



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 08:25 PM EST

PDB ID : 4FZG
Title : 20S yeast proteasome in complex with glidobactin
Authors : Stein, M.; Beck, P.; Kaiser, M.; Dudler, R.; Becker, C.F.W.; Groll, M.
Deposited on : 2012-07-06
Resolution : 3.00 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)
Xtrriage (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

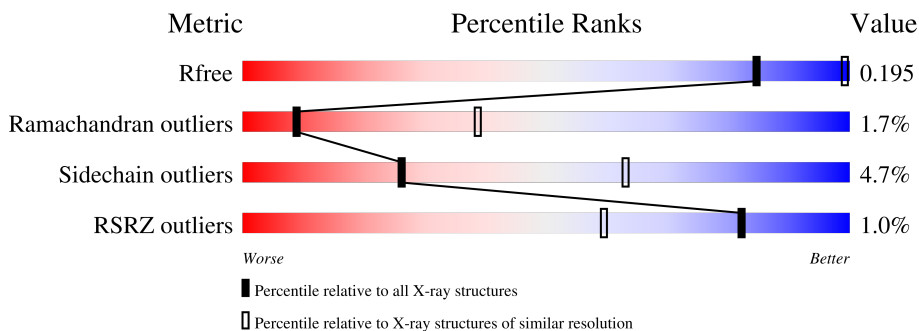
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R _{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	96% .
1	O	250	96% .
2	B	244	93% 7%
2	P	244	93% 7%
3	C	241	95% 5%
3	Q	241	95% 5%


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Mol	Chain	Length	Quality of chain
4	D	242	2% 94% 6%
4	R	242	2% 94% 6%
5	E	233	2% 90% 9%
5	S	233	2% 91% 9%
6	F	244	2% 93% 7%
6	T	244	2% 92% 8%
7	G	243	2% 94% 6%
7	U	243	2% 94% 6%
8	H	222	0% 95% 5%
8	V	222	0% 95% 5%
9	I	204	0% 97% 0%
9	W	204	0% 97% 0%
10	J	198	2% 97% 0%
10	X	198	2% 97% 0%
11	K	212	0% 97% 0%
11	Y	212	0% 97% 0%
12	L	222	0% 92% 8%
12	Z	222	0% 92% 7%
13	M	233	0% 93% 7%
13	a	233	0% 94% 6%
14	N	196	0% 96% 0%
14	b	196	0% 95% 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 50986 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
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			

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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	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
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 Glidobactin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			37	27	4	6			
15	d	4	Total	C	N	O	0	0	0
			37	27	4	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	0	0	0
			37	27	4	6			
15	f	4	Total	C	N	O	0	0	0
			37	27	4	6			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	35	Total	O	0	0
			35	35		
16	C	41	Total	O	0	0
			41	41		
16	D	39	Total	O	0	0
			39	39		
16	E	25	Total	O	0	0
			25	25		
16	F	45	Total	O	0	0
			45	45		
16	G	59	Total	O	0	0
			59	59		
16	H	52	Total	O	0	0
			52	52		
16	I	61	Total	O	0	0
			61	61		
16	J	55	Total	O	0	0
			55	55		
16	K	41	Total	O	0	0
			41	41		
16	L	57	Total	O	0	0
			57	57		
16	M	63	Total	O	0	0
			63	63		
16	N	61	Total	O	0	0
			61	61		
16	O	34	Total	O	0	0
			34	34		
16	P	27	Total	O	0	0
			27	27		
16	Q	29	Total	O	0	0
			29	29		

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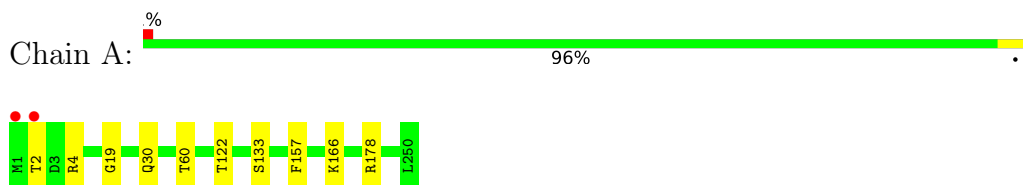
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	31	Total 31	O 31	0	0
16	S	21	Total 21	O 21	0	0
16	T	36	Total 36	O 36	0	0
16	U	63	Total 63	O 63	0	0
16	V	46	Total 46	O 46	0	0
16	W	47	Total 47	O 47	0	0
16	X	47	Total 47	O 47	0	0
16	Y	44	Total 44	O 44	0	0
16	Z	49	Total 49	O 49	0	0
16	a	72	Total 72	O 72	0	0
16	b	54	Total 54	O 54	0	0

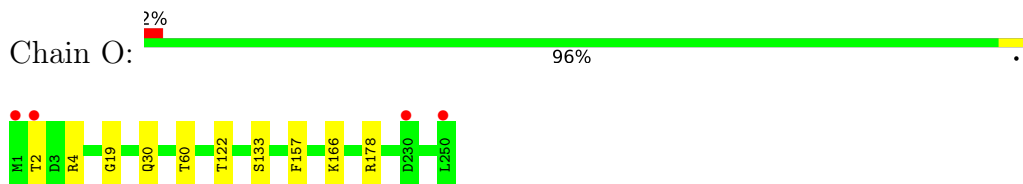
3 Residue-property plots [i](#)

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.

