n	0.26	0/1536	0.49	0/2080
15	O	0.26	0/1672	0.54	0/2267
15	o	0.26	0/1686	0.54	0/2282
16	P	0.26	0/1616	0.51	0/2180
16	p	0.27	0/1620	0.52	0/2184
17	Q	0.27	0/1621	0.51	0/2194
17	q	0.27	0/1611	0.52	0/2182
18	R	0.27	0/1590	0.52	0/2147
18	r	0.27	0/1580	0.54	0/2135
19	S	0.27	0/1671	0.55	0/2252
19	s	0.27	0/1680	0.54	1/2264 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.27	0/1716	0.55	0/2323
20	t	0.26	0/1720	0.53	0/2328
21	U	0.27	0/6575	0.53	0/8897
22	V	0.26	0/3681	0.53	0/4969
23	W	0.27	0/3683	0.61	0/4952
24	X	0.26	0/3053	0.56	1/4115 (0.0%)
25	Y	0.28	0/3173	0.63	1/4273 (0.0%)
26	Z	0.28	0/2324	0.61	0/3150
27	a	0.26	0/3053	0.58	1/4133 (0.0%)
28	b	0.26	0/1478	0.57	0/2001
29	c	0.28	0/2302	0.58	0/3110
30	d	0.27	0/2162	0.56	1/2919 (0.0%)
31	f	0.27	0/6980	0.61	2/9433 (0.0%)
33	x	0.25	0/3202	0.50	0/4310
34	y	0.26	0/607	0.57	0/816
35	e	0.27	0/437	0.51	0/595
All	All	0.27	0/111064	0.55	13/149980 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	190	LEU	CA-CB-CG	5.97	129.03	115.30
6	F	317	LEU	CA-CB-CG	5.80	128.64	115.30
3	C	134	LEU	CA-CB-CG	5.63	128.24	115.30
25	Y	377	LEU	CA-CB-CG	5.63	128.24	115.30
24	X	69	LEU	CA-CB-CG	5.52	128.01	115.30

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	365 (89%)	45 (11%)	1 (0%)	47	79
2	B	397/440 (90%)	359 (90%)	38 (10%)	0	100	100
3	C	394/398 (99%)	354 (90%)	40 (10%)	0	100	100
4	D	378/418 (90%)	347 (92%)	31 (8%)	0	100	100
5	E	387/403 (96%)	346 (89%)	38 (10%)	3 (1%)	19	59
6	F	391/439 (89%)	362 (93%)	28 (7%)	1 (0%)	41	75
7	G	238/246 (97%)	227 (95%)	11 (5%)	0	100	100
7	g	242/246 (98%)	233 (96%)	9 (4%)	0	100	100
8	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
8	h	230/234 (98%)	213 (93%)	17 (7%)	0	100	100
9	I	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
9	i	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	228 (96%)	9 (4%)	0	100	100
11	K	236/241 (98%)	224 (95%)	11 (5%)	1 (0%)	34	71
11	k	232/241 (96%)	222 (96%)	10 (4%)	0	100	100
12	L	238/269 (88%)	230 (97%)	8 (3%)	0	100	100
12	l	236/269 (88%)	227 (96%)	9 (4%)	0	100	100
13	M	240/255 (94%)	230 (96%)	10 (4%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	196 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
19	s	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
20	T	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
21	U	821/953 (86%)	765 (93%)	56 (7%)	0	100	100
22	V	442/534 (83%)	433 (98%)	9 (2%)	0	100	100
23	W	444/456 (97%)	415 (94%)	28 (6%)	1 (0%)	47	79
24	X	378/422 (90%)	358 (95%)	20 (5%)	0	100	100
25	Y	376/389 (97%)	338 (90%)	38 (10%)	0	100	100
26	Z	284/324 (88%)	256 (90%)	28 (10%)	0	100	100
27	a	371/376 (99%)	336 (91%)	34 (9%)	1 (0%)	41	75
28	b	189/377 (50%)	173 (92%)	16 (8%)	0	100	100
29	c	285/310 (92%)	248 (87%)	37 (13%)	0	100	100
30	d	255/350 (73%)	221 (87%)	34 (13%)	0	100	100
31	f	887/908 (98%)	778 (88%)	109 (12%)	0	100	100
33	x	390/494 (79%)	372 (95%)	18 (5%)	0	100	100
34	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
35	e	48/70 (69%)	41 (85%)	6 (12%)	1 (2%)	7	40
All	All	13813/15458 (89%)	12929 (94%)	875 (6%)	9 (0%)	54	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	LYS
5	E	248	SER
5	E	180	LYS
6	F	344	ARG
35	e	28	ALA

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	348/372 (94%)	347 (100%)	1 (0%)	92	97
2	B	349/385 (91%)	348 (100%)	1 (0%)	92	97
3	C	340/346 (98%)	339 (100%)	1 (0%)	92	97
4	D	333/366 (91%)	331 (99%)	2 (1%)	86	94
5	E	341/353 (97%)	340 (100%)	1 (0%)	92	97
6	F	340/379 (90%)	337 (99%)	3 (1%)	78	90
7	G	202/210 (96%)	202 (100%)	0	100	100
7	g	201/210 (96%)	201 (100%)	0	100	100
8	H	187/191 (98%)	186 (100%)	1 (0%)	88	95
8	h	188/191 (98%)	187 (100%)	1 (0%)	88	95
9	I	202/221 (91%)	201 (100%)	1 (0%)	88	95
9	i	206/221 (93%)	205 (100%)	1 (0%)	88	95
10	J	197/211 (93%)	197 (100%)	0	100	100
10	j	196/211 (93%)	193 (98%)	3 (2%)	65	84
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/230 (88%)	200 (99%)	2 (1%)	76	88
12	l	201/230 (87%)	200 (100%)	1 (0%)	88	95
13	M	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	197 (100%)	1 (0%)	88	95
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	178 (99%)	1 (1%)	86	94
21	U	707/816 (87%)	703 (99%)	4 (1%)	86	94
22	V	390/460 (85%)	387 (99%)	3 (1%)	81	91
23	W	410/416 (99%)	404 (98%)	6 (2%)	65	84
24	X	327/362 (90%)	327 (100%)	0	100	100
25	Y	334/344 (97%)	330 (99%)	4 (1%)	71	87
26	Z	257/295 (87%)	256 (100%)	1 (0%)	91	97
27	a	333/336 (99%)	331 (99%)	2 (1%)	86	94
28	b	167/312 (54%)	166 (99%)	1 (1%)	86	94
29	c	252/268 (94%)	249 (99%)	3 (1%)	71	87
30	d	231/294 (79%)	231 (100%)	0	100	100
31	f	745/763 (98%)	742 (100%)	3 (0%)	91	97
33	x	353/439 (80%)	349 (99%)	4 (1%)	73	88
34	y	68/68 (100%)	68 (100%)	0	100	100
35	e	44/63 (70%)	43 (98%)	1 (2%)	50	76
All	All	11810/13133 (90%)	11757 (100%)	53 (0%)	91	97

