wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 06:42 PM EDT

PDB ID	:	1JD2
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 (i) 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 (i)) were used in the production of this report:

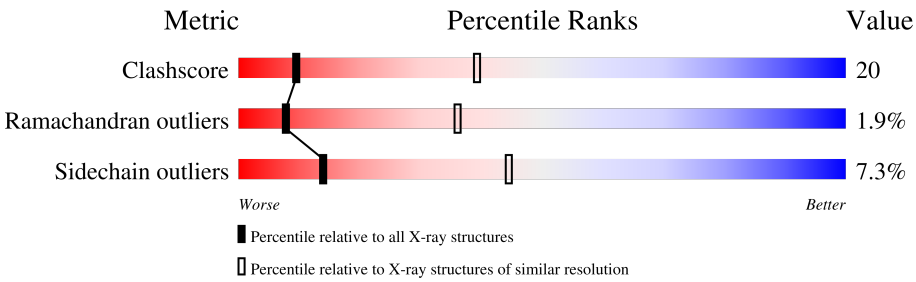
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	66% 32% •
1	V	250	66% 33% •
2	B	244	59% 38% •
2	W	244	61% 34% 5%
3	C	241	63% 33% •
3	X	241	56% 40% •
4	D	242	65% 31% •
4	Y	242	66% 31% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	233	57% 38% 5%
5	Z	233	54% 40% 6%
6	1	244	48% 48% •
6	F	244	53% 44% •
7	2	243	51% 43% 6%
7	G	243	60% 35% 5%
8	H	222	61% 36% •
8	O	222	57% 37% 5%
9	I	204	67% 31% •
9	P	204	63% 33% •
10	J	198	63% 32% 6%
10	Q	198	62% 35% •
11	K	212	64% 32% •
11	R	212	70% 27% •
12	L	222	60% 37% •
12	S	222	66% 31% •
13	M	233	57% 40% •
13	T	233	55% 42% •
14	N	196	56% 42% •
14	U	196	53% 43% 5%
15	8	5	40% 20% 20% 20%
15	9	5	40% 20% 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	1915	1219	315	377	4	0	0	0
1	V	250	1915	1219	315	377	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	1905	1201	321	380	3	0	0	0
2	W	244	1905	1201	321	380	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	1891	1181	331	375	4	0	0	0
3	X	241	1891	1181	331	375	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	1862	1162	314	379	7	0	0	0
4	Y	242	1862	1162	314	379	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
			Total	C	N	O	S			
5	E	233	1795	1129	312	350	4	0	0	0
			Total	C	N	O	S			
5	Z	233	1795	1129	312	350	4	0	0	0

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
			Total	C	N	O	S			
6	F	244	1897	1205	330	358	4	0	0	0
6	1	244	1897	1205	330	358	4	0	0	0

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

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

- Molecule 8 is a protein called PROTEASOME COMPONENT PUP1.

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

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP3.

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

- Molecule 10 is a protein called PROTEASOME COMPONENT C11.

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

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE2.

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

Continued on next page...

Continued from previous page...

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

- Molecule 12 is a protein called PROTEASOME COMPONENT C5.

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

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE4.

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

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE3.

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

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

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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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

- Molecule 17 is water.

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

Continued on next page...

Continued from previous page...

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

3 Residue-property plots (i)

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

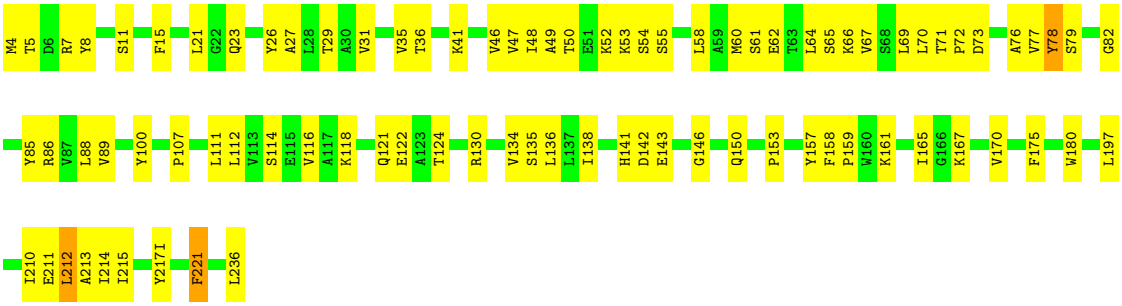
Note EDS was not executed.

