Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 01:34 am GMT

PDB ID	:	4YA0
Title	:	Yeast 20S proteasome beta2-H116E mutant in complex with Ac-PAE-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-17
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (i)) were used in the production of this report:

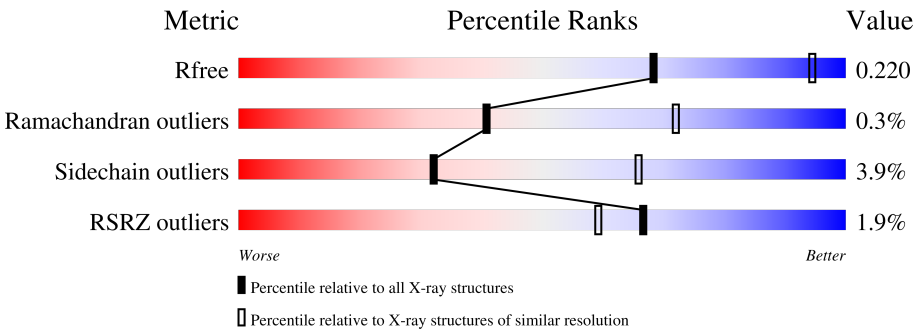
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 >=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 <=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	2%, 98%, •
1	O	250	2%, 98%, •
2	B	258	2%, 90%, •, 5%
2	P	258	3%, 90%, •, 5%
3	C	254	5%, 89%, 6%, 6%
3	Q	254	6%, 88%, 6%, 6%

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Mol	Chain	Length	Quality of chain
4	D	260	%; 86%; 5%; 10%
4	R	260	2%; 86%; 5%; 10%
5	E	234	3%; 94%; 5%
5	S	234	3%; 94%; 5%
6	F	288	2%; 81%; 16%
6	T	288	2%; 81%; 16%
7	G	252	2%; 91%; 5%
7	U	252	2%; 91%; 5%
8	H	232	3%; 96%
8	V	232	3%; 96%
9	I	205	99%
9	W	205	%; 99%
10	J	198	%; 95%
10	X	198	%; 95%
11	K	212	97%
11	Y	212	97%
12	L	222	97%
12	Z	222	%; 97%
13	M	246	92%; 5%
13	a	246	92%; 5%
14	N	196	%; 97%
14	b	196	%; 97%
15	1	5	60%; 20%; 20%
15	2	5	60%; 40%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49761 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	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	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	1904	1201	321	379	3	0	0	0
2	P	244	1904	1201	321	379	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	1881	1176	329	372	4	0	0	0
3	Q	240	1881	1176	329	372	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	1813	1136	304	366	7	0	0	0
4	R	235	1813	1136	304	366	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	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	1892	1203	329	356	4	0	0	0
6	T	243	1892	1203	329	356	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	1907	1214	320	365	8	0	0	0
7	U	241	1907	1214	320	365	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	226	1718	1081	296	334	7	0	0	0
8	V	226	1718	1081	296	334	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	GLU	HIS	engineered mutation	UNP P25043
V	116	GLU	HIS	engineered mutation	UNP P25043

- 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	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	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	1561	992	264	299	6	0	0	0
10	X	195	1561	992	264	299	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
11	Y	212	1644	1045	280	312	7	0	0	0

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

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

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

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

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

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

- Molecule 15 is a protein called Ac-PAE-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	1	5	28	18	3	7	0	0	0
15	2	5	28	18	3	7	0	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
16	G	1	1	1	0	0
16	I	2	2	2	0	0
16	K	1	1	1	0	0
16	L	1	1	1	0	0
16	N	1	1	1	0	0
16	Z	1	1	1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	11	11	11	0	0
18	B	13	13	13	0	0
18	C	10	10	10	0	0
18	D	7	7	7	0	0
18	E	4	4	4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	F	12	12	12	0	0
			Total	O		
18	G	18	18	18	0	0
			Total	O		
18	H	20	20	20	0	0
			Total	O		
18	I	7	7	7	0	0
			Total	O		
18	J	15	15	15	0	0
			Total	O		
18	K	16	16	16	0	0
			Total	O		
18	L	19	19	19	0	0
			Total	O		
18	M	19	19	19	0	0
			Total	O		
18	N	15	15	15	0	0
			Total	O		
18	O	4	4	4	0	0
			Total	O		
18	P	11	11	11	0	0
			Total	O		
18	Q	6	6	6	0	0
			Total	O		
18	R	10	10	10	0	0
			Total	O		
18	S	3	3	3	0	0
			Total	O		
18	T	11	11	11	0	0
			Total	O		
18	U	13	13	13	0	0
			Total	O		
18	V	16	16	16	0	0
			Total	O		
18	W	8	8	8	0	0
			Total	O		
18	X	14	14	14	0	0
			Total	O		
18	Y	14	14	14	0	0
			Total	O		
18	Z	13	13	13	0	0

