



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:02 pm BST

PDB ID : 4Y6A  
Title : Yeast 20S proteasome beta2-H114D mutant in complex with Ac-PAD-ep  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-02-12  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

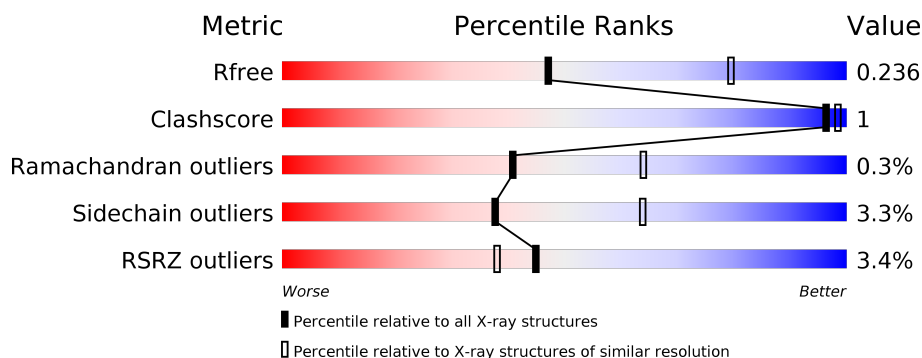
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>5%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>4%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>5%</div> <div>88%</div> <div>6% • 5%</div> </div>
2	P	258	<div> <div>8%</div> <div>88%</div> <div>6% • 5%</div> </div>
3	C	254	<div> <div>5%</div> <div>87%</div> <div>6% • 6%</div> </div>
3	Q	254	<div> <div>12%</div> <div>87%</div> <div>6% • 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	c	4	
15	d	4	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50213 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	226	Total	C	N	O	S	0	0	0
			1717	1080	296	334	7			
8	V	226	Total	C	N	O	S	0	0	0
			1717	1080	296	334	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	114	ASP	HIS	conflict	UNP P25043
V	114	ASP	HIS	conflict	UNP P25043

- 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			
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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			27	17	3	7			
15	d	4	Total	C	N	O	0	0	0
			27	17	3	7			

- 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	K	1	Total	Mg	0	0
			1	1		
16	I	2	Total	Mg	0	0
			2	2		
16	Z	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	L	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	35	Total	O	0	0
			35	35		
18	B	28	Total	O	0	0
			28	28		
18	C	32	Total	O	0	0
			32	32		
18	D	22	Total	O	0	0
			22	22		
18	E	13	Total	O	0	0
			13	13		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	F	23	Total O 23 23	0	0
18	G	33	Total O 33 33	0	0
18	H	39	Total O 39 39	0	0
18	I	37	Total O 37 37	0	0
18	J	26	Total O 26 26	0	0
18	K	27	Total O 27 27	0	0
18	L	38	Total O 38 38	0	0
18	M	32	Total O 32 32	0	0
18	N	28	Total O 28 28	0	0
18	O	20	Total O 20 20	0	0
18	P	22	Total O 22 22	0	0
18	Q	22	Total O 22 22	0	0
18	R	16	Total O 16 16	0	0
18	S	12	Total O 12 12	0	0
18	T	23	Total O 23 23	0	0
18	U	41	Total O 41 41	0	0
18	V	28	Total O 28 28	0	0
18	W	27	Total O 27 27	0	0
18	X	30	Total O 30 30	0	0
18	Y	34	Total O 34 34	0	0
18	Z	32	Total O 32 32	0	0

*Continued on next page...*



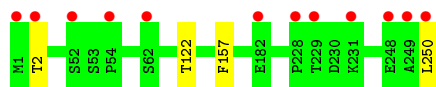
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	a	40	Total 40	O 40	0	0
18	b	23	Total 23	O 23	0	0
18	c	2	Total 2	O 2	0	0
18	d	3	Total 3	O 3	0	0

### 3 Residue-property plots [i](#)

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

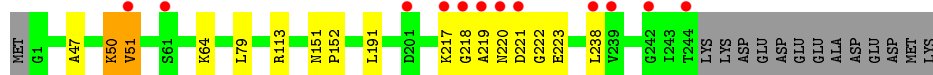
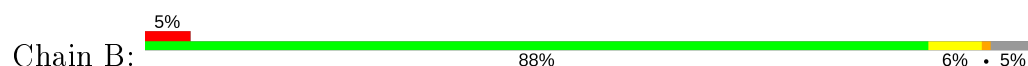
- Molecule 1: Proteasome subunit alpha type-2



