



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2025 – 10:32 am BST

PDB ID : 9QC9 / pdb_00009qc9
Title : Yeast 20S proteasome double mutant: beta5_F(-46)S / beta5_G128V
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-04
Resolution : 2.60 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

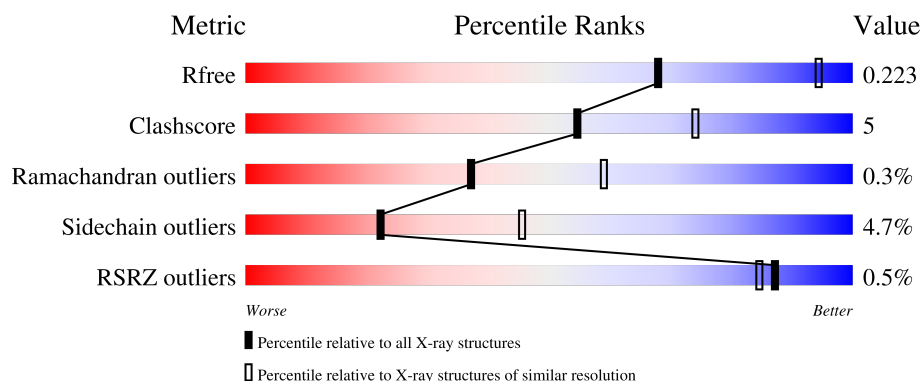
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.










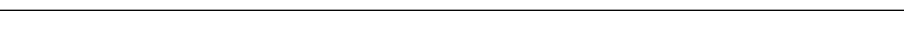
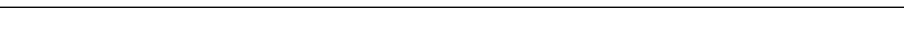

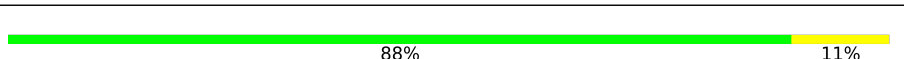


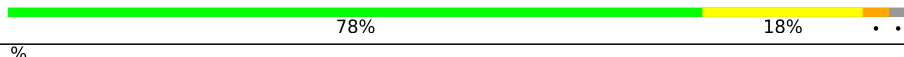

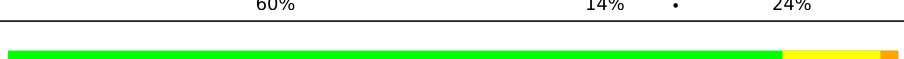




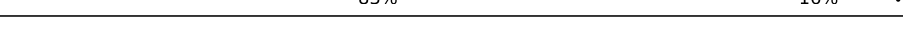
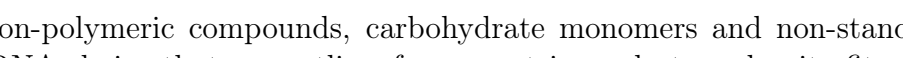

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 style="width: 92%;"></div> <div style="width: 5%;"></div> <div style="width: 3%;"></div> </div> 92% 5% ..
1	O	250	<div> <div style="width: 94%;"></div> <div style="width: 6%;"></div> <div style="width: 0%;"></div> </div> 94% 6% .
2	B	258	<div> <div style="width: 83%;"></div> <div style="width: 10%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div> 83% 10% 5%
2	P	258	<div> <div style="width: 85%;"></div> <div style="width: 9%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> 85% 9% 5%
3	C	254	<div> <div style="width: 85%;"></div> <div style="width: 7%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div> 85% 7% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	287	
11	Y	287	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	W	301	-	-	-	X
17	MES	b	201	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50416 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	248	Total	C	N	O	S	0	0	0
			1900	1210	313	374	3			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	219	Total	C	N	O	S	0	0	0
			1700	1083	291	319	7			
11	Y	219	Total	C	N	O	S	0	0	0
			1700	1083	291	319	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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

