



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 9QBW / pdb_00009qbw
Title : Yeast 20S proteasome mutant: beta5_G128V (b5-propeptide in trans) in complex with Carfilzomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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

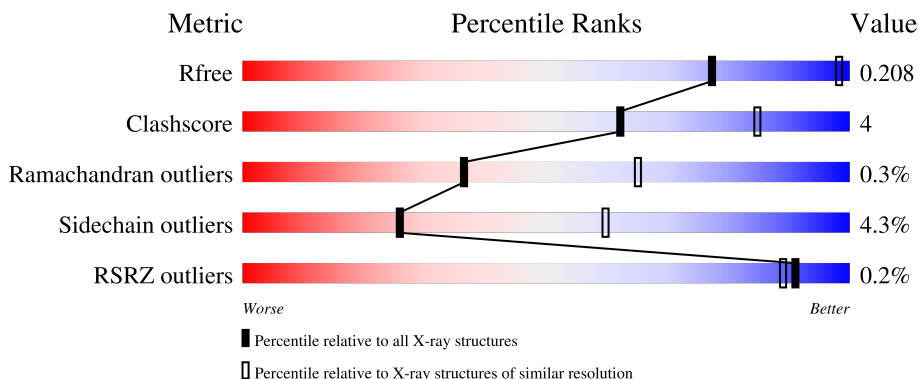
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div style="width: 96%;">96%</div> <div style="width: 96%; background-color: #00FF00;">96%</div> <div style="width: 96%; background-color: #FF0000;">.</div> </div>
1	O	250	<div> <div style="width: 96%;">96%</div> <div style="width: 96%; background-color: #00FF00;">96%</div> <div style="width: 96%; background-color: #FF0000;">.</div> </div>
2	B	258	<div> <div style="width: 86%;">86%</div> <div style="width: 86%; background-color: #00FF00;">86%</div> <div style="width: 86%; background-color: #FF0000;">7%</div> <div style="width: 86%; background-color: #FFA500;">5%</div> <div style="width: 86%; background-color: #808080;">.</div> </div>
2	P	258	<div> <div style="width: 86%;">86%</div> <div style="width: 86%; background-color: #00FF00;">86%</div> <div style="width: 86%; background-color: #FF0000;">7%</div> <div style="width: 86%; background-color: #FFA500;">5%</div> <div style="width: 86%; background-color: #808080;">.</div> </div>
3	C	254	<div> <div style="width: 87%;">87%</div> <div style="width: 87%; background-color: #00FF00;">87%</div> <div style="width: 87%; background-color: #FF0000;">6%</div> <div style="width: 87%; background-color: #FFA500;">6%</div> <div style="width: 87%; background-color: #808080;">.</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	254	87% 5% • 6%
4	D	260	85% 5% • 10%
4	R	260	85% 5% 10%
5	E	234	93% • •
5	S	234	93% 5% •
6	F	288	% 80% • • 16%
6	T	288	79% 5% • 16%
7	G	252	88% 7% • •
7	U	252	86% 9% • •
8	H	231	84% 11% • •
8	V	231	86% 10% • •
9	I	205	87% 11% •
9	W	205	87% 12% •
10	J	198	81% 15% • •
10	X	198	81% 15% • •
11	K	211	74% 21% 5%
11	Y	211	76% 19% 5%
12	L	222	% 75% 22% •
12	Z	222	78% 19% •
13	M	246	85% 9% • 5%
13	a	246	86% 8% • 5%
14	N	195	88% 10% •
14	b	195	89% 9% •
15	f	5	60% 40%
15	g	5	40% 40% 20%

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Mol	Chain	Length	Quality of chain
15	h	5	
15	i	5	
15	j	5	
15	k	5	

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
20	SO4	U	302	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 49952 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	130	VAL	GLY	engineered mutation	UNP P30656
Y	130	VAL	GLY	engineered mutation	UNP P30656

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	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	f	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	g	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	h	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	i	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	j	5	Total	C	N	O	0	0	0
			59	44	6	9			
15	k	5	Total	C	N	O	0	0	0
			59	44	6	9			

