



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:20 AM GMT

PDB ID : 3DY3
Title : Crystal structure of yeast 20S proteasome in complex with the epimer form of spiro lactacystin
Authors : Groll, M.; Balskus, E.; Jacobsen, E.
Deposited on : 2008-07-25
Resolution : 2.81 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

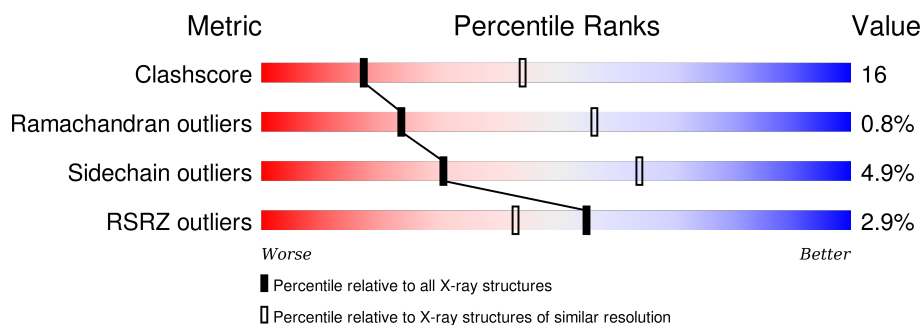
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>3%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	O	250	<div> <div>6%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
2	B	244	<div> <div>5%</div> <div>63%</div> <div>33%</div> <div>.</div> </div>
2	P	244	<div> <div>6%</div> <div>63%</div> <div>33%</div> <div>.</div> </div>
3	C	241	<div> <div>7%</div> <div>63%</div> <div>36%</div> <div>.</div> </div>
3	Q	241	<div> <div>9%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>
4	D	242	<div> <div>5%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SLR	Y	301	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50584 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
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- 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	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- 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	T	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	U	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	V	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	W	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	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			
11	Y	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	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

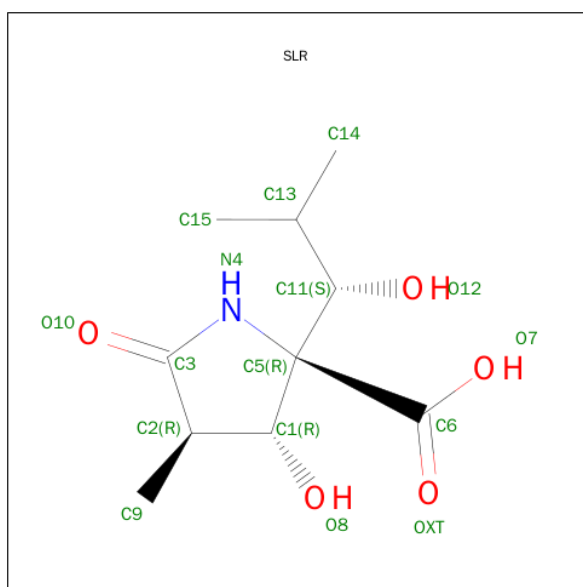
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	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	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is (3R,4R)-3-HYDROXY-2-[(1S)-1-HYDROXY-2-METHYLPROPYL]-4-METHYL-5-OXO-D-PROLINE (three-letter code: SLR) (formula: C₁₀H₁₇NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			15	10	1	4		
15	Y	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 16 is water.

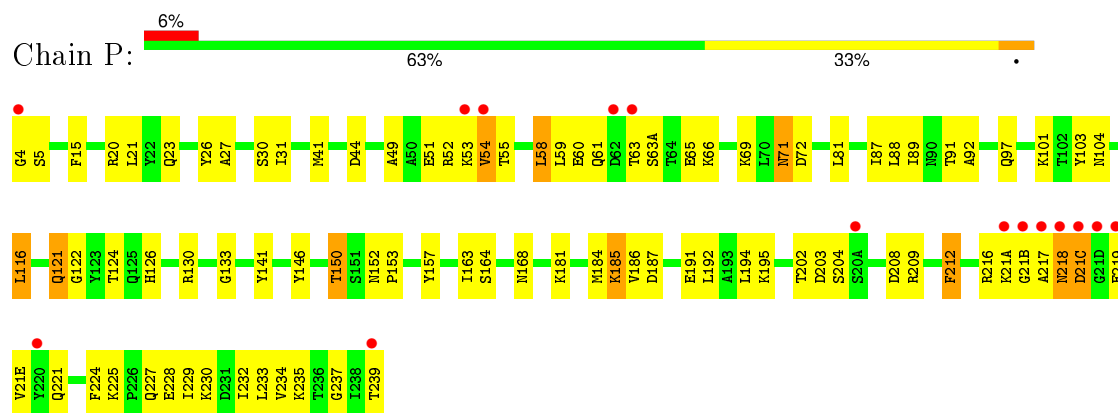
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	35	Total	O	0	0
			35	35		
16	B	27	Total	O	0	0
			27	27		
16	C	32	Total	O	0	0
			32	32		
16	D	23	Total	O	0	0
			23	23		
16	E	15	Total	O	0	0
			15	15		
16	F	35	Total	O	0	0
			35	35		
16	G	51	Total	O	0	0
			51	51		
16	H	41	Total	O	0	0
			41	41		
16	I	51	Total	O	0	0
			51	51		
16	J	38	Total	O	0	0
			38	38		

Continued on next page...

