



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:13 PM BST

PDB ID : 4J70
Title : Yeast 20S proteasome in complex with the belactosin derivative 3e
Authors : Kawamura, S.; Unno, Y.; List, A.; Tanaka, M.; Sasaki, T.; Arisawa, M.; Asai, A.; Groll, M.; Shuto, S.
Deposited on : 2013-02-12
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 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
buster-report : 1.1.7 (2018)
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

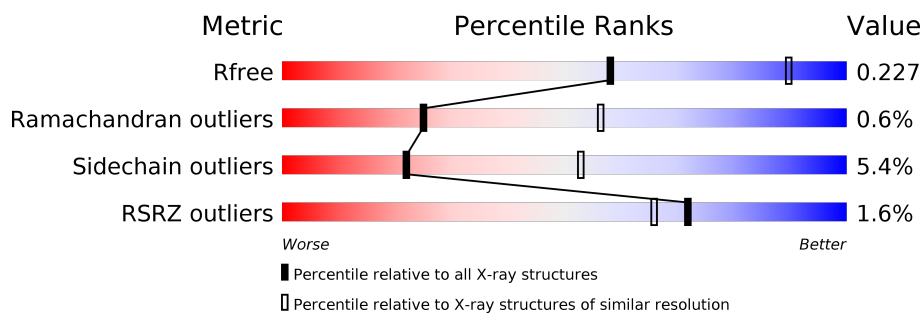
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 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>%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
3	Q	254	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
4	D	260	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	R	260	 3% 87% 6% 7%
5	E	234	 2% 89% 10%
5	S	234	 2% 88% 11%
6	F	288	 2% 80% 5% 15%
6	T	288	 2% 80% 5% 15%
7	G	252	 2% 92% 6%
7	U	252	 % 91% 6%
8	H	232	 % 90% 6%
8	V	232	 % 91% 5%
9	I	205	 97%
9	W	205	 98%
10	J	198	 2% 96%
10	X	198	 2% 95%
11	K	212	 96%
11	Y	212	 96%
12	L	222	 96%
12	Z	222	 95%
13	M	233	 96%
13	a	233	 96%
14	N	196	 97%
14	b	196	 95% 5%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			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 component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	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
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	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
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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			

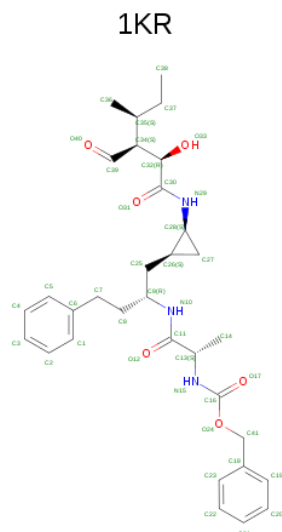
- Molecule 13 is a protein called Proteasome component PRE4.

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 benzyl [(2S)-1-({(2R)-1-[(1S,2S)-2-{{(2R,3S,4S)-3-formyl-2-hydroxy-4-methylhexanoyl}amino}cyclopropyl]-4-phenylbutan-2-yl}amino)-1-oxopropan-2-yl]carbamate (three-letter code: 1KR) (formula: C₃₂H₄₃N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total 41	C 32	N 3	O 6	0	0
15	Y	1	Total 41	C 32	N 3	O 6	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	55	Total O 55 55	0	0
16	B	37	Total O 37 37	0	0
16	C	45	Total O 45 45	0	0
16	D	39	Total O 39 39	0	0
16	E	22	Total O 22 22	0	0
16	F	46	Total O 46 46	0	0
16	G	63	Total O 63 63	0	0
16	H	52	Total O 52 52	0	0
16	I	67	Total O 67 67	0	0
16	J	55	Total O 55 55	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	40	Total 40	O 40	0	0
16	L	57	Total 57	O 57	0	0
16	M	75	Total 75	O 75	0	0
16	N	54	Total 54	O 54	0	0
16	O	31	Total 31	O 31	0	0
16	P	31	Total 31	O 31	0	0
16	Q	26	Total 26	O 26	0	0
16	R	30	Total 30	O 30	0	0
16	S	23	Total 23	O 23	0	0
16	T	43	Total 43	O 43	0	0
16	U	59	Total 59	O 59	0	0
16	V	51	Total 51	O 51	0	0
16	W	62	Total 62	O 62	0	0
16	X	46	Total 46	O 46	0	0
16	Y	49	Total 49	O 49	0	0
16	Z	51	Total 51	O 51	0	0
16	a	72	Total 72	O 72	0	0
16	b	55	Total 55	O 55	0	0

3 Residue-property plots

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.

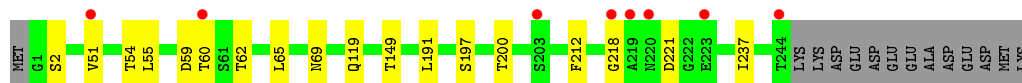
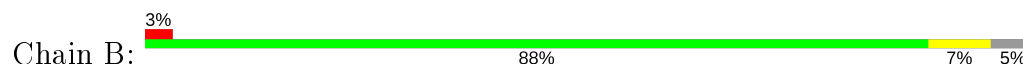
- Molecule 1: Proteasome component Y7



