



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:07 PM UTC

PDB ID : 1JD2 / pdb_00001jd2
Title : Crystal Structure of the yeast 20S Proteasome:TMC-95A complex: A non-covalent Proteasome Inhibitor
Authors : Groll, M.; Koguchi, Y.; Huber, R.; Kohno, J.
Deposited on : 2001-06-12
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

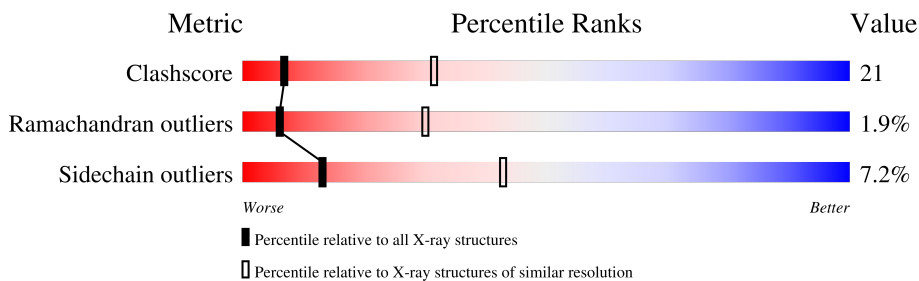
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)











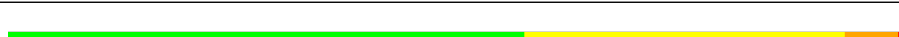


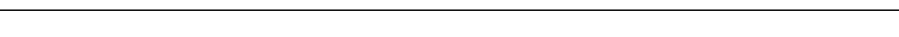
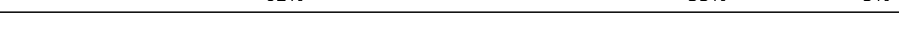
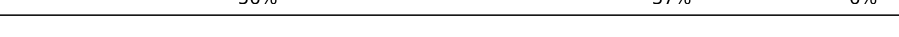






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	V	250	
2	B	244	
2	W	244	
3	C	241	
3	X	241	
4	D	242	
4	Y	242	

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Mol	Chain	Length	Quality of chain
5	E	233	 54% 38% 7%
5	Z	233	 49% 40% 11%
6	1	244	 45% 47% 8%
6	F	244	 49% 46%
7	2	243	 43% 49% 9%
7	G	243	 53% 40% 7%
8	H	222	 53% 41% 6%
8	O	222	 48% 42% 10%
9	I	204	 62% 31% 6%
9	P	204	 57% 38% 5%
10	J	198	 58% 36% 6%
10	Q	198	 57% 37% 6%
11	K	212	 57% 37% 6%
11	R	212	 62% 33% 5%
12	L	222	 56% 37% 6%
12	S	222	 63% 28% 9%
13	M	233	 54% 39% 7%
13	T	233	 52% 44% 5%
14	N	196	 48% 45% 6%
14	U	196	 45% 51% 5%
15	8	5	 20% 40% 20% 20%
15	9	5	 20% 40% 20% 20%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 52549 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 COMPONENT Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0
1	V	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0

- Molecule 2 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	Total 1905	C 1201	N 321	O 380	S 3	0	0	0
2	W	244	Total 1905	C 1201	N 321	O 380	S 3	0	0	0

- Molecule 3 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	Total 1891	C 1181	N 331	O 375	S 4	0	0	0
3	X	241	Total 1891	C 1181	N 331	O 375	S 4	0	0	0

- Molecule 4 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	Total 1862	C 1162	N 314	O 379	S 7	0	0	0
4	Y	242	Total 1862	C 1162	N 314	O 379	S 7	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	LEU	-	insertion	UNP P32379
D	122	ARG	-	insertion	UNP P32379
D	123	PHE	-	insertion	UNP P32379
D	123A	GLY	-	insertion	UNP P32379
D	123B	GLU	-	insertion	UNP P32379
D	123C	GLY	-	insertion	UNP P32379
D	123E	SER	-	insertion	UNP P32379
D	123F	GLY	-	insertion	UNP P32379
D	123G	GLU	-	insertion	UNP P32379
D	125	GLU	ALA	conflict	UNP P32379
D	126	ARG	ALA	conflict	UNP P32379
D	127	LEU	ALA	conflict	UNP P32379
Y	121	LEU	-	insertion	UNP P32379
Y	122	ARG	-	insertion	UNP P32379
Y	123	PHE	-	insertion	UNP P32379
Y	123A	GLY	-	insertion	UNP P32379
Y	123B	GLU	-	insertion	UNP P32379
Y	123C	GLY	-	insertion	UNP P32379
Y	123E	SER	-	insertion	UNP P32379
Y	123F	GLY	-	insertion	UNP P32379
Y	123G	GLU	-	insertion	UNP P32379
Y	125	GLU	ALA	conflict	UNP P32379
Y	126	ARG	ALA	conflict	UNP P32379
Y	127	LEU	ALA	conflict	UNP P32379

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	Z	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	127	TYR	ALA	conflict	UNP P40302
Z	127	TYR	ALA	conflict	UNP P40302

- Molecule 6 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	1	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called PROTEASOME COMPONENT C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	2	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	O	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	P	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
10	Q	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	S	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	T	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	U	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	8	5	Total	C	N	O	0	0	0
			49	33	6	10			
15	9	5	Total	C	N	O	0	0	0
			49	33	6	10			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	1	Total	Mg	0	0
			1	1		
16	F	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	H	1	Total 1	Mg 1	0	0
16	I	2	Total 2	Mg 2	0	0
16	L	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	P	1	Total 1	Mg 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	105	Total 105	O 105	0	0
17	B	80	Total 80	O 80	0	0
17	C	69	Total 69	O 69	0	0
17	D	90	Total 90	O 90	0	0
17	E	55	Total 55	O 55	0	0
17	F	99	Total 99	O 99	0	0
17	G	106	Total 106	O 106	0	0
17	H	114	Total 114	O 114	0	0
17	I	107	Total 107	O 107	0	0
17	J	116	Total 116	O 116	0	0
17	K	103	Total 103	O 103	0	0
17	L	140	Total 140	O 140	0	0
17	M	150	Total 150	O 150	0	0

