



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 07:57 AM EDT

PDB ID : 5FMG
EMDB ID: : EMD-3231
Title : Structure and function based design of Plasmodium-selective proteasome inhibitors
Authors : Li, H.; O'Donoghue, A.J.; van der Linden, W.A.; Xie, S.C.; Yoo, E.; Foe, I.T.; Tilley, L.; Craik, C.S.; da Fonseca, P.C.A.; Bogoy, M.
Deposited on : unknown
Resolution : 3.60 Å(reported)
Based on PDB ID : 1IRU

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

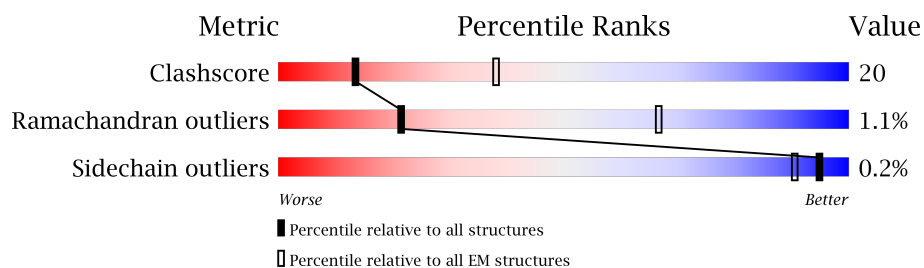
1 Overall quality at a glance

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)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	260	
1	O	260	
2	B	235	
2	P	235	
3	C	246	
3	Q	246	
4	D	241	
4	R	241	
5	E	256	

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Mol	Chain	Length	Quality of chain
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	211	
12	Z	211	
13	M	240	
13	a	240	
14	N	265	
14	b	265	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 39334 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEASOME SUBUNIT ALPHA, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	219	Total	C	N	O	S	0	0
			1440	907	251	274	8		
1	O	219	Total	C	N	O	S	0	0
			1440	907	251	274	8		

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	212	Total	C	N	O	S	0	0
			1381	895	232	250	4		
2	P	212	Total	C	N	O	S	0	0
			1381	895	232	250	4		

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	220	Total	C	N	O	S	0	0
			1527	984	251	289	3		
3	Q	220	Total	C	N	O	S	0	0
			1527	984	251	289	3		

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1409	904	241	259	5		
4	R	215	Total	C	N	O	S	0	0
			1409	904	241	259	5		

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	217	Total	C	N	O	S	0	0
			1440	914	241	277	8		
5	S	217	Total	C	N	O	S	0	0
			1440	914	241	277	8		

- Molecule 6 is a protein called PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	219	Total	C	N	O	S	0	0
			1492	956	244	287	5		
6	T	219	Total	C	N	O	S	0	0
			1492	956	244	287	5		

- Molecule 7 is a protein called PROTEASOME COMPONENT C8, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total	C	N	O	S	0	0
			1542	988	265	281	8		
7	U	219	Total	C	N	O	S	0	0
			1542	988	265	281	8		

- Molecule 8 is a protein called PROTEASOME, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1316	832	224	253	7		
8	V	191	Total	C	N	O	S	0	0
			1316	832	224	253	7		

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	186	Total	C	N	O	S	0	0
			1241	774	218	236	13		
9	W	186	Total	C	N	O	S	0	0
			1241	774	218	236	13		

- Molecule 10 is a protein called BETA3 PROTEASOME SUBUNIT, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	191	Total	C	N	O	S	0	0
			1273	803	215	243	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	191	Total	C	N	O	S	0	0
			1273	803	215	243	12		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q8I261
J	2	GLY	-	expression tag	UNP Q8I261
J	3	SER	-	expression tag	UNP Q8I261
J	4	ILE	-	expression tag	UNP Q8I261
J	5	TYR	-	expression tag	UNP Q8I261
J	6	ASN	-	expression tag	UNP Q8I261
J	7	TYR	-	expression tag	UNP Q8I261
J	8	ASN	-	expression tag	UNP Q8I261
J	9	GLY	-	expression tag	UNP Q8I261
J	10	GLY	-	expression tag	UNP Q8I261
J	11	CYS	-	expression tag	UNP Q8I261
J	12	VAL	-	expression tag	UNP Q8I261
J	13	LEU	-	expression tag	UNP Q8I261
J	14	GLY	-	expression tag	UNP Q8I261
X	1	MET	-	initiating methionine	UNP Q8I261
X	2	GLY	-	expression tag	UNP Q8I261
X	3	SER	-	expression tag	UNP Q8I261
X	4	ILE	-	expression tag	UNP Q8I261
X	5	TYR	-	expression tag	UNP Q8I261
X	6	ASN	-	expression tag	UNP Q8I261
X	7	TYR	-	expression tag	UNP Q8I261
X	8	ASN	-	expression tag	UNP Q8I261
X	9	GLY	-	expression tag	UNP Q8I261
X	10	GLY	-	expression tag	UNP Q8I261
X	11	CYS	-	expression tag	UNP Q8I261
X	12	VAL	-	expression tag	UNP Q8I261
X	13	LEU	-	expression tag	UNP Q8I261
X	14	GLY	-	expression tag	UNP Q8I261

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	194	Total	C	N	O	S	0	0
			1452	932	240	273	7		
11	Y	194	Total	C	N	O	S	0	0
			1452	932	240	273	7		

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	189	Total	C	N	O	S	0	0
			1355	870	223	256	6		
12	Z	189	Total	C	N	O	S	0	0
			1355	870	223	256	6		

