



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2025 – 11:15 am BST

PDB ID : 9QBY / pdb_00009qby
Title : Yeast 20S proteasome mutant: beta5_G128V (b5-propeptide in trans) in complex with ONX0914
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-04
Resolution : 2.90 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

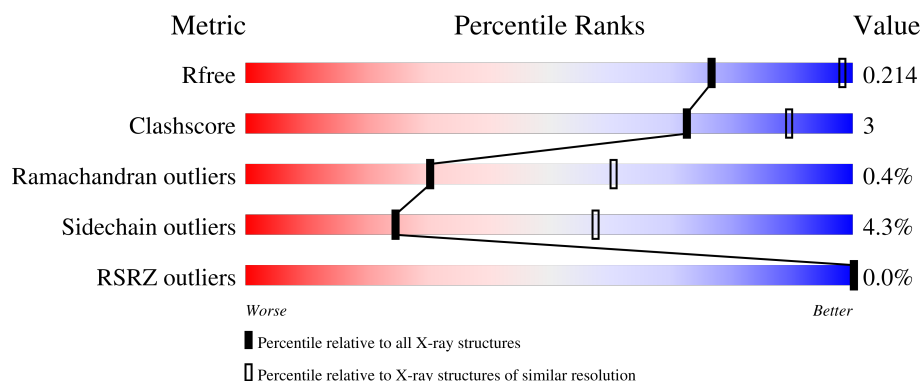
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	 97%
1	O	250	 96%
2	B	258	 87% 7% 5%
2	P	258	 87% 7% 5%
3	C	254	 87% 6% 6%





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Mol	Chain	Length	Quality of chain
3	Q	254	 87% 6% • 6%
4	D	260	 85% 5% • 10%
4	R	260	 85% 5% • 10%
5	E	234	 92% 5% • •
5	S	234	 92% 5% • •
6	F	288	 80% • • 16%
6	T	288	 80% • • 16%
7	G	252	 87% 8% • •
7	U	252	 87% 8% • •
8	H	231	 87% 9% • •
8	V	231	 88% 8% • •
9	I	205	 92% 7%
9	W	205	 91% 9%
10	J	198	 89% 6% • •
10	X	198	 87% 8% • •
11	K	211	 78% 19% •
11	Y	211	 80% 17% •
12	L	222	 84% 13% •
12	Z	222	 84% 14% •
13	M	246	 80% 11% • 6%
13	a	246	 82% 12% • 5%
14	N	195	 89% 10% •
14	b	195	 88% 11% •
15	d	4	 50% 50%
15	e	4	 50% 50%

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Mol	Chain	Length	Quality of chain
15	f	4	 50%50%
15	g	4	 50%50%
15	h	4	 50%50%
15	i	4	 50%50%

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
19	MPD	a	302	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49907 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
			1640	1044	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	130	VAL	GLY	engineered mutation	UNP P30656
Y	130	VAL	GLY	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	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	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	d	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	e	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	f	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	g	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	h	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	i	4	Total	C	N	O	0	0	0
			49	35	5	9			

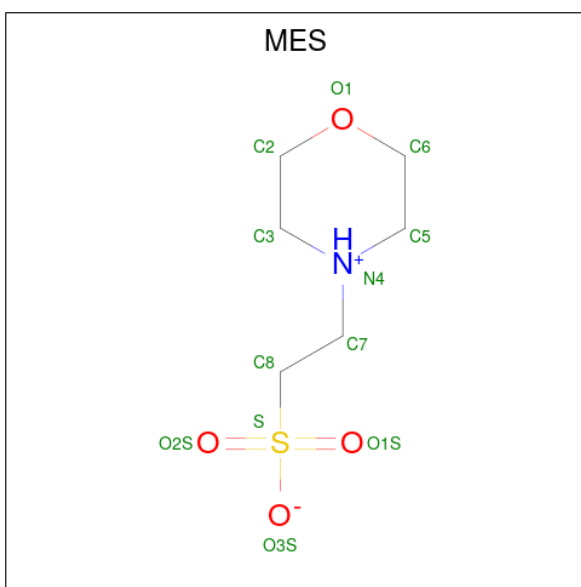
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	W	1	Total	Mg	0	0
			1	1		

