



wwPDB X-ray Structure Validation Summary Report

Apr 23, 2024 – 10:10 pm BST

PDB ID : 8RHL
Title : Yeast 20S proteasome in complex with a linear biarylether epoxyketone (compound 15a)
Authors : Goetz, M.G.; Godwin, K.; Price, R.; Dorn, R.; Merrill-Steskal, G.; Hansen, H.; Klemmer, W.; Produturi, G.; Rocha, M.; Palmer, M.; Molacek, L.; Strater, Z.; Groll, M.
Deposited on : 2023-12-15
Resolution : 3.20 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

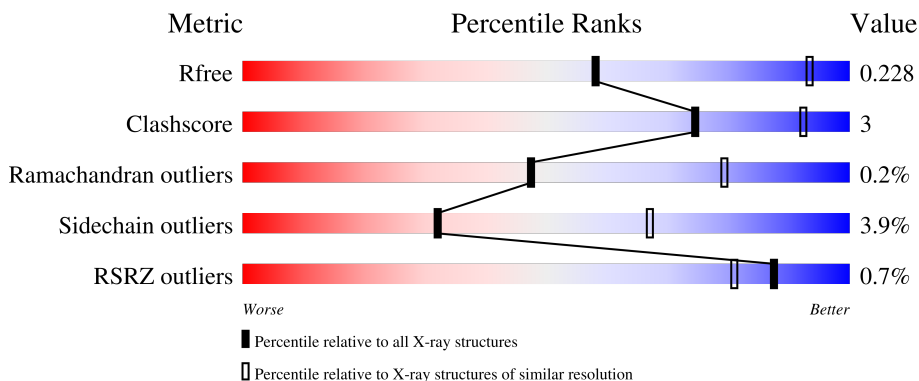
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.








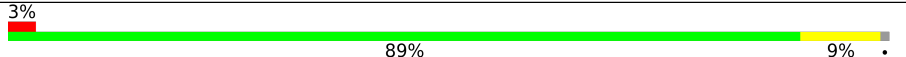

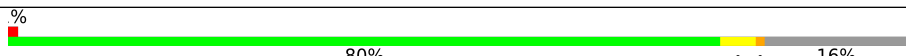


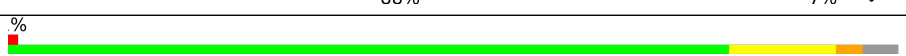


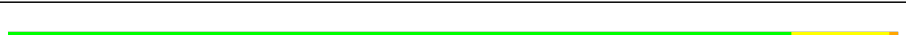
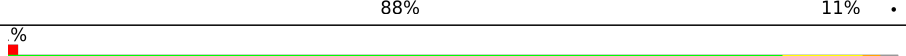
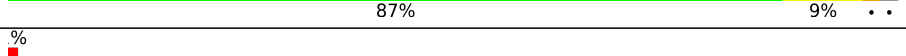
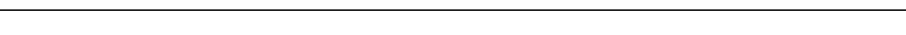

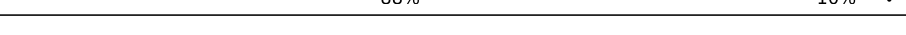
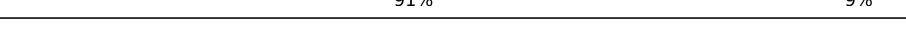
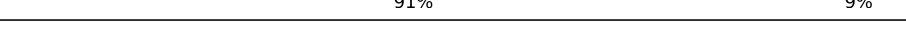
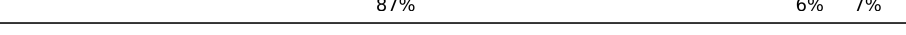


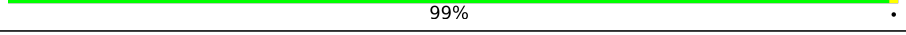
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

