



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:58 PM BST

PDB ID : 5LAI
Title : Ligand-induced aziridine-formation at the yeast proteasomal subunit beta5 by sulfonate esters
Authors : Groll, M.; Dubiella, C.; Cui, H.
Deposited on : 2016-06-14
Resolution : 2.50 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 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	:	2.13
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)	:	2.13

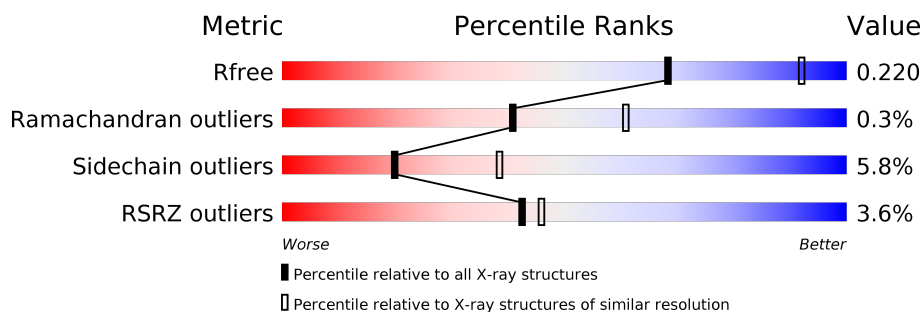
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	O	250	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
2	B	258	<div> <div>5%</div> <div>89%</div> <div>5% 5%</div> </div>
2	P	258	<div> <div>6%</div> <div>89%</div> <div>5% 5%</div> </div>
3	C	254	<div> <div>8%</div> <div>86%</div> <div>9% 6%</div> </div>
3	Q	254	<div> <div>9%</div> <div>86%</div> <div>9% 6%</div> </div>
4	D	260	<div> <div>2%</div> <div>84%</div> <div>7% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	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	MG	I	302	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50312 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 subunit alpha type-2.

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 subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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 subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

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 subunit beta type-7.

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 subunit beta type-1.

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

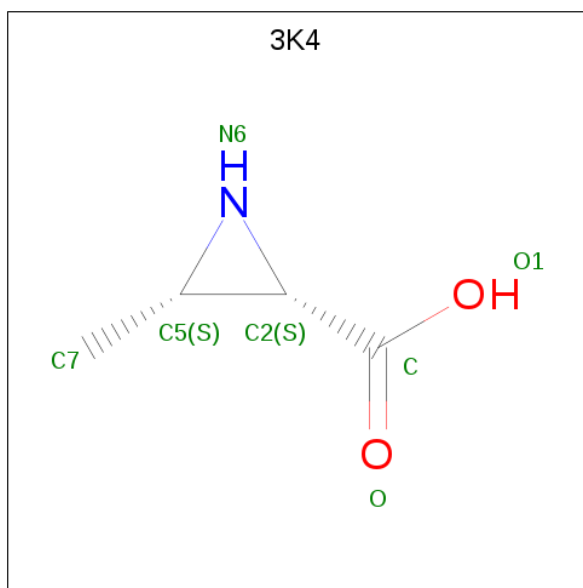
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	2	Total 2	Mg 2	0	0
15	H	1	Total 1	Mg 1	0	0
15	I	2	Total 2	Mg 2	0	0
15	V	1	Total 1	Mg 1	0	0
15	Z	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0

- Molecule 16 is (2S,3S)-3-methylaziridine-2-carboxylic acid (three-letter code: 3K4) (formula: $C_4H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total 6	C 4	N 1	O 1	0	0
16	Y	1	Total 6	C 4	N 1	O 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	51	Total O 51 51	0	0
17	B	31	Total O 31 31	0	0
17	C	25	Total O 25 25	0	0
17	D	21	Total O 21 21	0	0
17	E	24	Total O 24 24	0	0
17	F	28	Total O 28 28	0	0
17	G	42	Total O 42 42	0	0
17	H	41	Total O 41 41	0	0
17	I	34	Total O 34 34	0	0
17	J	39	Total O 39 39	0	0
17	K	40	Total O 40 40	0	0
17	L	47	Total O 47 47	0	0
17	M	46	Total O 46 46	0	0
17	N	33	Total O 33 33	0	0
17	O	23	Total O 23 23	0	0
17	P	28	Total O 28 28	0	0
17	Q	23	Total O 23 23	0	0
17	R	24	Total O 24 24	0	0
17	S	8	Total O 8 8	0	0
17	T	35	Total O 35 35	0	0
17	U	38	Total O 38 38	0	0
17	V	23	Total O 23 23	0	0

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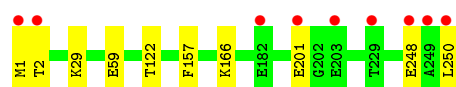
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	39	Total 39	O 39	0	0
17	X	34	Total 34	O 34	0	0
17	Y	30	Total 30	O 30	0	0
17	Z	35	Total 35	O 35	0	0
17	a	55	Total 55	O 55	0	0
17	b	40	Total 40	O 40	0	0

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.

