



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2025 – 11:16 am BST

PDB ID : 9QBE / pdb\_00009qbe  
Title : Yeast 20S proteasome mutant: beta5\_T3M in complex with ONX0914  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2025-03-02  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

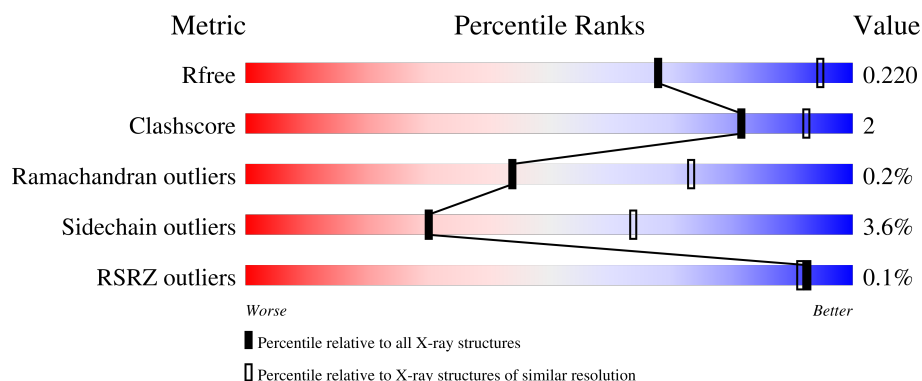
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






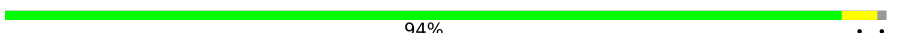














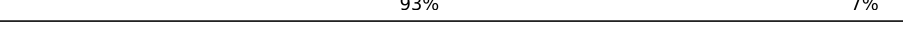






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 95% .
1	O	250	 95% 5%
2	B	258	 % 87% 7% . 5%
2	P	258	 89% 5% . 5%
3	C	254	 87% 5% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 89% . . 6%
4	D	260	 82% 8% 10%
4	R	260	 84% 6% 10%
5	E	234	 94% . .
5	S	234	 94% . .
6	F	288	 81% . . 16%
6	T	288	 81% . . 16%
7	G	252	 89% 6% .
7	U	252	 90% 6% .
8	H	231	 88% 6% . .
8	V	231	 88% 6% . .
9	I	205	 91% 8% .
9	W	205	 90% 8% .
10	J	198	 % 90% 6% . .
10	X	198	 % 89% 8% . .
11	K	211	 83% 15% .
11	Y	211	 82% 16% .
12	L	222	 93% 7%
12	Z	222	 91% 9%
13	M	246	 87% 6% . 5%
13	a	246	 87% 7% 5%
14	N	195	 91% 9%
14	b	195	 91% 9%
15	e	4	 50% 50%
15	f	4	 25% 50% 25%

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Mol	Chain	Length	Quality of chain
15	g	4	
15	h	4	
15	i	4	
15	j	4	

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	00E	e	1	-	-	X	-
15	0A1	e	3	-	-	X	-

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49833 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
			1638	1042	279	309	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1638	1042	279	309	8			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

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

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	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			
15	j	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	I	1	Total	Mg	0	0
			1	1		
16	K	2	Total	Mg	0	0
			2	2		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	X	1	Total	Mg	0	0
			1	1		
16	Y	2	Total	Mg	0	0
			2	2		
16	Z	1	Total	Mg	0	0
			1	1		

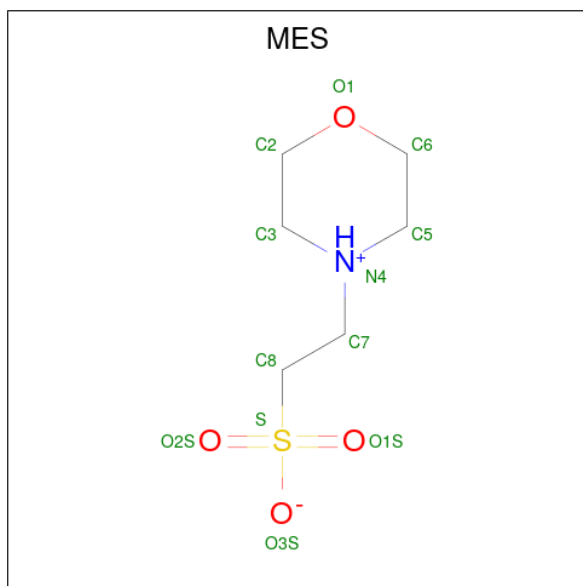
- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



(formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	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		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	7	Total	O	0	0
			7	7		
19	B	11	Total	O	0	0
			11	11		
19	C	8	Total	O	0	0
			8	8		
19	D	5	Total	O	0	0
			5	5		
19	E	6	Total	O	0	0
			6	6		
19	F	7	Total	O	0	0
			7	7		
19	G	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	H	11	Total O 11 11	0	0
19	I	4	Total O 4 4	0	0
19	J	15	Total O 15 15	0	0
19	K	5	Total O 5 5	0	0
19	L	12	Total O 12 12	0	0
19	M	13	Total O 13 13	0	0
19	N	8	Total O 8 8	0	0
19	O	5	Total O 5 5	0	0
19	P	7	Total O 7 7	0	0
19	Q	5	Total O 5 5	0	0
19	R	10	Total O 10 10	0	0
19	S	4	Total O 4 4	0	0
19	T	6	Total O 6 6	0	0
19	U	12	Total O 12 12	0	0
19	V	8	Total O 8 8	0	0
19	W	3	Total O 3 3	0	0
19	X	9	Total O 9 9	0	0
19	Y	2	Total O 2 2	0	0
19	Z	7	Total O 7 7	0	0
19	a	8	Total O 8 8	0	0
19	b	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	g	2	Total	O	0	0
			2	2		
19	j	2	Total	O	0	0
			2	2		

### 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:  95%




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95%




- Molecule 2: Proteasome subunit alpha type-3

Chain B:  87%




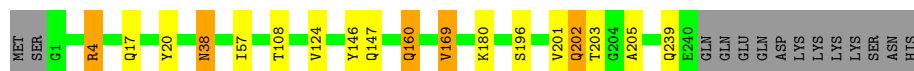
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  89%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87%



- Molecule 3: Proteasome subunit alpha type-4

MET	SER	G1	R4	F9	N38	L50	T108	V146	Q147	Q160	V169	K180	S196	V201	Q202	T203	G204	A205	Q239	Q240	GLN	GLN	GLU	GLN	GLN	ASP	LYS	LYS	LYS	LYS	LYS	LYS	ASN	HS
-----	-----	----	----	----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----

- |     |      |      |
|-----|------|------|
| GLU | GLU  | MET  |
| GLU | PHE  | L20  |
| ALA | LEU  | R24  |
| ASP | THR  | L40  |
| VAL | ARG  | L51  |
| GLU | SER  | V60  |
| MET | GLU  | A88  |
| SER | TYR  | H91  |
|     | D1   | I99  |
|     | R2   | L104 |
|     | L20  | L113 |
|     | R24  | E117 |
|     | L40  | GLY  |
|     | L51  | ALA  |
|     | V60  | SER  |
|     | A88  | GLY  |
|     | H91  | GLU  |
|     | I99  | GLU  |
|     | L104 | ARG  |
|     | L113 | L125 |
|     | E117 | N160 |
|     | GLY  | S166 |
|     | ALA  | L176 |
|     | SER  | W179 |
|     | GLY  | L193 |
|     | GLU  | K197 |
|     | GLU  | T214 |
|     | ARG  | K236 |
|     | L125 | E242 |
|     | N160 | SER  |
|     | S166 |      |
|     | L176 |      |
|     | W179 |      |
|     | L193 |      |
|     | K197 |      |
|     | T214 |      |
|     | K236 |      |
|     | E242 |      |
|     | SER  |      |


- |     |     |     |     |     |     |     |     |     |    |     |     |     |     |     |     |     |      |      |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | MET | PHE | LEU | THR | ARG | SER | GLU | TYR | D1 | Q15 | L20 | L40 | L51 | V60 | A88 | I99 | L104 | E117 | GLY | ALA | SER | GLY | GLU | GLU | ARG | L125 | N160 | L176 | W179 | L193 | K197 | T214 | K236 | E242 | SER | PRO | GLU | GLU | ALA | ASP | VAL | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|