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



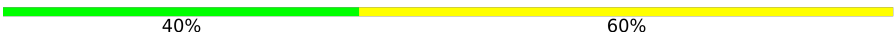
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Mol	Chain	Length	Quality of chain
3	C	254	 87% 6% • 6%
3	Q	254	 4% 87% 5% • 6%
4	D	260	 84% 6% 10%
4	R	260	 84% 6% 10%
5	E	234	 89% 9% •
5	S	234	 3% 89% 9% •
6	F	288	 78% 5% • 16%
6	T	288	 1% 80% • • 16%
7	G	252	 89% 6% •
7	U	252	 88% 7% •
8	H	232	 1% 81% 12% • •
8	V	232	 1% 81% 12% • •
9	I	205	 88% 10% •
9	W	205	 88% 11% •
10	J	198	 1% 87% 9% • •
10	X	198	 1% 88% 9% • •
11	K	212	 89% 10% •
11	Y	212	 88% 10% •
12	L	222	 91% 9%
12	Z	222	 91% 9%
13	M	246	 87% 6% 7%
13	a	246	 91% • 7%
14	N	196	 91% 8% •
14	b	196	 99% •
15	e	5	 40% 60%

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Mol	Chain	Length	Quality of chain	
15	f	5	 40%	60%
15	g	5	 40%	60%
15	h	5	 40%	60%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49514 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
			Total	C	N	O	S			
1	A	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0
1	O	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	Total 1684	C 1061	N 293	O 323	S 7	0	0	0
8	V	222	Total 1684	C 1061	N 293	O 323	S 7	0	0	0

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

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

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

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

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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	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	229	Total	C	N	O	S	0	0	0
			1790	1133	306	344	7			
13	a	229	Total	C	N	O	S	0	0	0
			1790	1133	306	344	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 a protein called Linear biarylether epoxyketone.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	0	0	0
			49	35	5	9			
15	f	5	Total	C	N	O	0	0	0
			49	35	5	9			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	g	5	Total	C	N	O	0	0	0
			49	35	5	9			
15	h	5	Total	C	N	O	0	0	0
			49	35	5	9			

- Molecule 16 is MAGNESIUM ION (three-letter code: 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	1	Total	Mg	0	0
			1	1		
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	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (three-letter code: 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 (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			1	1		
19	B	2	Total	O	0	0
			2	2		
19	C	2	Total	O	0	0
			2	2		
19	D	1	Total	O	0	0
			1	1		
19	F	1	Total	O	0	0
			1	1		
19	G	1	Total	O	0	0
			1	1		
19	H	1	Total	O	0	0
			1	1		
19	J	5	Total	O	0	0
			5	5		
19	K	2	Total	O	0	0
			2	2		
19	L	3	Total	O	0	0
			3	3		
19	M	9	Total	O	0	0
			9	9		

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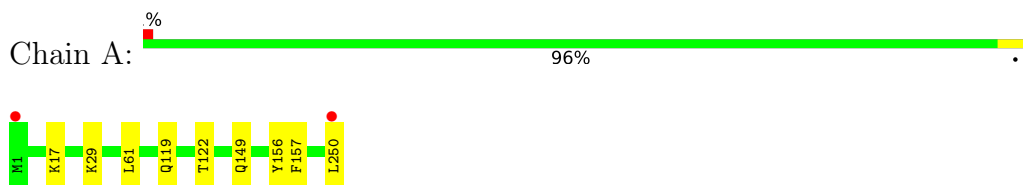
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	N	6	Total O 6 6	0	0
19	O	1	Total O 1 1	0	0
19	P	2	Total O 2 2	0	0
19	Q	5	Total O 5 5	0	0
19	R	1	Total O 1 1	0	0
19	S	2	Total O 2 2	0	0
19	U	2	Total O 2 2	0	0
19	V	2	Total O 2 2	0	0
19	W	2	Total O 2 2	0	0
19	X	5	Total O 5 5	0	0
19	Z	1	Total O 1 1	0	0
19	a	5	Total O 5 5	0	0
19	b	2	Total O 2 2	0	0
19	e	1	Total O 1 1	0	0
19	f	1	Total O 1 1	0	0
19	g	1	Total O 1 1	0	0
19	h	1	Total O 1 1	0	0

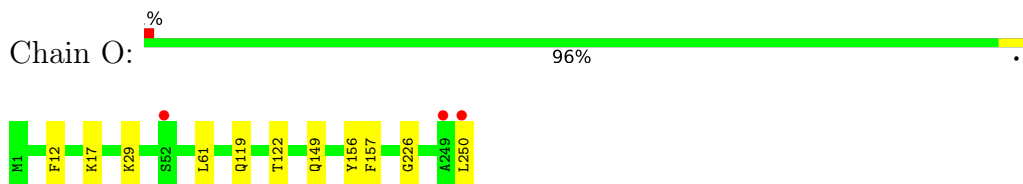
3 Residue-property plots [i](#)

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.

