



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:51 am BST

PDB ID : 4GFB
Title : Rap1/DNA complex
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Deposited on : 2012-08-03
Resolution : 2.99 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	:	2.11
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)	:	2.11

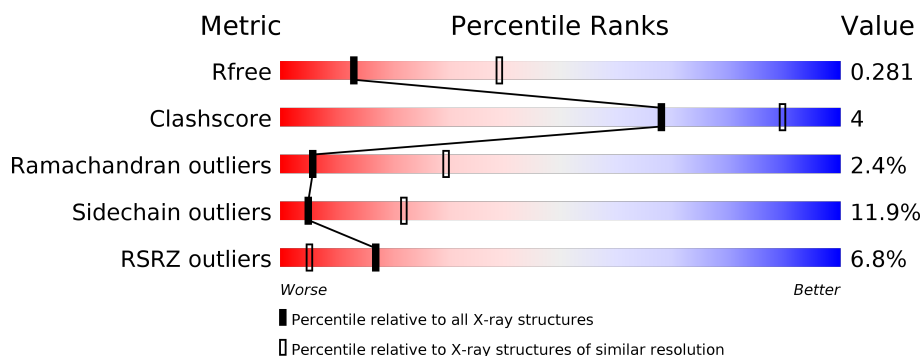
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	A	272	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>•</div> <div>20%</div> </div> </div>
2	C	31	<div> <div>16%</div> <div> <div>23%</div> <div>61%</div> <div>10%</div> <div>6%</div> </div> </div>
3	D	31	<div> <div>6%</div> <div> <div>16%</div> <div>58%</div> <div>26%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3057 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 DNA-binding protein RAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1813	1147	329	336	1			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	LYS	-	EXPRESSION TAG	UNP P11938
A	332	HIS	-	EXPRESSION TAG	UNP P11938
A	333	HIS	-	EXPRESSION TAG	UNP P11938
A	334	HIS	-	EXPRESSION TAG	UNP P11938
A	335	HIS	-	EXPRESSION TAG	UNP P11938
A	336	HIS	-	EXPRESSION TAG	UNP P11938
A	337	HIS	-	EXPRESSION TAG	UNP P11938
A	338	PRO	-	EXPRESSION TAG	UNP P11938
A	339	MET	-	EXPRESSION TAG	UNP P11938
A	340	SER	-	EXPRESSION TAG	UNP P11938
A	341	ASP	-	EXPRESSION TAG	UNP P11938
A	342	TYR	-	EXPRESSION TAG	UNP P11938
A	343	ASP	-	EXPRESSION TAG	UNP P11938
A	344	ILE	-	EXPRESSION TAG	UNP P11938
A	345	PRO	-	EXPRESSION TAG	UNP P11938
A	346	THR	-	EXPRESSION TAG	UNP P11938
A	347	THR	-	EXPRESSION TAG	UNP P11938
A	348	GLU	-	EXPRESSION TAG	UNP P11938
A	349	ASN	-	EXPRESSION TAG	UNP P11938
A	350	LEU	-	EXPRESSION TAG	UNP P11938
A	351	TYR	-	EXPRESSION TAG	UNP P11938
A	352	PHE	-	EXPRESSION TAG	UNP P11938
A	353	GLN	-	EXPRESSION TAG	UNP P11938
A	354	GLY	-	EXPRESSION TAG	UNP P11938
A	355	ALA	-	EXPRESSION TAG	UNP P11938
A	356	MET	-	EXPRESSION TAG	UNP P11938
A	357	ALA	-	EXPRESSION TAG	UNP P11938

- Molecule 2 is a DNA chain called telomeric DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	29	Total	C	N	O	P	0	0	0
			587	278	115	165	29			

- Molecule 3 is a DNA chain called telomeric DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	31	Total	C	N	O	P	0	0	0
			644	306	111	196	31			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	D	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 122.65Å 149.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.27 – 2.99 39.27 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.27-2.99) 98.8 (39.27-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.204 , 0.269 0.214 , 0.281	Depositor DCC
R_{free} test set	603 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3057	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.53	0/1860	0.76	0/2513
2	C	1.15	0/658	2.16	29/1007 (2.9%)
3	D	1.12	1/720 (0.1%)	2.19	37/1113 (3.3%)
All	All	0.84	1/3238 (0.0%)	1.57	66/4633 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	DT	C3'-O3'	-6.13	1.35	1.44

