Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2023 – 04:53 am GMT

PDB ID	:	2JGR
Title	:	Crystal structure of YegS in complex with ADP
Authors	:	Bakali, H.M.; Herman, M.D.; Johnson, K.A.; Kelly, A.A.; Wieslander, A.; Hallberg, B.M.; Nordlund, P.
Deposited on	:	2007-02-14
Resolution	:	2.65 Å(reported)

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

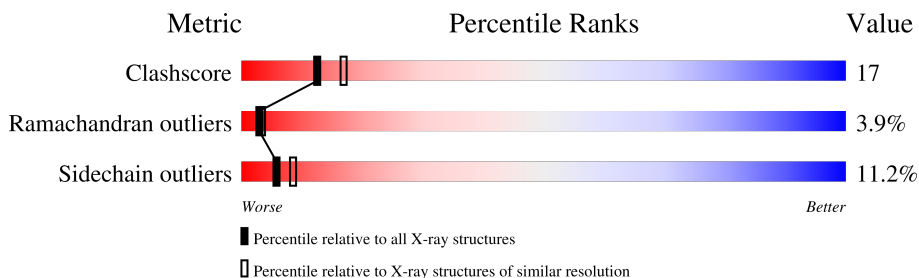|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		3.9%
Sidechain outliers		11.2%

Worse _____ *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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%

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	299	58% 22% 7% 13%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2001 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 YEGS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total 1966	C 1235	N 347	O 372	S 6	Se 6	0	1	0

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).
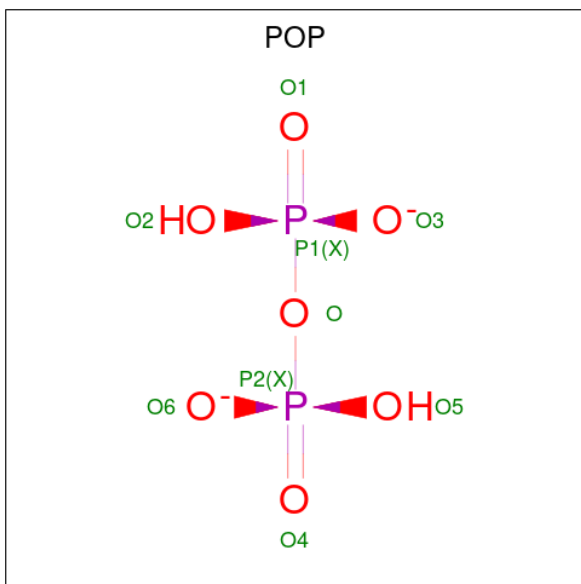
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 9	O 7	P 2	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS was not executed.

• Molecule 1: YEGS

Chain A:
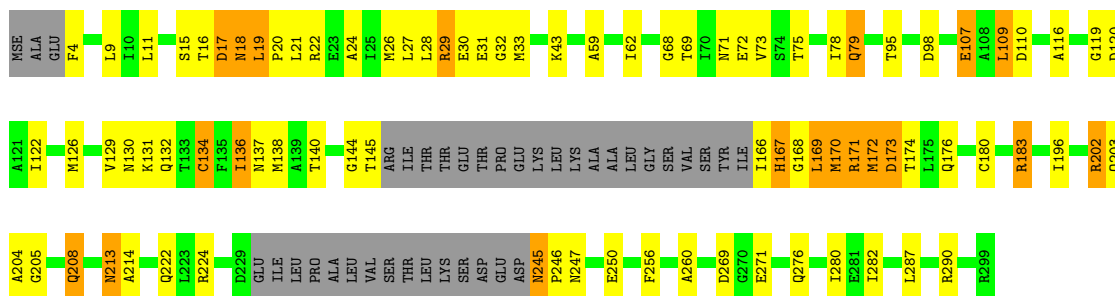
4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.97Å 124.97Å 54.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.39 – 2.65	Depositor
% Data completeness (in resolution range)	95.8 (88.39-2.65)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2001	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.04	3/1997 (0.2%)	1.00	2/2697 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	CYS	CB-SG	-11.85	1.62	1.82
1	A	107	GLU	CG-CD	5.63	1.60	1.51
1	A	180	CYS	CB-SG	-5.63	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	LEU	CA-CB-CG	7.72	133.06	115.30
1	A	120	ASP	CB-CG-OD1	5.46	123.21	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	THR	Peptide