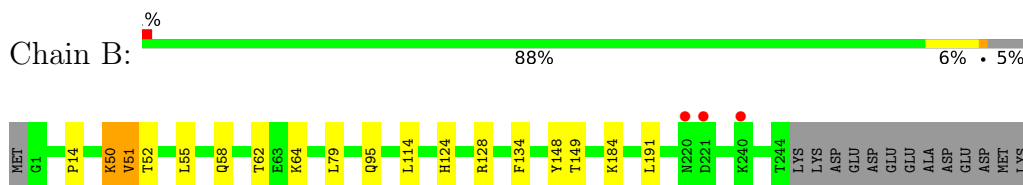
- Molecule 1: Proteasome subunit alpha type-2



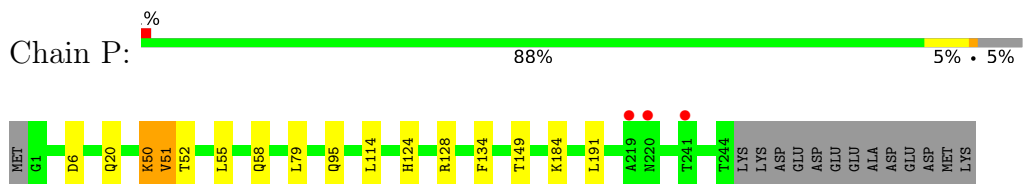
- Molecule 1: Proteasome subunit alpha type-2



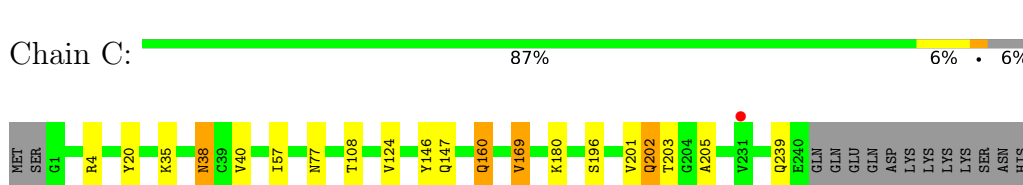
- Molecule 2: Proteasome subunit alpha type-3



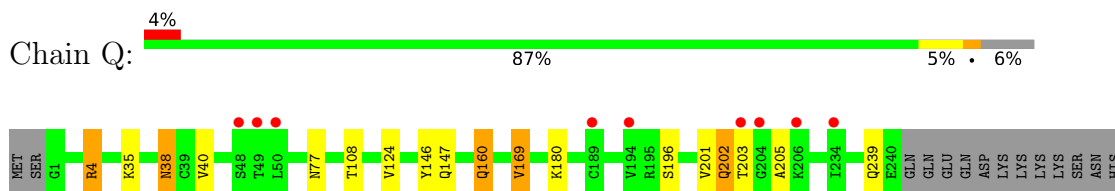
- Molecule 2: Proteasome subunit alpha type-3



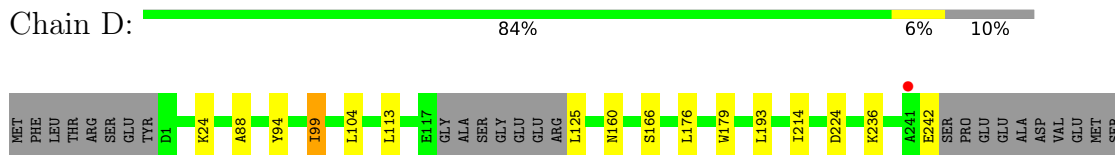
- Molecule 3: Proteasome subunit alpha type-4