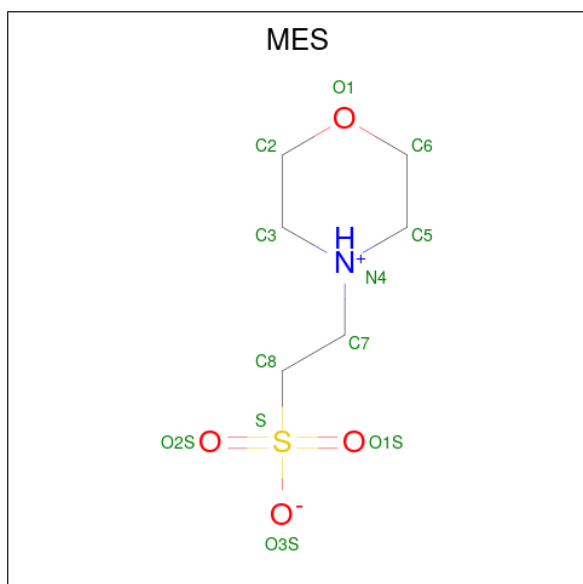
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



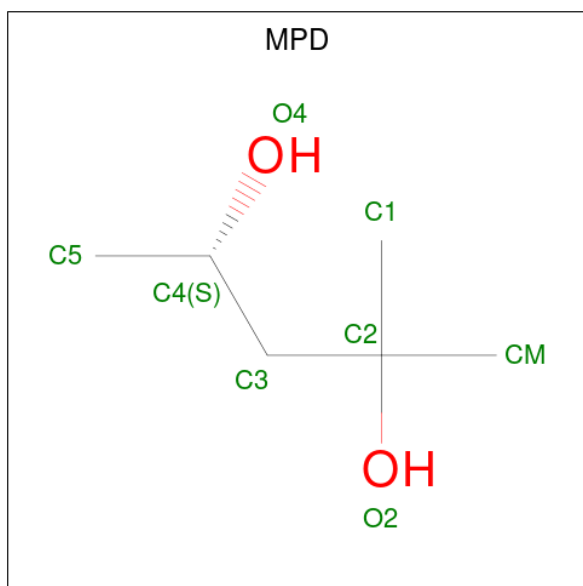
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	U	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Z	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	b	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	40	Total O 40 40	0	0
19	B	24	Total O 24 24	0	0
19	C	34	Total O 34 34	0	0
19	D	26	Total O 26 26	0	0
19	E	20	Total O 20 20	0	0
19	F	30	Total O 30 30	0	0
19	G	44	Total O 44 44	0	0
19	H	40	Total O 40 40	0	0
19	I	40	Total O 40 40	0	0
19	J	18	Total O 18 18	0	0
19	K	22	Total O 22 22	0	0
19	L	29	Total O 29 29	0	0
19	M	47	Total O 47 47	0	0
19	N	41	Total O 41 41	0	0
19	O	31	Total O 31 31	0	0
19	P	21	Total O 21 21	0	0
19	Q	19	Total O 19 19	0	0
19	R	22	Total O 22 22	0	0
19	S	23	Total O 23 23	0	0
19	T	27	Total O 27 27	0	0
19	U	45	Total O 45 45	0	0
19	V	29	Total O 29 29	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	W	26	Total 26	O 26	0	0
19	X	10	Total 10	O 10	0	0
19	Y	19	Total 19	O 19	0	0
19	Z	22	Total 22	O 22	0	0
19	a	43	Total 43	O 43	0	0
19	b	41	Total 41	O 41	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

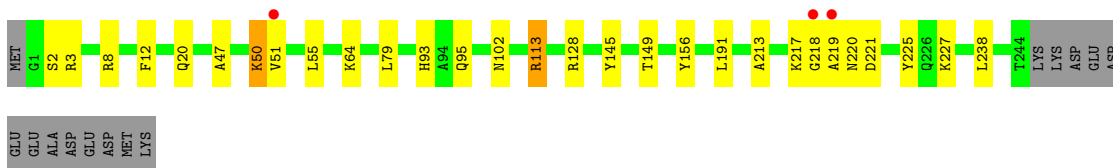
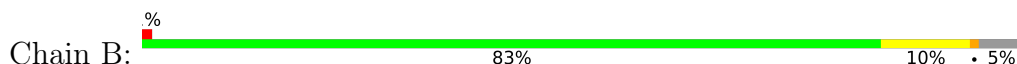
- Molecule 1: Proteasome subunit alpha type-2