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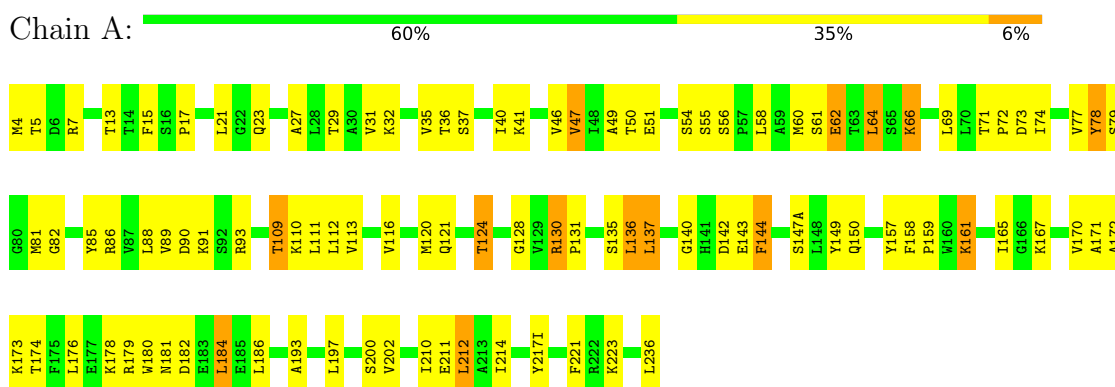
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	N	116	Total O 116 116	0	0
17	O	121	Total O 121 121	0	0
17	P	101	Total O 101 101	0	0
17	Q	121	Total O 121 121	0	0
17	R	107	Total O 107 107	0	0
17	S	144	Total O 144 144	0	0
17	T	142	Total O 142 142	0	0
17	U	118	Total O 118 118	0	0
17	V	104	Total O 104 104	0	0
17	W	74	Total O 74 74	0	0
17	X	70	Total O 70 70	0	0
17	Y	89	Total O 89 89	0	0
17	Z	53	Total O 53 53	0	0
17	1	93	Total O 93 93	0	0
17	2	103	Total O 103 103	0	0
17	8	2	Total O 2 2	0	0
17	9	1	Total O 1 1	0	0

3 Residue-property plots

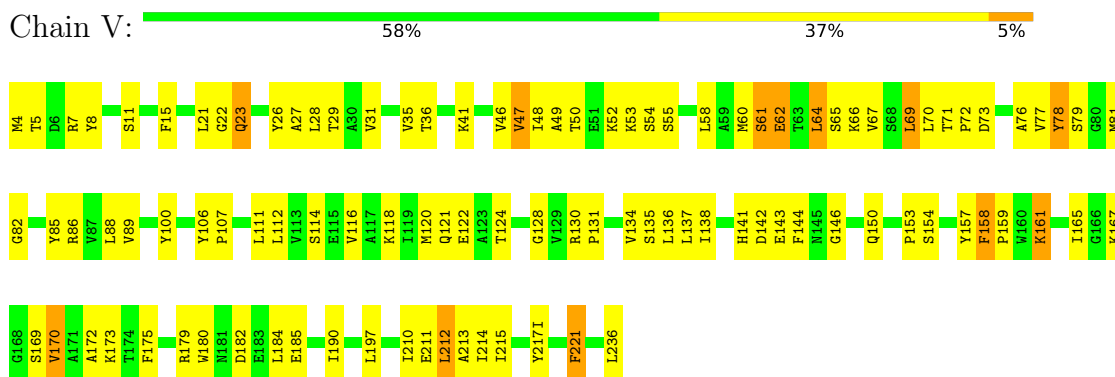
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

