



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 02:21 PM EST

PDB ID : 4FZC
Title : 20S yeast proteasome in complex with cepafungin I
Authors : Stein, M.; Beck, P.; Kaiser, M.; Dudler, R.; Becker, C.F.W.; Groll, M.
Deposited on : 2012-07-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

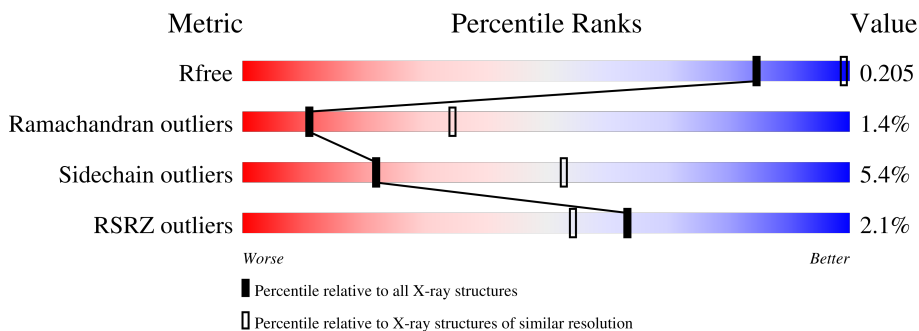
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

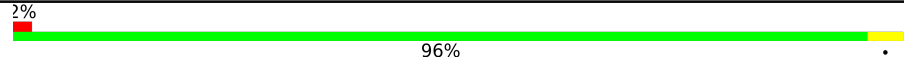
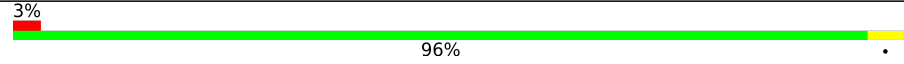
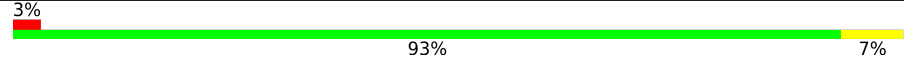
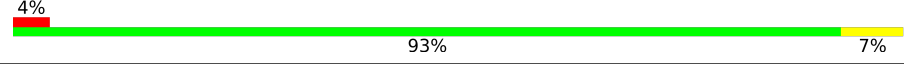
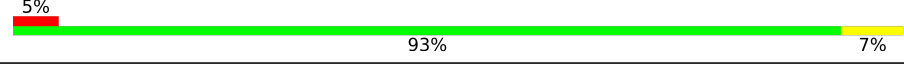
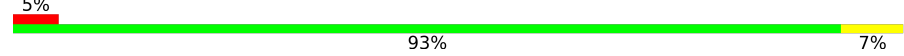
The reported resolution of this entry is 2.80 Å.

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.



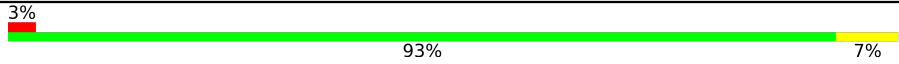
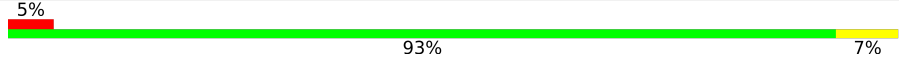
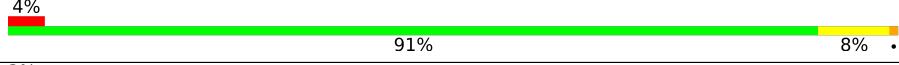
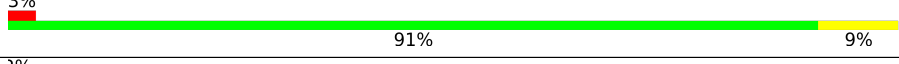
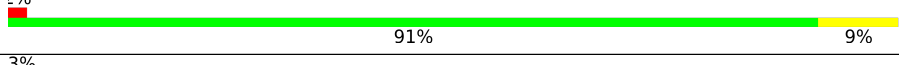
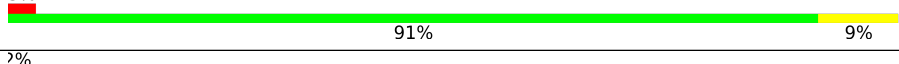
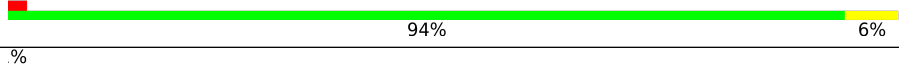
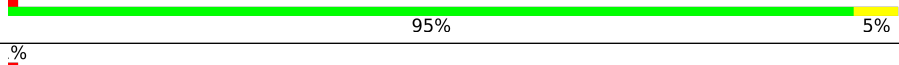
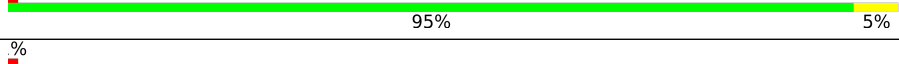
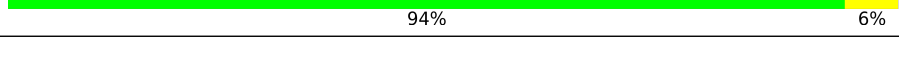
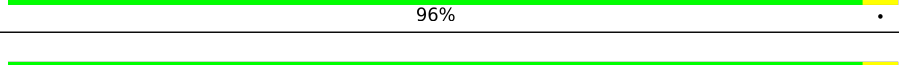
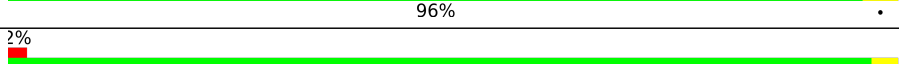
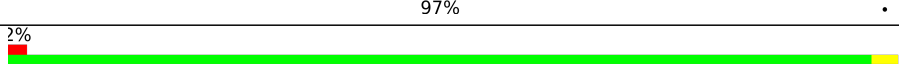
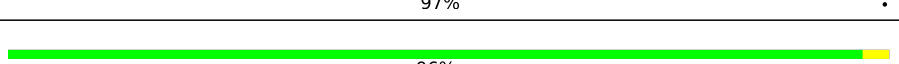
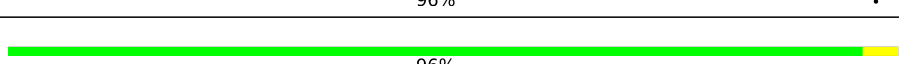
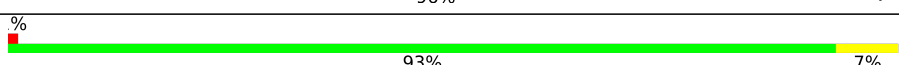
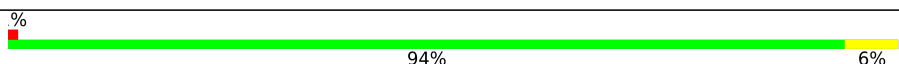
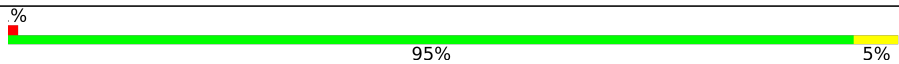
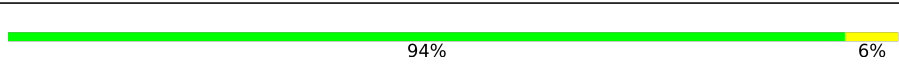
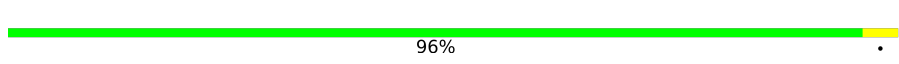
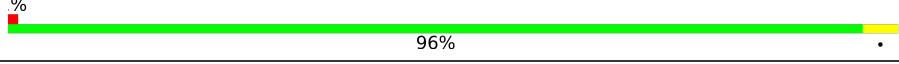
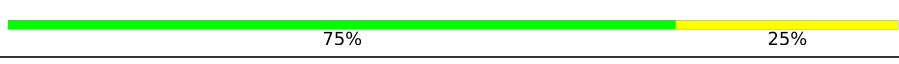
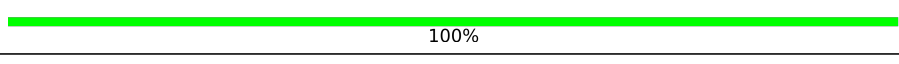
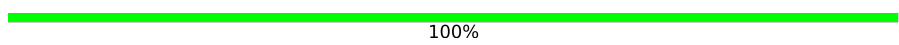