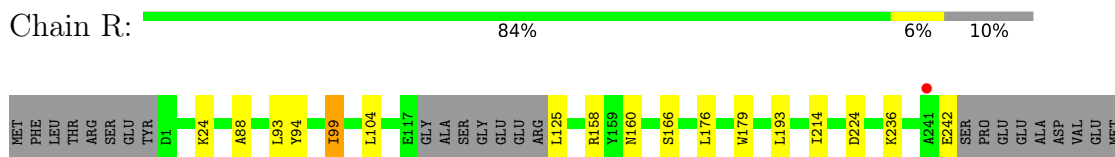
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5

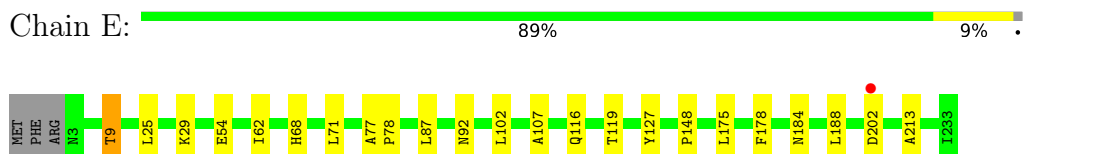


- Molecule 4: Proteasome subunit alpha type-5

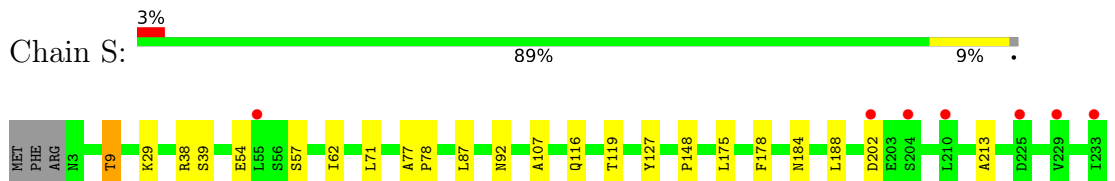


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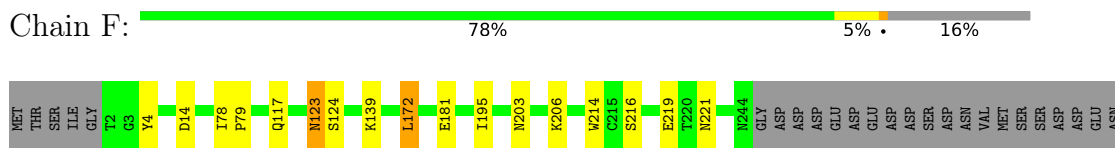
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

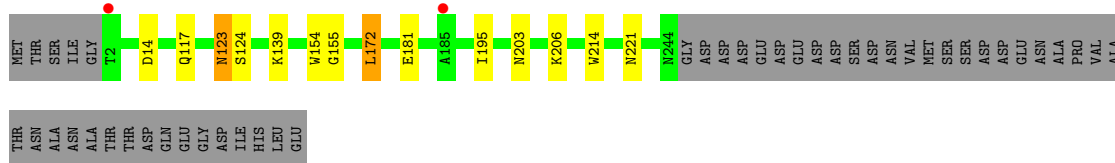
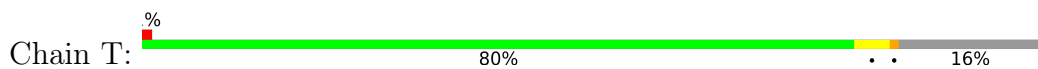


- Molecule 6: Probable proteasome subunit alpha type-7

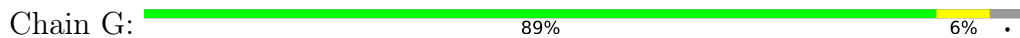


ALA
PRO
VAL
ALA
THR
ASN
ASN
ALA
ALA
THR
THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

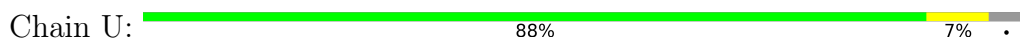
- Molecule 6: Probable proteasome subunit alpha type-7



