



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 09:03 PM UTC

PDB ID : 9QD2 / pdb_00009qd2
Title : Yeast 20S proteasome mutant: beta1_G128V (b1-propeptide deleted) in complex with MG132
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-05
Resolution : 2.70 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

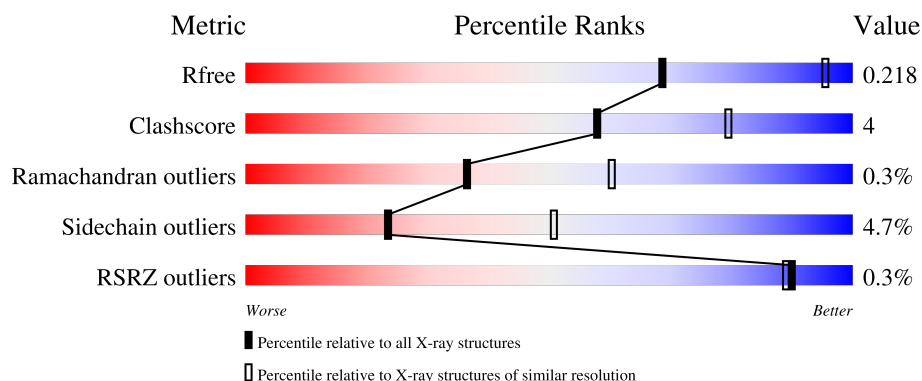
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	250	96%
1	O	250	95%
2	B	258	% 88% 5% 5%
2	P	258	% 88% 5% 5%
3	C	254	89% ••6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 2% 90% 6%
4	D	260	 84% 6% 10%
4	R	260	 85% 5% 10%
5	E	234	 92% 6%
5	S	234	 92% 6%
6	F	288	 80% 16%
6	T	288	 79% 16%
7	G	252	 88% 6%
7	U	252	 87% 8%
8	H	231	 80% 15%
8	V	231	 81% 14%
9	I	205	 94% 5%
9	W	205	 93% 6%
10	J	198	 82% 13%
10	X	198	 82% 14%
11	K	211	 70% 27%
11	Y	211	 74% 22%
12	L	222	 89% 9%
12	Z	222	 86% 13%
13	M	246	 74% 17% 5%
13	a	246	 74% 19% 5%
14	N	195	 74% 18% 7%
14	b	195	 76% 19% 5%
15	d	4	 50% 25% 25%
15	e	4	 50% 50%

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Mol	Chain	Length	Quality of chain
15	f	4	 50%25%25%
15	g	4	 50%25%25%
15	h	4	 50%50%
15	i	4	 50%25%25%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49779 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	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	VAL	GLY	engineered mutation	UNP P38624
b	128	VAL	GLY	engineered mutation	UNP P38624

- 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
			41	30	4	7			
15	e	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	f	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	g	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	h	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	i	4	Total	C	N	O	0	0	0
			41	30	4	7			

- 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	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	2	Total	Cl	0	0
			2	2		
17	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		
17	b	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	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	6	Total	O	0	0
			6	6		
19	B	13	Total	O	0	0
			13	13		
19	C	12	Total	O	0	0
			12	12		
19	D	9	Total	O	0	0
			9	9		
19	E	4	Total	O	0	0
			4	4		
19	F	6	Total	O	0	0
			6	6		
19	G	7	Total	O	0	0
			7	7		
19	H	16	Total	O	0	0
			16	16		
19	I	8	Total	O	0	0
			8	8		
19	J	13	Total	O	0	0
			13	13		
19	K	9	Total	O	0	0
			9	9		

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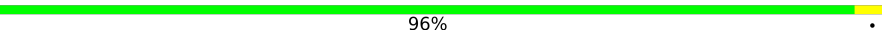
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	18	Total 18	O 18	0	0
19	M	9	Total 9	O 9	0	0
19	N	5	Total 5	O 5	0	0
19	O	5	Total 5	O 5	0	0
19	P	5	Total 5	O 5	0	0
19	Q	8	Total 8	O 8	0	0
19	R	3	Total 3	O 3	0	0
19	S	4	Total 4	O 4	0	0
19	T	8	Total 8	O 8	0	0
19	U	11	Total 11	O 11	0	0
19	V	9	Total 9	O 9	0	0
19	W	9	Total 9	O 9	0	0
19	X	14	Total 14	O 14	0	0
19	Y	11	Total 11	O 11	0	0
19	Z	7	Total 7	O 7	0	0
19	a	9	Total 9	O 9	0	0
19	b	9	Total 9	O 9	0	0
19	d	1	Total 1	O 1	0	0
19	e	1	Total 1	O 1	0	0
19	g	1	Total 1	O 1	0	0
19	h	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