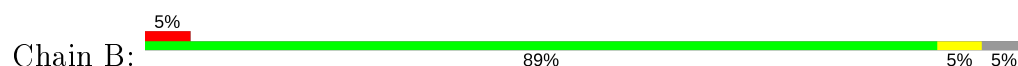
- Molecule 1: Proteasome subunit alpha type-2



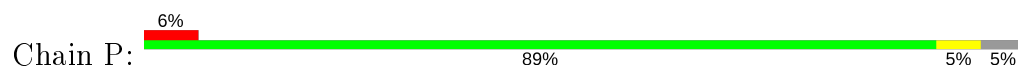
- Molecule 1: Proteasome subunit alpha type-2



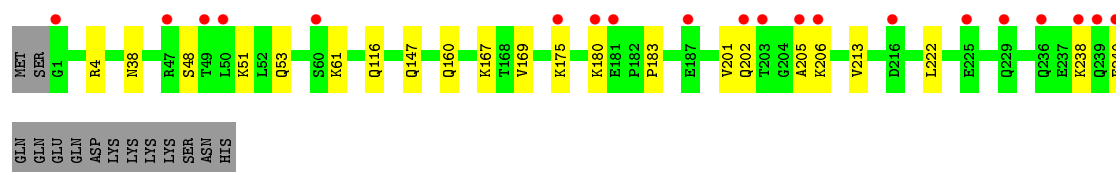
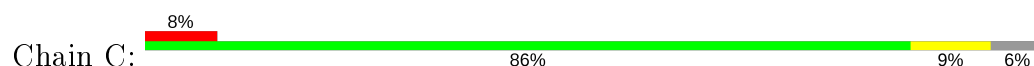
- Molecule 2: Proteasome subunit alpha type-3



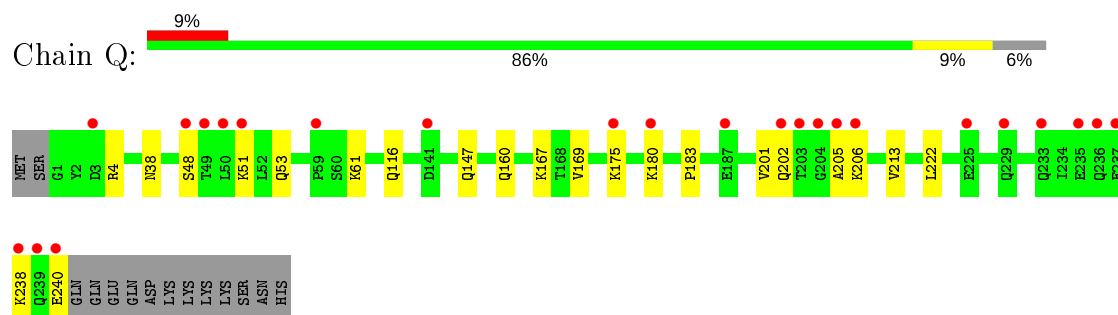
- Molecule 2: Proteasome subunit alpha type-3



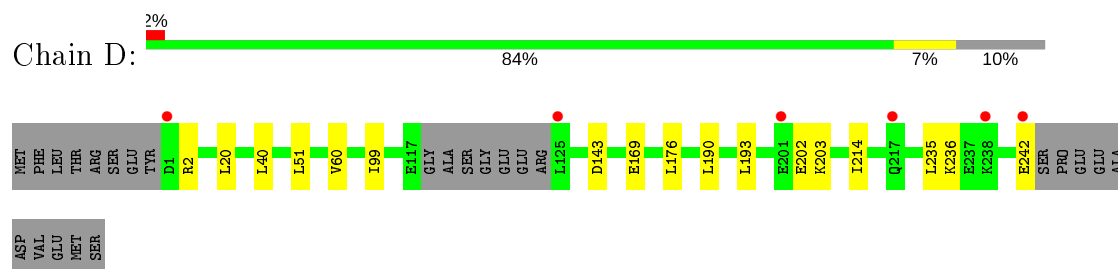
- Molecule 3: Proteasome subunit alpha type-4



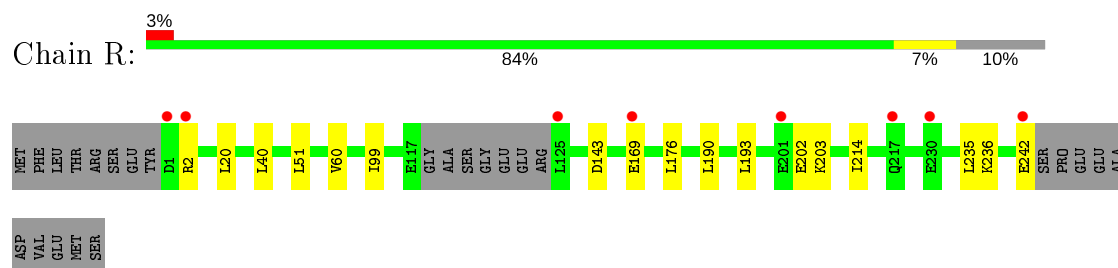
- Molecule 3: Proteasome subunit alpha type-4