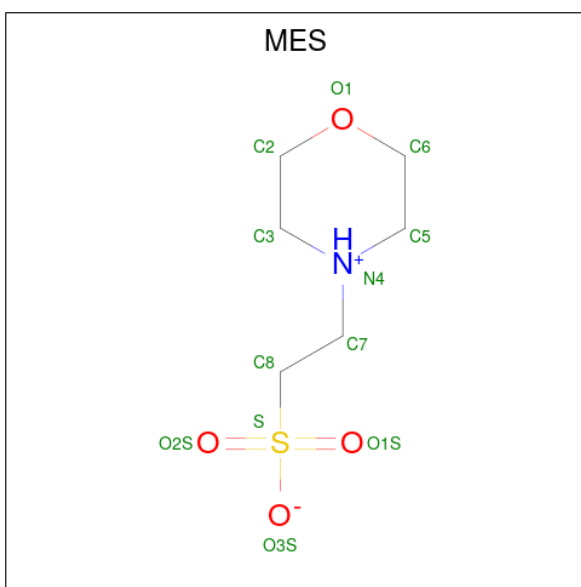
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

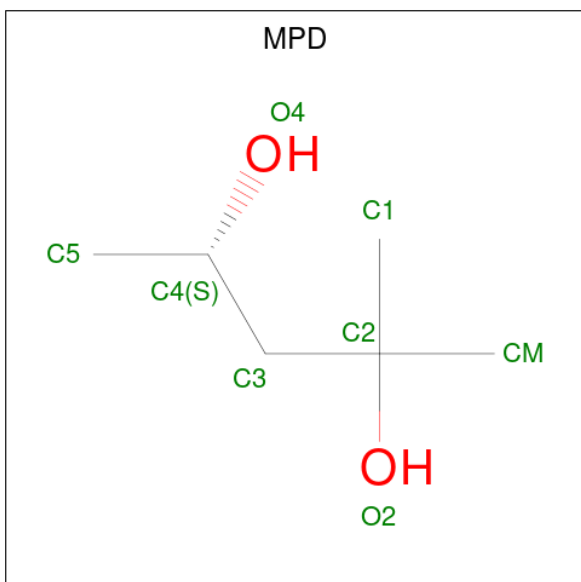
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		
17	b	1	Total	Cl	0	0
			1	1		

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



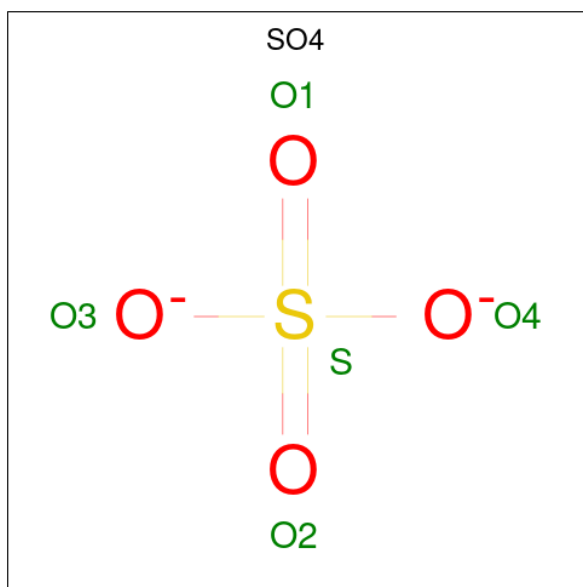
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	L	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	i	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



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

- Molecule 20 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	U	1	Total	O	S	0	0
			5	4	1		

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	4	Total	O	0	0
			4	4		
21	B	6	Total	O	0	0
			6	6		
21	C	2	Total	O	0	0
			2	2		
21	D	5	Total	O	0	0
			5	5		
21	E	5	Total	O	0	0
			5	5		
21	F	6	Total	O	0	0
			6	6		
21	G	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	H	8	Total O 8 8	0	0
21	I	5	Total O 5 5	0	0
21	J	5	Total O 5 5	0	0
21	K	5	Total O 5 5	0	0
21	L	9	Total O 9 9	0	0
21	M	5	Total O 5 5	0	0
21	N	7	Total O 7 7	0	0
21	O	2	Total O 2 2	0	0
21	P	8	Total O 8 8	0	0
21	Q	4	Total O 4 4	0	0
21	R	5	Total O 5 5	0	0
21	S	5	Total O 5 5	0	0
21	T	3	Total O 3 3	0	0
21	U	14	Total O 14 14	0	0
21	V	8	Total O 8 8	0	0
21	W	4	Total O 4 4	0	0
21	X	5	Total O 5 5	0	0
21	Y	7	Total O 7 7	0	0
21	Z	11	Total O 11 11	0	0
21	a	17	Total O 17 17	0	0
21	b	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	h	2	Total	O	0	0
			2	2		
21	k	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:  96% .