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

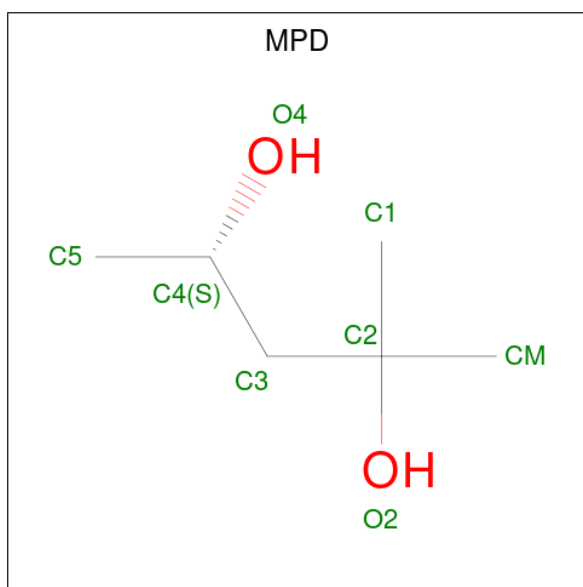
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	U	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	K	1	Total	C	O	0	0
			8	6	2		
19	a	1	Total	C	O	0	0
			8	6	2		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	6	Total	O	0	0
			6	6		
20	B	8	Total	O	0	0
			8	8		
20	C	5	Total	O	0	0
			5	5		
20	D	2	Total	O	0	0
			2	2		
20	E	7	Total	O	0	0
			7	7		
20	F	10	Total	O	0	0
			10	10		
20	G	8	Total	O	0	0
			8	8		
20	H	16	Total	O	0	0
			16	16		
20	I	4	Total	O	0	0
			4	4		
20	J	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	K	6	Total 6	O 6	0	0
20	L	7	Total 7	O 7	0	0
20	M	10	Total 10	O 10	0	0
20	N	9	Total 9	O 9	0	0
20	O	2	Total 2	O 2	0	0
20	P	7	Total 7	O 7	0	0
20	Q	6	Total 6	O 6	0	0
20	R	4	Total 4	O 4	0	0
20	S	5	Total 5	O 5	0	0
20	T	8	Total 8	O 8	0	0
20	U	11	Total 11	O 11	0	0
20	V	12	Total 12	O 12	0	0
20	W	5	Total 5	O 5	0	0
20	X	4	Total 4	O 4	0	0
20	Y	8	Total 8	O 8	0	0
20	Z	10	Total 10	O 10	0	0
20	a	6	Total 6	O 6	0	0
20	b	4	Total 4	O 4	0	0
20	f	2	Total 2	O 2	0	0
20	h	1	Total 1	O 1	0	0
20	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:  97%




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  96%




- Molecule 2: Proteasome subunit alpha type-3

Chain B:  87% 7% 5%




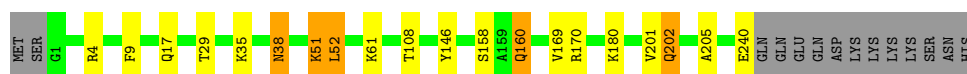
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  87% 7% 5%




- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% 6%



- Molecule 3: Proteasome subunit alpha type-4


Chain Q:  87% 6% 6%

- Molecule 7: Proteasome subunit alpha type-1

Chain G:  87% 8% . .




- Molecule 7: Proteasome subunit alpha type-1

Chain U:  87% 8% . .