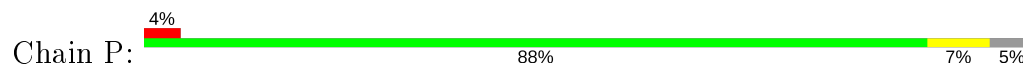
- Molecule 1: Proteasome component Y7



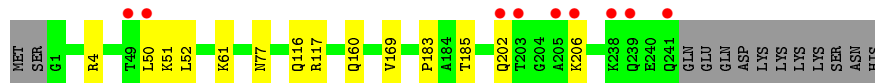
- Molecule 2: Proteasome component Y13



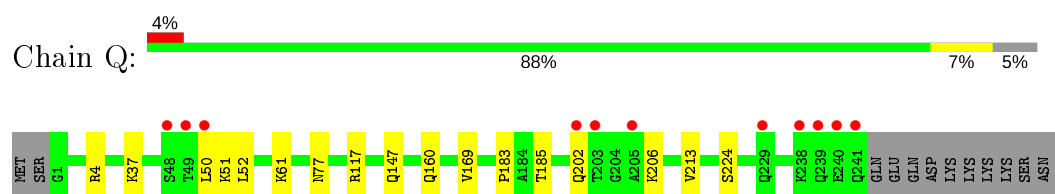
- Molecule 2: Proteasome component Y13



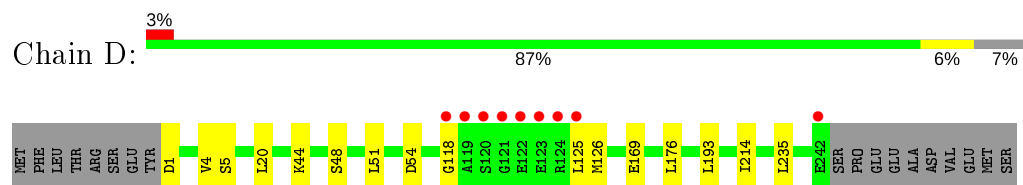
- Molecule 3: Proteasome component PRE6



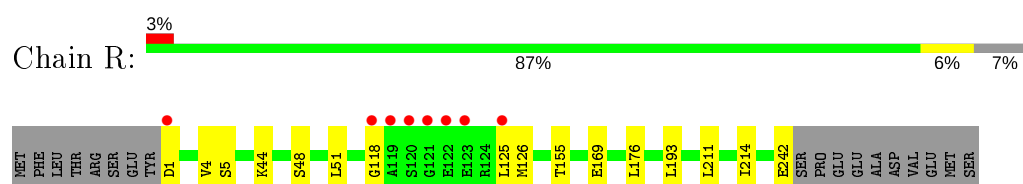
- Molecule 3: Proteasome component PRE6



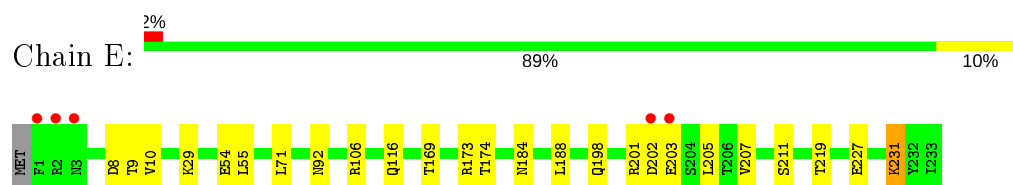
- Molecule 4: Proteasome component PUP2



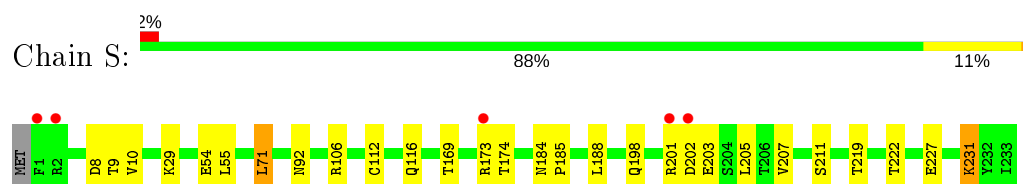
- Molecule 4: Proteasome component PUP2



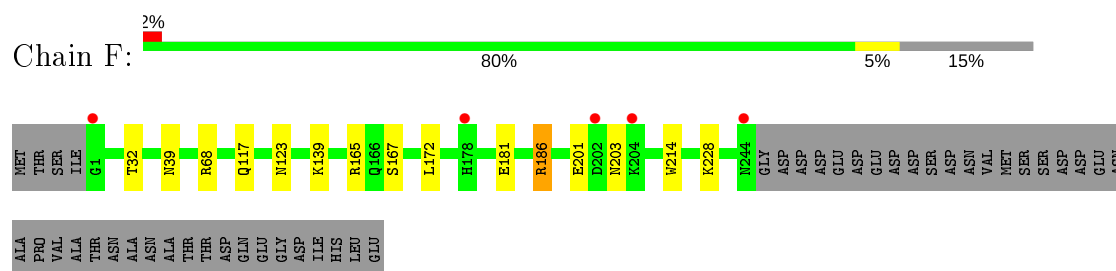
- Molecule 5: Proteasome component PRE5



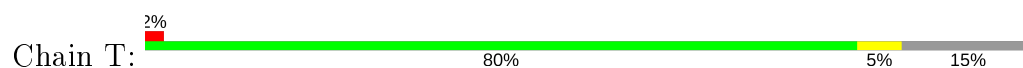
- Molecule 5: Proteasome component PRE5

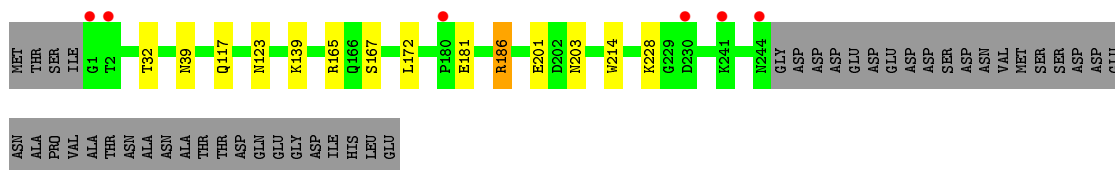


- Molecule 6: Proteasome component C1

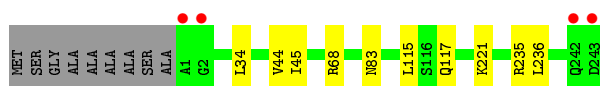
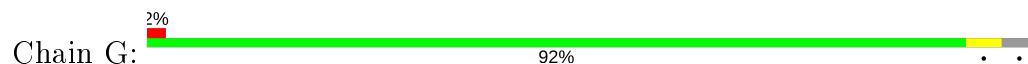


- Molecule 6: Proteasome component C1

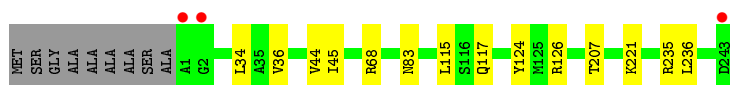
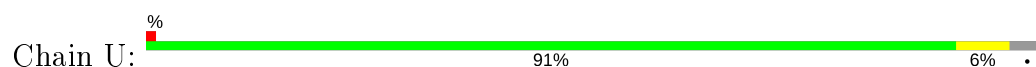




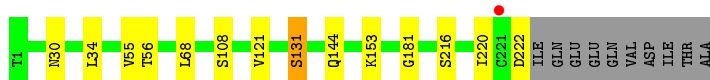
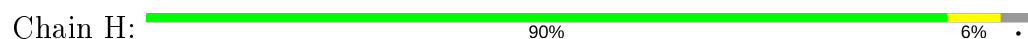
- Molecule 7: Proteasome component C7-alpha



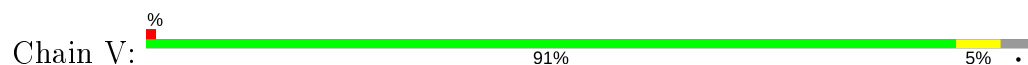
- Molecule 7: Proteasome component C7-alpha