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 $\leq 5\%$. 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	 2% 96%
1	O	250	 3% 96%
2	B	244	 3% 93% 7%
2	P	244	 4% 93% 7%
3	C	241	 5% 93% 7%
3	Q	241	 5% 93% 7%


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Mol	Chain	Length	Quality of chain
4	D	242	 3% 93% 7%
4	R	242	 5% 93% 7%
5	E	233	 4% 91% 8%
5	S	233	 3% 91% 9%
6	F	244	 2% 91% 9%
6	T	244	 3% 91% 9%
7	G	243	 2% 94% 6%
7	U	243	 1% 95% 5%
8	H	222	 1% 95% 5%
8	V	222	 1% 94% 6%
9	I	204	 0% 96% 5%
9	W	204	 0% 96% 5%
10	J	198	 2% 97% 5%
10	X	198	 2% 97% 5%
11	K	212	 0% 96% 5%
11	Y	212	 0% 96% 5%
12	L	222	 1% 93% 7%
12	Z	222	 1% 94% 6%
13	M	233	 1% 95% 5%
13	a	233	 0% 94% 6%
14	N	196	 0% 96% 5%
14	b	196	 1% 96% 5%
15	c	4	 0% 75% 25%
15	d	4	 0% 100% 0%
15	e	4	 0% 100% 0%

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Mol	Chain	Length	Quality of chain
15	f	4	 100%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51020 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	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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
5	E	233	Total 1795	C 1129	N 312	O 350	S 4	0	0	0
5	S	233	Total 1795	C 1129	N 312	O 350	S 4	0	0	0

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	Total 1897	C 1205	N 330	O 358	S 4	0	0	0
6	T	244	Total 1897	C 1205	N 330	O 358	S 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	Total 1921	C 1221	N 322	O 370	S 8	0	0	0
7	U	243	Total 1921	C 1221	N 322	O 370	S 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	Total 1685	C 1061	N 293	O 324	S 7	0	0	0
8	V	222	Total 1685	C 1061	N 293	O 324	S 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	Total 1581	C 1010	N 258	O 305	S 8	0	0	0
9	W	204	Total 1581	C 1010	N 258	O 305	S 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	Total 1585	C 1005	N 269	O 305	S 6	0	0	0

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

- Molecule 15 is a protein called Cepafungin I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	c	4	Total	C	N	O	0	0	0
			38	28	4	6			
15	d	4	Total	C	N	O	0	0	0
			38	28	4	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	0	0	0
			38	28	4	6			
15	f	4	Total	C	N	O	0	0	0
			38	28	4	6			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	55	Total	O	0	0
			55	55		
16	B	37	Total	O	0	0
			37	37		
16	C	41	Total	O	0	0
			41	41		
16	D	40	Total	O	0	0
			40	40		
16	E	23	Total	O	0	0
			23	23		
16	F	46	Total	O	0	0
			46	46		
16	G	59	Total	O	0	0
			59	59		
16	H	53	Total	O	0	0
			53	53		
16	I	68	Total	O	0	0
			68	68		
16	J	51	Total	O	0	0
			51	51		
16	K	43	Total	O	0	0
			43	43		
16	L	58	Total	O	0	0
			58	58		
16	M	71	Total	O	0	0
			71	71		
16	N	58	Total	O	0	0
			58	58		
16	O	33	Total	O	0	0
			33	33		
16	P	27	Total	O	0	0
			27	27		
16	Q	26	Total	O	0	0
			26	26		

