

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 - 04:14 AM EDT

PDB ID	:	3E9R
Title	:	Crystal structure of purine nucleoside phosphorylase from Schistosoma man-
		soni in complex with adenine
Authors	:	Pereira, H.M.; Rezende, M.M.; Oliva, G.; Garratt, R.C.
Deposited on		
Resolution	:	1.85 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 (1)) were used in the production of this report:

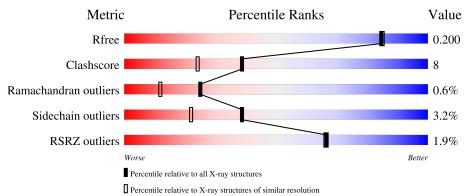
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.85 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2469(1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592(1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	А	287	85%	14% ••
1	В	287	5%	12% • 5%
1	С	287	87%	11% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	А	291	-	Х	-	-
2	SO4	А	704	-	Х	-	-
2	SO4	В	291	-	Х	-	-
2	SO4	С	291	-	Х	-	-
3	ACT	С	700	-	-	Х	-



2 Entry composition (i)

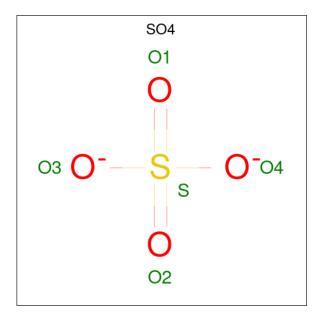
There are 6 unique types of molecules in this entry. The entry contains 7206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	285	Total	С	Ν	0	S	0	0	0
	A	200	2161	1376	372	399	14	0		0
1	Р	273	Total	С	Ν	0	S	0	1	0
	D	213	2066	1316	355	381	14	0		
1	С	284	Total	С	Ν	0	S	0	2	0
		204	2161	1378	373	396	14	0		U

• Molecule 1 is a protein called Purine-nucleoside phosphorylase.

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

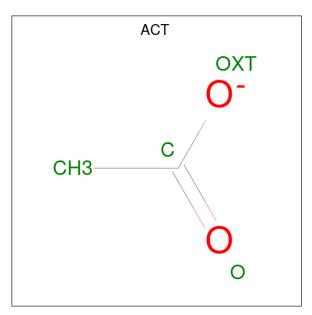
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	С	1	Total 5	0 4	S 1	0	0

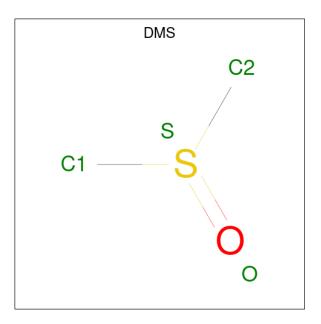
• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



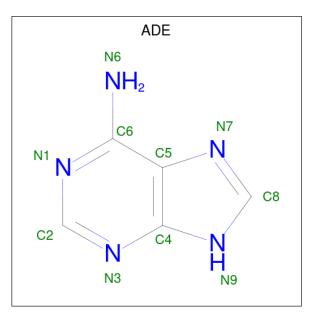
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	В	1	Total 10	С 5	N 5	0	0



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	270	Total O 270 270	0	0
6	В	240	Total O 240 240	0	0
6	С	258	Total O 258 258	0	0

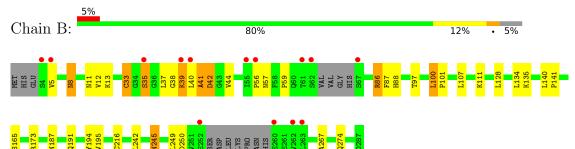


3 Residue-property plots (i)

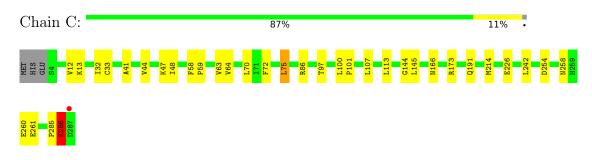
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Purine-nucleoside phosphorylase

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• Molecule 1: Purine-nucleoside phosphorylase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.99Å 120.00Å 130.98Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.03 - 1.85	Depositor
Resolution (A)	41.03 - 1.85	EDS
% Data completeness	96.6 (41.03-1.85)	Depositor
(in resolution range)	96.6 (41.03-1.85)	EDS
R _{merge}	0.08	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$2.96 (at 1.86 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
D D.	0.162 , 0.201	Depositor
R, R_{free}	0.161 , 0.200	DCC
R_{free} test set	3266 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.2	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 49.8	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7206	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: ACT, SO4, DMS, ADE

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.38	0/2199	0.54	0/2978	
1	В	0.37	0/2100	0.56	0/2840	
1	С	0.39	0/2206	0.56	0/2988	
All	All	0.38	0/6505	0.55	0/8806	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2161	0	2211	32	0
1	В	2066	0	2101	36	0
1	С	2161	0	2214	29	0
2	А	10	0	0	1	0
2	В	5	0	0	1	0
2	С	5	0	0	0	0
3	А	4	0	3	1	0
3	С	4	0	3	2	0
4	А	4	0	6	0	0
4	В	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	С	4	0	6	0	0
5	В	10	0	4	0	0
6	А	270	0	0	6	0
6	В	240	0	0	8	0
6	С	258	0	0	9	0
All	All	7206	0	6554	98	0

