



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PNR
Title : PURINE REPRESSOR-HYPOXANTHINE-PURF-OPERATOR COMPLEX
Authors : Schumacher, M.A.; Choi, K.Y.; Zalkin, H.; Brennan, R.G.
Deposited on : 1995-03-29
Resolution : 2.70 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

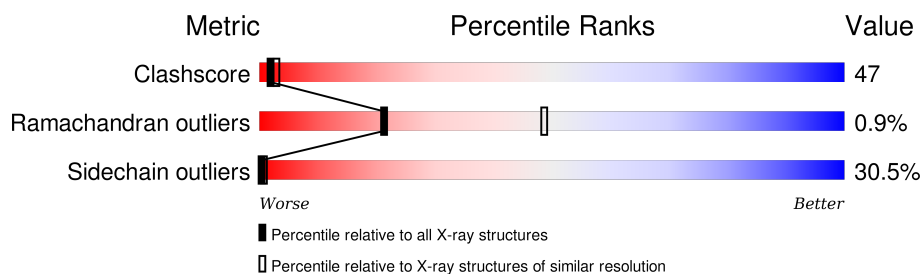
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.


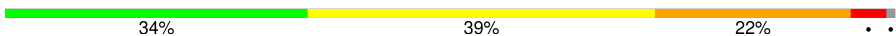
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	
2	A	340	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3054 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.

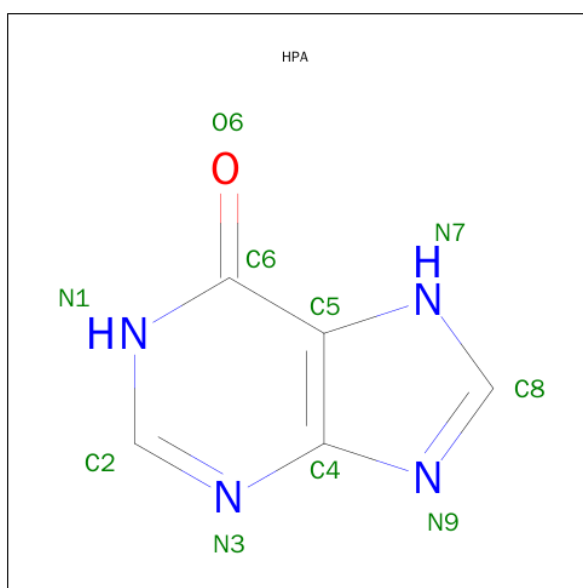
- Molecule 1 is a DNA chain called DNA (5'-D(*AP*AP*CP*GP*AP*AP*AP*AP*CP*GP*TP*TP*TP*TP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	17	Total	C	N	O	P	0	0	0
			346	167	64	99	16			

- Molecule 2 is a protein called PROTEIN (PURINE REPRESSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	338	Total	C	N	O	S	0	0	0
			2652	1671	469	493	19			

- Molecule 3 is HYPOXANTHINE (three-letter code: HPA) (formula: C₅H₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	2	Total 2	O 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(*AP*AP*CP*GP*AP*AP*AP*AP*CP*GP*TP*TP*TP*TP*CP*GP*T)-3')

Chain B: 

A699
A700
C701
G702
A703
A704
A705
A706
C707
G708
T709
T710
T711
T712
C713
G714
T715

- Molecule 2: PROTEIN (PURINE REPRESSOR)

Chain A: 

ALA
T3
I4
K5
R10
S14
T17
V18
S19
H20
V21
I22
N23
K24
T25
R26
F27
K103
Y107
L108
S109
A35
V36
M111
W37
A38
A39
I40
K41
E42
L43
H44
Y45
S46
P47
V50
A51
R52
S53
L54
K55
V56
N57
H58
T59
K60
S61
I62
G63
L64
L65
A71
F74

E79
E82
K83
R84
C85
F86
Q87
K88
Y90
T91
L92
N99
M100
L101
E102
K103
Y107
L108
S109
A110
A112
Q113
K114
R115
V116
D117
G118
L119
H120
V121
M122
C123
S124
P127
E128
L129
K130
V131
M132
H133
L134
E135
R138
H139
I140
P141
M142
V143
I144
M145