• Molecule 1: PROTEASOME COMPONENT Y7

Chain A: 66% 32% •

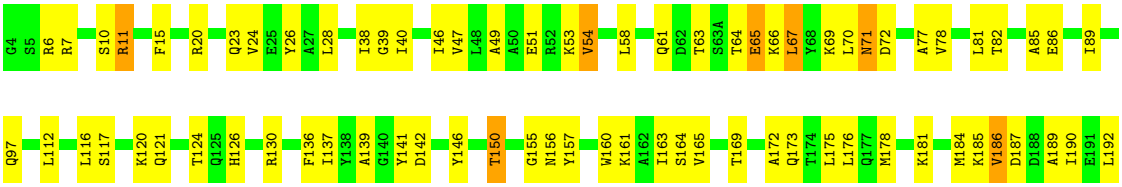
• Molecule 1: PROTEASOME COMPONENT Y7

Chain V: 66% 33% •



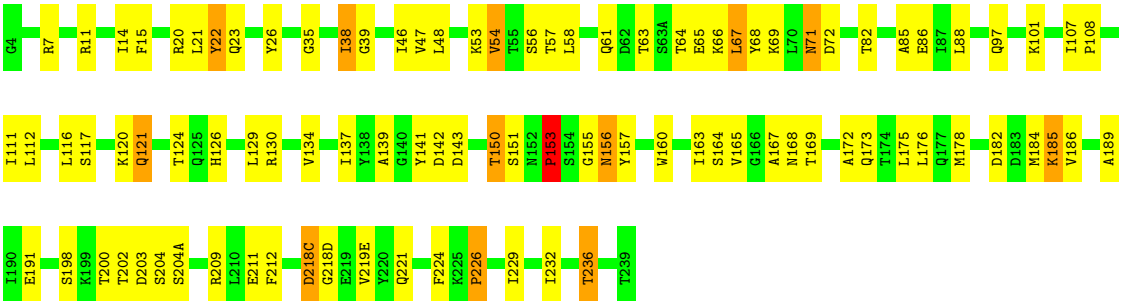
• Molecule 2: PROTEASOME COMPONENT Y13

Chain B: 59% 38% •



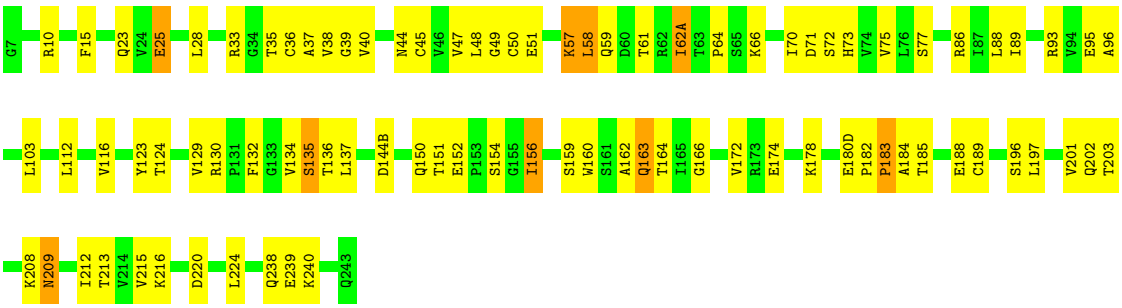
• Molecule 2: PROTEASOME COMPONENT Y13

Chain W:



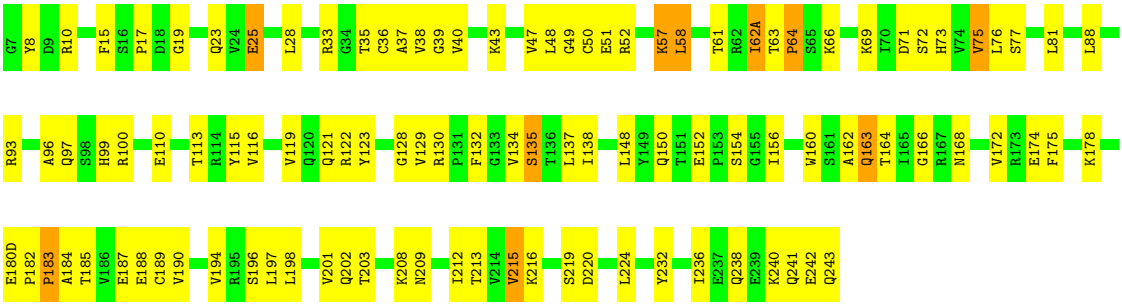
• Molecule 3: PROTEASOME COMPONENT PRE6

Chain C:



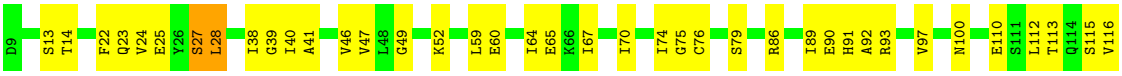
• Molecule 3: PROTEASOME COMPONENT PRE6

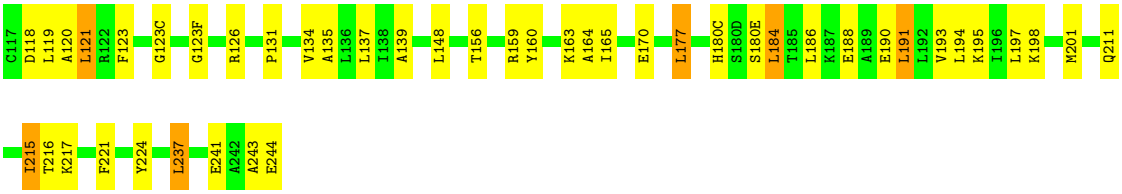
Chain X:



• Molecule 4: PROTEASOME COMPONENT PUP2

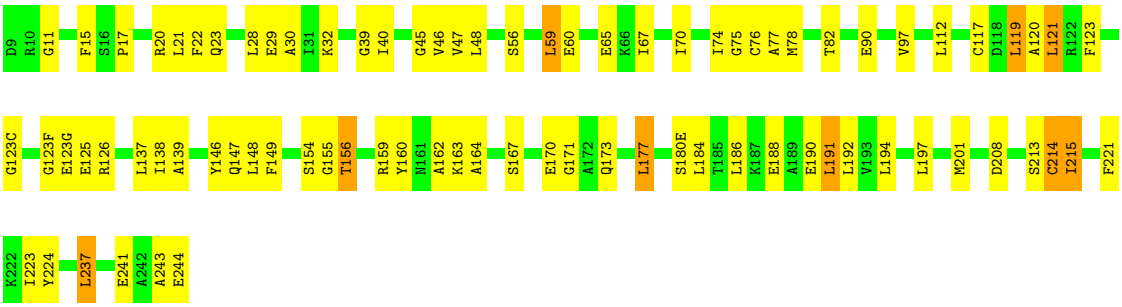
Chain D:





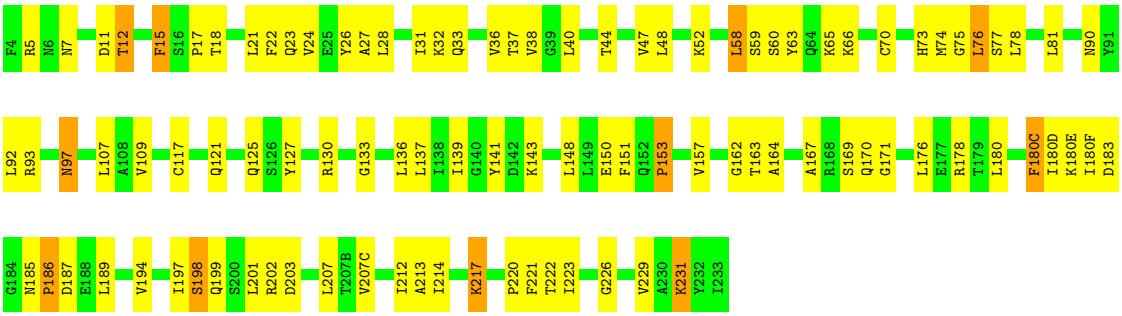
• Molecule 4: PROTEASOME COMPONENT PUP2

Chain Y: 66% 31% •



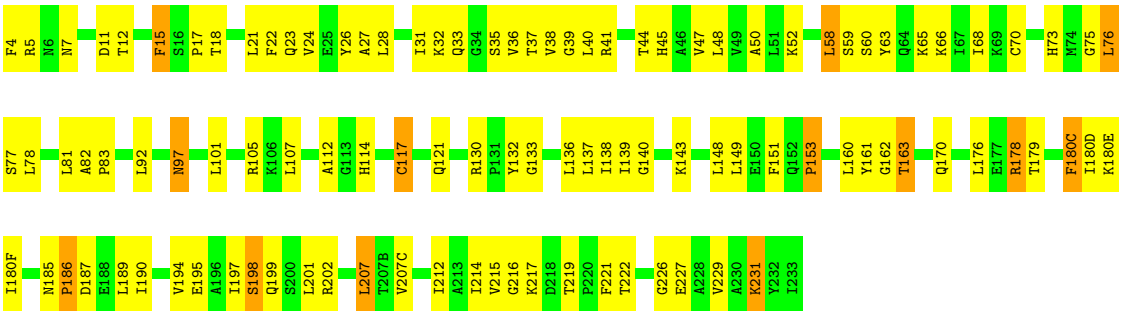
• Molecule 5: PROTEASOME COMPONENT PRE5

Chain E: 57% 38% 5%



• Molecule 5: PROTEASOME COMPONENT PRE5

Chain Z: 54% 40% 6%



• Molecule 6: PROTEASOME COMPONENT C1

Chain F: 53% 44% •

G5 S11 N12 S13 V14 P17 D18 G19 R20 N21 F22 Q23 V24 E25 Y26 A27 V31 E32 N33 G34 T35 T36 S37 I38 C42 N43 V50 E51 K52 L53 I54 K66 I67 Q68 V69 V70 D71 R72 H73 I74 Y78 L81 I82 P83 D84 G85 R86 V89 I107 P108

I109 P110 A111 F112 A113 D114 R115 L116 Y119 V120 Q121 A122 L125 Y126 N127 R130 P131 F132 G133 V134 S135 T136 I137 V141 H147 L148 Y149 M150 L151 E152 P153 S154 G155 S156 Y157 W158 G159 Y160 K161 G162 A163 A164 T165 R169 Q170 S171 A172 K173 A174 E175 L176 E180E G180F

L184 S185 A186 R187 E188 A189 V190 K191 Q192 K195 I196 I197 Y198 L199 E203 D204 N205 K206 E206B K206C D207 F208 E209 L210 E211 I212 S213 W214 C215 S216 E218A T218B N218C H221 K222 F223 D227 I233 A236 Q237 K238 N241

- Molecule 6: PROTEASOME COMPONENT C1

Chain 1:

G5 T6 G7 Y8 D9 N12 S13 V14 F15 D18 G19 R20 Q23 V24 E25 Y26 A27 E32 N33 G34 T35 T36 S37 I38 C42 N43 V46 V47 F48 A49 V50 E51 K52 L53 I54 L59 V60 P61 Q62 K63 N64 V65 K66 I67 Q68 V69 V70 D71 R72 H73 I74 V77

L81 I82 P83 R86 H87 L88 V89 E95 A96 A97 S98 F99 L102 I107 P108 I109 P110 A111 R115 L116 Y119 V120 Q121 A122 L125 Y126 N127 R130 G133 V134 S135 T136 V141 D142 K143 M150 L151 E152 P153 S156 Y157 W158 G159 Y160 K161 G162 A163