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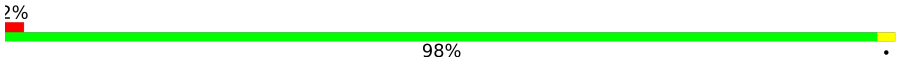
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	a	14	14	14	0	0
			Total	O		
18	b	8	8	8	0	0
			Total	O		
18	2	1	1	1	0	0

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.

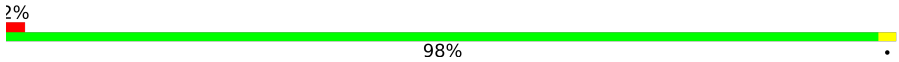
• Molecule 1: Proteasome subunit alpha type-2

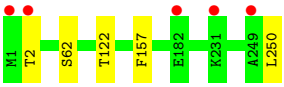
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

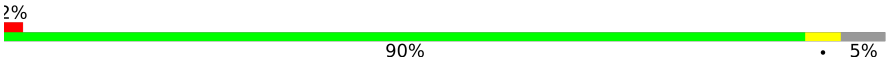
Chain O:

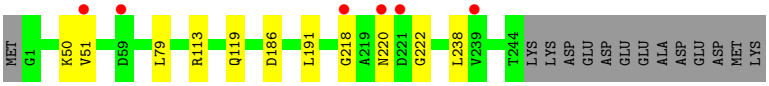




• Molecule 2: Proteasome subunit alpha type-3

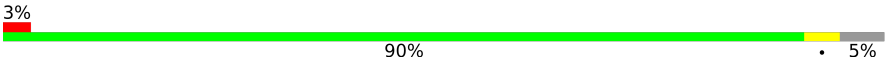
Chain B:

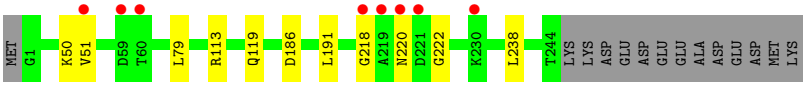




• Molecule 2: Proteasome subunit alpha type-3

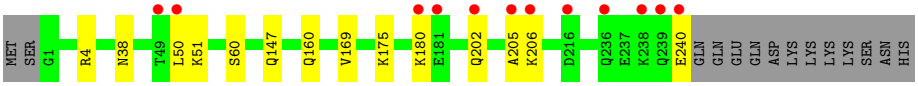
Chain P:





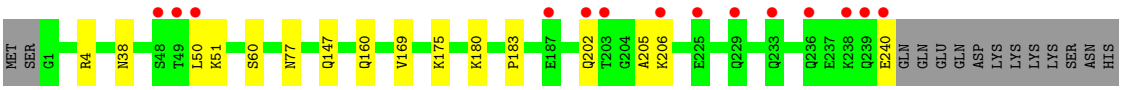
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



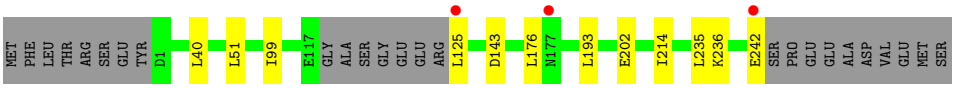
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



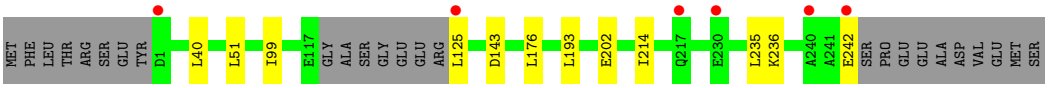
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