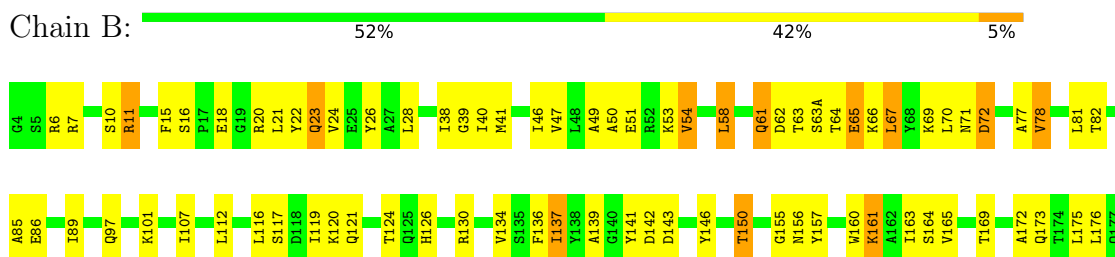
- Molecule 1: PROTEASOME COMPONENT Y7

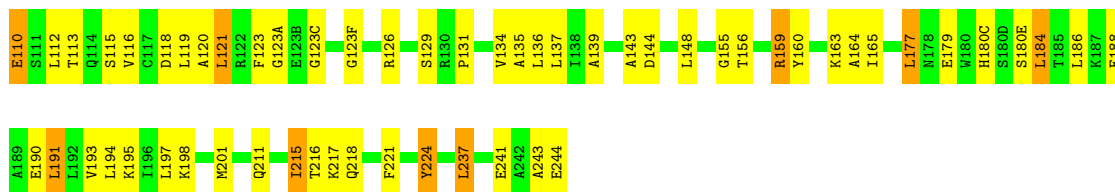


- Molecule 1: PROTEASOME COMPONENT Y7



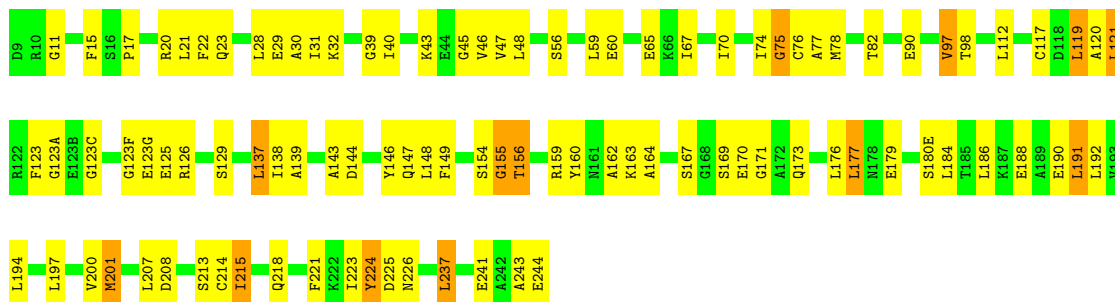
- Molecule 2: PROTEASOME COMPONENT Y13





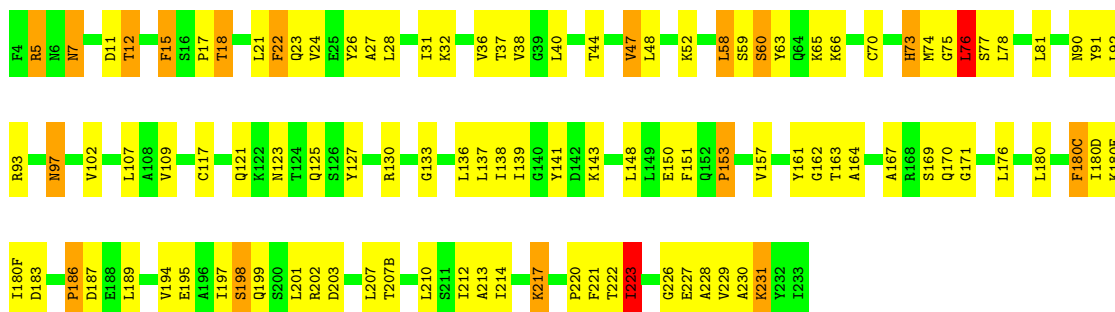
- Molecule 4: PROTEASOME COMPONENT PUP2

Chain Y: 60% 35% 5%



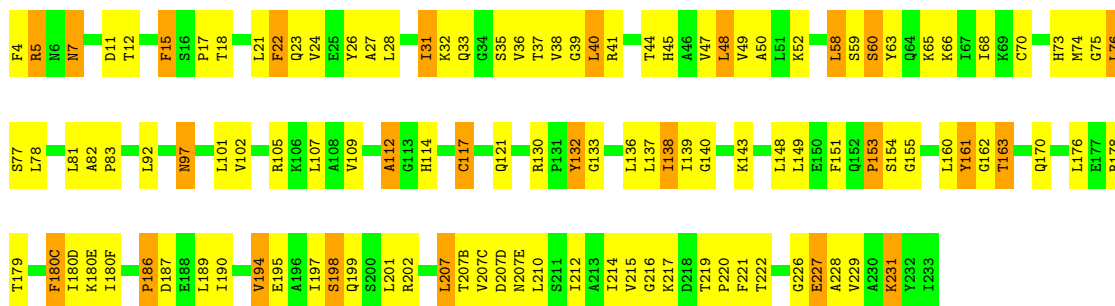
- Molecule 5: PROTEASOME COMPONENT PRE5

Chain E: 54% 38% 7%



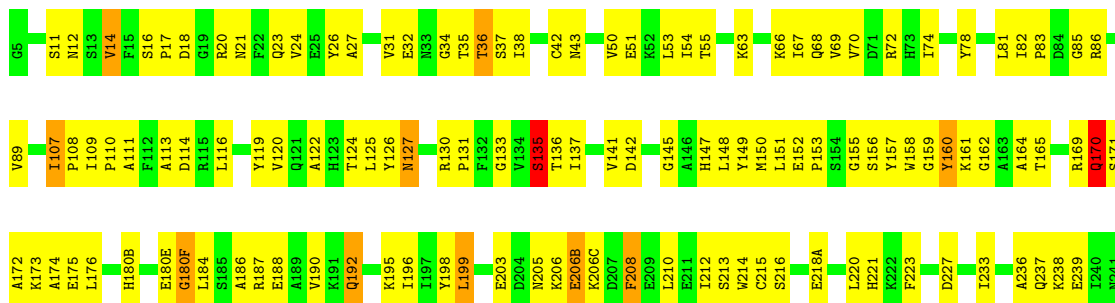