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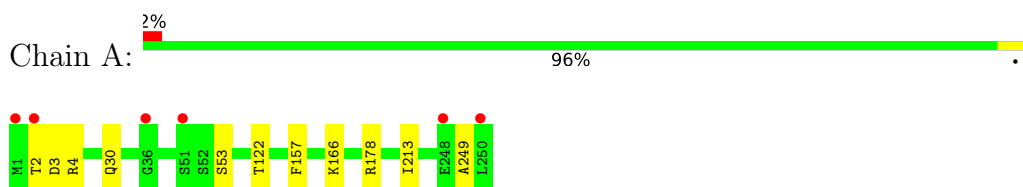
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	28	Total 28	O 28	0	0
16	S	21	Total 21	O 21	0	0
16	T	38	Total 38	O 38	0	0
16	U	62	Total 62	O 62	0	0
16	V	47	Total 47	O 47	0	0
16	W	57	Total 57	O 57	0	0
16	X	47	Total 47	O 47	0	0
16	Y	41	Total 41	O 41	0	0
16	Z	55	Total 55	O 55	0	0
16	a	74	Total 74	O 74	0	0
16	b	60	Total 60	O 60	0	0
16	f	1	Total 1	O 1	0	0

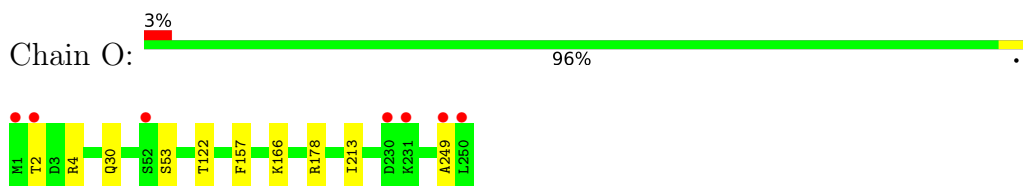
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

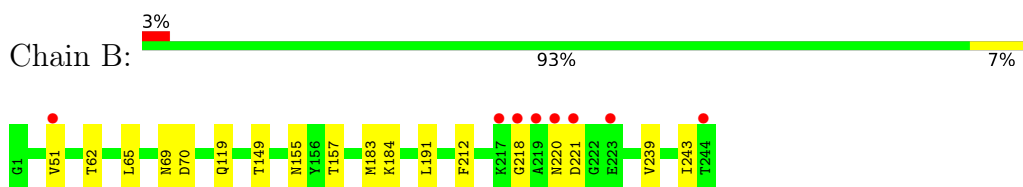
- Molecule 1: Proteasome component Y7



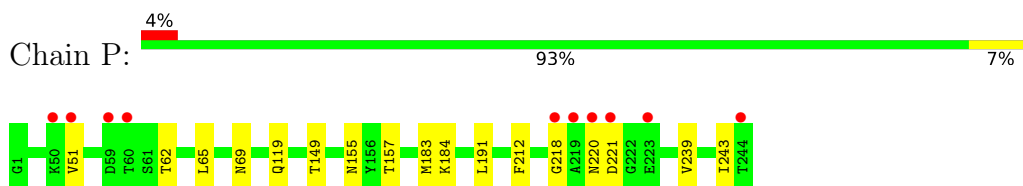
- Molecule 1: Proteasome component Y7



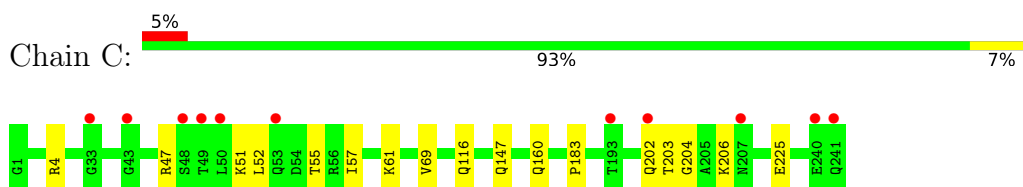
- Molecule 2: Proteasome component Y13



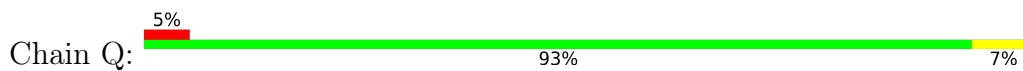
- Molecule 2: Proteasome component Y13



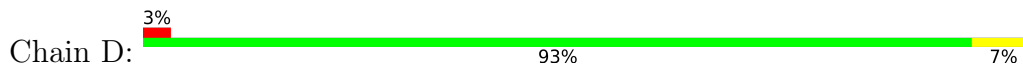
- Molecule 3: Proteasome component PRE6



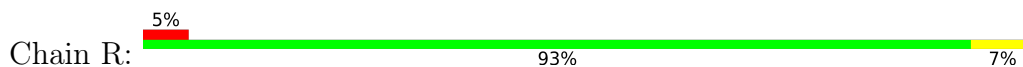
- Molecule 3: Proteasome component PRE6



- Molecule 4: Proteasome component PUP2



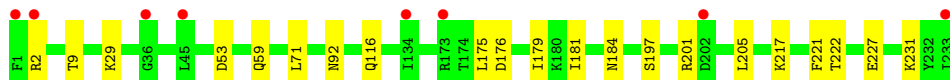
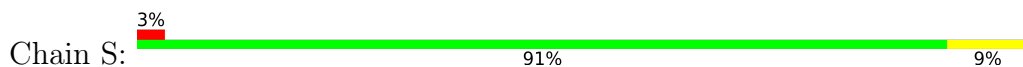
- Molecule 4: Proteasome component PUP2