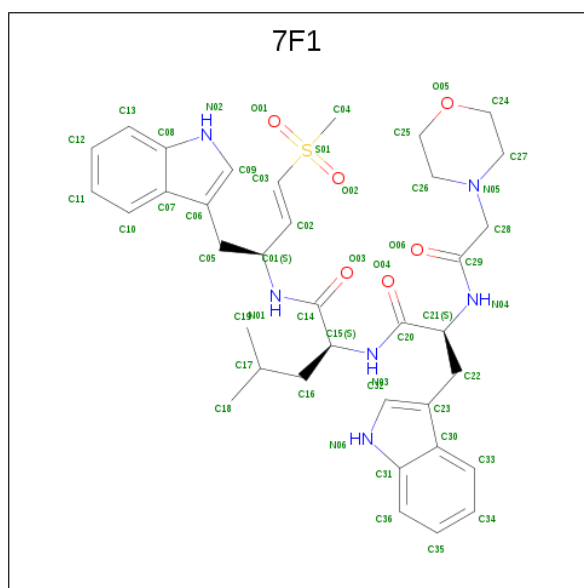
- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	199	Total	C	N	O	S	0	0
			1413	908	236	263	6		
13	a	199	Total	C	N	O	S	0	0
			1413	908	236	263	6		

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	187	Total	C	N	O	S	0	0
			1337	852	233	249	3		
14	b	187	Total	C	N	O	S	0	0
			1337	852	233	249	3		

- Molecule 15 is (2S)-N-[(E,2S)-1-(1H-indol-3-yl)-4-methylsulfonyl-but-3-en-2-yl]-2-[[(2S)-3-(1H-indol-3-yl)-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]-4-methyl-pentanamide (three-letter code: 7F1) (formula: C₃₆H₄₆N₆O₆S).

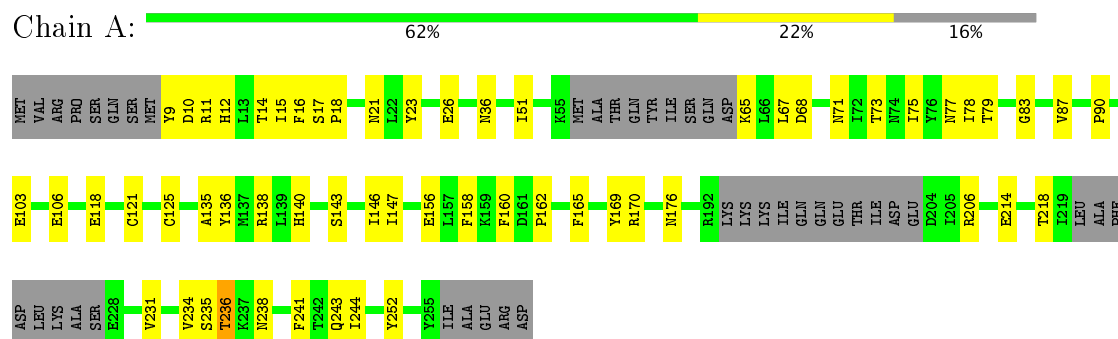


Mol	Chain	Residues	Atoms					AltConf
15	I	1	Total 49	C 36	N 6	O 6	S 1	0
15	W	1	Total 49	C 36	N 6	O 6	S 1	0

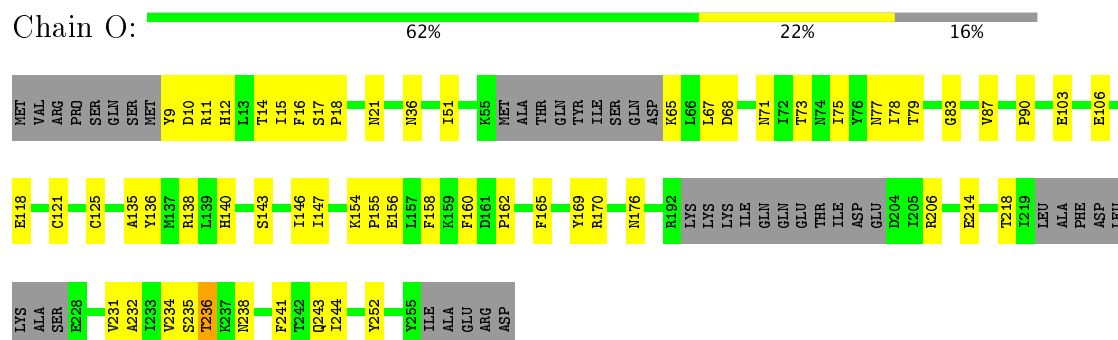
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

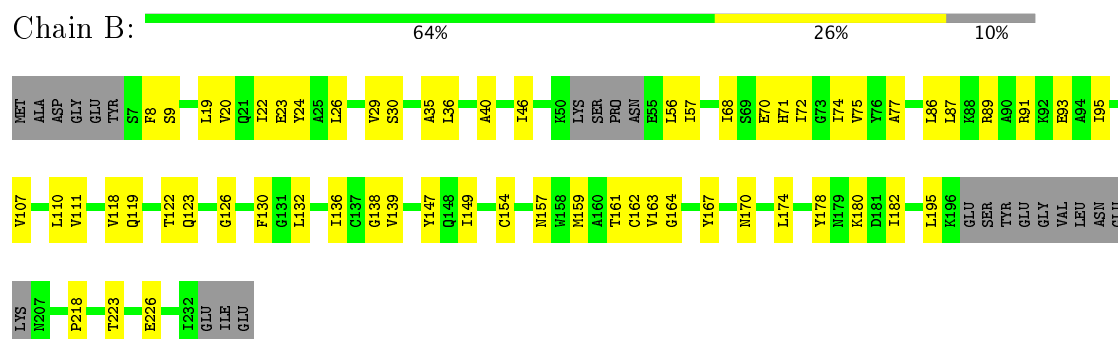
- Molecule 1: PROTEASOME SUBUNIT ALPHA, PUTATIVE