- Molecule 8: Proteasome subunit beta type-2

Chain H:  87% 9% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V:  88% 8% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I:  92% 7%




- Molecule 9: Proteasome subunit beta type-3

Chain W:  91% 9%

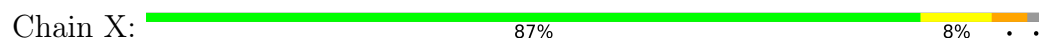


- Molecule 10: Proteasome subunit beta type-4

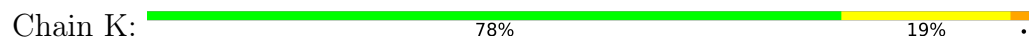
Chain J:  89% 6% . .



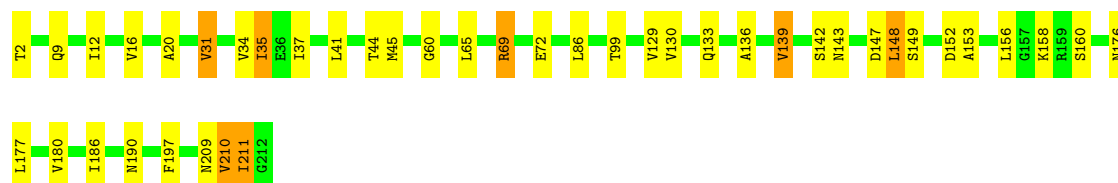
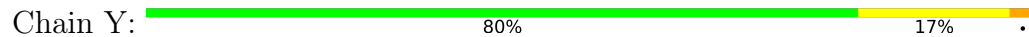
- Molecule 10: Proteasome subunit beta type-4



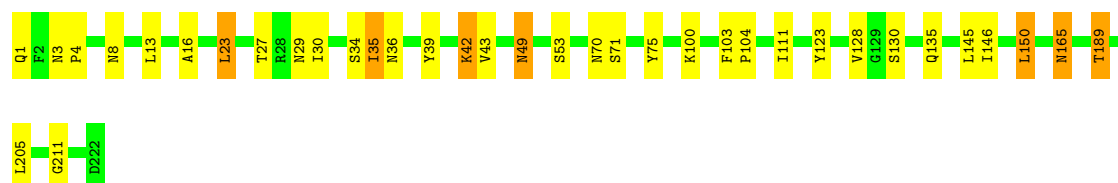
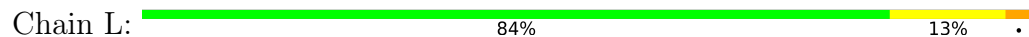
- Molecule 11: Proteasome subunit beta type-5



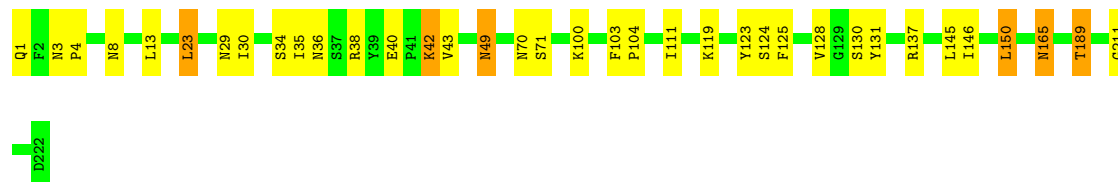
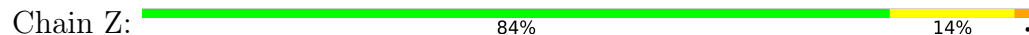
- Molecule 11: Proteasome subunit beta type-5



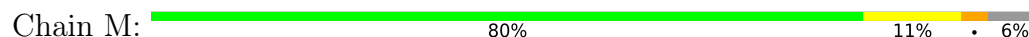
- Molecule 12: Proteasome subunit beta type-6