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	DA	O4'-C1'-N9	19.34	121.53	108.00
3	D	28	DT	O4'-C1'-N1	18.25	120.78	108.00
2	C	10	DC	P-O3'-C3'	11.97	134.06	119.70
2	C	5	DG	O4'-C1'-N9	11.65	116.16	108.00
2	C	28	DC	P-O3'-C3'	11.45	133.44	119.70
3	D	2	DC	P-O3'-C3'	10.87	132.74	119.70
2	C	12	DA	P-O3'-C3'	10.67	132.51	119.70
3	D	26	DG	P-O3'-C3'	10.54	132.35	119.70
3	D	22	DT	O4'-C1'-N1	9.57	114.70	108.00
3	D	1	DA	P-O3'-C3'	9.27	130.82	119.70
2	C	27	DA	P-O3'-C3'	9.23	130.78	119.70
2	C	9	DA	C1'-O4'-C4'	-9.19	100.91	110.10
2	C	13	DC	P-O3'-C3'	9.08	130.60	119.70
2	C	27	DA	O4'-C1'-N9	9.06	114.34	108.00
3	D	13	DG	O4'-C1'-N9	8.76	114.13	108.00
2	C	23	DA	P-O3'-C3'	8.71	130.15	119.70
3	D	25	DT	O4'-C1'-N1	8.61	114.03	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	26	DC	P-O3'-C3'	8.59	130.00	119.70
3	D	24	DG	O4'-C1'-N9	8.17	113.72	108.00
3	D	23	DG	P-O3'-C3'	8.12	129.45	119.70
3	D	28	DT	P-O3'-C3'	7.90	129.18	119.70
2	C	9	DA	P-O3'-C3'	7.85	129.12	119.70
3	D	7	DT	O4'-C1'-N1	7.84	113.48	108.00
3	D	16	DG	P-O3'-C3'	7.78	129.03	119.70
3	D	1	DA	O4'-C1'-N9	7.76	113.43	108.00
3	D	5	DG	P-O3'-C3'	7.74	128.98	119.70
2	C	10	DC	O4'-C1'-N1	7.69	113.38	108.00
3	D	21	DG	P-O3'-C3'	7.68	128.92	119.70
2	C	26	DC	O4'-C1'-N1	7.67	113.37	108.00
2	C	11	DC	P-O3'-C3'	7.39	128.57	119.70
2	C	22	DC	O4'-C1'-N1	7.34	113.14	108.00
2	C	4	DT	P-O3'-C3'	7.31	128.48	119.70
3	D	27	DT	P-O3'-C3'	7.28	128.43	119.70
2	C	2	DT	O4'-C1'-N1	6.88	112.81	108.00
2	C	14	DA	P-O3'-C3'	6.82	127.88	119.70
2	C	5	DG	P-O3'-C3'	6.81	127.88	119.70
3	D	29	DC	O4'-C1'-N1	6.78	112.74	108.00
3	D	19	DG	O4'-C1'-N9	-6.73	103.29	108.00
2	C	1	DG	P-O3'-C3'	6.64	127.66	119.70
3	D	12	DG	O4'-C1'-N9	-6.44	103.49	108.00
3	D	27	DT	O4'-C1'-N1	6.29	112.41	108.00
3	D	10	DG	P-O3'-C3'	6.25	127.20	119.70
3	D	18	DT	P-O3'-C3'	6.18	127.12	119.70
3	D	26	DG	O4'-C1'-N9	6.10	112.27	108.00
3	D	24	DG	P-O3'-C3'	5.94	126.83	119.70
2	C	26	DC	C1'-O4'-C4'	-5.93	104.17	110.10
3	D	28	DT	C1'-O4'-C4'	-5.92	104.17	110.10
2	C	31	DG	O4'-C1'-N9	5.80	112.06	108.00
3	D	28	DT	C3'-C2'-C1'	-5.78	95.56	102.50
2	C	18	DC	P-O3'-C3'	5.75	126.59	119.70
3	D	15	DT	P-O3'-C3'	5.65	126.48	119.70
2	C	6	DA	O4'-C1'-N9	5.63	111.94	108.00
3	D	25	DT	P-O3'-C3'	5.61	126.43	119.70
3	D	19	DG	N3-C4-C5	-5.60	125.80	128.60
3	D	17	DT	C6-C5-C7	-5.46	119.63	122.90
2	C	9	DA	N9-C1'-C2'	5.45	122.95	112.60
3	D	10	DG	O4'-C1'-N9	5.36	111.75	108.00
2	C	2	DT	P-O3'-C3'	5.33	126.09	119.70
3	D	20	DT	O4'-C1'-N1	5.32	111.72	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	16	DG	C8-N9-C4	-5.24	104.30	106.40
2	C	21	DC	O4'-C1'-N1	5.23	111.66	108.00
3	D	30	DA	P-O3'-C3'	5.19	125.93	119.70
2	C	3	DG	O4'-C1'-N9	5.14	111.60	108.00
3	D	19	DG	N3-C4-N9	5.09	129.05	126.00
3	D	11	DT	N3-C2-O2	-5.07	119.26	122.30
3	D	19	DG	P-O3'-C3'	5.06	125.77	119.70

There are no chirality outliers.