5.2 Too-close contacts ⓘ

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	1966	0	1955	66	0
2	A	9	0	0	0	0
3	A	26	0	0	4	0
All	All	2001	0	1955	66	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 17.

All (66) 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:170:MSE:CE	1:A:170:MSE:SE	2.15	1.44
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.21	1.02
1:A:24:ALA:O	1:A:28:LEU:HD13	1.70	0.90
1:A:26:MSE:HE1	1:A:29:ARG:HH21	1.42	0.85
1:A:202:ARG:NH1	1:A:214:ALA:O	2.09	0.84
1:A:126:MSE:SE	1:A:136:ILE:HG13	2.30	0.82
1:A:144:GLY:HA3	1:A:172:MSE:HE1	1.64	0.80
1:A:202:ARG:HH11	1:A:202:ARG:CG	1.98	0.76
1:A:18:ASN:OD1	1:A:20:PRO:HG2	1.89	0.72
1:A:69:THR:O	1:A:73:VAL:HG23	1.92	0.70
1:A:144:GLY:HA3	1:A:172:MSE:CE	2.24	0.68
1:A:31:GLU:HB2	3:A:2005:HOH:O	1.96	0.66
1:A:29:ARG:HD2	3:A:2004:HOH:O	1.95	0.64
1:A:138:MSE:HG2	1:A:204:ALA:HB2	1.80	0.62
1:A:202:ARG:HG3	1:A:202:ARG:NH1	2.03	0.62
1:A:109:LEU:HD22	1:A:109:LEU:O	1.99	0.61
1:A:129:VAL:HG22	1:A:280:ILE:HG12	1.82	0.60
1:A:213:ASN:HD21	1:A:224[B]:ARG:HH12	1.49	0.60
1:A:19:LEU:N	1:A:20:PRO:HD2	2.16	0.60
1:A:68:GLY:O	1:A:72:GLU:HG3	2.03	0.59
1:A:71:ASN:HD21	1:A:269:ASP:CB	2.18	0.57
1:A:245:ASN:HD22	1:A:246:PRO:HD2	1.70	0.56
1:A:245:ASN:HD22	1:A:246:PRO:CD	2.19	0.56
1:A:166:ILE:O	1:A:169:LEU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:ND2	1:A:224[B]:ARG:HH12	2.04	0.56
1:A:126:MSE:HE3	1:A:134:CYS:HB3	1.86	0.56
1:A:208:GLN:HE21	1:A:208:GLN:N	2.04	0.56
1:A:245:ASN:HD22	1:A:246:PRO:N	2.04	0.54
1:A:245:ASN:HD22	1:A:245:ASN:C	2.11	0.54
1:A:137:ASN:HB3	1:A:269:ASP:OD1	2.09	0.53
1:A:144:GLY:CA	1:A:172:MSE:HE1	2.37	0.53
1:A:71:ASN:ND2	1:A:269:ASP:HB2	2.23	0.53
1:A:107:GLU:HG2	3:A:2016:HOH:O	2.09	0.52
1:A:166:ILE:C	1:A:169:LEU:HB2	2.30	0.50
1:A:71:ASN:HD21	1:A:269:ASP:HB2	1.76	0.50
1:A:71:ASN:ND2	1:A:269:ASP:CB	2.75	0.50
1:A:75:THR:O	1:A:79:GLN:HG2	2.13	0.49
1:A:245:ASN:HD21	1:A:247:ASN:HB2	1.76	0.48
1:A:26:MSE:CE	1:A:29:ARG:HH21	2.22	0.48
1:A:222:GLN:NE2	1:A:224[B]:ARG:HH22	2.12	0.48
1:A:22:ARG:O	1:A:26:MSE:HG2	2.14	0.47
1:A:183:ARG:O	1:A:256:PHE:HA	2.15	0.47
1:A:173:ASP:OD2	1:A:173:ASP:N	2.47	0.46
1:A:245:ASN:C	1:A:245:ASN:ND2	2.68	0.46
1:A:78:ILE:HD12	1:A:78:ILE:O	2.16	0.46
