



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:21 AM UTC

PDB ID : 9QB1 / pdb_00009qb1
Title : Yeast 20S proteasome mutant: beta5_T3M in complex with Bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-02-28
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

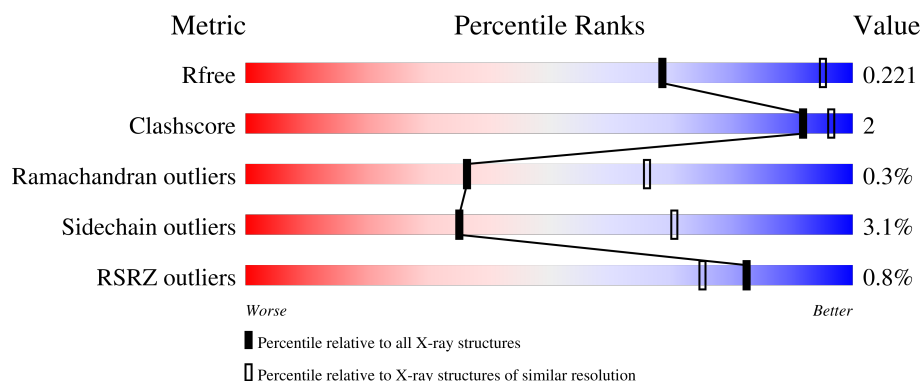
1 Overall quality at a glance ⓘ

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div></div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>2%</div> <div>88%</div> <div>7% 5%</div> </div>
2	P	258	<div> <div>%</div> <div>87%</div> <div>7% 5%</div> </div>
3	C	254	<div> <div></div> <div>88%</div> <div>. . 6%</div> </div>



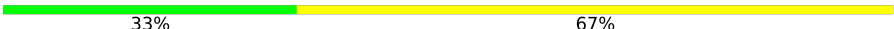
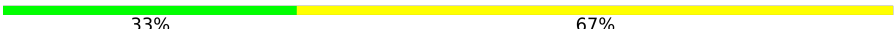
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Mol	Chain	Length	Quality of chain
3	Q	254	 2% 87% 5% 6%
4	D	260	 % 85% 5% 10%
4	R	260	 84% 6% 10%
5	E	234	 95% . .
5	S	234	 95% . .
6	F	288	 % 82% . 16%
6	T	288	 % 81% . 16%
7	G	252	 90% 5% .
7	U	252	 90% 6% .
8	H	231	 93% . .
8	V	231	 92% 5% .
9	I	204	 93% 6%
9	W	204	 93% 6% .
10	J	198	 % 89% 7% . .
10	X	198	 % 87% 9% . .
11	K	211	 % 87% 12% .
11	Y	211	 2% 87% 12% .
12	L	222	 2% 95% 5%
12	Z	222	 % 94% 5%
13	M	246	 % 91% . . 5%
13	a	246	 % 90% . . 5%
14	N	195	 94% 5% .
14	b	195	 % 94% 5% .
15	e	3	 67% 33%
15	f	3	 33% 67%

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Mol	Chain	Length	Quality of chain
15	g	3	 67% 33%
15	h	3	 33% 67%
15	i	3	 33% 67%
15	j	3	 33% 67%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49925 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	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	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
			1638	1042	279	309	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1638	1042	279	309	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	3	MET	THR	engineered mutation	UNP P30656
Y	3	MET	THR	engineered mutation	UNP P30656