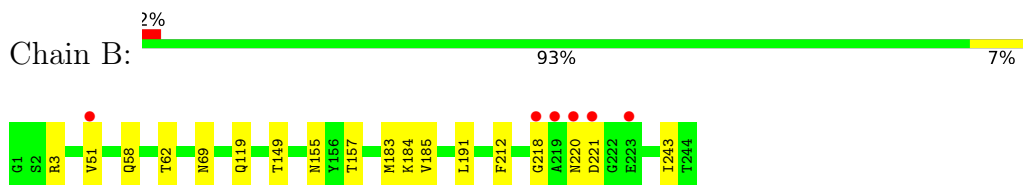
- Molecule 1: Proteasome component Y7



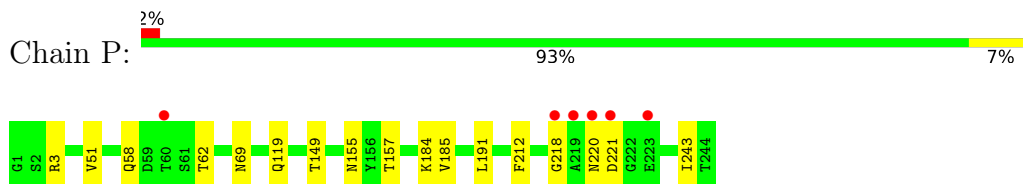
- Molecule 1: Proteasome component Y7



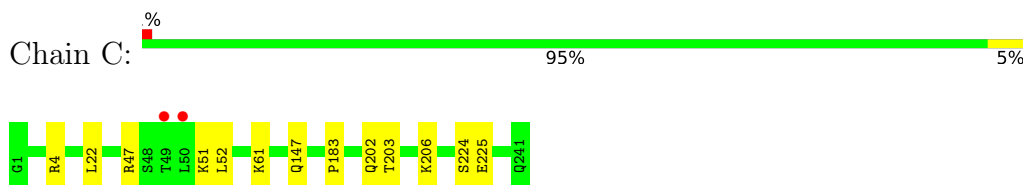
- Molecule 2: Proteasome component Y13



- Molecule 2: Proteasome component Y13



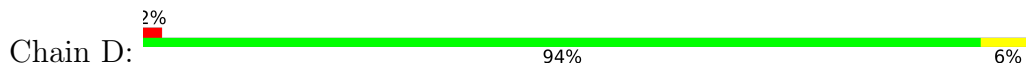
- Molecule 3: Proteasome component PRE6



- Molecule 3: Proteasome component PRE6



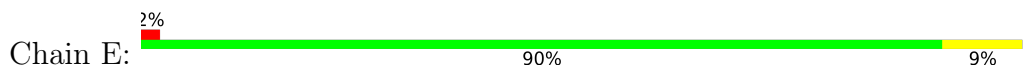
- Molecule 4: Proteasome component PUP2



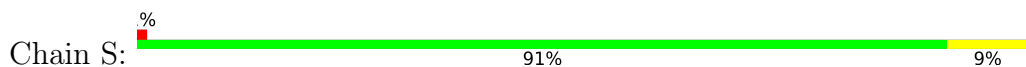
- Molecule 4: Proteasome component PUP2



- Molecule 5: Proteasome component PRE5



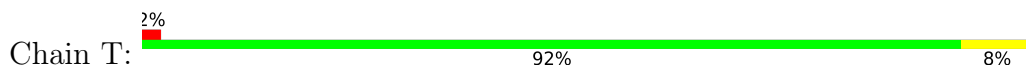
- Molecule 5: Proteasome component PRE5



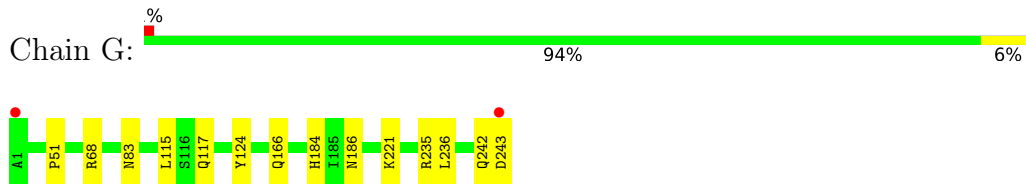
- Molecule 6: Proteasome component C1



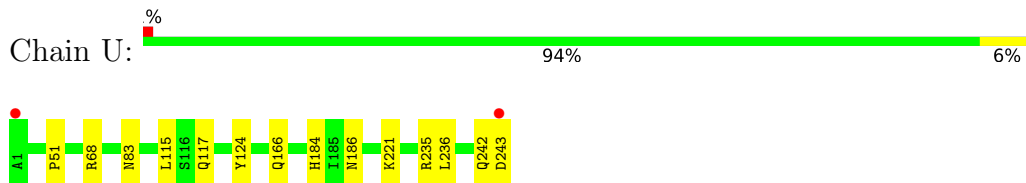
- Molecule 6: Proteasome component C1



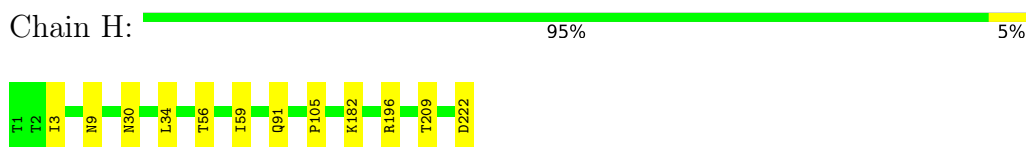
- Molecule 7: Proteasome component C7-alpha



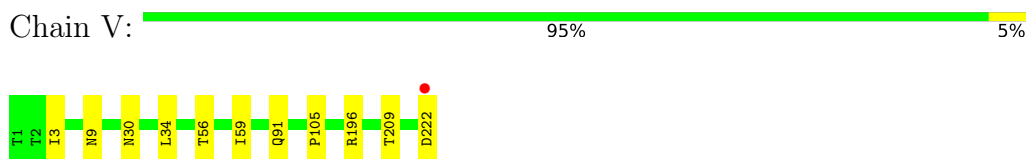
- Molecule 7: Proteasome component C7-alpha