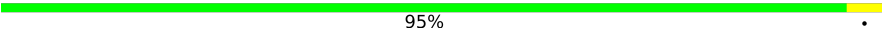
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

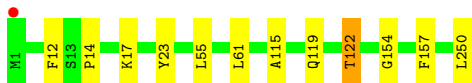
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  96%



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95%



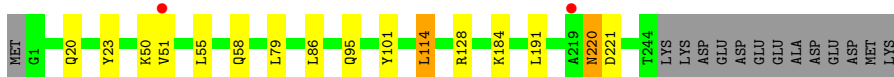
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 5% • 5%



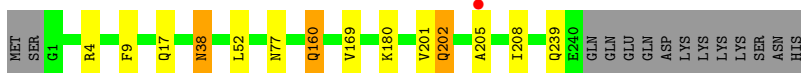
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 5% • 5%

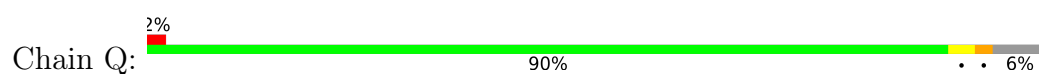


- Molecule 3: Proteasome subunit alpha type-4

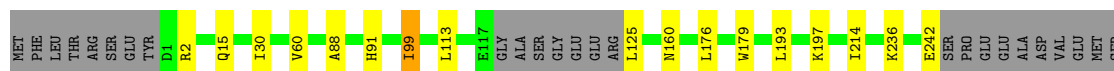
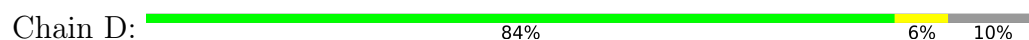
Chain C:  89% • • 6%



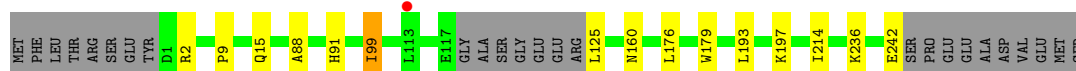
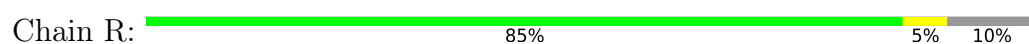
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



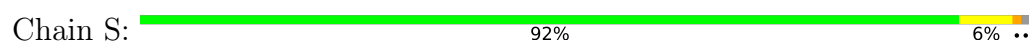
- Molecule 4: Proteasome subunit alpha type-5



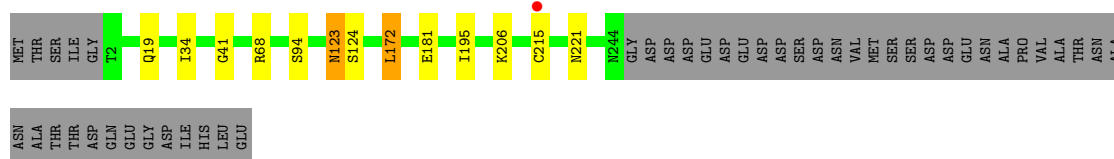
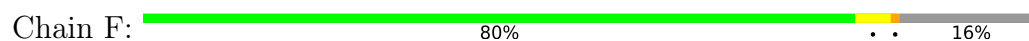
- Molecule 5: Proteasome subunit alpha type-6



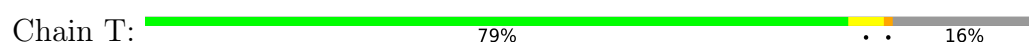
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 88% 6% . .