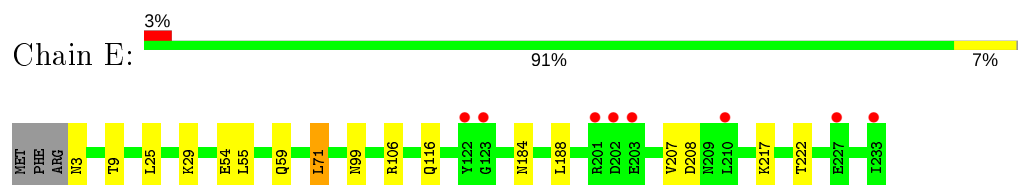
- Molecule 4: Proteasome subunit alpha type-5



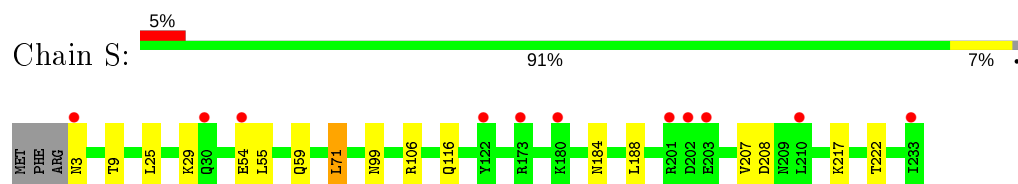
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-6

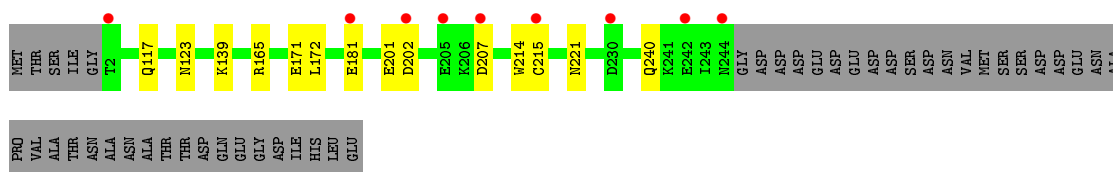


- Molecule 5: Proteasome subunit alpha type-6

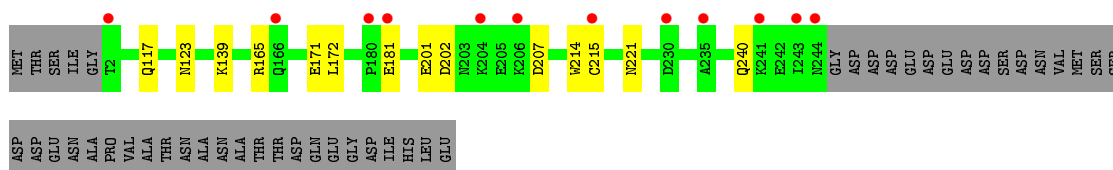
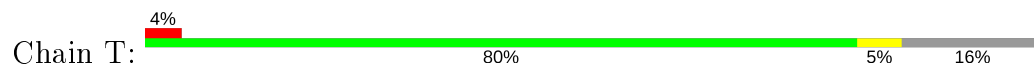


- Molecule 6: Probable proteasome subunit alpha type-7





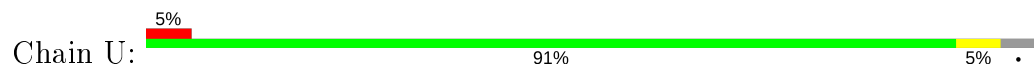
- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 7: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

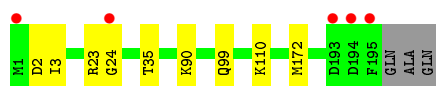




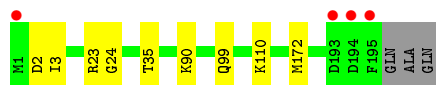
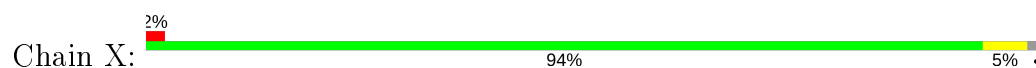
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



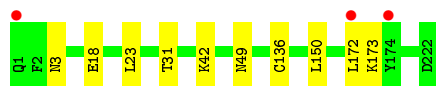
- Molecule 11: Proteasome subunit beta type-5