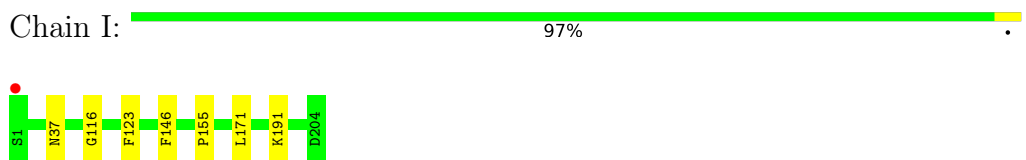
- Molecule 8: Proteasome component PUP1



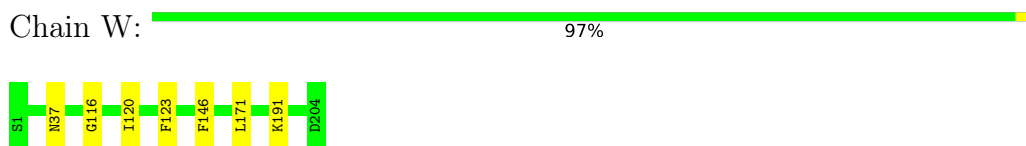
- Molecule 8: Proteasome component PUP1



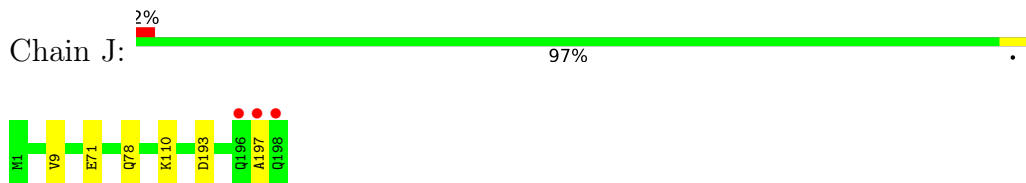
- Molecule 9: Proteasome component PUP3



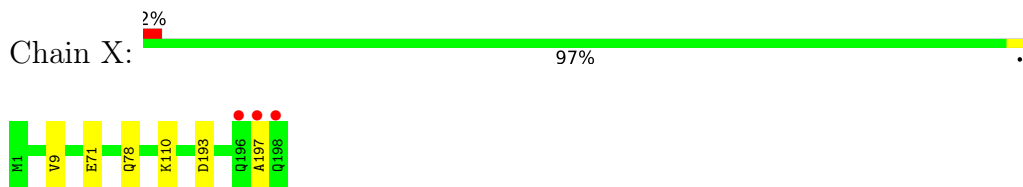
- Molecule 9: Proteasome component PUP3



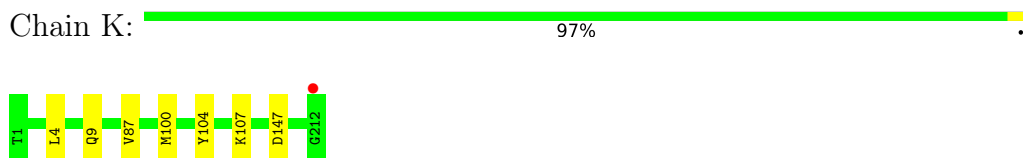
- Molecule 10: Proteasome component C11



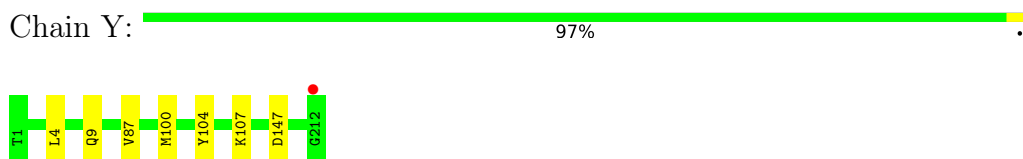
- Molecule 10: Proteasome component C11



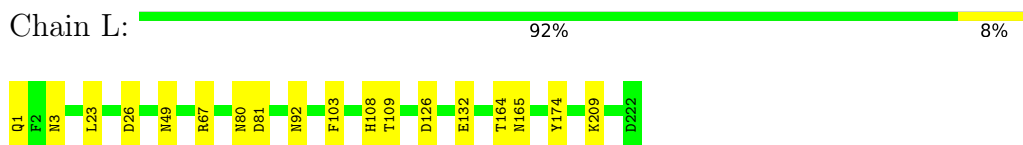
- Molecule 11: Proteasome component PRE2



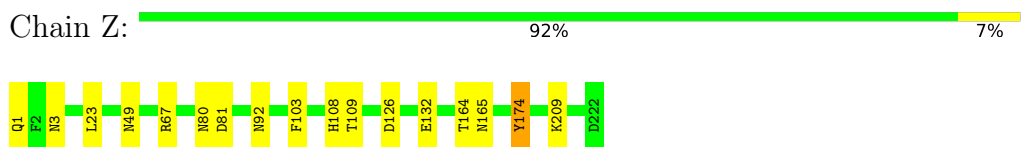
- Molecule 11: Proteasome component PRE2



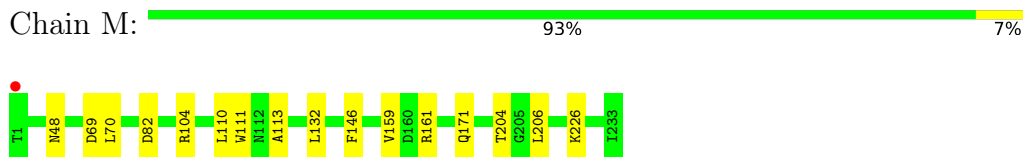
- Molecule 12: Proteasome component C5



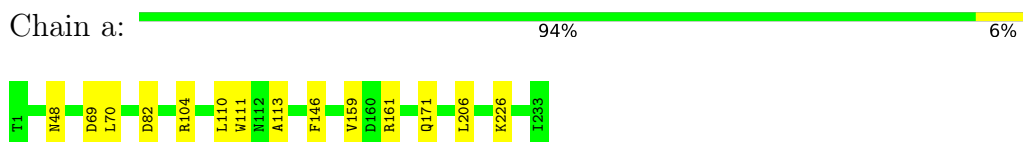
- Molecule 12: Proteasome component C5



- Molecule 13: Proteasome component PRE4



- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3

Chain N:  96%



- Molecule 14: Proteasome component PRE3

Chain b:  95%



- Molecule 15: Glidobactin

Chain c:  75%



- Molecule 15: Glidobactin

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Glidobactin

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Glidobactin

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	134.77Å 300.35Å 144.49Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 24.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-3.00) 99.6 (24.92-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.99Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.226 0.195 , 0.195	Depositor DCC
R_{free} test set	10479 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtrriage
Anisotropy	0.875	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.0	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	50986	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: MH9, 0W6, LYO