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Y	375	LEU
29	c	161	ARG
33	x	240	LYS
25	Y	377	LEU
27	a	289	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
31	f	180	GLN
31	f	329	ASN
33	x	281	GLN
20	t	188	GLN
21	U	115	ASN

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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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$
36	ATP	C	501	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
36	ATP	D	501	-	26,33,33	0.61	0	31,52,52	0.82	1 (3%)
37	ADP	F	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
36	ATP	E	501	-	26,33,33	0.61	0	31,52,52	0.72	1 (3%)

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
36	ATP	C	501	-	-	3/18/38/38	0/3/3/3
36	ATP	D	501	-	-	7/18/38/38	0/3/3/3
37	ADP	F	501	-	-	6/12/32/32	0/3/3/3
36	ATP	E	501	-	-	8/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	501	ADP	C5-C4	2.46	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	F	501	ADP	C3'-C2'-C1'	3.57	106.35	100.98
37	F	501	ADP	PA-O3A-PB	-3.27	121.61	132.83
37	F	501	ADP	N3-C2-N1	-2.79	124.31	128.68
37	F	501	ADP	C4-C5-N7	-2.73	106.55	109.40
36	E	501	ATP	C5-C6-N6	2.28	123.82	120.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

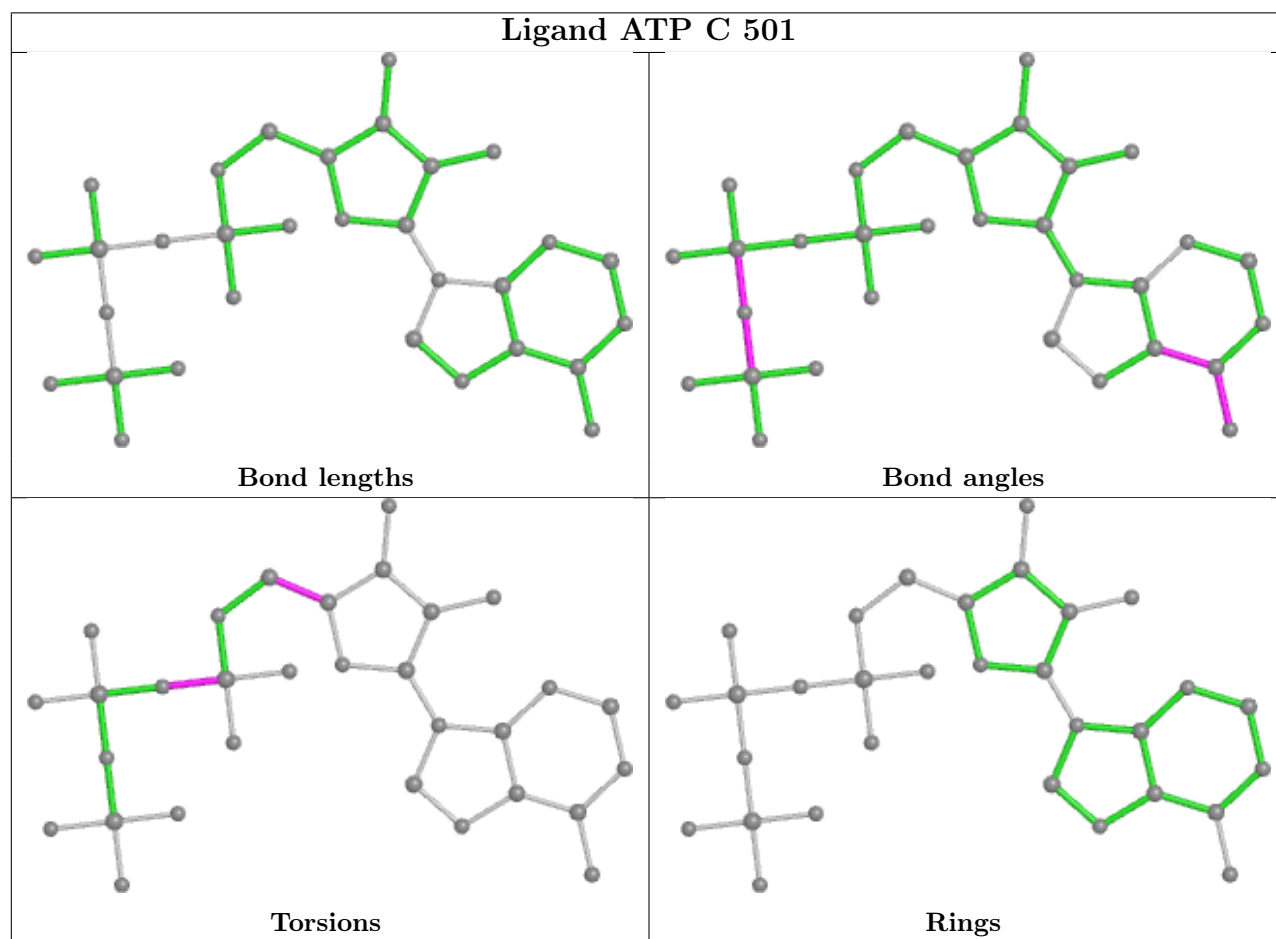
Mol	Chain	Res	Type	Atoms
36	C	501	ATP	PB-O3A-PA-O5'
36	D	501	ATP	O4'-C4'-C5'-O5'
36	D	501	ATP	C3'-C4'-C5'-O5'
36	E	501	ATP	C5'-O5'-PA-O2A
37	F	501	ADP	C5'-O5'-PA-O1A