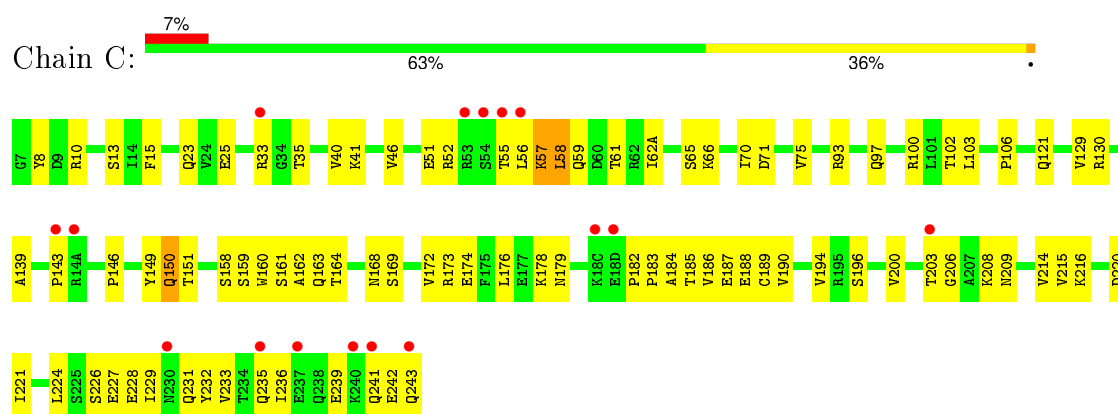
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	33	Total 33	O 33	0	0
16	L	43	Total 43	O 43	0	0
16	M	56	Total 56	O 56	0	0
16	N	49	Total 49	O 49	0	0
16	O	28	Total 28	O 28	0	0
16	P	18	Total 18	O 18	0	0
16	Q	19	Total 19	O 19	0	0
16	R	19	Total 19	O 19	0	0
16	S	16	Total 16	O 16	0	0
16	T	30	Total 30	O 30	0	0
16	U	48	Total 48	O 48	0	0
16	V	36	Total 36	O 36	0	0
16	W	40	Total 40	O 40	0	0
16	X	36	Total 36	O 36	0	0
16	Y	36	Total 36	O 36	0	0
16	Z	36	Total 36	O 36	0	0
16	1	64	Total 64	O 64	0	0
16	2	51	Total 51	O 51	0	0