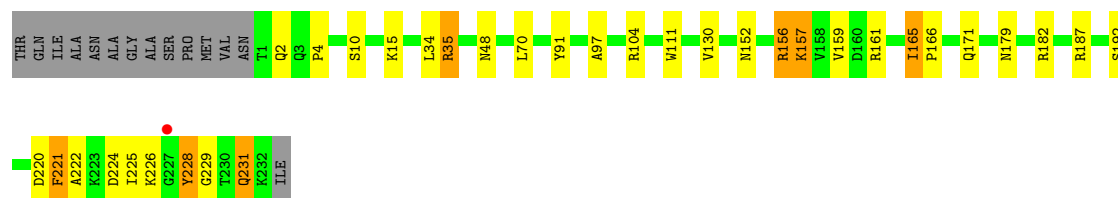


- Molecule 12: Proteasome subunit beta type-6



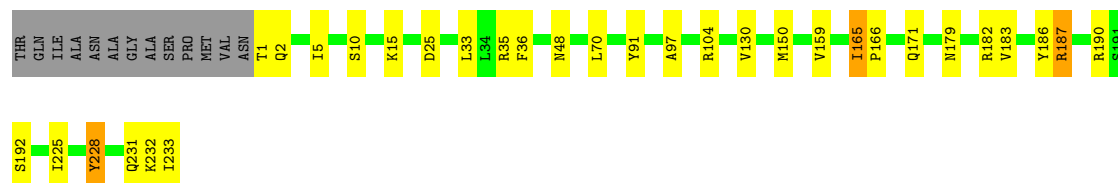
- Molecule 13: Proteasome subunit beta type-7





• Molecule 13: Proteasome subunit beta type-7

Chain a: 82% 12% 5%



• Molecule 14: Proteasome subunit beta type-1

Chain N: 89% 10%



• Molecule 14: Proteasome subunit beta type-1

Chain b: 88% 11%



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

Chain d: 50% 50%



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

Chain e: 50% 50%



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

Chain f: 50% 50%

00E1
A2
Y3
A11444

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

Chain g:  50% 50%

00E1
A2
Y3
A11444

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

Chain h:  50% 50%

00E1
A2
Y3
A11444

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

Chain i:  50% 50%

00E1
A2
Y3
A11444

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.44Å 300.23Å 146.21Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-2.90) 96.4 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.177 , 0.211 0.157 , 0.214	Depositor DCC
R_{free} test set	11466 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.983	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49907	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: MPD, CL, MG, MES, 0A1, 00E, A1I44

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	1.04	0/1952	1.41	0/2642
1	O	1.04	0/1952	1.41	0/2642
2	B	1.02	0/1934	1.42	0/2618
2	P	1.03	0/1934	1.43	0/2618
3	C	1.03	0/1910	1.46	0/2586
3	Q	1.03	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.45	0/2475
4	R	1.03	0/1837	1.45	0/2475
5	E	1.04	0/1800	1.43	2/2433 (0.1%)
5	S	1.04	0/1800	1.44	0/2433
6	F	1.03	0/1932	1.44	2/2609 (0.1%)
6	T	1.02	0/1932	1.44	2/2609 (0.1%)
7	G	1.01	0/1945	1.40	0/2634
7	U	1.02	0/1945	1.41	0/2634
8	H	1.03	0/1743	1.42	0/2363
8	V	1.03	0/1743	1.42	0/2363
9	I	1.02	0/1611	1.42	1/2174 (0.0%)
9	W	1.02	0/1611	1.42	0/2174
10	J	1.00	0/1589	1.42	2/2142 (0.1%)
10	X	1.00	0/1589	1.41	2/2142 (0.1%)
11	K	1.01	0/1677	1.41	0/2269
11	Y	1.00	0/1677	1.39	0/2269
12	L	1.00	0/1795	1.40	0/2420
12	Z	1.01	0/1795	1.40	2/2420 (0.1%)
13	M	1.01	0/1846	1.39	3/2503 (0.1%)
13	a	1.01	0/1855	1.39	2/2514 (0.1%)
14	N	1.00	0/1534	1.39	0/2077
14	b	1.01	0/1534	1.40	0/2077
15	d	0.21	0/4	0.81	0/4
15	e	0.57	0/4	0.47	0/4
15	f	0.95	0/4	0.75	0/4
15	g	0.29	0/4	0.74	0/4