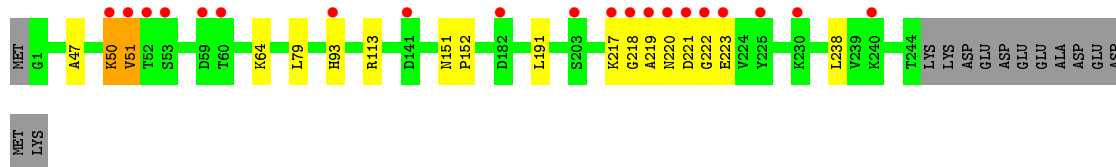
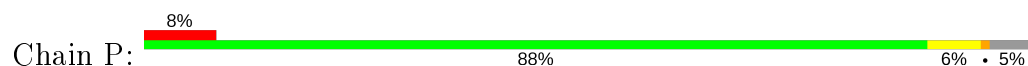
- Molecule 1: Proteasome subunit alpha type-2



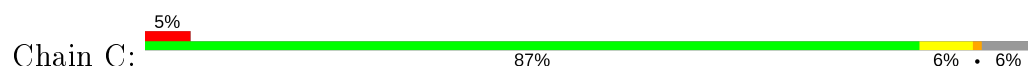
- Molecule 2: Proteasome subunit alpha type-3



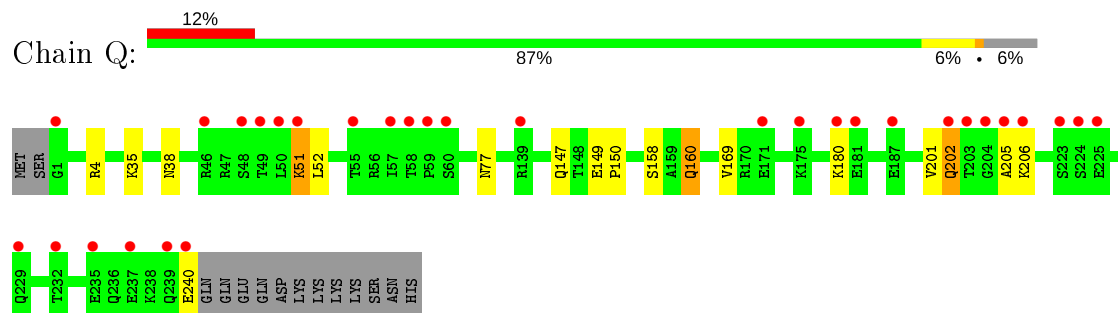
- Molecule 2: Proteasome subunit alpha type-3



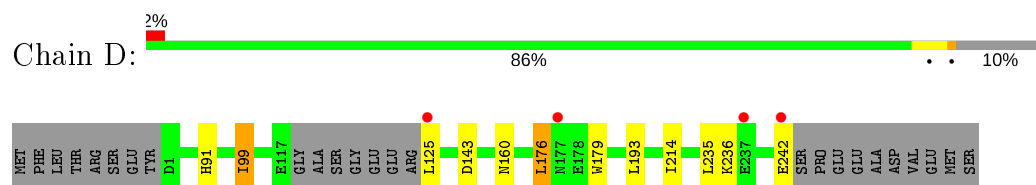
- Molecule 3: Proteasome subunit alpha type-4



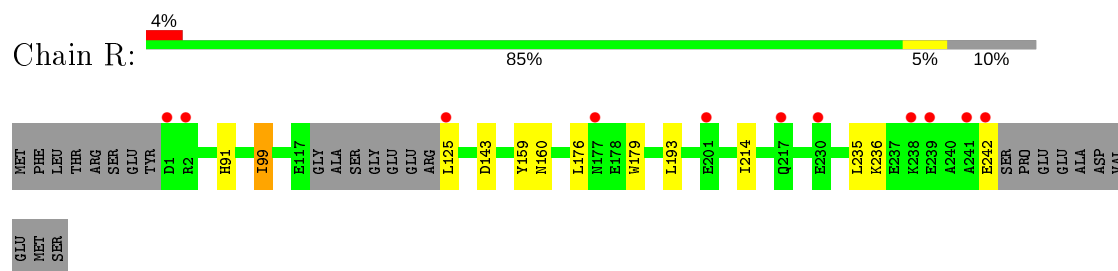
- Molecule 3: Proteasome subunit alpha type-4



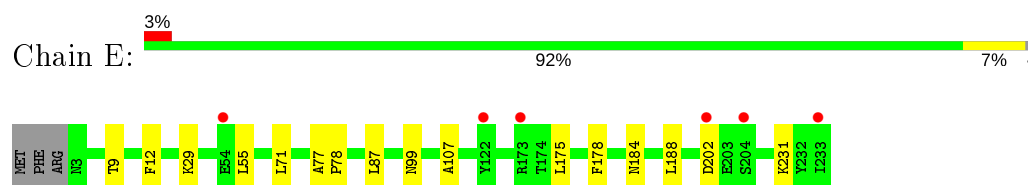
- Molecule 4: Proteasome subunit alpha type-5