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	0.39	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.38	0/1935	0.63	0/2618
2	P	0.39	0/1935	0.64	0/2618
3	C	0.35	0/1920	0.61	0/2598
3	Q	0.36	0/1920	0.62	0/2598
4	D	0.36	0/1887	0.63	0/2541
4	R	0.38	0/1887	0.64	0/2541
5	E	0.36	0/1823	0.59	0/2463
5	S	0.37	0/1823	0.59	0/2463
6	F	0.39	0/1937	0.61	0/2614
6	T	0.39	0/1937	0.61	0/2614
7	G	0.39	0/1959	0.62	0/2652
7	U	0.38	0/1959	0.62	0/2652
8	H	0.39	0/1716	0.66	0/2326
8	V	0.38	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.65	0/2174
9	W	0.42	0/1611	0.65	0/2174
10	J	0.42	0/1613	0.64	0/2173
10	X	0.42	0/1613	0.64	0/2173
11	K	0.41	0/1681	0.65	0/2274
11	Y	0.42	0/1681	0.65	0/2274
12	L	0.41	0/1795	0.66	0/2420
12	Z	0.41	0/1795	0.66	0/2420
13	M	0.40	0/1855	0.67	2/2514 (0.1%)
13	a	0.40	0/1855	0.67	2/2514 (0.1%)
14	N	0.41	0/1541	0.64	0/2087
14	b	0.40	0/1541	0.64	0/2087
15	c	1.04	0/6	0.80	0/7
15	d	1.14	0/6	1.13	0/7
15	e	1.08	0/6	0.74	0/7
15	f	0.86	0/6	1.12	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/50474	0.64	4/68220 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	110	LEU	N-CA-C	-5.98	94.85	111.00
13	M	110	LEU	N-CA-C	-5.75	95.47	111.00
13	a	113	ALA	N-CA-C	-5.25	96.83	111.00
13	M	113	ALA	N-CA-C	-5.02	97.44	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%)	18 (7%)	4 (2%)	9	40
1	O	248/250 (99%)	224 (90%)	20 (8%)	4 (2%)	9	40
2	B	242/244 (99%)	213 (88%)	21 (9%)	8 (3%)	4	21
2	P	242/244 (99%)	212 (88%)	23 (10%)	7 (3%)	4	24
3	C	239/241 (99%)	214 (90%)	20 (8%)	5 (2%)	7	33
3	Q	239/241 (99%)	215 (90%)	19 (8%)	5 (2%)	7	33
4	D	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	3	18
4	R	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	3	18
5	E	231/233 (99%)	202 (87%)	21 (9%)	8 (4%)	3	20
5	S	231/233 (99%)	202 (87%)	22 (10%)	7 (3%)	4	24
6	F	242/244 (99%)	224 (93%)	16 (7%)	2 (1%)	19	57
6	T	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	19	57
7	G	241/243 (99%)	219 (91%)	19 (8%)	3 (1%)	13	48
7	U	241/243 (99%)	218 (90%)	20 (8%)	3 (1%)	13	48
8	H	220/222 (99%)	197 (90%)	20 (9%)	3 (1%)	11	43
8	V	220/222 (99%)	195 (89%)	22 (10%)	3 (1%)	11	43
9	I	202/204 (99%)	185 (92%)	14 (7%)	3 (2%)	10	42
9	W	202/204 (99%)	185 (92%)	15 (7%)	2 (1%)	15	53
