



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2020 – 09:38 PM EST

PDB ID : 6WS0
Title : Rational drug design of phenazopyridine derivatives as novel inhibitors of Rev1-CT
Authors : McPherson, K.S.; Korzhnev, D.M.
Deposited on : 2020-04-30
Resolution : 2.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.15.1
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)	:	2.15.1

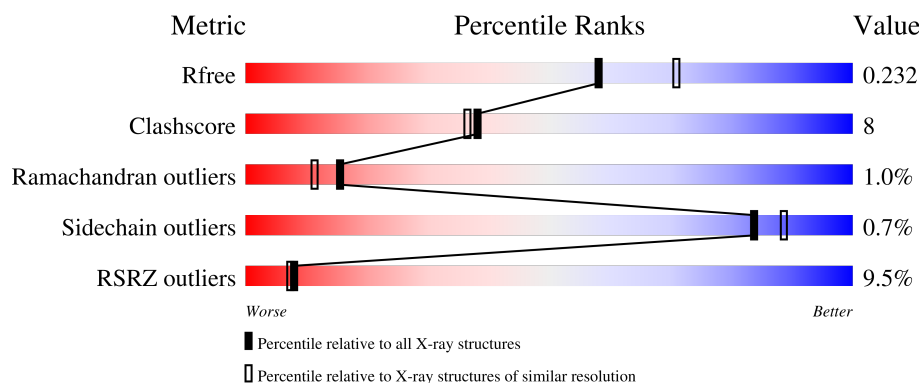
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 $\leq 5\%$. 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	HHH	95	<div> <div>9%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
2	CCC	227	<div> <div>7%</div> <div>68%</div> <div>16%</div> <div>16%</div> </div>
3	ZZZ	52	<div> <div>10%</div> <div>33%</div> <div>6%</div> <div>62%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5050 atoms, of which 2558 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 DNA repair protein REV1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	94	Total	C	H	N	O	S	34	0	0
			1539	490	776	119	149	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HHH	1157	GLY	-	expression tag	UNP Q9UBZ9

- Molecule 2 is a protein called Mitotic spindle assembly checkpoint protein MAD2B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	CCC	191	Total	C	H	N	O	S	73	1	0
			3178	1008	1615	266	279	10			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-15	MET	-	expression tag	UNP Q9UI95
CCC	-14	GLY	-	expression tag	UNP Q9UI95
CCC	-13	SER	-	expression tag	UNP Q9UI95
CCC	-12	SER	-	expression tag	UNP Q9UI95
CCC	-11	HIS	-	expression tag	UNP Q9UI95
CCC	-10	HIS	-	expression tag	UNP Q9UI95
CCC	-9	HIS	-	expression tag	UNP Q9UI95
CCC	-8	HIS	-	expression tag	UNP Q9UI95
CCC	-7	HIS	-	expression tag	UNP Q9UI95
CCC	-6	HIS	-	expression tag	UNP Q9UI95
CCC	-5	SER	-	expression tag	UNP Q9UI95
CCC	-4	GLN	-	expression tag	UNP Q9UI95
CCC	-3	ASP	-	expression tag	UNP Q9UI95
CCC	-2	PRO	-	expression tag	UNP Q9UI95
CCC	-1	ASN	-	expression tag	UNP Q9UI95

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	0	SER	-	expression tag	UNP Q9UI95
CCC	124	ALA	ARG	engineered mutation	UNP Q9UI95

- Molecule 3 is a protein called DNA polymerase zeta catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	ZZZ	20	Total	C	H	N	O	S	5	0	0
			322	97	167	28	28	2			

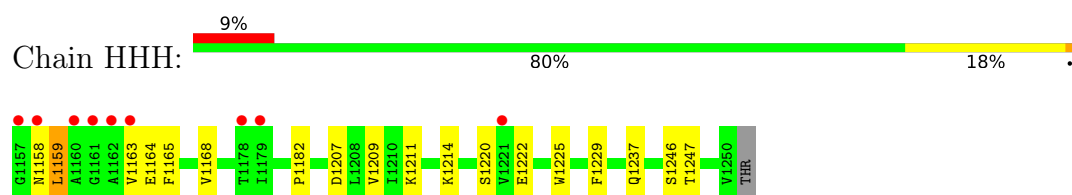
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	HHH	2	Total	O	0	0
			2	2		
4	CCC	9	Total	O	0	0
			9	9		