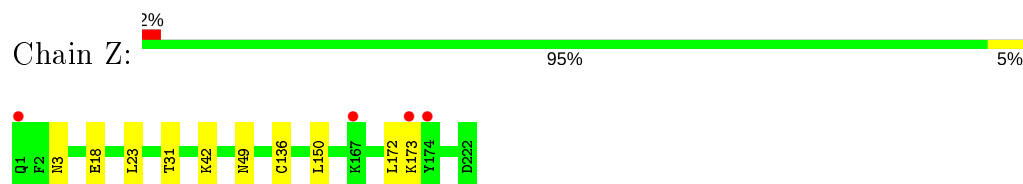
- Molecule 11: Proteasome subunit beta type-5



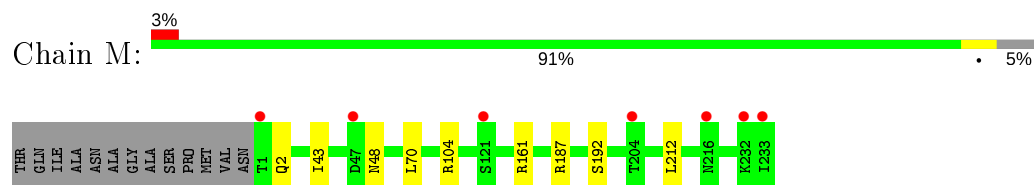
- Molecule 12: Proteasome subunit beta type-6



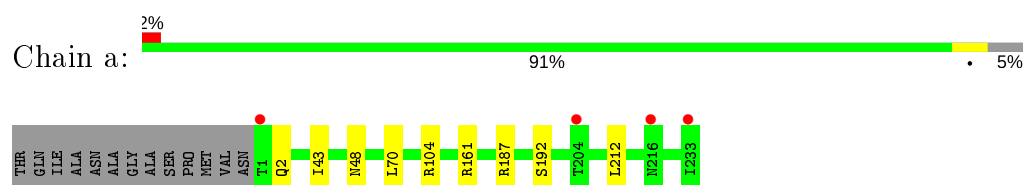
- Molecule 12: Proteasome subunit beta type-6



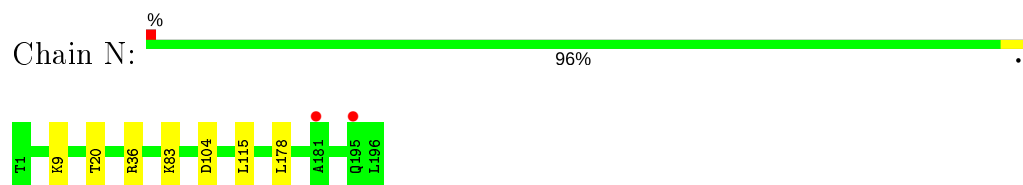
- Molecule 13: Proteasome subunit beta type-7



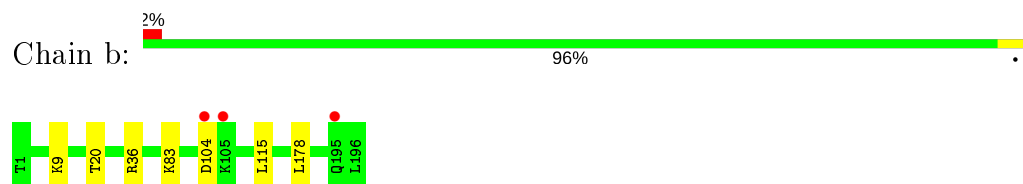
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.15Å 300.75Å 145.66Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.50) 97.5 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.219 0.204 , 0.220	Depositor DCC
R_{free} test set	17995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50312	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3K4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1952	0.50	0/2642
1	O	0.28	0/1952	0.50	0/2642
2	B	0.29	0/1934	0.54	0/2618
2	P	0.29	0/1934	0.54	0/2618
3	C	0.29	0/1910	0.55	0/2586
3	Q	0.30	0/1910	0.55	0/2586
4	D	0.28	0/1837	0.53	0/2475
4	R	0.28	0/1837	0.52	0/2475
5	E	0.29	0/1800	0.52	1/2433 (0.0%)
5	S	0.29	0/1800	0.52	1/2433 (0.0%)
6	F	0.29	0/1932	0.50	0/2609
6	T	0.29	0/1932	0.50	0/2609
7	G	0.28	0/1945	0.51	0/2634
7	U	0.28	0/1945	0.51	0/2634
8	H	0.25	0/1750	0.52	0/2373
8	V	0.25	0/1750	0.52	0/2373
9	I	0.27	0/1611	0.53	0/2174
9	W	0.27	0/1611	0.53	0/2174
10	J	0.28	0/1589	0.51	0/2142
10	X	0.28	0/1589	0.51	0/2142
11	K	0.26	0/1674	0.55	1/2264 (0.0%)
11	Y	0.26	0/1674	0.56	1/2264 (0.0%)
12	L	0.27	0/1795	0.53	0/2420
12	Z	0.27	0/1795	0.53	0/2420
13	M	0.27	0/1855	0.55	0/2514
13	a	0.26	0/1855	0.55	0/2514
14	N	0.25	0/1541	0.51	0/2087
14	b	0.25	0/1541	0.51	0/2087
All	All	0.28	0/50250	0.52	4/67942 (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
1	A	0	1
1	O	0	1
2	B	0	1
2	P	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.40	127.73	115.30
11	K	4	LEU	CA-CB-CG	5.40	127.71	115.30
5	E	71	LEU	CA-CB-CG	5.15	127.14	115.30
5	S	71	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
2	B	50	LYS	Peptide
1	O	1	MET	Peptide
2	P	50	LYS	Peptide