10	J	196/198 (99%)	183 (93%)	10 (5%)	3 (2%)	10	42
10	X	196/198 (99%)	182 (93%)	11 (6%)	3 (2%)	10	42
11	K	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
11	Y	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
12	L	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	6	30
12	Z	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	8	37
13	M	231/233 (99%)	206 (89%)	24 (10%)	1 (0%)	34	72
13	a	231/233 (99%)	206 (89%)	24 (10%)	1 (0%)	34	72
14	N	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	29	68
14	b	194/196 (99%)	183 (94%)	9 (5%)	2 (1%)	15	53
15	c	1/4 (25%)	1 (100%)	0	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6316/6384 (99%)	5724 (91%)	485 (8%)	107 (2%)	9	39

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	62	THR
2	B	221	ASP
3	C	52	LEU
4	D	122	GLU
5	E	2	ARG
5	E	201	ARG
5	E	217	LYS
6	F	8	ASN
6	F	9	SER
7	G	242	GLN
12	L	81	ASP
2	P	51	VAL
2	P	62	THR
2	P	221	ASP
3	Q	52	LEU
4	R	122	GLU
5	S	2	ARG
5	S	201	ARG
5	S	217	LYS
6	T	8	ASN
6	T	9	SER
7	U	242	GLN
12	Z	81	ASP
2	B	3	ARG
2	B	218	GLY
3	C	203	THR
4	D	53	SER
4	D	126	MET
4	D	181	SER
4	D	206	GLU
5	E	175	LEU
5	E	176	ASP
9	I	191	LYS

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Mol	Chain	Res	Type
10	J	193	ASP
10	J	197	ALA
12	L	164	THR
2	P	3	ARG
2	P	218	GLY
3	Q	203	THR
4	R	53	SER
4	R	126	MET
4	R	181	SER
4	R	206	GLU
5	S	175	LEU
5	S	176	ASP
8	V	9	ASN
8	V	91	GLN
9	W	191	LYS
10	X	193	ASP
10	X	197	ALA
12	Z	164	THR
14	b	191	ASP
1	A	60	THR
3	C	202	GLN
3	C	224	SER
4	D	2	ARG
5	E	227	GLU
8	H	9	ASN
8	H	91	GLN
8	H	105	PRO
12	L	103	PHE
14	N	191	ASP
1	O	2	THR
1	O	60	THR
3	Q	202	GLN
4	R	2	ARG
8	V	105	PRO
12	Z	209	LYS
1	A	2	THR
2	B	183	MET
5	E	221	PHE
10	J	9	VAL
12	L	209	LYS
3	Q	224	SER
5	S	221	PHE

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Mol	Chain	Res	Type
10	X	9	VAL
12	Z	103	PHE
13	a	111	TRP
1	A	166	LYS
2	B	243	ILE
4	D	112	ALA
4	D	118	GLY
7	G	51	PRO
7	G	184	HIS
9	I	116	GLY
12	L	26	ASP
13	M	111	TRP
1	O	19	GLY
1	O	166	LYS
2	P	243	ILE
4	R	112	ALA
4	R	118	GLY
5	S	227	GLU
7	U	51	PRO
7	U	184	HIS
9	W	116	GLY
1	A	19	GLY
4	D	121	GLY
5	E	186	ASP
4	R	121	GLY
14	b	145	ASN
3	C	183	PRO
3	Q	183	PRO
9	I	155	PRO
2	B	185	VAL
2	P	185	VAL

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.