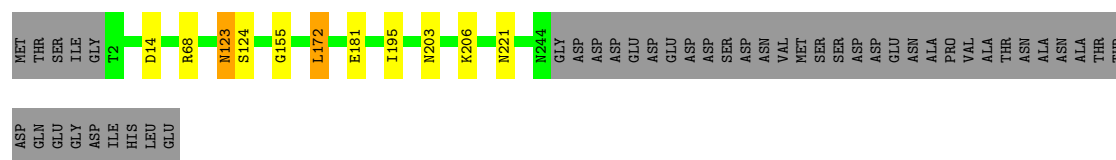
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- | Amino Acid | Percentage |
|------------|------------|
| MET        | 10%        |
| PHE        | 10%        |
| ARG        | 10%        |
| N3         | 10%        |
| T9         | 10%        |
| L25        | 10%        |
| K29        | 10%        |
| E54        | 10%        |
| L71        | 10%        |
| A77        | 10%        |
| P78        | 10%        |
| L87        | 10%        |
| F98        | 10%        |
| A107       | 10%        |
| L188       | 10%        |
| I233       | 10%        |

- 
- | Protein | Number of Amino Acids |
|---------|-----------------------|
| MET     | 10                    |
| PHE     | 10                    |
| ARG     | 10                    |
| N3      | 10                    |
| T9      | 10                    |
| L25     | 10                    |
| K29     | 10                    |
| E54     | 10                    |
| L71     | 10                    |
| A77     | 10                    |
| P78     | 10                    |
| L87     | 10                    |
| F98     | 10                    |
| A107    | 10                    |
| L188    | 10                    |
| I233    | 10                    |


- |     |      |
|-----|------|
| GLU | MET  |
| GLY | THR  |
| ASP | SER  |
| ILE | ILE  |
| HIS | GLY  |
| LEU | T2   |
| GLU | R68  |
|     | N123 |
|     | S124 |
|     | G158 |
|     | L172 |
|     | E181 |
|     | I195 |
|     | N203 |
|     | K206 |
|     | N221 |
|     | N244 |
|     | GLY  |
|     | ASP  |
|     | ASP  |
|     | ASP  |
|     | GLU  |
|     | ASP  |
|     | GLU  |
|     | ASP  |
|     | ASP  |
|     | SER  |
|     | ASP  |
|     | ASN  |
|     | ASN  |
|     | VAL  |
|     | MET  |
|     | SER  |
|     | SER  |
|     | ASP  |
|     | ASP  |
|     | GLU  |
|     | ASN  |
|     | ALA  |
|     | PRO  |
|     | VAL  |
|     | ALA  |
|     | THR  |
|     | ASN  |
|     | ALA  |
|     | ASN  |
|     | ALA  |
|     | THR  |
|     | THR  |
|     | ASP  |

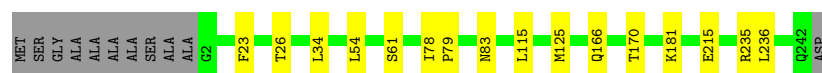
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Chain T:  81% 16%



- Molecule 7: Proteasome subunit alpha type-1

Chain G:  89% 6%



- Molecule 7: Proteasome subunit alpha type-1

Chain U:  90% 6%




- Molecule 8: Proteasome subunit beta type-2

Chain H:  88% 6%




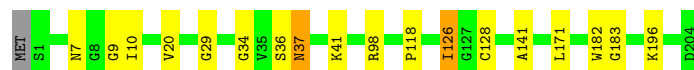
- Molecule 8: Proteasome subunit beta type-2