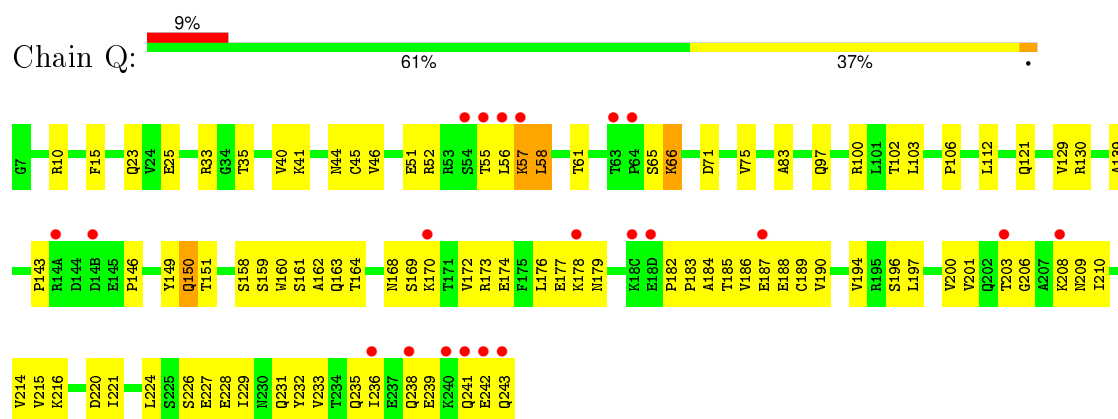
- Molecule 2: Proteasome component Y13



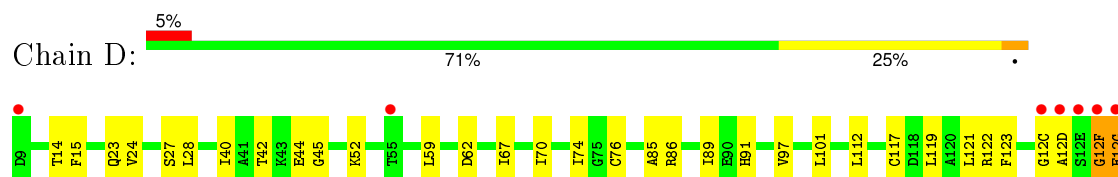
- Molecule 3: Proteasome component PRE6

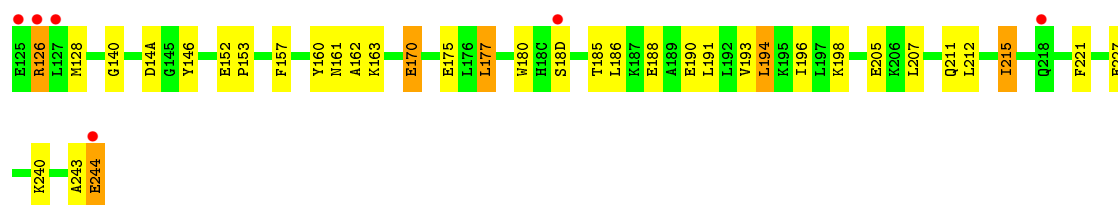


- Molecule 3: Proteasome component PRE6

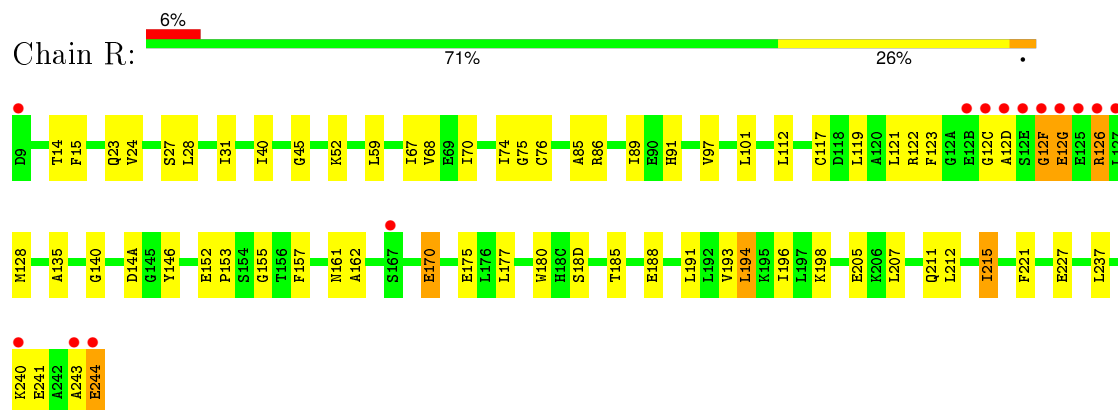


- Molecule 4: Proteasome component PUP2

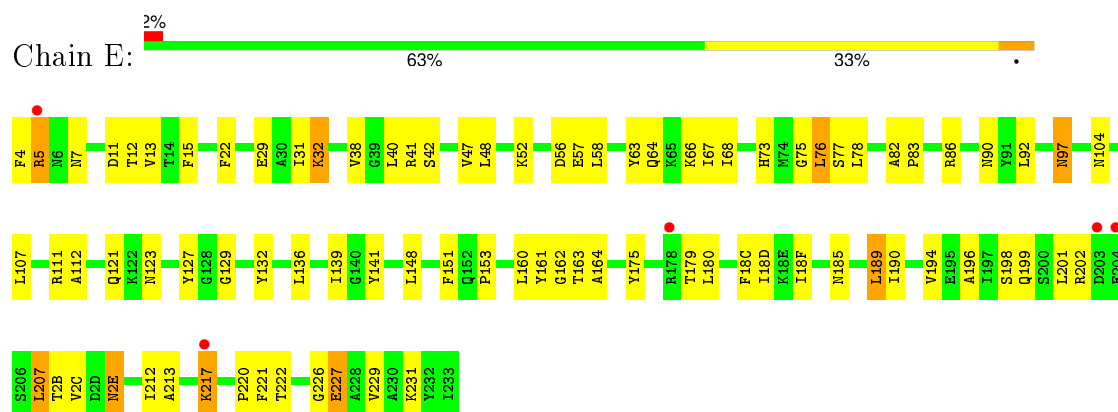




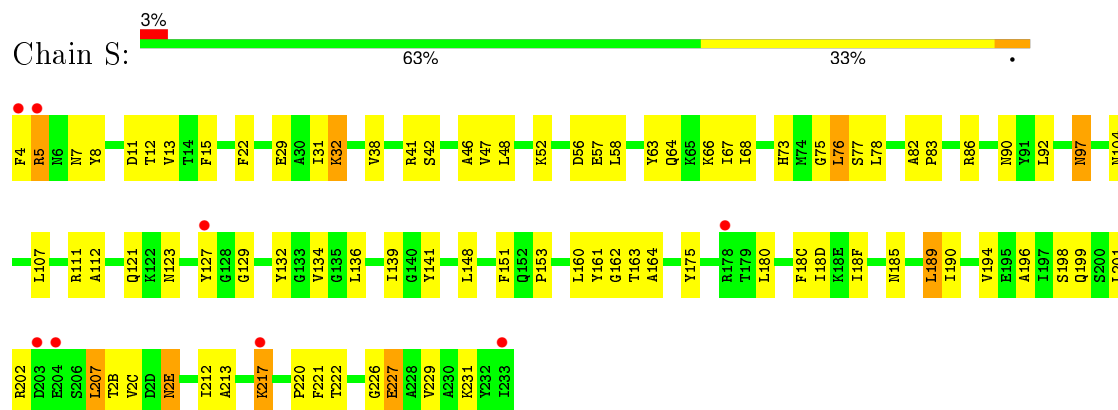
• Molecule 4: Proteasome component PUP2



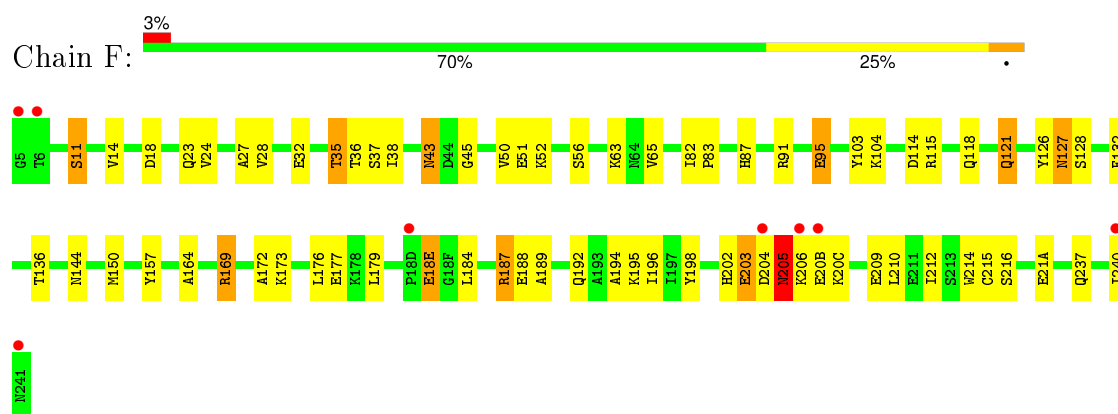