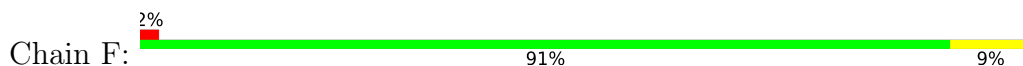
- Molecule 5: Proteasome component PRE5



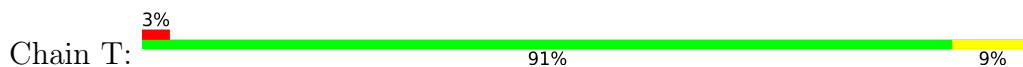
- Molecule 5: Proteasome component PRE5



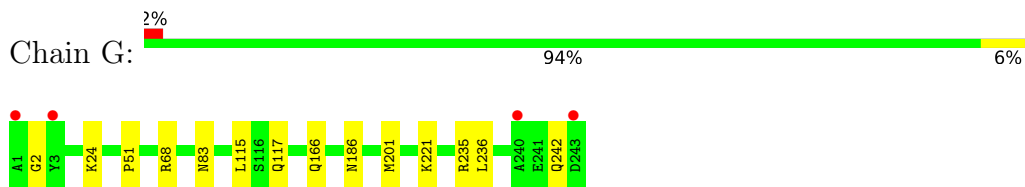
- Molecule 6: Proteasome component C1



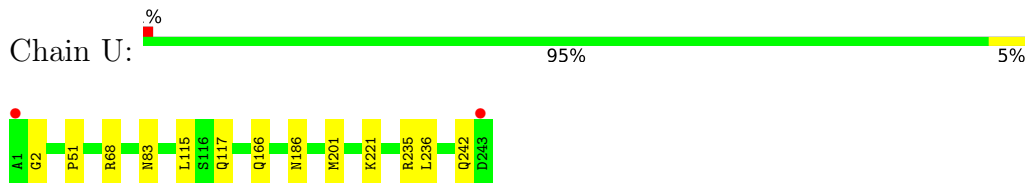
- Molecule 6: Proteasome component C1



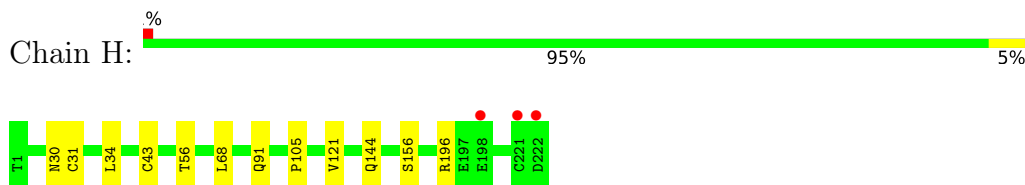
- Molecule 7: Proteasome component C7-alpha



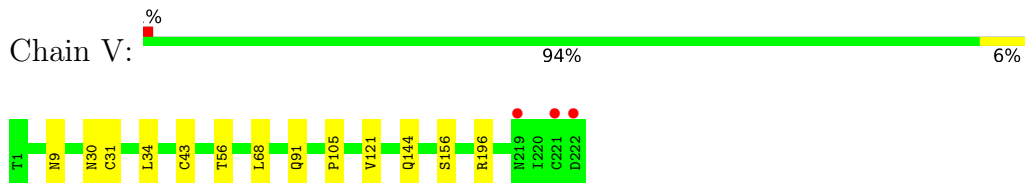
- Molecule 7: Proteasome component C7-alpha



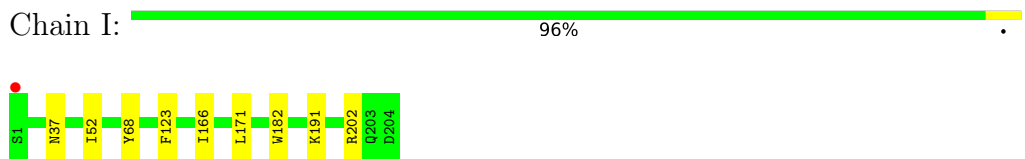
- Molecule 8: Proteasome component PUP1



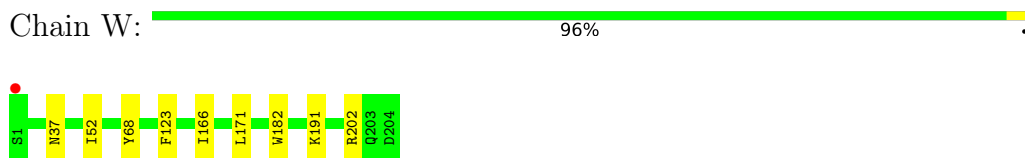
- Molecule 8: Proteasome component PUP1



- Molecule 9: Proteasome component PUP3

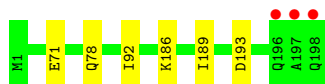


- Molecule 9: Proteasome component PUP3



- Molecule 10: Proteasome component C11





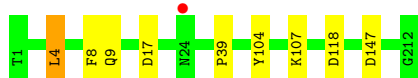
- Molecule 10: Proteasome component C11



- Molecule 11: Proteasome component PRE2



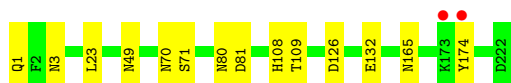
- Molecule 11: Proteasome component PRE2



- Molecule 12: Proteasome component C5



- Molecule 12: Proteasome component C5



- Molecule 13: Proteasome component PRE4



- Molecule 13: Proteasome component PRE4

Chain a:  94% 6%



- Molecule 14: Proteasome component PRE3

Chain N:  96%



- Molecule 14: Proteasome component PRE3

Chain b:  96%



- Molecule 15: Cepafungin I

Chain c:  75% 25%



- Molecule 15: Cepafungin I

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Cepafungin I

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Cepafungin I

Chain f:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 301.02Å 144.83Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 24.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.80) 98.1 (24.96-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.244 0.205 , 0.205	Depositor DCC
R_{free} test set	12823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtrriage
Anisotropy	0.765	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51020	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0W5, LY0, 0W6