- Molecule 5: PROTEASOME COMPONENT PRE5

Chain Z: 49% 40% 11%

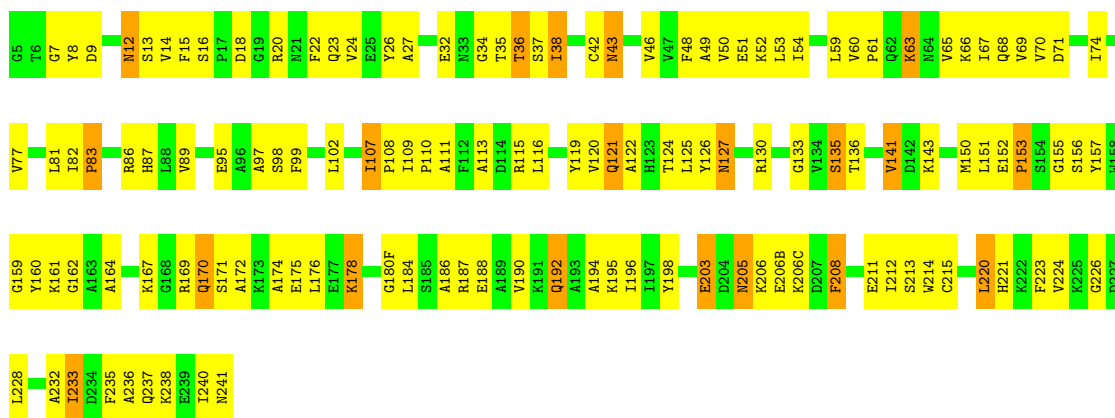


- Molecule 6: PROTEASOME COMPONENT C1

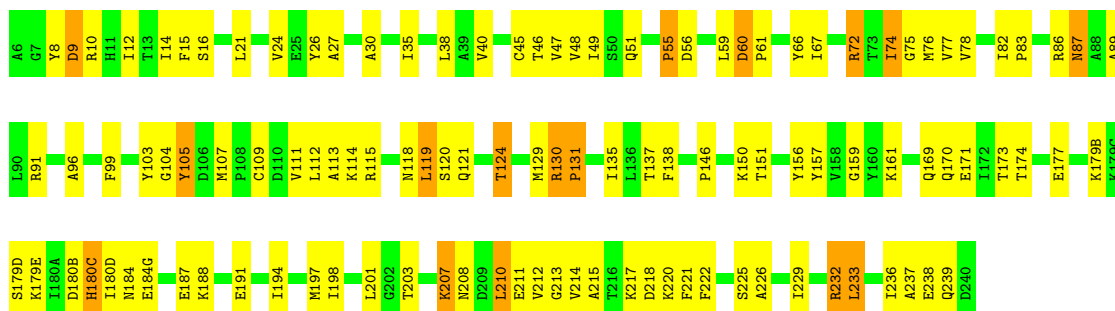
Chain F: 49% 46% 5%



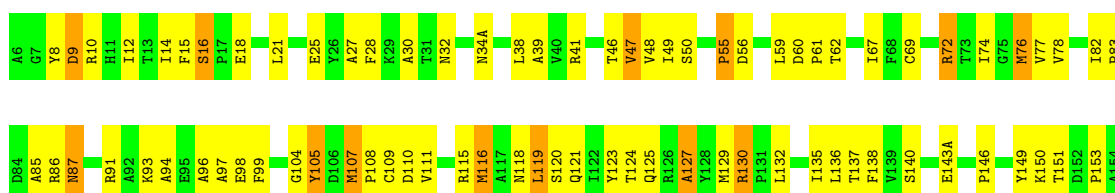
- Molecule 6: PROTEASOME COMPONENT C1

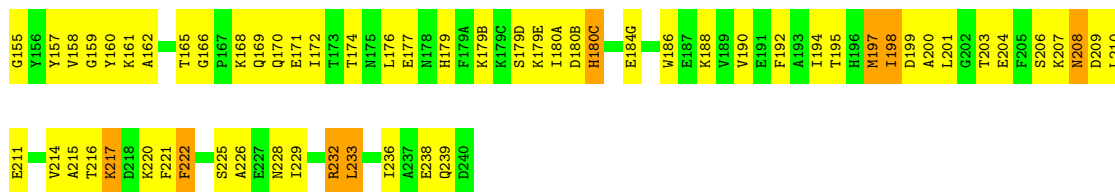


- Molecule 7: PROTEASOME COMPONENT C7-ALPHA



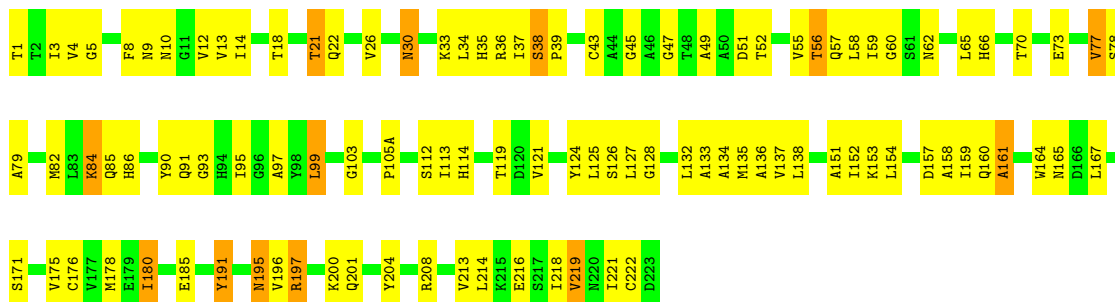
- Molecule 7: PROTEASOME COMPONENT C7-ALPHA





