wwPDB X-ray Structure Validation Summary Report (i)

Jul 28, 2016 – 05:59 PM EDT

PDB ID	:	5G35
Title	:	Structure of Rad14 in complex with acetylaminopyren-C8-guanine containing DNA
Authors	:	Simon, N.; Ebert, C.; Schneider, S.
Deposited on	:	2016-04-18
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

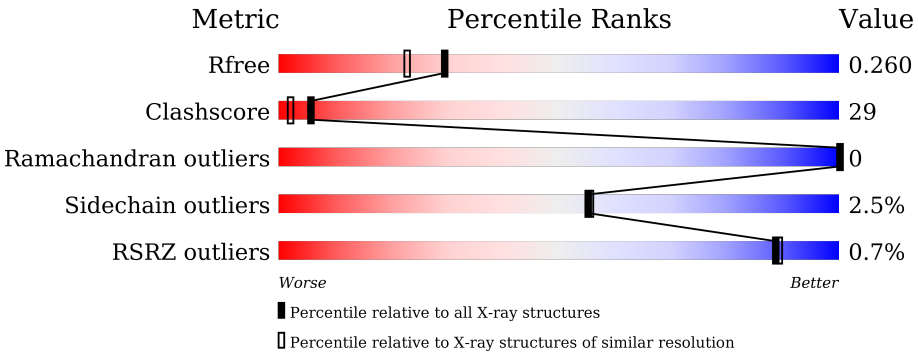
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	131	80% 7% 13%
1	B	131	77% 10% • 12%
2	C	15	7% 80% 7% 7%
2	E	15	13% 73% 7% 7%
3	D	14	7% 93%
3	F	14	93% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3093 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 RAD14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			930	588	162	172	8			
1	B	115	Total	C	N	O	S	0	0	0
			939	592	162	177	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	MET	-	INITIATING METHIONINE	UNP P28519
A	307	GLY	-	EXPRESSION TAG	UNP P28519
A	308	SER	-	EXPRESSION TAG	UNP P28519
A	309	ALA	-	EXPRESSION TAG	UNP P28519
A	310	TRP	-	EXPRESSION TAG	UNP P28519
A	311	SER	-	EXPRESSION TAG	UNP P28519
A	312	HIS	-	EXPRESSION TAG	UNP P28519
A	313	PRO	-	EXPRESSION TAG	UNP P28519
A	314	GLN	-	EXPRESSION TAG	UNP P28519
A	315	PHE	-	EXPRESSION TAG	UNP P28519
A	316	GLU	-	EXPRESSION TAG	UNP P28519
A	317	LYS	-	EXPRESSION TAG	UNP P28519
B	187	MET	-	INITIATING METHIONINE	UNP P28519
B	307	GLY	-	EXPRESSION TAG	UNP P28519
B	308	SER	-	EXPRESSION TAG	UNP P28519
B	309	ALA	-	EXPRESSION TAG	UNP P28519
B	310	TRP	-	EXPRESSION TAG	UNP P28519
B	311	SER	-	EXPRESSION TAG	UNP P28519
B	312	HIS	-	EXPRESSION TAG	UNP P28519
B	313	PRO	-	EXPRESSION TAG	UNP P28519
B	314	GLN	-	EXPRESSION TAG	UNP P28519
B	315	PHE	-	EXPRESSION TAG	UNP P28519
B	316	GLU	-	EXPRESSION TAG	UNP P28519
B	317	LYS	-	EXPRESSION TAG	UNP P28519

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*TP*CP*TP*AP*8PYP*TP*CP*AP*TP*CP*AP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			299	153	49	84	13			
2	E	14	Total	C	N	O	P	0	0	0
			299	153	49	84	13			

- Molecule 3 is a DNA chain called 5'-D(*GP*TP*GP*AP*TP*GP*AP*CP*GP*TP*AP*GP*AP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	57	80	13			
3	F	14	Total	C	N	O	P	0	0	0
			285	135	57	80	13			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

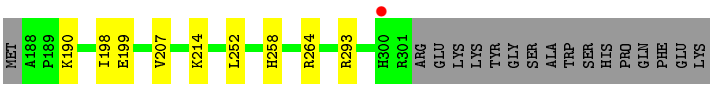
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	25	Total	O	0	0
			25	25		
5	C	4	Total	O	0	0
			4	4		
5	D	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

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.

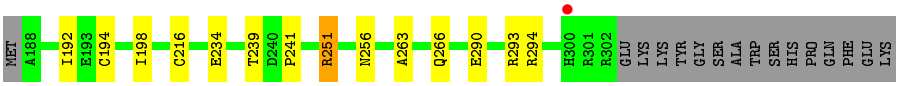
- Molecule 1: RAD14

Chain A:



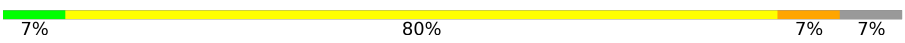
- Molecule 1: RAD14

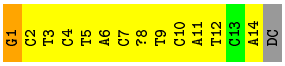
Chain B:



- Molecule 2: 5'-D(*GP*CP*TP*CP*TP*AP*8PYP*TP*CP*AP*TP*CP*AP*CP)-3'

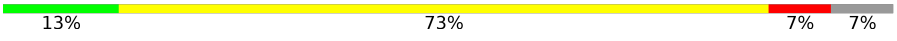
Chain C:

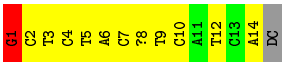




- Molecule 2: 5'-D(*GP*CP*TP*CP*TP*AP*8PYP*TP*CP*AP*TP*CP*AP*CP)-3'