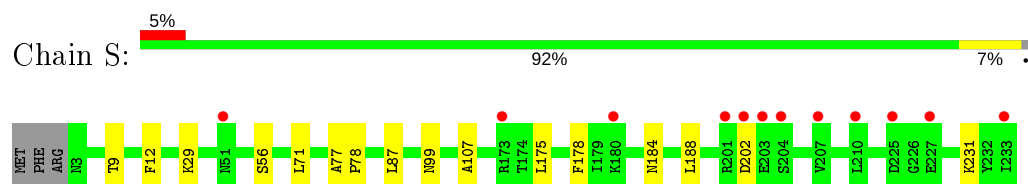
- Molecule 4: Proteasome subunit alpha type-5



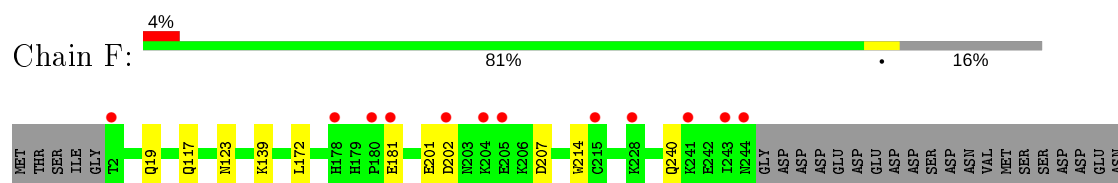
- Molecule 5: Proteasome subunit alpha type-6



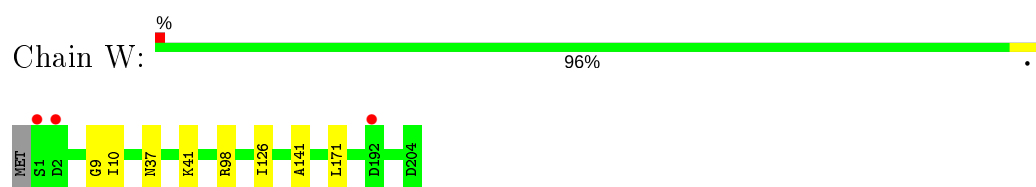
- Molecule 5: Proteasome subunit alpha type-6



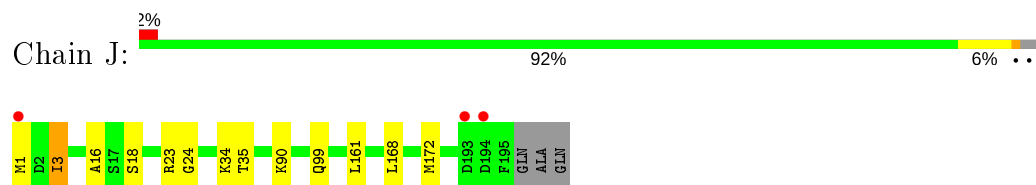
- Molecule 6: Probable proteasome subunit alpha type-7



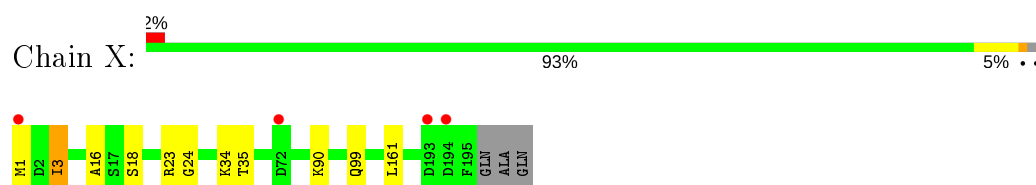




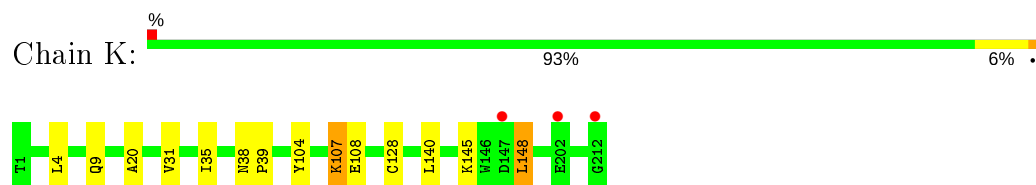
- Molecule 10: Proteasome subunit beta type-4



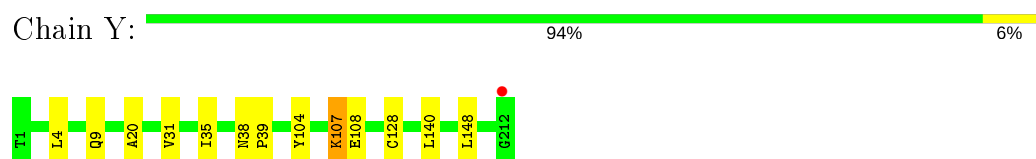
- Molecule 10: Proteasome subunit beta type-4



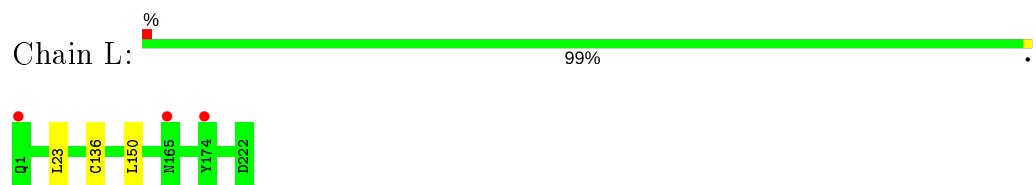
- Molecule 11: Proteasome subunit beta type-5