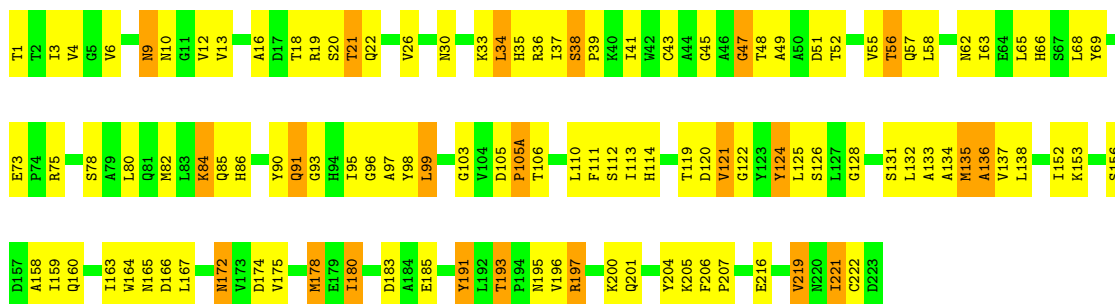
- Molecule 8: PROTEASOME COMPONENT PUP1

Chain H: 53% 41% 6%



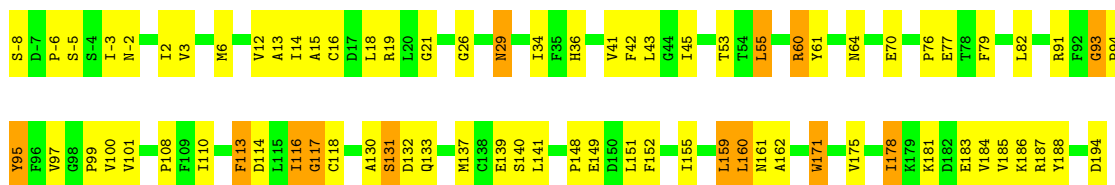
- Molecule 8: PROTEASOME COMPONENT PUP1

Chain O: 48% 42% 10%



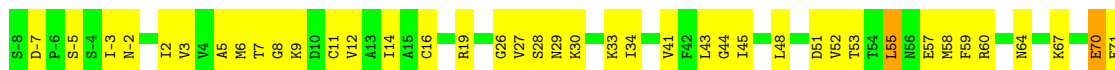
- Molecule 9: PROTEASOME COMPONENT PUP3

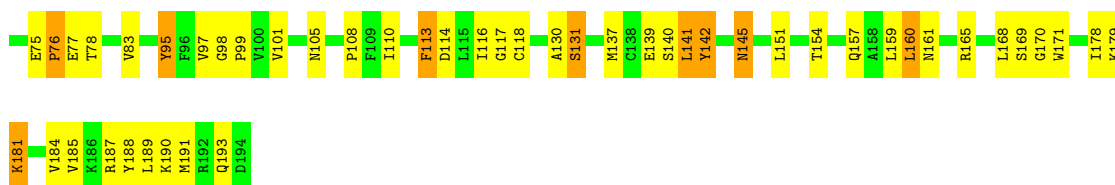
Chain I: 62% 31% 6%



- Molecule 9: PROTEASOME COMPONENT PUP3

Chain P: 57% 38% 5%





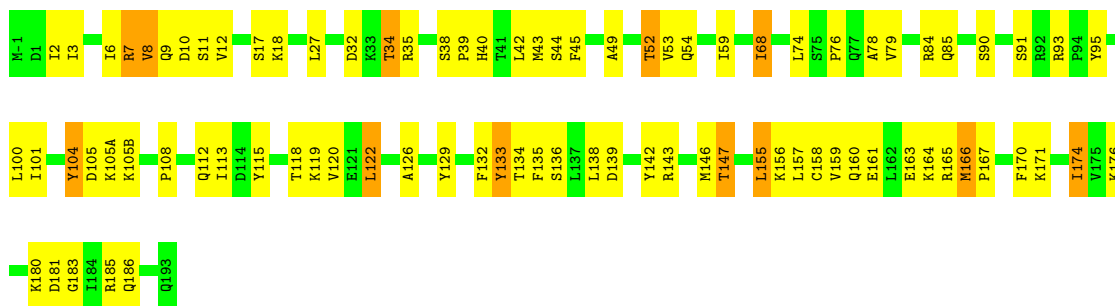
- Molecule 10: PROTEASOME COMPONENT C11

Chain J: 58% 36% 6%



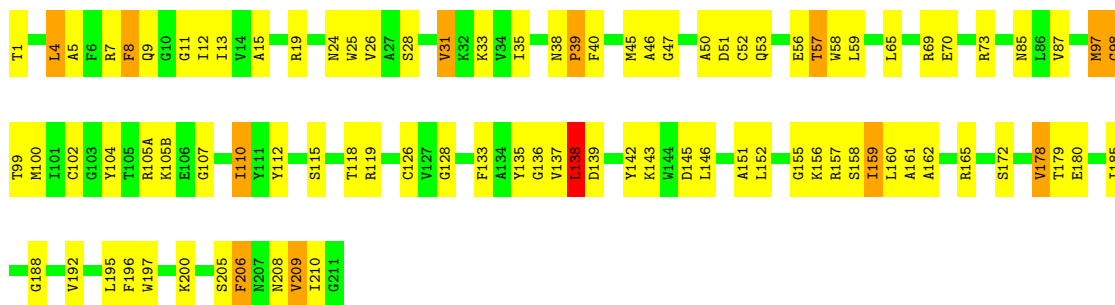
- Molecule 10: PROTEASOME COMPONENT C11

Chain Q: 57% 37% 6%



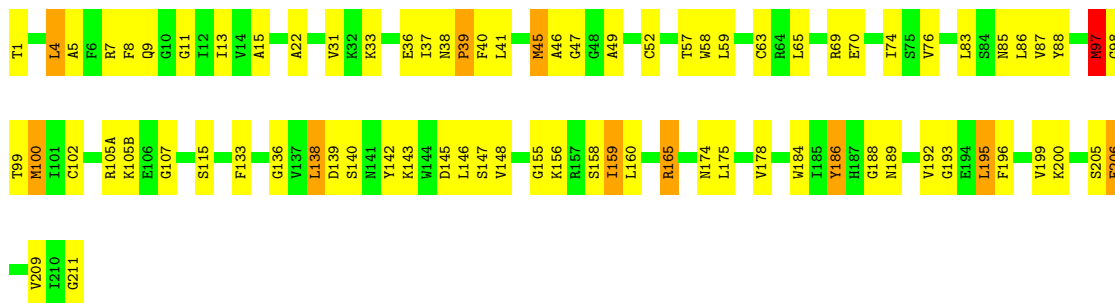
- Molecule 11: PROTEASOME COMPONENT PRE2

Chain K: 57% 37% 6%



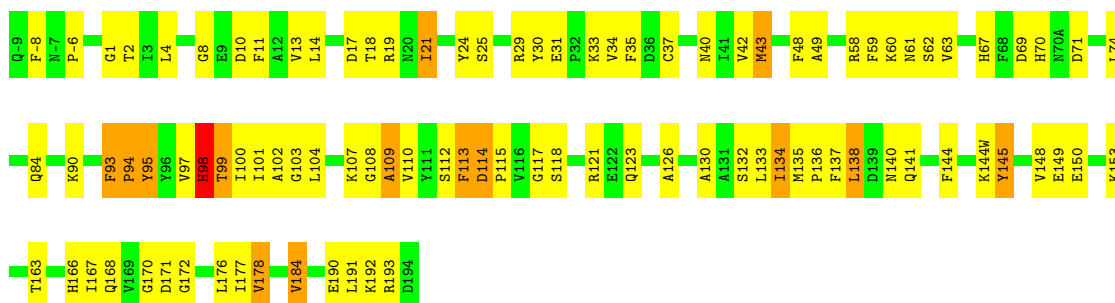
- Molecule 11: PROTEASOME COMPONENT PRE2