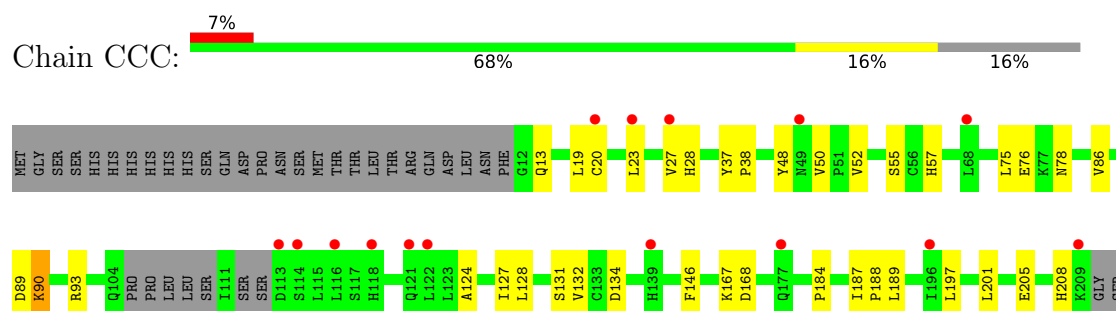
3 Residue-property plots

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 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.

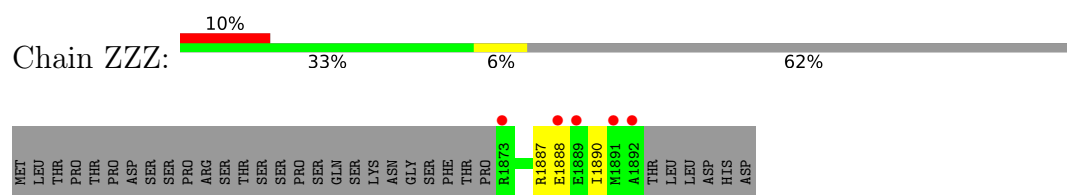
- Molecule 1: DNA repair protein REV1



- Molecule 2: Mitotic spindle assembly checkpoint protein MAD2B



- Molecule 3: DNA polymerase zeta catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.38Å 69.38Å 106.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.07 – 2.24 29.06 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.07-2.24) 99.5 (29.06-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.204 , 0.221 0.208 , 0.232	Depositor DCC
R_{free} test set	771 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.041 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5050	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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](#)

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	HHH	0.73	0/773	0.93	0/1046
2	CCC	0.76	0/1594	0.99	0/2162
3	ZZZ	0.71	0/157	0.89	0/211
All	All	0.75	0/2524	0.97	0/3419

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	HHH	763	776	773	12	0
2	CCC	1563	1615	1602	28	0
3	ZZZ	155	167	166	5	0
4	CCC	9	0	0	0	0
4	HHH	2	0	0	0	0
All	All	2492	2558	2541	38	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.