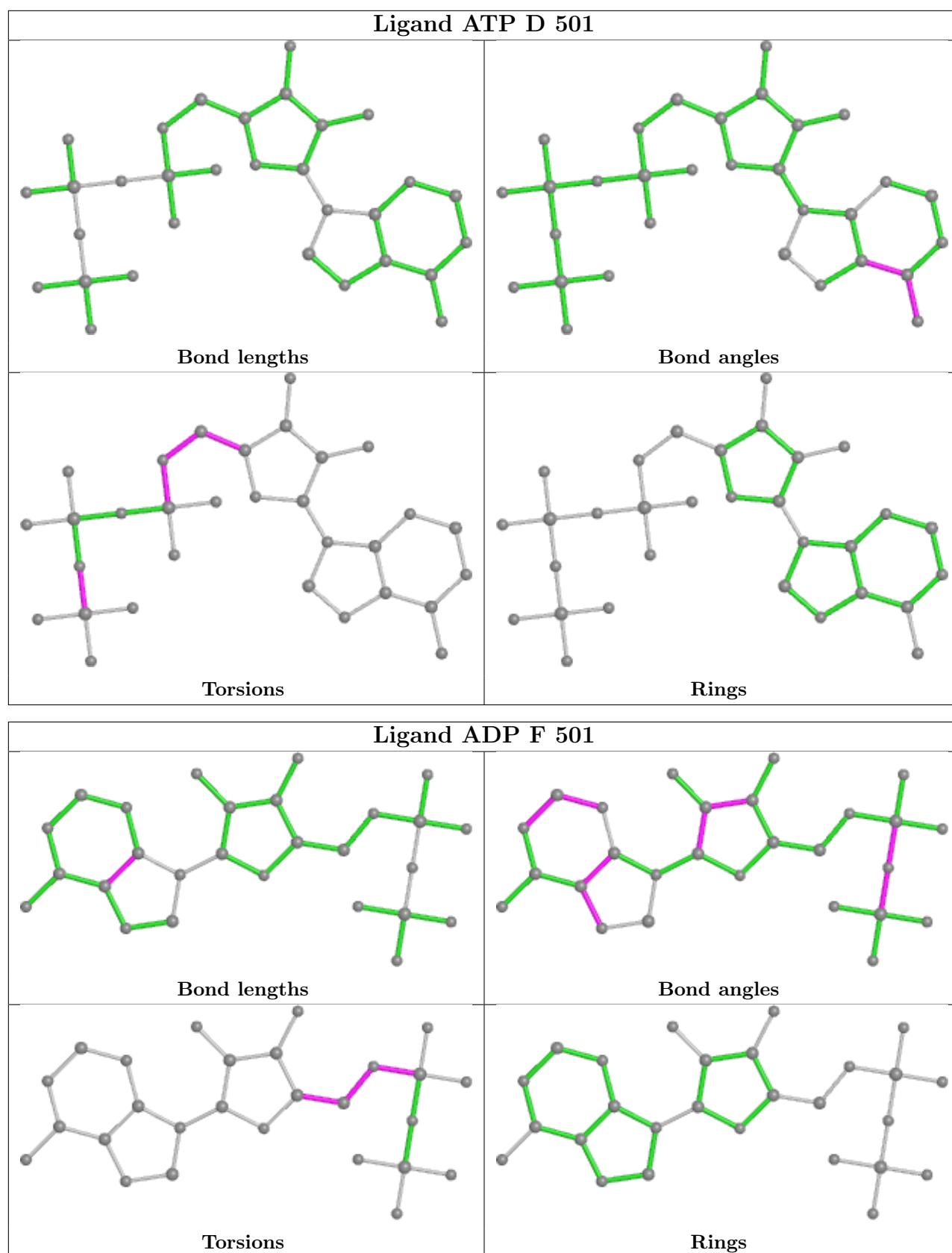
There are no ring outliers.

