wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2024 – 03:46 PM EDT

PDB ID	:	4PKN
Title	:	Crystal structure of the football-shaped GroEL-GroES2-(ADPBeFx)14 complex containing substrate Rubisco
Authors	:	Fei, X.; Ye, X.; Laronde-Leblanc, N.; Lorimer, G.H.
Deposited on	:	2014-05-15
Resolution	:	3.66 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 (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	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.66 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 64579 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.

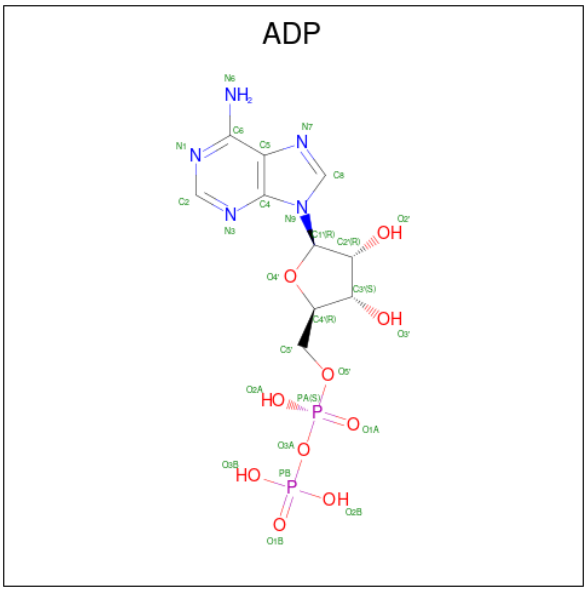
- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	A	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	B	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	F	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	E	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	C	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	D	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	K	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	J	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	I	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	L	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	M	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	H	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	N	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0

- Molecule 2 is a protein called 10 kDa chaperonin.

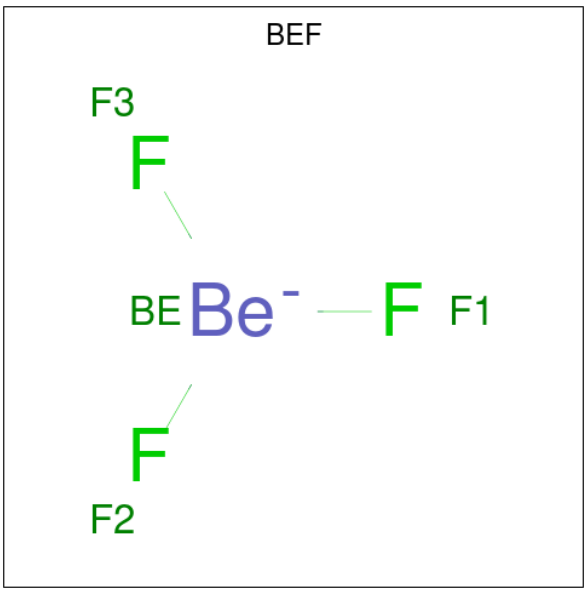
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	P	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Q	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	U	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	T	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	R	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	S	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	X	95	Total	C	N	O	S	0	0	0
			714	446	125	142	1			
2	W	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	V	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Y	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Z	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	2	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	1	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Be F 4 1 3	0	0
4	A	1	Total Be F 4 1 3	0	0
4	B	1	Total Be F 4 1 3	0	0
4	F	1	Total Be F 4 1 3	0	0
4	E	1	Total Be F 4 1 3	0	0
4	C	1	Total Be F 4 1 3	0	0
4	D	1	Total Be F 4 1 3	0	0
4	K	1	Total Be F 4 1 3	0	0
4	J	1	Total Be F 4 1 3	0	0
4	I	1	Total Be F 4 1 3	0	0
4	L	1	Total Be F 4 1 3	0	0
4	M	1	Total Be F 4 1 3	0	0
4	H	1	Total Be F 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total Be F 4 1 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	I	1	Total Mg 1 1	0	0
5	L	1	Total Mg 1 1	0	0
5	M	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	N	1	Total Mg 1 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	F	1	Total K 1 1	0	0
6	E	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	K	1	Total K 1 1	0	0
6	J	1	Total K 1 1	0	0
6	I	1	Total K 1 1	0	0
6	L	1	Total K 1 1	0	0
6	M	1	Total K 1 1	0	0
6	H	1	Total K 1 1	0	0
6	N	1	Total K 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	171.95Å 173.65Å 411.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.19 – 3.66	Depositor
% Data completeness (in resolution range)	99.5 (122.19-3.66)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.188 , 0.241	Depositor
Wilson B-factor (Å^2)	87.5	Xtriage
Anisotropy	0.664	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.190 for k,h,-l	Xtriage
Total number of atoms	64579	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.