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	h	0.63	0/4	0.46	0/4
15	i	0.85	0/4	0.72	0/4
All	All	1.02	0/50243	1.42	18/67925 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	5.46	124.70	120.33
6	T	77	LEU	C-N-CA	5.46	124.70	120.33
13	M	157	LYS	N-CA-C	-5.33	105.52	112.23
9	I	9	GLY	CA-C-O	-5.22	118.11	122.33
10	J	134	GLY	CA-C-N	5.20	127.24	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	11	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	13	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	13	0
8	H	1712	0	1709	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1712	0	1709	9	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	13	0
10	X	1561	0	1569	15	0
11	K	1640	0	1591	25	0
11	Y	1640	0	1591	23	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	20	0
13	M	1815	0	1821	27	0
13	a	1824	0	1832	19	0
14	N	1505	0	1471	17	0
14	b	1505	0	1471	15	0
15	d	49	0	25	2	0
15	e	49	0	25	0	0
15	f	49	0	25	0	0
15	g	49	0	25	2	0
15	h	49	0	25	0	0
15	i	49	0	25	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	G	12	0	13	1	0
18	H	12	0	13	0	0
18	M	12	0	13	0	0
18	U	12	0	13	0	0
18	V	12	0	13	0	0
18	a	12	0	13	0	0
19	K	8	0	14	1	0
19	a	8	0	14	7	0
20	A	6	0	0	0	0
20	B	8	0	0	0	0
20	C	5	0	0	0	0
20	D	2	0	0	0	0
20	E	7	0	0	0	0
20	F	10	0	0	0	0
20	G	8	0	0	0	0
20	H	16	0	0	0	0
20	I	4	0	0	0	0
20	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	K	6	0	0	0	0
20	L	7	0	0	0	0
20	M	10	0	0	0	0
20	N	9	0	0	1	0
20	O	2	0	0	0	0
20	P	7	0	0	0	0
20	Q	6	0	0	0	0
20	R	4	0	0	0	0
20	S	5	0	0	0	0
20	T	8	0	0	0	0
20	U	11	0	0	0	0
20	V	12	0	0	0	0
20	W	5	0	0	0	0
20	X	4	0	0	0	0
20	Y	8	0	0	0	0
20	Z	10	0	0	0	0
20	a	6	0	0	0	0
20	b	4	0	0	0	0
20	f	2	0	0	0	0
20	h	1	0	0	0	0
20	i	2	0	0	0	0
All	All	49907	0	49327	302	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 3.

The worst 5 of 302 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)
13:M:152:ASN:O	13:M:156:ARG:HG3	1.43	1.18
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.35	0.91
13:M:152:ASN:O	13:M:156:ARG:CG	2.20	0.88
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.37	0.88
13:M:161:ARG:HG2	13:M:161:ARG:HH11	1.37	0.86

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%)	240 (97%)	7 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	27
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	27
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	45
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	45
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	223/231 (96%)	221 (99%)	2 (1%)	0	100	100
8	V	223/231 (96%)	221 (99%)	2 (1%)	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	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	25	56
10	X	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	25	56
11	K	209/211 (99%)	199 (95%)	8 (4%)	2 (1%)	13	40
11	Y	209/211 (99%)	198 (95%)	9 (4%)	2 (1%)	13	40
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	230/246 (94%)	220 (96%)	8 (4%)	2 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	b	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
15	g	1/4 (25%)	1 (100%)	0	0	100	100
15	h	1/4 (25%)	1 (100%)	0	0	100	100
15	i	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6283/6632 (95%)	6100 (97%)	161 (3%)	22 (0%)	30	60