Chain R: 62% 33% 5%



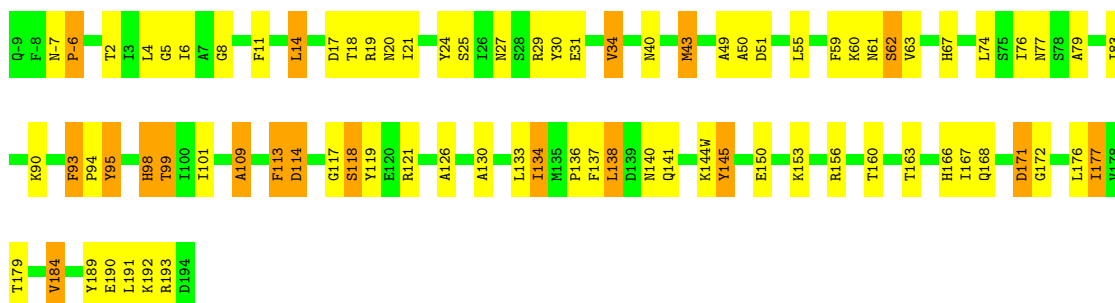
- Molecule 12: PROTEASOME COMPONENT C5

Chain L: 56% 37% 6%



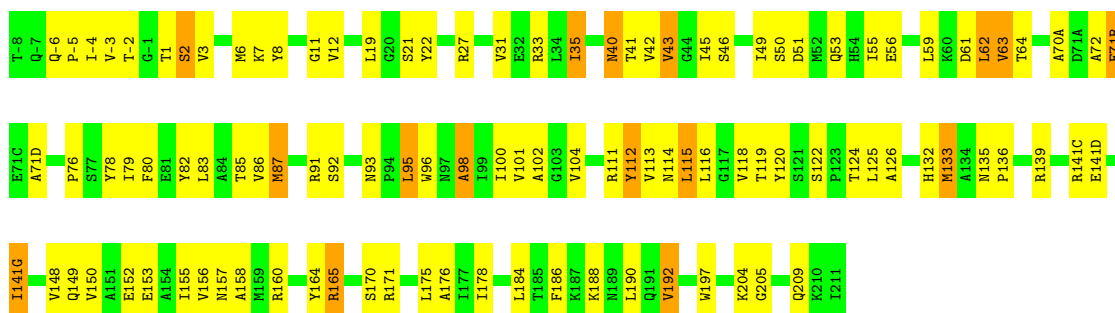
- Molecule 12: PROTEASOME COMPONENT C5

Chain S: 63% 28% 9%



- Molecule 13: PROTEASOME COMPONENT PRE4

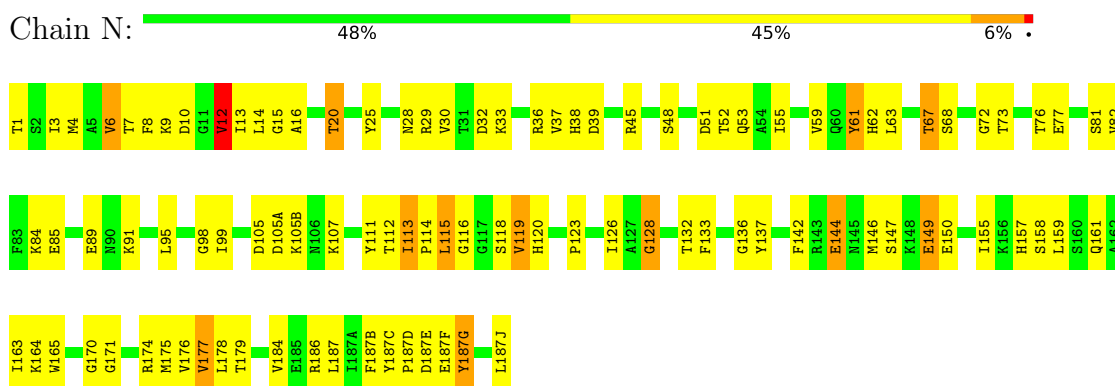
Chain M: 54% 39% 7%



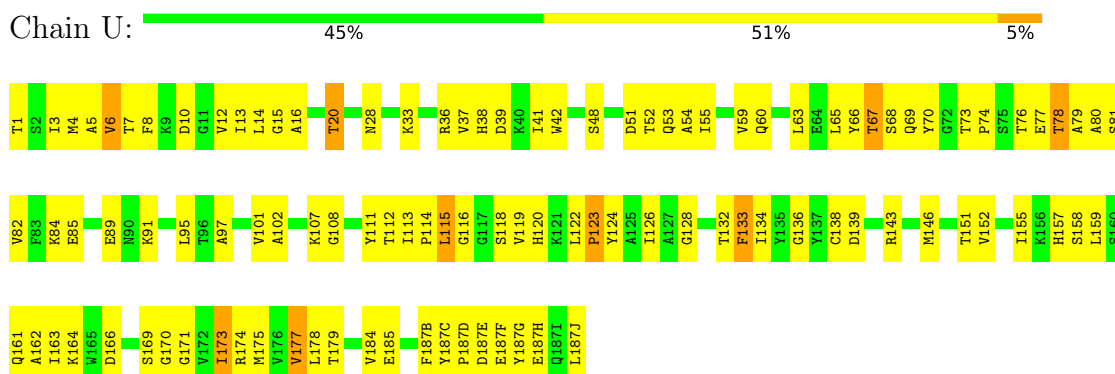
- Molecule 13: PROTEASOME COMPONENT PRE4



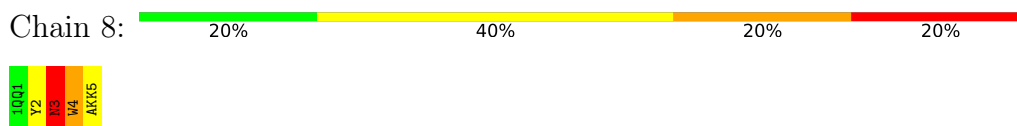
- Molecule 14: PROTEASOME COMPONENT PRE3



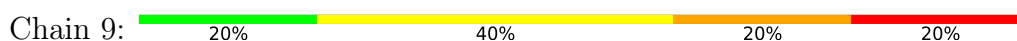
- Molecule 14: PROTEASOME COMPONENT PRE3



- Molecule 15: TMC-95A inhibitor



- Molecule 15: TMC-95A inhibitor





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 301.30Å 144.80Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.251 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	52549	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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: R4K, 1QQ, AKK, MG