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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%)	193 (95%)	10 (5%)	25	61
2	P	203/203 (100%)	193 (95%)	10 (5%)	25	61
3	C	213/213 (100%)	205 (96%)	8 (4%)	33	69
3	Q	213/213 (100%)	205 (96%)	8 (4%)	33	69
4	D	198/198 (100%)	193 (98%)	5 (2%)	47	79
4	R	198/198 (100%)	193 (98%)	5 (2%)	47	79
5	E	192/192 (100%)	176 (92%)	16 (8%)	11	39
5	S	192/192 (100%)	176 (92%)	16 (8%)	11	39
6	F	201/201 (100%)	186 (92%)	15 (8%)	13	43
6	T	201/201 (100%)	184 (92%)	17 (8%)	10	38
7	G	207/207 (100%)	196 (95%)	11 (5%)	22	58
7	U	207/207 (100%)	196 (95%)	11 (5%)	22	58
8	H	181/181 (100%)	172 (95%)	9 (5%)	24	60
8	V	181/181 (100%)	173 (96%)	8 (4%)	28	65
9	I	172/172 (100%)	168 (98%)	4 (2%)	50	80
9	W	172/172 (100%)	167 (97%)	5 (3%)	42	76
10	J	175/175 (100%)	172 (98%)	3 (2%)	60	85
10	X	175/175 (100%)	172 (98%)	3 (2%)	60	85
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	67
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	67
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	50
12	Z	185/185 (100%)	172 (93%)	13 (7%)	15	47
13	M	199/199 (100%)	186 (94%)	13 (6%)	17	50
13	a	199/199 (100%)	188 (94%)	11 (6%)	21	57
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	66
14	b	162/162 (100%)	155 (96%)	7 (4%)	29	66
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	5083 (95%)	253 (5%)	26	63

All (253) 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	133	SER
1	A	157	PHE
1	A	178	ARG
2	B	58	GLN
2	B	69	ASN
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
3	C	4	ARG
3	C	22	LEU
3	C	47	ARG
3	C	51	LYS
3	C	61	LYS
3	C	147	GLN
3	C	206	LYS
3	C	225	GLU
4	D	68	CYS
4	D	124	ARG
4	D	169	GLU
4	D	176	LEU
4	D	193	LEU
5	E	9	THR
5	E	10	VAL
5	E	12	PHE
5	E	29	LYS
5	E	53	ASP

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Mol	Chain	Res	Type
5	E	71	LEU
5	E	92	ASN
5	E	112	CYS
5	E	116	GLN
5	E	184	ASN
5	E	197	SER
5	E	198	GLN
5	E	205	LEU
5	E	222	THR
5	E	227	GLU
5	E	231	LYS
6	F	32	THR
6	F	39	ASN
6	F	68	ARG
6	F	94	SER
6	F	101	THR
6	F	117	GLN
6	F	123	ASN
6	F	165	ARG
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	124	TYR
7	G	166	GLN
7	G	186	ASN
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
7	G	243	ASP
8	H	3	ILE
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	59	ILE

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Mol	Chain	Res	Type
8	H	182	LYS
8	H	196	ARG
8	H	209	THR
8	H	222	ASP
9	I	37	ASN
9	I	123	PHE
9	I	146	PHE
9	I	171	LEU
10	J	71	GLU
10	J	78	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	87	VAL
11	K	100	MET
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	67	ARG
12	L	80	ASN
12	L	92	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
12	L	132	GLU
12	L	165	ASN
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	82	ASP
13	M	104	ARG
13	M	132	LEU
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	171	GLN
13	M	204	THR
13	M	206	LEU

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Mol	Chain	Res	Type
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	119	VAL
14	N	144	GLU
1	O	4	ARG
1	O	30	GLN
1	O	122	THR
1	O	133	SER
1	O	157	PHE
1	O	178	ARG
2	P	58	GLN
2	P	69	ASN
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
3	Q	4	ARG
3	Q	22	LEU
3	Q	47	ARG
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	206	LYS
3	Q	225	GLU
4	R	68	CYS
4	R	124	ARG
4	R	169	GLU
4	R	176	LEU
4	R	193	LEU
5	S	9	THR
5	S	10	VAL
5	S	12	PHE
5	S	29	LYS
5	S	53	ASP