• Molecule 5: Proteasome component PRE5



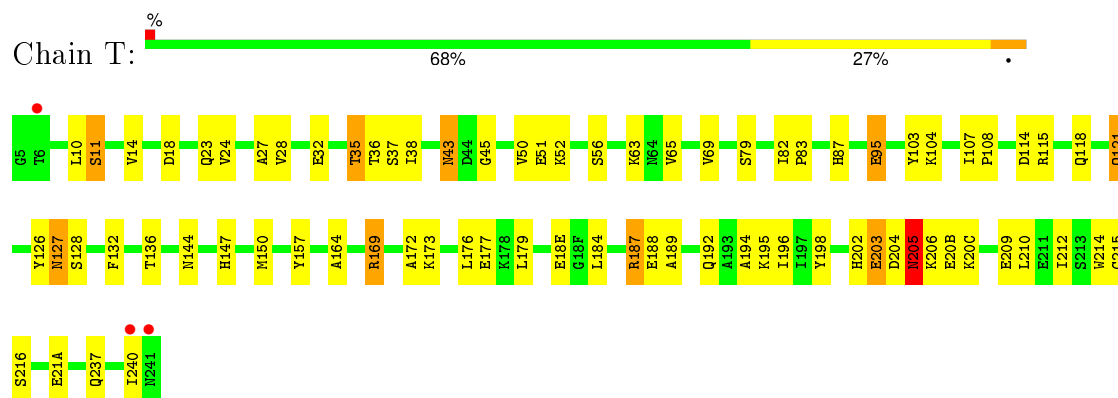
• Molecule 5: Proteasome component PRE5



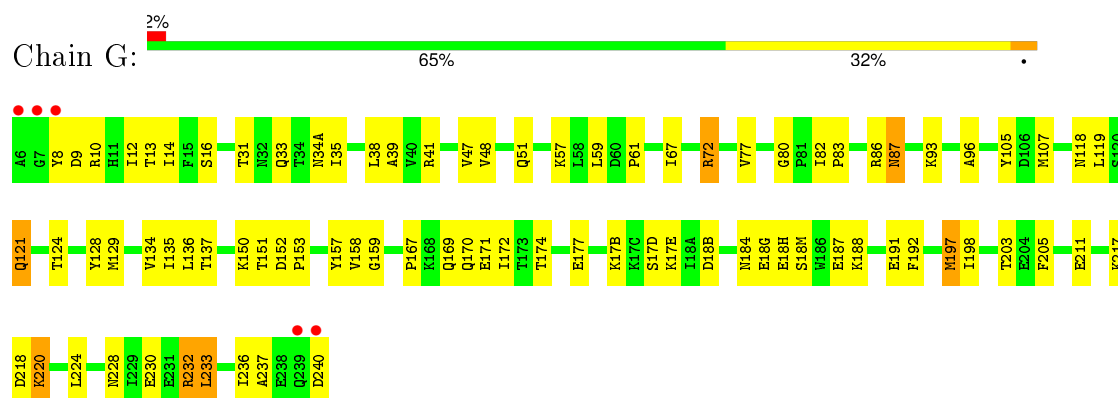
• Molecule 6: Proteasome component C1



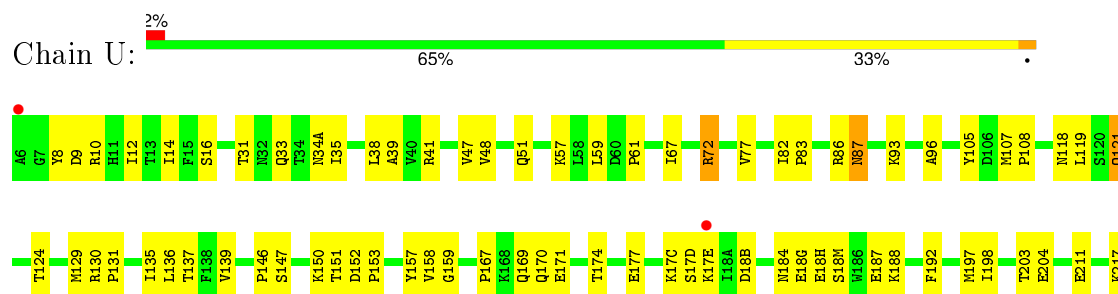
• Molecule 6: Proteasome component C1

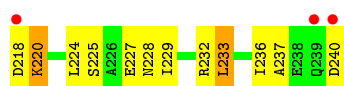


• Molecule 7: Proteasome component C7-alpha



• Molecule 7: Proteasome component C7-alpha





• Molecule 8: Proteasome component PUP1