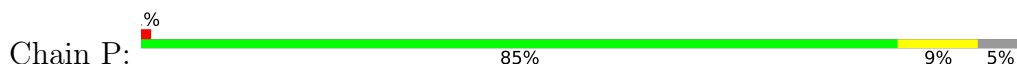
- Molecule 1: Proteasome subunit alpha type-2



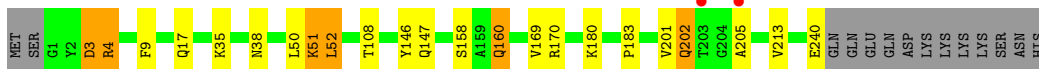
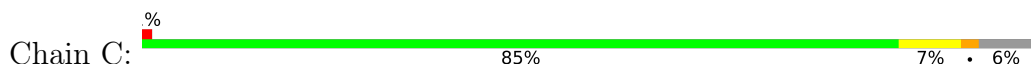
- Molecule 2: Proteasome subunit alpha type-3



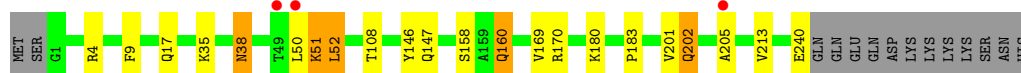
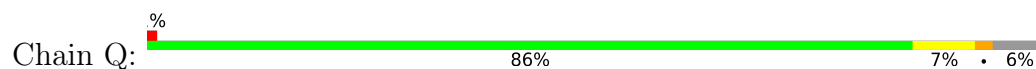
- Molecule 2: Proteasome subunit alpha type-3



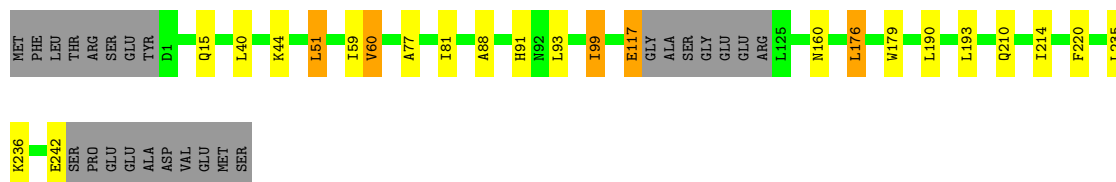
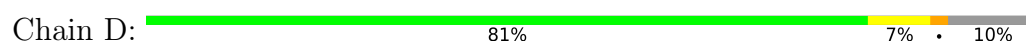
- Molecule 3: Proteasome subunit alpha type-4



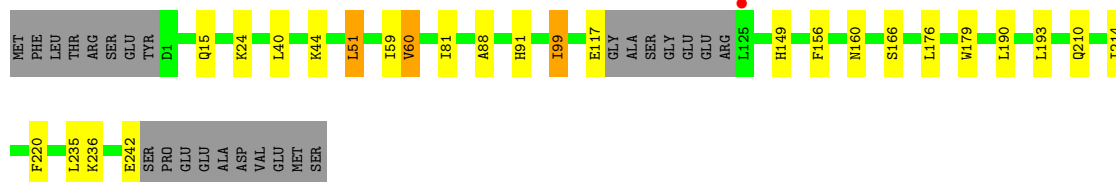
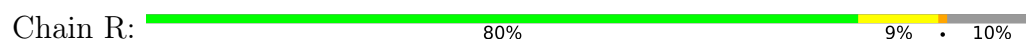
- Molecule 3: Proteasome subunit alpha type-4



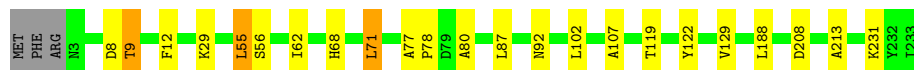
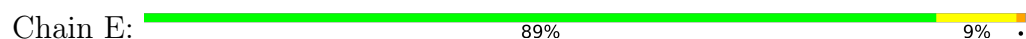
- Molecule 4: Proteasome subunit alpha type-5