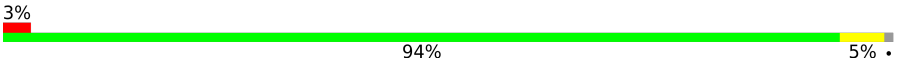
• Molecule 4: Proteasome subunit alpha type-5

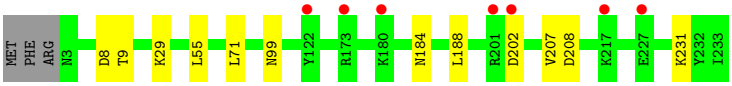
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

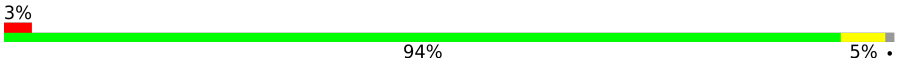
Chain E:

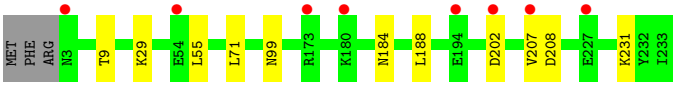




• Molecule 5: Proteasome subunit alpha type-6

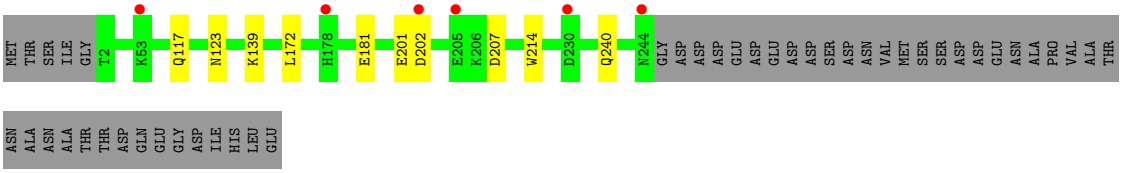
Chain S:





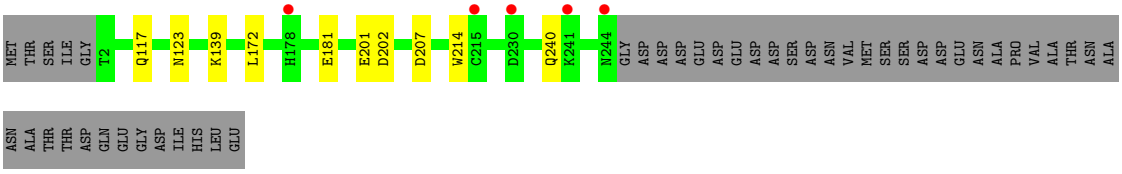
• Molecule 6: Proteasome subunit alpha type-7

Chain F:



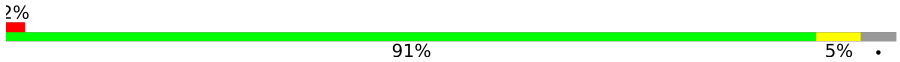
• Molecule 6: Proteasome subunit alpha type-7

Chain T:



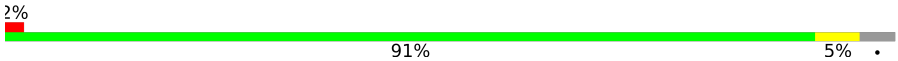
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



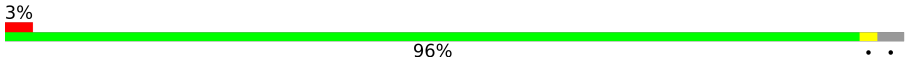
• Molecule 7: Proteasome subunit alpha type-1

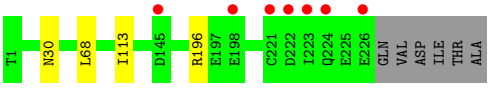
Chain U:



• Molecule 8: Proteasome subunit beta type-2

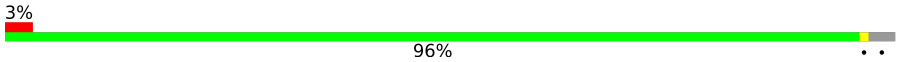
Chain H:

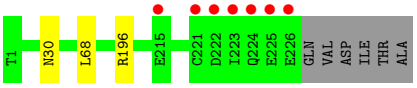




• Molecule 8: Proteasome subunit beta type-2

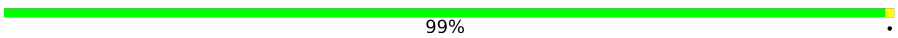
Chain V:

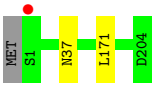




• Molecule 9: Proteasome subunit beta type-3

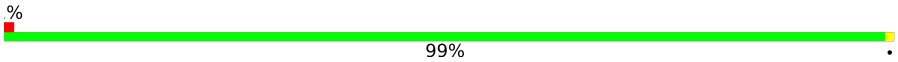
Chain I:

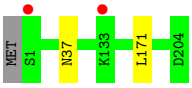




• Molecule 9: Proteasome subunit beta type-3

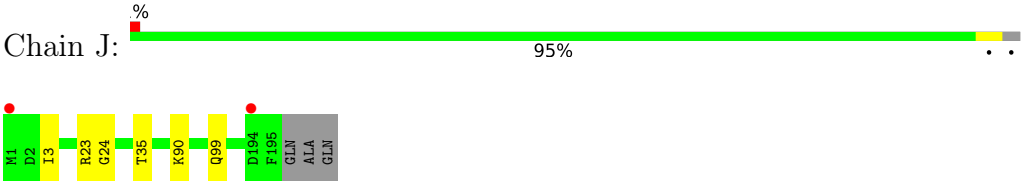
Chain W:





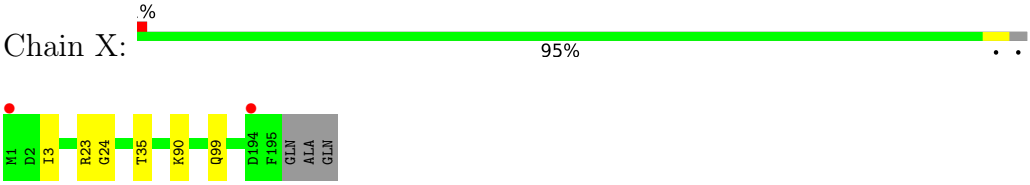
• Molecule 10: Proteasome subunit beta type-4

Chain J:



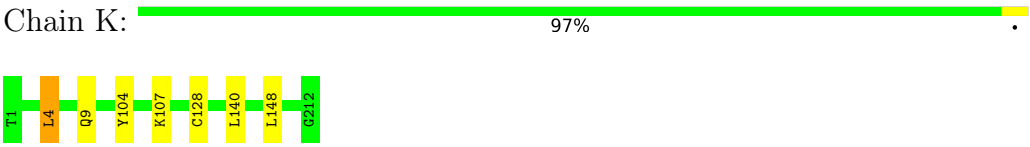
• Molecule 10: Proteasome subunit beta type-4

Chain X:



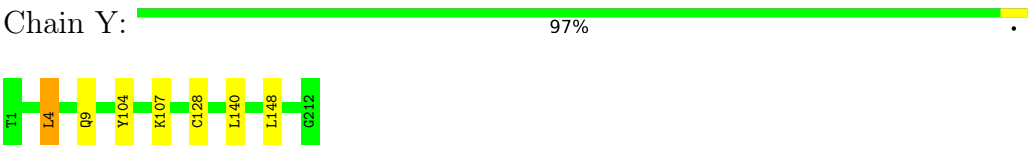
• Molecule 11: Proteasome subunit beta type-5

Chain K:



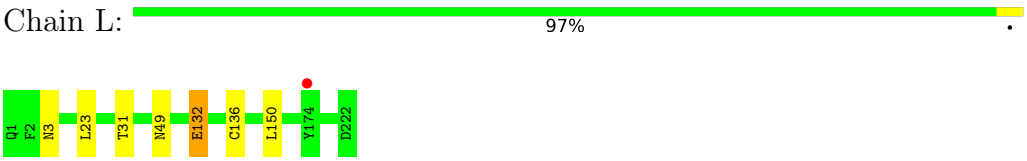
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