- Molecule 1: PROTEASOME SUBUNIT ALPHA, PUTATIVE

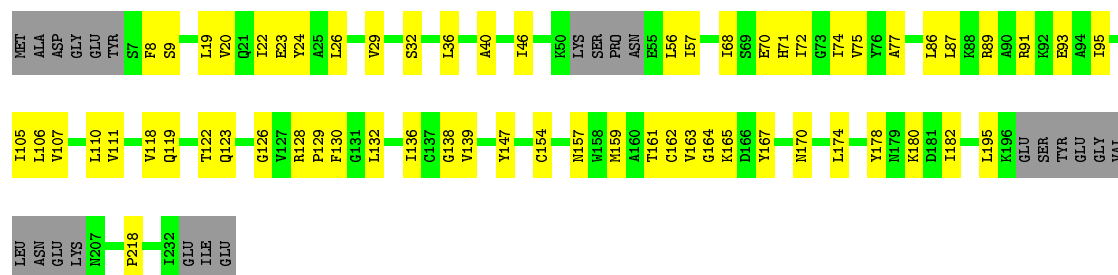


- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE



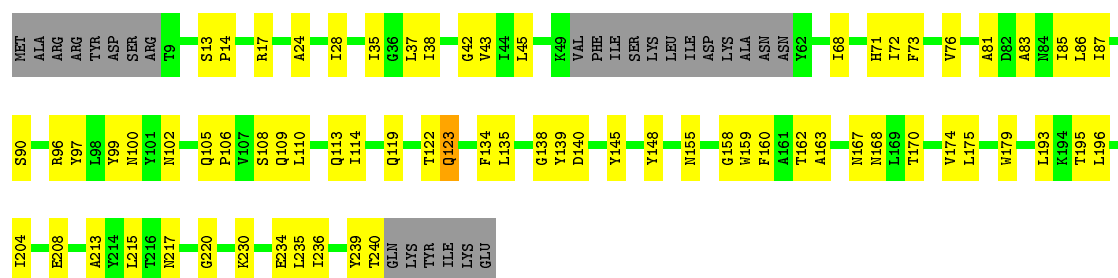
- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE

Chain P: 



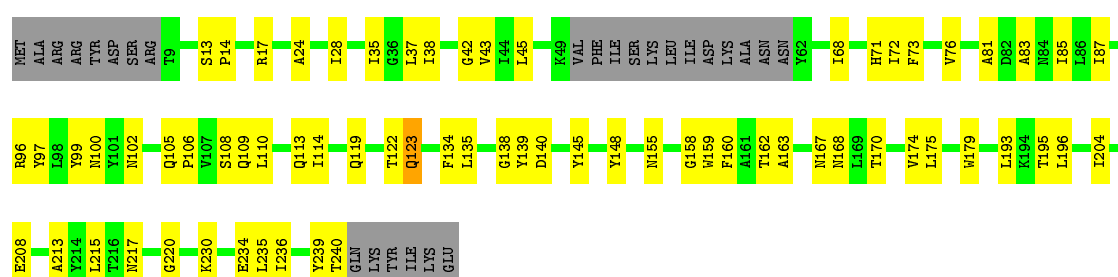
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE

Chain C: 



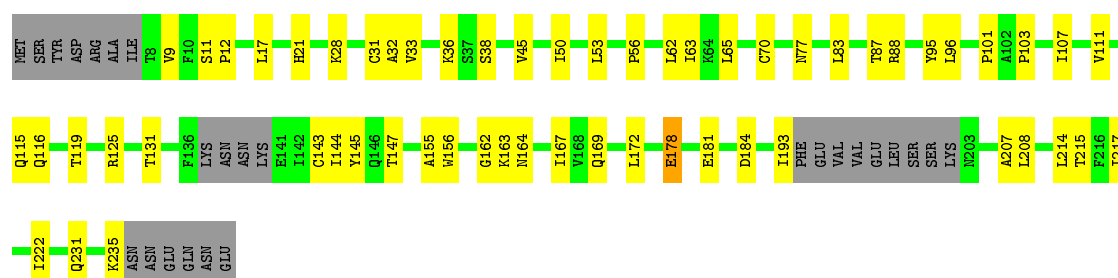
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE

Chain Q: 



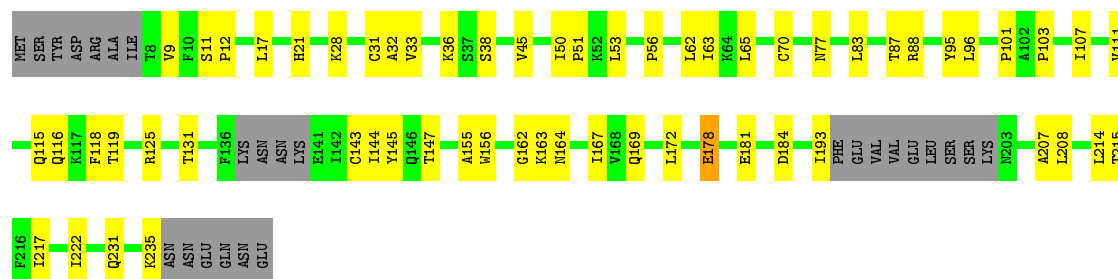
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE

Chain D: 



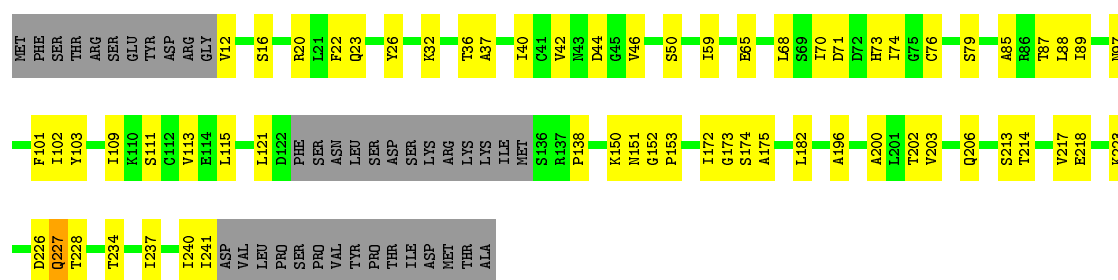
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE