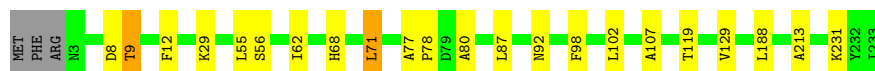
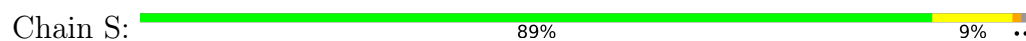
- Molecule 4: Proteasome subunit alpha type-5



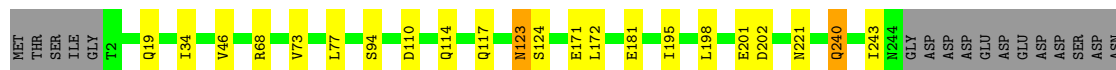
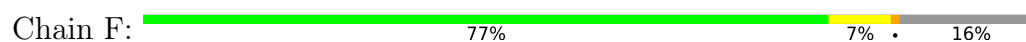
- Molecule 5: Proteasome subunit alpha type-6



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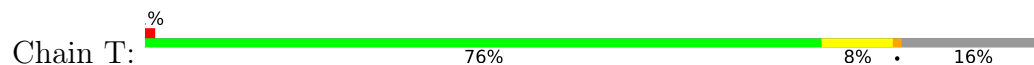


- Molecule 6: Probable proteasome subunit alpha type-7



VAL MET THR SER SER ILE GLY ASP ASP GLU ASN ALA PRO VAL THR ALA THR ASN ALA THR THR THR THR GLN GLY GLY ASP ASP ILE HIS LEU GLU

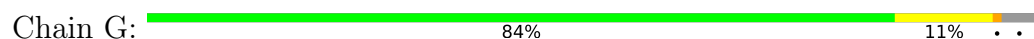
- Molecule 6: Probable proteasome subunit alpha type-7



MET THR SER SER ILE GLY ASP ASP GLU ASN ALA PRO VAL THR ALA THR ASN ALA THR THR THR THR GLN GLY GLY ASP ASP ILE HIS LEU GLU

GLU ASP GLU GLY ASP ASP ASP ASN VAL MET SER SER ASP ASP GLU ASN ALA PRO VAL THR THR ASN ALA THR THR THR THR GLN GLY GLY ASP ASP ILE HIS LEU GLU

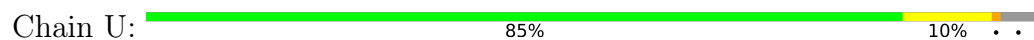
- Molecule 7: Proteasome subunit alpha type-1



MET SER GLY ALA ALA ALA SER SER ALA MET G2 E13 F23 T26 L34 V43 S61 R68 M72 V73 W74 N75 G76 P77 I78 P79 N83 N114 L115 R122 M125 T133 K165 Q166 Q167 T171 V194 L205 E215 K223

R235 L236 Q242 ASP

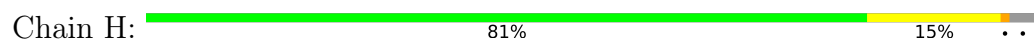
- Molecule 7: Proteasome subunit alpha type-1



MET SER GLY ALA ALA ALA SER SER ALA MET G2 P12 E13 F23 T26 L34 V43 S61 R68 V73 W74 N75 G76 P77 I78 P79 N83 N114 L115 R122 M125 T133 K165 Q166 Q167 T171 V194 L205 E215 K223

R235 L236 Q242 ASP

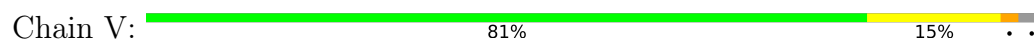
- Molecule 8: Proteasome subunit beta type-2



T1 T2 I3 V4 I14 R19 S20 T21 Q22 A27 D28 K29 N30 K33 L34 K40 C43 A44 E53 A54 V55 T56 Q57 I63 L68 P74 L80 K84 L98 I99 D104 P105 I113 L127 G128 I163 W164 N165 D166 L167 G170