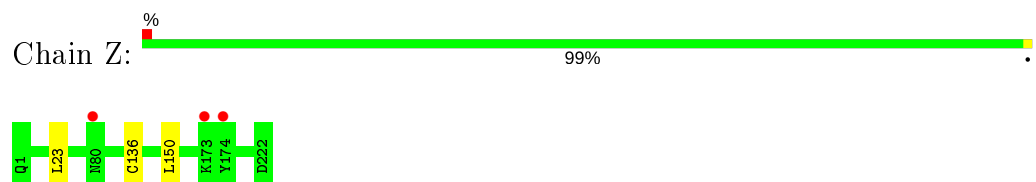
- Molecule 11: Proteasome subunit beta type-5



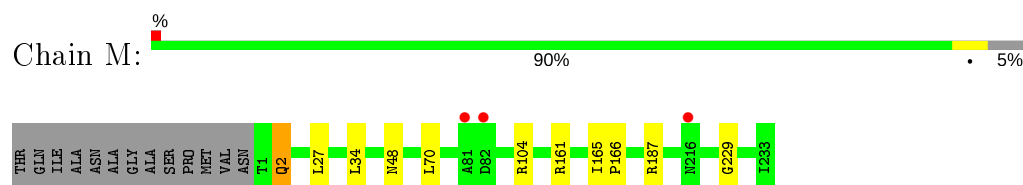
- Molecule 12: Proteasome subunit beta type-6



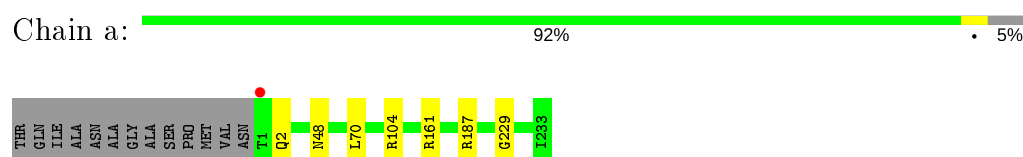
- Molecule 12: Proteasome subunit beta type-6



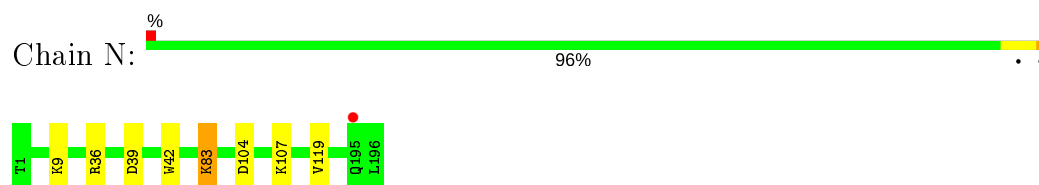
- Molecule 13: Proteasome subunit beta type-7



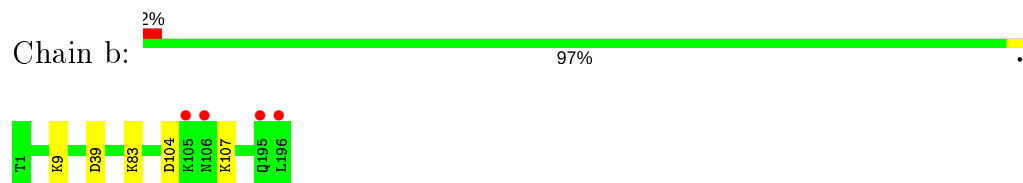
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



- Molecule 15: Ac-PAD-ep



There are no outlier residues recorded for this chain.

- Molecule 15: Ac-PAD-ep



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.77Å 302.73Å 145.98Å 90.00° 113.19° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (15.00-2.60) 96.5 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.217 , 0.232 0.222 , 0.236	Depositor DCC
$R_{free}$ test set	15990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	50213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ASJ, MG, N7P, POL, 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	0.46	0/2642
1	O	0.28	0/1952	0.46	0/2642
2	B	0.28	0/1934	0.49	0/2618
2	P	0.28	0/1934	0.50	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.28	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.28	0/1800	0.47	0/2433
5	S	0.28	0/1800	0.47	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.28	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.46	0/2634
7	U	0.28	0/1945	0.46	0/2634
8	H	0.28	0/1747	0.56	2/2369 (0.1%)
8	V	0.28	0/1747	0.57	1/2369 (0.0%)
9	I	0.30	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.28	0/1589	0.48	0/2142
10	X	0.28	0/1589	0.48	0/2142
11	K	0.28	0/1681	0.50	0/2274
11	Y	0.27	0/1681	0.50	0/2274
12	L	0.28	0/1795	0.48	0/2420
12	Z	0.28	0/1795	0.48	0/2420
13	M	0.29	0/1855	0.50	0/2514
13	a	0.29	0/1855	0.50	0/2514
14	N	0.30	0/1541	0.49	0/2087
14	b	0.31	0/1541	0.49	0/2087
15	c	0.95	0/4	0.93	0/4
15	d	1.17	0/4	0.99	0/4
All	All	0.28	0/50266	0.49	3/67962 (0.0%)