Chain R:  64% 24% 11%



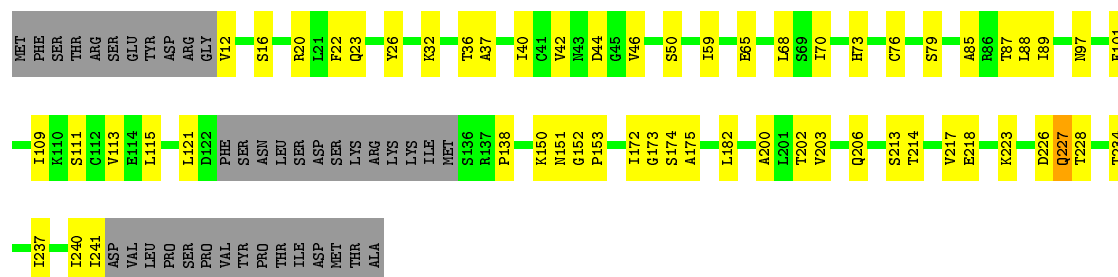
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE

Chain E:  60% 24% 15%



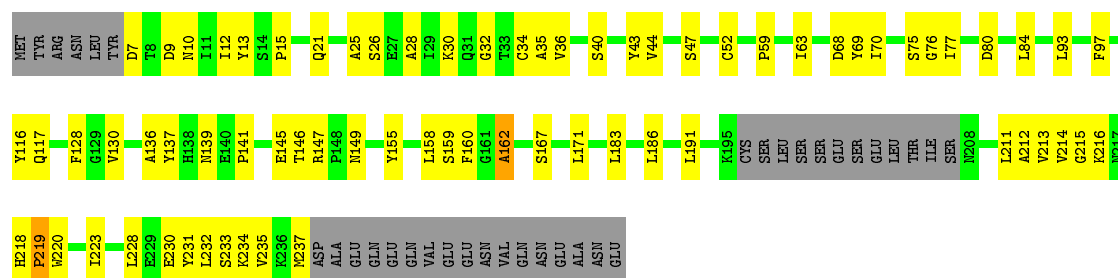
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE

Chain S:  62% 22% 15%



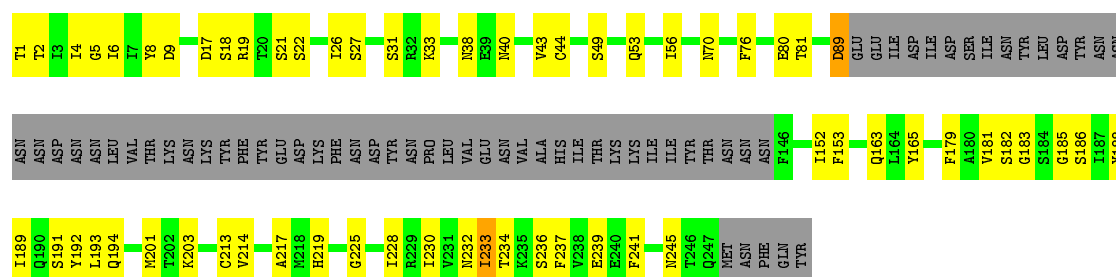
• Molecule 6: PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE

Chain F:  58% 28% 14%



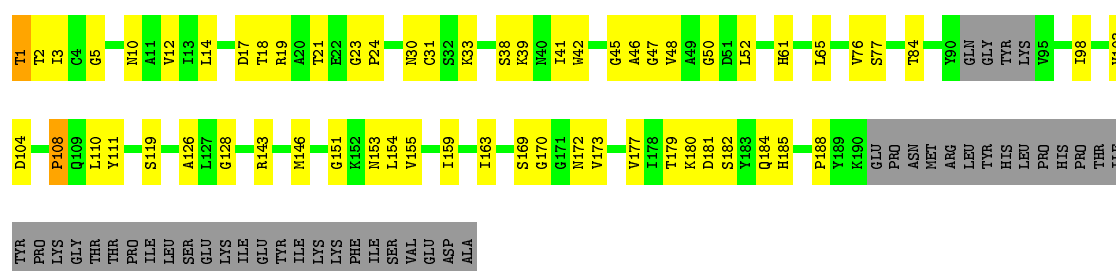
• Molecule 6: PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE

Chain V:  52% 23% 1% 24%



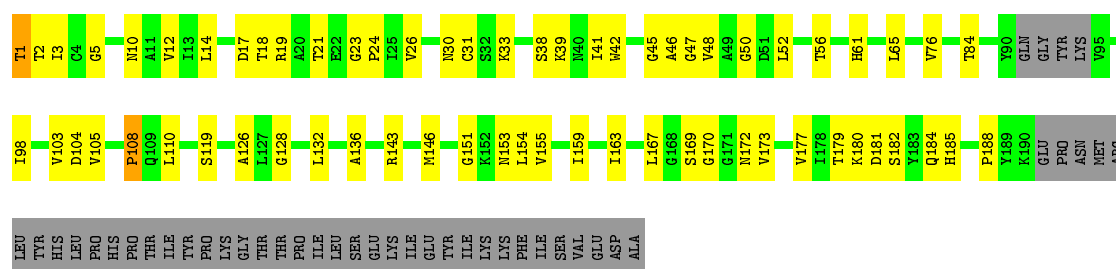
• Molecule 9: PROTEASOME SUBUNIT BETA TYPE