1:A:24:ALA:O	1:A:28:LEU:CD1	2.55	0.45
1:A:245:ASN:ND2	1:A:247:ASN:H	2.13	0.45
1:A:224[A]:ARG:HD2	1:A:250:GLU:HG2	1.98	0.45
1:A:29:ARG:HA	1:A:33:MSE:O	2.17	0.45
1:A:140:THR:HA	1:A:196:ILE:O	2.17	0.45
1:A:260:ALA:O	1:A:276:GLN:HB3	2.17	0.44
1:A:98:ASP:HB3	1:A:203:GLN:HG3	2.00	0.44
1:A:78:ILE:HD12	1:A:78:ILE:C	2.37	0.43
1:A:78:ILE:HG22	1:A:287:LEU:HB3	2.00	0.43
1:A:9:LEU:HD12	1:A:62:ILE:O	2.18	0.43
1:A:116:ALA:O	1:A:290:ARG:HD2	2.18	0.43
1:A:166:ILE:N	1:A:169:LEU:HD22	2.35	0.42
1:A:30:GLU:C	1:A:32:GLY:N	2.74	0.41
1:A:28:LEU:HB3	1:A:33:MSE:HE3	2.02	0.41
1:A:167:HIS:HB3	1:A:168:GLY:H	1.58	0.41
1:A:28:LEU:HD12	1:A:28:LEU:N	2.36	0.40
1:A:11:LEU:HD21	1:A:21:LEU:HD21	2.02	0.40
1:A:176:GLN:HE21	1:A:176:GLN:HB3	1.67	0.40
1:A:202:ARG:NH1	1:A:202:ARG:CG	2.69	0.40
1:A:59:ALA:HB3	3:A:2002:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:O	1:A:132:GLN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	256/299 (86%)	230 (90%)	16 (6%)	10 (4%)	3 3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	167	HIS
1	A	170	MSE
1	A	119	GLY
1	A	131	LYS
1	A	169	LEU
1	A	171	ARG
1	A	205	GLY
1	A	15	SER
1	A	17	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	206/231 (89%)	183 (89%)	23 (11%)	6 8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	17	ASP
1	A	19	LEU
1	A	29	ARG
1	A	43	LYS
1	A	79	GLN
1	A	95	THR
1	A	109	LEU
1	A	110	ASP
1	A	122	ILE
1	A	136	ILE
1	A	145	THR
1	A	171	ARG
1	A	172	MSE
1	A	173	ASP
1	A	174	THR
1	A	183	ARG
1	A	202	ARG
1	A	208	GLN
1	A	213	ASN
1	A	245	ASN
1	A	271	GLU
1	A	282	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	176	GLN
1	A	203	GLN
1	A	208	GLN
1	A	209	GLN
1	A	213	ASN
1	A	222	GLN
1	A	245	ASN
1	A	276	GLN

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 monosaccharides 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	POP	A	1300	-	6,8,8	0.40	0	13,13,13	1.50	2 (15%)

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	POP	A	1300	-	-	1/6/6/6	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1300	POP	O6-P2-O	3.33	115.80	104.64
2	A	1300	POP	O2-P1-O	2.60	113.36	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1300	POP	P2-O-P1-O3

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.