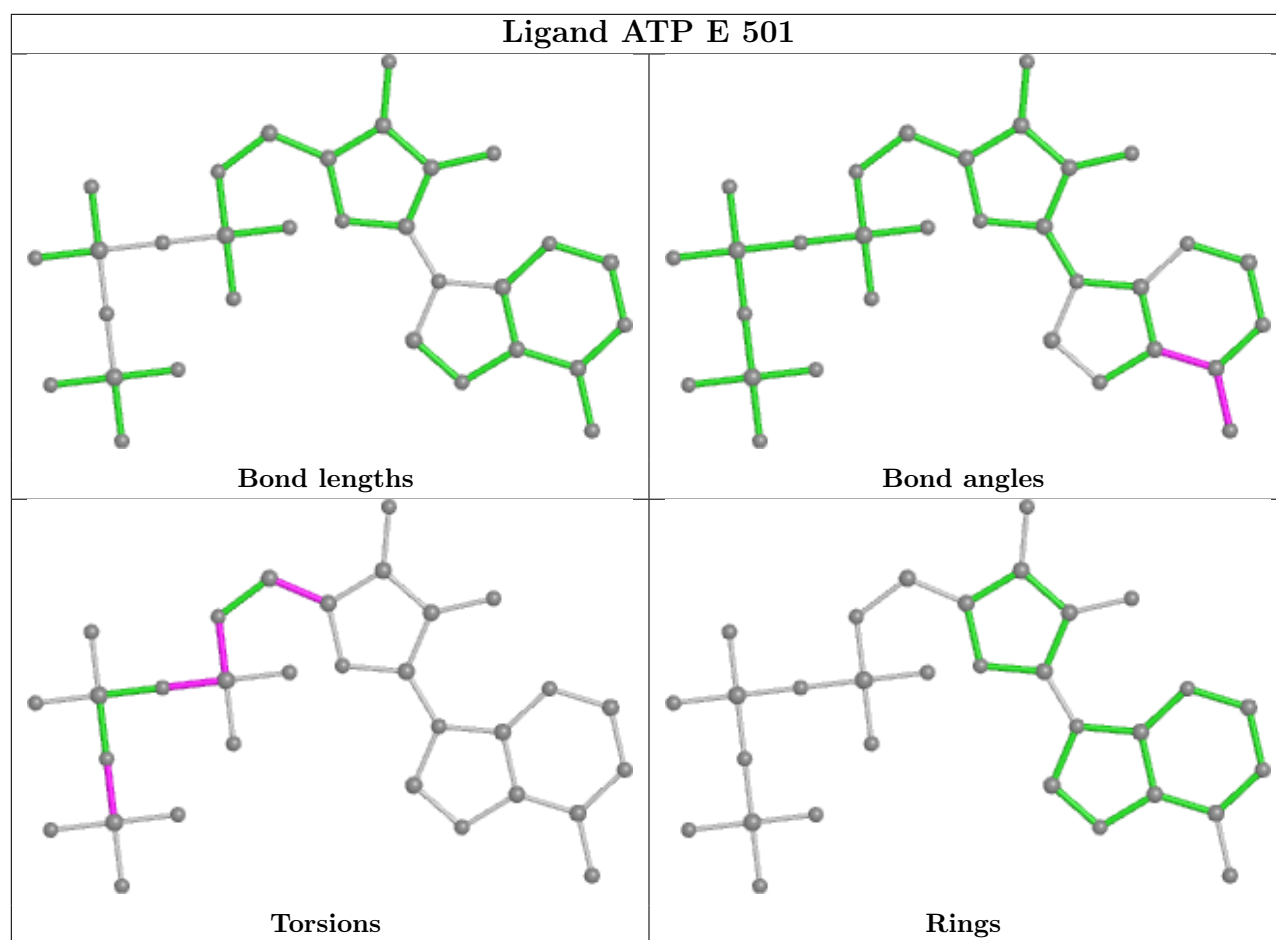
No monomer is involved in short contacts.

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.

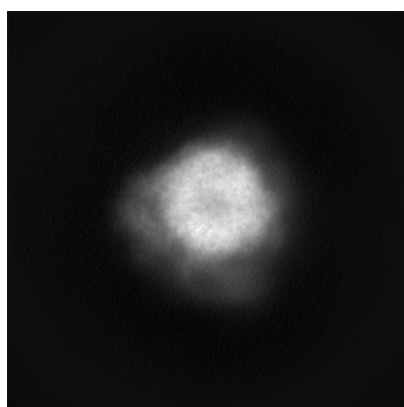
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32276. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

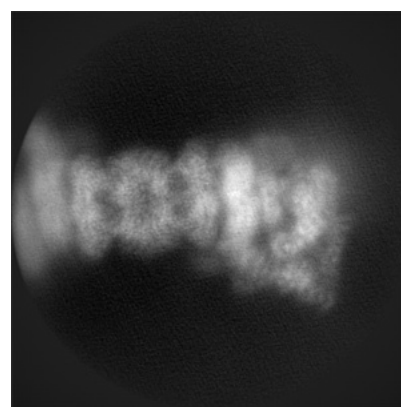
6.1.1 Primary map



X



Y

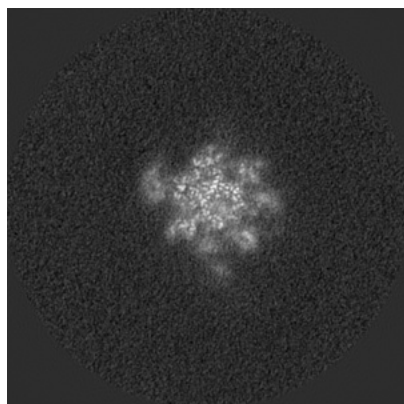


Z

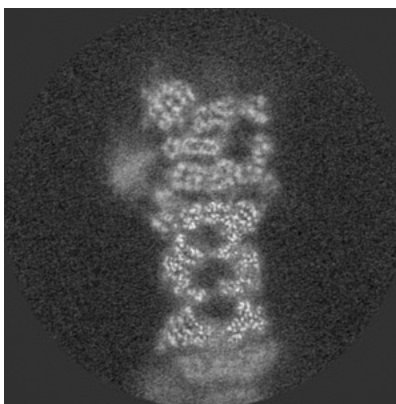
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

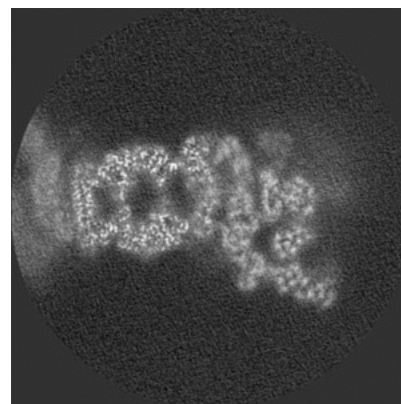
6.2.1 Primary map



X Index: 320



Y Index: 320

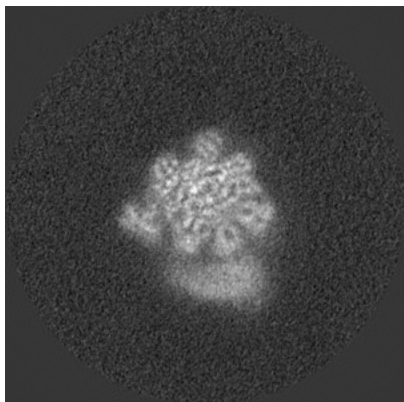


Z Index: 320

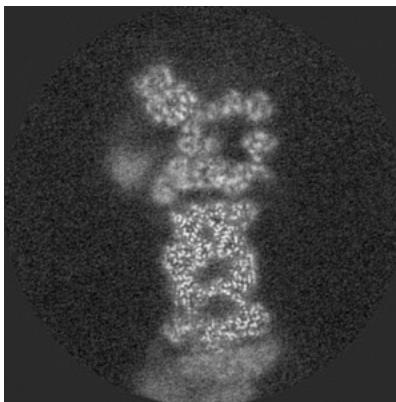
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