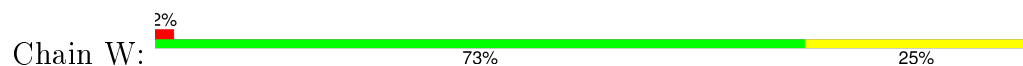
• Molecule 8: Proteasome component PUP1



• Molecule 9: Proteasome component PUP3

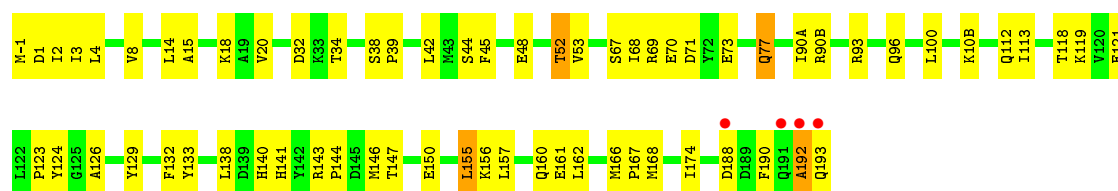


• Molecule 9: Proteasome component PUP3

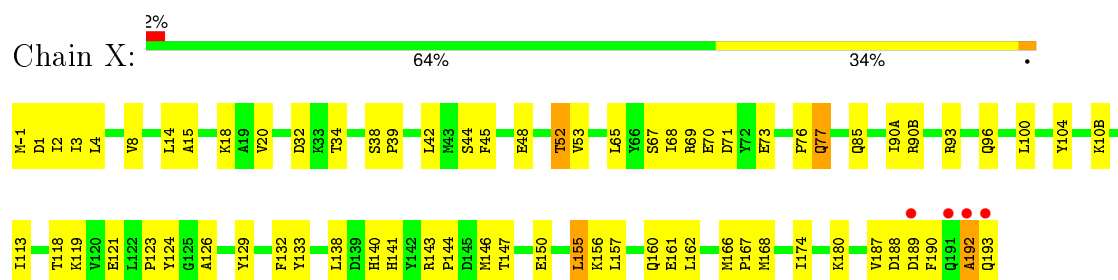


• Molecule 10: Proteasome component C11

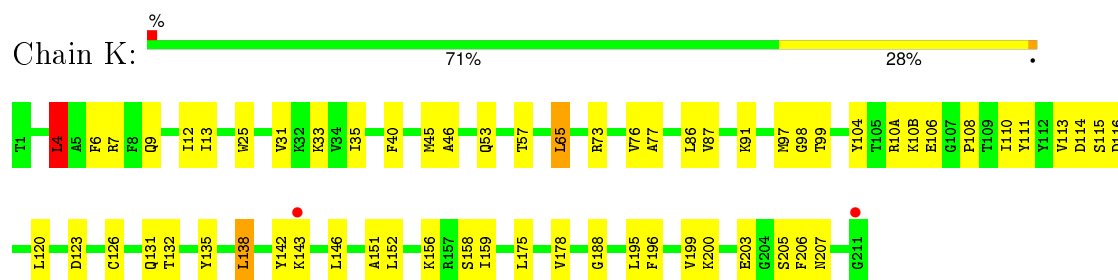




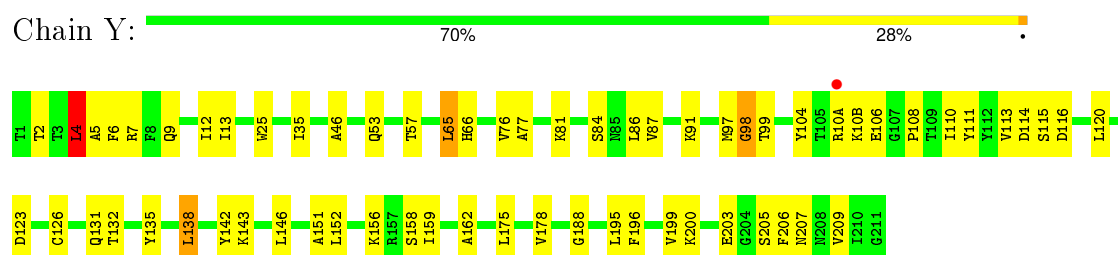
• Molecule 10: Proteasome component C11



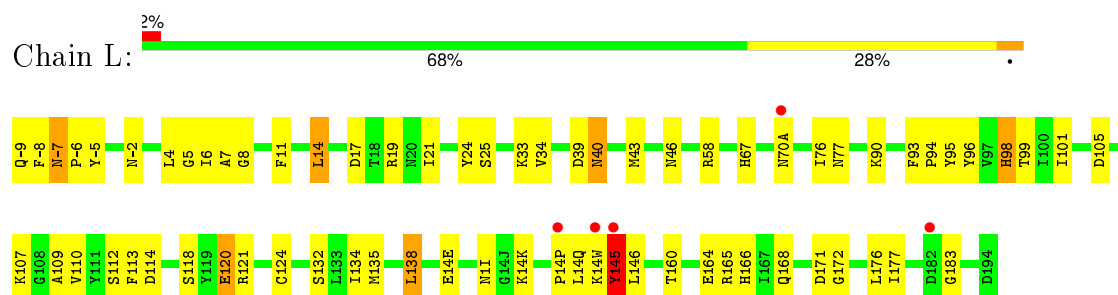
• Molecule 11: Proteasome component PRE2