Chain V:  88% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  91% 8%

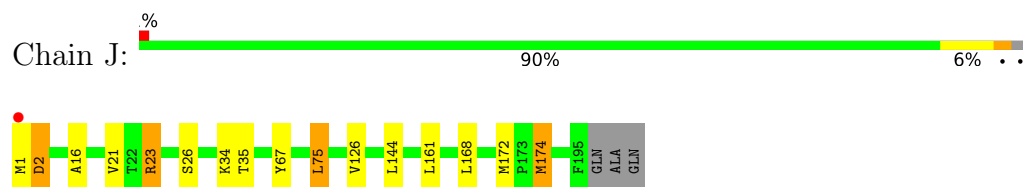


- Molecule 9: Proteasome subunit beta type-3

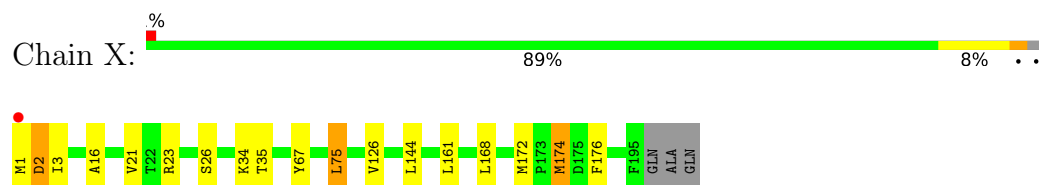
Chain W:  90% 8%



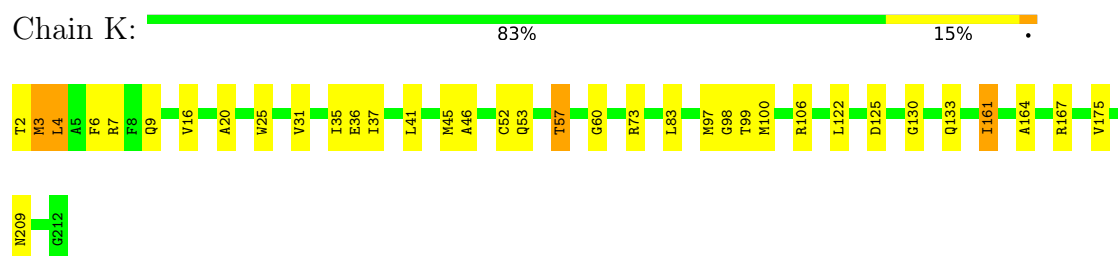
- Molecule 10: Proteasome subunit beta type-4



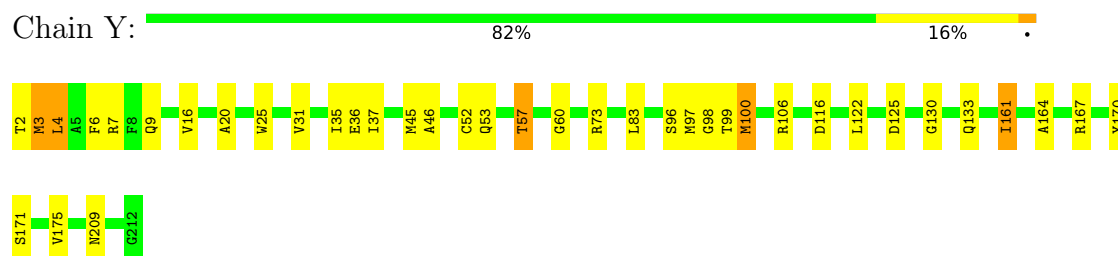
- Molecule 10: Proteasome subunit beta type-4



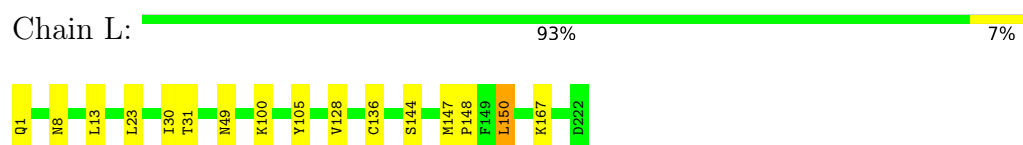
- Molecule 11: Proteasome subunit beta type-5



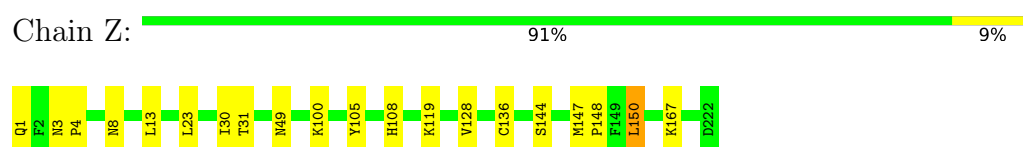
- Molecule 11: Proteasome subunit beta type-5




- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6




- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 6% • 5%




- Molecule 13: Proteasome subunit beta type-7

Chain a:  87% 7% 5%




- Molecule 14: Proteasome subunit beta type-1

Chain N:  91% 9%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  91% 9%

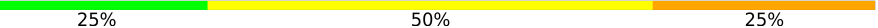


- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain e:  50% 50%



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

Chain f:  25% 50% 25%




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

Chain g:  25% 25% 50%



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



Chain h:  25% 25% 50%



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

Chain i:  25% 50% 25%



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

Chain j:  25% 50% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.08Å 299.85Å 145.33Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (15.00-2.80) 94.7 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.175 , 0.211 0.172 , 0.220	Depositor DCC
$R_{free}$ test set	12407 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	49833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1I44, MES, 0A1, 00E, MG, CL

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	1.00	0/1952	1.39	0/2642
1	O	1.01	0/1952	1.40	0/2642
2	B	1.00	0/1934	1.40	1/2618 (0.0%)
2	P	1.01	0/1934	1.41	0/2618
3	C	1.00	0/1910	1.43	0/2586
3	Q	1.01	0/1910	1.43	0/2586
4	D	1.01	0/1837	1.42	2/2475 (0.1%)
4	R	1.01	0/1837	1.43	0/2475
5	E	1.01	0/1800	1.41	0/2433
5	S	1.01	0/1800	1.40	0/2433
6	F	0.99	0/1932	1.41	0/2609
6	T	1.00	0/1932	1.41	0/2609
7	G	0.99	0/1945	1.38	0/2634
7	U	0.99	0/1945	1.39	0/2634
8	H	1.00	0/1708	1.36	0/2316
8	V	1.00	0/1708	1.37	0/2316
9	I	0.97	0/1611	1.37	1/2174 (0.0%)
9	W	0.98	0/1611	1.38	1/2174 (0.0%)
10	J	0.98	0/1589	1.38	0/2142
10	X	0.98	0/1589	1.38	0/2142
11	K	0.97	0/1675	1.42	0/2264
11	Y	0.98	0/1675	1.41	0/2264
12	L	0.96	0/1795	1.35	0/2420
12	Z	0.97	0/1795	1.36	2/2420 (0.1%)
13	M	0.98	0/1855	1.37	3/2514 (0.1%)
13	a	0.98	0/1855	1.36	1/2514 (0.0%)
14	N	0.97	0/1534	1.38	0/2077
14	b	0.98	0/1534	1.38	0/2077
15	e	0.95	0/4	1.22	0/4
15	f	0.42	0/4	0.85	0/4
15	g	0.62	0/4	1.22	0/4
15	h	0.65	0/4	1.18	0/4

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	i	0.61	0/4	1.25	0/4
15	j	1.06	0/4	1.83	0/4
All	All	0.99	0/50178	1.39	11/67832 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	N-CA-C	7.04	118.75	111.14
13	M	35	ARG	N-CA-C	6.78	118.32	111.07
9	W	183	GLY	CA-C-O	-5.99	118.33	122.22
9	I	183	GLY	CA-C-O	-5.84	118.42	122.22
12	Z	119	LYS	CA-C-N	5.52	125.22	119.92

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	6	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	5	0
8	H	1677	0	1678	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1677	0	1678	9	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	12	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	11	0
11	K	1638	0	1587	29	0
11	Y	1638	0	1587	30	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	8	0
14	N	1505	0	1471	9	0
14	b	1505	0	1471	11	0
15	e	49	0	25	6	0
15	f	49	0	25	5	0
15	g	49	0	25	3	0
15	h	49	0	25	2	0
15	i	49	0	25	8	0
15	j	49	0	25	3	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	2	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	X	1	0	0	0	0
16	Y	2	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	H	12	0	13	0	0
18	K	12	0	13	4	0
18	Y	12	0	13	3	0
18	h	12	0	13	1	0
19	A	7	0	0	0	0
19	B	11	0	0	0	0
19	C	8	0	0	0	0
19	D	5	0	0	0	0
19	E	6	0	0	0	0
19	F	7	0	0	0	0
19	G	12	0	0	0	0
19	H	11	0	0	0	0
19	I	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	15	0	0	0	0
19	K	5	0	0	0	0
19	L	12	0	0	0	0
19	M	13	0	0	1	0
19	N	8	0	0	0	0
19	O	5	0	0	0	0
19	P	7	0	0	0	0
19	Q	5	0	0	0	0
19	R	10	0	0	0	0
19	S	4	0	0	0	0
19	T	6	0	0	0	0
19	U	12	0	0	0	0
19	V	8	0	0	0	0
19	W	3	0	0	0	0
19	X	9	0	0	0	0
19	Y	2	0	0	0	0
19	Z	7	0	0	1	0
19	a	8	0	0	0	0
19	b	9	0	0	0	0
19	g	2	0	0	0	0
19	j	2	0	0	0	0
All	All	49833	0	49214	234	0