- Molecule 8: Proteasome component PUP1



- Molecule 8: Proteasome component PUP1



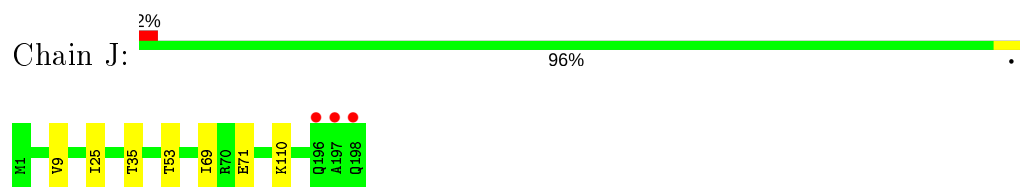
- Molecule 9: Proteasome component PUP3



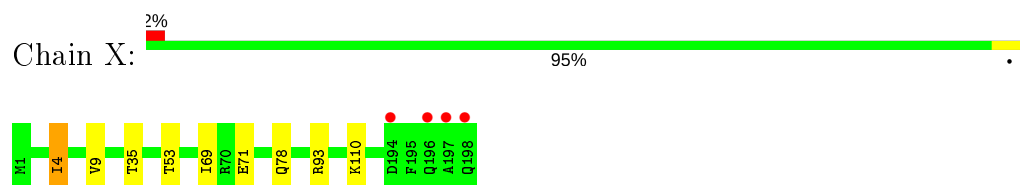
- Molecule 9: Proteasome component PUP3



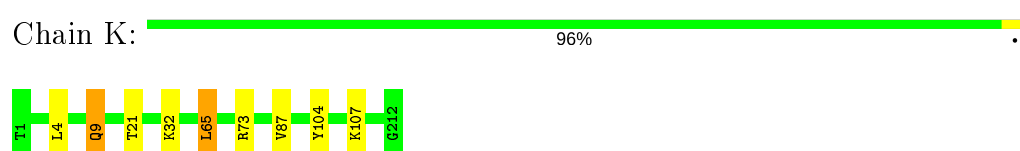
- Molecule 10: Proteasome component C11



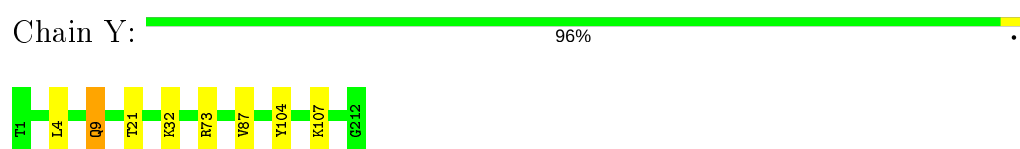
- Molecule 10: Proteasome component C11



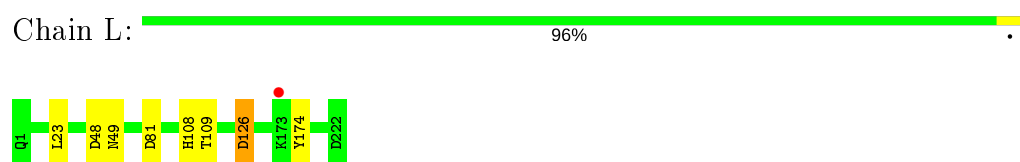
- Molecule 11: Proteasome component PRE2



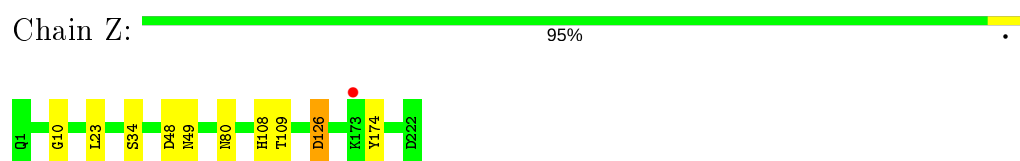
- Molecule 11: Proteasome component PRE2



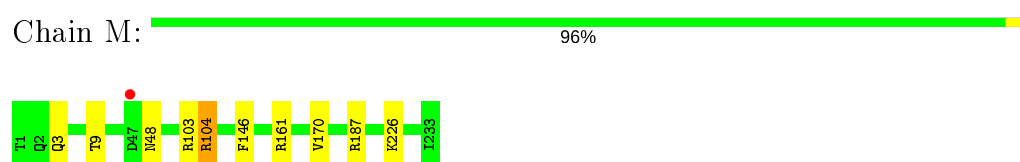
- Molecule 12: Proteasome component C5



- Molecule 12: Proteasome component C5



- Molecule 13: Proteasome component PRE4



- Molecule 13: Proteasome component PRE4

Chain a:  96% .



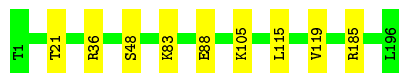
- Molecule 14: Proteasome component PRE3

Chain N:  97% .



- Molecule 14: Proteasome component PRE3

Chain b:  95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.08Å 301.71Å 146.23Å 90.00° 113.69° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.80) 98.9 (15.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.224 0.175 , 0.227	Depositor DCC
R_{free} test set	13052 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	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	50956	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: 1KR