- 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	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	f	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	g	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	h	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	i	3	Total	C	N	O	0	0	0
			35	24	5	6			
15	j	3	Total	C	N	O	0	0	0
			35	24	5	6			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	J	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	b	1	Total	Cl	0	0
			1	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	16	Total	O	0	0
			16	16		
18	B	15	Total	O	0	0
			15	15		
18	C	13	Total	O	0	0
			13	13		
18	D	5	Total	O	0	0
			5	5		
18	E	5	Total	O	0	0
			5	5		
18	F	14	Total	O	0	0
			14	14		
18	G	19	Total	O	0	0
			19	19		
18	H	23	Total	O	0	0
			23	23		
18	I	12	Total	O	0	0
			12	12		
18	J	16	Total	O	0	0
			16	16		
18	K	8	Total	O	0	0
			8	8		
18	L	14	Total	O	0	0
			14	14		
18	M	21	Total	O	0	0
			21	21		
18	N	13	Total	O	0	0
			13	13		
18	O	5	Total	O	0	0
			5	5		
18	P	11	Total	O	0	0
			11	11		
18	Q	14	Total	O	0	0
			14	14		
18	R	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	S	7	Total 7	O 7	0	0
18	T	6	Total 6	O 6	0	0
18	U	18	Total 18	O 18	0	0
18	V	25	Total 25	O 25	0	0
18	W	12	Total 12	O 12	0	0
18	X	13	Total 13	O 13	0	0
18	Y	13	Total 13	O 13	0	0
18	Z	12	Total 12	O 12	0	0
18	a	21	Total 21	O 21	0	0
18	b	13	Total 13	O 13	0	0
18	e	1	Total 1	O 1	0	0
18	g	1	Total 1	O 1	0	0
18	i	2	Total 2	O 2	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.

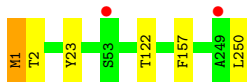
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98% .




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .




- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 7% 5% 2%




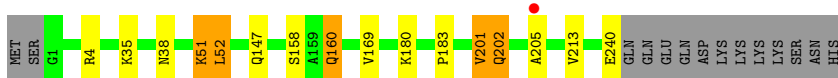
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  87% 7% 5% 2%

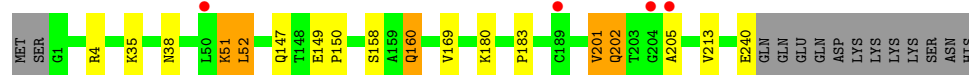
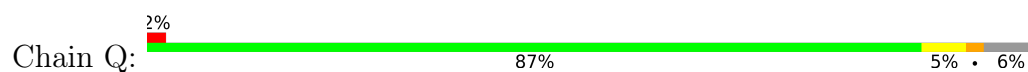


- Molecule 3: Proteasome subunit alpha type-4

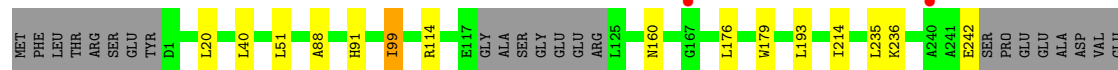
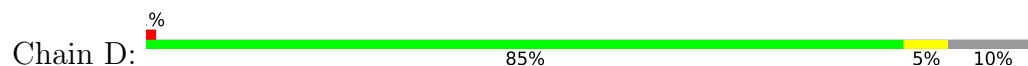
Chain C:  88% . . 6%



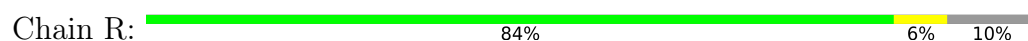
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



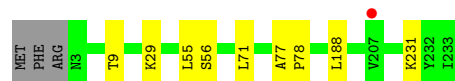
- Molecule 4: Proteasome subunit alpha type-5



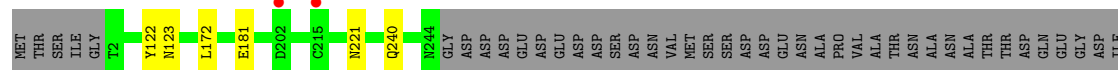
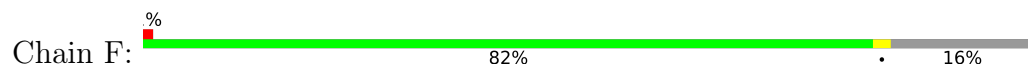
- Molecule 5: Proteasome subunit alpha type-6



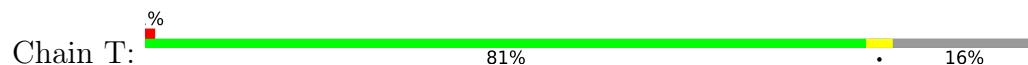
- Molecule 5: Proteasome subunit alpha type-6

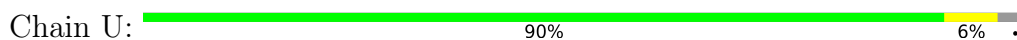


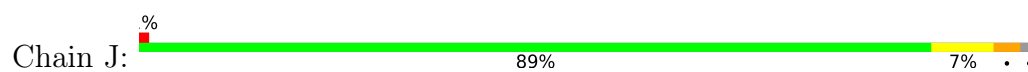
- Molecule 6: Probable proteasome subunit alpha type-7