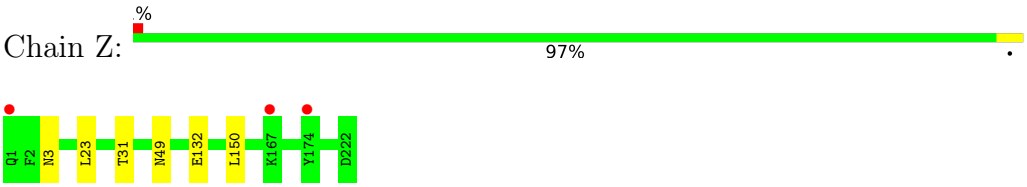
• Molecule 12: Proteasome subunit beta type-6

Chain L:



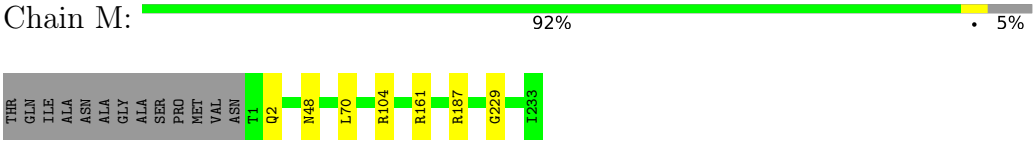
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



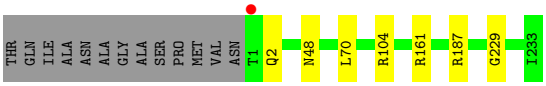
• Molecule 13: Proteasome subunit beta type-7

Chain M:



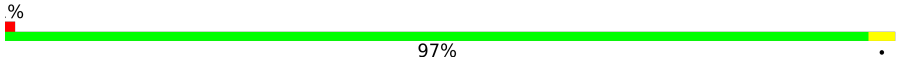
• Molecule 13: Proteasome subunit beta type-7

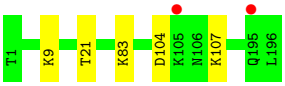
Chain a:



• Molecule 14: Proteasome subunit beta type-1

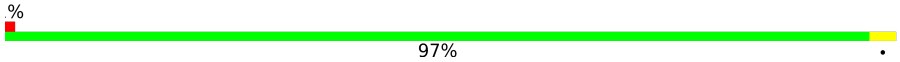
Chain N:

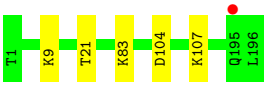




• Molecule 14: Proteasome subunit beta type-1

Chain b:





• Molecule 15: Ac-PAE-ep

Chain 1:

• Molecule 15: Ac-PAE-ep

Chain 2:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.60Å 299.89Å 145.92Å 90.00° 113.15° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (15.00-2.80) 93.3 (14.99-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.216 0.198 , 0.220	Depositor DCC
R_{free} test set	12322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49761	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: POL, GAU, MG, ACE, 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	0.28	0/1952	0.47	0/2642
1	O	0.28	0/1952	0.47	0/2642
2	B	0.29	0/1934	0.51	0/2618
2	P	0.29	0/1934	0.51	0/2618
3	C	0.29	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.49	0/2475
4	R	0.28	0/1837	0.49	0/2475
5	E	0.28	0/1800	0.48	0/2433
5	S	0.28	0/1800	0.48	0/2433
6	F	0.28	0/1932	0.46	0/2609
6	T	0.28	0/1932	0.46	0/2609
7	G	0.28	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.30	0/1748	0.49	0/2370
8	V	0.29	0/1748	0.48	0/2370
9	I	0.30	0/1611	0.50	0/2174
9	W	0.30	0/1611	0.50	0/2174
10	J	0.28	0/1589	0.49	0/2142
10	X	0.28	0/1589	0.49	0/2142
11	K	0.27	0/1681	0.50	1/2274 (0.0%)
11	Y	0.27	0/1681	0.50	1/2274 (0.0%)
12	L	0.29	0/1795	0.50	1/2420 (0.0%)
12	Z	0.30	0/1795	0.50	0/2420
13	M	0.29	0/1855	0.52	0/2514
13	a	0.29	0/1855	0.52	0/2514
14	N	0.31	0/1541	0.50	0/2087
14	b	0.34	0/1541	0.50	0/2087
15	1	2.83	1/13 (7.7%)	1.43	0/18
15	2	2.78	1/13 (7.7%)	1.11	0/18
All	All	0.29	2/50286 (0.0%)	0.49	3/67992 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	2	PRO	CA-C	-8.12	1.36	1.52
15	2	2	PRO	CA-C	-8.03	1.36	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	132	GLU	CA-CB-CG	5.14	124.71	113.40
11	Y	4	LEU	CA-CB-CG	5.12	127.07	115.30
11	K	4	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	8 (3%)	1 (0%)	34	66
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	66
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	29
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	29
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	49
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	36
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	66
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	66
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	1	2/5 (40%)	2 (100%)	0	0	100	100
15	2	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6288/6624 (95%)	6136 (98%)	133 (2%)	19 (0%)	41	72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR

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Mol	Chain	Res	Type
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
10	J	24	GLY
10	X	24	GLY
13	M	229	GLY
13	a	229	GLY
3	Q	183	PRO

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%)	205 (98%)	4 (2%)	57	85
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	85
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	71
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	71
3	C	212/226 (94%)	200 (94%)	12 (6%)	20	50
3	Q	212/226 (94%)	199 (94%)	13 (6%)	18	48
4	D	194/215 (90%)	182 (94%)	12 (6%)	18	47
4	R	194/215 (90%)	182 (94%)	12 (6%)	18	47
5	E	190/193 (98%)	178 (94%)	12 (6%)	18	46
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	50
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	56
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	56
7	G	206/210 (98%)	194 (94%)	12 (6%)	20	50
7	U	206/210 (98%)	194 (94%)	12 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	185/190 (97%)	181 (98%)	4 (2%)	52	83
8	V	185/190 (97%)	182 (98%)	3 (2%)	62	88
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	92
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	92
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	64
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	67
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	73
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
15	1	1/1 (100%)	0	1 (100%)	0	0
15	2	1/1 (100%)	1 (100%)	0	100	100
All	All	5322/5542 (96%)	5113 (96%)	209 (4%)	32	66

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS

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Mol	Chain	Res	Type
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN

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Mol	Chain	Res	Type
7	G	13	GLU
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	178	LYS
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	68	LEU
8	H	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	107	LYS
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	132	GLU
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG

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Mol	Chain	Res	Type
13	M	187	ARG
14	N	9	LYS
14	N	21	THR
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU

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Mol	Chain	Res	Type
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	178	LYS
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS

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Mol	Chain	Res	Type
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	132	GLU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	21	THR
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
15	1	2	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN

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Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
8	H	66	HIS
8	H	114	HIS
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
10	J	147	HIS
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN

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Mol	Chain	Res	Type
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
8	V	66	HIS
8	V	114	HIS
8	V	165	ASN

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Mol	Chain	Res	Type
9	W	37	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
14	b	161	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)

2 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	GAU	1	4	15,14	8,8,8	1.38	2 (25%)	8,9,9	1.60	2 (25%)
15	GAU	2	4	15,14	8,8,8	1.47	2 (25%)	8,9,9	1.54	2 (25%)

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	GAU	1	4	15,14	-	3/7/7/7	-
15	GAU	2	4	15,14	-	2/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	4	GAU	C-CA	3.27	1.57	1.52
15	1	4	GAU	C-CA	2.98	1.57	1.52
15	2	4	GAU	OE2-CD	-2.28	1.23	1.30
15	1	4	GAU	OE2-CD	-2.12	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	4	GAU	CB-CA-N	-3.16	99.84	109.03
15	2	4	GAU	CB-CA-N	-2.59	101.52	109.03
15	2	4	GAU	CG-CB-CA	-2.41	107.69	112.74
15	1	4	GAU	CG-CB-CA	-2.01	108.51	112.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	1	4	GAU	O-C-CA-CB
15	2	4	GAU	O-C-CA-CB
15	1	4	GAU	O-C-CA-N
15	2	4	GAU	O-C-CA-N
15	1	4	GAU	OE2-CD-CG-CB