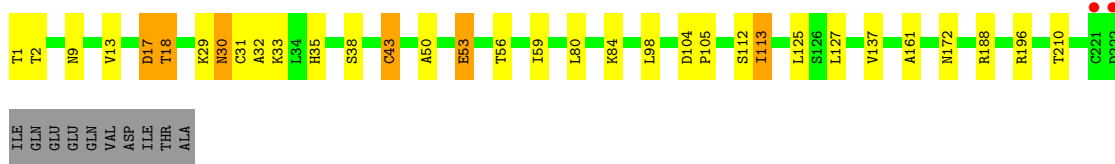
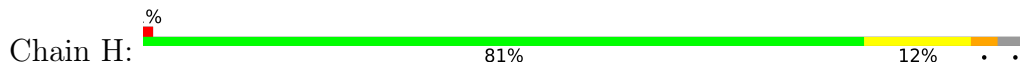
- Molecule 7: Proteasome subunit alpha type-1



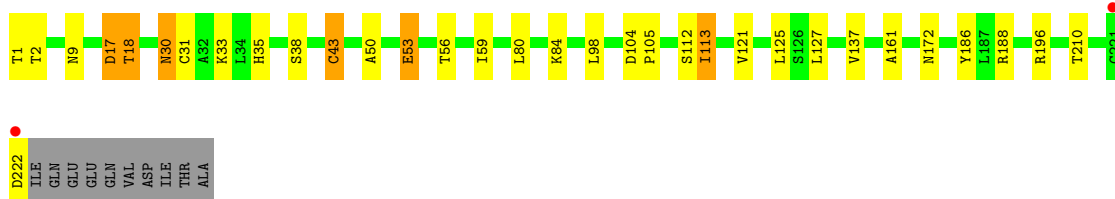
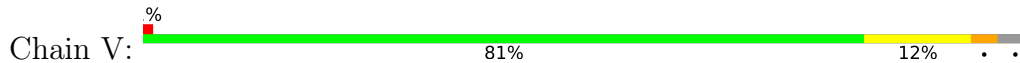
- Molecule 7: Proteasome subunit alpha type-1



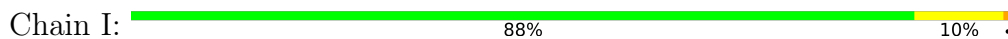
- Molecule 8: Proteasome subunit beta type-2




- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3




- Molecule 9: Proteasome subunit beta type-3

Chain W:  88% 11%




- Molecule 10: Proteasome subunit beta type-4

Chain J:  87% 9%




- Molecule 10: Proteasome subunit beta type-4

Chain X:  88% 9%




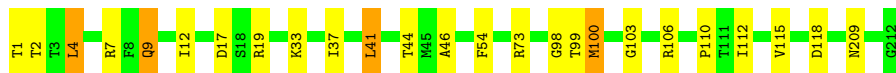
- Molecule 11: Proteasome subunit beta type-5

Chain K:  89% 10%




- Molecule 11: Proteasome subunit beta type-5

Chain Y:  88% 10%



- Molecule 12: Proteasome subunit beta type-6

Chain L:  91% 9%




- Molecule 12: Proteasome subunit beta type-6

Chain Z:  91% 9%




- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 6% 7%




- Molecule 13: Proteasome subunit beta type-7

Chain a:  91% 7%



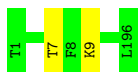
- Molecule 14: Proteasome subunit beta type-1

Chain N:  91% 8%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  99%



- Molecule 15: Linear biarylether epoxyketone

Chain e:  40% 60%



- Molecule 15: Linear biarylether epoxyketone

Chain f:  40% 60%



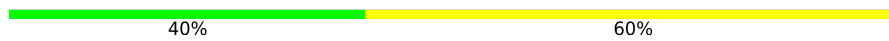
- Molecule 15: Linear biarylether epoxyketone

Chain g:  40% 60%



- Molecule 15: Linear biarylether epoxyketone

Chain h:



ACE1
F2
L3
Y4
6VU5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.21Å 303.14Å 143.23Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 49.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-3.20) 97.7 (49.72-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.184 , 0.228 0.189 , 0.228	Depositor DCC
R_{free} test set	8498 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtrriage
Anisotropy	0.646	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49514	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: ACE, CL, PPN, MES, 6VO, MG