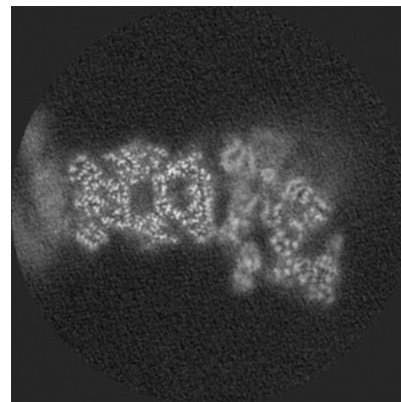
6.3.1 Primary map



X Index: 364



Y Index: 303



Z Index: 300

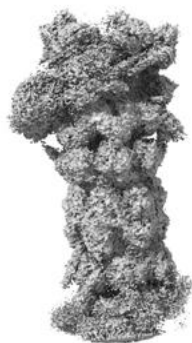
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

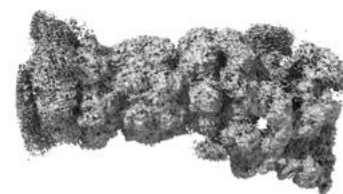
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

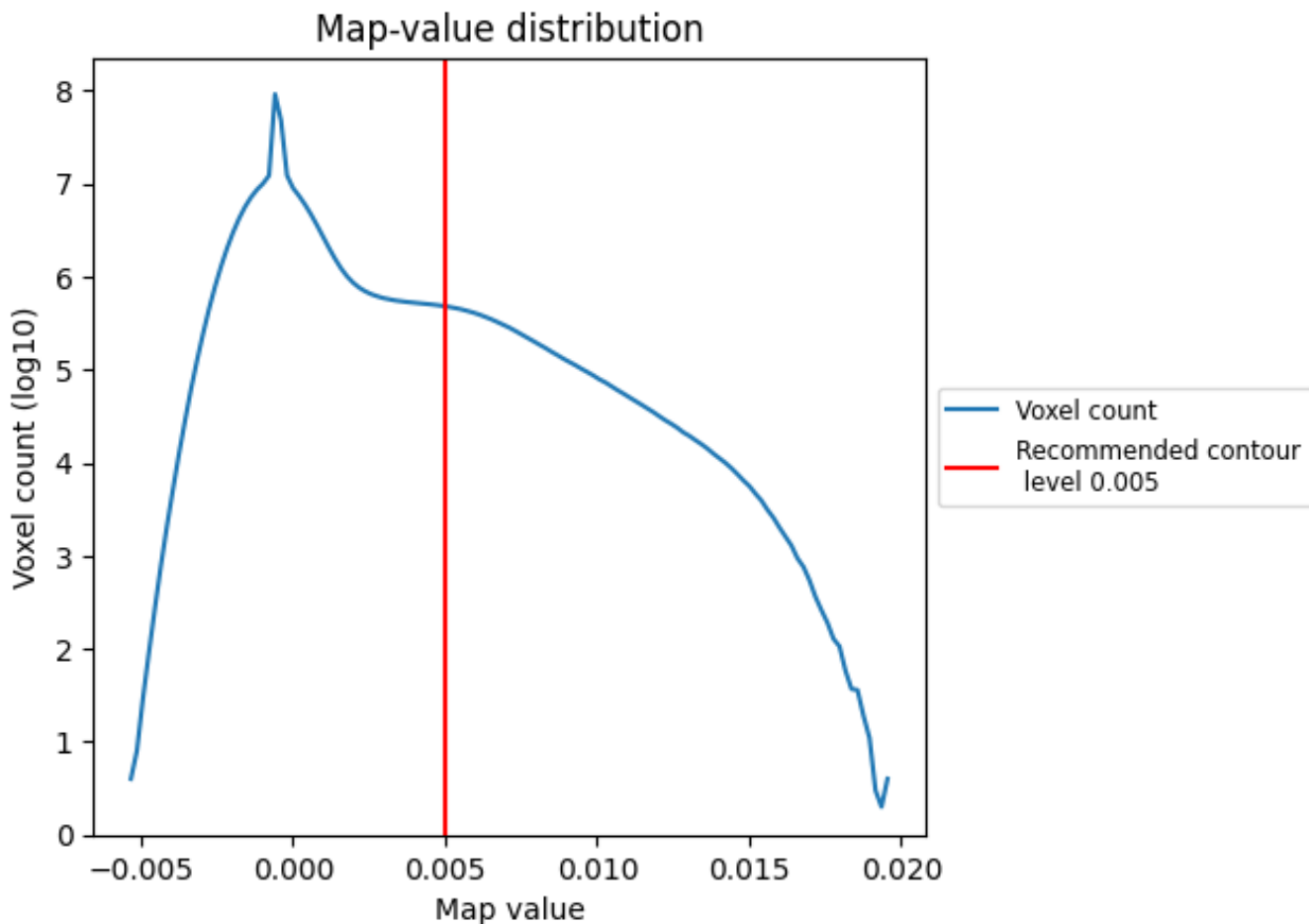
6.5 Mask visualisation