• Molecule 11: Proteasome component PRE2

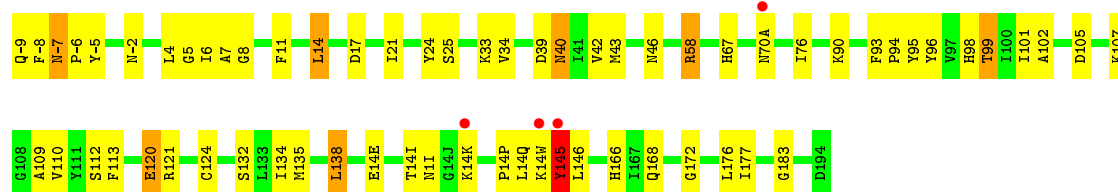


• Molecule 12: Proteasome component C5

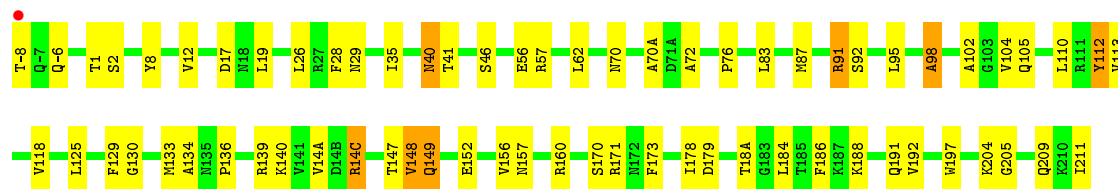


• Molecule 12: Proteasome component C5

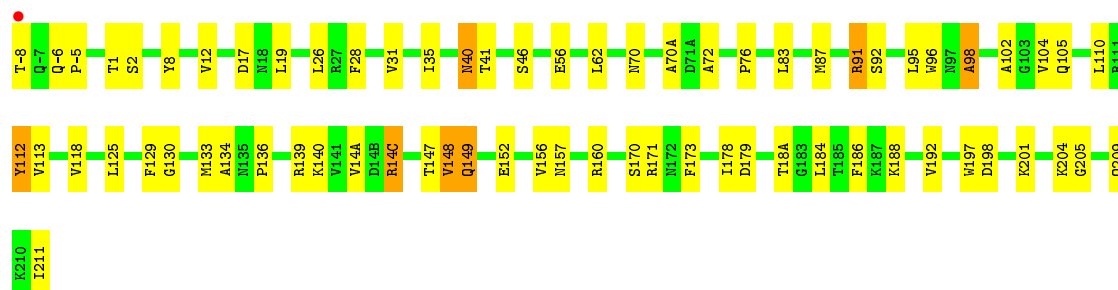




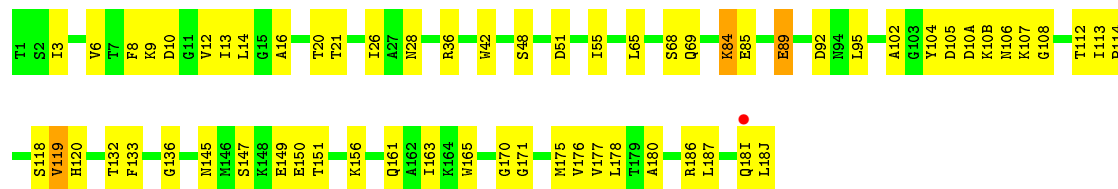
• Molecule 13: Proteasome component PRE4



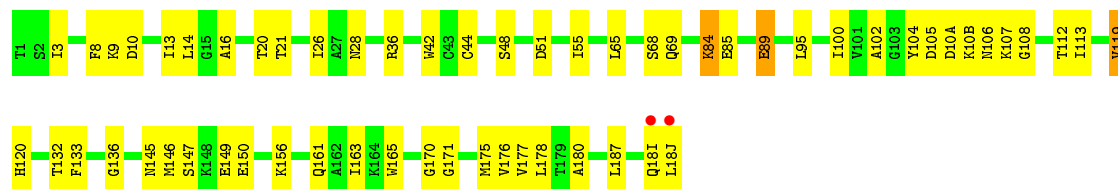
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.15Å 301.86Å 144.08Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.81 20.02 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.81) 98.7 (20.02-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.245 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 252651 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50584	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: SLR

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	0.38	0/1952	0.63	0/2642
1	O	0.37	0/1952	0.63	0/2642
2	B	0.38	0/1935	0.63	0/2618
2	P	0.38	0/1935	0.64	0/2618
3	C	0.35	0/1920	0.61	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.36	0/1887	0.63	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.35	0/1823	0.61	0/2463
5	S	0.35	0/1823	0.61	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.38	0/1937	0.63	0/2614
7	G	0.40	0/1959	0.63	0/2652
7	U	0.39	0/1959	0.63	0/2652
8	H	0.40	0/1716	0.66	0/2326
8	V	0.37	0/1716	0.65	0/2326
9	I	0.39	0/1611	0.64	0/2174
9	W	0.40	0/1611	0.65	0/2174
10	J	0.37	0/1613	0.64	0/2173
10	X	0.38	0/1613	0.64	0/2173
11	K	0.40	0/1681	0.67	2/2274 (0.1%)
11	Y	0.38	0/1681	0.66	3/2274 (0.1%)
12	L	0.40	0/1795	0.65	0/2420
12	Z	0.39	0/1795	0.65	0/2420
13	1	0.41	0/1855	0.67	2/2514 (0.1%)
13	M	0.39	0/1855	0.66	2/2514 (0.1%)
14	2	0.40	0/1541	0.65	0/2087
14	N	0.41	0/1541	0.65	0/2087
All	All	0.38	0/50450	0.64	9/68192 (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
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.58	128.13	115.30
11	K	4	LEU	CA-CB-CG	5.35	127.61	115.30
13	1	95	LEU	N-CA-C	-5.16	97.07	111.00
11	Y	188	GLY	N-CA-C	5.12	125.91	113.10
11	Y	98	GLY	N-CA-C	-5.09	100.37	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