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	0.87	1/1952 (0.1%)	1.13	13/2642 (0.5%)
1	V	0.82	1/1952 (0.1%)	1.14	17/2642 (0.6%)
2	B	0.89	0/1935	1.11	14/2618 (0.5%)
2	W	0.84	0/1935	1.13	14/2618 (0.5%)
3	C	0.85	1/1920 (0.1%)	1.11	16/2598 (0.6%)
3	X	0.76	0/1920	1.10	16/2598 (0.6%)
4	D	0.82	1/1887 (0.1%)	1.08	14/2541 (0.6%)
4	Y	0.80	1/1887 (0.1%)	1.06	14/2541 (0.6%)
5	E	0.73	0/1823	1.12	15/2463 (0.6%)
5	Z	0.74	0/1823	1.13	14/2463 (0.6%)
6	1	0.81	1/1937 (0.1%)	1.15	16/2614 (0.6%)
6	F	0.78	0/1937	1.15	16/2614 (0.6%)
7	2	0.96	4/1959 (0.2%)	1.17	14/2652 (0.5%)
7	G	0.86	1/1959 (0.1%)	1.15	18/2652 (0.7%)
8	H	0.97	0/1716	1.18	13/2326 (0.6%)
8	O	0.96	2/1716 (0.1%)	1.16	19/2326 (0.8%)
9	I	1.00	0/1611	1.20	15/2174 (0.7%)
9	P	1.02	0/1611	1.17	12/2174 (0.6%)
10	J	0.96	0/1613	1.13	12/2173 (0.6%)
10	Q	0.93	0/1613	1.14	15/2173 (0.7%)
11	K	0.96	0/1681	1.13	14/2274 (0.6%)
11	R	0.93	1/1681 (0.1%)	1.13	15/2274 (0.7%)
12	L	1.00	0/1795	1.19	15/2420 (0.6%)
12	S	0.92	0/1795	1.19	18/2420 (0.7%)
13	M	0.98	3/1855 (0.2%)	1.15	12/2514 (0.5%)
13	T	0.98	1/1855 (0.1%)	1.17	14/2514 (0.6%)
14	N	1.03	1/1541 (0.1%)	1.16	15/2087 (0.7%)
14	U	0.99	1/1541 (0.1%)	1.14	10/2087 (0.5%)
15	8	2.17	1/20 (5.0%)	3.13	2/26 (7.7%)
15	9	2.59	2/20 (10.0%)	3.59	2/26 (7.7%)
All	All	0.90	23/50490 (0.0%)	1.14	414/68244 (0.6%)

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
11	R	0	1
15	8	0	1
15	9	0	1
All	All	0	3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	107	MET	SD-CE	-7.95	1.59	1.79
13	M	141(G)	ILE	CA-CB	-6.81	1.50	1.54
7	2	76	MET	SD-CE	-6.50	1.63	1.79
13	M	87	MET	SD-CE	-6.15	1.64	1.79
1	A	120	MET	SD-CE	-5.95	1.64	1.79

The worst 5 of 414 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	9	3	ASN	OD1-CG-ND2	-14.75	107.85	122.60
15	8	3	ASN	OD1-CG-ND2	-13.11	109.49	122.60
13	T	27	ARG	N-CA-C	11.40	123.68	111.03
13	M	27	ARG	N-CA-C	11.12	123.37	111.03
2	B	107	ILE	N-CA-C	10.76	117.89	108.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	8	3	ASN	Sidechain
15	9	3	ASN	Sidechain
11	R	186	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	67	0
1	V	1915	0	1926	77	0
2	B	1905	0	1901	81	0
2	W	1905	0	1901	75	0
3	C	1891	0	1900	75	0
3	X	1891	0	1900	97	0
4	D	1862	0	1836	78	0
4	Y	1862	0	1836	73	0
5	E	1795	0	1797	86	0
5	Z	1795	0	1797	117	0
6	1	1897	0	1886	120	0
6	F	1897	0	1886	110	0
7	2	1921	0	1910	110	0
7	G	1921	0	1910	90	0
8	H	1685	0	1688	87	0
8	O	1685	0	1688	92	0
9	I	1581	0	1574	61	0
9	P	1581	0	1574	73	0
10	J	1585	0	1590	57	0
10	Q	1585	0	1590	65	0
11	K	1644	0	1595	80	0
11	R	1644	0	1595	60	0
12	L	1757	0	1711	84	0
12	S	1757	0	1711	83	0
13	M	1824	0	1832	78	0
13	T	1824	0	1832	96	0
14	N	1512	0	1481	77	0
14	U	1512	0	1481	84	0
15	8	49	0	36	8	0
15	9	49	0	36	7	0
16	D	1	0	0	0	0
16	F	2	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	P	1	0	0	0	0
17	1	93	0	0	3	0
17	2	103	0	0	7	0
17	8	2	0	0	0	0
17	9	1	0	0	0	0
17	A	105	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	80	0	0	1	0
17	C	69	0	0	3	0
17	D	90	0	0	6	0
17	E	55	0	0	3	0
17	F	99	0	0	6	0
17	G	106	0	0	3	0
17	H	114	0	0	2	0
17	I	107	0	0	3	0
17	J	116	0	0	6	0
17	K	103	0	0	4	0
17	L	140	0	0	8	0
17	M	150	0	0	3	0
17	N	116	0	0	5	0
17	O	121	0	0	3	0
17	P	101	0	0	4	0
17	Q	121	0	0	5	0
17	R	107	0	0	4	0
17	S	144	0	0	6	0
17	T	142	0	0	8	0
17	U	118	0	0	1	0
17	V	104	0	0	2	0
17	W	74	0	0	2	0
17	X	70	0	0	4	0
17	Y	89	0	0	5	0
17	Z	53	0	0	2	0
All	All	52549	0	49326	2108	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 21.

The worst 5 of 2108 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)
7:2:123:TYR:O	17:2:2009:HOH:O	1.54	1.25
14:N:136:GLY:HA2	14:U:161:GLN:HE21	1.13	1.10
8:H:21:THR:O	15:8:4:R4K:O33	1.75	1.05
14:N:161:GLN:HE21	14:U:136:GLY:HA2	1.21	1.05
8:O:21:THR:O	15:9:4:R4K:O33	1.75	1.04

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 X-ray entries followed by that with respect to entries of similar resolution.