All (38) 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)
2:CCC:89:ASP:O	2:CCC:90:LYS:HB2	1.81	0.81
2:CCC:50:VAL:HG21	2:CCC:124:ALA:HB1	1.66	0.78
2:CCC:37:TYR:CE1	3:ZZZ:1890:ILE:HD12	2.31	0.66
2:CCC:28:HIS:CD2	2:CCC:55:SER:H	2.18	0.62
2:CCC:50:VAL:CG2	2:CCC:124:ALA:HB1	2.31	0.61
1:HHH:1207:ASP:OD1	1:HHH:1211:LYS:HE2	2.04	0.58
2:CCC:28:HIS:HD2	2:CCC:55:SER:H	1.52	0.57
1:HHH:1165:PHE:O	1:HHH:1168:VAL:N	2.40	0.55
2:CCC:13:GLN:HG2	2:CCC:76:GLU:HG2	1.88	0.55
1:HHH:1165:PHE:CE2	1:HHH:1209:VAL:HG23	2.43	0.54
1:HHH:1246:SER:HB3	2:CCC:184:PRO:HG2	1.93	0.51
2:CCC:128:LEU:O	2:CCC:131:SER:OG	2.25	0.51
2:CCC:23:LEU:O	2:CCC:27:VAL:HG23	2.10	0.50
2:CCC:167:LYS:O	2:CCC:168:ASP:HB2	2.12	0.49
1:HHH:1220:SER:HB3	1:HHH:1222:GLU:OE2	2.12	0.49
2:CCC:37:TYR:CD1	3:ZZZ:1890:ILE:HD12	2.48	0.49
2:CCC:37:TYR:CE1	3:ZZZ:1890:ILE:CD1	2.95	0.48
1:HHH:1158:ASN:OD1	1:HHH:1159:LEU:N	2.48	0.47
1:HHH:1165:PHE:HE2	1:HHH:1209:VAL:HG23	1.79	0.46
2:CCC:189:LEU:HD12	2:CCC:201:LEU:HG	1.98	0.46
2:CCC:78:ASN:O	2:CCC:78:ASN:CG	2.55	0.45
1:HHH:1182:PRO:HB3	1:HHH:1225:TRP:CH2	2.52	0.45
2:CCC:57:HIS:CE1	3:ZZZ:1890:ILE:HG12	2.52	0.45
2:CCC:13:GLN:CG	2:CCC:76:GLU:HG2	2.49	0.43
1:HHH:1214:LYS:HB2	1:HHH:1229:PHE:CZ	2.54	0.43
2:CCC:52:VAL:HG12	2:CCC:127:ILE:HG21	1.99	0.43
1:HHH:1237:GLN:NE2	1:HHH:1247:THR:HG23	2.34	0.42
2:CCC:86:VAL:O	2:CCC:146:PHE:HA	2.19	0.42
2:CCC:167:LYS:HA	2:CCC:167:LYS:HD3	1.86	0.42
1:HHH:1163:VAL:HG23	1:HHH:1164:GLU:N	2.35	0.42
2:CCC:20:CYS:SG	2:CCC:75:LEU:HD12	2.59	0.42
2:CCC:132:VAL:HG23	2:CCC:132:VAL:O	2.19	0.42
2:CCC:38:PRO:HD3	3:ZZZ:1887:ARG:HG3	2.03	0.41
2:CCC:89:ASP:OD1	2:CCC:93[A]:ARG:NH2	2.54	0.41
2:CCC:48:TYR:C	2:CCC:50:VAL:H	2.24	0.41
2:CCC:187:ILE:CD1	2:CCC:205:GLU:HG2	2.51	0.41
2:CCC:19:LEU:HD21	2:CCC:197:LEU:HD11	2.03	0.40
1:HHH:1207:ASP:HB2	2:CCC:188:PRO:HG2	2.03	0.40

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	HHH	92/95 (97%)	86 (94%)	5 (5%)	1 (1%)	14	9
2	CCC	187/227 (82%)	175 (94%)	11 (6%)	1 (0%)	29	28
3	ZZZ	18/52 (35%)	15 (83%)	2 (11%)	1 (6%)	2	0
All	All	297/374 (79%)	276 (93%)	18 (6%)	3 (1%)	15	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	ZZZ	1888	GLU
1	HHH	1159	LEU
2	CCC	90	LYS

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	
1	HHH	88/89 (99%)	88 (100%)	0	100	100
2	CCC	180/213 (84%)	178 (99%)	2 (1%)	73	80
3	ZZZ	18/49 (37%)	18 (100%)	0	100	100
All	All	286/351 (82%)	284 (99%)	2 (1%)	84	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	134	ASP
2	CCC	208	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

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

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	HHH	94/95 (98%)	0.30	9 (9%) 8 7	28, 48, 88, 102	0
2	CCC	191/227 (84%)	0.25	15 (7%) 12 12	25, 44, 84, 120	0
3	ZZZ	20/52 (38%)	0.75	5 (25%) 0 0	28, 48, 108, 112	0
All	All	305/374 (81%)	0.30	29 (9%) 8 7	25, 46, 92, 120	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	HHH	1162	ALA	6.4
1	HHH	1163	VAL	4.7
3	ZZZ	1892	ALA	4.3
1	HHH	1161	GLY	4.3
2	CCC	113	ASP	4.2
3	ZZZ	1873	ARG	4.1
1	HHH	1157	GLY	4.1
1	HHH	1158	ASN	3.3
2	CCC	118	HIS	3.2
2	CCC	122	LEU	3.0
3	ZZZ	1889	GLU	3.0
1	HHH	1160	ALA	3.0
3	ZZZ	1891	MET	2.8
3	ZZZ	1888	GLU	2.8
1	HHH	1179	ILE	2.7
1	HHH	1221	VAL	2.7
1	HHH	1178	THR	2.7
2	CCC	49	ASN	2.6
2	CCC	68	LEU	2.6
2	CCC	209	LYS	2.5
2	CCC	121	GLN	2.5
2	CCC	116	LEU	2.5
2	CCC	23	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	CCC	196	ILE	2.4
2	CCC	139	HIS	2.3
2	CCC	20	CYS	2.3
2	CCC	27	VAL	2.2
2	CCC	114	SER	2.1
2	CCC	177	GLN	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.