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  96% .



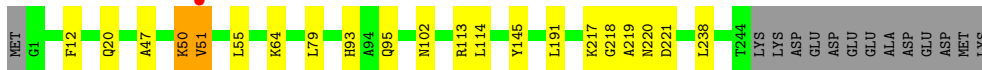
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  86% 7% • 5%




- Molecule 2: Proteasome subunit alpha type-3

Chain P:  86% 7% • 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% • 6%



- Molecule 3: Proteasome subunit alpha type-4



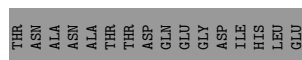
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | Phe | Leu | Thr | Arg | Ser | Glu | Tyr | D1 | Q15 | V60 | A88 | H91 | E97 | D98 | I99 | E117 | GLY | ALA | SER | GLY | GLY | GLU | GLU | ARG | L125 | M160 | L176 | M179 | L193 | I214 | L235 | K236 | E242 | SER | PRO | GLU | GLU | ASP | ASP | VAL | GLU | MET |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | PHE | LEU | THR | ARG | SER | GLU | TYR | D1 | Q15 | V60 | A88 | H91 | I99 | E117 | GLY | ALA | SER | GLY | GLU | GLU | ARG | L125 | N160 | L176 | W179 | L193 | I214 | L235 | K236 | E242 | PRO | GLU | GLU | ALA | ASP | VAL | GLU | MET |
|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|

-
- | Amino Acid | Percentage (%) |
|------------|----------------|
| MET | 10 |
| PHE | 10 |
| ARG | 10 |
| N3 | 5 |
| T9 | 10 |
| F12 | 10 |
| K29 | 10 |
| L55 | 10 |
| L71 | 10 |
| A77 | 10 |
| P78 | 10 |
| L87 | 10 |
| N92 | 10 |
| A107 | 10 |
| N118 | 10 |
| L188 | 10 |
| K231 | 10 |
| T232 | 10 |
| T233 | 10 |

- | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| Met | Phe | Arg | N3 | T9 | F12 | K29 | V35 | L55 | L71 | A77 | P78 | L87 | N92 | A107 | N118 | L188 | K231 | Y232 | I233 |
|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|


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|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | THR | SER | ILE | GLY | T2 | Q19 | R68 | T78 | P79 | S94 | M23 | S124 | G158 | E171 | L172 | E181 | E201 | D202 | C215 | N221 | Q240 | T244 | GLY | ASP | ASP | ASP | ASP | GLU | GLU | ASP | ASP | ASP | ASP | ASN | VAL | MET | SER | SER | ASP | ASP | ASP | ASN | ALA | PRO | VAL |
|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



- | MET |
|------|
| TMR |
| SER |
| IIE |
| GLY |
| T2 |
| Q19 |
| R68 |
| L78 |
| P79 |
| S94 |
| M23 |
| S124 |
| G155 |
| G158 |
| E171 |
| L172 |
| E181 |
| E201 |
| N221 |
| Q240 |
| N244 |
| GLY |
| ASP |
| ASP |
| ASP |
| GLU |
| GLU |
| GLU |
| ASP |
| ASP |
| ASP |
| SER |
| ASN |
| VAL |
| MET |
| SER |
| SER |
| ASP |
| ASP |
| GLU |
| ALA |
| ALA |
| PRO |
| VAL |
| ALA |


ASN
ALA
ASN
GLY
ALA
THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

• Molecule 7: Proteasome subunit alpha type-1

Chain G:  88% 7% . .


MET SER GLY ALA ALA THR ASP GLN SER ALA ALA G2 E13 F23 T26 L34 L54 C65 I78 P79 N83 N114 L115 R122 M125 K165 Q166 Q167 T171 L205 E208 R235 L236 Q242 ASP

• Molecule 7: Proteasome subunit alpha type-1

Chain U:  86% 9% . .

MET SER GLY ALA ALA THR ASP GLN SER ALA ALA G2 P12 E13 F23 T26 L34 L54 T59 F64 C65 I78 P79 N83 N114 L115 R122 M125 A159 K165 Q166 Q167 T171 L205 E208 R235 L236 Q242 ASP

• Molecule 8: Proteasome subunit beta type-2

Chain H:  84% 11% . .