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Mol	Chain	Res	Type
5	S	71	LEU
5	S	92	ASN
5	S	112	CYS
5	S	116	GLN
5	S	184	ASN
5	S	197	SER
5	S	198	GLN
5	S	205	LEU
5	S	222	THR
5	S	227	GLU
5	S	231	LYS
6	T	14	ASP
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	94	SER
6	T	101	THR
6	T	117	GLN
6	T	123	ASN
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	214	TRP
6	T	221	ASN
6	T	228	LYS
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	124	TYR
7	U	166	GLN
7	U	186	ASN
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
7	U	243	ASP
8	V	3	ILE
8	V	30	ASN
8	V	34	LEU

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Mol	Chain	Res	Type
8	V	56	THR
8	V	59	ILE
8	V	196	ARG
8	V	209	THR
8	V	222	ASP
9	W	37	ASN
9	W	120	ILE
9	W	123	PHE
9	W	146	PHE
9	W	171	LEU
10	X	71	GLU
10	X	78	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	87	VAL
11	Y	100	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	147	ASP
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	67	ARG
12	Z	80	ASN
12	Z	92	ASN
12	Z	108	HIS
12	Z	109	THR
12	Z	126	ASP
12	Z	132	GLU
12	Z	165	ASN
12	Z	174	TYR
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	82	ASP
13	a	104	ARG
13	a	146	PHE
13	a	159	VAL
13	a	161	ARG
13	a	171	GLN

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Mol	Chain	Res	Type
13	a	206	LEU
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	119	VAL
14	b	144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
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
3	C	17	GLN
3	C	92	GLN
3	C	147	GLN
3	C	160	GLN
3	C	207	ASN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN

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Mol	Chain	Res	Type
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	224	HIS
7	G	6	HIS
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	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	172	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	146	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	188	HIS

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Mol	Chain	Res	Type
11	K	191	HIS
11	K	208	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	92	ASN
12	L	135	GLN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	165	ASN
12	L	195	HIS
12	L	197	GLN
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	194	ASN
13	M	213	GLN
14	N	60	GLN
14	N	69	GLN
14	N	157	HIS
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	69	ASN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	92	GLN

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Mol	Chain	Res	Type
3	Q	147	GLN
3	Q	160	GLN
3	Q	207	ASN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	4	ASN
5	S	30	GLN
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	151	ASN
5	S	184	ASN
5	S	198	GLN
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	6	HIS
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	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN

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Mol	Chain	Res	Type
8	V	172	ASN
9	W	37	ASN
9	W	71	ASN
9	W	88	GLN
9	W	156	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
10	X	146	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	188	HIS
11	Y	191	HIS
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	92	ASN
12	Z	135	GLN
12	Z	152	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	165	ASN
12	Z	195	HIS
12	Z	197	GLN
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	194	ASN
13	a	213	GLN
14	b	60	GLN
14	b	69	GLN

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Mol	Chain	Res	Type
14	b	145	ASN
14	b	157	HIS
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	OW6	d	4	15,11	6,6,7	1.10	0	5,6,8	0.69	0
15	OW6	f	4	15,11	6,6,7	1.12	0	5,6,8	0.65	0
15	LYO	d	3	15	7,9,10	0.87	0	6,10,12	0.54	0
15	LYO	c	3	15	7,9,10	0.97	0	6,10,12	0.56	0
15	OW6	e	4	8,15	6,6,7	1.08	0	5,6,8	0.91	0
15	LYO	f	3	15	7,9,10	0.95	0	6,10,12	0.51	0
15	OW6	c	4	8,15	6,6,7	1.45	1 (16%)	5,6,8	0.86	0
15	LYO	e	3	15	7,9,10	0.92	0	6,10,12	0.45	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	OW6	d	4	15,11	-	1/3/4/5	-
15	OW6	f	4	15,11	-	1/3/4/5	-
15	LYO	d	3	15	-	3/8/9/11	-
15	LYO	c	3	15	-	4/8/9/11	-