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

The worst 5 of 234 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)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.49	0.78
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.49	0.77
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.65	0.77
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.66	0.75
15:e:1:00E:HD1A	15:e:3:0A1:CE2	2.21	0.71

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%)	240 (97%)	8 (3%)	0	100	100
1	O	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	61
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	61
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	32
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	10	32
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (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
8	H	219/231 (95%)	216 (99%)	2 (1%)	1 (0%)	25	56
8	V	219/231 (95%)	216 (99%)	2 (1%)	1 (0%)	25	56
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%)	190 (98%)	2 (1%)	1 (0%)	25	56
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	25	56
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	61
14	N	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
14	b	193/195 (99%)	186 (96%)	7 (4%)	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
15	j	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6276/6632 (95%)	6095 (97%)	167 (3%)	14 (0%)	44	73

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN

### 5.3.2 Protein sidechains [i](#)

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%)	44	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	44	77
2	B	203/216 (94%)	194 (96%)	9 (4%)	24	56
2	P	203/216 (94%)	194 (96%)	9 (4%)	24	56
3	C	212/226 (94%)	205 (97%)	7 (3%)	33	67
3	Q	212/226 (94%)	205 (97%)	7 (3%)	33	67
4	D	194/215 (90%)	182 (94%)	12 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	194/215 (90%)	182 (94%)	12 (6%)	15	43
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	68
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	68
6	F	201/239 (84%)	194 (96%)	7 (4%)	31	65
6	T	201/239 (84%)	193 (96%)	8 (4%)	27	60
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	66
8	H	180/189 (95%)	175 (97%)	5 (3%)	38	72
8	V	180/189 (95%)	174 (97%)	6 (3%)	33	67
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	78
9	W	172/173 (99%)	168 (98%)	4 (2%)	45	78
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	71
11	K	168/168 (100%)	157 (94%)	11 (6%)	14	40
11	Y	168/168 (100%)	157 (94%)	11 (6%)	14	40
12	L	185/185 (100%)	177 (96%)	8 (4%)	25	57
12	Z	185/185 (100%)	177 (96%)	8 (4%)	25	57
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	75
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	75
14	N	161/161 (100%)	157 (98%)	4 (2%)	42	75
14	b	161/161 (100%)	158 (98%)	3 (2%)	52	82
All	All	5306/5534 (96%)	5115 (96%)	191 (4%)	30	64

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	203	THR
7	U	115	LEU
4	R	60	VAL
5	S	29	LYS
8	V	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	167	GLN
13	a	102	GLN
8	V	86	HIS
10	X	146	HIS
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	g	1	15	9,9,10	0.65	0	10,10,12	1.91	4 (40%)
15	00E	h	1	15	9,9,10	0.67	0	10,10,12	1.40	1 (10%)
15	0A1	j	3	15	12,13,14	1.74	1 (8%)	13,16,18	1.15	2 (15%)
15	0A1	f	3	15	12,13,14	1.88	1 (8%)	13,16,18	1.71	2 (15%)
15	00E	f	1	15	9,9,10	0.59	0	10,10,12	1.10	0
15	0A1	g	3	15	12,13,14	1.62	1 (8%)	13,16,18	1.03	1 (7%)
15	00E	j	1	15	9,9,10	0.81	0	10,10,12	1.62	1 (10%)
15	00E	e	1	15	9,9,10	0.59	0	10,10,12	1.43	1 (10%)
15	0A1	h	3	15	12,13,14	1.77	1 (8%)	13,16,18	1.51	2 (15%)
15	0A1	e	3	15	12,13,14	1.80	1 (8%)	13,16,18	1.56	1 (7%)
15	0A1	i	3	15	12,13,14	1.66	1 (8%)	13,16,18	1.28	1 (7%)
15	00E	i	1	15	9,9,10	0.45	0	10,10,12	0.90	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	g	1	15	-	2/2/11/12	0/1/1/1
15	00E	h	1	15	-	1/2/11/12	0/1/1/1
15	0A1	j	3	15	-	2/7/8/10	0/1/1/1
15	0A1	f	3	15	-	4/7/8/10	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1
15	0A1	g	3	15	-	2/7/8/10	0/1/1/1
15	00E	j	1	15	-	2/2/11/12	0/1/1/1
15	00E	e	1	15	-	2/2/11/12	0/1/1/1
15	0A1	h	3	15	-	4/7/8/10	0/1/1/1
15	0A1	e	3	15	-	4/7/8/10	0/1/1/1
15	0A1	i	3	15	-	4/7/8/10	0/1/1/1
15	00E	i	1	15	-	0/2/11/12	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	3	0A1	CB-CG	-6.14	1.36	1.51
15	e	3	0A1	CB-CG	-5.79	1.37	1.51
15	j	3	0A1	CB-CG	-5.76	1.37	1.51
15	h	3	0A1	CB-CG	-5.72	1.37	1.51
15	i	3	0A1	CB-CG	-5.49	1.38	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	3	0A1	CM-OH-CZ	-5.12	106.39	117.51
15	h	3	0A1	CM-OH-CZ	-4.76	107.18	117.51
15	f	3	0A1	CM-OH-CZ	-4.24	108.32	117.51
15	f	3	0A1	CG-CB-CA	-3.68	106.65	114.10
15	i	3	0A1	CM-OH-CZ	-3.60	109.70	117.51