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	0.69	0/1952	0.81	1/2642 (0.0%)
1	O	0.64	0/1952	0.79	0/2642
2	B	0.67	0/1934	0.80	0/2618
2	P	0.66	0/1934	0.82	0/2618
3	C	0.65	0/1919	0.82	2/2598 (0.1%)
3	Q	0.61	0/1919	0.79	3/2598 (0.1%)
4	D	0.65	0/1886	0.84	2/2541 (0.1%)
4	R	0.65	0/1886	0.86	3/2541 (0.1%)
5	E	0.64	0/1823	0.82	0/2463
5	S	0.64	0/1823	0.80	1/2463 (0.0%)
6	F	0.68	0/1936	0.82	3/2614 (0.1%)
6	T	0.65	0/1936	0.81	1/2614 (0.0%)
7	G	0.72	0/1959	0.82	0/2652
7	U	0.69	1/1959 (0.1%)	0.80	1/2652 (0.0%)
8	H	0.71	0/1715	0.83	0/2326
8	V	0.70	0/1715	0.82	0/2326
9	I	0.76	0/1611	0.84	1/2174 (0.0%)
9	W	0.72	0/1611	0.83	0/2174
10	J	0.72	0/1613	0.87	0/2173
10	X	0.72	0/1613	0.87	2/2173 (0.1%)
11	K	0.72	0/1681	0.85	1/2274 (0.0%)
11	Y	0.70	0/1681	0.83	0/2274
12	L	0.73	0/1795	0.84	1/2420 (0.0%)
12	Z	0.72	0/1795	0.83	1/2420 (0.0%)
13	M	0.70	0/1855	0.89	2/2514 (0.1%)
13	a	0.71	0/1855	0.90	2/2514 (0.1%)
14	N	0.75	0/1541	0.84	0/2087
14	b	0.70	0/1541	0.84	1/2087 (0.0%)
All	All	0.69	1/50440 (0.0%)	0.83	28/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
12	L	0	1
12	Z	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	124	TYR	CE1-CZ	5.06	1.45	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	128	ARG	NE-CZ-NH1	7.11	123.85	120.30
11	K	65	LEU	CB-CG-CD2	-6.93	99.22	111.00
13	M	104	ARG	NE-CZ-NH1	6.61	123.61	120.30
3	C	50	LEU	CA-CB-CG	6.26	129.69	115.30
6	T	186	ARG	NE-CZ-NH1	6.21	123.40	120.30
3	Q	117	ARG	NE-CZ-NH2	-6.16	117.22	120.30
4	R	125	LEU	CA-CB-CG	6.12	129.38	115.30
10	X	4	ILE	CG1-CB-CG2	-6.10	97.98	111.40
3	C	117	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	Q	50	LEU	CA-CB-CG	6.05	129.21	115.30
4	D	51	LEU	CA-CB-CG	5.97	129.04	115.30
4	R	51	LEU	CA-CB-CG	5.84	128.74	115.30
6	F	186	ARG	NE-CZ-NH1	5.80	123.20	120.30
13	M	103	ARG	NE-CZ-NH2	-5.79	117.41	120.30
7	U	126	ARG	NE-CZ-NH2	-5.78	117.41	120.30
3	Q	117	ARG	NE-CZ-NH1	5.73	123.17	120.30
6	F	186	ARG	NE-CZ-NH2	-5.60	117.50	120.30
6	F	68	ARG	NE-CZ-NH1	5.60	123.10	120.30
10	X	93	ARG	NE-CZ-NH1	-5.53	117.54	120.30
13	a	187	ARG	NE-CZ-NH1	5.52	123.06	120.30
4	D	125	LEU	CA-CB-CG	5.49	127.92	115.30
12	Z	126	ASP	CB-CA-C	-5.39	99.62	110.40
1	A	99	ARG	NE-CZ-NH1	-5.29	117.66	120.30
12	L	126	ASP	CB-CA-C	-5.25	99.90	110.40
5	S	71	LEU	CA-CB-CG	5.23	127.33	115.30
9	I	28	LEU	CA-CB-CG	5.14	127.12	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	211	LEU	CA-CB-CG	5.09	127.02	115.30
14	b	115	LEU	C-N-CA	-5.09	111.61	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	181	GLY	Peptide
12	L	174	TYR	Peptide
12	Z	174	TYR	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%)	7 (3%)	1 (0%)	34	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	226 (93%)	13 (5%)	3 (1%)	13	39
2	P	242/258 (94%)	225 (93%)	14 (6%)	3 (1%)	13	39
3	C	239/254 (94%)	232 (97%)	4 (2%)	3 (1%)	12	36
3	Q	239/254 (94%)	231 (97%)	5 (2%)	3 (1%)	12	36
4	D	240/260 (92%)	225 (94%)	13 (5%)	2 (1%)	19	49
4	R	240/260 (92%)	229 (95%)	9 (4%)	2 (1%)	19	49
5	E	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	12	36
5	S	231/234 (99%)	216 (94%)	11 (5%)	4 (2%)	9	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	242/288 (84%)	230 (95%)	12 (5%)	0	100	100
6	T	242/288 (84%)	228 (94%)	14 (6%)	0	100	100
7	G	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
7	U	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
8	H	220/232 (95%)	211 (96%)	8 (4%)	1 (0%)	29	61
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	196/198 (99%)	190 (97%)	5 (3%)	1 (0%)	29	61
10	X	196/198 (99%)	191 (97%)	4 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	29	61
11	Y	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	29	61
12	L	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	17	46
12	Z	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	17	46
13	M	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	34	66
13	a	231/233 (99%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6312/6588 (96%)	6027 (96%)	250 (4%)	35 (1%)	25	56

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	52	LEU
2	P	51	VAL
3	Q	52	LEU
2	B	218	GLY
3	C	202	GLN
4	D	118	GLY
4	D	126	MET
11	K	9	GLN
2	P	218	GLY
3	Q	183	PRO
3	Q	202	GLN
4	R	118	GLY

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Mol	Chain	Res	Type
12	Z	48	ASP
1	A	2	THR
2	B	221	ASP
3	C	183	PRO
5	E	202	ASP
12	L	81	ASP
1	O	2	THR
5	S	202	ASP
5	S	231	LYS
11	Y	9	GLN
5	E	201	ARG
12	L	48	ASP
2	P	221	ASP
4	R	126	MET
5	S	201	ARG
5	E	231	LYS
8	H	131	SER
13	M	9	THR
5	S	185	PRO
10	J	9	VAL
10	X	9	VAL
12	Z	10	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%)	204 (98%)	5 (2%)	49	81
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	81
2	B	203/216 (94%)	188 (93%)	15 (7%)	13	37
2	P	203/216 (94%)	189 (93%)	14 (7%)	15	41
3	C	213/226 (94%)	204 (96%)	9 (4%)	30	63
3	Q	213/226 (94%)	201 (94%)	12 (6%)	21	51
4	D	198/215 (92%)	186 (94%)	12 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	198/215 (92%)	187 (94%)	11 (6%)	21	51
5	E	192/193 (100%)	169 (88%)	23 (12%)	5	15
5	S	192/193 (100%)	167 (87%)	25 (13%)	4	13
6	F	201/239 (84%)	187 (93%)	14 (7%)	15	40
6	T	201/239 (84%)	187 (93%)	14 (7%)	15	40
7	G	207/210 (99%)	197 (95%)	10 (5%)	25	58
7	U	207/210 (99%)	195 (94%)	12 (6%)	20	50
8	H	181/190 (95%)	168 (93%)	13 (7%)	14	38
8	V	181/190 (95%)	169 (93%)	12 (7%)	16	44
9	I	172/173 (99%)	167 (97%)	5 (3%)	42	76
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	82
10	J	175/175 (100%)	169 (97%)	6 (3%)	37	71
10	X	175/175 (100%)	168 (96%)	7 (4%)	31	65
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	54
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	180 (97%)	5 (3%)	44	78
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	67
13	M	199/199 (100%)	191 (96%)	8 (4%)	31	65
13	a	199/199 (100%)	191 (96%)	8 (4%)	31	65
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	68
14	b	162/162 (100%)	154 (95%)	8 (5%)	25	57
All	All	5332/5522 (97%)	5045 (95%)	287 (5%)	22	53