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	218	GLY
3	C	202	GLN
2	P	51	VAL
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%)	205 (98%)	4 (2%)	52	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	52	81
2	B	203/216 (94%)	198 (98%)	5 (2%)	42	75
2	P	203/216 (94%)	198 (98%)	5 (2%)	42	75
3	C	212/226 (94%)	204 (96%)	8 (4%)	28	63
3	Q	212/226 (94%)	204 (96%)	8 (4%)	28	63
4	D	194/215 (90%)	186 (96%)	8 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	194/215 (90%)	185 (95%)	9 (5%)	23	55
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	69
5	S	190/193 (98%)	185 (97%)	5 (3%)	41	74
6	F	201/239 (84%)	193 (96%)	8 (4%)	27	61
6	T	201/239 (84%)	193 (96%)	8 (4%)	27	61
7	G	206/210 (98%)	197 (96%)	9 (4%)	24	57
7	U	206/210 (98%)	197 (96%)	9 (4%)	24	57
8	H	184/189 (97%)	173 (94%)	11 (6%)	16	44
8	V	184/189 (97%)	172 (94%)	12 (6%)	14	40
9	I	172/173 (99%)	169 (98%)	3 (2%)	56	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	56	83
10	J	173/175 (99%)	165 (95%)	8 (5%)	23	55
10	X	173/175 (99%)	164 (95%)	9 (5%)	19	50
11	K	169/169 (100%)	157 (93%)	12 (7%)	12	36
11	Y	169/169 (100%)	157 (93%)	12 (7%)	12	36
12	L	185/185 (100%)	173 (94%)	12 (6%)	14	40
12	Z	185/185 (100%)	172 (93%)	13 (7%)	12	36
13	M	198/208 (95%)	183 (92%)	15 (8%)	11	32
13	a	199/208 (96%)	185 (93%)	14 (7%)	12	36
14	N	161/161 (100%)	157 (98%)	4 (2%)	42	75
14	b	161/161 (100%)	156 (97%)	5 (3%)	35	70
All	All	5315/5536 (96%)	5086 (96%)	229 (4%)	25	57