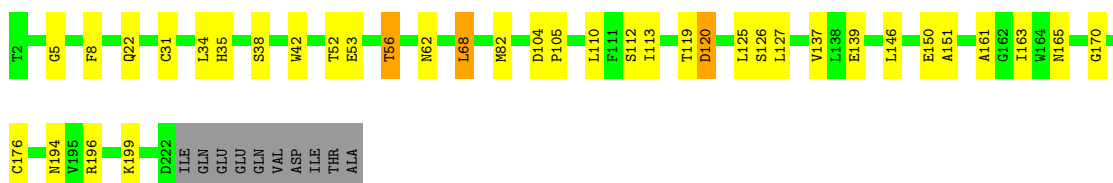
- Molecule 7: Proteasome subunit alpha type-1

Chain U: 87% 8% . .



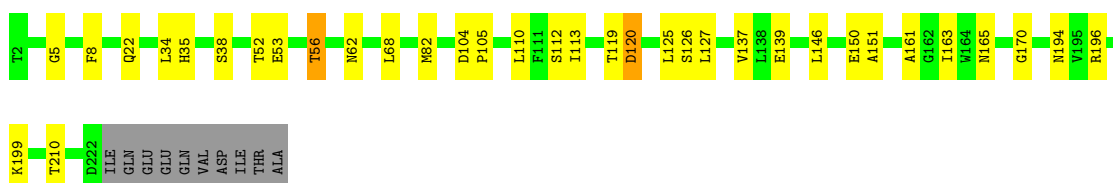
- Molecule 8: Proteasome subunit beta type-2

Chain H: 80% 15% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 81% 14% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 94% 5%

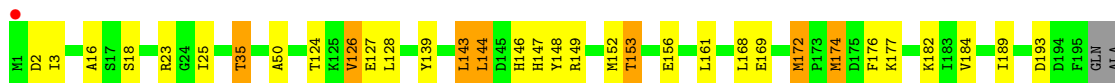
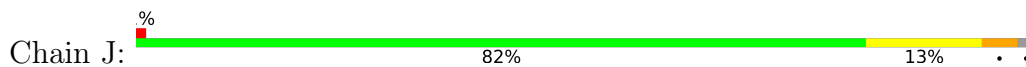


- Molecule 9: Proteasome subunit beta type-3

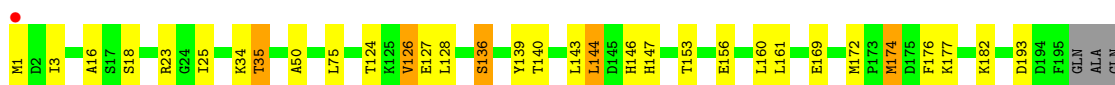
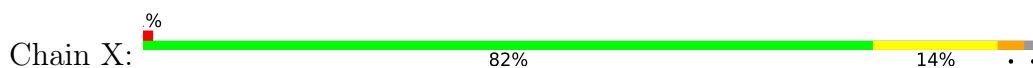
Chain W: 93% 6%



- Molecule 10: Proteasome subunit beta type-4



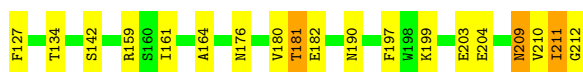
- Molecule 10: Proteasome subunit beta type-4



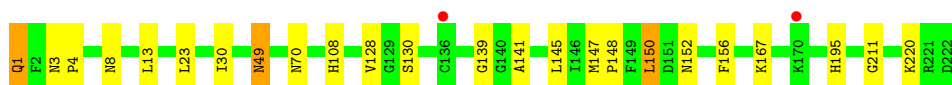
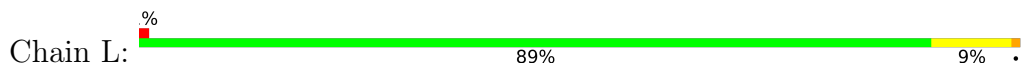
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



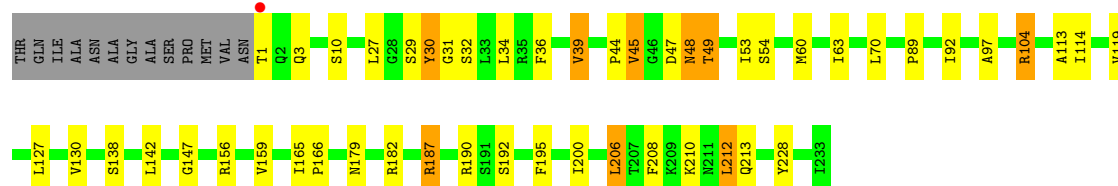
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  86% 13% .