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	248/250 (99%)	207 (84%)	38 (15%)	3 (1%)	10	40
1	V	248/250 (99%)	212 (86%)	32 (13%)	4 (2%)	7	34
2	B	242/244 (99%)	210 (87%)	26 (11%)	6 (2%)	4	23
2	W	242/244 (99%)	209 (86%)	24 (10%)	9 (4%)	2	15
3	C	239/241 (99%)	207 (87%)	25 (10%)	7 (3%)	3	20
3	X	239/241 (99%)	203 (85%)	29 (12%)	7 (3%)	3	20
4	D	240/242 (99%)	205 (85%)	30 (12%)	5 (2%)	5	27
4	Y	240/242 (99%)	210 (88%)	24 (10%)	6 (2%)	4	23
5	E	231/233 (99%)	196 (85%)	30 (13%)	5 (2%)	5	26
5	Z	231/233 (99%)	196 (85%)	28 (12%)	7 (3%)	3	19
6	1	242/244 (99%)	203 (84%)	33 (14%)	6 (2%)	4	23
6	F	242/244 (99%)	206 (85%)	34 (14%)	2 (1%)	16	50
7	2	241/243 (99%)	211 (88%)	24 (10%)	6 (2%)	4	23
7	G	241/243 (99%)	209 (87%)	27 (11%)	5 (2%)	5	27
8	H	220/222 (99%)	192 (87%)	25 (11%)	3 (1%)	9	36
8	O	220/222 (99%)	198 (90%)	17 (8%)	5 (2%)	5	25
9	I	202/204 (99%)	181 (90%)	20 (10%)	1 (0%)	24	60
9	P	202/204 (99%)	185 (92%)	16 (8%)	1 (0%)	24	60
10	J	196/198 (99%)	175 (89%)	17 (9%)	4 (2%)	6	28
10	Q	196/198 (99%)	175 (89%)	16 (8%)	5 (3%)	4	23
11	K	210/212 (99%)	190 (90%)	17 (8%)	3 (1%)	9	36
11	R	210/212 (99%)	187 (89%)	21 (10%)	2 (1%)	12	45
12	L	220/222 (99%)	191 (87%)	27 (12%)	2 (1%)	14	48
12	S	220/222 (99%)	196 (89%)	23 (10%)	1 (0%)	24	60
13	M	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	T	231/233 (99%)	200 (87%)	29 (13%)	2 (1%)	14	48
14	N	194/196 (99%)	175 (90%)	16 (8%)	3 (2%)	8	35
14	U	194/196 (99%)	171 (88%)	20 (10%)	3 (2%)	8	35
15	8	1/5 (20%)	1 (100%)	0	0	100	100
15	9	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6314/6378 (99%)	5504 (87%)	693 (11%)	117 (2%)	6	30

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	167	LYS
2	B	54	VAL
2	B	204(A)	SER
3	C	58	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	209/209 (100%)	197 (94%)	12 (6%)	18	52
1	V	209/209 (100%)	196 (94%)	13 (6%)	16	49
2	B	203/203 (100%)	187 (92%)	16 (8%)	11	39
2	W	203/203 (100%)	185 (91%)	18 (9%)	9	34
3	C	213/213 (100%)	199 (93%)	14 (7%)	15	46
3	X	213/213 (100%)	195 (92%)	18 (8%)	10	36
4	D	198/198 (100%)	186 (94%)	12 (6%)	17	49
4	Y	198/198 (100%)	184 (93%)	14 (7%)	13	43
5	E	192/192 (100%)	175 (91%)	17 (9%)	9	34
5	Z	192/192 (100%)	169 (88%)	23 (12%)	5	22
6	1	201/201 (100%)	184 (92%)	17 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/201 (100%)	184 (92%)	17 (8%)	10	36
7	2	207/207 (100%)	194 (94%)	13 (6%)	16	48
7	G	207/207 (100%)	193 (93%)	14 (7%)	14	45
8	H	181/181 (100%)	172 (95%)	9 (5%)	22	56
8	O	181/181 (100%)	167 (92%)	14 (8%)	12	40
9	I	172/172 (100%)	160 (93%)	12 (7%)	14	44
9	P	172/172 (100%)	161 (94%)	11 (6%)	16	48
10	J	175/175 (100%)	165 (94%)	10 (6%)	18	52
10	Q	175/175 (100%)	164 (94%)	11 (6%)	16	48
11	K	169/169 (100%)	157 (93%)	12 (7%)	13	43
11	R	169/169 (100%)	159 (94%)	10 (6%)	18	50
12	L	185/185 (100%)	172 (93%)	13 (7%)	14	44
12	S	185/185 (100%)	173 (94%)	12 (6%)	15	47
13	M	199/199 (100%)	187 (94%)	12 (6%)	17	50
13	T	199/199 (100%)	188 (94%)	11 (6%)	19	53
14	N	162/162 (100%)	145 (90%)	17 (10%)	6	27
14	U	162/162 (100%)	149 (92%)	13 (8%)	11	38
15	8	2/2 (100%)	2 (100%)	0	100	100
15	9	2/2 (100%)	2 (100%)	0	100	100
All	All	5336/5336 (100%)	4951 (93%)	385 (7%)	13	43

5 of 385 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	R	138	LEU
2	W	63	THR
12	S	99	THR
14	U	115	LEU
3	X	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 210 such sidechains are listed below:

Mol	Chain	Res	Type
8	O	114	HIS

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Mol	Chain	Res	Type
13	T	40	ASN
7	2	33	GLN
9	P	36	HIS
11	R	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	R4K	9	4	15	17,18,19	3.97	9 (52%)	21,27,29	3.44	9 (42%)
15	R4K	8	4	15	17,18,19	3.10	6 (35%)	21,27,29	2.36	11 (52%)

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	R4K	9	4	15	-	3/11/28/30	0/2/2/2
15	R4K	8	4	15	-	2/11/28/30	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	9	4	R4K	C32-N31	-9.31	1.24	1.35
15	9	4	R4K	C55-C50	-8.66	1.30	1.39
15	8	4	R4K	C29-C50	-7.49	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	8	4	R4K	C55-C50	-6.62	1.32	1.39
15	8	4	R4K	C32-N31	-5.59	1.28	1.35

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	9	4	R4K	C51-C50-C55	10.35	128.82	119.81
15	9	4	R4K	C54-C55-C50	-6.80	115.56	121.92
15	8	4	R4K	C51-C50-C55	4.63	123.84	119.81
15	9	4	R4K	C50-C55-N31	4.42	112.56	109.60
15	9	4	R4K	C51-C50-C29	-4.21	124.91	130.81

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	8	4	R4K	O-C-CA-CB
15	8	4	R4K	N-CA-CB-C29
15	9	4	R4K	N-CA-CB-C29
15	9	4	R4K	O-C-CA-CB
15	9	4	R4K	C-CA-CB-C29

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	9	4	R4K	2	0
15	8	4	R4K	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.