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%)	240 (97%)	6 (2%)	2 (1%)	19	35
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19	35
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	35
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	35
3	C	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	12	21
3	Q	238/254 (94%)	227 (95%)	8 (3%)	3 (1%)	12	21
4	D	231/260 (89%)	229 (99%)	1 (0%)	1 (0%)	34	54
4	R	231/260 (89%)	229 (99%)	1 (0%)	1 (0%)	34	54
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	48
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	48
11	K	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6282/6614 (95%)	6117 (97%)	147 (2%)	18 (0%)	41	61

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
3	C	202	GLN
3	C	205	ALA
1	O	2	THR
3	Q	202	GLN
3	Q	205	ALA
4	D	2	ARG
4	R	2	ARG
1	A	166	LYS
1	O	166	LYS
2	B	51	VAL
2	P	51	VAL
3	C	183	PRO
10	J	24	GLY
3	Q	183	PRO
10	X	24	GLY
2	B	218	GLY
2	P	218	GLY

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%)	202 (97%)	7 (3%)	38	64
1	O	209/209 (100%)	202 (97%)	7 (3%)	38	64
2	B	203/216 (94%)	191 (94%)	12 (6%)	19	37
2	P	203/216 (94%)	191 (94%)	12 (6%)	19	37
3	C	212/226 (94%)	193 (91%)	19 (9%)	9	19
3	Q	212/226 (94%)	193 (91%)	19 (9%)	9	19
4	D	194/215 (90%)	178 (92%)	16 (8%)	11	22
4	R	194/215 (90%)	178 (92%)	16 (8%)	11	22
5	E	190/193 (98%)	173 (91%)	17 (9%)	9	19
5	S	190/193 (98%)	173 (91%)	17 (9%)	9	19
6	F	201/239 (84%)	187 (93%)	14 (7%)	15	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	187 (93%)	14 (7%)	15	29
7	G	206/210 (98%)	195 (95%)	11 (5%)	22	43
7	U	206/210 (98%)	195 (95%)	11 (5%)	22	43
8	H	185/190 (97%)	176 (95%)	9 (5%)	25	47
8	V	185/190 (97%)	176 (95%)	9 (5%)	25	47
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	62
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	62
10	J	173/175 (99%)	165 (95%)	8 (5%)	27	50
10	X	173/175 (99%)	165 (95%)	8 (5%)	27	50
11	K	168/169 (99%)	160 (95%)	8 (5%)	25	48
11	Y	168/169 (99%)	160 (95%)	8 (5%)	25	48
12	L	185/185 (100%)	175 (95%)	10 (5%)	22	42
12	Z	185/185 (100%)	175 (95%)	10 (5%)	22	42
13	M	199/208 (96%)	190 (96%)	9 (4%)	27	51
13	a	199/208 (96%)	190 (96%)	9 (4%)	27	51
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	53
14	b	162/162 (100%)	155 (96%)	7 (4%)	29	53
All	All	5318/5540 (96%)	5012 (94%)	306 (6%)	20	38

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	59	GLU
1	A	122	THR
1	A	157	PHE
1	A	201	GLU
1	A	248	GLU
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	63	GLU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG

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Mol	Chain	Res	Type
2	B	119	GLN
2	B	191	LEU
2	B	203	SER
2	B	237	ILE
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	48	SER
3	C	51	LYS
3	C	53	GLN
3	C	61	LYS
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	201	VAL
3	C	206	LYS
3	C	213	VAL
3	C	222	LEU
3	C	238	LYS
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	143	ASP
4	D	169	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	203	LYS
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	9	THR

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Mol	Chain	Res	Type
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	59	GLN
5	E	71	LEU
5	E	99	ASN
5	E	106	ARG
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	217	LYS
5	E	222	THR
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	215	CYS
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	166	GLN
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU

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Mol	Chain	Res	Type
8	H	55	VAL
8	H	63	ILE
8	H	68	LEU
8	H	106	THR
8	H	127	LEU
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	96	GLU
9	I	126	ILE
9	I	133	LYS
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	172	MET
11	K	4	LEU
11	K	7	ARG
11	K	35	ILE
11	K	57	THR
11	K	104	TYR
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	42	LYS
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	83	LYS
14	N	104	ASP
14	N	115	LEU
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	122	THR
1	O	157	PHE
1	O	201	GLU
1	O	248	GLU
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	63	GLU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	203	SER
2	P	237	ILE
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER
3	Q	51	LYS
3	Q	53	GLN
3	Q	61	LYS
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS

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Mol	Chain	Res	Type
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	201	VAL
3	Q	206	LYS
3	Q	213	VAL
3	Q	222	LEU
3	Q	238	LYS
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	143	ASP
4	R	169	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	203	LYS
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	59	GLN
5	S	71	LEU
5	S	99	ASN
5	S	106	ARG
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	217	LYS
5	S	222	THR

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Mol	Chain	Res	Type
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	215	CYS
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	63	ILE
8	V	68	LEU
8	V	106	THR
8	V	127	LEU
8	V	153	LYS
8	V	196	ARG
9	W	37	ASN
9	W	96	GLU
9	W	126	ILE
9	W	133	LYS
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE

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Mol	Chain	Res	Type
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	172	MET
11	Y	4	LEU
11	Y	7	ARG
11	Y	35	ILE
11	Y	57	THR
11	Y	104	TYR
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	212	LEU
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	83	LYS
14	b	104	ASP
14	b	115	LEU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	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
8	H	30	ASN
8	H	66	HIS
8	H	114	HIS

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Mol	Chain	Res	Type
8	H	116	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS

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Mol	Chain	Res	Type
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	66	HIS
8	V	114	HIS
8	V	116	HIS
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN

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Mol	Chain	Res	Type
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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$
16	3K4	Y	301	11	5,6,7	3.99	3 (60%)	4,8,10	4.99	3 (75%)
16	3K4	K	301	11	5,6,7	3.72	3 (60%)	4,8,10	5.17	3 (75%)

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
16	3K4	Y	301	11	-	1/1/7/9	0/1/1/1
16	3K4	K	301	11	-	1/1/7/9	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	3K4	C5-N6	-7.27	1.42	1.48
16	K	301	3K4	C5-N6	-6.47	1.43	1.48
16	K	301	3K4	C2-C5	-4.16	1.39	1.48
16	Y	301	3K4	C2-C5	-4.07	1.39	1.48
16	K	301	3K4	C7-C5	-2.58	1.47	1.52
16	Y	301	3K4	C7-C5	-2.41	1.47	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	301	3K4	C7-C5-C2	6.60	133.85	122.56
16	Y	301	3K4	C7-C5-N6	6.32	136.13	117.83
16	K	301	3K4	C7-C5-N6	6.21	135.82	117.83
16	Y	301	3K4	C7-C5-C2	6.20	133.16	122.56
16	K	301	3K4	C2-C5-N6	4.81	61.64	59.79
16	Y	301	3K4	C2-C5-N6	4.42	61.49	59.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	3K4	O-C-C2-C5
16	Y	301	3K4	O-C-C2-C5

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%)	-0.13	9 (3%) 42 46	34, 46, 78, 120	0
1	O	250/250 (100%)	-0.03	11 (4%) 34 37	38, 52, 94, 128	0
2	B	244/258 (94%)	0.02	13 (5%) 26 28	34, 51, 90, 149	0
2	P	244/258 (94%)	0.12	16 (6%) 18 19	38, 54, 95, 143	0
3	C	240/254 (94%)	0.13	20 (8%) 11 11	33, 54, 117, 137	0
3	Q	240/254 (94%)	0.34	24 (10%) 7 6	39, 62, 132, 163	0
4	D	235/260 (90%)	-0.09	6 (2%) 56 59	39, 54, 84, 125	0
4	R	235/260 (90%)	0.03	8 (3%) 45 48	42, 59, 90, 123	0
5	E	231/234 (98%)	0.04	8 (3%) 44 47	41, 57, 94, 140	0
5	S	231/234 (98%)	0.17	11 (4%) 30 32	45, 65, 98, 146	0
6	F	243/288 (84%)	-0.09	9 (3%) 41 45	36, 53, 99, 126	0
6	T	243/288 (84%)	0.03	12 (4%) 29 31	37, 59, 108, 131	0
7	G	241/252 (95%)	-0.16	9 (3%) 41 45	32, 47, 79, 129	0
7	U	241/252 (95%)	-0.08	12 (4%) 28 30	37, 50, 78, 112	0
8	H	226/232 (97%)	-0.00	11 (4%) 29 31	33, 46, 76, 136	0
8	V	226/232 (97%)	0.09	9 (3%) 38 41	37, 50, 80, 146	0
9	I	204/205 (99%)	-0.39	3 (1%) 73 75	32, 44, 71, 90	0
9	W	204/205 (99%)	-0.37	2 (0%) 82 84	34, 46, 71, 98	0
10	J	195/198 (98%)	-0.18	5 (2%) 56 59	33, 47, 73, 134	0
10	X	195/198 (98%)	-0.19	4 (2%) 63 66	34, 48, 73, 132	0
11	K	211/212 (99%)	-0.34	2 (0%) 84 86	35, 46, 66, 84	0
11	Y	211/212 (99%)	-0.29	1 (0%) 91 91	37, 46, 69, 85	0
12	L	222/222 (100%)	-0.30	3 (1%) 75 77	34, 47, 74, 106	0
12	Z	222/222 (100%)	-0.25	4 (1%) 68 71	35, 48, 74, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	M	233/246 (94%)	-0.31	7 (3%)	50	53	31, 47, 70, 87	0
13	a	233/246 (94%)	-0.26	4 (1%)	70	72	32, 46, 66, 83	0
14	N	196/196 (100%)	-0.33	2 (1%)	82	84	33, 43, 70, 97	0
14	b	196/196 (100%)	-0.29	3 (1%)	73	75	34, 44, 69, 103	0
All	All	6342/6614 (95%)	-0.10	228 (3%)	42	46	31, 50, 88, 163	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	12.9
2	P	222	GLY	10.7
8	V	223	ILE	9.7
8	V	224	GLN	8.5
10	X	1	MET	7.6
8	V	221	CYS	7.3
2	B	221	ASP	7.2
10	J	1	MET	7.1
2	B	219	ALA	6.8
3	Q	206	LYS	6.4
2	B	218	GLY	6.3
8	H	226	GLU	6.1
2	P	51	VAL	6.0
8	V	226	GLU	5.8
3	Q	239	GLN	5.6
8	H	223	ILE	5.5
8	H	221	CYS	5.4
8	H	224	GLN	5.4
2	P	221	ASP	5.3
5	S	202	ASP	5.3
6	T	243	ILE	5.3
12	L	174	TYR	5.2
3	C	49	THR	5.0
12	Z	174	TYR	4.9
8	V	222	ASP	4.9
3	C	238	LYS	4.8
6	F	244	ASN	4.7
2	P	220	ASN	4.6
3	C	236	GLN	4.6
3	Q	50	LEU	4.6
3	C	240	GLU	4.6
1	A	2	THR	4.5