D146
E149
A150
K151
A152
D153
F154
T155
D156
A157
V158
I159
D160
N161
A162
F163
E164
G165
G166
R171
Y172
L173
I174
R176
R179
E180
I181
G182
V183
I184
P185
G186
P187
R190
N191
T192
G193
R196
L197
A198
G199
F200
M201
R202
A203
M204
E205
E206
A207
M208
I209
K210

V211
F212
S213
S214
W215
I216
V217
Q218
G219
D220
F221
E222
P223
E224
S225
G226
Y227
R228
A229
M230
Q231
Q232
I233
L234
S235
Q236
P237
H238
R239
P240
T241
A242
V243
F244
I249
M250
A251
R252
L255
C256
A257
E260
M261
G262
L263
R264
V265
Y269
S270
L271
I272
G273
Y274
D275
I276
V277

R278
M279
A280
R281
Y282
F283
T284
F285
A286
L287
L288
T289
I290
H291
Q292
P293
K294
D295
S296
L297
G298
E299
T300
T301
A302
R303
M304
L305
L306
D307
R308
I309
V310
N311
K312
R313
R314
E315
P316
Q317
S318
I319
E320
V321
H322
L325
I326
E327
R328
R329
R337
R340
ARG

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	175.85Å 94.79Å 81.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: HPA

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	B	0.87	0/388	2.80	33/597 (5.5%)
2	A	1.31	5/2706 (0.2%)	1.64	43/3660 (1.2%)
All	All	1.26	5/3094 (0.2%)	1.85	76/4257 (1.8%)

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
2	A	2	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	37	TRP	CB-CG	-6.38	1.38	1.50
2	A	213	GLU	CG-CD	6.07	1.61	1.51
2	A	244	PHE	CE2-CZ	5.76	1.48	1.37
2	A	243	VAL	CB-CG1	-5.62	1.41	1.52
2	A	243	VAL	CA-CB	-5.16	1.44	1.54

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	DA	C4-N9-C1'	-18.56	92.89	126.30
1	B	703	DA	C8-N9-C1'	18.32	160.68	127.70
1	B	705	DA	C8-N9-C1'	13.55	152.08	127.70
1	B	705	DA	C4-N9-C1'	-13.51	101.98	126.30
1	B	706	DA	C8-N9-C1'	12.45	150.11	127.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	211	VAL	CA
2	A	294	LYS	CA

There are no planarity outliers.

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	B	346	0	194	25	2
2	A	2652	0	2636	254	0
3	A	10	0	4	0	0
4	A	44	0	0	0	1
4	B	2	0	0	0	0
All	All	3054	0	2834	275	3

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 47.

The worst 5 of 275 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:B:713:DC:H2"	1:B:714:DG:H5"	1.25	1.16
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.16	1.08
2:A:61:SER:HB2	2:A:91:THR:HG22	1.16	1.08
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.26	1.01
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.81	0.95

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:718:HOH:O	4:A:718:HOH:O[4_555]	1.83	0.37
1:B:703:DA:N6	1:B:712:DT:O4[4_555]	2.07	0.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:DG:O6	1:B:713:DC:N4[4_555]	2.19	0.01

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
2	A	336/340 (99%)	302 (90%)	31 (9%)	3 (1%)	21 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	311	ASN

5.3.2 Protein sidechains [i](#)

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
2	A	279/280 (100%)	194 (70%)	85 (30%)	0 1

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	145	MET
2	A	205	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	312	LYS
2	A	151	LYS
2	A	176	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
2	A	96	ASN
2	A	291	HIS
2	A	218	GLN
2	A	58	HIS
2	A	99	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	HPA	A	599	-	8,11,11	1.55	2 (25%)	4,15,15	4.21	2 (50%)

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
3	HPA	A	599	-	-	0/0/0/0	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C2-N1	2.01	1.37	1.33
3	A	599	HPA	C6-N1	3.12	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	HPA	N3-C2-N1	-5.99	124.31	128.89
3	A	599	HPA	C2-N1-C6	5.79	124.82	116.04

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 [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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.