There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	V	84	LYS	CD-CE-NZ	14.99	146.18	111.70
8	H	84	LYS	CD-CE-NZ	14.04	143.98	111.70
8	H	84	LYS	CG-CD-CE	5.62	128.76	111.90

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	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1717	0	1716	11	0
8	V	1717	0	1716	9	0
9	I	1581	0	1574	3	0
9	W	1581	0	1574	3	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	3	0
11	K	1644	0	1595	4	0
11	Y	1644	0	1595	3	0
12	L	1757	0	1711	0	0
12	Z	1757	0	1711	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1479	3	0
14	b	1512	0	1478	0	0
15	c	27	0	14	0	0
15	d	27	0	14	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	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	A	35	0	0	0	0
18	B	28	0	0	0	0
18	C	32	0	0	0	0
18	D	22	0	0	0	0
18	E	13	0	0	0	0
18	F	23	0	0	0	0
18	G	33	0	0	0	0
18	H	39	0	0	1	0
18	I	37	0	0	0	0
18	J	26	0	0	0	0
18	K	27	0	0	0	0
18	L	38	0	0	0	0
18	M	32	0	0	1	0
18	N	28	0	0	0	0
18	O	20	0	0	0	0
18	P	22	0	0	1	0
18	Q	22	0	0	0	0
18	R	16	0	0	0	0
18	S	12	0	0	0	0
18	T	23	0	0	0	0
18	U	41	0	0	0	0
18	V	28	0	0	0	0
18	W	27	0	0	0	0
18	X	30	0	0	0	0
18	Y	34	0	0	0	0
18	Z	32	0	0	0	0
18	a	40	0	0	0	0
18	b	23	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	c	2	0	0	0	0
18	d	3	0	0	0	0
All	All	50213	0	49147	91	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 1.

All (91) 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)
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.81	0.61
8:V:112:SER:OG	8:V:120:ASP:OD1	2.17	0.61
2:P:93:HIS:HB3	18:P:301:HOH:O	2.00	0.60
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.81	0.60
8:H:112:SER:OG	8:H:120:ASP:OD1	2.17	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.84	0.58
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.57
8:H:53:GLU:O	8:H:57:GLN:HG3	2.10	0.52
8:V:53:GLU:O	8:V:57:GLN:HG3	2.10	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
13:M:2:GLN:NE2	18:M:301:HOH:O	2.44	0.49
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
8:H:120:ASP:OD1	8:H:120:ASP:N	2.46	0.49
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.95	0.48
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.78	0.48
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.95	0.48
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.48
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.61	0.48
8:V:120:ASP:OD1	8:V:120:ASP:N	2.46	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.79	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.98	0.46
2:B:221:ASP:O	2:B:223:GLU:N	2.49	0.46
2:P:221:ASP:O	2:P:223:GLU:N	2.49	0.46
8:V:35:HIS:CE1	8:V:53:GLU:HG2	2.51	0.46
8:H:35:HIS:CE1	8:H:53:GLU:HG2	2.51	0.46
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.97	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.50	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.45
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.97	0.45
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.98	0.45
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.16	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.99	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
2:B:217:LYS:C	2:B:219:ALA:H	2.22	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.01	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.43
5:E:12:PHE:H	6:F:19:GLN:HE22	1.66	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.42
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.87	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.01	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.50	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.42
2:P:217:LYS:C	2:P:219:ALA:H	2.22	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.01	0.42
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.01	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
8:H:84:LYS:HG3	8:H:85:GLN:N	2.34	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.21	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.41
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.03	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.52	0.40
8:H:116:HIS:HB2	18:H:301:HOH:O	2.21	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.40
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.57	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	0.40
10:J:168:LEU:O	10:J:172:MET:HB2	2.21	0.40
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.03	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
9:W:98:ARG:O	9:W:126:ILE:HD11	2.22	0.40
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40
5:S:12:PHE:H	6:T:19:GLN:HE22	1.69	0.40

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%)	8 (3%)	1 (0%)	34 57
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34 57
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 18
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 18
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19 39

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	39
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	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%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (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%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	52
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	57
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	34	57
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	c	1/4 (25%)	1 (100%)	0	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6286/6622 (95%)	6133 (98%)	135 (2%)	18 (0%)	41	64

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR
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
13	M	229	GLY
13	a	229	GLY
10	X	24	GLY