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

Mol	Chain	Res	Type
1	A	58	SER
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	2	SER
2	B	54	THR
2	B	55	LEU
2	B	59	ASP

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Mol	Chain	Res	Type
2	B	60	THR
2	B	62	THR
2	B	65	LEU
2	B	69	ASN
2	B	119	GLN
2	B	149	THR
2	B	191	LEU
2	B	197	SER
2	B	200	THR
2	B	212	PHE
2	B	237	ILE
3	C	4	ARG
3	C	51	LYS
3	C	61	LYS
3	C	77	ASN
3	C	116	GLN
3	C	160	GLN
3	C	169	VAL
3	C	185	THR
3	C	206	LYS
4	D	1	ASP
4	D	4	VAL
4	D	5	SER
4	D	20	LEU
4	D	44	LYS
4	D	48	SER
4	D	54	ASP
4	D	169	GLU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	92	ASN
5	E	106	ARG
5	E	116	GLN

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Mol	Chain	Res	Type
5	E	169	THR
5	E	173	ARG
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	198	GLN
5	E	203	GLU
5	E	205	LEU
5	E	207	VAL
5	E	211	SER
5	E	219	THR
5	E	227	GLU
5	E	231	LYS
6	F	32	THR
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	167	SER
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	214	TRP
6	F	228	LYS
7	G	34	LEU
7	G	44	VAL
7	G	45	ILE
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU

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Mol	Chain	Res	Type
8	H	108	SER
8	H	121	VAL
8	H	131	SER
8	H	144	GLN
8	H	153	LYS
8	H	216	SER
8	H	220	ILE
8	H	222	ASP
9	I	37	ASN
9	I	133	LYS
9	I	171	LEU
9	I	191	LYS
9	I	195	VAL
10	J	25	ILE
10	J	35	THR
10	J	53	THR
10	J	69	ILE
10	J	71	GLU
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	21	THR
11	K	32	LYS
11	K	65	LEU
11	K	73	ARG
11	K	87	VAL
11	K	104	TYR
11	K	107	LYS
12	L	23	LEU
12	L	49	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
13	M	3	GLN
13	M	48	ASN
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	170	VAL
13	M	187	ARG
13	M	226	LYS
14	N	36	ARG

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Mol	Chain	Res	Type
14	N	83	LYS
14	N	88	GLU
14	N	105	LYS
14	N	119	VAL
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	61	LEU
1	O	157	PHE
1	O	231	LYS
2	P	2	SER
2	P	54	THR
2	P	55	LEU
2	P	59	ASP
2	P	60	THR
2	P	62	THR
2	P	65	LEU
2	P	69	ASN
2	P	119	GLN
2	P	149	THR
2	P	191	LEU
2	P	197	SER
2	P	212	PHE
2	P	217	LYS
3	Q	4	ARG
3	Q	37	LYS
3	Q	51	LYS
3	Q	61	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	185	THR
3	Q	206	LYS
3	Q	213	VAL
3	Q	224	SER
4	R	1	ASP
4	R	4	VAL
4	R	5	SER
4	R	44	LYS
4	R	48	SER
4	R	155	THR

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Mol	Chain	Res	Type
4	R	169	GLU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	92	ASN
5	S	106	ARG
5	S	112	CYS
5	S	116	GLN
5	S	169	THR
5	S	173	ARG
5	S	174	THR
5	S	184	ASN
5	S	188	LEU
5	S	198	GLN
5	S	203	GLU
5	S	205	LEU
5	S	207	VAL
5	S	211	SER
5	S	219	THR
5	S	222	THR
5	S	227	GLU
5	S	231	LYS
6	T	32	THR
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	167	SER
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	203	ASN

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Mol	Chain	Res	Type
6	T	214	TRP
6	T	228	LYS
7	U	34	LEU
7	U	36	VAL
7	U	44	VAL
7	U	45	ILE
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	207	THR
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	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	153	LYS
8	V	216	SER
8	V	220	ILE
8	V	222	ASP
9	W	37	ASN
9	W	133	LYS
9	W	171	LEU
9	W	195	VAL
10	X	4	ILE
10	X	35	THR
10	X	53	THR
10	X	69	ILE
10	X	71	GLU
10	X	78	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	21	THR
11	Y	32	LYS
11	Y	73	ARG

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Mol	Chain	Res	Type
11	Y	87	VAL
11	Y	104	TYR
11	Y	107	LYS
12	Z	23	LEU
12	Z	34	SER
12	Z	49	ASN
12	Z	80	ASN
12	Z	108	HIS
12	Z	109	THR
12	Z	126	ASP
13	a	3	GLN
13	a	48	ASN
13	a	57	ILE
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	170	VAL
13	a	226	LYS
14	b	21	THR
14	b	36	ARG
14	b	48	SER
14	b	83	LYS
14	b	88	GLU
14	b	105	LYS
14	b	119	VAL
14	b	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) 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	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

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Mol	Chain	Res	Type
3	C	77	ASN
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	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	210	GLN
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	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
6	F	240	GLN
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	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN

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Mol	Chain	Res	Type
9	I	156	ASN
9	I	172	ASN
10	J	55	GLN
10	J	86	GLN
10	J	166	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	79	HIS
12	L	80	ASN
12	L	95	HIS
12	L	108	HIS
12	L	135	GLN
12	L	165	ASN
12	L	195	HIS
13	M	2	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	38	HIS
14	N	157	HIS
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN

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Mol	Chain	Res	Type
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
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	6	HIS
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	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	156	ASN
9	W	172	ASN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	166	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	188	HIS
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	135	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	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	69	GLN
14	b	157	HIS
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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	1KR	K	301	11	43,43,43	1.66	5 (11%)	51,57,57	1.86	11 (21%)
15	1KR	Y	301	11	43,43,43	1.69	7 (16%)	51,57,57	1.87	10 (19%)