Chain I:  55% 25% . 19%



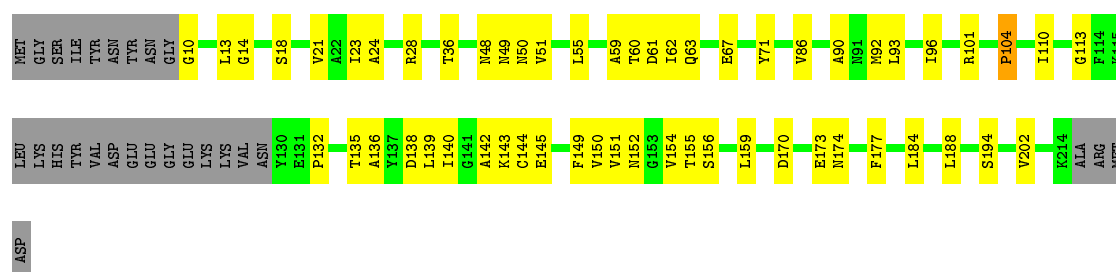
- Molecule 9: PROTEASOME SUBUNIT BETA TYPE

Chain W:  53% 27% 1% 19%

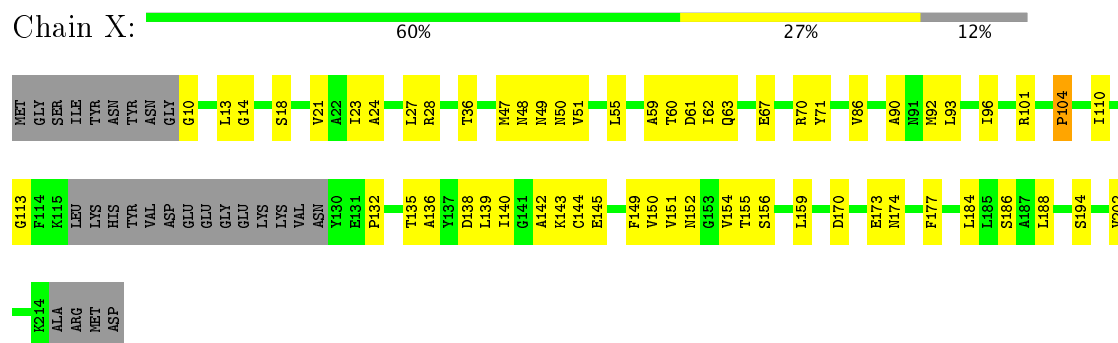


- Molecule 10: BETA3 PROTEASOME SUBUNIT, PUTATIVE

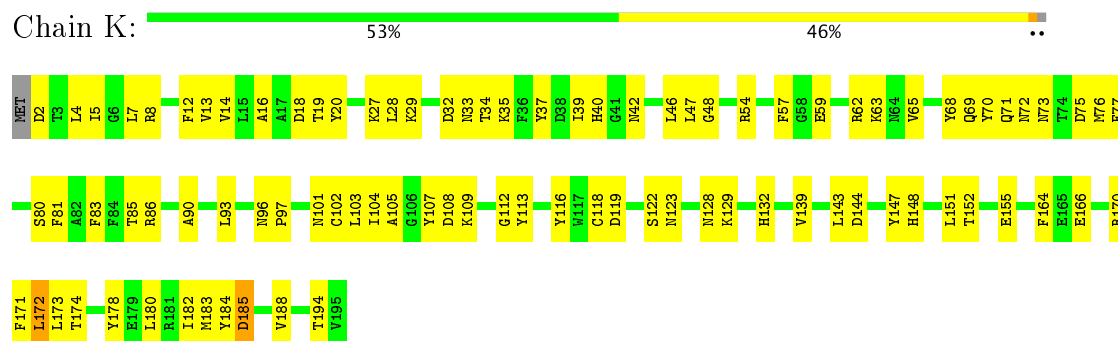
Chain J:  62% 25% 12%



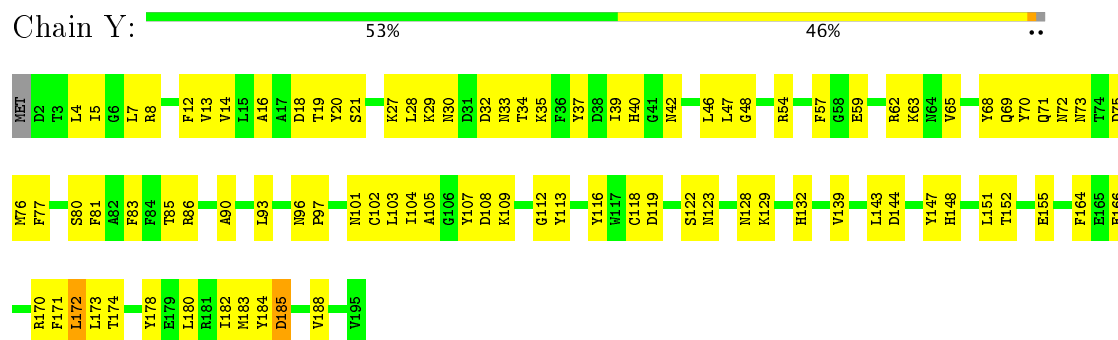
- Molecule 10: BETA3 PROTEASOME SUBUNIT, PUTATIVE