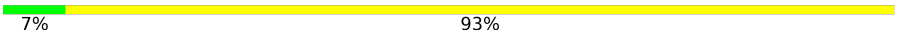
Chain E:

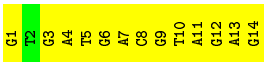




- Molecule 3: 5'-D(*GP*TP*GP*AP*TP*GP*AP*CP*GP*TP*AP*GP*AP*GP)-3'

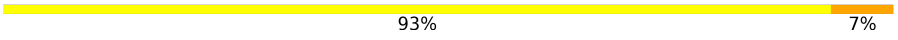
Chain D:

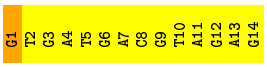




- Molecule 3: 5'-D(*GP*TP*GP*AP*TP*GP*AP*CP*GP*TP*AP*GP*AP*GP)-3'

Chain F:




G1
T2
G3
A4
T5
G6
A7
C8
G9
T10
A11
G12
A13
G14

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	53.17Å 53.17Å 131.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.17 – 2.00 41.32 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (53.17-2.00) 98.5 (41.32-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.217 , 0.254 0.227 , 0.260	Depositor DCC
R_{free} test set	1255 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3093	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 8PY

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	1.02	1/954 (0.1%)	1.00	1/1285 (0.1%)
1	B	0.95	0/963	0.93	0/1298
2	C	0.60	1/285 (0.4%)	1.17	0/434
2	E	0.72	1/285 (0.4%)	1.10	0/434
3	D	0.63	0/322	1.00	0/497
3	F	0.61	1/321 (0.3%)	1.19	0/496
All	All	0.87	4/3130 (0.1%)	1.03	1/4444 (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
2	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	GLU	CD-OE1	5.93	1.32	1.25
3	F	1	DG	O3'-P	-5.39	1.54	1.61
2	E	1	DG	C2'-C1'	5.16	1.57	1.52
2	C	1	DG	O3'-P	-5.04	1.55	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	ARG	NE-CZ-NH1	6.25	123.42	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1	DG	Sidechain

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	930	0	875	3	0
1	B	939	0	874	11	0
2	C	299	0	137	52	0
2	E	299	0	138	56	0
3	D	286	0	141	62	0
3	F	285	0	140	64	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	22	0	0	1	0
5	B	25	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
All	All	3093	0	2305	154	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 29.

The worst 5 of 154 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:C:8:8PY:C1'	2:E:8:8PY:C31	2.03	1.29
3:D:4:DA:N1	3:F:12:DG:N1	1.63	1.17
3:F:6:DG:C2'	3:F:7:DA:H5'	1.76	1.13
3:D:1:DG:C8	2:E:1:DG:C8	2.37	1.12
3:D:6:DG:H2"	3:D:7:DA:H5'	1.21	1.11

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	112/131 (86%)	109 (97%)	3 (3%)	0	100	100
1	B	113/131 (86%)	109 (96%)	4 (4%)	0	100	100
All	All	225/262 (86%)	218 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	99/118 (84%)	97 (98%)	2 (2%)	63	65
1	B	100/118 (85%)	97 (97%)	3 (3%)	48	47
All	All	199/236 (84%)	194 (98%)	5 (2%)	55	55

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	LYS
1	A	293	ARG
1	B	192	ILE
1	B	198	ILE
1	B	251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	266	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	8PY	C	8	3,2	40,48,49	1.73	6 (15%)	54,73,76	3.44	12 (22%)
2	8PY	E	8	3,2	40,48,49	1.55	6 (15%)	54,73,76	2.26	11 (20%)

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	8PY	C	8	3,2	-	0/11/33/34	0/7/7/7
2	8PY	E	8	3,2	-	0/11/33/34	0/7/7/7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	8PY	C11-N8	-7.09	1.34	1.44
2	E	8	8PY	C11-N8	-4.70	1.37	1.44
2	C	8	8PY	C12-C13	-3.09	1.34	1.42
2	E	8	8PY	C7-N8	-2.87	1.33	1.38
2	E	8	8PY	C12-C13	-2.26	1.36	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	8	8PY	C2'-C1'-N9	-13.60	102.36	115.77
2	C	8	8PY	C12-C11-N8	-8.07	108.64	121.35
2	E	8	8PY	C2'-C1'-N9	-7.71	108.16	115.77
2	E	8	8PY	C12-C11-N8	-7.26	109.91	121.35
2	C	8	8PY	C5-C6-N1	-6.66	114.82	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	8	8PY	10	0
2	E	8	8PY	17	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	114/131 (87%)	-0.20	1 (0%) 85 86	25, 39, 80, 94	0
1	B	115/131 (87%)	-0.22	1 (0%) 85 86	25, 40, 78, 99	0
2	C	13/15 (86%)	-0.49	0 100 100	27, 54, 62, 65	13 (100%)
2	E	13/15 (86%)	-0.34	0 100 100	39, 52, 59, 61	13 (100%)
3	D	14/14 (100%)	-0.22	0 100 100	33, 58, 71, 78	14 (100%)
3	F	14/14 (100%)	-0.38	0 100 100	34, 58, 75, 80	14 (100%)
All	All	283/320 (88%)	-0.24	2 (0%) 89 89	25, 41, 78, 99	54 (19%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	HIS	2.6
1	A	300	HIS	2.1

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

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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	8PY	E	8	42/43	0.84	0.16	-	47,51,60,63	42
2	8PY	C	8	42/43	0.83	0.20	-	46,49,65,69	42

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	A	338	1/1	1.00	0.10	1.07	32,32,32,32	0
4	ZN	B	338	1/1	1.00	0.08	-1.23	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.