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	1KR	K	301	11	-	18/46/51/51	0/3/3/3
15	1KR	Y	301	11	-	16/46/51/51	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	1KR	C5-C6	5.62	1.51	1.38
15	K	301	1KR	C5-C6	5.22	1.50	1.38
15	Y	301	1KR	O40-C39	3.61	1.34	1.19
15	K	301	1KR	C27-C28	3.46	1.54	1.49
15	Y	301	1KR	C27-C28	3.35	1.54	1.49
15	K	301	1KR	O40-C39	3.28	1.33	1.19
15	K	301	1KR	C34-C39	2.77	1.54	1.50
15	Y	301	1KR	C13-N15	2.64	1.51	1.45
15	Y	301	1KR	C34-C39	2.56	1.54	1.50
15	K	301	1KR	C4-C5	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	1KR	C16-N15	2.03	1.39	1.34
15	Y	301	1KR	C14-C13	2.02	1.58	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	1KR	C28-N29-C30	-6.75	111.15	123.07
15	K	301	1KR	C28-N29-C30	-5.86	112.71	123.07
15	K	301	1KR	C14-C13-C11	4.90	119.46	110.14
15	Y	301	1KR	C26-C25-C9	-4.66	107.84	115.56
15	Y	301	1KR	C13-N15-C16	4.08	128.14	120.49
15	K	301	1KR	C26-C25-C9	-3.84	109.20	115.56
15	Y	301	1KR	O24-C16-N15	3.77	118.17	110.50
15	K	301	1KR	C7-C8-C9	3.59	121.98	112.70
15	Y	301	1KR	C14-C13-N15	3.50	116.95	110.38
15	K	301	1KR	C13-C11-N10	3.40	124.67	116.75
15	K	301	1KR	O12-C11-N10	-3.22	116.96	122.93
15	K	301	1KR	O24-C16-N15	3.03	116.66	110.50
15	Y	301	1KR	O24-C41-C18	2.66	115.78	109.39
15	K	301	1KR	O17-C16-N15	-2.57	120.64	124.85
15	K	301	1KR	C25-C26-C27	-2.36	115.76	120.68
15	Y	301	1KR	C3-C2-C1	2.32	123.73	120.19
15	Y	301	1KR	O17-C16-N15	-2.29	121.09	124.85
15	K	301	1KR	C23-C18-C19	2.28	121.76	118.17
15	Y	301	1KR	C25-C26-C27	-2.13	116.25	120.68
15	Y	301	1KR	C41-O24-C16	2.13	120.68	115.93
15	K	301	1KR	O33-C32-C34	2.05	113.18	109.28

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	301	1KR	O17-C16-O24-C41
15	K	301	1KR	N15-C16-O24-C41
15	K	301	1KR	O24-C16-N15-C13
15	K	301	1KR	O12-C11-C13-C14
15	K	301	1KR	N10-C11-C13-C14
15	K	301	1KR	C13-C11-N10-C9
15	K	301	1KR	C26-C28-N29-C30
15	K	301	1KR	C9-C25-C26-C27
15	K	301	1KR	C26-C25-C9-N10
15	K	301	1KR	N29-C30-C32-O33

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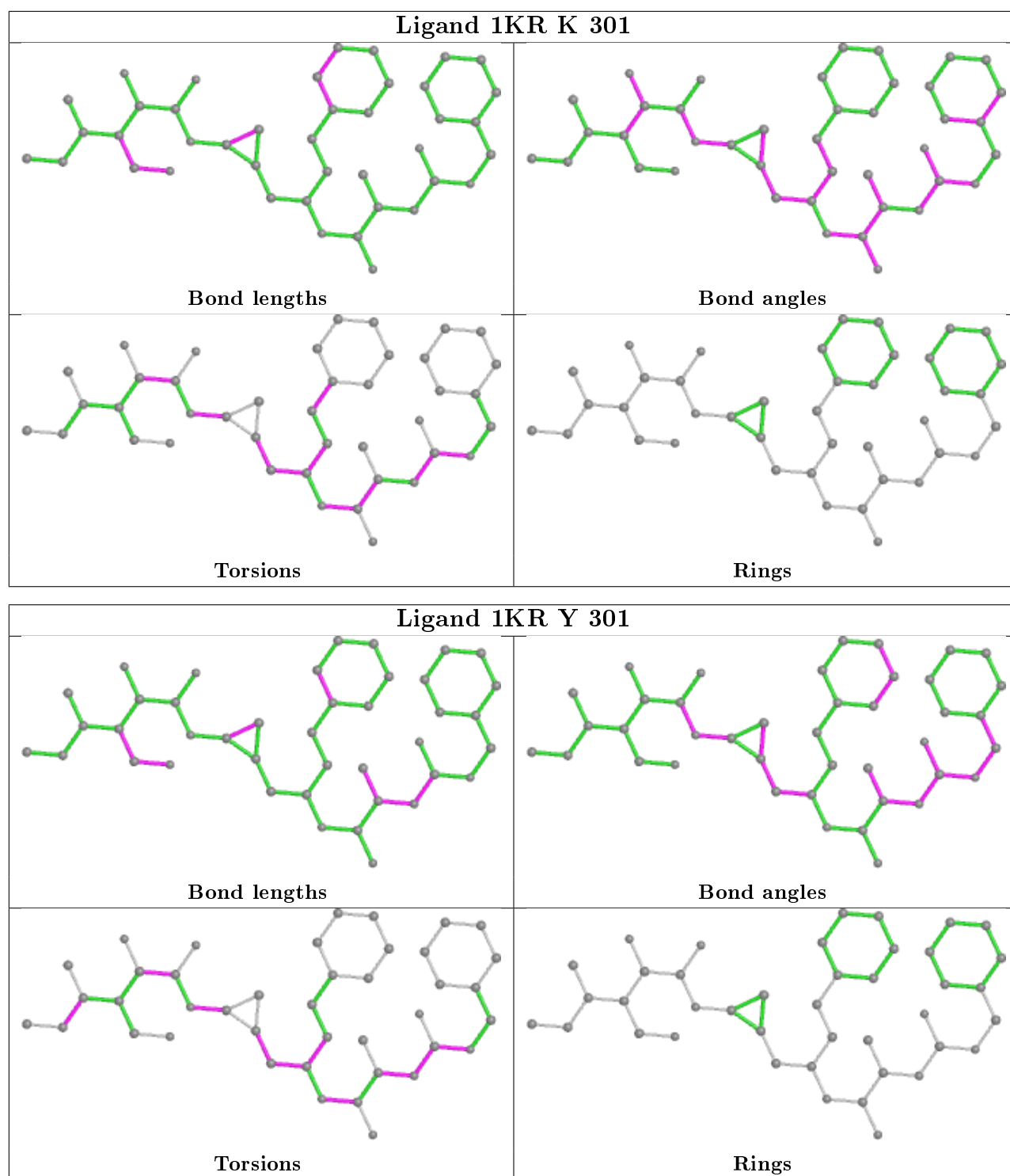
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Mol	Chain	Res	Type	Atoms
15	Y	301	1KR	O17-C16-O24-C41
15	Y	301	1KR	N15-C16-O24-C41
15	Y	301	1KR	O24-C16-N15-C13
15	Y	301	1KR	C9-C25-C26-C27
15	Y	301	1KR	C7-C8-C9-N10
15	K	301	1KR	O12-C11-N10-C9
15	K	301	1KR	O17-C16-N15-C13
15	Y	301	1KR	O17-C16-N15-C13
15	K	301	1KR	C7-C8-C9-C25
15	Y	301	1KR	O12-C11-N10-C9
15	Y	301	1KR	C13-C11-N10-C9
15	K	301	1KR	O31-C30-C32-O33
15	K	301	1KR	C26-C25-C9-C8
15	Y	301	1KR	C34-C35-C37-C38
15	K	301	1KR	C7-C8-C9-N10
15	Y	301	1KR	C7-C8-C9-C25
15	Y	301	1KR	C26-C25-C9-N10
15	Y	301	1KR	C14-C13-N15-C16
15	Y	301	1KR	O31-C30-C32-O33
15	Y	301	1KR	N29-C30-C32-O33
15	Y	301	1KR	C26-C28-N29-C30
15	K	301	1KR	C1-C6-C7-C8
15	K	301	1KR	C9-C25-C26-C28
15	Y	301	1KR	C9-C25-C26-C28