A164 K167 G168 R169 Q170 S171 A172 K173 A174 E175 L176 E177 K178 L184 S185 A186 R187 E188 A189 V190 K191 Q192 A193 A194 K195 I196 I197 Y198 E203 D204 N205 K206 E206B K206C D207 F208 E211 I212 S213 W214 C215 N218C G219 L220 H221 K222 F223 V224 D227 L228 A232 I233 D234

F235 A236 Q237 K238 E239 I240 N241

- Molecule 7: PROTEASOME COMPONENT C7-ALPHA

Chain G:

A6 G7 Y8 D9 R10 H11 I12 T13 I14 F15 L21 Y26 A27 A30 I35 V40 C45 T46 V47 V48 I49 S50 Q51 P55 D56 L59 D60 P61 R72 T73 I74 G75 M76 V77 I82 P83 R86 N87 A88 A89 L90 R91 A96 F99 Y105 D106

M107 P108 C109 D110 V111 L112 R115 N118 L119 S120 Q121 T124 M129 R130 P131 T137 F138 P146 K150 T151 Y156 Y157 V158 G159 Q169 Q170 E171 I172 T173 T174 E177 S179D K179E I180A D180B H180C I180D N184 E184G E187 K188 E191 I194 I198

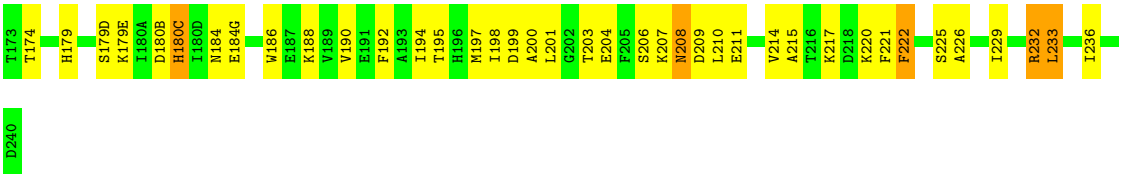
L201 G202 T203 E204 K207 N208 D209 L210 E211 V212 G213 V214 A215 T216 K217 D218 K220 F221 F222 S225 A226 I229 R232 L233 I236 A237 E238 Q239 D240

- Molecule 7: PROTEASOME COMPONENT C7-ALPHA

Chain 2:

A6 D9 I12 T13 I14 F15 S16 P17 E18 L21 E25 Y26 A27 F28 K29 L38 A39 V40 R41 T46 V47 V48 I49 S50 P55 D56 L59 D60 P61 T62 I67 F68 C69 R72 M76 V77 V78 I82 P83 D84 A85 R86 N87 R91 A92 K93

A96 F99 Y105 D106 M107 P108 C109 D110 V111 R115 N118 L119 S120 Q121 I122 Y123 T124 A127 Y128 M129 R130 P131 L132 L136 T137 F138 V139 S140 E143A P146 Y149 K150 T151 D152 P153 Y157 V158 G159 Y160 K161 A162 T165 G166 P167 K168 Q169 Q170 E171 I172

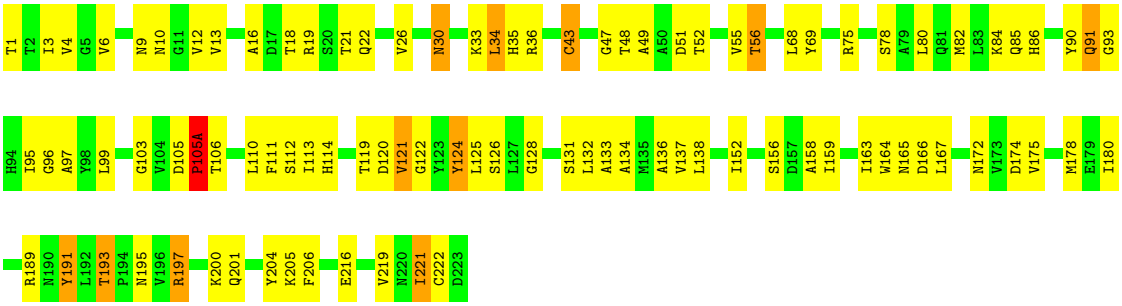


• Molecule 8: PROTEASOME COMPONENT PUP1

Chain H:

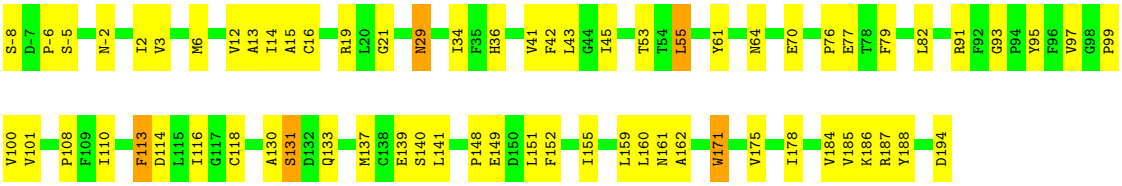
• Molecule 8: PROTEASOME COMPONENT PUP1

Chain O:



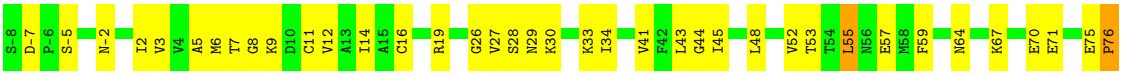
• Molecule 9: PROTEASOME COMPONENT PUP3

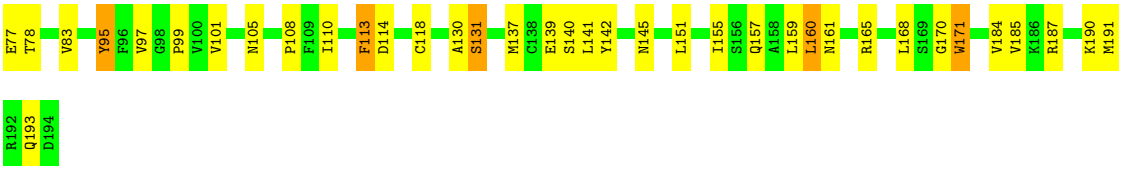
Chain I:



• Molecule 9: PROTEASOME COMPONENT PUP3

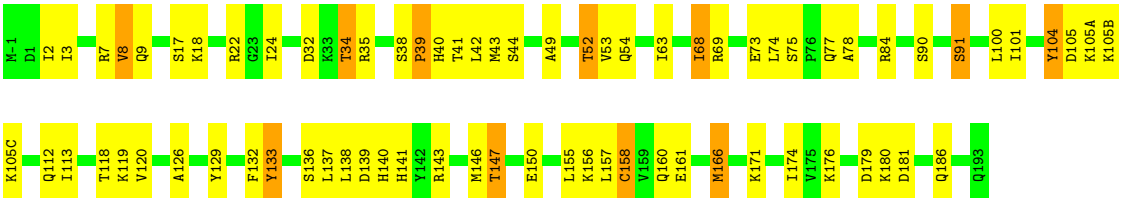
Chain P:





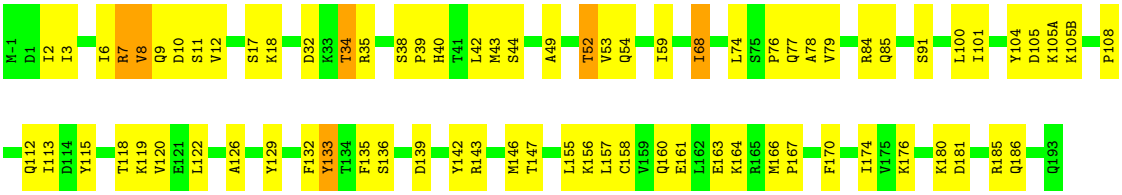
• Molecule 10: PROTEASOME COMPONENT C11

Chain J: 63% 32% 6%



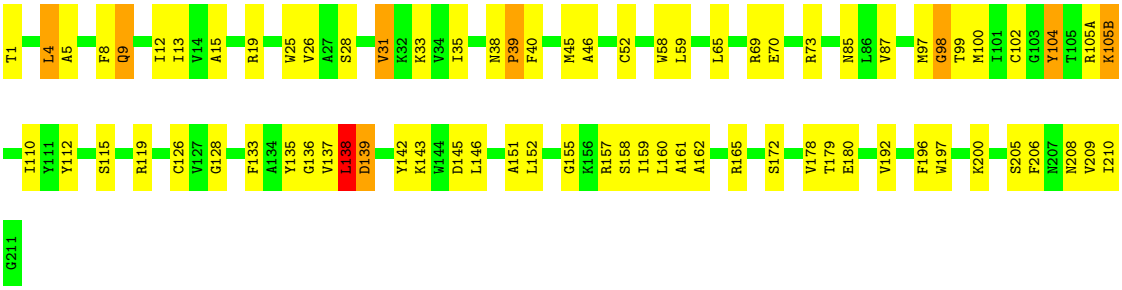
• Molecule 10: PROTEASOME COMPONENT C11

Chain Q: 62% 35% •



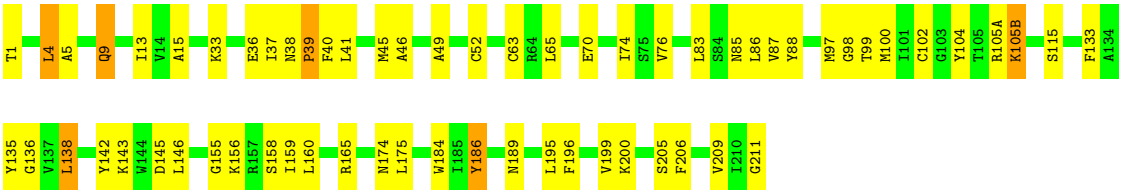
• Molecule 11: PROTEASOME COMPONENT PRE2