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Mol	Chain	Res	Type	RSRZ
9	I	1	SER	4.5
6	F	205	GLU	4.5
2	B	222	GLY	4.4
8	H	222	ASP	4.4
3	C	206	LYS	4.4
3	Q	238	LYS	4.4
3	C	202	GLN	4.4
3	Q	202	GLN	4.4
9	W	1	SER	4.3
1	O	231	LYS	4.3
5	E	123	GLY	4.3
10	X	194	ASP	4.3
3	C	50	LEU	4.3
3	C	239	GLN	4.2
2	B	51	VAL	4.2
1	O	249	ALA	4.2
1	O	1	MET	4.1
1	A	1	MET	4.1
5	E	202	ASP	4.1
3	Q	240	GLU	4.0
6	F	202	ASP	3.9
5	S	233	ILE	3.9
1	A	249	ALA	3.9
4	D	242	GLU	3.8
7	U	242	GLN	3.8
3	C	203	THR	3.8
3	Q	236	GLN	3.8
2	P	218	GLY	3.8
2	P	52	THR	3.8
6	T	180	PRO	3.7
3	Q	225	GLU	3.7
1	O	2	THR	3.6
4	R	1	ASP	3.6
10	J	194	ASP	3.6
7	G	242	GLN	3.6
2	P	59	ASP	3.6
1	O	52	SER	3.6
14	N	195	GLN	3.6
2	B	59	ASP	3.6
4	R	125	LEU	3.5
14	b	195	GLN	3.5
13	M	233	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
9	W	133	LYS	3.4
3	Q	51	LYS	3.4
7	G	241	GLU	3.4
6	T	181	GLU	3.4
10	X	193	ASP	3.4
6	T	241	LYS	3.3
14	b	105	LYS	3.3
8	H	225	GLU	3.3
8	V	225	GLU	3.2
2	B	52	THR	3.2
2	B	220	ASN	3.2
6	T	244	ASN	3.2
10	J	193	ASP	3.2
3	Q	49	THR	3.2
9	I	133	LYS	3.2
11	K	212	GLY	3.1
5	E	122	TYR	3.1
7	G	3	TYR	3.1
3	Q	229	GLN	3.1
3	C	180	LYS	3.1
12	Z	167	LYS	3.1
1	A	248	GLU	3.0
3	Q	203	THR	3.0
11	Y	212	GLY	3.0
1	O	250	LEU	3.0
1	A	250	LEU	3.0
1	A	201	GLU	3.0
5	E	233	ILE	3.0
3	C	225	GLU	3.0
2	B	60	THR	3.0
5	S	3	ASN	3.0
5	S	173	ARG	3.0
3	Q	237	GLU	2.9
7	U	188	GLU	2.9
2	B	203	SER	2.9
3	Q	48	SER	2.9
5	S	54	GLU	2.9
7	U	222	ASP	2.8
1	A	203	GLU	2.8
6	F	242	GLU	2.8
7	G	188	GLU	2.8
5	E	201	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
3	Q	204	GLY	2.8
9	I	131	GLU	2.8
3	Q	205	ALA	2.8
7	G	240	ALA	2.8
8	V	145	ASP	2.7
3	Q	180	LYS	2.7
13	a	1	THR	2.7
6	F	181	GLU	2.7
7	U	181	LYS	2.7
4	R	169	GLU	2.7
4	R	242	GLU	2.7
2	P	225	TYR	2.7
1	A	229	THR	2.6
2	P	240	LYS	2.6
13	M	1	THR	2.6
8	V	219	ASN	2.6
2	B	240	LYS	2.6
2	P	244	THR	2.6
1	O	50	LYS	2.6
8	H	198	GLU	2.6
13	a	216	ASN	2.6
7	U	2	GLY	2.6
8	H	219	ASN	2.6
3	C	229	GLN	2.5
5	E	203	GLU	2.5
8	V	198	GLU	2.5
6	T	2	THR	2.5
5	S	201	ARG	2.5
13	a	233	ILE	2.5
7	U	51	PRO	2.5
3	Q	233	GLN	2.5
2	P	182	ASP	2.5
2	P	242	GLY	2.4
5	E	210	LEU	2.4
13	M	204	THR	2.4