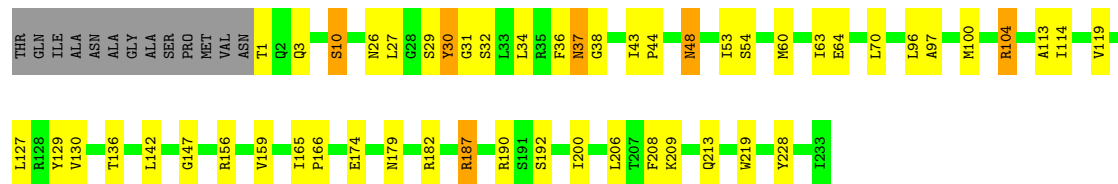
• Molecule 13: Proteasome subunit beta type-7

Chain M:  74% 17% . 5%



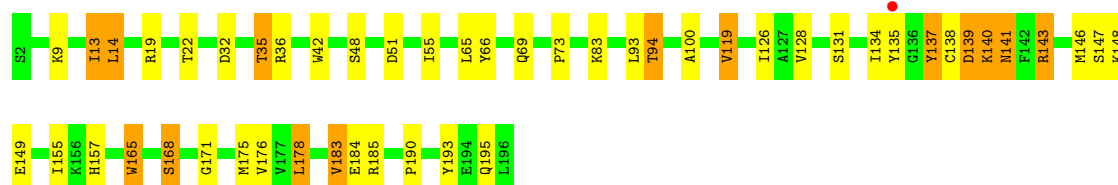
• Molecule 13: Proteasome subunit beta type-7

Chain a:  74% 19% . 5%



• Molecule 14: Proteasome subunit beta type-1

Chain N:  74% 18% 7%



• Molecule 14: Proteasome subunit beta type-1

Chain b:  76% 19% 5%



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

Chain d:  50% 25% 25%



- 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% 25% 25%



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

Chain g:  50% 25% 25%



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

Chain h:  50% 50%



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

Chain i:  50% 25% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.23Å 300.11Å 145.77Å 90.00° 113.25° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.70) 97.2 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.214 0.180 , 0.218	Depositor DCC
R_{free} test set	14253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.6	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	0.97	EDS
Total number of atoms	49779	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P6S, CL, MG, A1I48, MES

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	1.03	0/1952	1.43	0/2642
1	O	1.03	0/1952	1.43	0/2642
2	B	1.03	0/1934	1.44	0/2618
2	P	1.03	0/1934	1.44	0/2618
3	C	1.03	0/1910	1.47	0/2586
3	Q	1.03	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.47	4/2475 (0.2%)
4	R	1.03	0/1837	1.47	2/2475 (0.1%)
5	E	1.04	0/1800	1.45	4/2433 (0.2%)
5	S	1.04	0/1800	1.45	2/2433 (0.1%)
6	F	1.02	0/1932	1.46	2/2609 (0.1%)
6	T	1.02	0/1932	1.47	4/2609 (0.2%)
7	G	1.01	0/1945	1.42	0/2634
7	U	1.01	0/1945	1.43	0/2634
8	H	1.00	0/1708	1.41	1/2316 (0.0%)
8	V	1.00	0/1708	1.42	1/2316 (0.0%)
9	I	1.01	0/1611	1.42	1/2174 (0.0%)
9	W	1.01	0/1611	1.42	1/2174 (0.0%)
10	J	1.00	0/1589	1.40	0/2142
10	X	1.00	0/1589	1.38	0/2142
11	K	0.97	0/1674	1.38	1/2264 (0.0%)
11	Y	0.97	0/1674	1.39	1/2264 (0.0%)
12	L	1.00	0/1795	1.38	0/2420
12	Z	1.00	0/1795	1.38	1/2420 (0.0%)
13	M	0.98	0/1855	1.38	0/2514
13	a	0.99	0/1855	1.39	0/2514
14	N	0.97	0/1537	1.40	2/2082 (0.1%)
14	b	0.98	0/1537	1.39	1/2082 (0.0%)
15	d	0.70	0/15	0.76	0/19
15	e	0.79	0/15	0.78	0/19
15	f	0.61	0/15	0.83	0/19
15	g	0.63	0/15	0.75	0/19