Chain K: 64% 32% •



• Molecule 11: PROTEASOME COMPONENT PRE2

Chain R: 70% 27% •

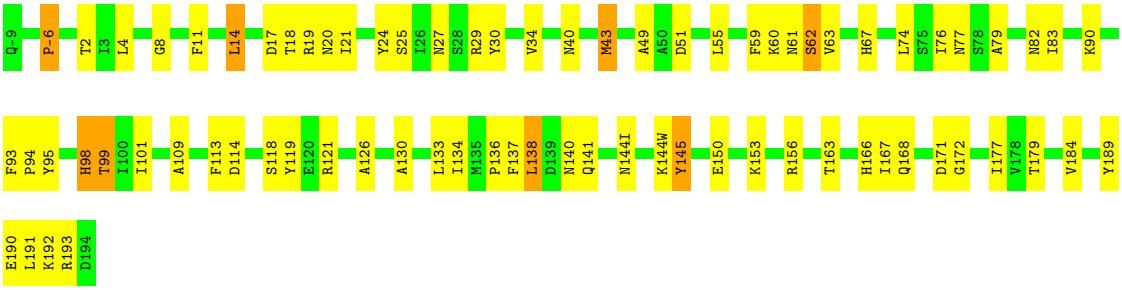


• Molecule 12: PROTEASOME COMPONENT C5

Chain L:

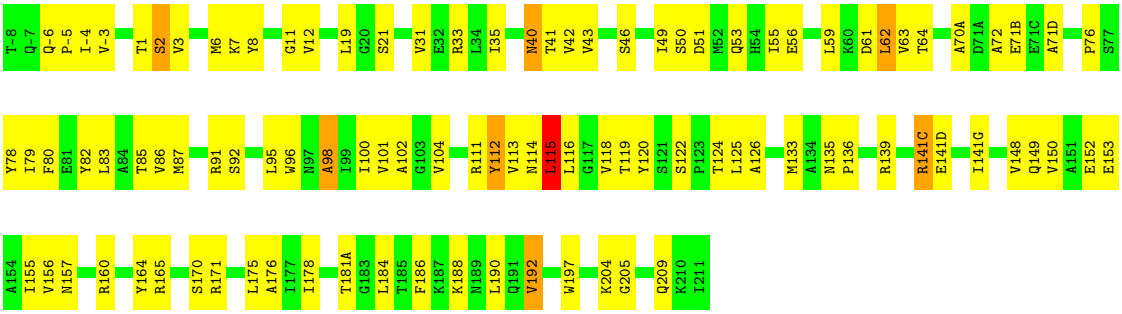
• Molecule 12: PROTEASOME COMPONENT C5

Chain S:



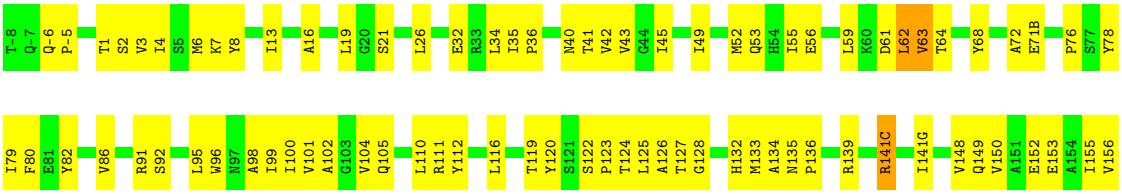
• Molecule 13: PROTEASOME COMPONENT PRE4

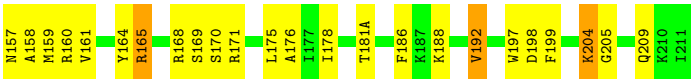
Chain M:



• Molecule 13: PROTEASOME COMPONENT PRE4

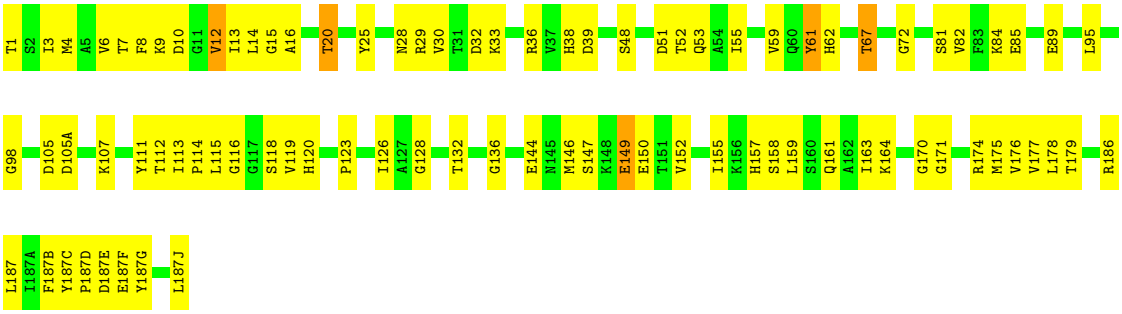
Chain T:





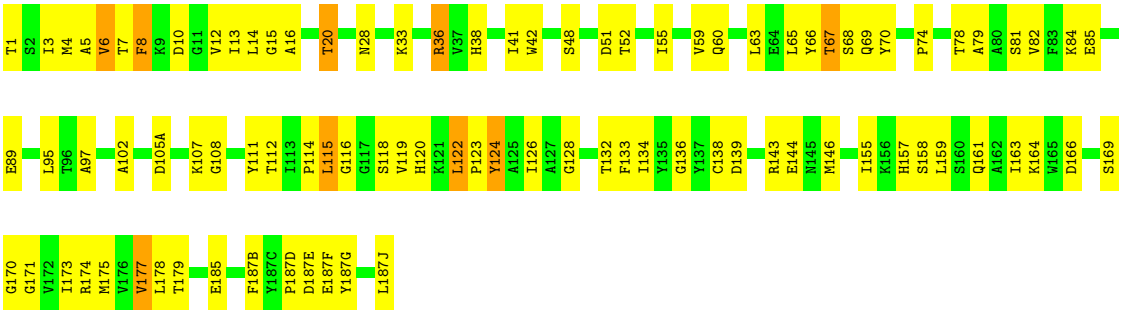
• Molecule 14: PROTEASOME COMPONENT PRE3

