



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2018 – 11:39 AM EST

PDB ID : 5H7J
Title : Crystal structure of Elongation factor 2
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Deposited on : 2016-11-18
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

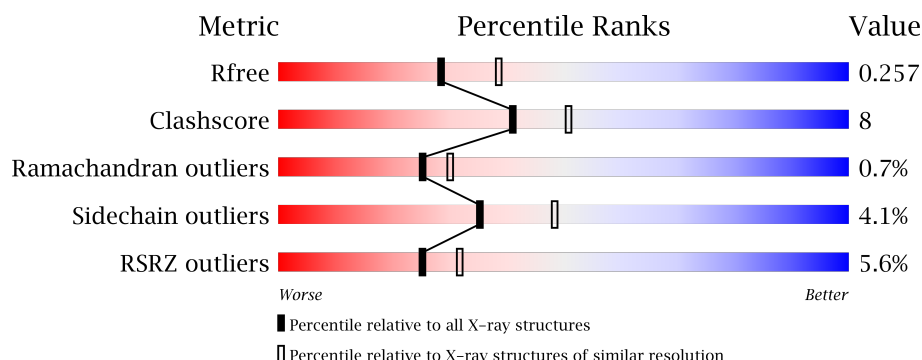
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	743	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>••</div> <div>8%</div> </div> </div>
1	B	743	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11116 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.

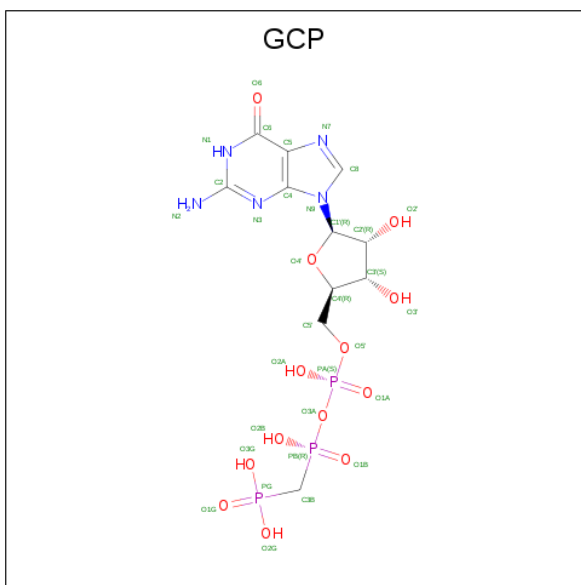
- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5419	3444	951	991	33			
1	B	692	Total	C	N	O	S	0	0	0
			5460	3467	957	1002	34			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O59521
A	2	VAL	-	expression tag	UNP O59521
A	3	GLU	-	expression tag	UNP O59521
A	736	LEU	-	expression tag	UNP O59521
A	737	GLU	-	expression tag	UNP O59521
A	738	HIS	-	expression tag	UNP O59521
A	739	HIS	-	expression tag	UNP O59521
A	740	HIS	-	expression tag	UNP O59521
A	741	HIS	-	expression tag	UNP O59521
A	742	HIS	-	expression tag	UNP O59521
A	743	HIS	-	expression tag	UNP O59521
B	1	MET	-	expression tag	UNP O59521
B	2	VAL	-	expression tag	UNP O59521
B	3	GLU	-	expression tag	UNP O59521
B	736	LEU	-	expression tag	UNP O59521
B	737	GLU	-	expression tag	UNP O59521
B	738	HIS	-	expression tag	UNP O59521
B	739	HIS	-	expression tag	UNP O59521
B	740	HIS	-	expression tag	UNP O59521
B	741	HIS	-	expression tag	UNP O59521
B	742	HIS	-	expression tag	UNP O59521
B	743	HIS	-	expression tag	UNP O59521