K182 V195 R196 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2



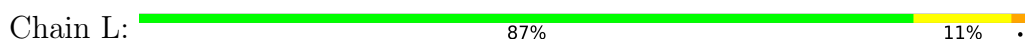
T1 T2 I3 I14 R19 S20 T21 Q22 A27 N30 K33 L34 K40 C43 A44 E53 A54 V55 T56 Q57 I63 L68 P74 L80 K84 L98 I99 D104 P105 F111 S112 I113 T119 L127 G128 Q144 I163 L167



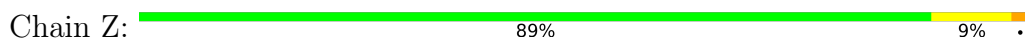
• Molecule 11: Proteasome subunit beta type-5



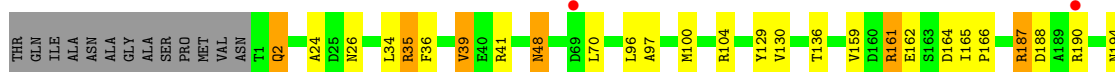
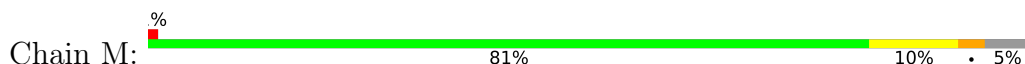
• Molecule 12: Proteasome subunit beta type-6



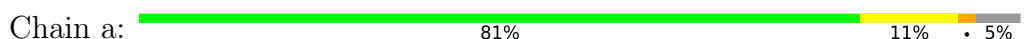
• Molecule 12: Proteasome subunit beta type-6



• Molecule 13: Proteasome subunit beta type-7

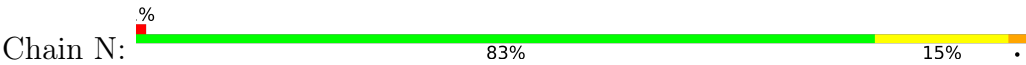


• Molecule 13: Proteasome subunit beta type-7

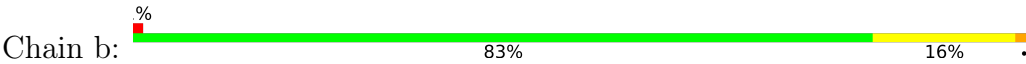




● Molecule 14: Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.72Å 300.35Å 144.55Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.60) 97.4 (15.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.186 , 0.224 0.185 , 0.223	Depositor DCC
R_{free} test set	15744 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	1.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	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	0.96	EDS
Total number of atoms	50416	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CL, MPD, MG, 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	1.02	0/1937	1.42	0/2622
1	O	1.02	0/1952	1.41	0/2642
2	B	1.01	0/1934	1.44	0/2618
2	P	1.02	0/1934	1.45	0/2618
3	C	1.02	0/1910	1.46	1/2586 (0.0%)
3	Q	1.02	0/1910	1.46	0/2586
4	D	1.02	0/1837	1.46	0/2475
4	R	1.02	0/1837	1.47	0/2475
5	E	1.02	0/1800	1.41	0/2433
5	S	1.02	0/1800	1.42	0/2433
6	F	1.01	0/1932	1.44	4/2609 (0.2%)
6	T	1.01	0/1932	1.46	4/2609 (0.2%)
7	G	1.00	0/1945	1.44	2/2634 (0.1%)
7	U	1.01	0/1945	1.42	2/2634 (0.1%)
8	H	1.01	0/1750	1.42	2/2373 (0.1%)
8	V	1.02	0/1750	1.41	0/2373
9	I	1.00	0/1611	1.40	1/2174 (0.0%)
9	W	1.01	0/1611	1.41	3/2174 (0.1%)
10	J	0.96	0/1589	1.40	0/2142
10	X	0.97	0/1589	1.40	2/2142 (0.1%)
11	K	0.99	1/1738 (0.1%)	1.46	2/2350 (0.1%)
11	Y	0.99	1/1738 (0.1%)	1.46	3/2350 (0.1%)
12	L	0.99	0/1795	1.38	0/2420
12	Z	0.99	0/1795	1.39	0/2420
13	M	1.02	0/1855	1.41	5/2514 (0.2%)
13	a	1.01	0/1855	1.39	3/2514 (0.1%)
14	N	1.00	0/1541	1.42	0/2087
14	b	1.00	0/1541	1.41	0/2087
All	All	1.01	2/50363 (0.0%)	1.43	34/68094 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	140	LEU	N-CA	5.58	1.49	1.46
11	K	140	LEU	N-CA	5.53	1.49	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	7.35	124.87	120.24
6	T	77	LEU	C-N-CA	7.35	124.87	120.24
7	G	77	PRO	CA-C-N	6.50	124.33	120.24
7	G	77	PRO	C-N-CA	6.50	124.33	120.24
11	Y	2	THR	CB-CA-C	6.42	123.20	110.42