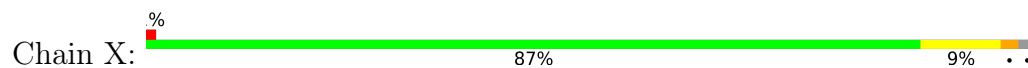
- Molecule 6: Probable proteasome subunit alpha type-7



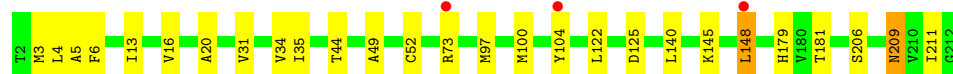
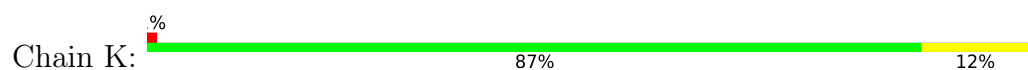




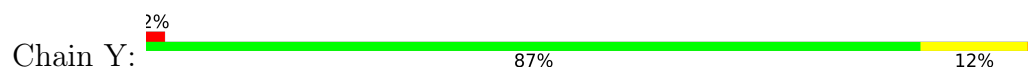
- Molecule 10: Proteasome subunit beta type-4



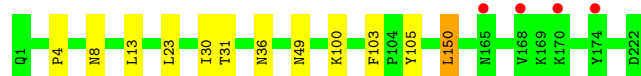
- Molecule 11: Proteasome subunit beta type-5



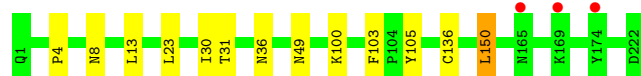
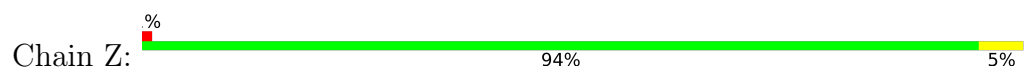
- Molecule 11: Proteasome subunit beta type-5



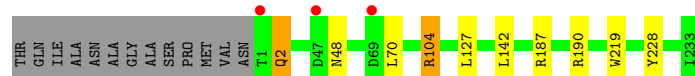
- Molecule 12: Proteasome subunit beta type-6



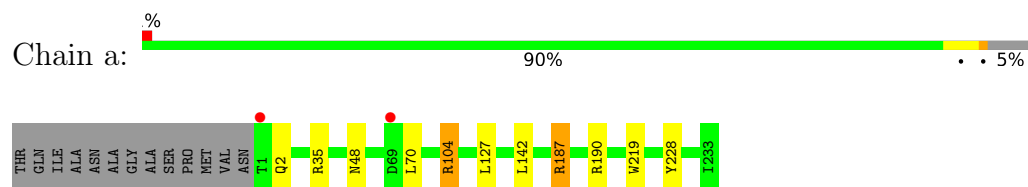
- Molecule 12: Proteasome subunit beta type-6



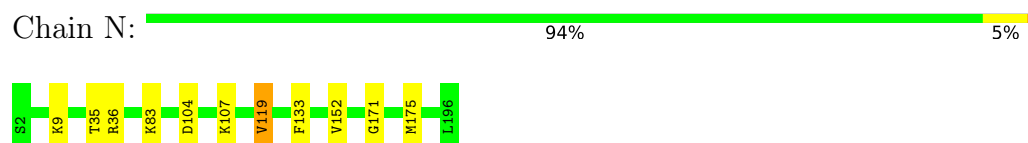
- Molecule 13: Proteasome subunit beta type-7



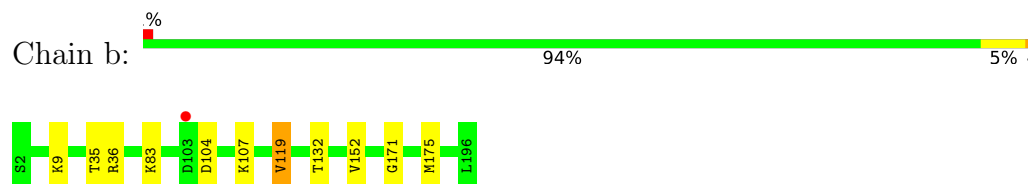
- Molecule 13: Proteasome subunit beta type-7