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	0.65	0/1952	0.70	0/2642
1	O	0.65	0/1952	0.70	0/2642
2	B	0.65	0/1934	0.71	0/2618
2	P	0.66	0/1934	0.71	0/2618
3	C	0.66	0/1910	0.72	0/2586
3	Q	0.66	0/1910	0.72	0/2586
4	D	0.66	0/1837	0.71	0/2475
4	R	0.66	0/1837	0.71	0/2475
5	E	0.66	0/1800	0.71	0/2433
5	S	0.66	0/1800	0.71	0/2433
6	F	0.65	0/1932	0.70	0/2609
6	T	0.65	0/1932	0.70	0/2609
7	G	0.64	0/1945	0.70	0/2634
7	U	0.64	0/1945	0.70	0/2634
8	H	0.65	0/1715	0.75	0/2326
8	V	0.66	0/1715	0.74	0/2326
9	I	0.65	0/1611	0.72	0/2174
9	W	0.65	0/1611	0.72	0/2174
10	J	0.64	0/1589	0.70	0/2142
10	X	0.64	0/1589	0.70	0/2142
11	K	0.65	0/1681	0.73	0/2274
11	Y	0.65	0/1681	0.73	0/2274
12	L	0.64	0/1795	0.71	0/2420
12	Z	0.64	0/1795	0.71	0/2420
13	M	0.65	0/1821	0.72	0/2470
13	a	0.65	0/1821	0.72	0/2470
14	N	0.65	0/1541	0.70	0/2087
14	b	0.65	0/1541	0.70	0/2087
15	e	3.01	3/20 (15.0%)	1.40	0/26
15	f	3.16	3/20 (15.0%)	1.41	0/26
15	g	2.87	3/20 (15.0%)	1.23	0/26
15	h	3.30	3/20 (15.0%)	1.75	0/26

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.66	12/50206 (0.0%)	0.71	0/67884

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	4	TYR	CB-CG	-10.67	1.35	1.51
15	f	4	TYR	CB-CG	-9.94	1.36	1.51
15	e	4	TYR	CB-CG	-9.53	1.37	1.51
15	g	4	TYR	CB-CG	-8.85	1.38	1.51
15	f	3	LEU	CA-C	-7.18	1.34	1.52

There are no bond angle outliers.

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	3	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	8	0
4	R	1813	0	1797	10	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	6	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	7	0
8	H	1684	0	1686	23	0
8	V	1684	0	1686	24	0
9	I	1581	0	1574	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	1581	0	1574	17	0
10	J	1561	0	1569	18	0
10	X	1561	0	1569	15	0
11	K	1644	0	1593	19	0
11	Y	1644	0	1592	29	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	17	0
13	M	1790	0	1793	6	0
13	a	1790	0	1793	0	0
14	N	1512	0	1481	10	0
14	b	1512	0	1481	0	0
15	e	49	0	28	0	0
15	f	49	0	28	0	0
15	g	49	0	28	0	0
15	h	49	0	28	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	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	1	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	K	12	0	13	0	0
19	A	1	0	0	0	0
19	B	2	0	0	2	0
19	C	2	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
19	G	1	0	0	0	0
19	H	1	0	0	0	0
19	J	5	0	0	0	0
19	K	2	0	0	0	0
19	L	3	0	0	0	0
19	M	9	0	0	0	0
19	N	6	0	0	0	0
19	O	1	0	0	0	0
19	P	2	0	0	0	0
19	Q	5	0	0	0	0
19	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	2	0	0	0	0
19	U	2	0	0	0	0
19	V	2	0	0	0	0
19	W	2	0	0	0	0
19	X	5	0	0	0	0
19	Z	1	0	0	0	0
19	a	5	0	0	0	0
19	b	2	0	0	0	0
19	e	1	0	0	0	0
19	f	1	0	0	0	0
19	g	1	0	0	0	0
19	h	1	0	0	0	0
All	All	49514	0	49106	266	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 266 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)
10:X:101:ASN:HB3	10:X:133:HIS:CD2	1.83	1.14
10:J:101:ASN:HB3	10:J:133:HIS:CD2	1.83	1.13
11:Y:1:THR:HG22	11:Y:2:THR:N	1.75	0.98
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	1.90	0.87
4:R:94:TYR:HD1	12:Z:95:HIS:HD1	1.17	0.86