Chain N:



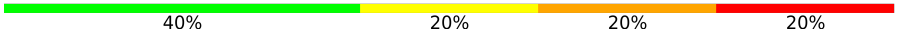
• Molecule 14: PROTEASOME COMPONENT PRE3

Chain U:



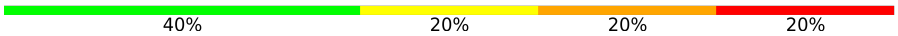
• Molecule 15: TMC-95A inhibitor

Chain 8:



• Molecule 15: TMC-95A inhibitor

Chain 9:



4 Data and refinement statistics (i)

Xtriage (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.	Xtriage
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: AKK, R4K, 1QQ, 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	0.65	0/1952	0.81	0/2642
1	V	0.62	0/1952	0.79	0/2642
2	B	0.65	0/1935	0.79	0/2618
2	W	0.62	0/1935	0.79	0/2618
3	C	0.65	0/1920	0.80	1/2598 (0.0%)
3	X	0.59	0/1920	0.78	0/2598
4	D	0.63	0/1887	0.78	1/2541 (0.0%)
4	Y	0.63	0/1887	0.78	2/2541 (0.1%)
5	E	0.57	0/1823	0.77	0/2463
5	Z	0.57	0/1823	0.78	0/2463
6	1	0.64	0/1937	0.79	0/2614
6	F	0.61	0/1937	0.78	1/2614 (0.0%)
7	2	0.71	0/1959	0.80	0/2652
7	G	0.65	0/1959	0.80	0/2652
8	H	0.72	0/1716	0.85	0/2326
8	O	0.69	1/1716 (0.1%)	0.81	0/2326
9	I	0.72	0/1611	0.84	0/2174
9	P	0.76	0/1611	0.85	2/2174 (0.1%)
10	J	0.70	1/1613 (0.1%)	0.82	0/2173
10	Q	0.69	0/1613	0.80	0/2173
11	K	0.71	0/1681	0.81	1/2274 (0.0%)
11	R	0.69	0/1681	0.80	0/2274
12	L	0.75	1/1795 (0.1%)	0.82	2/2420 (0.1%)
12	S	0.68	0/1795	0.83	1/2420 (0.0%)
13	M	0.68	0/1855	0.80	1/2514 (0.0%)
13	T	0.70	0/1855	0.84	3/2514 (0.1%)
14	N	0.75	0/1541	0.81	1/2087 (0.0%)
14	U	0.73	0/1541	0.78	1/2087 (0.0%)
15	8	1.96	0/20	2.20	2/26 (7.7%)
15	9	2.53	0/20	2.48	2/26 (7.7%)
All	All	0.67	3/50490 (0.0%)	0.81	21/68244 (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
11	R	0	1
15	8	0	1
15	9	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	37	CYS	CB-SG	-5.27	1.73	1.81
8	O	43	CYS	CB-SG	-5.14	1.73	1.81
10	J	158	CYS	CB-SG	-5.06	1.73	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	9	3	ASN	CB-CG-OD1	-7.24	107.12	121.60
15	8	3	ASN	CB-CG-OD1	-7.21	107.18	121.60
13	T	98	ALA	N-CA-C	-6.22	94.20	111.00
15	9	3	ASN	OD1-CG-ND2	-6.11	107.85	121.90
9	P	95	TYR	N-CA-C	-6.02	94.74	111.00

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	59	0
1	V	1915	0	1926	71	0
2	B	1905	0	1901	75	0
2	W	1905	0	1901	75	0
3	C	1891	0	1900	68	0
3	X	1891	0	1900	92	0
4	D	1862	0	1836	75	0
4	Y	1862	0	1836	67	0
5	E	1795	0	1797	78	0
5	Z	1795	0	1797	111	0
6	1	1897	0	1886	111	0
6	F	1897	0	1886	101	0
7	2	1921	0	1910	95	0
7	G	1921	0	1910	83	0
8	H	1685	0	1688	75	0
8	O	1685	0	1688	83	0
9	I	1581	0	1574	56	0
9	P	1581	0	1574	67	0
10	J	1585	0	1590	55	0
10	Q	1585	0	1590	62	0
11	K	1644	0	1595	72	0
11	R	1644	0	1595	54	0
12	L	1757	0	1711	79	0
12	S	1757	0	1711	80	0
13	M	1824	0	1832	74	0
13	T	1824	0	1832	90	0
14	N	1512	0	1481	75	0
14	U	1512	0	1481	71	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	6	0
17	8	2	0	0	0	0
17	9	1	0	0	0	0
17	A	105	0	0	1	0

Continued on next page...

Continued from previous page...