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	0.37	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.37	0/1935	0.63	0/2618
2	P	0.38	0/1935	0.63	0/2618
3	C	0.35	0/1920	0.62	0/2598
3	Q	0.36	0/1920	0.62	0/2598
4	D	0.35	0/1887	0.63	0/2541
4	R	0.36	0/1887	0.63	0/2541
5	E	0.35	0/1823	0.60	0/2463
5	S	0.35	0/1823	0.60	0/2463
6	F	0.38	0/1937	0.61	0/2614
6	T	0.37	0/1937	0.62	0/2614
7	G	0.40	0/1959	0.63	0/2652
7	U	0.39	0/1959	0.62	0/2652
8	H	0.38	0/1716	0.66	0/2326
8	V	0.37	0/1716	0.66	0/2326
9	I	0.38	0/1611	0.65	0/2174
9	W	0.39	0/1611	0.66	0/2174
10	J	0.39	0/1613	0.64	0/2173
10	X	0.40	0/1613	0.65	0/2173
11	K	0.40	0/1681	0.67	1/2274 (0.0%)
11	Y	0.40	0/1681	0.67	1/2274 (0.0%)
12	L	0.39	0/1795	0.66	1/2420 (0.0%)
12	Z	0.39	0/1795	0.67	0/2420
13	M	0.39	0/1855	0.65	1/2514 (0.0%)
13	a	0.39	0/1855	0.66	1/2514 (0.0%)
14	N	0.40	0/1541	0.65	0/2087
14	b	0.39	0/1541	0.65	0/2087
15	c	1.45	0/6	1.00	0/7
15	d	1.58	0/6	0.69	0/7
15	e	1.53	0/6	1.01	0/7
15	f	1.38	0/6	0.86	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.38	0/50474	0.64	5/68220 (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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	110	LEU	N-CA-C	-5.40	96.42	111.00
13	a	110	LEU	N-CA-C	-5.39	96.46	111.00
11	K	4	LEU	CA-CB-CG	5.35	127.60	115.30
11	Y	4	LEU	CA-CB-CG	5.25	127.39	115.30
12	L	105	TYR	N-CA-C	-5.16	97.06	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	174	TYR	Sidechain
12	Z	174	TYR	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [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%)	226 (91%)	17 (7%)	5 (2%)	7	24
1	O	248/250 (99%)	226 (91%)	18 (7%)	4 (2%)	9	31
2	B	242/244 (99%)	212 (88%)	24 (10%)	6 (2%)	5	19
2	P	242/244 (99%)	213 (88%)	23 (10%)	6 (2%)	5	19
3	C	239/241 (99%)	218 (91%)	15 (6%)	6 (2%)	5	19
3	Q	239/241 (99%)	217 (91%)	16 (7%)	6 (2%)	5	19
4	D	240/242 (99%)	218 (91%)	17 (7%)	5 (2%)	7	23
4	R	240/242 (99%)	218 (91%)	17 (7%)	5 (2%)	7	23
5	E	231/233 (99%)	207 (90%)	15 (6%)	9 (4%)	3	10
5	S	231/233 (99%)	204 (88%)	20 (9%)	7 (3%)	4	15
6	F	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	19	49
6	T	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	19	49
7	G	241/243 (99%)	223 (92%)	15 (6%)	3 (1%)	13	39
7	U	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	13	39
8	H	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	17	46
8	V	220/222 (99%)	201 (91%)	16 (7%)	3 (1%)	11	34
9	I	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	29	61
9	W	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	29	61
10	J	196/198 (99%)	183 (93%)	11 (6%)	2 (1%)	15	44
10	X	196/198 (99%)	182 (93%)	13 (7%)	1 (0%)	29	61
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	61
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	29	61
12	L	220/222 (99%)	199 (90%)	20 (9%)	1 (0%)	29	61
12	Z	220/222 (99%)	199 (90%)	20 (9%)	1 (0%)	29	61
13	M	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	34	66
13	a	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	17	46
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6312/6368 (99%)	5794 (92%)	432 (7%)	86 (1%)	11	34

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
2	B	51	VAL
2	B	221	ASP
3	C	52	LEU
3	C	203	THR
4	D	122	GLU
5	E	2	ARG
7	G	242	GLN
1	O	53	SER
2	P	51	VAL
2	P	221	ASP
3	Q	52	LEU
4	R	122	GLU
5	S	2	ARG
7	U	242	GLN
2	B	62	THR
2	B	218	GLY
3	C	183	PRO
4	D	181	SER
5	E	175	LEU
5	E	201	ARG
5	E	217	LYS
9	I	191	LYS
10	J	193	ASP
12	L	81	ASP
2	P	62	THR
2	P	218	GLY
3	Q	183	PRO
3	Q	203	THR
4	R	181	SER
5	S	175	LEU
5	S	201	ARG
5	S	217	LYS
6	T	139	LYS
9	W	191	LYS
10	X	193	ASP
12	Z	81	ASP
2	B	183	MET
3	C	202	GLN
4	D	121	GLY
5	E	176	ASP
5	E	221	PHE
6	F	139	LYS

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Mol	Chain	Res	Type
6	F	203	ASN
7	G	51	PRO
1	O	166	LYS
2	P	183	MET
3	Q	202	GLN
4	R	120	SER
4	R	121	GLY
5	S	176	ASP
5	S	221	PHE
6	T	203	ASN
7	U	51	PRO
1	A	2	THR
1	A	166	LYS
1	A	249	ALA
3	C	47	ARG
4	D	120	SER
8	H	105	PRO
10	J	186	LYS
1	O	2	THR
1	O	249	ALA
3	Q	47	ARG
8	V	91	GLN
8	V	105	PRO
1	A	3	ASP
5	E	227	GLU
8	H	91	GLN
13	M	10	SER
13	a	111	TRP
4	D	118	GLY
5	E	231	LYS
7	G	2	GLY
4	R	118	GLY
8	V	9	ASN
13	a	10	SER
5	S	181	ILE
7	U	2	GLY
5	E	181	ILE
11	Y	39	PRO
2	B	243	ILE
3	C	204	GLY
11	K	39	PRO
2	P	243	ILE

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Mol	Chain	Res	Type
3	Q	204	GLY

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%)	203 (97%)	6 (3%)	42	76
1	O	209/209 (100%)	203 (97%)	6 (3%)	42	76
2	B	203/203 (100%)	191 (94%)	12 (6%)	19	49
2	P	203/203 (100%)	192 (95%)	11 (5%)	22	53
3	C	213/213 (100%)	202 (95%)	11 (5%)	23	55
3	Q	213/213 (100%)	202 (95%)	11 (5%)	23	55
4	D	198/198 (100%)	186 (94%)	12 (6%)	18	48
4	R	198/198 (100%)	186 (94%)	12 (6%)	18	48
5	E	192/192 (100%)	179 (93%)	13 (7%)	16	42
5	S	192/192 (100%)	178 (93%)	14 (7%)	14	38
6	F	201/201 (100%)	180 (90%)	21 (10%)	7	21
6	T	201/201 (100%)	180 (90%)	21 (10%)	7	21
7	G	207/207 (100%)	196 (95%)	11 (5%)	22	54
7	U	207/207 (100%)	197 (95%)	10 (5%)	25	58
8	H	181/181 (100%)	171 (94%)	10 (6%)	21	52
8	V	181/181 (100%)	171 (94%)	10 (6%)	21	52
9	I	172/172 (100%)	164 (95%)	8 (5%)	26	59
9	W	172/172 (100%)	164 (95%)	8 (5%)	26	59
10	J	175/175 (100%)	171 (98%)	4 (2%)	50	82
10	X	175/175 (100%)	171 (98%)	4 (2%)	50	82
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	44
13	M	199/199 (100%)	190 (96%)	9 (4%)	27	60
13	a	199/199 (100%)	189 (95%)	10 (5%)	24	56
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	62
14	b	162/162 (100%)	155 (96%)	7 (4%)	29	62
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
All	All	5336/5336 (100%)	5049 (95%)	287 (5%)	22	53