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

7 Map analysis [i](#)

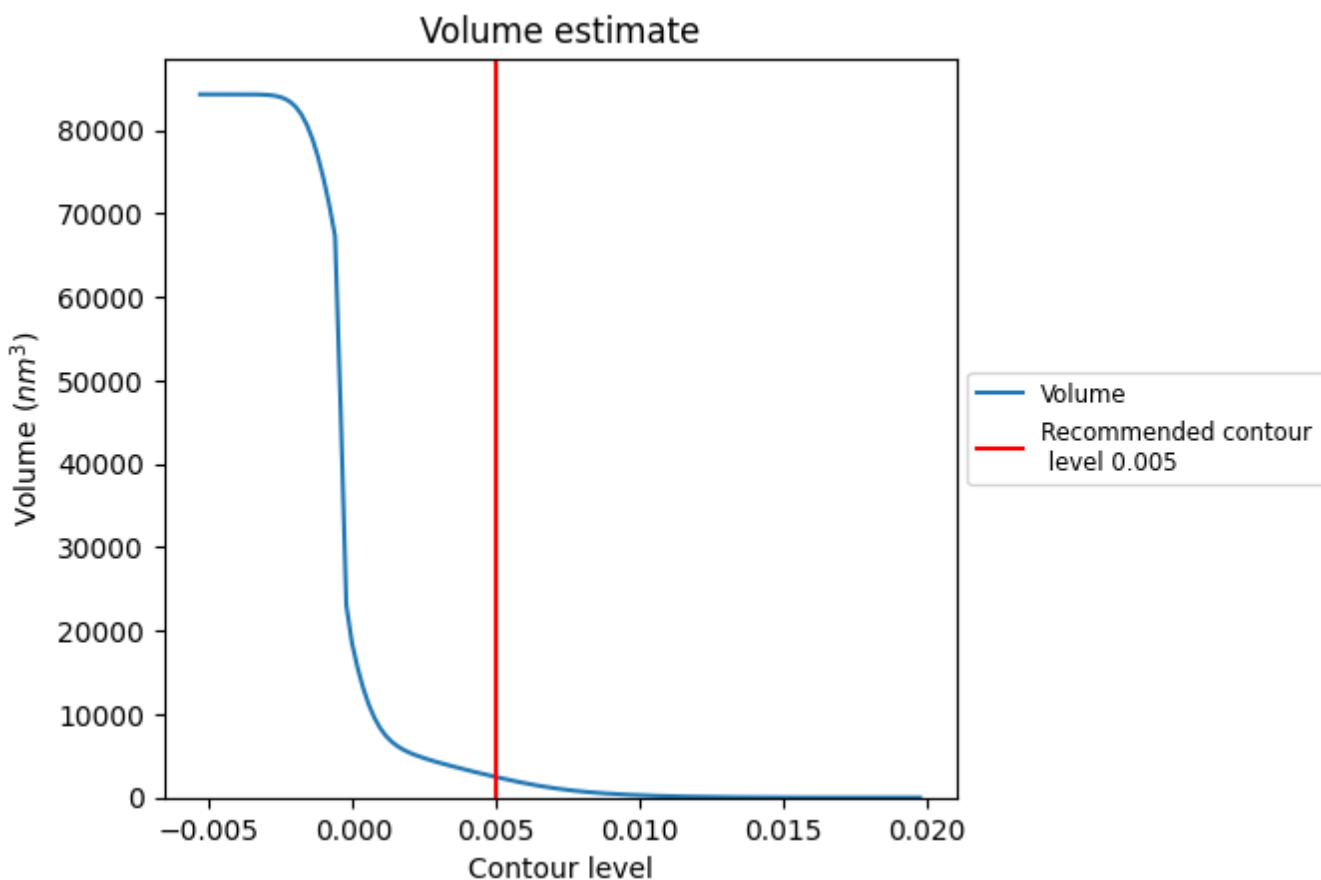
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

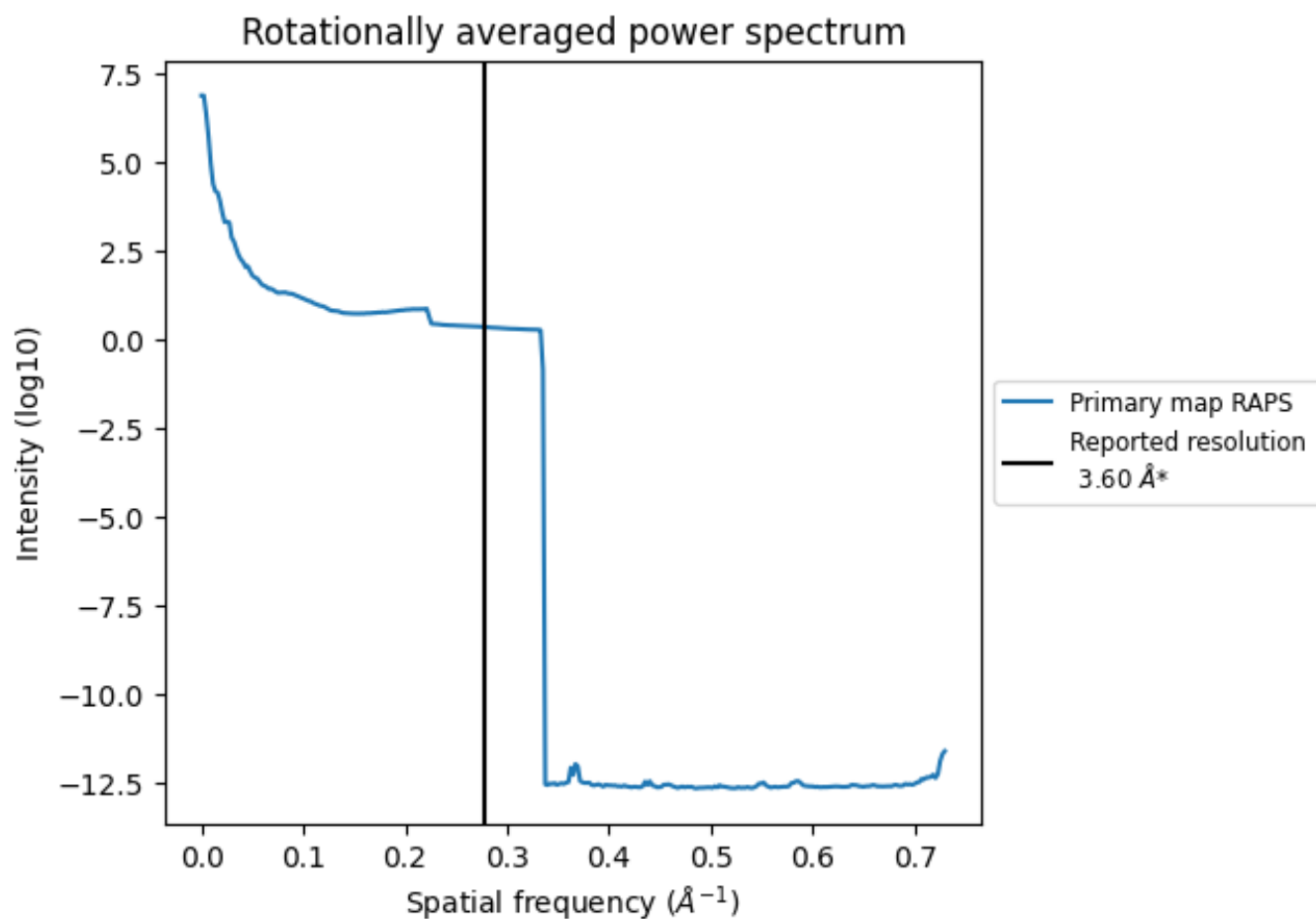
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2452 nm³; this corresponds to an approximate mass of 2215 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 0.278\AA^{-1}