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	h	0.76	0/15	0.78	0/19
15	i	0.64	0/15	0.85	0/19
All	All	1.01	0/50248	1.42	28/67932 (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
15	d	0	1
15	e	0	1
15	f	0	1
15	g	0	1
15	h	0	1
15	i	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	120	ASP	CA-CB-CG	9.68	122.28	112.60
8	H	120	ASP	CA-CB-CG	9.33	121.93	112.60
14	b	94	THR	CB-CA-C	8.53	124.66	111.70
14	N	94	THR	CB-CA-C	7.85	123.34	111.95
14	N	168	SER	N-CA-C	-6.12	104.53	111.14

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	d	3	LEU	Peptide
15	e	3	LEU	Peptide
15	f	3	LEU	Peptide
15	g	3	LEU	Peptide
15	h	3	LEU	Peptide

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	5	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	10	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	6	0
7	G	1907	0	1900	12	0
7	U	1907	0	1901	12	0
8	H	1677	0	1678	19	0
8	V	1677	0	1678	19	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	30	0
10	X	1561	0	1569	26	0
11	K	1637	0	1585	50	0
11	Y	1637	0	1585	45	0
12	L	1757	0	1711	20	0
12	Z	1757	0	1711	21	0
13	M	1824	0	1832	41	0
13	a	1824	0	1832	35	0
14	N	1508	0	1477	45	0
14	b	1508	0	1477	41	0
15	d	41	0	21	0	0
15	e	41	0	21	0	0
15	f	41	0	21	0	0
15	g	41	0	21	0	0
15	h	41	0	21	0	0
15	i	41	0	21	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Z	1	0	0	0	0
17	G	2	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	12	0	13	0	0
19	A	6	0	0	0	0
19	B	13	0	0	0	0
19	C	12	0	0	1	0
19	D	9	0	0	0	0
19	E	4	0	0	0	0
19	F	6	0	0	0	0
19	G	7	0	0	0	0
19	H	16	0	0	0	0
19	I	8	0	0	0	0
19	J	13	0	0	1	0
19	K	9	0	0	0	0
19	L	18	0	0	0	0
19	M	9	0	0	0	0
19	N	5	0	0	0	0
19	O	5	0	0	0	0
19	P	5	0	0	0	0
19	Q	8	0	0	0	0
19	R	3	0	0	0	0
19	S	4	0	0	0	0
19	T	8	0	0	1	0
19	U	11	0	0	0	0
19	V	9	0	0	0	0
19	W	9	0	0	0	0
19	X	14	0	0	0	0
19	Y	11	0	0	0	0
19	Z	7	0	0	0	0
19	a	9	0	0	0	0
19	b	9	0	0	0	0
19	d	1	0	0	0	0
19	e	1	0	0	0	0
19	g	1	0	0	0	0
19	h	2	0	0	0	0
All	All	49779	0	49158	444	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 4.

The worst 5 of 444 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)
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.21	1.17
14:b:143:ARG:H	14:b:146:MET:CE	1.67	1.08
13:M:45:VAL:HG11	13:M:92:ILE:HD13	1.30	1.08
14:b:143:ARG:H	14:b:146:MET:HE2	1.15	1.06
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.27	1.04

There are no symmetry-related clashes.

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%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	37
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	37
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	25
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
7	U	239/252 (95%)	233 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
8	V	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	209/211 (99%)	201 (96%)	6 (3%)	2 (1%)	12	32
11	Y	209/211 (99%)	203 (97%)	5 (2%)	1 (0%)	24	48
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	231/246 (94%)	220 (95%)	10 (4%)	1 (0%)	30	54
13	a	231/246 (94%)	218 (94%)	12 (5%)	1 (0%)	30	54
14	N	193/195 (99%)	183 (95%)	9 (5%)	1 (0%)	24	48
14	b	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	48
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	6276/6632 (95%)	6095 (97%)	164 (3%)	17 (0%)	36	60

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
11	K	37	ILE
2	P	51	VAL
3	Q	202	GLN