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	1	00E	C-CA-NB-CD1
15	g	1	00E	C-CA-NB-CD1
15	g	1	00E	C-CA-NB-CD2
15	j	1	00E	C-CA-NB-CD1
15	j	1	00E	C-CA-NB-CD2

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	g	1	00E	1	0
15	h	1	00E	1	0
15	j	3	0A1	1	0
15	f	3	0A1	3	0
15	g	3	0A1	2	0
15	e	1	00E	6	0
15	h	3	0A1	1	0
15	e	3	0A1	6	0
15	i	3	0A1	3	0
15	i	1	00E	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	H	301	-	12,12,12	0.71	0	14,16,16	0.42	0
18	MES	K	303	-	12,12,12	0.73	0	14,16,16	0.39	0
18	MES	h	101	-	12,12,12	0.75	0	14,16,16	0.39	0
18	MES	Y	303	-	12,12,12	0.74	0	14,16,16	0.35	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	H	301	-	-	3/6/14/14	0/1/1/1
18	MES	K	303	-	-	5/6/14/14	0/1/1/1
18	MES	h	101	-	-	1/6/14/14	0/1/1/1
18	MES	Y	303	-	-	1/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	303	MES	N4-C7-C8-S
18	Y	303	MES	N4-C7-C8-S
18	h	101	MES	N4-C7-C8-S
18	K	303	MES	C7-C8-S-O3S
18	H	301	MES	C7-C8-S-O3S