4	R	230	GLU	2.4
14	N	181	ALA	2.4
7	G	68	ARG	2.4
2	B	244	THR	2.4
2	P	54	THR	2.4
6	T	204	LYS	2.4
3	Q	187	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
7	U	206	GLY	2.3
5	E	227	GLU	2.3
2	P	203	SER	2.3
3	C	181	GLU	2.3
5	S	210	LEU	2.3
6	T	230	ASP	2.3
4	D	238	LYS	2.3
3	C	216	ASP	2.3
4	R	217	GLN	2.3
12	L	1	GLN	2.3
12	Z	1	GLN	2.3
13	M	47	ASP	2.3
13	a	204	THR	2.3
3	C	47	ARG	2.2
3	C	175	LYS	2.2
7	G	51	PRO	2.2
7	U	203	ASP	2.2
7	U	230	GLU	2.2
5	S	180	LYS	2.2
7	G	222	ASP	2.2
4	D	201	GLU	2.2
5	S	203	GLU	2.2
7	U	241	GLU	2.2
10	J	195	PHE	2.2
3	Q	141	ASP	2.2
5	S	30	GLN	2.2
6	T	166	GLN	2.2
6	F	230	ASP	2.2
1	O	201	GLU	2.2
3	C	205	ALA	2.2
3	Q	175	LYS	2.2
7	G	179	LYS	2.2
14	b	104	ASP	2.2
3	Q	59	PRO	2.2
7	U	3	TYR	2.2
6	F	2	THR	2.2
4	D	125	LEU	2.2
4	R	201	GLU	2.1
8	H	215	GLU	2.1
6	F	215	CYS	2.1
1	A	182	GLU	2.1
11	K	22	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	235	ALA	2.1
13	M	232	LYS	2.1
2	P	60	THR	2.1
2	B	93	HIS	2.1
4	R	2	ARG	2.1
12	L	172	LEU	2.1
3	C	60	SER	2.1
4	D	1	ASP	2.1
1	O	229	THR	2.1
3	Q	235	GLU	2.1
6	F	207	ASP	2.1
10	X	195	PHE	2.1
13	M	216	ASN	2.1
3	C	1	GLY	2.1
8	H	32	ALA	2.1
7	U	183	ASP	2.1
1	O	182	GLU	2.1
6	T	215	CYS	2.1
10	J	24	GLY	2.1
1	O	203	GLU	2.0
12	Z	173	LYS	2.0
8	H	145	ASP	2.0
4	D	217	GLN	2.0
6	T	206	LYS	2.0
13	M	121	SER	2.0
3	Q	3	ASP	2.0
3	C	187	GLU	2.0
5	S	122	TYR	2.0

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 monosaccharides 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. 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	MG	I	302	1/1	0.69	0.41	81,81,81,81	0
15	MG	H	301	1/1	0.82	0.24	74,74,74,74	0
15	MG	I	301	1/1	0.83	0.11	53,53,53,53	0
15	MG	Y	302	1/1	0.86	0.09	47,47,47,47	0
15	MG	N	201	1/1	0.88	0.11	48,48,48,48	0
16	3K4	Y	301	6/7	0.90	0.17	48,54,57,58	0
16	3K4	K	301	6/7	0.92	0.17	45,50,53,55	0
15	MG	Z	301	1/1	0.94	0.07	46,46,46,46	0
15	MG	J	201	1/1	0.95	0.37	55,55,55,55	0
15	MG	V	301	1/1	0.98	0.07	44,44,44,44	0
15	MG	K	303	1/1	0.98	0.34	45,45,45,45	0
15	MG	G	301	1/1	0.98	0.10	41,41,41,41	0
15	MG	K	302	1/1	0.99	0.11	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.