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	157	PHE
13	a	231	GLN
5	S	188	LEU
13	a	225	ILE
12	Z	34	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	99	ASN
8	V	189	ASN
5	S	151	ASN
7	U	83	ASN
10	X	63	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	00E	d	1	15	9,9,10	0.81	0	10,10,12	1.37	2 (20%)
15	0A1	e	3	15	12,13,14	1.52	1 (8%)	13,16,18	1.17	2 (15%)
15	0A1	h	3	15	12,13,14	1.44	1 (8%)	13,16,18	1.11	1 (7%)
15	00E	i	1	15	9,9,10	0.87	0	10,10,12	1.34	1 (10%)
15	00E	f	1	15	9,9,10	0.89	1 (11%)	10,10,12	1.33	1 (10%)
15	0A1	f	3	15	12,13,14	1.52	1 (8%)	13,16,18	1.23	1 (7%)
15	00E	g	1	15	9,9,10	0.74	0	10,10,12	1.39	1 (10%)
15	00E	e	1	15	9,9,10	0.89	0	10,10,12	1.32	1 (10%)
15	00E	h	1	15	9,9,10	0.85	0	10,10,12	1.40	1 (10%)
15	0A1	g	3	15	12,13,14	1.41	1 (8%)	13,16,18	0.91	0
15	0A1	i	3	15	12,13,14	1.52	1 (8%)	13,16,18	1.25	1 (7%)
15	0A1	d	3	15	12,13,14	1.51	1 (8%)	13,16,18	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	00E	d	1	15	-	0/2/11/12	0/1/1/1
15	0A1	e	3	15	-	0/7/8/10	0/1/1/1
15	0A1	h	3	15	-	0/7/8/10	0/1/1/1
15	00E	i	1	15	-	0/2/11/12	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1
15	0A1	f	3	15	-	2/7/8/10	0/1/1/1
15	00E	g	1	15	-	0/2/11/12	0/1/1/1
15	00E	e	1	15	-	0/2/11/12	0/1/1/1
15	00E	h	1	15	-	0/2/11/12	0/1/1/1
15	0A1	g	3	15	-	0/7/8/10	0/1/1/1
15	0A1	i	3	15	-	2/7/8/10	0/1/1/1
15	0A1	d	3	15	-	0/7/8/10	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	3	0A1	CB-CG	-4.91	1.39	1.51
15	e	3	0A1	CB-CG	-4.86	1.39	1.51
15	f	3	0A1	CB-CG	-4.83	1.39	1.51
15	d	3	0A1	CB-CG	-4.77	1.39	1.51
15	h	3	0A1	CB-CG	-4.56	1.40	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	3	0A1	CB-CA-C	-3.77	104.40	111.47
15	f	3	0A1	CB-CA-C	-3.67	104.59	111.47
15	e	3	0A1	CG-CB-CA	-2.69	108.65	114.10
15	g	1	00E	C-CA-NB	-2.66	107.50	112.84
15	h	3	0A1	CG-CB-CA	-2.62	108.79	114.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	f	3	0A1	C-CA-CB-CG
15	i	3	0A1	C-CA-CB-CG
15	f	3	0A1	N-CA-CB-CG
15	i	3	0A1	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	d	1	00E	2	0
15	g	1	00E	2	0
15	g	3	0A1	1	0
15	d	3	0A1	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
18	MES	U	302	-	12,12,12	0.77	0	14,16,16	0.45	0
19	MPD	a	302	-	7,7,7	0.34	0	9,10,10	0.36	0
18	MES	M	301	-	12,12,12	0.68	0	14,16,16	0.46	0
18	MES	a	301	-	12,12,12	0.72	0	14,16,16	0.40	0
18	MES	G	303	-	12,12,12	0.78	0	14,16,16	0.36	0
18	MES	H	301	-	12,12,12	0.75	0	14,16,16	0.36	0
19	MPD	K	301	-	7,7,7	0.11	0	9,10,10	0.48	0
18	MES	V	301	-	12,12,12	0.74	0	14,16,16	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	U	302	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MPD	a	302	-	-	0/5/5/5	-
18	MES	M	301	-	-	0/6/14/14	0/1/1/1
18	MES	a	301	-	-	0/6/14/14	0/1/1/1
18	MES	G	303	-	-	1/6/14/14	0/1/1/1
18	MES	H	301	-	-	1/6/14/14	0/1/1/1
19	MPD	K	301	-	-	2/5/5/5	-
18	MES	V	301	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	U	302	MES	C7-C8-S-O2S
18	U	302	MES	C7-C8-S-O3S
18	G	303	MES	N4-C7-C8-S
18	H	301	MES	N4-C7-C8-S
19	K	301	MPD	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	302	MPD	7	0
18	G	303	MES	1	0
19	K	301	MPD	1	0