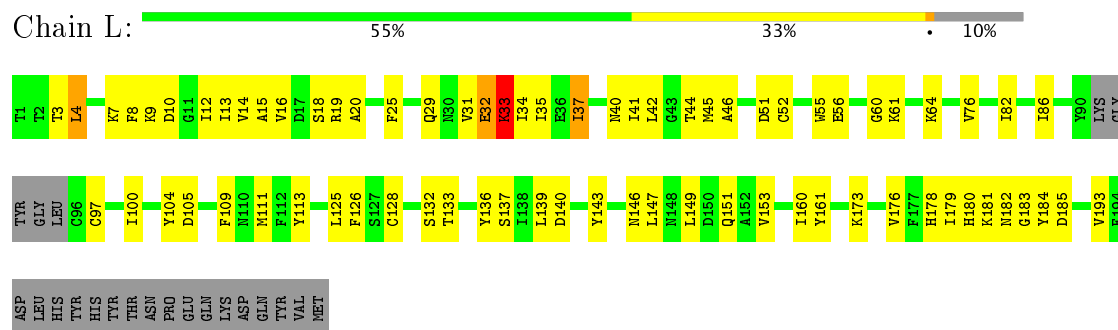
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE

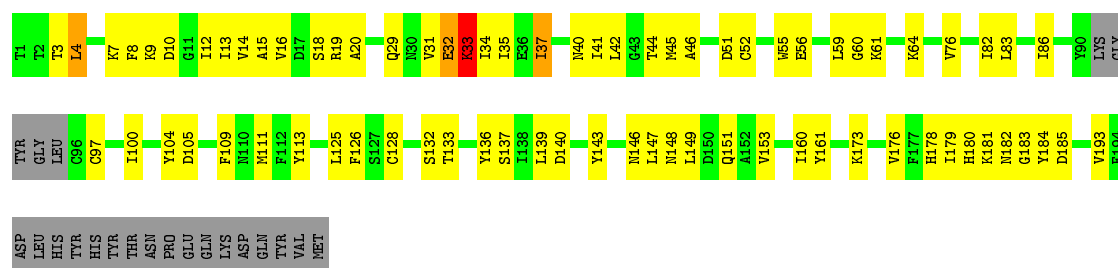


- Molecule 12: PROTEASOME SUBUNIT BETA TYPE



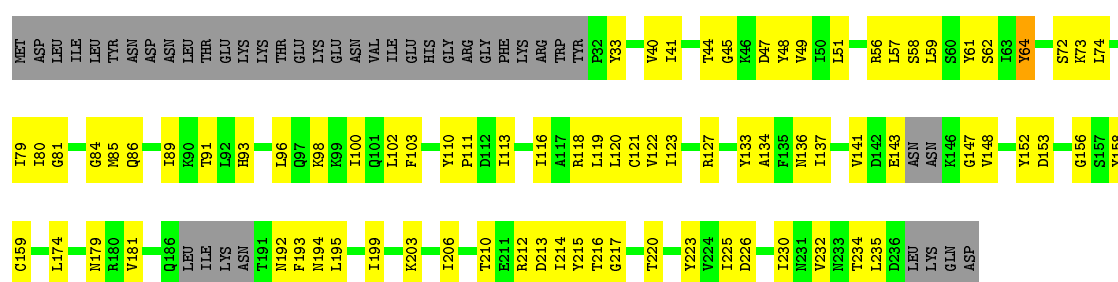
- Molecule 12: PROTEASOME SUBUNIT BETA TYPE

Chain Z:  54% 34% 10%




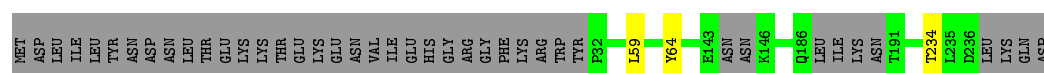
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE

Chain M:  49% 34% 17%



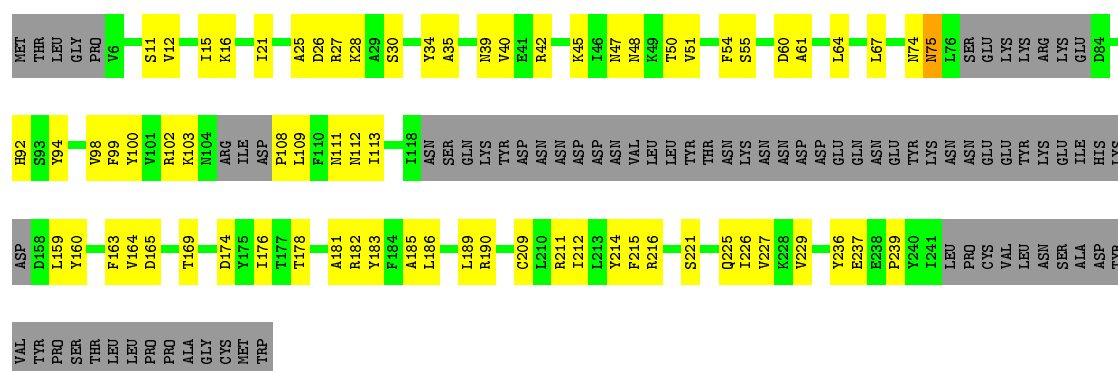
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE