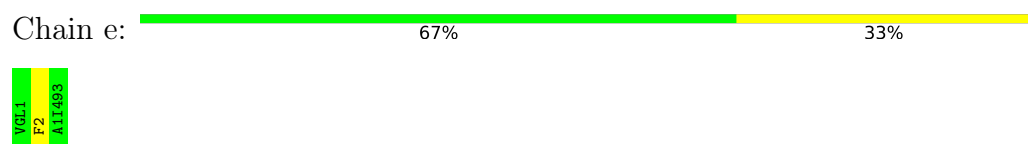
- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



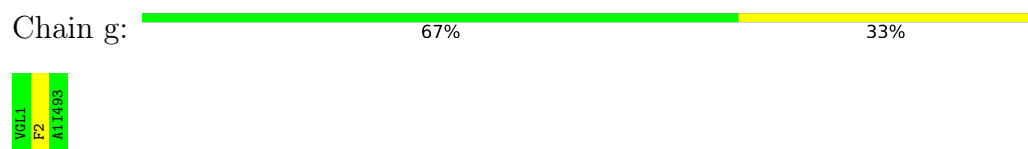
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

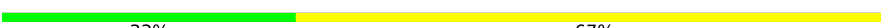


- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain i:  33% 67%

VGL1
F2
A11493

- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain j:  33% 67%

VGL1
F2
A11493

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.49Å 300.56Å 145.08Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.80) 95.4 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.215 0.200 , 0.221	Depositor DCC
R_{free} test set	12379 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49925	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: VGL, MG, CL, A1I49

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/1952	0.67	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.39	0/1934	0.66	0/2618
2	P	0.39	0/1934	0.67	0/2618
3	C	0.38	0/1910	0.68	1/2586 (0.0%)
3	Q	0.39	0/1910	0.68	1/2586 (0.0%)
4	D	0.38	0/1837	0.65	0/2475
4	R	0.38	0/1837	0.64	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.38	0/1800	0.65	0/2433
6	F	0.39	0/1932	0.68	0/2609
6	T	0.38	0/1932	0.69	0/2609
7	G	0.38	0/1945	0.66	0/2634
7	U	0.38	0/1945	0.67	0/2634
8	H	0.33	0/1743	0.66	0/2363
8	V	0.33	0/1743	0.66	0/2363
9	I	0.34	0/1611	0.69	0/2174
9	W	0.36	0/1611	0.71	0/2174
10	J	0.45	0/1589	0.73	2/2142 (0.1%)
10	X	0.46	0/1589	0.74	0/2142
11	K	0.39	0/1675	0.72	0/2264
11	Y	0.34	0/1675	0.68	0/2264
12	L	0.33	0/1795	0.69	2/2420 (0.1%)
12	Z	0.33	0/1795	0.69	2/2420 (0.1%)
13	M	0.35	0/1855	0.69	0/2514
13	a	0.36	0/1855	0.70	1/2514 (0.0%)
14	N	0.34	0/1534	0.68	0/2077
14	b	0.33	0/1534	0.68	0/2077
15	e	1.35	0/11	1.91	1/13 (7.7%)
15	f	1.29	0/11	1.58	1/13 (7.7%)
15	g	1.32	0/11	1.89	1/13 (7.7%)
15	h	1.27	0/11	1.52	1/13 (7.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	i	1.33	0/11	1.74	1/13 (7.7%)
15	j	1.32	0/11	1.82	1/13 (7.7%)
All	All	0.38	0/50290	0.68	15/67980 (0.0%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	N-CA-C	6.67	118.21	111.07
15	e	2	PHE	CA-CB-CG	-6.51	107.29	113.80
15	g	2	PHE	CA-CB-CG	-6.42	107.38	113.80
12	Z	103	PHE	CA-C-N	6.09	126.05	119.78
12	Z	103	PHE	C-N-CA	6.09	126.05	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	5	0
8	H	1712	0	1709	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1712	0	1709	10	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	20	0
10	X	1561	0	1569	15	0
11	K	1638	0	1587	14	0
11	Y	1638	0	1587	18	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	5	0
14	N	1505	0	1471	5	0
14	b	1505	0	1471	5	0
15	e	35	0	11	0	0
15	f	35	0	11	1	0
15	g	35	0	11	0	0
15	h	35	0	11	1	0
15	i	35	0	11	1	0
15	j	35	0	11	1	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	A	16	0	0	0	0
18	B	15	0	0	0	0
18	C	13	0	0	0	0
18	D	5	0	0	1	0
18	E	5	0	0	0	0
18	F	14	0	0	0	0
18	G	19	0	0	0	0
18	H	23	0	0	0	0
18	I	12	0	0	0	0
18	J	16	0	0	0	0
18	K	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	14	0	0	0	0
18	M	21	0	0	1	0
18	N	13	0	0	0	0
18	O	5	0	0	0	0
18	P	11	0	0	1	0
18	Q	14	0	0	0	0
18	R	9	0	0	0	0
18	S	7	0	0	0	0
18	T	6	0	0	1	0
18	U	18	0	0	0	0
18	V	25	0	0	0	0
18	W	12	0	0	0	0
18	X	13	0	0	1	0
18	Y	13	0	0	0	0
18	Z	12	0	0	0	0
18	a	21	0	0	0	0
18	b	13	0	0	0	0
18	e	1	0	0	0	0
18	g	1	0	0	0	0
18	i	2	0	0	0	0
All	All	49925	0	49140	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 159 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:149:ARG:NE	11:Y:205:GLY:O	2.21	0.72
10:X:25:ILE:O	10:X:25:ILE:HG12	1.90	0.71
10:J:149:ARG:HH11	11:Y:206:SER:HA	1.54	0.71
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.25	0.68
10:J:139:TYR:HE1	10:J:171:ARG:HB3	1.59	0.68