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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 98 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:4:SER:HB3	6:A:937:HOH:O	1.75	0.87
1:A:173:ARG:HH11	1:A:191:GLN:HE22	1.25	0.84
1:A:76:SER:HB3	1:A:282:GLU:HG3	1.60	0.84
1:B:12:VAL:HG12	1:B:107:LEU:HD22	1.60	0.81
1:C:59:PRO:HB3	1:C:97:THR:HG23	1.63	0.81

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	Analysed Favoured Al		Outliers	Percentiles
1	А	283/287~(99%)	277~(98%)	5(2%)	1 (0%)	34 19
1	В	268/287~(93%)	258 (96%)	7 (3%)	3 (1%)	14 4
1	С	284/287~(99%)	279~(98%)	4 (1%)	1 (0%)	34 19
All	All	835/861~(97%)	814 (98%)	16 (2%)	5 (1%)	25 12

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	41	ALA
1	В	42	ASP
1	С	286	LYS
1	А	64	VAL
1	В	35	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	238/242~(98%)	232~(98%)	6(2%)	47 31		
1	В	224/242~(93%)	213~(95%)	11 (5%)	25 9		
1	С	238/242~(98%)	233~(98%)	5(2%)	53 38		
All	All	700/726~(96%)	678~(97%)	22 (3%)	39 23		

5 of 22 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	245	ASN
1	С	70	LEU
1	В	250	ASP
1	С	75	LEU
1	В	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	274	GLN
1	С	57	ASN
1	С	20	GLN
1	С	146	ASN
1	А	258	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands 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	Turne	Chain	Res	Link	B	ond len	gths	E	ond ang	gles
MOI	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	ACT	А	700	-	3,3,3	1.44	1 (33%)	$3,\!3,\!3$	0.38	0
4	DMS	А	703	-	3,3,3	1.46	1 (33%)	3,3,3	0.52	0
5	ADE	В	288	-	9,11,11	1.03	1 (11%)	7,15,15	1.07	0
2	SO4	А	291	-	4,4,4	2.95	4 (100%)	6,6,6	0.25	0
2	SO4	А	704	-	4,4,4	3.10	4 (100%)	6,6,6	0.14	0
2	SO4	В	291	-	4,4,4	2.90	4 (100%)	6,6,6	0.25	0
3	ACT	С	700	-	3,3,3	1.32	0	3,3,3	0.41	0
4	DMS	В	703	-	3,3,3	1.35	0	3,3,3	0.65	0
4	DMS	С	703	-	3,3,3	1.43	1 (33%)	3,3,3	0.75	0
2	SO4	С	291	-	4,4,4	2.91	4 (100%)	$6,\!6,\!6$	0.20	0

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
5	ADE	В	288	-	-	-	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	704	SO4	O1-S	3.81	1.66	1.46
2	А	704	SO4	O2-S	3.70	1.66	1.46
2	А	291	SO4	O1-S	3.66	1.65	1.46
2	А	291	SO4	O2-S	3.58	1.65	1.46
2	С	291	SO4	O2-S	3.54	1.65	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	700	ACT	1	0
2	А	291	SO4	1	0
2	В	291	SO4	1	0
3	С	700	ACT	2	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, 95^{th} 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	$\langle RSRZ \rangle$	$\#RSRZ{>}2$		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	285/287~(99%)	-0.38	1 (0%) 92	92	13, 24, 51, 102	0
1	В	273/287~(95%)	-0.08	14 (5%) 28	26	15, 26, 63, 147	1 (0%)
1	С	284/287~(98%)	-0.38	1 (0%) 92	92	13, 24, 51, 113	1 (0%)
All	All	842/861~(97%)	-0.28	16 (1%) 66	66	13, 25, 54, 147	2(0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	40	LEU	12.1
1	С	287	ASP	6.4
1	В	252	GLU	4.7
1	В	35	SER	4.0
1	В	56	PRO	3.3

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 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, 95^{th} 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	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
2	SO4	А	704	5/5	0.87	0.20	57,63,68,74	0
3	ACT	С	700	4/4	0.88	0.24	22,28,40,45	0
3	ACT	А	700	4/4	0.93	0.13	14,14,16,38	0
5	ADE	В	288	10/10	0.94	0.10	20,31,37,37	0
2	SO4	С	291	5/5	0.95	0.20	38,39,45,65	0
2	SO4	А	291	5/5	0.98	0.15	32,35,44,45	0
4	DMS	А	703	4/4	0.99	0.07	$14,\!15,\!17,\!18$	0
4	DMS	В	703	4/4	0.99	0.05	17,17,19,21	0
4	DMS	С	703	4/4	0.99	0.07	20,20,20,20	0
2	SO4	В	291	5/5	0.99	0.09	26,28,37,40	0

6.5 Other polymers (i)

There are no such residues in this entry.