T2 K7 V13 R19 Q22 L34 S38 P39 V55 L68 K84 L98 D104 P105 L110 F111 S112 I113 S118 L125 S126 L127 G128 V137 L138 E139 A161 G162 I163 W164 N165 D166 L167 G170 R196 T210 L213 K214 E215 S216


E226 GLN VAL ASP ILE THR ALA

• Molecule 8: Proteasome subunit beta type-2

Chain V:  86% 10% . .

T2 K7 V13 Q22 L34 R35 R36 I37 S38 P39 V55 L68 L80 K84 L98 L113 S118 S126 L127 V137 L138 E139 A161 G162 I163 W164 N165 G170 R196 T210 L213 E226 GLN VAL ASP ILE THR ALA

• Molecule 9: Proteasome subunit beta type-3

Chain I:  87% 11% .


MET S1 N7 G8 G9 I10 V20 G29 G34 N37 K41 D58 L62 N71 V104 P118 F123 C128 A141 S151 S167 L171 D177 G183 R197 Y198 L199 K200 R201 R202 Q203 D204

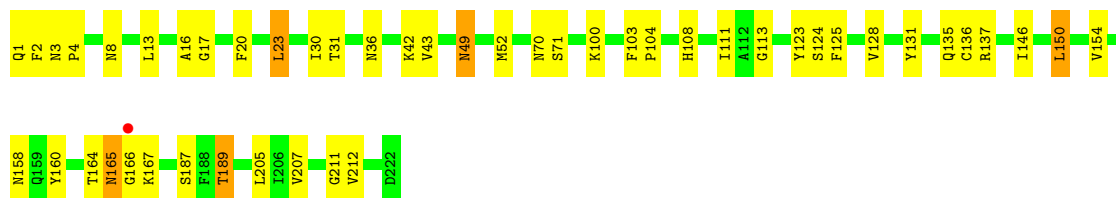
• Molecule 9: Proteasome subunit beta type-3

Chain W:  87% 12% .


MET S1 N7 G8 G9 I10 V20 G29 G34 N37 K41 D58 L62 N71 V104 P118 F123 C128 A141 G147 S151 S167 L171 D177 G183 Y198 L199 K200 W201 R202 Q203 D204

• Molecule 10: Proteasome subunit beta type-4

Chain Z:  78% 19%




- Molecule 13: Proteasome subunit beta type-7

Chain M:  85% 9% 5%




- Molecule 13: Proteasome subunit beta type-7

Chain a:  86% 8% 5%




- Molecule 14: Proteasome subunit beta type-1

Chain N:  88% 10%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  89% 9%



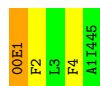
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZOLE

Chain f:  60% 40%

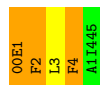


- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZOLE

Chain g:  40% 40% 20%



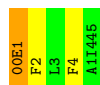
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



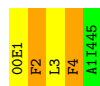
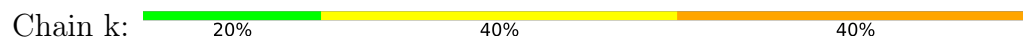
- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.00Å 300.83Å 145.58Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.90) 96.9 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.171 , 0.207 0.175 , 0.208	Depositor DCC
R_{free} test set	11542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49952	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, SO4, CL, MES, A1I44, MG, HPE, 00E

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	1.01	0/1952	1.42	0/2642
1	O	1.02	0/1952	1.43	0/2642
2	B	1.02	0/1934	1.44	0/2618
2	P	1.02	0/1934	1.44	0/2618
3	C	1.02	0/1910	1.47	0/2586
3	Q	1.02	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.49	0/2475
4	R	1.03	0/1837	1.49	0/2475
5	E	1.03	0/1800	1.45	0/2433
5	S	1.03	0/1800	1.46	2/2433 (0.1%)
6	F	1.01	0/1932	1.45	0/2609
6	T	1.01	0/1932	1.45	0/2609
7	G	1.00	0/1945	1.42	0/2634
7	U	1.01	0/1945	1.43	0/2634
8	H	1.01	0/1743	1.42	0/2363
8	V	1.01	0/1743	1.43	0/2363
9	I	1.01	0/1611	1.43	1/2174 (0.0%)
9	W	1.01	0/1611	1.43	1/2174 (0.0%)
10	J	0.98	0/1589	1.42	0/2142
10	X	0.99	0/1589	1.41	0/2142
11	K	0.98	0/1677	1.41	0/2269
11	Y	0.97	0/1677	1.42	0/2269
12	L	0.98	0/1795	1.41	0/2420
12	Z	0.98	0/1795	1.40	0/2420
13	M	1.01	0/1855	1.40	0/2514
13	a	1.00	0/1855	1.38	0/2514
14	N	1.00	0/1534	1.41	1/2077 (0.0%)
14	b	1.00	0/1534	1.43	0/2077
15	f	1.15	0/19	1.19	0/24
15	g	1.27	1/19 (5.3%)	1.62	1/24 (4.2%)
15	h	1.32	1/19 (5.3%)	1.00	0/24
15	i	1.12	0/19	1.20	0/24