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%)	-1.00	0 100 100	43, 60, 91, 131	0
1	O	250/250 (100%)	-1.00	0 100 100	46, 66, 100, 156	0
2	B	244/258 (94%)	-0.91	0 100 100	45, 66, 112, 154	0
2	P	244/258 (94%)	-0.90	0 100 100	48, 69, 110, 149	0
3	C	240/254 (94%)	-0.93	0 100 100	46, 70, 126, 143	0
3	Q	240/254 (94%)	-0.85	1 (0%) 89 86	53, 80, 142, 168	0
4	D	235/260 (90%)	-1.01	0 100 100	49, 71, 99, 123	0
4	R	235/260 (90%)	-0.95	0 100 100	49, 72, 102, 126	0
5	E	231/234 (98%)	-0.94	0 100 100	51, 74, 106, 137	0
5	S	231/234 (98%)	-0.89	0 100 100	51, 80, 116, 141	0
6	F	243/288 (84%)	-1.01	0 100 100	44, 67, 101, 141	0
6	T	243/288 (84%)	-0.96	0 100 100	46, 70, 117, 134	0
7	G	241/252 (95%)	-1.06	0 100 100	43, 60, 92, 145	0
7	U	241/252 (95%)	-1.02	0 100 100	44, 62, 95, 125	0
8	H	225/231 (97%)	-1.06	0 100 100	41, 56, 87, 123	0
8	V	225/231 (97%)	-1.02	0 100 100	46, 59, 92, 149	0
9	I	204/205 (99%)	-1.08	0 100 100	42, 60, 86, 108	0
9	W	204/205 (99%)	-1.09	0 100 100	43, 60, 88, 114	0
10	J	195/198 (98%)	-1.03	0 100 100	43, 64, 94, 123	0
10	X	195/198 (98%)	-1.05	0 100 100	46, 67, 94, 134	0
11	K	211/211 (100%)	-0.91	0 100 100	46, 68, 110, 129	0
11	Y	211/211 (100%)	-0.94	0 100 100	47, 67, 113, 133	0
12	L	222/222 (100%)	-1.04	0 100 100	47, 61, 92, 115	0
12	Z	222/222 (100%)	-1.04	0 100 100	44, 60, 88, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	232/246 (94%)	-0.96	1 (0%) 89 86	41, 59, 87, 109	0
13	a	233/246 (94%)	-1.00	0 100 100	40, 58, 84, 120	0
14	N	195/195 (100%)	-1.13	0 100 100	41, 55, 85, 106	0
14	b	195/195 (100%)	-1.10	0 100 100	40, 55, 84, 110	0
15	d	1/4 (25%)	-0.40	0 100 100	59, 59, 59, 59	0
15	e	1/4 (25%)	-0.26	0 100 100	71, 71, 71, 71	0
15	f	1/4 (25%)	0.56	0 100 100	92, 92, 92, 92	0
15	g	1/4 (25%)	-0.50	0 100 100	61, 61, 61, 61	0
15	h	1/4 (25%)	-0.71	0 100 100	75, 75, 75, 75	0
15	i	1/4 (25%)	-0.54	0 100 100	84, 84, 84, 84	0
All	All	6343/6632 (95%)	-0.99	2 (0%) 100 100	40, 64, 106, 168	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	3.5
13	M	227	GLY	2.5

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

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	00E	f	1	9/10	0.90	0.11	98,115,123,125	0
15	00E	i	1	9/10	0.90	0.11	88,113,120,122	0
15	00E	h	1	9/10	0.92	0.09	80,85,89,90	0
15	0A1	h	3	13/14	0.93	0.08	66,71,93,101	0
15	0A1	e	3	13/14	0.96	0.07	64,69,86,89	0
15	0A1	f	3	13/14	0.96	0.08	81,91,97,97	0
15	00E	d	1	9/10	0.96	0.07	73,81,83,85	0
15	0A1	i	3	13/14	0.96	0.07	80,86,98,99	0
15	00E	e	1	9/10	0.97	0.06	72,80,94,97	0
15	00E	g	1	9/10	0.97	0.06	65,77,84,85	0
15	0A1	d	3	13/14	0.98	0.04	53,58,65,66	0
15	0A1	g	3	13/14	0.98	0.05	61,63,67,68	0

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(Å ²)	Q<0.9
19	MPD	K	301	8/8	0.88	0.15	90,97,98,111	0
18	MES	G	303	12/12	0.91	0.13	92,153,170,176	0
18	MES	a	301	12/12	0.92	0.10	125,129,133,133	0
16	MG	W	301	1/1	0.93	0.18	143,143,143,143	0
18	MES	M	301	12/12	0.93	0.12	126,137,147,151	0
19	MPD	a	302	8/8	0.93	0.10	80,102,107,111	0
18	MES	U	302	12/12	0.95	0.10	108,131,136,141	0
18	MES	V	301	12/12	0.96	0.10	92,106,111,115	0
18	MES	H	301	12/12	0.96	0.09	79,94,99,100	0
17	CL	U	301	1/1	0.99	0.05	60,60,60,60	0
16	MG	N	201	1/1	0.99	0.06	72,72,72,72	0
17	CL	G	302	1/1	0.99	0.06	59,59,59,59	0
16	MG	G	301	1/1	1.00	0.02	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.