### 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%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	198 (98%)	5 (2%)	47	73
2	P	203/216 (94%)	198 (98%)	5 (2%)	47	73
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	50
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	50
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	51
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	51
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	55
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	55
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	47
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	48
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	53
8	H	185/190 (97%)	180 (97%)	5 (3%)	44	71
8	V	185/190 (97%)	180 (97%)	5 (3%)	44	71
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	87
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	87
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	68
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	68
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	50
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	50
12	L	185/185 (100%)	182 (98%)	3 (2%)	62	82
12	Z	185/185 (100%)	182 (98%)	3 (2%)	62	82
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	67
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	67
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	66
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	66
All	All	5320/5540 (96%)	5143 (97%)	177 (3%)	38	64

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	99	ASN
5	E	184	ASN
5	E	188	LEU
5	E	202	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
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	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	55	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	68	LEU
8	H	84	LYS
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	35	ILE
11	K	104	TYR
11	K	107	LYS
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
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
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
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	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	99	ASN
5	S	184	ASN
5	S	188	LEU
5	S	202	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	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	55	VAL
8	V	68	LEU
8	V	84	LYS
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
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	104	TYR
11	Y	107	LYS
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	136	CYS
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	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
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	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	35	HIS
8	H	66	HIS
9	I	37	ASN
9	I	203	GLN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
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	38	ASN
3	Q	77	ASN
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	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	143	HIS
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	35	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	W	37	ASN
10	X	55	GLN
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
13	a	179	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	N7P	c	1	15	9,10,11	2.04	4 (44%)	9,13,15	1.73	2 (22%)
15	N7P	d	1	15	9,10,11	1.57	2 (22%)	9,13,15	1.90	3 (33%)
15	ASJ	d	3	15,14	4,7,7	1.79	1 (25%)	3,8,8	2.63	2 (66%)
15	ASJ	c	3	15,14	4,7,7	1.58	1 (25%)	3,8,8	2.07	2 (66%)