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%)	239 (96%)	9 (4%)	0	100	100
1	O	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	69
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	69
3	C	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	12	47
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	12	47
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	216 (98%)	4 (2%)	0	100	100
8	V	220/232 (95%)	216 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	67
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	67
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	M	227/246 (92%)	218 (96%)	9 (4%)	0	100	100
13	a	227/246 (92%)	218 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6276/6634 (95%)	6090 (97%)	176 (3%)	10 (0%)	47 79

5 of 10 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%)	49 77
1	O	209/209 (100%)	204 (98%)	5 (2%)	49 77
2	B	203/216 (94%)	195 (96%)	8 (4%)	32 67
2	P	203/216 (94%)	195 (96%)	8 (4%)	32 67
3	C	212/226 (94%)	204 (96%)	8 (4%)	33 67
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33 67
4	D	194/215 (90%)	186 (96%)	8 (4%)	30 66
4	R	194/215 (90%)	186 (96%)	8 (4%)	30 66
5	E	190/193 (98%)	181 (95%)	9 (5%)	26 62
5	S	190/193 (98%)	182 (96%)	8 (4%)	30 65
6	F	201/239 (84%)	191 (95%)	10 (5%)	24 60
6	T	201/239 (84%)	191 (95%)	10 (5%)	24 60
7	G	206/210 (98%)	198 (96%)	8 (4%)	32 67
7	U	206/210 (98%)	197 (96%)	9 (4%)	28 64
8	H	181/190 (95%)	167 (92%)	14 (8%)	13 44
8	V	181/190 (95%)	168 (93%)	13 (7%)	14 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	69
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	69
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	66
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	66
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	69
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	69
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	67
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	67
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	72
13	a	195/208 (94%)	189 (97%)	6 (3%)	40	72
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	88
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	88
15	e	2/2 (100%)	2 (100%)	0	100	100
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
All	All	5312/5548 (96%)	5105 (96%)	207 (4%)	32	67

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	184	LYS
6	T	123	ASN
13	a	43	ILE
3	Q	77	ASN
4	R	224	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	60	GLN
12	Z	3	ASN
4	R	15	GLN
12	Z	1	GLN
13	a	102	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	PPN	g	2	15	12,14,15	2.68	3 (25%)	13,18,20	1.16	1 (7%)
15	PPN	h	2	15	12,14,15	2.47	2 (16%)	13,18,20	1.85	4 (30%)
15	PPN	f	2	15	12,14,15	3.32	3 (25%)	13,18,20	1.63	3 (23%)
15	PPN	e	2	15	12,14,15	2.87	3 (25%)	13,18,20	1.02	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	PPN	g	2	15	-	5/7/10/12	0/1/1/1
15	PPN	h	2	15	-	4/7/10/12	0/1/1/1
15	PPN	f	2	15	-	4/7/10/12	0/1/1/1
15	PPN	e	2	15	-	2/7/10/12	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	2	PPN	O1-N1	7.91	1.36	1.22
15	f	2	PPN	CB-CG	-6.08	1.36	1.51
15	g	2	PPN	CB-CG	-6.08	1.36	1.51
15	h	2	PPN	CB-CG	-5.90	1.37	1.51
15	e	2	PPN	CB-CG	-5.87	1.37	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	2	PPN	CB-CG-CD2	-3.75	113.47	120.91
15	f	2	PPN	CB-CG-CD2	-3.19	114.56	120.91
15	h	2	PPN	CB-CG-CD1	2.80	126.47	120.91
15	h	2	PPN	CG-CB-CA	2.67	119.51	114.10
15	f	2	PPN	CE1-CD1-CG	-2.49	117.60	121.03