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	1915	0	1926	53	0
1	O	1915	0	1926	65	0
2	B	1905	0	1901	87	0
2	P	1905	0	1901	94	0
3	C	1891	0	1900	92	0
3	Q	1891	0	1900	90	0
4	D	1862	0	1836	53	0
4	R	1862	0	1836	50	0
5	E	1795	0	1797	67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1795	0	1797	70	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	68	0
7	G	1921	0	1910	62	0
7	U	1921	0	1910	69	0
8	H	1685	0	1688	47	0
8	V	1685	0	1688	45	0
9	I	1581	0	1574	51	0
9	W	1581	0	1574	50	0
10	J	1585	0	1590	67	0
10	X	1585	0	1590	66	0
11	K	1644	0	1594	53	0
11	Y	1644	0	1594	52	0
12	L	1757	0	1711	62	0
12	Z	1757	0	1711	63	0
13	1	1824	0	1832	57	0
13	M	1824	0	1832	61	0
14	2	1512	0	1481	50	0
14	N	1512	0	1481	52	0
15	K	15	0	16	0	0
15	Y	15	0	16	0	0
16	1	64	0	0	1	0
16	2	51	0	0	1	0
16	A	35	0	0	2	0
16	B	27	0	0	3	0
16	C	32	0	0	5	0
16	D	23	0	0	1	0
16	E	15	0	0	0	0
16	F	35	0	0	1	0
16	G	51	0	0	2	0
16	H	41	0	0	4	0
16	I	51	0	0	1	0
16	J	38	0	0	1	0
16	K	33	0	0	0	0
16	L	43	0	0	2	0
16	M	56	0	0	4	0
16	N	49	0	0	3	0
16	O	28	0	0	2	0
16	P	18	0	0	2	0
16	Q	19	0	0	4	0
16	R	19	0	0	0	0
16	S	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	T	30	0	0	5	0
16	U	48	0	0	6	0
16	V	36	0	0	1	0
16	W	40	0	0	1	0
16	X	36	0	0	3	0
16	Y	36	0	0	2	0
16	Z	36	0	0	7	0
All	All	50584	0	49284	1590	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 16.

The worst 5 of 1590 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:U:96:ALA:HA	7:U:107:MET:HE2	1.27	1.16
7:G:96:ALA:HA	7:G:107:MET:HE2	1.27	1.14
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.22	1.02
2:B:71:ASN:ND2	2:B:72:ASP:H	1.60	0.99
2:P:202:THR:HG22	2:P:204:SER:H	1.26	0.99

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%)	231 (93%)	15 (6%)	2 (1%)	24 56
1	O	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	24 56
2	B	242/244 (99%)	221 (91%)	18 (7%)	3 (1%)	16 45
2	P	242/244 (99%)	220 (91%)	19 (8%)	3 (1%)	16 45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	239/241 (99%)	216 (90%)	19 (8%)	4 (2%)	11	34
3	Q	239/241 (99%)	216 (90%)	19 (8%)	4 (2%)	11	34
4	D	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	9	28
4	R	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	9	28
5	E	231/233 (99%)	211 (91%)	17 (7%)	3 (1%)	15	42
5	S	231/233 (99%)	211 (91%)	17 (7%)	3 (1%)	15	42
6	F	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	24	56
6	T	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	24	56
7	G	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	39	73
7	U	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	39	73
8	H	220/222 (99%)	205 (93%)	15 (7%)	0	100	100
8	V	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	34	68
9	I	202/204 (99%)	193 (96%)	7 (4%)	2 (1%)	19	51
9	W	202/204 (99%)	192 (95%)	8 (4%)	2 (1%)	19	51
10	J	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	13	38
10	X	196/198 (99%)	183 (93%)	10 (5%)	3 (2%)	13	38
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
12	Z	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
13	1	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	39	73
13	M	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	39	73
14	2	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
14	N	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
All	All	6312/6368 (99%)	5895 (93%)	364 (6%)	53 (1%)	24	56

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA
1	O	5	THR

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 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%)	205 (98%)	4 (2%)	65	90
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	90
2	B	203/203 (100%)	194 (96%)	9 (4%)	35	68
2	P	203/203 (100%)	194 (96%)	9 (4%)	35	68
3	C	213/213 (100%)	203 (95%)	10 (5%)	32	66
3	Q	213/213 (100%)	203 (95%)	10 (5%)	32	66
4	D	198/198 (100%)	188 (95%)	10 (5%)	29	62
4	R	198/198 (100%)	188 (95%)	10 (5%)	29	62
5	E	192/192 (100%)	172 (90%)	20 (10%)	9	25
5	S	192/192 (100%)	172 (90%)	20 (10%)	9	25
6	F	201/201 (100%)	185 (92%)	16 (8%)	15	39
6	T	201/201 (100%)	185 (92%)	16 (8%)	15	39
7	G	207/207 (100%)	196 (95%)	11 (5%)	28	60
7	U	207/207 (100%)	196 (95%)	11 (5%)	28	60
8	H	181/181 (100%)	174 (96%)	7 (4%)	39	73
8	V	181/181 (100%)	174 (96%)	7 (4%)	39	73
9	I	172/172 (100%)	166 (96%)	6 (4%)	43	76
9	W	172/172 (100%)	166 (96%)	6 (4%)	43	76
10	J	175/175 (100%)	170 (97%)	5 (3%)	50	82
10	X	175/175 (100%)	170 (97%)	5 (3%)	50	82
11	K	169/169 (100%)	164 (97%)	5 (3%)	48	81
11	Y	169/169 (100%)	164 (97%)	5 (3%)	48	81
12	L	185/185 (100%)	173 (94%)	12 (6%)	21	50
12	Z	185/185 (100%)	173 (94%)	12 (6%)	21	50
13	1	199/199 (100%)	189 (95%)	10 (5%)	30	63
13	M	199/199 (100%)	189 (95%)	10 (5%)	30	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	162/162 (100%)	156 (96%)	6 (4%)	41	75
14	N	162/162 (100%)	156 (96%)	6 (4%)	41	75
All	All	5332/5332 (100%)	5070 (95%)	262 (5%)	31	64