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	1900	0	1910	19	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	26	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	14	0
3	Q	1881	0	1895	10	0
4	D	1813	0	1797	15	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	18	0
5	S	1773	0	1775	14	0
6	F	1892	0	1883	8	0
6	T	1892	0	1883	13	0
7	G	1907	0	1901	15	0
7	U	1907	0	1901	14	0
8	H	1719	0	1719	18	0
8	V	1719	0	1719	20	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	17	0
10	J	1561	0	1569	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1561	0	1569	32	0
11	K	1700	0	1664	45	0
11	Y	1700	0	1664	28	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	19	0
13	M	1824	0	1832	22	0
13	a	1824	0	1832	20	0
14	N	1512	0	1481	24	0
14	b	1512	0	1481	28	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	G	12	0	13	0	0
17	H	12	0	13	1	0
17	M	12	0	13	1	0
17	N	12	0	13	4	0
17	U	12	0	13	0	0
17	V	12	0	13	1	0
17	Z	12	0	13	0	0
17	b	12	0	13	6	0
18	K	8	0	14	2	0
18	a	8	0	14	0	0
19	A	40	0	0	0	0
19	B	24	0	0	2	0
19	C	34	0	0	0	0
19	D	26	0	0	0	0
19	E	20	0	0	0	0
19	F	30	0	0	0	0
19	G	44	0	0	0	0
19	H	40	0	0	0	0
19	I	40	0	0	0	0
19	J	18	0	0	0	0
19	K	22	0	0	1	0
19	L	29	0	0	0	0
19	M	47	0	0	2	0
19	N	41	0	0	0	0
19	O	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	21	0	0	2	0
19	Q	19	0	0	0	0
19	R	22	0	0	0	0
19	S	23	0	0	0	0
19	T	27	0	0	0	0
19	U	45	0	0	0	0
19	V	29	0	0	0	0
19	W	26	0	0	0	0
19	X	10	0	0	0	0
19	Y	19	0	0	0	0
19	Z	22	0	0	0	0
19	a	43	0	0	3	0
19	b	41	0	0	0	0
All	All	50416	0	49381	468	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 5.

The worst 5 of 468 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)
11:K:133:GLN:HB3	11:K:135:PHE:CE1	1.75	1.19
11:K:133:GLN:HB3	11:K:135:PHE:CZ	1.91	1.05
14:b:128:GLY:HA2	17:b:201:MES:H82	1.38	1.04
11:K:73:ARG:HH21	11:K:105:THR:HG22	1.20	1.02
1:A:4:ARG:HB2	2:B:2:SER:OG	1.65	0.94

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	246/250 (98%)	239 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	237 (96%)	10 (4%)	1 (0%)	30	52
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	16
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	16
3	C	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	10	21
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	21
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (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%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	217/287 (76%)	209 (96%)	7 (3%)	1 (0%)	25	47
11	Y	217/287 (76%)	207 (95%)	9 (4%)	1 (0%)	25	47
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%)	222 (96%)	8 (4%)	1 (0%)	30	52
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	30	52
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6296/6764 (93%)	6123 (97%)	154 (2%)	19 (0%)	37	59