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	j	1.22	0/19	1.55	1/24 (4.2%)
15	k	1.40	1/19 (5.3%)	1.10	0/24
All	All	1.01	3/50342 (0.0%)	1.43	7/68056 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	k	4	PHE	CB-CG	-5.50	1.38	1.50
15	h	4	PHE	CB-CG	-5.26	1.38	1.50
15	g	4	PHE	CB-CG	-5.06	1.39	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	4	PHE	CA-CB-CG	-6.93	106.87	113.80
15	j	4	PHE	CA-CB-CG	-6.58	107.22	113.80
9	W	183	GLY	CA-C-O	-5.68	118.53	122.22
9	I	183	GLY	CA-C-O	-5.63	118.56	122.22
14	N	128	GLY	CA-C-O	-5.09	118.50	122.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	4	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	13	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	12	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1773	0	1775	11	0
6	F	1892	0	1883	8	0
6	T	1892	0	1883	7	0
7	G	1907	0	1901	14	0
7	U	1907	0	1901	16	0
8	H	1712	0	1709	23	0
8	V	1712	0	1709	14	0
9	I	1581	0	1574	26	0
9	W	1581	0	1574	21	0
10	J	1561	0	1569	28	0
10	X	1561	0	1569	26	0
11	K	1640	0	1591	41	0
11	Y	1640	0	1591	42	0
12	L	1757	0	1711	43	0
12	Z	1757	0	1711	39	0
13	M	1824	0	1832	14	0
13	a	1824	0	1832	16	0
14	N	1505	0	1471	16	0
14	b	1505	0	1471	15	0
15	f	59	0	40	0	0
15	g	59	0	40	2	0
15	h	59	0	40	5	0
15	i	59	0	40	0	0
15	j	59	0	40	2	0
15	k	59	0	40	4	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	1	0
18	G	12	0	13	2	0
18	H	12	0	13	1	0
18	L	12	0	13	2	0
18	a	12	0	13	0	0
18	i	12	0	13	0	0
19	K	8	0	14	0	0
19	a	8	0	14	0	0
20	U	5	0	0	3	0
21	A	4	0	0	0	0
21	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	2	0	0	0	0
21	D	5	0	0	0	0
21	E	5	0	0	0	0
21	F	6	0	0	0	0
21	G	7	0	0	0	0
21	H	8	0	0	0	0
21	I	5	0	0	0	0
21	J	5	0	0	0	0
21	K	5	0	0	0	0
21	L	9	0	0	0	0
21	M	5	0	0	0	0
21	N	7	0	0	0	0
21	O	2	0	0	0	0
21	P	8	0	0	0	0
21	Q	4	0	0	0	0
21	R	5	0	0	0	0
21	S	5	0	0	0	0
21	T	3	0	0	0	0
21	U	14	0	0	0	0
21	V	8	0	0	0	0
21	W	4	0	0	0	0
21	X	5	0	0	0	0
21	Y	7	0	0	0	0
21	Z	11	0	0	0	0
21	a	17	0	0	1	0
21	b	4	0	0	0	0
21	h	2	0	0	0	0
21	k	2	0	0	0	0
All	All	49952	0	49415	408	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 408 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)
15:h:2:HPE:HE2	15:h:4:PHE:CZ	1.92	1.04
15:k:2:HPE:HE2	15:k:4:PHE:CZ	1.93	1.03
12:L:158:ASN:HD22	9:W:171:LEU:HB3	1.26	1.00
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.34	0.92
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.34	0.92