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	30	GLN
1	A	122	THR
1	A	157	PHE
1	A	178	ARG
1	A	213	ILE
2	B	65	LEU
2	B	69	ASN
2	B	70	ASP
2	B	119	GLN
2	B	149	THR
2	B	155	ASN
2	B	157	THR
2	B	184	LYS
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
2	B	239	VAL
3	C	4	ARG
3	C	51	LYS
3	C	55	THR
3	C	57	ILE
3	C	61	LYS
3	C	69	VAL
3	C	116	GLN

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Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	206	LYS
3	C	225	GLU
4	D	20	LEU
4	D	40	LEU
4	D	68	CYS
4	D	99	ILE
4	D	102	GLU
4	D	124	ARG
4	D	143	ASP
4	D	169	GLU
4	D	176	LEU
4	D	182	SER
4	D	183	LEU
4	D	214	ILE
5	E	9	THR
5	E	29	LYS
5	E	53	ASP
5	E	59	GLN
5	E	71	LEU
5	E	92	ASN
5	E	116	GLN
5	E	179	ILE
5	E	184	ASN
5	E	205	LEU
5	E	222	THR
5	E	227	GLU
5	E	231	LYS
6	F	7	SER
6	F	32	THR
6	F	39	ASN
6	F	68	ARG
6	F	78	ILE
6	F	94	SER
6	F	101	THR
6	F	103	ILE
6	F	117	GLN
6	F	123	ASN
6	F	131	SER
6	F	165	ARG
6	F	181	GLU

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Mol	Chain	Res	Type
6	F	186	ARG
6	F	201	GLU
6	F	202	ASP
6	F	203	ASN
6	F	208	PHE
6	F	214	TRP
6	F	221	ASN
6	F	243	ILE
7	G	24	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	166	GLN
7	G	186	ASN
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	31	CYS
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
8	H	156	SER
8	H	196	ARG
9	I	37	ASN
9	I	52	ILE
9	I	68	TYR
9	I	123	PHE
9	I	166	ILE
9	I	171	LEU
9	I	182	TRP
9	I	202	ARG
10	J	71	GLU
10	J	78	GLN
10	J	92	ILE
10	J	189	ILE
11	K	4	LEU

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Mol	Chain	Res	Type
11	K	8	PHE
11	K	9	GLN
11	K	17	ASP
11	K	104	TYR
11	K	107	LYS
11	K	147	ASP
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	70	ASN
12	L	71	SER
12	L	80	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
12	L	132	GLU
12	L	165	ASN
13	M	37	ASN
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	159	VAL
13	M	161	ARG
13	M	171	GLN
13	M	226	LYS
14	N	36	ARG
14	N	83	LYS
14	N	88	GLU
14	N	104	ASP
14	N	105	LYS
14	N	115	LEU
14	N	144	GLU
1	O	4	ARG
1	O	30	GLN
1	O	122	THR
1	O	157	PHE
1	O	178	ARG
1	O	213	ILE
2	P	65	LEU
2	P	69	ASN

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Mol	Chain	Res	Type
2	P	119	GLN
2	P	149	THR
2	P	155	ASN
2	P	157	THR
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
2	P	239	VAL
3	Q	4	ARG
3	Q	51	LYS
3	Q	55	THR
3	Q	57	ILE
3	Q	61	LYS
3	Q	69	VAL
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	206	LYS
3	Q	225	GLU
4	R	20	LEU
4	R	40	LEU
4	R	68	CYS
4	R	99	ILE
4	R	102	GLU
4	R	124	ARG
4	R	143	ASP
4	R	169	GLU
4	R	176	LEU
4	R	182	SER
4	R	183	LEU
4	R	214	ILE
5	S	9	THR
5	S	29	LYS
5	S	53	ASP
5	S	59	GLN
5	S	71	LEU
5	S	92	ASN
5	S	116	GLN
5	S	179	ILE
5	S	184	ASN
5	S	197	SER

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Mol	Chain	Res	Type
5	S	205	LEU
5	S	222	THR
5	S	227	GLU
5	S	231	LYS
6	T	7	SER
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	78	ILE
6	T	94	SER
6	T	101	THR
6	T	103	ILE
6	T	117	GLN
6	T	123	ASN
6	T	131	SER
6	T	165	ARG
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	202	ASP
6	T	203	ASN
6	T	208	PHE
6	T	214	TRP
6	T	221	ASN
6	T	243	ILE
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	166	GLN
7	U	186	ASN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	31	CYS
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	121	VAL

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Mol	Chain	Res	Type
8	V	144	GLN
8	V	156	SER
8	V	196	ARG
9	W	37	ASN
9	W	52	ILE
9	W	68	TYR
9	W	123	PHE
9	W	166	ILE
9	W	171	LEU
9	W	182	TRP
9	W	202	ARG
10	X	71	GLU
10	X	78	GLN
10	X	92	ILE
10	X	189	ILE
11	Y	4	LEU
11	Y	8	PHE
11	Y	9	GLN
11	Y	17	ASP
11	Y	104	TYR
11	Y	107	LYS
11	Y	118	ASP
11	Y	147	ASP
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	70	ASN
12	Z	71	SER
12	Z	80	ASN
12	Z	108	HIS
12	Z	109	THR
12	Z	126	ASP
12	Z	132	GLU
12	Z	165	ASN
13	a	37	ASN
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	82	ASP
13	a	104	ARG
13	a	159	VAL