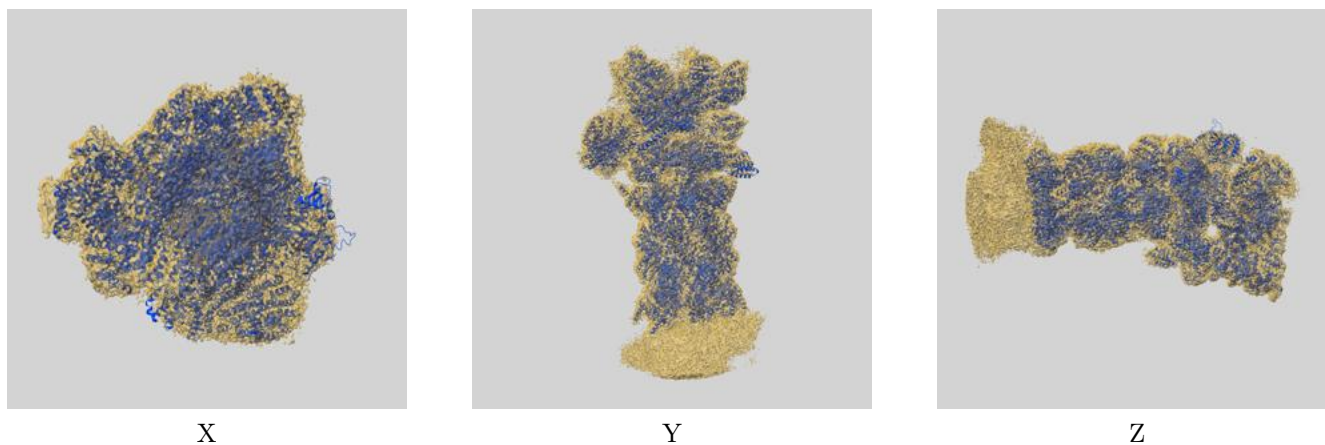
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

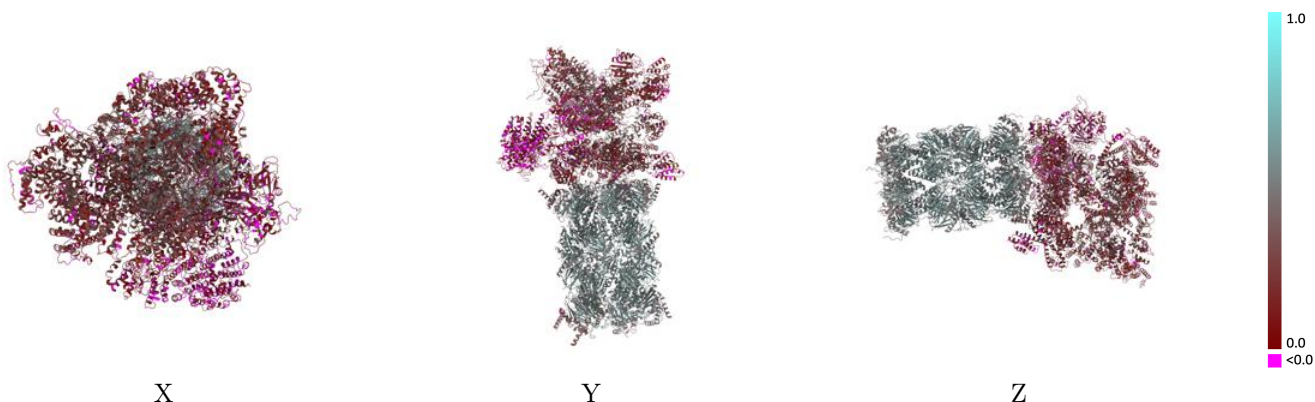
This section contains information regarding the fit between EMDB map EMD-32276 and PDB model 7W3B. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



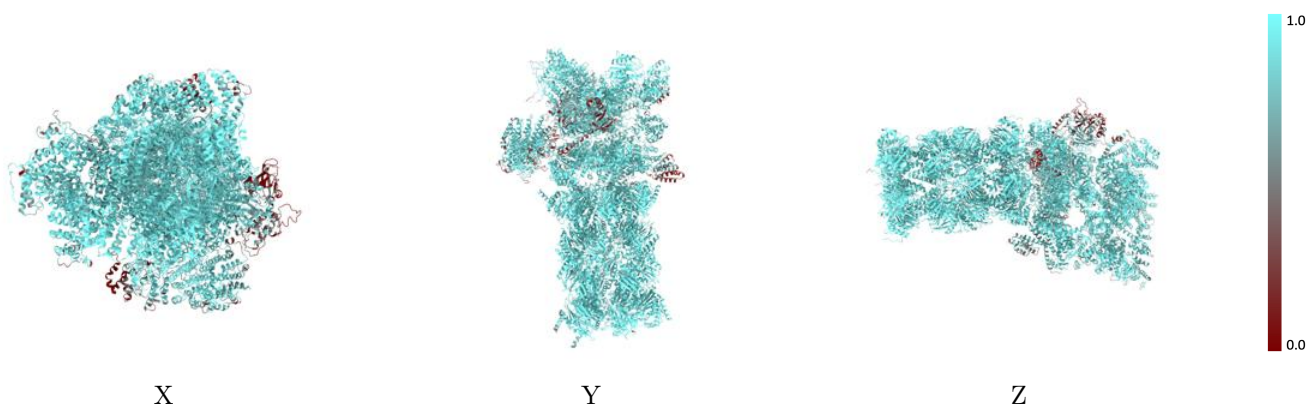
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