Chain a:  82% 17%



• Molecule 14: PROTEASOME SUBUNIT BETA TYPE

Chain N:  44% 26% 29%



• Molecule 14: PROTEASOME SUBUNIT BETA TYPE

Chain b:  70% 29%

ILE	HIS	LYS	ASP	D153	V6	THR	LEU	GLY	PRO	MET
LEU	VAL	CYS	PRO	I241	N75	GLU	LYS	ARG	LYS	THR
LEU	ASP	SER	ALA	ASP	L76	LEU	GLY	ASP	ASP	LEU
VAL	THR	THR	VAL	D84	N104	ARG	ILE	ASP	P108	THR
PRO	PRO	LEU	PRO	ALA	I118	ASN	SER	GLN	LYS	ASP
ALA	GLY	CYS	GLY	GLY	ASN	SER	GLN	LYS	THR	ASP
MET	TRP				ASP	ASN	ASN	ASN	ASP	ASN
					ASP	ASP	VAL	LEU	LEU	THR
					ASN	LEU	LEU	TYR	THR	ASN
					LYS	ASN	LEU	LYS	ASN	LYS
					ASN	ASP	ASP	ASP	ASP	ASN
					GLU	GLN	GLU	GLU	GLU	GLU
					ASN	ASN	TYR	TYR	TYR	TYR
					LYS	LYS	LYS	LYS	LYS	LYS
					ASN	ASN	ASN	ASN	ASN	ASN
					GLU	GLU	GLU	GLU	GLU	GLU
					LYS	LYS	LYS	LYS	LYS	LYS
					THR	THR	THR	THR	THR	THR
					ASP	ASP	ASP	ASP	ASP	ASP
					GLY	GLY	GLY	GLY	GLY	GLY
					VAL	VAL	VAL	VAL	VAL	VAL
					ASN	ASN	ASN	ASN	ASN	ASN
					THR	THR				

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	97720	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FULL RECORDED IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.8	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7F1

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 >2	RMSZ	# Z >2
1	A	0.49	0/1455	0.60	0/1988
1	O	0.49	0/1455	0.60	0/1988
10	J	0.53	0/1283	0.66	0/1751
10	X	0.53	0/1283	0.66	0/1751
11	K	0.56	0/1482	0.68	1/2017 (0.0%)
11	Y	0.56	0/1482	0.68	1/2017 (0.0%)
12	L	0.54	0/1378	0.71	4/1866 (0.2%)
12	Z	0.54	0/1378	0.71	4/1866 (0.2%)
13	M	0.54	0/1434	0.65	0/1956
13	a	0.54	0/1434	0.65	0/1956
14	N	0.53	0/1355	0.64	0/1844
14	b	0.53	0/1355	0.64	0/1844
2	B	0.50	0/1400	0.62	0/1921
2	P	0.50	0/1400	0.62	0/1921
3	C	0.52	0/1554	0.64	1/2131 (0.0%)
3	Q	0.52	0/1554	0.64	1/2131 (0.0%)
4	D	0.49	0/1427	0.59	0/1964
4	R	0.49	0/1427	0.59	0/1964
5	E	0.49	0/1457	0.60	0/1997
5	S	0.49	0/1457	0.60	0/1997
6	F	0.49	0/1519	0.58	0/2082
6	T	0.49	0/1519	0.58	0/2082
7	G	0.51	0/1571	0.61	0/2150
7	U	0.51	0/1571	0.61	0/2150
8	H	0.57	0/1332	0.63	0/1814
8	V	0.57	0/1332	0.63	0/1814
9	I	0.69	1/1257 (0.1%)	0.71	1/1721 (0.1%)
9	W	0.69	1/1257 (0.1%)	0.71	1/1721 (0.1%)
All	All	0.53	2/39808 (0.0%)	0.64	14/54404 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
11	K	0	1
11	Y	0	1
12	L	0	2
12	Z	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	THR	C-N	15.29	1.69	1.34
9	W	1	THR	C-N	15.29	1.69	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	THR	O-C-N	-13.05	101.81	122.70
9	W	1	THR	O-C-N	-13.05	101.81	122.70
12	L	32	GLU	O-C-N	-6.86	111.73	122.70
12	Z	32	GLU	O-C-N	-6.86	111.73	122.70
12	L	33	LYS	CA-C-N	-5.63	104.82	117.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
11	K	12	PHE	Peptide
12	L	32	GLU	Mainchain
12	L	33	LYS	Mainchain
1	O	236	THR	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1440	0	1220	40	0
1	O	1440	0	1220	40	0
2	B	1381	0	1212	48	0
2	P	1381	0	1212	48	0
3	C	1527	0	1339	64	0
3	Q	1527	0	1339	60	0
4	D	1409	0	1210	47	0
4	R	1409	0	1210	47	0
5	E	1440	0	1279	42	0
5	S	1440	0	1279	37	0
6	F	1492	0	1278	54	0
6	T	1492	0	1278	50	0
7	G	1542	0	1357	78	0
7	U	1542	0	1357	78	0
8	H	1316	0	1153	59	0
8	V	1316	0	1153	61	0
9	I	1241	0	1143	44	0
9	W	1241	0	1143	52	0
10	J	1273	0	1171	49	0
10	X	1273	0	1171	51	0
11	K	1452	0	1292	97	0
11	Y	1452	0	1292	95	0
12	L	1355	0	1254	74	0
12	Z	1355	0	1254	75	0
13	M	1413	0	1334	72	0
13	a	1413	0	1334	0	0
14	N	1337	0	1220	59	0
14	b	1337	0	1220	0	0
15	I	49	0	0	17	0
15	W	49	0	0	17	0
All	All	39334	0	34924	1377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1377 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:THR:C	9:I:2:THR:N	1.69	1.43
9:W:1:THR:C	9:W:2:THR:N	1.69	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:ILE:HD11	8:H:193:LEU:CD1	1.69	1.23
8:V:4:ILE:HD11	8:V:193:LEU:CD1	1.69	1.20
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.29	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/260 (81%)	202 (96%)	7 (3%)	2 (1%)	20	64
1	O	211/260 (81%)	202 (96%)	7 (3%)	2 (1%)	20	64
2	B	206/235 (88%)	200 (97%)	5 (2%)	1 (0%)	32	73
2	P	206/235 (88%)	200 (97%)	5 (2%)	1 (0%)	32	73
3	C	216/246 (88%)	202 (94%)	12 (6%)	2 (1%)	20	64
3	Q	216/246 (88%)	202 (94%)	12 (6%)	2 (1%)	20	64
4	D	209/241 (87%)	200 (96%)	7 (3%)	2 (1%)	18	62
4	R	209/241 (87%)	200 (96%)	7 (3%)	2 (1%)	18	62
5	E	213/256 (83%)	201 (94%)	8 (4%)	4 (2%)	9	50
5	S	213/256 (83%)	201 (94%)	8 (4%)	4 (2%)	9	50
6	F	215/254 (85%)	196 (91%)	16 (7%)	3 (1%)	13	56
6	T	215/254 (85%)	196 (91%)	16 (7%)	3 (1%)	13	56
7	G	213/252 (84%)	200 (94%)	12 (6%)	1 (0%)	32	73
7	U	213/252 (84%)	200 (94%)	12 (6%)	1 (0%)	32	73
8	H	187/252 (74%)	170 (91%)	14 (8%)	3 (2%)	11	53
8	V	187/252 (74%)	170 (91%)	14 (8%)	3 (2%)	11	53
9	I	182/229 (80%)	164 (90%)	14 (8%)	4 (2%)	8	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	182/229 (80%)	164 (90%)	14 (8%)	4 (2%)	8	47
10	J	187/218 (86%)	178 (95%)	7 (4%)	2 (1%)	17	61
10	X	187/218 (86%)	178 (95%)	7 (4%)	2 (1%)	17	61
11	K	192/195 (98%)	181 (94%)	8 (4%)	3 (2%)	11	53
11	Y	192/195 (98%)	181 (94%)	8 (4%)	3 (2%)	11	53
12	L	185/211 (88%)	174 (94%)	9 (5%)	2 (1%)	17	61
12	Z	185/211 (88%)	174 (94%)	9 (5%)	2 (1%)	17	61
13	M	193/240 (80%)	176 (91%)	15 (8%)	2 (1%)	18	62
13	a	193/240 (80%)	176 (91%)	15 (8%)	2 (1%)	18	62
14	N	179/265 (68%)	171 (96%)	8 (4%)	0	100	100
14	b	179/265 (68%)	171 (96%)	8 (4%)	0	100	100
All	All	5576/6708 (83%)	5230 (94%)	284 (5%)	62 (1%)	21	61