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Mol	Chain	Res	Type
13	a	161	ARG
13	a	171	GLN
13	a	226	LYS
14	b	36	ARG
14	b	83	LYS
14	b	88	GLU
14	b	104	ASP
14	b	105	LYS
14	b	115	LEU
14	b	144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	143	ASN
2	B	20	GLN
2	B	58	GLN
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	77	ASN
3	C	92	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	139	HIS
4	D	160	ASN
4	D	210	GLN
4	D	225	ASN

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Mol	Chain	Res	Type
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
8	H	189	ASN
8	H	219	ASN
9	I	37	ASN
9	I	71	ASN
9	I	88	GLN
9	I	156	ASN
10	J	55	GLN
10	J	78	GLN
10	J	86	GLN
10	J	118	GLN
10	J	146	HIS

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Mol	Chain	Res	Type
10	J	147	HIS
10	J	191	GLN
10	J	198	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	208	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	95	HIS
12	L	152	ASN
12	L	153	GLN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	145	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
1	O	143	ASN
2	P	20	GLN
2	P	58	GLN
2	P	69	ASN
2	P	93	HIS
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
2	P	232	GLN

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Mol	Chain	Res	Type
3	Q	17	GLN
3	Q	77	ASN
3	Q	92	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	139	HIS
4	R	160	ASN
4	R	210	GLN
4	R	225	ASN
5	S	4	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	30	ASN
8	V	66	HIS

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Mol	Chain	Res	Type
8	V	144	GLN
8	V	172	ASN
8	V	189	ASN
8	V	219	ASN
9	W	37	ASN
9	W	88	GLN
9	W	156	ASN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
10	X	198	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	95	HIS
12	Z	152	ASN
12	Z	153	GLN
12	Z	159	GLN
12	Z	165	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	145	ASN

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Mol	Chain	Res	Type
14	b	161	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](#)

8 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	LYO	c	3	15	7,9,10	0.99	0	6,10,12	0.46	0
15	OW6	d	4	11,15	6,6,7	1.04	0	5,6,8	0.86	0
15	LYO	d	3	15	7,9,10	0.99	0	6,10,12	0.82	0
15	OW6	f	4	11,15	6,6,7	1.02	0	5,6,8	0.83	0
15	LYO	e	3	15	7,9,10	1.01	0	6,10,12	0.45	0
15	OW6	e	4	8,15	6,6,7	0.95	0	5,6,8	0.81	0
15	OW6	c	4	8,15	6,6,7	1.23	1 (16%)	5,6,8	0.78	0
15	LYO	f	3	15	7,9,10	0.90	0	6,10,12	0.82	0

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	LYO	c	3	15	-	3/8/9/11	-
15	OW6	d	4	11,15	-	1/3/4/5	-
15	LYO	d	3	15	-	3/8/9/11	-
15	OW6	f	4	11,15	-	1/3/4/5	-
15	LYO	e	3	15	-	3/8/9/11	-
15	OW6	e	4	8,15	-	1/3/4/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	0W6	c	4	8,15	-	1/3/4/5	-
15	LYO	f	3	15	-	3/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	0W6	C17-CA	2.32	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	3	LYO	C-CA-CB-CG
15	c	3	LYO	CG-CD-CE-NZ
15	d	3	LYO	C-CA-CB-CG
15	d	3	LYO	CG-CD-CE-NZ
15	e	3	LYO	N-CA-CB-CG
15	e	3	LYO	C-CA-CB-CG
15	e	3	LYO	CG-CD-CE-NZ
15	f	3	LYO	C-CA-CB-CG
15	f	3	LYO	CG-CD-CE-NZ
15	c	4	0W6	CA-C17-C18-C
15	e	4	0W6	CA-C17-C18-C
15	d	4	0W6	CA-C17-C18-C
15	f	4	0W6	CA-C17-C18-C
15	c	3	LYO	N-CA-CB-CG
15	d	3	LYO	N-CA-CB-CG
15	f	3	LYO	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