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%)	240 (97%)	7 (3%)	1 (0%)	30	59
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	59
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	26
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	26
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	16	44
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%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	223/231 (96%)	219 (98%)	4 (2%)	0	100	100
8	V	223/231 (96%)	219 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	192 (100%)	1 (0%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	209/211 (99%)	198 (95%)	7 (3%)	4 (2%)	6	23
11	Y	209/211 (99%)	198 (95%)	8 (4%)	3 (1%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	225 (97%)	6 (3%)	0	100	100
13	a	231/246 (94%)	225 (97%)	6 (3%)	0	100	100
14	N	193/195 (99%)	190 (98%)	3 (2%)	0	100	100
14	b	193/195 (99%)	190 (98%)	3 (2%)	0	100	100
15	f	1/5 (20%)	1 (100%)	0	0	100	100
15	g	1/5 (20%)	1 (100%)	0	0	100	100
15	h	1/5 (20%)	1 (100%)	0	0	100	100
15	i	1/5 (20%)	1 (100%)	0	0	100	100
15	j	1/5 (20%)	1 (100%)	0	0	100	100
15	k	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6284/6638 (95%)	6124 (98%)	139 (2%)	21 (0%)	36	65

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
11	K	207	PHE
11	K	210	VAL

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%)	203 (97%)	6 (3%)	37	71
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	75
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	204 (96%)	8 (4%)	29	64
3	Q	212/226 (94%)	204 (96%)	8 (4%)	29	64
4	D	194/215 (90%)	186 (96%)	8 (4%)	27	61
4	R	194/215 (90%)	186 (96%)	8 (4%)	27	61
5	E	190/193 (98%)	183 (96%)	7 (4%)	30	64
5	S	190/193 (98%)	183 (96%)	7 (4%)	30	64
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	58
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	58
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	184/189 (97%)	172 (94%)	12 (6%)	15	44
8	V	184/189 (97%)	170 (92%)	14 (8%)	12	36
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	82
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	82
10	J	173/175 (99%)	165 (95%)	8 (5%)	24	57
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	52
11	K	169/169 (100%)	154 (91%)	15 (9%)	9	28
11	Y	169/169 (100%)	156 (92%)	13 (8%)	12	35
12	L	185/185 (100%)	173 (94%)	12 (6%)	15	44
12	Z	185/185 (100%)	175 (95%)	10 (5%)	20	51
13	M	199/208 (96%)	192 (96%)	7 (4%)	32	66
13	a	199/208 (96%)	193 (97%)	6 (3%)	36	70
14	N	161/161 (100%)	156 (97%)	5 (3%)	35	69
14	b	161/161 (100%)	156 (97%)	5 (3%)	35	69
15	f	2/2 (100%)	2 (100%)	0	100	100
15	g	2/2 (100%)	2 (100%)	0	100	100
15	h	2/2 (100%)	2 (100%)	0	100	100
15	i	2/2 (100%)	2 (100%)	0	100	100
15	j	2/2 (100%)	2 (100%)	0	100	100
15	k	2/2 (100%)	2 (100%)	0	100	100
All	All	5328/5548 (96%)	5101 (96%)	227 (4%)	26	60

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	1	MET
13	a	187	ARG
5	S	29	LYS
13	a	70	LEU
11	Y	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
4	R	225	ASN
8	V	66	HIS
5	S	116	GLN
6	T	240	GLN
9	W	88	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	j	1	15	9,9,10	0.70	0	10,10,12	1.09	1 (10%)
15	HPE	g	2	15	11,12,13	1.42	1 (9%)	9,14,16	0.75	0
15	HPE	j	2	15	11,12,13	1.46	1 (9%)	9,14,16	0.76	0
15	00E	g	1	15	9,9,10	0.69	0	10,10,12	1.18	1 (10%)
15	HPE	h	2	15	11,12,13	1.32	1 (9%)	9,14,16	1.78	3 (33%)
15	HPE	f	2	15	11,12,13	1.36	1 (9%)	9,14,16	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	00E	f	1	15	9,9,10	0.72	0	10,10,12	1.18	1 (10%)
15	HPE	k	2	15	11,12,13	1.28	1 (9%)	9,14,16	1.67	3 (33%)
15	HPE	i	2	15	11,12,13	1.32	1 (9%)	9,14,16	0.45	0
15	00E	k	1	15	9,9,10	0.72	0	10,10,12	3.95	5 (50%)
15	00E	i	1	15	9,9,10	0.77	0	10,10,12	1.10	1 (10%)
15	00E	h	1	15	9,9,10	0.65	0	10,10,12	4.59	6 (60%)