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	6 (2%)	59	49	43, 56, 91, 132	0
1	O	250/250 (100%)	-0.30	5 (2%)	65	56	48, 65, 108, 138	0
2	B	244/258 (94%)	-0.32	6 (2%)	57	47	43, 61, 105, 153	0
2	P	244/258 (94%)	-0.24	8 (3%)	46	36	50, 68, 112, 162	0
3	C	240/254 (94%)	-0.22	12 (5%)	28	19	44, 67, 128, 153	0
3	Q	240/254 (94%)	0.02	14 (5%)	23	15	53, 79, 156, 174	0
4	D	235/260 (90%)	-0.32	3 (1%)	77	72	53, 71, 103, 141	0
4	R	235/260 (90%)	-0.24	6 (2%)	56	46	54, 75, 112, 147	0
5	E	231/234 (98%)	-0.16	7 (3%)	50	40	54, 73, 111, 159	0
5	S	231/234 (98%)	-0.11	8 (3%)	44	34	56, 80, 122, 167	0
6	F	243/288 (84%)	-0.37	6 (2%)	57	47	46, 64, 115, 146	0
6	T	243/288 (84%)	-0.22	5 (2%)	63	54	49, 73, 130, 158	0
7	G	241/252 (95%)	-0.44	4 (1%)	70	63	40, 60, 92, 143	0
7	U	241/252 (95%)	-0.40	4 (1%)	70	63	44, 60, 94, 137	0
8	H	226/232 (97%)	-0.41	7 (3%)	49	39	37, 54, 89, 152	0
8	V	226/232 (97%)	-0.31	7 (3%)	49	39	44, 58, 92, 170	0
9	I	204/205 (99%)	-0.63	1 (0%)	91	88	40, 53, 82, 107	0
9	W	204/205 (99%)	-0.60	2 (0%)	82	77	44, 57, 87, 112	0
10	J	195/198 (98%)	-0.48	2 (1%)	82	77	43, 59, 83, 140	0
10	X	195/198 (98%)	-0.47	2 (1%)	82	77	44, 60, 85, 145	0
11	K	212/212 (100%)	-0.50	0	100	100	41, 58, 82, 104	0
11	Y	212/212 (100%)	-0.52	0	100	100	45, 59, 83, 104	0
12	L	222/222 (100%)	-0.48	1 (0%)	91	88	43, 59, 91, 123	0
12	Z	222/222 (100%)	-0.49	3 (1%)	75	70	37, 58, 90, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.54	0 100 100	40, 56, 79, 98	0
13	a	233/246 (94%)	-0.52	1 (0%) 92 91	40, 56, 77, 94	0
14	N	196/196 (100%)	-0.60	2 (1%) 82 77	39, 51, 78, 106	0
14	b	196/196 (100%)	-0.58	1 (0%) 91 88	41, 54, 80, 115	0
15	1	2/5 (40%)	-0.56	0 100 100	62, 62, 62, 63	0
15	2	2/5 (40%)	-0.79	0 100 100	56, 56, 56, 62	0
All	All	6348/6624 (95%)	-0.38	123 (1%) 66 59	37, 62, 107, 174	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	6.3
3	C	206	LYS	6.1
3	Q	206	LYS	5.9
9	W	1	SER	5.8
8	V	226	GLU	5.3
10	J	1	MET	5.1
5	E	202	ASP	4.8
2	B	220	ASN	4.7
3	Q	239	GLN	4.7
3	Q	49	THR	4.6
3	C	49	THR	4.6
10	X	1	MET	4.4
10	X	194	ASP	4.3
3	Q	50	LEU	4.3
5	S	202	ASP	4.2
3	Q	236	GLN	4.1
2	B	221	ASP	4.0
8	H	226	GLU	3.8
14	b	195	GLN	3.8
1	O	2	THR	3.8
2	P	220	ASN	3.7
2	P	59	ASP	3.7
3	Q	240	GLU	3.7
10	J	194	ASP	3.6
2	P	221	ASP	3.6
8	V	221	CYS	3.5
6	F	244	ASN	3.5