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%)	-0.23	6 (2%) 59 49	44, 65, 95, 118	0
1	O	250/250 (100%)	-0.26	7 (2%) 53 43	43, 66, 96, 118	0
2	B	244/244 (100%)	-0.07	8 (3%) 46 36	45, 67, 107, 132	0
2	P	244/244 (100%)	-0.11	10 (4%) 37 27	46, 68, 107, 133	0
3	C	241/241 (100%)	-0.02	11 (4%) 32 22	48, 71, 119, 140	0
3	Q	241/241 (100%)	0.01	12 (4%) 28 19	49, 74, 120, 140	0
4	D	242/242 (100%)	0.01	7 (2%) 51 41	50, 72, 105, 139	0
4	R	242/242 (100%)	0.01	11 (4%) 33 23	51, 73, 106, 139	0
5	E	233/233 (100%)	-0.07	10 (4%) 35 25	51, 77, 102, 124	0
5	S	233/233 (100%)	0.06	8 (3%) 45 35	50, 77, 103, 124	0
6	F	244/244 (100%)	-0.17	5 (2%) 65 56	47, 67, 103, 117	0
6	T	244/244 (100%)	-0.02	8 (3%) 46 36	47, 67, 102, 117	0
7	G	243/243 (100%)	-0.28	4 (1%) 72 66	43, 63, 92, 124	0
7	U	243/243 (100%)	-0.25	2 (0%) 86 81	45, 63, 92, 123	0
8	H	222/222 (100%)	-0.47	3 (1%) 75 70	41, 57, 79, 118	0
8	V	222/222 (100%)	-0.50	3 (1%) 75 70	43, 58, 79, 117	0
9	I	204/204 (100%)	-0.51	1 (0%) 91 88	40, 59, 80, 97	0
9	W	204/204 (100%)	-0.48	1 (0%) 91 88	40, 59, 81, 97	0
10	J	198/198 (100%)	-0.41	3 (1%) 73 68	41, 57, 77, 137	0
10	X	198/198 (100%)	-0.44	4 (2%) 65 56	42, 58, 78, 137	0
11	K	212/212 (100%)	-0.42	1 (0%) 91 88	41, 58, 79, 86	0
11	Y	212/212 (100%)	-0.44	1 (0%) 91 88	40, 58, 80, 87	0
12	L	222/222 (100%)	-0.47	2 (0%) 84 80	41, 60, 84, 108	0
12	Z	222/222 (100%)	-0.44	2 (0%) 84 80	40, 60, 84, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.49	2 (0%) 84 80	39, 59, 76, 83	0
13	a	233/233 (100%)	-0.46	1 (0%) 92 91	39, 58, 76, 82	0
14	N	196/196 (100%)	-0.52	0 100 100	36, 54, 78, 90	0
14	b	196/196 (100%)	-0.49	1 (0%) 91 88	37, 54, 78, 90	0
15	c	1/4 (25%)	-0.32	0 100 100	63, 63, 63, 63	0
15	d	1/4 (25%)	0.00	0 100 100	53, 53, 53, 53	0
15	e	1/4 (25%)	-0.23	0 100 100	64, 64, 64, 64	0
15	f	1/4 (25%)	-0.66	0 100 100	53, 53, 53, 53	0
All	All	6372/6384 (99%)	-0.27	134 (2%) 63 54	36, 63, 99, 140	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	121	GLY	7.8
4	D	120	SER	7.8
2	B	220	ASN	7.6
4	R	121	GLY	7.3
7	U	243	ASP	7.0
4	R	120	SER	6.9
3	C	49	THR	6.8
3	C	50	LEU	6.7
2	P	220	ASN	6.6
10	X	198	GLN	6.3
4	D	118	GLY	6.1
2	P	219	ALA	5.6
10	X	197	ALA	5.4
4	D	122	GLU	5.4
5	E	202	ASP	5.3
5	S	2	ARG	5.1
2	B	51	VAL	5.1
10	J	198	GLN	5.1
6	F	1	GLY	5.1
3	Q	49	THR	5.0
4	D	119	ALA	4.9
10	J	197	ALA	4.9
3	Q	50	LEU	4.8
4	R	118	GLY	4.8
7	G	243	ASP	4.7
8	H	221	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	4.7
5	E	1	PHE	4.4
2	B	219	ALA	4.4
8	V	222	ASP	4.3
1	O	2	THR	4.3
4	R	119	ALA	4.2
5	S	1	PHE	4.1
5	E	2	ARG	4.0
1	O	1	MET	4.0
2	B	244	THR	4.0
7	U	1	ALA	4.0
6	T	1	GLY	4.0
3	Q	48	SER	3.9
2	P	223	GLU	3.7
12	L	174	TYR	3.7
9	I	1	SER	3.7
5	S	202	ASP	3.7
1	A	2	THR	3.6
12	Z	173	LYS	3.6
13	M	1	THR	3.5
10	X	196	GLN	3.5
6	F	202	ASP	3.4
4	R	124	ARG	3.4
13	a	1	THR	3.4
1	A	1	MET	3.4
1	O	249	ALA	3.3
12	Z	174	TYR	3.3
1	A	250	LEU	3.3
8	H	222	ASP	3.3
6	T	2	THR	3.3
3	Q	241	GLN	3.3
3	C	241	GLN	3.2
8	V	221	CYS	3.2
4	D	124	ARG	3.2
3	Q	240	GLU	3.2
2	P	60	THR	3.2
3	Q	239	GLN	3.2
10	J	196	GLN	3.1
3	Q	58	THR	3.1
3	Q	203	THR	3.1
5	S	173	ARG	3.1
2	P	221	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	2.9
5	S	36	GLY	2.9
4	R	49	PRO	2.9
6	T	51	THR	2.9
6	T	53	LYS	2.8
1	O	230	ASP	2.8
6	F	2	THR	2.8
4	R	125	LEU	2.8
3	Q	236	GLN	2.8
5	S	45	LEU	2.7
3	C	240	GLU	2.7
1	O	250	LEU	2.7
3	C	48	SER	2.7
1	O	52	SER	2.7
5	E	3	ASN	2.7
7	G	3	TYR	2.7
5	E	233	ILE	2.7
5	S	233	ILE	2.7
8	V	219	ASN	2.6
2	P	218	GLY	2.6
12	L	173	LYS	2.6
3	Q	47	ARG	2.6
6	T	244	ASN	2.6
6	T	178	HIS	2.6
3	C	202	GLN	2.5
5	E	203	GLU	2.5
4	R	123	GLU	2.5
2	P	59	ASP	2.5
2	B	223	GLU	2.4
3	C	33	GLY	2.4
3	Q	202	GLN	2.4
6	T	181	GLU	2.4
4	R	240	ALA	2.4
1	A	36	GLY	2.4
5	E	36	GLY	2.4
3	C	193	THR	2.4
4	D	31	GLY	2.3
5	E	30	GLN	2.3
1	A	248	GLU	2.3
6	T	35	GLY	2.3
2	P	50	LYS	2.3
4	R	31	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
9	W	1	SER	2.3
11	K	212	GLY	2.3
11	Y	24	ASN	2.3
5	E	201	ARG	2.3
1	O	231	LYS	2.3
3	C	43	GLY	2.2
7	G	240	ALA	2.2
4	R	122	GLU	2.2
2	B	218	GLY	2.2
3	C	53	GLN	2.2
2	P	51	VAL	2.2
5	E	54	GLU	2.2
6	F	241	LYS	2.2
14	b	195	GLN	2.1
3	Q	57	ILE	2.1
5	S	134	ILE	2.1
2	P	244	THR	2.1
6	F	243	ILE	2.1
2	B	217	LYS	2.1
3	C	207	ASN	2.1
1	A	51	SER	2.0
10	X	194	ASP	2.0
8	H	198	GLU	2.0
13	M	81	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
15	LYO	e	3	10/11	0.93	0.17	60,61,62,63	0
15	0W6	c	4	7/8	0.93	0.15	57,58,61,63	0
15	LYO	c	3	10/11	0.95	0.17	59,60,63,63	0
15	LYO	d	3	10/11	0.95	0.17	48,51,53,54	0
15	0W6	e	4	7/8	0.95	0.15	57,59,61,62	0
15	0W6	f	4	7/8	0.95	0.13	49,50,56,56	0
15	LYO	f	3	10/11	0.96	0.16	48,51,53,54	0
15	0W6	d	4	7/8	0.97	0.11	49,50,56,56	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.