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	j	1	15	-	1/2/11/12	0/1/1/1
15	HPE	g	2	15	-	0/6/7/9	0/1/1/1
15	HPE	j	2	15	-	0/6/7/9	0/1/1/1
15	00E	g	1	15	-	1/2/11/12	0/1/1/1
15	HPE	h	2	15	-	4/6/7/9	0/1/1/1
15	HPE	f	2	15	-	2/6/7/9	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1
15	HPE	k	2	15	-	4/6/7/9	0/1/1/1
15	HPE	i	2	15	-	2/6/7/9	0/1/1/1
15	00E	k	1	15	-	1/2/11/12	0/1/1/1
15	00E	i	1	15	-	0/2/11/12	0/1/1/1
15	00E	h	1	15	-	1/2/11/12	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	j	2	HPE	CG-CD	-4.48	1.39	1.51
15	g	2	HPE	CG-CD	-4.40	1.39	1.51
15	f	2	HPE	CG-CD	-3.97	1.40	1.51
15	i	2	HPE	CG-CD	-3.83	1.40	1.51
15	h	2	HPE	CG-CD	-3.77	1.41	1.51

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	k	1	00E	CD2-NB-CD1	9.81	129.98	108.84
15	h	1	00E	CD2-NB-CD1	9.61	129.55	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	1	00E	CA-NB-CD2	7.17	117.97	110.49
15	h	1	00E	CE2-OZ-CE1	5.54	127.79	109.88
15	k	1	00E	CE2-OZ-CE1	5.32	127.10	109.88

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	h	1	00E	C-CA-NB-CD1
15	k	1	00E	C-CA-NB-CD1
15	h	2	HPE	N-CA-CB-CG
15	h	2	HPE	C-CA-CB-CG
15	k	2	HPE	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	j	1	00E	2	0
15	g	1	00E	2	0
15	h	2	HPE	2	0
15	k	2	HPE	2	0
15	h	1	00E	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	SO4	U	302	-	4,4,4	0.55	0	6,6,6	0.21	0
18	MES	H	301	-	12,12,12	0.73	0	15,16,16	0.42	0
19	MPD	K	301	-	7,7,7	0.14	0	9,10,10	0.43	0
18	MES	a	301	-	12,12,12	0.71	0	15,16,16	0.35	0
18	MES	i	101	-	12,12,12	0.82	0	15,16,16	0.46	0
18	MES	G	303	-	12,12,12	0.77	0	15,16,16	0.37	0
19	MPD	a	302	-	7,7,7	0.13	0	9,10,10	0.32	0
18	MES	L	301	-	12,12,12	0.70	0	15,16,16	0.42	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	-	-	0/6/14/14	0/1/1/1
19	MPD	K	301	-	-	2/5/5/5	-
18	MES	a	301	-	-	0/6/14/14	0/1/1/1
18	MES	i	101	-	-	0/6/14/14	0/1/1/1
18	MES	G	303	-	-	1/6/14/14	0/1/1/1
19	MPD	a	302	-	-	1/5/5/5	-
18	MES	L	301	-	-	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 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	L	301	MES	C8-C7-N4-C5
19	K	301	MPD	C2-C3-C4-O4
19	K	301	MPD	C2-C3-C4-C5
18	G	303	MES	N4-C7-C8-S
18	L	301	MES	N4-C7-C8-S