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	A	1813	0	1754	13	0
2	C	587	0	323	3	0
3	D	644	0	354	7	0
4	A	1	0	0	0	0
5	A	11	0	0	0	1
5	D	1	0	0	0	0
All	All	3057	0	2431	20	1

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 4.

All (20) 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)
3:D:10:DG:H2"	3:D:11:DT:H72	1.77	0.64
1:A:542:ARG:NH1	1:A:546:ARG:HD2	2.15	0.61
3:D:20:DT:H2"	3:D:21:DG:N7	2.23	0.53
1:A:423:LYS:HZ3	1:A:423:LYS:H	1.57	0.53
1:A:583:ARG:HD2	1:A:584:PRO:HD2	1.93	0.50
1:A:580:ARG:HD2	3:D:7:DT:H72	1.93	0.49
1:A:444:SER:HB2	3:D:12:DG:OP1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HD12	1:A:506:GLU:HG3	1.95	0.48
3:D:9:DT:H2"	3:D:10:DG:C8	2.49	0.47
3:D:20:DT:H2"	3:D:21:DG:C8	2.49	0.47
1:A:398:HIS:ND1	2:C:18:DC:OP2	2.47	0.46
2:C:9:DA:H1'	2:C:10:DC:OP2	2.16	0.45
1:A:469:LEU:HG	1:A:517:ARG:NH1	2.31	0.45
1:A:422:ASP:HB2	1:A:423:LYS:HZ1	1.81	0.44
1:A:517:ARG:HH21	1:A:520:PRO:HD2	1.83	0.44
1:A:466:TYR:HE1	1:A:472:ILE:HG22	1.85	0.42
1:A:479:SER:OG	1:A:481:ILE:HD12	2.20	0.41
3:D:4:DT:H2"	3:D:5:DG:C8	2.56	0.41
1:A:399:THR:O	1:A:403:ILE:HD12	2.21	0.41
2:C:29:DC:H2"	2:C:30:DA:C8	2.56	0.40

All (1) 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)
5:A:805:HOH:O	5:A:805:HOH:O[7_556]	2.10	0.10

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	212/272 (78%)	185 (87%)	22 (10%)	5 (2%)	6	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	THR
1	A	515	GLN
1	A	477	GLY

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Mol	Chain	Res	Type
1	A	504	GLY
1	A	584	PRO

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	194/241 (80%)	171 (88%)	23 (12%)	5 22

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

Mol	Chain	Res	Type
1	A	358	HIS
1	A	359	ASN
1	A	362	SER
1	A	402	SER
1	A	415	LEU
1	A	420	GLU
1	A	423	LYS
1	A	430	ASP
1	A	431	ASP
1	A	469	LEU
1	A	481	ILE
1	A	482	THR
1	A	505	SER
1	A	521	ILE
1	A	537	THR
1	A	542	ARG
1	A	543	ASP
1	A	556	ASP
1	A	569	ARG
1	A	570	GLU
1	A	571	PRO
1	A	575	LYS
1	A	583	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	A	405	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is 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, 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	A	218/272 (80%)	0.10	12 (5%) 25 9	25, 49, 91, 121	0
2	C	29/31 (93%)	0.47	5 (17%) 1 0	31, 60, 160, 165	0
3	D	31/31 (100%)	0.43	2 (6%) 18 5	35, 62, 184, 188	0
All	All	278/334 (83%)	0.18	19 (6%) 17 5	25, 52, 148, 188	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	PRO	6.8
1	A	503	PRO	5.7
3	D	29	DC	5.6
1	A	584	PRO	5.0
3	D	30	DA	4.3
1	A	502	VAL	4.2
1	A	585	GLY	4.1
2	C	6	DA	4.1
1	A	359	ASN	3.4
1	A	504	GLY	3.3
1	A	586	VAL	3.0
1	A	583	ARG	2.9
1	A	358	HIS	2.8
2	C	11	DC	2.7
2	C	9	DA	2.4
2	C	5	DG	2.3
1	A	569	ARG	2.2
2	C	12	DA	2.2
1	A	481	ILE	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 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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
4	CA	A	701	1/1	0.92	0.20	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.