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	N7P	c	1	15	-	0/4/16/18	0/1/1/1
15	N7P	d	1	15	-	0/4/16/18	0/1/1/1
15	ASJ	d	3	15,14	-	0/4/6/6	-
15	ASJ	c	3	15,14	-	0/4/6/6	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	1	N7P	CB-CA	-3.37	1.45	1.53
15	d	3	ASJ	C-CA	2.97	1.57	1.52
15	d	1	N7P	CB-CA	-2.85	1.46	1.53
15	c	1	N7P	C1-N	-2.74	1.31	1.35
15	c	3	ASJ	C-CA	2.74	1.56	1.52
15	c	1	N7P	CA-N	-2.73	1.45	1.48
15	c	1	N7P	CG-CD	-2.52	1.43	1.51
15	d	1	N7P	CG-CD	-2.40	1.43	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	1	N7P	CB-CA-C	-3.92	107.31	112.70
15	d	1	N7P	CB-CA-C	-3.67	107.65	112.70
15	d	3	ASJ	CG-CB-CA	3.20	116.34	112.95
15	d	1	N7P	O1-C1-N	3.06	123.97	120.64
15	d	3	ASJ	CB-CA-C	-2.79	107.16	112.21
15	c	3	ASJ	CB-CA-C	-2.41	107.86	112.21
15	d	1	N7P	CA-N-C1	2.18	126.59	121.26
15	c	3	ASJ	CG-CB-CA	2.12	115.20	112.95
15	c	1	N7P	O1-C1-N	2.09	122.92	120.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.19	12 (4%)	30 24	34, 47, 84, 123	0
1	O	250/250 (100%)	-0.05	11 (4%)	34 27	37, 56, 102, 132	0
2	B	244/258 (94%)	0.00	12 (4%)	29 23	35, 54, 100, 148	0
2	P	244/258 (94%)	0.11	20 (8%)	11 8	39, 59, 103, 146	0
3	C	240/254 (94%)	0.11	13 (5%)	25 20	34, 58, 121, 148	0
3	Q	240/254 (94%)	0.46	31 (12%)	3 2	41, 70, 151, 175	0
4	D	235/260 (90%)	-0.06	4 (1%)	70 66	41, 60, 95, 137	0
4	R	235/260 (90%)	0.06	11 (4%)	31 25	44, 65, 106, 143	0
5	E	231/234 (98%)	0.04	6 (2%)	56 50	41, 62, 102, 145	0
5	S	231/234 (98%)	0.19	12 (5%)	27 21	42, 68, 115, 155	0
6	F	243/288 (84%)	-0.08	12 (4%)	29 23	35, 53, 107, 135	0
6	T	243/288 (84%)	0.06	13 (5%)	26 20	37, 63, 118, 150	0
7	G	241/252 (95%)	-0.22	8 (3%)	46 39	30, 49, 83, 130	0
7	U	241/252 (95%)	-0.10	9 (3%)	41 34	36, 53, 88, 133	0
8	H	226/232 (97%)	-0.20	6 (2%)	54 48	28, 45, 80, 142	0
8	V	226/232 (97%)	-0.13	5 (2%)	62 56	34, 49, 82, 156	0
9	I	204/205 (99%)	-0.50	1 (0%)	91 89	30, 42, 74, 95	0
9	W	204/205 (99%)	-0.41	3 (1%)	73 70	32, 46, 79, 105	0
10	J	195/198 (98%)	-0.27	3 (1%)	73 70	32, 48, 73, 123	0
10	X	195/198 (98%)	-0.32	4 (2%)	63 58	33, 49, 75, 136	0
11	K	212/212 (100%)	-0.30	3 (1%)	75 71	30, 48, 71, 92	0
11	Y	212/212 (100%)	-0.35	1 (0%)	91 89	33, 48, 73, 95	0
12	L	222/222 (100%)	-0.32	3 (1%)	75 71	32, 50, 83, 119	0
12	Z	222/222 (100%)	-0.29	3 (1%)	75 71	29, 48, 81, 114	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.40	3 (1%) 77 73	31, 47, 70, 90	0
13	a	233/246 (94%)	-0.37	1 (0%) 92 91	30, 46, 68, 84	0
14	N	196/196 (100%)	-0.42	1 (0%) 91 89	30, 41, 70, 99	0
14	b	196/196 (100%)	-0.39	4 (2%) 65 60	30, 43, 72, 107	0
15	c	1/4 (25%)	-0.32	0 100 100	53, 53, 53, 53	0
15	d	1/4 (25%)	-0.30	0 100 100	49, 49, 49, 49	0
All	All	6346/6622 (95%)	-0.14	215 (3%) 45 38	28, 52, 99, 175	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	8.9
2	B	221	ASP	8.4
3	Q	50	LEU	8.2
10	J	1	MET	7.2
2	P	51	VAL	7.0
6	T	178	HIS	6.2
8	V	221	CYS	6.2
7	U	2	GLY	6.2
12	Z	174	TYR	6.0
2	B	51	VAL	5.9
14	b	195	GLN	5.9
2	P	218	GLY	5.8
8	H	226	GLU	5.8
3	C	236	GLN	5.7
8	V	226	GLU	5.6
14	N	195	GLN	5.6
1	A	2	THR	5.6
3	C	50	LEU	5.6
5	S	233	ILE	5.4
5	S	202	ASP	5.3
10	X	194	ASP	5.3
3	C	49	THR	5.3
10	X	1	MET	5.2
7	U	242	GLN	5.1
1	O	1	MET	5.0
10	J	194	ASP	5.0
3	Q	206	LYS	4.9
12	L	174	TYR	4.9
3	Q	48	SER	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	4.8
3	Q	229	GLN	4.8
2	P	182	ASP	4.7
6	F	244	ASN	4.7
3	Q	60	SER	4.7
3	C	240	GLU	4.7
1	O	250	LEU	4.7
9	W	1	SER	4.7
6	T	243	ILE	4.6
6	T	244	ASN	4.5
6	F	178	HIS	4.5
3	C	203	THR	4.4
3	C	238	LYS	4.4
3	Q	240	GLU	4.4
3	C	202	GLN	4.3
5	E	202	ASP	4.3
2	B	218	GLY	4.2
5	S	203	GLU	4.2