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%)	43	72
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	72
2	B	203/216 (94%)	195 (96%)	8 (4%)	28	57
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	57
3	C	212/226 (94%)	207 (98%)	5 (2%)	43	72
3	Q	212/226 (94%)	206 (97%)	6 (3%)	38	68
4	D	194/215 (90%)	185 (95%)	9 (5%)	24	51
4	R	194/215 (90%)	186 (96%)	8 (4%)	27	56
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	70
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	70
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	61
6	T	201/239 (84%)	193 (96%)	8 (4%)	28	56
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	62
7	U	206/210 (98%)	198 (96%)	8 (4%)	28	57
8	H	180/189 (95%)	172 (96%)	8 (4%)	25	53
8	V	180/189 (95%)	173 (96%)	7 (4%)	28	57
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	84
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	84
10	J	173/175 (99%)	162 (94%)	11 (6%)	16	38
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	47
11	K	168/168 (100%)	152 (90%)	16 (10%)	8	20
11	Y	168/168 (100%)	152 (90%)	16 (10%)	8	20
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	64
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	54
13	M	199/208 (96%)	184 (92%)	15 (8%)	12	31
13	a	199/208 (96%)	187 (94%)	12 (6%)	17	41
14	N	162/162 (100%)	142 (88%)	20 (12%)	4	12
14	b	162/162 (100%)	143 (88%)	19 (12%)	5	13
15	d	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	e	2/2 (100%)	2 (100%)	0	100	100
15	f	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	g	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	h	2/2 (100%)	2 (100%)	0	100	100
15	i	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	5320/5548 (96%)	5071 (95%)	249 (5%)	23	51

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	140	LYS
13	a	70	LEU
4	R	99	ILE
13	a	37	ASN
14	b	141	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 195 such sidechains are listed below:

Mol	Chain	Res	Type
4	R	100	ASN
8	V	22	GLN
4	R	225	ASN
6	T	117	GLN
8	V	189	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	A1I48	h	4	15,11	12,14,15	1.37	1 (8%)	10,18,20	1.48	3 (30%)
15	A1I48	i	4	15,14	12,14,15	1.55	1 (8%)	10,18,20	1.53	1 (10%)
15	A1I48	e	4	15,11	12,14,15	1.12	1 (8%)	10,18,20	1.24	1 (10%)
15	A1I48	f	4	15,14	12,14,15	1.18	1 (8%)	10,18,20	1.12	1 (10%)
15	A1I48	d	4	15,8	12,14,15	1.38	1 (8%)	10,18,20	1.58	2 (20%)
15	A1I48	g	4	15,8	12,14,15	1.38	1 (8%)	10,18,20	1.55	2 (20%)

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	A1I48	h	4	15,11	-	4/15/18/20	-
15	A1I48	i	4	15,14	-	3/15/18/20	-
15	A1I48	e	4	15,11	-	4/15/18/20	-
15	A1I48	f	4	15,14	-	3/15/18/20	-
15	A1I48	d	4	15,8	-	4/15/18/20	-
15	A1I48	g	4	15,8	-	4/15/18/20	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	4	A1I48	CA-N2	-4.93	1.33	1.47
15	g	4	A1I48	CA-N2	-4.25	1.35	1.47
15	h	4	A1I48	CA-N2	-4.23	1.35	1.47
15	d	4	A1I48	CA-N2	-4.22	1.35	1.47
15	f	4	A1I48	CA-N2	-3.44	1.37	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	4	A1I48	CB-CA-N2	-3.65	90.29	114.17
15	g	4	A1I48	CB-CA-N2	-3.33	92.44	114.17
15	d	4	A1I48	CB-CA-N2	-3.33	92.44	114.17
15	h	4	A1I48	CB-CA-N2	-2.61	97.13	114.17
15	f	4	A1I48	O-C-CA	-2.25	119.00	124.77

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	d	4	A1I48	O23-C22-OG1-CB
15	d	4	A1I48	O-C-CA-CB
15	e	4	A1I48	O23-C22-OG1-CB
15	e	4	A1I48	O-C-CA-CB
15	f	4	A1I48	O23-C22-OG1-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	a	301	-	12,12,12	0.67	0	15,16,16	0.34	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	a	301	-	-	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	301	MES	C7-C8-S-O2S
18	a	301	MES	C7-C8-S-O3S
18	a	301	MES	C7-C8-S-O1S