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.77	3 (1%) 79 73	28, 43, 74, 146	0
1	O	250/250 (100%)	-0.68	2 (0%) 86 81	30, 51, 87, 142	0
2	B	244/258 (94%)	-0.58	8 (3%) 46 36	27, 48, 104, 154	0
2	P	244/258 (94%)	-0.53	10 (4%) 37 27	33, 52, 105, 156	0
3	C	241/254 (94%)	-0.49	9 (3%) 41 31	28, 52, 111, 147	0
3	Q	241/254 (94%)	-0.33	11 (4%) 32 22	33, 58, 125, 153	0
4	D	242/260 (93%)	-0.55	9 (3%) 41 31	32, 51, 89, 185	0
4	R	242/260 (93%)	-0.51	8 (3%) 46 36	34, 54, 94, 195	0
5	E	233/234 (99%)	-0.58	5 (2%) 63 54	36, 55, 87, 152	0
5	S	233/234 (99%)	-0.52	5 (2%) 63 54	35, 58, 97, 146	0
6	F	244/288 (84%)	-0.71	5 (2%) 65 56	30, 47, 92, 128	0
6	T	244/288 (84%)	-0.59	6 (2%) 57 47	31, 52, 98, 134	0
7	G	243/252 (96%)	-0.74	4 (1%) 72 66	24, 43, 80, 157	0
7	U	243/252 (96%)	-0.70	3 (1%) 79 73	29, 46, 83, 149	0
8	H	222/232 (95%)	-0.87	1 (0%) 91 88	26, 40, 65, 99	0
8	V	222/232 (95%)	-0.84	2 (0%) 84 80	29, 42, 70, 113	0
9	I	204/205 (99%)	-0.98	1 (0%) 91 88	26, 40, 64, 99	0
9	W	204/205 (99%)	-0.95	1 (0%) 91 88	27, 41, 66, 115	0
10	J	198/198 (100%)	-0.79	3 (1%) 73 68	28, 42, 68, 184	0
10	X	198/198 (100%)	-0.76	4 (2%) 65 56	30, 43, 71, 162	0
11	K	212/212 (100%)	-0.91	0 100 100	27, 42, 61, 76	0
11	Y	212/212 (100%)	-0.90	0 100 100	29, 43, 64, 80	0
12	L	222/222 (100%)	-0.87	1 (0%) 91 88	27, 44, 73, 117	0
12	Z	222/222 (100%)	-0.88	1 (0%) 91 88	28, 43, 70, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.89	1 (0%) 92 91	29, 44, 61, 83	0
13	a	233/233 (100%)	-0.86	0 100 100	26, 43, 60, 77	0
14	N	196/196 (100%)	-0.92	0 100 100	27, 39, 63, 91	0
14	b	196/196 (100%)	-0.92	0 100 100	24, 40, 66, 90	0
All	All	6368/6588 (96%)	-0.73	103 (1%) 72 66	24, 46, 87, 195	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	197	ALA	9.9
2	P	220	ASN	9.2
4	D	119	ALA	9.1
7	U	1	ALA	8.6
4	R	121	GLY	8.6
2	B	220	ASN	8.5
4	D	120	SER	8.1
3	C	49	THR	8.0
2	P	219	ALA	7.4
2	B	219	ALA	7.2
10	X	197	ALA	7.2
10	X	198	GLN	6.9
10	J	198	GLN	6.9
7	G	1	ALA	6.3
7	U	243	ASP	6.1
7	G	243	ASP	5.9
4	D	118	GLY	5.8
4	D	121	GLY	5.7
4	R	118	GLY	5.6
4	R	119	ALA	5.6
4	R	120	SER	5.5
4	D	122	GLU	5.5
9	W	1	SER	5.3
2	B	218	GLY	5.1
3	Q	240	GLU	4.9
1	O	1	MET	4.8
3	Q	49	THR	4.8
3	C	238	LYS	4.7
3	Q	203	THR	4.3
3	Q	241	GLN	4.3
6	F	1	GLY	4.2
3	C	50	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
9	I	1	SER	3.9
5	E	1	PHE	3.9
3	Q	50	LEU	3.8
5	S	1	PHE	3.8
3	Q	48	SER	3.8
6	T	244	ASN	3.7
3	C	239	GLN	3.7
5	S	2	ARG	3.7
2	B	51	VAL	3.6
10	J	196	GLN	3.6
3	C	203	THR	3.5
2	P	60	THR	3.3
3	C	205	ALA	3.3
7	G	242	GLN	3.3
1	A	1	MET	3.2
2	P	59	ASP	3.2
8	V	221	CYS	3.2
3	C	241	GLN	3.2
3	C	206	LYS	3.1
8	V	222	ASP	3.1
2	B	203	SER	2.9
2	P	221	ASP	2.8
8	H	221	CYS	2.8
10	X	194	ASP	2.8
4	D	124	ARG	2.8
5	S	173	ARG	2.7
4	D	123	GLU	2.7
3	Q	238	LYS	2.7
3	Q	239	GLN	2.7
4	R	1	ASP	2.7
4	D	125	LEU	2.6
7	G	2	GLY	2.6
6	F	178	HIS	2.6
5	E	202	ASP	2.6
2	P	203	SER	2.6
6	T	180	PRO	2.6
7	U	2	GLY	2.5
2	P	51	VAL	2.5
2	P	223	GLU	2.5
10	X	196	GLN	2.5
6	F	202	ASP	2.4
6	T	1	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	203	GLU	2.3
2	P	218	GLY	2.3
12	L	173	LYS	2.3
5	S	202	ASP	2.3
4	D	242	GLU	2.3
4	R	123	GLU	2.3
5	S	201	ARG	2.3
2	B	244	THR	2.2
5	E	3	ASN	2.2
4	R	122	GLU	2.2
6	F	244	ASN	2.2
6	T	241	LYS	2.2
4	R	125	LEU	2.2
3	Q	202	GLN	2.2
1	A	2	THR	2.2
2	B	60	THR	2.2
2	P	240	LYS	2.2
1	A	249	ALA	2.1
12	Z	173	LYS	2.1
2	B	223	GLU	2.1
3	Q	205	ALA	2.1
1	O	249	ALA	2.1
6	T	2	THR	2.1
5	E	2	ARG	2.1
13	M	47	ASP	2.0
3	C	202	GLN	2.0
6	T	230	ASP	2.0
3	Q	229	GLN	2.0
6	F	204	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