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	303	MES	4	0
18	h	101	MES	1	0
18	Y	303	MES	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-1.00	1 (0%) 89 85	56, 72, 102, 161	0
1	O	250/250 (100%)	-0.96	0 100 100	60, 80, 115, 170	0
2	B	244/258 (94%)	-0.88	2 (0%) 82 77	58, 77, 123, 169	0
2	P	244/258 (94%)	-0.88	0 100 100	61, 82, 122, 158	0
3	C	240/254 (94%)	-0.92	0 100 100	60, 84, 141, 158	0
3	Q	240/254 (94%)	-0.86	1 (0%) 89 85	65, 93, 154, 177	0
4	D	235/260 (90%)	-0.96	0 100 100	65, 84, 111, 140	0
4	R	235/260 (90%)	-0.94	0 100 100	62, 86, 117, 143	0
5	E	231/234 (98%)	-0.87	0 100 100	65, 86, 118, 145	0
5	S	231/234 (98%)	-0.81	0 100 100	66, 90, 126, 148	0
6	F	243/288 (84%)	-0.96	0 100 100	56, 78, 117, 145	0
6	T	243/288 (84%)	-0.93	0 100 100	57, 83, 126, 147	0
7	G	241/252 (95%)	-1.01	0 100 100	52, 70, 106, 150	0
7	U	241/252 (95%)	-1.04	0 100 100	58, 73, 103, 127	0
8	H	221/231 (95%)	-0.99	0 100 100	56, 71, 103, 130	0
8	V	221/231 (95%)	-0.96	0 100 100	59, 73, 103, 135	0
9	I	204/205 (99%)	-1.04	0 100 100	55, 73, 99, 121	0
9	W	204/205 (99%)	-1.05	0 100 100	58, 76, 105, 128	0
10	J	195/198 (98%)	-1.02	1 (0%) 87 83	54, 72, 98, 135	0
10	X	195/198 (98%)	-1.04	1 (0%) 87 83	59, 75, 97, 157	0
11	K	211/211 (100%)	-0.81	0 100 100	67, 83, 110, 127	0
11	Y	211/211 (100%)	-0.78	0 100 100	66, 83, 112, 135	0
12	L	222/222 (100%)	-0.93	0 100 100	61, 78, 118, 138	0
12	Z	222/222 (100%)	-0.89	0 100 100	59, 76, 110, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.98	0 100 100	56, 72, 108, 124	0
13	a	233/246 (94%)	-1.00	1 (0%) 89 85	54, 71, 102, 131	0
14	N	195/195 (100%)	-1.06	0 100 100	56, 66, 94, 117	0
14	b	195/195 (100%)	-1.01	0 100 100	53, 67, 93, 116	0
15	e	1/4 (25%)	0.75	0 100 100	80, 80, 80, 80	0
15	f	1/4 (25%)	0.75	0 100 100	100, 100, 100, 100	0
15	g	1/4 (25%)	0.70	0 100 100	93, 93, 93, 93	0
15	h	1/4 (25%)	1.01	0 100 100	85, 85, 85, 85	0
15	i	1/4 (25%)	0.61	0 100 100	111, 111, 111, 111	0
15	j	1/4 (25%)	-0.11	0 100 100	91, 91, 91, 91	0
All	All	6336/6632 (95%)	-0.95	7 (0%) 92 91	52, 78, 117, 177	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	a	1	THR	2.5
10	X	1	MET	2.4
3	Q	50	LEU	2.3
2	B	219	ALA	2.2
2	B	51	VAL	2.2

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	00E	i	1	9/10	0.78	0.13	109,111,117,117	0
15	0A1	f	3	13/14	0.80	0.12	93,97,106,109	0
15	00E	e	1	9/10	0.89	0.10	92,110,113,114	0
15	0A1	e	3	13/14	0.89	0.10	78,82,86,89	0
15	00E	h	1	9/10	0.89	0.09	92,102,105,107	0
15	0A1	j	3	13/14	0.89	0.11	83,87,99,100	0
15	0A1	i	3	13/14	0.90	0.08	99,102,107,110	0
15	0A1	h	3	13/14	0.90	0.09	77,83,88,88	0
15	00E	g	1	9/10	0.91	0.10	97,114,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	00E	j	1	9/10	0.92	0.12	90,118,127,127	0
15	00E	f	1	9/10	0.92	0.11	100,108,112,115	0
15	0A1	g	3	13/14	0.93	0.08	81,86,91,92	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, 95<sup>th</sup> 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
18	MES	K	303	12/12	0.89	0.11	104,107,113,118	0
18	MES	h	101	12/12	0.93	0.09	109,112,119,119	0
18	MES	Y	303	12/12	0.94	0.10	100,109,114,117	0
18	MES	H	301	12/12	0.94	0.09	99,107,111,112	0
16	MG	Z	301	1/1	0.95	0.07	86,86,86,86	0
16	MG	I	301	1/1	0.96	0.12	83,83,83,83	0
16	MG	Y	302	1/1	0.97	0.11	69,69,69,69	0
16	MG	Y	301	1/1	0.97	0.04	80,80,80,80	0
16	MG	K	302	1/1	0.98	0.15	63,63,63,63	0
16	MG	G	301	1/1	0.98	0.04	70,70,70,70	0
17	CL	G	302	1/1	0.99	0.06	57,57,57,57	0
17	CL	U	301	1/1	0.99	0.06	62,62,62,62	0
16	MG	X	201	1/1	0.99	0.08	53,53,53,53	0
16	MG	K	301	1/1	0.99	0.06	80,80,80,80	0
16	MG	N	201	1/1	0.99	0.03	63,63,63,63	0
16	MG	V	301	1/1	0.99	0.06	97,97,97,97	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.