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%)	-0.64	1 (0%) 88 87	54, 70, 101, 177	0
1	O	250/250 (100%)	-0.59	1 (0%) 88 87	59, 77, 115, 172	0
2	B	244/258 (94%)	-0.48	3 (1%) 76 75	56, 74, 121, 169	0
2	P	244/258 (94%)	-0.44	2 (0%) 82 81	61, 79, 124, 173	0
3	C	240/254 (94%)	-0.53	1 (0%) 88 87	56, 77, 131, 156	0
3	Q	240/254 (94%)	-0.39	4 (1%) 69 67	60, 90, 152, 178	0
4	D	235/260 (90%)	-0.58	0 100 100	58, 79, 110, 151	0
4	R	235/260 (90%)	-0.50	1 (0%) 88 87	56, 80, 115, 151	0
5	E	231/234 (98%)	-0.57	0 100 100	59, 82, 114, 139	0
5	S	231/234 (98%)	-0.48	0 100 100	62, 86, 120, 157	0
6	F	243/288 (84%)	-0.55	1 (0%) 88 87	55, 77, 117, 140	0
6	T	243/288 (84%)	-0.50	0 100 100	58, 83, 128, 147	0
7	G	241/252 (95%)	-0.60	0 100 100	54, 70, 100, 134	0
7	U	241/252 (95%)	-0.60	0 100 100	58, 73, 104, 143	0
8	H	221/231 (95%)	-0.70	0 100 100	54, 66, 89, 120	0
8	V	221/231 (95%)	-0.66	0 100 100	56, 69, 91, 135	0
9	I	204/205 (99%)	-0.72	0 100 100	50, 65, 90, 117	0
9	W	204/205 (99%)	-0.73	0 100 100	51, 68, 96, 116	0
10	J	195/198 (98%)	-0.52	1 (0%) 87 86	52, 68, 95, 128	0
10	X	195/198 (98%)	-0.52	1 (0%) 87 86	55, 72, 94, 138	0
11	K	211/211 (100%)	-0.63	0 100 100	53, 66, 91, 177	0
11	Y	211/211 (100%)	-0.57	0 100 100	52, 67, 96, 181	0
12	L	222/222 (100%)	-0.52	2 (0%) 81 80	52, 70, 101, 121	0
12	Z	222/222 (100%)	-0.55	1 (0%) 87 86	53, 67, 99, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.66	1 (0%) 88 87	53, 71, 91, 111	0
13	a	233/246 (94%)	-0.69	0 100 100	51, 69, 91, 111	0
14	N	195/195 (100%)	-0.52	1 (0%) 87 86	53, 69, 117, 149	0
14	b	195/195 (100%)	-0.53	0 100 100	52, 69, 118, 151	0
15	d	2/4 (50%)	0.03	0 100 100	87, 87, 87, 96	0
15	e	2/4 (50%)	-0.69	0 100 100	71, 71, 71, 71	0
15	f	2/4 (50%)	-0.28	0 100 100	86, 86, 86, 89	0
15	g	2/4 (50%)	0.91	0 100 100	92, 92, 92, 101	0
15	h	2/4 (50%)	-1.14	0 100 100	77, 77, 77, 77	0
15	i	2/4 (50%)	-0.07	0 100 100	81, 81, 81, 84	0
All	All	6342/6632 (95%)	-0.57	21 (0%) 90 89	50, 73, 114, 181	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	205	ALA	4.2
10	X	1	MET	3.8
14	N	135	TYR	3.6
1	A	1	MET	3.4
2	B	219	ALA	3.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	A1I48	f	4	15/16	0.94	0.11	69,75,88,93	0
15	A1I48	d	4	15/16	0.95	0.11	62,76,89,90	0
15	A1I48	h	4	15/16	0.95	0.09	67,71,73,74	0
15	A1I48	g	4	15/16	0.96	0.09	66,77,86,90	0
15	A1I48	i	4	15/16	0.97	0.09	71,80,84,84	0
15	A1I48	e	4	15/16	0.98	0.06	62,67,70,71	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($\text{\AA}^2$)	Q<0.9
16	MG	I	301	1/1	0.85	0.17	109,109,109,109	0
18	MES	a	301	12/12	0.87	0.14	122,130,143,149	0
16	MG	Z	301	1/1	0.93	0.13	99,99,99,99	0
16	MG	G	301	1/1	0.93	0.11	82,82,82,82	0
16	MG	J	201	1/1	0.94	0.10	30,30,30,30	0
17	CL	G	303	1/1	0.95	0.21	30,30,30,30	0
17	CL	U	301	1/1	0.97	0.04	70,70,70,70	0
17	CL	G	302	1/1	0.98	0.03	64,64,64,64	0
17	CL	b	201	1/1	0.98	0.06	81,81,81,81	0
17	CL	N	201	1/1	0.98	0.04	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.