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	2	PPN	CE1-CZ-N1-O1
15	e	2	PPN	CE2-CZ-N1-O1
15	f	2	PPN	CE1-CZ-N1-O1
15	f	2	PPN	CE2-CZ-N1-O1
15	g	2	PPN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MES	K	301	-	12,12,12	0.84	0	14,16,16	0.29	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	K	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.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	301	MES	C8-C7-N4-C3
18	K	301	MES	C8-C7-N4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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%)	-0.35	2 (0%) 86 78	64, 84, 117, 167	0
1	O	250/250 (100%)	-0.20	3 (1%) 79 67	71, 92, 132, 162	0
2	B	244/258 (94%)	-0.10	3 (1%) 79 67	65, 92, 143, 194	0
2	P	244/258 (94%)	-0.13	3 (1%) 79 67	72, 91, 150, 173	0
3	C	240/254 (94%)	0.01	1 (0%) 92 89	67, 97, 146, 158	0
3	Q	240/254 (94%)	0.08	9 (3%) 40 26	76, 108, 167, 182	0
4	D	235/260 (90%)	-0.24	1 (0%) 92 89	66, 92, 120, 156	0
4	R	235/260 (90%)	-0.20	1 (0%) 92 89	71, 100, 138, 166	0
5	E	231/234 (98%)	-0.16	1 (0%) 92 89	70, 94, 121, 145	0
5	S	231/234 (98%)	0.01	7 (3%) 50 34	72, 104, 142, 175	0
6	F	243/288 (84%)	-0.33	0 100 100	64, 85, 126, 148	0
6	T	243/288 (84%)	-0.23	2 (0%) 86 78	68, 96, 135, 148	0
7	G	241/252 (95%)	-0.36	0 100 100	62, 81, 111, 142	0
7	U	241/252 (95%)	-0.28	0 100 100	64, 89, 116, 143	0
8	H	222/232 (95%)	-0.31	2 (0%) 84 75	65, 79, 105, 158	0
8	V	222/232 (95%)	-0.19	2 (0%) 84 75	72, 85, 108, 169	0
9	I	204/205 (99%)	-0.33	0 100 100	61, 78, 99, 128	0
9	W	204/205 (99%)	-0.36	0 100 100	60, 78, 101, 126	0
10	J	195/198 (98%)	-0.31	1 (0%) 91 86	62, 80, 106, 133	0
10	X	195/198 (98%)	-0.35	1 (0%) 91 86	64, 82, 105, 142	0
11	K	212/212 (100%)	-0.29	1 (0%) 91 86	61, 78, 103, 129	0
11	Y	212/212 (100%)	-0.36	0 100 100	68, 82, 110, 123	0
12	L	222/222 (100%)	-0.35	0 100 100	58, 79, 106, 117	0
12	Z	222/222 (100%)	-0.28	0 100 100	60, 80, 109, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	229/246 (93%)	-0.43	1 (0%) 92 89	59, 78, 99, 114	0
13	a	229/246 (93%)	-0.45	1 (0%) 92 89	61, 77, 100, 108	0
14	N	196/196 (100%)	-0.35	0 100 100	60, 75, 100, 124	0
14	b	196/196 (100%)	-0.19	0 100 100	65, 79, 105, 124	0
15	e	2/5 (40%)	-0.25	0 100 100	91, 91, 91, 92	0
15	f	2/5 (40%)	-0.99	0 100 100	74, 74, 74, 80	0
15	g	2/5 (40%)	-0.24	0 100 100	95, 95, 95, 96	0
15	h	2/5 (40%)	-0.95	0 100 100	80, 80, 80, 82	0
All	All	6336/6634 (95%)	-0.25	42 (0%) 87 81	58, 85, 129, 194	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	222	ASP	8.9
8	H	222	ASP	5.6
2	B	220	ASN	5.2
3	Q	50	LEU	4.3
3	Q	48	SER	4.2

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, 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	PPN	g	2	14/15	0.90	0.27	97,108,115,116	0
15	PPN	e	2	14/15	0.91	0.30	101,103,114,118	0
15	PPN	h	2	14/15	0.91	0.24	85,91,112,117	0
15	PPN	f	2	14/15	0.92	0.21	80,88,106,115	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
16	MG	G	301	1/1	0.86	0.06	74,74,74,74	0
16	MG	I	301	1/1	0.87	0.56	83,83,83,83	0
17	CL	G	302	1/1	0.88	0.12	67,67,67,67	0
18	MES	K	301	12/12	0.89	0.27	101,113,120,125	0
17	CL	U	301	1/1	0.93	0.14	88,88,88,88	0
16	MG	Z	301	1/1	0.94	0.21	98,98,98,98	0
16	MG	X	201	1/1	0.94	0.24	64,64,64,64	0
16	MG	K	302	1/1	0.96	0.20	100,100,100,100	0
16	MG	N	201	1/1	0.97	0.18	68,68,68,68	0
16	MG	V	301	1/1	0.98	0.16	104,104,104,104	0
16	MG	Y	301	1/1	0.99	0.07	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.