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	238 (96%)	9 (4%)	1 (0%)	30	60
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	60
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	25
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	31
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	31
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (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	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
8	V	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
11	K	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
11	Y	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
14	b	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
All	All	6278/6606 (95%)	6104 (97%)	158 (2%)	16 (0%)	36	66

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	50	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	57
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	57
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	53
4	R	194/215 (90%)	183 (94%)	11 (6%)	18	49
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	70
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	70
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	76
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	76
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	68
8	H	184/189 (97%)	182 (99%)	2 (1%)	65	87
8	V	184/189 (97%)	182 (99%)	2 (1%)	65	87
9	I	172/172 (100%)	169 (98%)	3 (2%)	53	83
9	W	172/172 (100%)	168 (98%)	4 (2%)	44	78
10	J	173/175 (99%)	166 (96%)	7 (4%)	28	63
10	X	173/175 (99%)	165 (95%)	8 (5%)	24	58
11	K	168/168 (100%)	161 (96%)	7 (4%)	26	61
11	Y	168/168 (100%)	161 (96%)	7 (4%)	26	61
12	L	185/185 (100%)	182 (98%)	3 (2%)	55	83
12	Z	185/185 (100%)	181 (98%)	4 (2%)	45	78
13	M	199/208 (96%)	193 (97%)	6 (3%)	36	72
13	a	199/208 (96%)	193 (97%)	6 (3%)	36	72
14	N	161/161 (100%)	156 (97%)	5 (3%)	35	70
14	b	161/161 (100%)	156 (97%)	5 (3%)	35	70
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
15	i	1/1 (100%)	1 (100%)	0	100	100
15	j	1/1 (100%)	1 (100%)	0	100	100
All	All	5320/5538 (96%)	5154 (97%)	166 (3%)	35	70