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	38	SER
5	E	151	ASN
9	I	24	PRO
9	I	188	PRO
13	M	64	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/231 (51%)	118 (100%)	0	100	100
1	O	118/231 (51%)	118 (100%)	0	100	100
2	B	111/205 (54%)	110 (99%)	1 (1%)	82	92
2	P	111/205 (54%)	110 (99%)	1 (1%)	82	92
3	C	129/213 (61%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	129/213 (61%)	129 (100%)	0	100	100
4	D	107/207 (52%)	107 (100%)	0	100	100
4	R	107/207 (52%)	107 (100%)	0	100	100
5	E	126/223 (56%)	126 (100%)	0	100	100
5	S	126/223 (56%)	126 (100%)	0	100	100
6	F	127/227 (56%)	127 (100%)	0	100	100
6	T	127/227 (56%)	127 (100%)	0	100	100
7	G	140/229 (61%)	140 (100%)	0	100	100
7	U	140/229 (61%)	140 (100%)	0	100	100
8	H	118/231 (51%)	117 (99%)	1 (1%)	85	94
8	V	118/231 (51%)	117 (99%)	1 (1%)	85	94
9	I	117/194 (60%)	117 (100%)	0	100	100
9	W	117/194 (60%)	117 (100%)	0	100	100
10	J	118/191 (62%)	118 (100%)	0	100	100
10	X	118/191 (62%)	118 (100%)	0	100	100
11	K	138/174 (79%)	138 (100%)	0	100	100
11	Y	138/174 (79%)	138 (100%)	0	100	100
12	L	127/176 (72%)	127 (100%)	0	100	100
12	Z	127/176 (72%)	127 (100%)	0	100	100
13	M	139/216 (64%)	138 (99%)	1 (1%)	87	95
13	a	139/216 (64%)	138 (99%)	1 (1%)	87	95
14	N	122/239 (51%)	121 (99%)	1 (1%)	85	94
14	b	122/239 (51%)	121 (99%)	1 (1%)	85	94
All	All	3474/5912 (59%)	3466 (100%)	8 (0%)	95	99

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	75	ASN
14	b	75	ASN
8	V	89	ASP
13	M	234	THR
2	P	163	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	182	ASN
3	Q	119	GLN
12	Z	182	ASN
13	M	107	HIS
2	P	71	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	7F1	I	300	9	50,53,53	3.55	17 (34%)	57,74,74	1.64	14 (24%)
15	7F1	W	300	9	50,53,53	3.55	17 (34%)	57,74,74	1.64	14 (24%)

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	7F1	I	300	9	-	0/39/50/50	0/5/5/5
15	7F1	W	300	9	-	0/39/50/50	0/5/5/5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	300	7F1	C28-N05	-7.35	1.32	1.46
15	W	300	7F1	C28-N05	-7.35	1.32	1.46
15	I	300	7F1	C27-N05	-5.01	1.33	1.47
15	W	300	7F1	C27-N05	-5.01	1.33	1.47
15	I	300	7F1	C26-N05	-4.71	1.34	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	300	7F1	C02-C03-S01	-4.85	109.64	122.16
15	W	300	7F1	C02-C03-S01	-4.85	109.64	122.16
15	I	300	7F1	C22-C23-C32	-3.80	123.28	127.97
15	W	300	7F1	C22-C23-C32	-3.80	123.28	127.97
15	I	300	7F1	C05-C06-C09	-3.68	123.42	127.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	I	300	7F1	17	0
15	W	300	7F1	17	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	1

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Mol	Chain	Number of breaks
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1:THR	C	2:THR	N	1.69
1	W	1:THR	C	2:THR	N	1.69