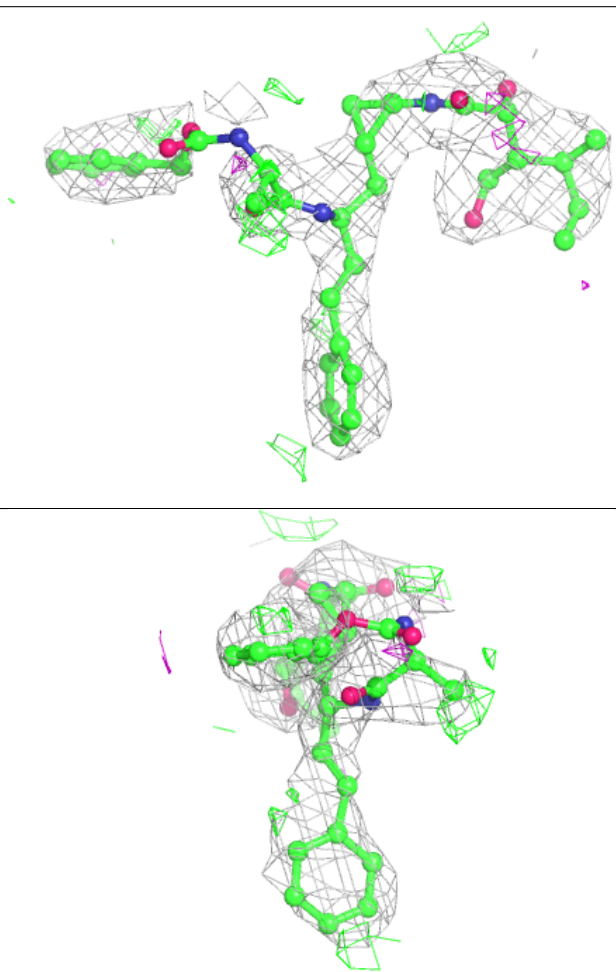
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

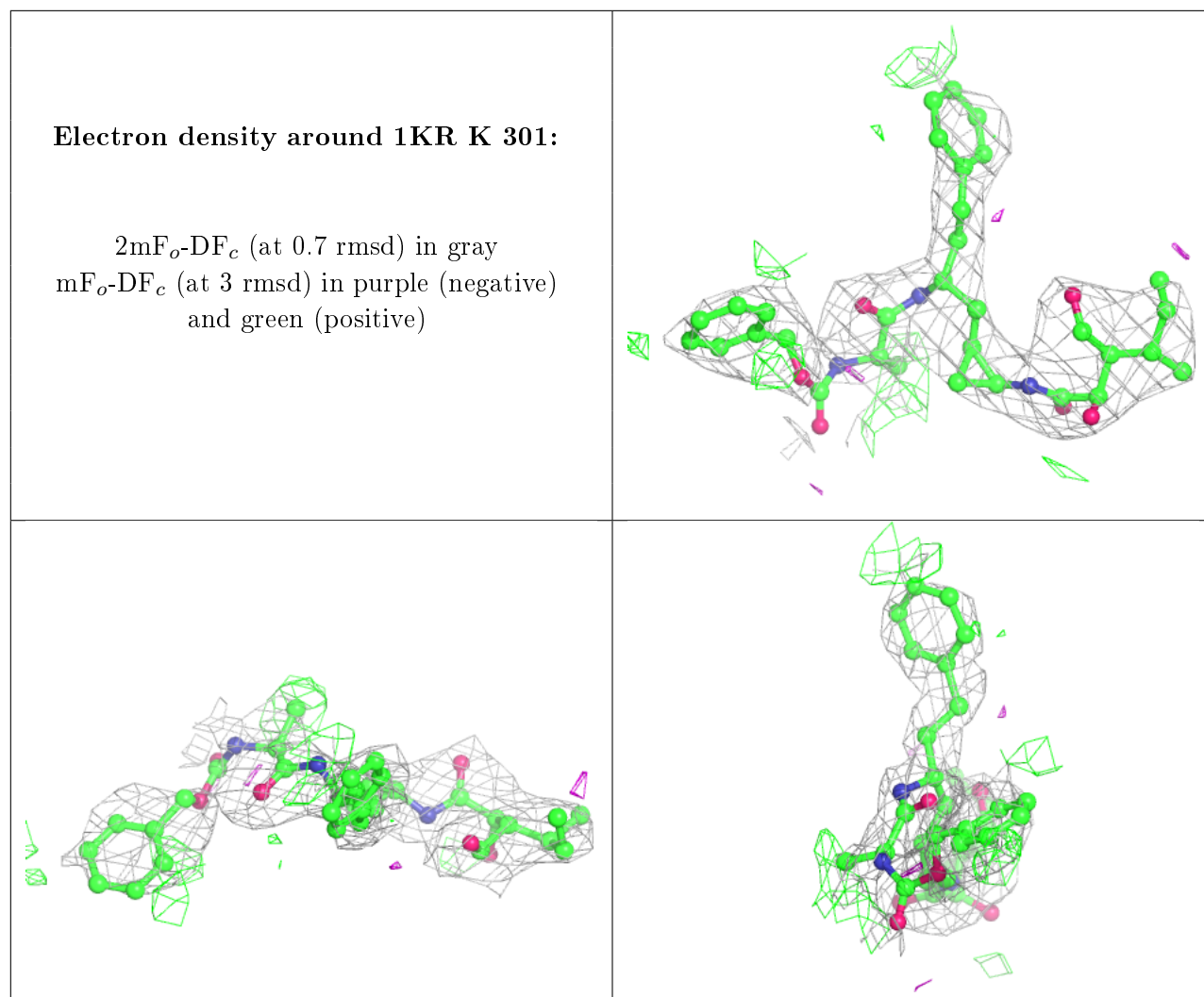
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	1KR	Y	301	41/41	0.88	0.25	37,81,137,168	0
15	1KR	K	301	41/41	0.90	0.23	40,81,141,150	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1KR Y 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.