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	71	LEU
10	X	147	HIS
6	T	172	LEU
8	V	68	LEU
11	Y	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	48	ASN
12	Z	79	HIS
3	Q	120	GLN
12	Z	49	ASN
13	a	149	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.35	0 100 100	43, 58, 96, 136	0
1	O	250/250 (100%)	-0.32	2 (0%) 82 75	47, 67, 110, 147	0
2	B	244/258 (94%)	-0.18	5 (2%) 65 56	48, 69, 116, 168	0
2	P	244/258 (94%)	-0.19	2 (0%) 82 75	52, 71, 113, 157	0
3	C	240/254 (94%)	-0.11	1 (0%) 88 84	46, 72, 133, 162	0
3	Q	240/254 (94%)	-0.00	4 (1%) 69 60	53, 83, 166, 186	0
4	D	235/260 (90%)	-0.22	2 (0%) 81 74	52, 73, 104, 147	0
4	R	235/260 (90%)	-0.07	0 100 100	60, 78, 120, 155	0
5	E	231/234 (98%)	-0.15	0 100 100	50, 74, 112, 154	0
5	S	231/234 (98%)	-0.01	1 (0%) 88 84	53, 80, 126, 160	0
6	F	243/288 (84%)	-0.21	2 (0%) 82 75	46, 69, 115, 144	0
6	T	243/288 (84%)	-0.07	3 (1%) 76 68	48, 76, 135, 164	0
7	G	241/252 (95%)	-0.35	0 100 100	42, 60, 98, 146	0
7	U	241/252 (95%)	-0.28	1 (0%) 88 84	47, 63, 100, 149	0
8	H	225/231 (97%)	-0.35	1 (0%) 88 84	38, 56, 96, 156	0
8	V	225/231 (97%)	-0.35	1 (0%) 88 84	42, 59, 92, 173	0
9	I	204/204 (100%)	-0.48	0 100 100	41, 58, 86, 114	0
9	W	204/204 (100%)	-0.44	0 100 100	45, 61, 91, 114	0
10	J	195/198 (98%)	-0.34	1 (0%) 87 82	43, 60, 90, 128	0
10	X	195/198 (98%)	-0.35	1 (0%) 87 82	45, 63, 90, 140	0
11	K	211/211 (100%)	-0.02	3 (1%) 73 64	51, 68, 105, 122	0
11	Y	211/211 (100%)	0.05	5 (2%) 59 49	52, 68, 110, 129	0
12	L	222/222 (100%)	-0.25	4 (1%) 67 58	44, 61, 111, 142	0
12	Z	222/222 (100%)	-0.24	3 (1%) 73 64	36, 62, 115, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.48	3 (1%) 75 66	39, 57, 80, 99	0
13	a	233/246 (94%)	-0.43	2 (0%) 81 74	40, 57, 78, 100	0
14	N	195/195 (100%)	-0.43	0 100 100	39, 52, 81, 107	0
14	b	195/195 (100%)	-0.38	1 (0%) 87 82	40, 54, 83, 113	0
15	e	1/3 (33%)	-0.12	0 100 100	56, 56, 56, 56	0
15	f	1/3 (33%)	0.07	0 100 100	60, 60, 60, 60	0
15	g	1/3 (33%)	0.16	0 100 100	60, 60, 60, 60	0
15	h	1/3 (33%)	0.35	0 100 100	65, 65, 65, 65	0
15	i	1/3 (33%)	1.90	0 100 100	55, 55, 55, 55	0
15	j	1/3 (33%)	0.91	0 100 100	57, 57, 57, 57	0
All	All	6344/6624 (95%)	-0.25	48 (0%) 82 75	36, 65, 113, 186	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.6
10	J	1	MET	4.3
12	Z	174	TYR	4.0
3	Q	50	LEU	4.0
2	B	219	ALA	3.9

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 oligosaccharides 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(\AA^2)	Q<0.9
16	MG	Z	301	1/1	0.92	0.12	67,67,67,67	0
16	MG	Y	301	1/1	0.93	0.07	63,63,63,63	0
16	MG	I	301	1/1	0.94	0.16	75,75,75,75	0
16	MG	V	301	1/1	0.94	0.09	71,71,71,71	0
17	CL	b	201	1/1	0.97	0.11	50,50,50,50	0
16	MG	G	301	1/1	0.98	0.03	51,51,51,51	0
16	MG	J	201	1/1	0.98	0.13	46,46,46,46	0
16	MG	K	301	1/1	0.99	0.06	66,66,66,66	0
17	CL	G	302	1/1	0.99	0.09	40,40,40,40	0
17	CL	N	202	1/1	0.99	0.05	49,49,49,49	0
17	CL	U	301	1/1	0.99	0.08	46,46,46,46	0
16	MG	N	201	1/1	0.99	0.06	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.