1	O	201	GLU	4.2
3	Q	204	GLY	4.2
2	P	53	SER	4.2
1	A	249	ALA	4.1
11	Y	212	GLY	4.1
5	S	173	ARG	4.0
1	A	1	MET	4.0
2	P	220	ASN	4.0
4	R	125	LEU	4.0
3	Q	225	GLU	4.0
4	D	242	GLU	3.9
5	S	227	GLU	3.9
5	E	173	ARG	3.9
2	B	219	ALA	3.9
3	C	206	LYS	3.8
2	P	52	THR	3.8
2	P	221	ASP	3.8
1	O	52	SER	3.7
3	Q	223	SER	3.7
6	T	2	THR	3.7
4	R	238	LYS	3.7
5	S	225	ASP	3.7
3	Q	237	GLU	3.6
6	T	230	ASP	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	X	193	ASP	3.5
2	P	222	GLY	3.5
9	I	1	SER	3.5
7	U	3	TYR	3.5
1	O	2	THR	3.4
2	B	220	ASN	3.4
3	Q	232	THR	3.4
2	P	59	ASP	3.4
3	Q	58	THR	3.3
3	Q	205	ALA	3.3
10	J	193	ASP	3.3
13	M	82	ASP	3.2
8	V	224	GLN	3.2
3	Q	187	GLU	3.2
2	P	240	LYS	3.2
1	O	248	GLU	3.2
8	H	198	GLU	3.2
3	Q	59	PRO	3.2
6	F	215	CYS	3.2
3	Q	55	THR	3.2
6	F	181	GLU	3.2
1	O	249	ALA	3.1
3	C	225	GLU	3.1
4	R	1	ASP	3.1
1	O	203	GLU	3.1
3	Q	1	GLY	3.1
7	G	240	ALA	3.1
8	V	222	ASP	3.1
5	E	233	ILE	3.0
6	F	228	LYS	3.0
2	P	203	SER	3.0
2	P	217	LYS	3.0
5	S	210	LEU	3.0
3	C	204	GLY	3.0
1	O	53	SER	3.0
9	W	192	ASP	3.0
1	A	250	LEU	3.0
3	Q	180	LYS	3.0
1	O	231	LYS	2.9
4	R	239	GLU	2.9
5	S	180	LYS	2.9
4	R	241	ALA	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	E	54	GLU	2.9
3	C	205	ALA	2.9
3	Q	202	GLN	2.9
1	A	62	SER	2.9
4	R	242	GLU	2.9
7	G	3	TYR	2.8
2	B	239	VAL	2.8
5	S	51	ASN	2.8
7	G	242	GLN	2.8
1	A	52	SER	2.8
4	R	230	GLU	2.8
6	T	241	LYS	2.8
5	E	204	SER	2.7
5	S	207	VAL	2.7
6	F	205	GLU	2.7
3	Q	224	SER	2.7
8	V	145	ASP	2.7
3	C	223	SER	2.7
4	R	201	GLU	2.7
1	A	228	PRO	2.6
5	S	201	ARG	2.6
13	a	1	THR	2.6
7	G	222	ASP	2.6
11	K	202	GLU	2.6
3	Q	46	ARG	2.6
4	R	217	GLN	2.6
3	Q	235	GLU	2.6
3	Q	239	GLN	2.6
6	T	206	LYS	2.6
3	Q	181	GLU	2.6
5	E	122	TYR	2.5
2	P	50	LYS	2.5
8	H	221	CYS	2.5
2	P	225	TYR	2.5
7	U	183	ASP	2.5
2	B	217	LYS	2.5
4	R	177	ASN	2.5
2	P	230	LYS	2.5
8	H	223	ILE	2.5
7	U	222	ASP	2.5
6	F	2	THR	2.5
3	C	180	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Q	175	LYS	2.5
9	W	2	ASP	2.5
6	F	241	LYS	2.5
5	S	204	SER	2.5
7	U	203	ASP	2.5
1	O	40	THR	2.4
6	F	204	LYS	2.4
11	K	147	ASP	2.4
8	H	222	ASP	2.4
12	Z	80	ASN	2.4
7	G	241	GLU	2.4
14	b	105	LYS	2.3
6	T	205	GLU	2.3
7	U	241	GLU	2.3
11	K	212	GLY	2.3
12	L	1	GLN	2.3
7	G	51	PRO	2.3
4	D	237	GLU	2.3
14	b	196	LEU	2.3
6	F	243	ILE	2.3
2	B	238	LEU	2.3
2	B	201	ASP	2.3
7	G	68	ARG	2.3
6	T	239	ALA	2.3
7	G	2	GLY	2.2
1	A	229	THR	2.2
1	A	231	LYS	2.2
7	U	206	GLY	2.2
3	Q	139	ARG	2.2
3	Q	203	THR	2.2
3	Q	51	LYS	2.2
13	M	216	ASN	2.2
7	U	230	GLU	2.2
8	H	224	GLN	2.2
2	B	242	GLY	2.2
2	B	244	THR	2.2
2	B	61	SER	2.2
6	T	139	LYS	2.2
2	P	60	THR	2.2
6	T	181	GLU	2.1
10	X	72	ASP	2.1
6	T	228	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	L	165	ASN	2.1
6	F	202	ASP	2.1
4	R	2	ARG	2.1
6	T	237	ASP	2.1
1	A	248	GLU	2.1
1	A	54	PRO	2.1
6	F	180	PRO	2.1
13	M	81	ALA	2.1
4	D	177	ASN	2.1
2	P	141	ASP	2.1
2	P	223	GLU	2.1
2	P	93	HIS	2.1
4	D	125	LEU	2.0
14	b	106	ASN	2.0
1	A	182	GLU	2.0
3	Q	57	ILE	2.0
3	Q	171	GLU	2.0
12	Z	173	LYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	ASJ	d	3	8/8	0.94	0.14	50,53,54,55	0
15	ASJ	c	3	8/8	0.95	0.14	52,57,60,61	0
15	N7P	d	1	10/11	0.96	0.15	42,46,50,54	0
15	N7P	c	1	10/11	0.97	0.15	47,52,56,60	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
16	MG	G	301	1/1	0.93	0.11	47,47,47,47	0
16	MG	I	301	1/1	0.94	0.08	50,50,50,50	0
16	MG	Z	301	1/1	0.94	0.10	52,52,52,52	0
16	MG	N	201	1/1	0.96	0.10	48,48,48,48	0
16	MG	K	301	1/1	0.97	0.12	47,47,47,47	0
16	MG	L	301	1/1	0.98	0.06	47,47,47,47	0
16	MG	I	302	1/1	0.99	0.08	44,44,44,44	0
17	CL	U	301	1/1	0.99	0.17	42,42,42,42	0
17	CL	G	302	1/1	1.00	0.10	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.