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	1936	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 1936 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%)	13	48
1	V	248/250 (99%)	212 (86%)	32 (13%)	4 (2%)	9	40
2	B	242/244 (99%)	210 (87%)	26 (11%)	6 (2%)	5	28
2	W	242/244 (99%)	209 (86%)	24 (10%)	9 (4%)	3	19
3	C	239/241 (99%)	207 (87%)	25 (10%)	7 (3%)	4	24
3	X	239/241 (99%)	203 (85%)	29 (12%)	7 (3%)	4	24
4	D	240/242 (99%)	205 (85%)	30 (12%)	5 (2%)	7	33
4	Y	240/242 (99%)	210 (88%)	24 (10%)	6 (2%)	5	28
5	E	231/233 (99%)	196 (85%)	30 (13%)	5 (2%)	6	31
5	Z	231/233 (99%)	196 (85%)	28 (12%)	7 (3%)	4	24
6	1	242/244 (99%)	203 (84%)	33 (14%)	6 (2%)	5	28
6	F	242/244 (99%)	206 (85%)	34 (14%)	2 (1%)	19	57
7	2	241/243 (99%)	211 (88%)	24 (10%)	6 (2%)	5	28
7	G	241/243 (99%)	209 (87%)	27 (11%)	5 (2%)	7	33
8	H	220/222 (99%)	192 (87%)	25 (11%)	3 (1%)	11	43
8	O	220/222 (99%)	198 (90%)	17 (8%)	5 (2%)	6	30
9	I	202/204 (99%)	181 (90%)	20 (10%)	1 (0%)	29	68
9	P	202/204 (99%)	185 (92%)	16 (8%)	1 (0%)	29	68
10	J	196/198 (99%)	175 (89%)	17 (9%)	4 (2%)	7	34
10	Q	196/198 (99%)	175 (89%)	16 (8%)	5 (3%)	5	27
11	K	210/212 (99%)	190 (90%)	17 (8%)	3 (1%)	11	43
11	R	210/212 (99%)	187 (89%)	21 (10%)	2 (1%)	15	53
12	L	220/222 (99%)	191 (87%)	27 (12%)	2 (1%)	17	55
12	S	220/222 (99%)	196 (89%)	23 (10%)	1 (0%)	29	68
13	M	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	9	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	T	231/233 (99%)	200 (87%)	29 (13%)	2 (1%)	17	55
14	N	194/196 (99%)	175 (90%)	16 (8%)	3 (2%)	10	42
14	U	194/196 (99%)	171 (88%)	20 (10%)	3 (2%)	10	42
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%)	8	36

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%)	198 (95%)	11 (5%)	22	58
1	V	209/209 (100%)	200 (96%)	9 (4%)	29	66
2	B	203/203 (100%)	188 (93%)	15 (7%)	13	44
2	W	203/203 (100%)	186 (92%)	17 (8%)	11	38
3	C	213/213 (100%)	194 (91%)	19 (9%)	9	35
3	X	213/213 (100%)	196 (92%)	17 (8%)	12	40
4	D	198/198 (100%)	185 (93%)	13 (7%)	16	49
4	Y	198/198 (100%)	185 (93%)	13 (7%)	16	49
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	25
5	Z	192/192 (100%)	173 (90%)	19 (10%)	8	30
6	1	201/201 (100%)	181 (90%)	20 (10%)	7	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/201 (100%)	183 (91%)	18 (9%)	9	35
7	2	207/207 (100%)	188 (91%)	19 (9%)	9	34
7	G	207/207 (100%)	191 (92%)	16 (8%)	13	42
8	H	181/181 (100%)	169 (93%)	12 (7%)	16	49
8	O	181/181 (100%)	167 (92%)	14 (8%)	13	42
9	I	172/172 (100%)	160 (93%)	12 (7%)	15	47
9	P	172/172 (100%)	163 (95%)	9 (5%)	23	59
10	J	175/175 (100%)	164 (94%)	11 (6%)	18	51
10	Q	175/175 (100%)	165 (94%)	10 (6%)	20	56
11	K	169/169 (100%)	156 (92%)	13 (8%)	13	42
11	R	169/169 (100%)	158 (94%)	11 (6%)	17	50
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	50
12	S	185/185 (100%)	173 (94%)	12 (6%)	17	50
13	M	199/199 (100%)	186 (94%)	13 (6%)	17	50
13	T	199/199 (100%)	188 (94%)	11 (6%)	21	57
14	N	162/162 (100%)	152 (94%)	10 (6%)	18	52
14	U	162/162 (100%)	147 (91%)	15 (9%)	9	33
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%)	4944 (93%)	392 (7%)	14	44

5 of 392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	R	39	PRO
1	V	236	LEU
11	R	138	LEU
13	T	181(A)	THR
2	W	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
12	S	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	W	156	ASN
12	S	144(B)	ASN
13	T	172	ASN
3	X	163	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	8	4	15	16,18,19	3.01	5 (31%)	18,27,29	2.51	8 (44%)
15	R4K	9	4	15	16,18,19	3.83	8 (50%)	18,27,29	3.62	10 (55%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	9	4	R4K	C32-N31	-9.11	1.24	1.35
15	9	4	R4K	C55-C50	-8.49	1.30	1.39
15	8	4	R4K	C29-C50	-6.85	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	8	4	R4K	C55-C50	-6.49	1.32	1.39
15	8	4	R4K	C32-N31	-5.46	1.28	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	9	4	R4K	C51-C50-C55	10.34	128.82	119.81
15	9	4	R4K	C54-C55-C50	-6.68	115.56	121.91
15	8	4	R4K	C51-C50-C55	4.63	123.84	119.81
15	9	4	R4K	C50-C55-N31	4.43	112.56	109.59
15	8	4	R4K	C54-C55-C50	-4.04	118.06	121.91

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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.