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	U	302	SO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	H	301	MES	1	0
18	G	303	MES	2	0
18	L	301	MES	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.62	0 100 100	47, 62, 94, 131	0
1	O	250/250 (100%)	-0.60	0 100 100	50, 70, 104, 148	0
2	B	244/258 (94%)	-0.47	1 (0%) 88 85	50, 67, 112, 152	0
2	P	244/258 (94%)	-0.45	1 (0%) 88 85	51, 71, 114, 155	0
3	C	240/254 (94%)	-0.50	1 (0%) 88 85	48, 72, 134, 151	0
3	Q	240/254 (94%)	-0.45	1 (0%) 88 85	54, 81, 146, 158	0
4	D	235/260 (90%)	-0.59	0 100 100	54, 74, 101, 130	0
4	R	235/260 (90%)	-0.51	0 100 100	54, 75, 106, 124	0
5	E	231/234 (98%)	-0.53	0 100 100	54, 76, 109, 135	0
5	S	231/234 (98%)	-0.47	0 100 100	58, 81, 116, 137	0
6	F	243/288 (84%)	-0.51	2 (0%) 82 77	47, 68, 108, 133	0
6	T	243/288 (84%)	-0.53	0 100 100	50, 73, 120, 136	0
7	G	241/252 (95%)	-0.62	0 100 100	44, 61, 94, 143	0
7	U	241/252 (95%)	-0.60	0 100 100	49, 63, 96, 128	0
8	H	225/231 (97%)	-0.60	1 (0%) 88 85	45, 57, 91, 132	0
8	V	225/231 (97%)	-0.56	0 100 100	48, 60, 94, 151	0
9	I	204/205 (99%)	-0.64	0 100 100	45, 61, 86, 113	0
9	W	204/205 (99%)	-0.67	0 100 100	46, 63, 94, 116	0
10	J	195/198 (98%)	-0.57	0 100 100	45, 67, 99, 130	0
10	X	195/198 (98%)	-0.59	0 100 100	51, 69, 96, 132	0
11	K	211/211 (100%)	-0.45	0 100 100	50, 70, 115, 130	0
11	Y	211/211 (100%)	-0.44	0 100 100	51, 70, 112, 131	0
12	L	222/222 (100%)	-0.60	2 (0%) 81 75	48, 63, 100, 120	0
12	Z	222/222 (100%)	-0.64	1 (0%) 87 83	46, 62, 94, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.70	0 100 100	44, 58, 82, 90	0
13	a	233/246 (94%)	-0.71	1 (0%) 88 85	43, 56, 78, 91	0
14	N	195/195 (100%)	-0.71	0 100 100	43, 54, 80, 104	0
14	b	195/195 (100%)	-0.74	0 100 100	44, 55, 86, 105	0
15	f	2/5 (40%)	-0.89	0 100 100	56, 56, 56, 58	0
15	g	2/5 (40%)	-0.27	0 100 100	57, 57, 57, 61	0
15	h	2/5 (40%)	-0.70	0 100 100	48, 48, 48, 52	0
15	i	2/5 (40%)	-0.31	0 100 100	63, 63, 63, 63	0
15	j	2/5 (40%)	-0.55	0 100 100	59, 59, 59, 65	0
15	k	2/5 (40%)	-0.65	0 100 100	48, 48, 48, 53	0
All	All	6350/6638 (95%)	-0.57	11 (0%) 91 89	43, 66, 108, 158	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	3.5
6	F	215	CYS	2.9
13	a	1	THR	2.8
2	P	51	VAL	2.4
2	B	218	GLY	2.4

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	00E	h	1	9/10	0.60	0.16	95,121,135,137	0
15	00E	k	1	9/10	0.62	0.16	88,122,128,130	0
15	00E	i	1	9/10	0.81	0.14	76,109,118,119	0
15	00E	j	1	9/10	0.83	0.13	82,105,112,114	0
15	00E	f	1	9/10	0.84	0.13	76,102,110,112	0
15	HPE	h	2	12/13	0.84	0.17	65,85,103,105	0
15	00E	g	1	9/10	0.87	0.11	84,108,114,116	0
15	HPE	j	2	12/13	0.89	0.10	71,74,76,79	0
15	HPE	k	2	12/13	0.89	0.14	60,80,99,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	HPE	g	2	12/13	0.92	0.09	67,71,75,81	0
15	HPE	i	2	12/13	0.96	0.07	65,71,73,73	0
15	HPE	f	2	12/13	0.97	0.06	64,71,77,78	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(\AA^2)	Q<0.9
16	MG	W	301	1/1	0.79	0.23	128,128,128,128	0
18	MES	L	301	12/12	0.80	0.16	120,143,147,151	0
19	MPD	a	302	8/8	0.84	0.16	100,117,120,125	0
18	MES	i	101	12/12	0.86	0.39	54,59,71,75	12
18	MES	H	301	12/12	0.86	0.36	56,63,80,81	12
18	MES	G	303	12/12	0.89	0.12	81,121,138,139	0
18	MES	a	301	12/12	0.89	0.13	125,130,134,134	0
19	MPD	K	301	8/8	0.92	0.14	80,88,90,93	0
20	SO4	U	302	5/5	0.93	0.41	20,20,20,20	0
17	CL	b	201	1/1	0.97	0.28	30,30,30,30	0
17	CL	G	302	1/1	0.97	0.06	57,57,57,57	0
17	CL	U	301	1/1	0.97	0.06	59,59,59,59	0
16	MG	N	201	1/1	0.98	0.09	71,71,71,71	0
17	CL	N	202	1/1	0.98	0.22	30,30,30,30	0
16	MG	G	301	1/1	0.99	0.03	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.