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	0W6	C17-CA	2.96	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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%)	-0.43	2 (0%) 86 65	61, 83, 116, 141	0
1	O	250/250 (100%)	-0.54	4 (1%) 72 44	61, 83, 117, 141	0
2	B	244/244 (100%)	-0.36	6 (2%) 57 29	61, 83, 131, 151	0
2	P	244/244 (100%)	-0.37	6 (2%) 57 29	61, 83, 131, 151	0
3	C	241/241 (100%)	-0.38	2 (0%) 86 65	63, 89, 135, 162	0
3	Q	241/241 (100%)	-0.32	4 (1%) 70 41	65, 91, 136, 162	0
4	D	242/242 (100%)	-0.30	6 (2%) 57 29	61, 90, 125, 155	0
4	R	242/242 (100%)	-0.29	5 (2%) 63 34	63, 91, 126, 155	0
5	E	233/233 (100%)	-0.34	4 (1%) 70 41	67, 95, 125, 145	0
5	S	233/233 (100%)	-0.31	3 (1%) 77 51	68, 95, 125, 145	0
6	F	244/244 (100%)	-0.37	3 (1%) 79 54	64, 87, 124, 141	0
6	T	244/244 (100%)	-0.29	4 (1%) 72 44	65, 87, 125, 140	0
7	G	243/243 (100%)	-0.48	2 (0%) 86 65	62, 84, 116, 152	0
7	U	243/243 (100%)	-0.47	2 (0%) 86 65	63, 83, 115, 153	0
8	H	222/222 (100%)	-0.67	0 100 100	59, 75, 98, 140	0
8	V	222/222 (100%)	-0.67	1 (0%) 91 75	61, 74, 98, 142	0
9	I	204/204 (100%)	-0.71	1 (0%) 91 75	57, 75, 99, 117	0
9	W	204/204 (100%)	-0.68	0 100 100	58, 75, 99, 116	0
10	J	198/198 (100%)	-0.58	3 (1%) 73 46	56, 76, 99, 161	0
10	X	198/198 (100%)	-0.60	3 (1%) 73 46	57, 77, 98, 162	0
11	K	212/212 (100%)	-0.63	1 (0%) 91 75	55, 75, 99, 115	0
11	Y	212/212 (100%)	-0.63	1 (0%) 91 75	56, 75, 101, 117	0
12	L	222/222 (100%)	-0.65	0 100 100	59, 77, 105, 129	0
12	Z	222/222 (100%)	-0.63	0 100 100	59, 77, 104, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.63	1 (0%) 92 79	59, 77, 99, 110	0
13	a	233/233 (100%)	-0.62	0 100 100	58, 77, 99, 110	0
14	N	196/196 (100%)	-0.65	0 100 100	58, 74, 100, 115	0
14	b	196/196 (100%)	-0.61	0 100 100	58, 74, 101, 114	0
15	c	1/4 (25%)	-0.79	0 100 100	75, 75, 75, 75	0
15	d	1/4 (25%)	-0.65	0 100 100	63, 63, 63, 63	0
15	e	1/4 (25%)	-0.57	0 100 100	75, 75, 75, 75	0
15	f	1/4 (25%)	-1.05	0 100 100	66, 66, 66, 66	0
All	All	6372/6384 (99%)	-0.50	64 (1%) 82 59	55, 81, 120, 162	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	118	GLY	6.2
7	U	243	ASP	6.1
4	R	121	GLY	6.0
4	D	121	GLY	5.6
2	B	220	ASN	5.5
4	D	120	SER	5.4
4	R	118	GLY	5.3
4	D	119	ALA	5.2
2	P	220	ASN	5.1
10	X	198	GLN	5.0
2	B	219	ALA	4.7
3	C	50	LEU	4.7
3	C	49	THR	4.7
2	P	219	ALA	4.6
4	R	119	ALA	4.3
10	X	197	ALA	4.1
10	J	197	ALA	4.0
10	J	198	GLN	3.9
5	E	1	PHE	3.8
3	Q	50	LEU	3.7
3	Q	48	SER	3.7
4	R	120	SER	3.7
7	G	1	ALA	3.5
8	V	222	ASP	3.3
2	B	221	ASP	3.1
5	E	2	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
6	F	202	ASP	3.1
10	J	196	GLN	3.1
6	T	1	GLY	3.0
3	Q	49	THR	3.0
1	O	1	MET	3.0
1	A	1	MET	2.9
5	S	1	PHE	2.8
7	G	243	ASP	2.8
5	E	233	ILE	2.8
6	F	203	ASN	2.8
11	Y	212	GLY	2.7
10	X	196	GLN	2.7
2	P	218	GLY	2.6
11	K	212	GLY	2.6
5	S	233	ILE	2.6
5	E	202	ASP	2.5
6	F	1	GLY	2.5
7	U	1	ALA	2.5
6	T	51	THR	2.4
4	D	124	ARG	2.4
2	B	51	VAL	2.4
2	P	221	ASP	2.3
2	B	218	GLY	2.3
1	A	2	THR	2.3
13	M	1	THR	2.3
6	T	2	THR	2.3
2	P	60	THR	2.2
9	I	1	SER	2.2
4	D	122	GLU	2.2
5	S	52	ALA	2.2
3	Q	203	THR	2.2
1	O	2	THR	2.1
2	P	223	GLU	2.1
1	O	250	LEU	2.1
2	B	223	GLU	2.1
6	T	201	GLU	2.1
1	O	230	ASP	2.1
4	R	122	GLU	2.1

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	0.18	73,75,78,79	0
15	0W6	c	4	7/8	0.95	0.14	70,72,76,77	0
15	0W6	e	4	7/8	0.95	0.15	71,73,77,77	0
15	LYO	d	3	10/11	0.96	0.13	64,68,71,71	0
15	0W6	d	4	7/8	0.96	0.13	67,67,72,72	0
15	LYO	c	3	10/11	0.96	0.12	72,74,78,78	0
15	LYO	f	3	10/11	0.97	0.13	64,67,71,72	0
15	0W6	f	4	7/8	0.97	0.12	67,68,72,73	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.