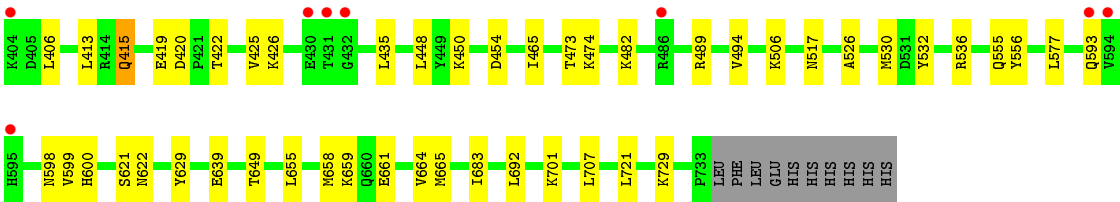
- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	113	Total O 113 113	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.22Å 116.13Å 189.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.30 46.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.59-2.30) 99.2 (46.29-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.257 0.215 , 0.257	Depositor DCC
R_{free} test set	4131 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11116	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	0.47	0/5519	0.66	6/7462 (0.1%)
1	B	0.47	0/5560	0.62	1/7519 (0.0%)
All	All	0.47	0/11079	0.64	7/14981 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	692	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	435	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	19	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	367	ARG	CA-CB-CG	5.51	125.53	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	GLN	Peptide

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	5419	0	5544	105	0
1	B	5460	0	5587	72	0
2	B	32	0	14	4	0
3	A	92	0	0	8	0
3	B	113	0	0	6	0
All	All	11116	0	11145	178	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 8.

The worst 5 of 178 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)
1:A:457:ILE:HG22	1:A:459:ILE:HG13	1.61	0.82
1:A:426:LYS:NZ	1:A:433:GLN:HE22	1.77	0.81
1:A:596:GLU:OE2	3:A:801:HOH:O	1.98	0.81
1:A:426:LYS:HZ2	1:A:433:GLN:HE22	1.29	0.80
1:A:622:ASN:ND2	3:A:803:HOH:O	2.13	0.80

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	678/743 (91%)	657 (97%)	17 (2%)	4 (1%)	28 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	686/743 (92%)	664 (97%)	17 (2%)	5 (1%)	25	30
All	All	1364/1486 (92%)	1321 (97%)	34 (2%)	9 (1%)	25	30

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	GLN
1	B	366	LEU
1	A	33	ILE
1	B	280	SER
1	B	281	ASP

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	589/638 (92%)	563 (96%)	26 (4%)	33	45
1	B	594/638 (93%)	571 (96%)	23 (4%)	37	51
All	All	1183/1276 (93%)	1134 (96%)	49 (4%)	35	48

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	577	LEU
1	B	22	GLU
1	B	649	THR
1	A	707	LEU
1	B	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	ASN
1	B	622	ASN

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Mol	Chain	Res	Type
1	B	433	GLN
1	A	433	GLN
1	B	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
2	GCP	B	801	-	25,34,34	2.91	8 (32%)	28,54,54	1.40	1 (3%)

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
2	GCP	B	801	-	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GCP	C4-N9	-11.58	1.32	1.47
2	B	801	GCP	C8-N9	-3.52	1.36	1.46
2	B	801	GCP	PG-O2G	-2.46	1.49	1.54
2	B	801	GCP	C2-N1	-2.21	1.35	1.44
2	B	801	GCP	C5-C6	-2.17	1.49	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GCP	PA-O3A-PB	-5.97	113.14	132.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GCP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	686/743 (92%)	0.60	59 (8%) 11 16	32, 60, 97, 115	0
1	B	692/743 (93%)	0.33	18 (2%) 56 63	26, 55, 85, 108	0
All	All	1378/1486 (92%)	0.46	77 (5%) 25 32	26, 57, 93, 115	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	ARG	5.9
1	A	413	LEU	5.7
1	A	403	VAL	5.5
1	B	388	TYR	5.4
1	A	405	ASP	5.1

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

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GCP	B	801	32/32	0.84	0.21	1.33	51,69,87,88	32

6.5 Other polymers ⓘ

There are no such residues in this entry.