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP

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	207/209 (99%)	198 (96%)	9 (4%)	25	49
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	64
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	58
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	58
3	C	212/226 (94%)	201 (95%)	11 (5%)	19	41
3	Q	212/226 (94%)	201 (95%)	11 (5%)	19	41
4	D	194/215 (90%)	182 (94%)	12 (6%)	15	33
4	R	194/215 (90%)	182 (94%)	12 (6%)	15	33
5	E	190/193 (98%)	181 (95%)	9 (5%)	22	45
5	S	190/193 (98%)	182 (96%)	8 (4%)	25	50
6	F	201/239 (84%)	191 (95%)	10 (5%)	20	43
6	T	201/239 (84%)	193 (96%)	8 (4%)	27	52
7	G	206/210 (98%)	197 (96%)	9 (4%)	24	48
7	U	206/210 (98%)	197 (96%)	9 (4%)	24	48
8	H	185/190 (97%)	173 (94%)	12 (6%)	14	31
8	V	185/190 (97%)	172 (93%)	13 (7%)	12	27
9	I	172/173 (99%)	170 (99%)	2 (1%)	67	85
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	85
10	J	173/175 (99%)	161 (93%)	12 (7%)	13	28
10	X	173/175 (99%)	164 (95%)	9 (5%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	175/236 (74%)	164 (94%)	11 (6%)	15	32
11	Y	175/236 (74%)	162 (93%)	13 (7%)	11	24
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	60
12	Z	185/185 (100%)	178 (96%)	7 (4%)	28	54
13	M	199/208 (96%)	188 (94%)	11 (6%)	18	38
13	a	199/208 (96%)	191 (96%)	8 (4%)	27	52
14	N	162/162 (100%)	155 (96%)	7 (4%)	25	49
14	b	162/162 (100%)	155 (96%)	7 (4%)	25	49
All	All	5330/5674 (94%)	5082 (95%)	248 (5%)	22	45

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	161	ARG
11	Y	133	GLN
3	Q	50	LEU
11	Y	130	VAL
13	a	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	123	ASN
11	Y	85	ASN
7	U	30	ASN
8	V	57	GLN
12	Z	36	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
17	MES	H	301	-	12,12,12	0.71	0	14,16,16	0.46	0
17	MES	N	202	-	12,12,12	0.77	0	14,16,16	0.86	0
17	MES	V	302	-	12,12,12	0.71	0	14,16,16	0.48	0
17	MES	b	201	-	12,12,12	0.69	0	14,16,16	0.53	0
18	MPD	K	301	-	7,7,7	0.13	0	9,10,10	0.48	0
17	MES	Z	302	-	12,12,12	0.74	0	14,16,16	0.43	0
17	MES	U	302	-	12,12,12	0.76	0	14,16,16	0.48	0
18	MPD	a	301	-	7,7,7	0.12	0	9,10,10	0.41	0
17	MES	M	301	-	12,12,12	0.73	0	14,16,16	0.43	0
17	MES	G	303	-	12,12,12	0.77	0	14,16,16	0.43	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
17	MES	H	301	-	-	0/6/14/14	0/1/1/1
17	MES	N	202	-	-	0/6/14/14	0/1/1/1
17	MES	V	302	-	-	3/6/14/14	0/1/1/1
17	MES	b	201	-	-	3/6/14/14	0/1/1/1
18	MPD	K	301	-	-	1/5/5/5	-
17	MES	Z	302	-	-	1/6/14/14	0/1/1/1
17	MES	U	302	-	-	3/6/14/14	0/1/1/1
18	MPD	a	301	-	-	0/5/5/5	-
17	MES	M	301	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	G	303	-	-	2/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	G	303	MES	C8-C7-N4-C5
17	G	303	MES	N4-C7-C8-S
17	M	301	MES	C7-C8-S-O1S
17	V	302	MES	C7-C8-S-O2S
17	Z	302	MES	C8-C7-N4-C5