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	112	TYR
3	Q	57	LYS
12	Z	112	SER
13	M	148	VAL
1	O	158	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	89	GLN
3	Q	82	ASN
12	Z	1(I)	ASN
13	M	149	GLN
1	O	227	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	SLR	K	301	11	14,15,16	2.81	4 (28%)	10,23,25	1.91	3 (30%)
15	SLR	Y	301	11	14,15,16	2.78	4 (28%)	10,23,25	1.88	3 (30%)

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	SLR	K	301	11	-	0/12/32/35	0/1/1/1
15	SLR	Y	301	11	-	0/12/32/35	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	SLR	O7-C6	-5.51	1.24	1.42
15	K	301	SLR	O7-C6	-5.45	1.24	1.42
15	Y	301	SLR	C5-C1	2.55	1.58	1.54
15	K	301	SLR	C5-C1	2.74	1.59	1.54
15	Y	301	SLR	C2-C1	3.09	1.56	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	SLR	O12-C11-C13	-2.81	103.92	109.92
15	K	301	SLR	O12-C11-C13	-2.77	104.00	109.92
15	K	301	SLR	O10-C3-C2	-2.60	124.16	126.25
15	Y	301	SLR	O10-C3-C2	-2.58	124.17	126.25
15	Y	301	SLR	O7-C6-C5	3.48	120.87	111.81

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.27	8 (3%)	51	39	27, 43, 74, 104	0
1	O	250/250 (100%)	-0.10	16 (6%)	23	13	31, 52, 78, 101	0
2	B	244/244 (100%)	-0.10	11 (4%)	37	26	29, 49, 82, 111	0
2	P	244/244 (100%)	0.01	15 (6%)	25	15	29, 51, 87, 113	0
3	C	241/241 (100%)	0.07	16 (6%)	22	12	31, 54, 102, 119	0
3	Q	241/241 (100%)	0.26	21 (8%)	13	6	37, 57, 105, 120	0
4	D	242/242 (100%)	0.00	13 (5%)	29	19	35, 51, 84, 116	0
4	R	242/242 (100%)	0.08	14 (5%)	26	17	36, 55, 89, 116	0
5	E	233/233 (100%)	-0.21	5 (2%)	67	56	34, 51, 77, 103	0
5	S	233/233 (100%)	-0.22	8 (3%)	49	37	33, 51, 79, 105	0
6	F	244/244 (100%)	-0.27	8 (3%)	50	38	30, 44, 86, 106	0
6	T	244/244 (100%)	-0.39	3 (1%)	81	73	26, 43, 82, 103	0
7	G	243/243 (100%)	-0.33	5 (2%)	67	56	23, 39, 68, 112	0
7	U	243/243 (100%)	-0.28	5 (2%)	67	56	27, 42, 69, 113	0
8	H	222/222 (100%)	-0.47	3 (1%)	78	69	25, 40, 58, 89	0
8	V	222/222 (100%)	-0.41	3 (1%)	78	69	33, 43, 60, 96	0
9	I	204/204 (100%)	-0.54	2 (0%)	84	77	28, 41, 59, 77	0
9	W	204/204 (100%)	-0.55	4 (1%)	68	58	30, 42, 61, 78	0
10	J	198/198 (100%)	-0.32	4 (2%)	68	58	30, 44, 61, 118	0
10	X	198/198 (100%)	-0.28	4 (2%)	68	58	28, 45, 62, 120	0
11	K	212/212 (100%)	-0.40	2 (0%)	85	79	28, 43, 61, 69	0
11	Y	212/212 (100%)	-0.46	1 (0%)	91	88	27, 44, 63, 72	0
12	L	222/222 (100%)	-0.37	5 (2%)	64	52	26, 43, 65, 86	0
12	Z	222/222 (100%)	-0.40	4 (1%)	71	61	28, 42, 68, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.54	1 (0%) 93 90	24, 38, 53, 60	0
13	M	233/233 (100%)	-0.51	1 (0%) 93 90	25, 39, 54, 61	0
14	2	196/196 (100%)	-0.52	2 (1%) 84 77	23, 37, 56, 77	0
14	N	196/196 (100%)	-0.53	1 (0%) 91 88	26, 36, 57, 74	0
All	All	6368/6368 (100%)	-0.28	185 (2%) 55 43	23, 45, 78, 120	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	U	240	ASP	11.6
4	R	12(D)	ALA	10.4
4	D	12(E)	SER	10.3
4	R	12(E)	SER	10.1
3	C	55	THR	9.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	SLR	Y	301	15/16	0.94	0.19	2.19	46,48,49,51	0
15	SLR	K	301	15/16	0.95	0.19	0.91	42,42,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.