12	L	174	TYR	3.5
1	A	249	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	P	218	GLY	3.4
3	C	239	GLN	3.4
7	U	242	GLN	3.3
8	V	222	ASP	3.3
2	B	218	GLY	3.3
3	C	236	GLN	3.3
1	A	2	THR	3.3
2	B	51	VAL	3.3
13	a	1	THR	3.3
4	R	230	GLU	3.3
8	H	224	GLN	3.2
1	O	249	ALA	3.2
4	R	242	GLU	3.2
8	H	221	CYS	3.1
8	H	222	ASP	3.1
12	Z	174	TYR	3.1
3	C	50	LEU	3.0
6	T	241	LYS	3.0
6	T	244	ASN	3.0
8	H	223	ILE	2.9
1	O	1	MET	2.9
5	S	180	LYS	2.9
4	D	242	GLU	2.9
2	P	51	VAL	2.9
6	T	230	ASP	2.8
8	V	223	ILE	2.8
8	H	145	ASP	2.8
2	P	219	ALA	2.8
3	Q	225	GLU	2.8
9	I	1	SER	2.8
3	C	205	ALA	2.7
12	Z	1	GLN	2.7
1	A	1	MET	2.7
5	S	227	GLU	2.7
3	Q	187	GLU	2.7
3	Q	202	GLN	2.6
14	N	195	GLN	2.6
4	R	1	ASP	2.6
1	O	231	LYS	2.6
5	S	207	VAL	2.5
6	T	178	HIS	2.5
6	T	215	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	229	GLN	2.5
5	E	227	GLU	2.5
9	W	133	LYS	2.4
6	F	230	ASP	2.4
7	G	3	TYR	2.4
5	S	3	ASN	2.4
4	R	240	ALA	2.4
4	R	217	GLN	2.4
7	U	181	LYS	2.4
5	S	173	ARG	2.4
1	O	182	GLU	2.3
2	P	230	LYS	2.3
3	Q	233	GLN	2.3
3	C	240	GLU	2.3
5	E	217	LYS	2.3
6	F	202	ASP	2.3
3	Q	238	LYS	2.3
5	S	54	GLU	2.3
6	F	205	GLU	2.2
3	C	202	GLN	2.2
4	D	177	ASN	2.2
7	U	188	GLU	2.2
1	A	250	LEU	2.2
3	C	181	GLU	2.2
2	B	59	ASP	2.2
3	Q	203	THR	2.2
2	B	239	VAL	2.2
6	F	53	LYS	2.1
8	V	215	GLU	2.1
6	F	178	HIS	2.1
5	E	180	LYS	2.1
1	A	201	GLU	2.1
4	D	125	LEU	2.1
5	S	194	GLU	2.1
7	G	240	ALA	2.1
5	E	201	ARG	2.1
4	R	125	LEU	2.1
12	Z	167	LYS	2.1
7	G	242	GLN	2.1
1	A	248	GLU	2.1
8	V	225	GLU	2.1
3	Q	48	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	60	THR	2.0
3	C	216	ASP	2.0
3	C	180	LYS	2.0
5	E	122	TYR	2.0
7	G	181	LYS	2.0
5	E	173	ARG	2.0
3	C	238	LYS	2.0
7	U	222	ASP	2.0
14	N	105	LYS	2.0
8	H	198	GLU	2.0

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	GAU	2	4	9/9	0.94	0.13	61,64,66,67	0
15	GAU	1	4	9/9	0.97	0.13	60,69,74,74	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	N	201	1/1	0.92	0.16	51,51,51,51	0
17	CL	U	301	1/1	0.93	0.28	30,30,30,30	0
16	MG	I	302	1/1	0.96	0.07	60,60,60,60	0
16	MG	G	301	1/1	0.96	0.06	61,61,61,61	0
16	MG	Z	301	1/1	0.96	0.23	68,68,68,68	0
16	MG	I	301	1/1	0.96	0.30	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	L	301	1/1	0.97	0.07	69,69,69,69	0
16	MG	K	301	1/1	0.98	0.05	56,56,56,56	0
17	CL	G	302	1/1	0.99	0.26	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.