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	MES	1	0
17	N	202	MES	4	0
17	V	302	MES	1	0
17	b	201	MES	6	0
18	K	301	MPD	2	0
17	M	301	MES	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	248/250 (99%)	-0.63	2 (0%) 82 79	37, 48, 77, 115	0
1	O	250/250 (100%)	-0.56	3 (1%) 76 72	42, 55, 89, 118	0
2	B	244/258 (94%)	-0.44	3 (1%) 76 72	38, 53, 87, 137	0
2	P	244/258 (94%)	-0.50	3 (1%) 76 72	41, 55, 88, 134	0
3	C	240/254 (94%)	-0.46	2 (0%) 82 79	40, 56, 109, 126	0
3	Q	240/254 (94%)	-0.34	3 (1%) 74 70	46, 63, 130, 150	0
4	D	235/260 (90%)	-0.57	0 100 100	42, 56, 78, 105	0
4	R	235/260 (90%)	-0.56	1 (0%) 89 86	44, 59, 82, 113	0
5	E	231/234 (98%)	-0.55	0 100 100	43, 57, 85, 104	0
5	S	231/234 (98%)	-0.49	0 100 100	43, 63, 90, 110	0
6	F	243/288 (84%)	-0.58	0 100 100	37, 52, 87, 119	0
6	T	243/288 (84%)	-0.59	2 (0%) 82 79	42, 59, 97, 113	0
7	G	241/252 (95%)	-0.66	0 100 100	36, 48, 72, 108	0
7	U	241/252 (95%)	-0.56	0 100 100	41, 53, 76, 114	0
8	H	226/232 (97%)	-0.58	0 100 100	37, 46, 72, 130	0
8	V	226/232 (97%)	-0.58	1 (0%) 89 86	40, 50, 75, 136	0
9	I	204/205 (99%)	-0.83	0 100 100	36, 45, 64, 84	0
9	W	204/205 (99%)	-0.80	0 100 100	37, 47, 69, 88	0
10	J	195/198 (98%)	-0.55	1 (0%) 87 84	37, 56, 83, 117	0
10	X	195/198 (98%)	-0.66	0 100 100	40, 59, 82, 105	0
11	K	219/287 (76%)	-0.50	2 (0%) 81 77	38, 51, 84, 112	0
11	Y	219/287 (76%)	-0.54	2 (0%) 81 77	40, 51, 83, 103	0
12	L	222/222 (100%)	-0.79	0 100 100	36, 48, 69, 89	0
12	Z	222/222 (100%)	-0.77	0 100 100	37, 49, 69, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.75	2 (0%) 81 77	36, 46, 63, 74	0
13	a	233/246 (94%)	-0.73	1 (0%) 89 86	36, 47, 61, 75	0
14	N	196/196 (100%)	-0.70	1 (0%) 87 84	36, 43, 61, 97	0
14	b	196/196 (100%)	-0.63	2 (1%) 79 75	36, 45, 62, 99	0
All	All	6356/6764 (93%)	-0.60	31 (0%) 87 84	36, 52, 85, 150	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	4.4
1	O	2	THR	4.1
10	J	1	MET	4.0
3	Q	50	LEU	3.5
8	V	223	ILE	3.2

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(Å ²)	Q<0.9
15	MG	W	301	1/1	0.71	0.41	127,127,127,127	0
15	MG	N	201	1/1	0.78	0.16	50,50,50,50	0
17	MES	M	301	12/12	0.83	0.17	102,108,113,113	0
17	MES	V	302	12/12	0.85	0.16	74,95,99,108	0
15	MG	Z	301	1/1	0.88	0.26	127,127,127,127	0
17	MES	Z	302	12/12	0.88	0.13	74,80,95,97	0
18	MPD	a	301	8/8	0.89	0.12	69,75,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	MES	b	201	12/12	0.92	0.16	59,72,79,81	0
18	MPD	K	301	8/8	0.92	0.11	60,64,66,66	0
17	MES	H	301	12/12	0.92	0.12	73,88,94,95	0
17	MES	N	202	12/12	0.93	0.11	65,75,87,87	0
17	MES	G	303	12/12	0.93	0.13	70,86,104,105	0
17	MES	U	302	12/12	0.95	0.11	71,82,87,90	0
15	MG	V	301	1/1	0.96	0.17	89,89,89,89	0
15	MG	I	301	1/1	0.97	0.18	125,125,125,125	0
15	MG	G	301	1/1	0.98	0.10	63,63,63,63	0
16	CL	U	301	1/1	0.98	0.10	69,69,69,69	0
16	CL	G	302	1/1	0.99	0.06	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.