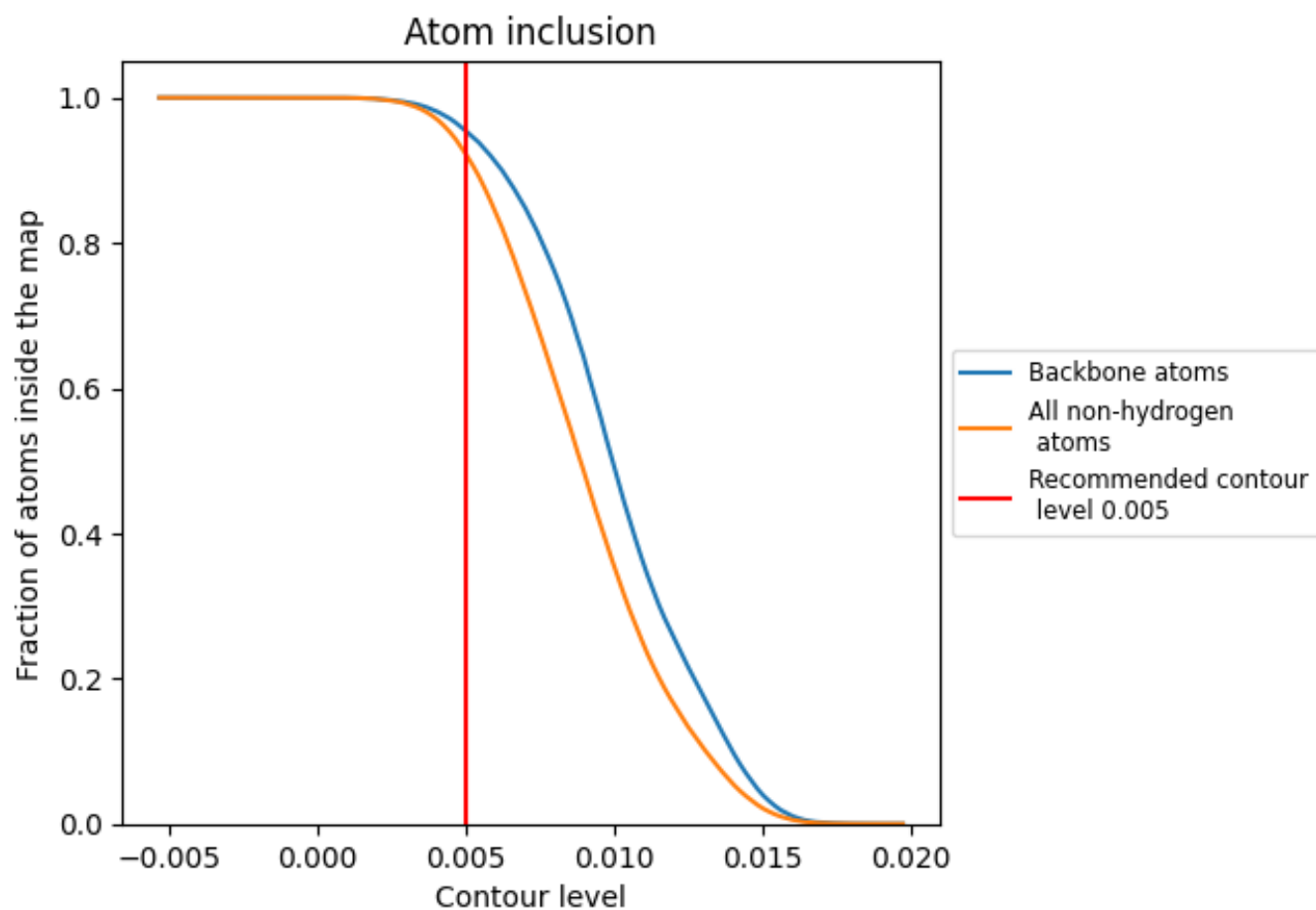
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9231	 0.3360
A	 0.9336	 0.1830
B	 0.9492	 0.1600
C	 0.9645	 0.2460
D	 0.9751	 0.2630
E	 0.9411	 0.2510
F	 0.9427	 0.2080
G	 0.9771	 0.4910
H	 0.9881	 0.4940
I	 0.9784	 0.4750
J	 0.9802	 0.4570
K	 0.9833	 0.4840
L	 0.9880	 0.5060
M	 0.9822	 0.5030
N	 0.9906	 0.5320
O	 0.9895	 0.5250
P	 0.9961	 0.5280
Q	 0.9929	 0.5250
R	 0.9980	 0.5280
S	 0.9888	 0.5240
T	 0.9896	 0.5330
U	 0.9312	 0.2450
V	 0.9213	 0.2390
W	 0.7789	 0.1970
X	 0.8660	 0.2060
Y	 0.9211	 0.2150
Z	 0.9698	 0.2590
a	 0.9037	 0.2080
b	 0.9466	 0.1970
c	 0.9628	 0.2690
d	 0.8338	 0.1960
e	 0.8592	 0.2320
f	 0.7504	 0.0770
g	 0.9745	 0.4940
h	 0.9842	 0.4980



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9650	 0.4750
j	 0.9565	 0.4430
k	 0.9734	 0.4780
l	 0.9857	 0.5170
m	 0.9761	 0.4930
n	 0.9892	 0.5330
o	 0.9945	 0.5250
p	 0.9936	 0.5250
q	 0.9948	 0.5250
r	 0.9940	 0.5250
s	 0.9895	 0.5240
t	 0.9890	 0.5350
v	 0.8714	 0.1670
x	 0.5360	 0.1270
y	 0.2872	 0.1460