



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:35 PM GMT

PDB ID : 1GDR
Title : MODEL FOR A DNA MEDIATED SYNAPTIC COMPLEX SUGGESTED
BY CRYSTAL PACKING OF GAMMA DELTA RESOLVASE SUBUNITS
Authors : Rice, P.A.; Steitz, T.A.
Deposited on : 1993-08-31
Resolution : 3.50 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
<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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

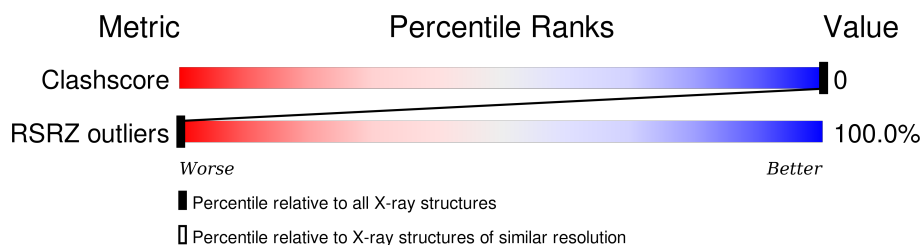
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1157 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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.

Mol	Chain	Length	Quality of chain
1	A	140	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 105 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.

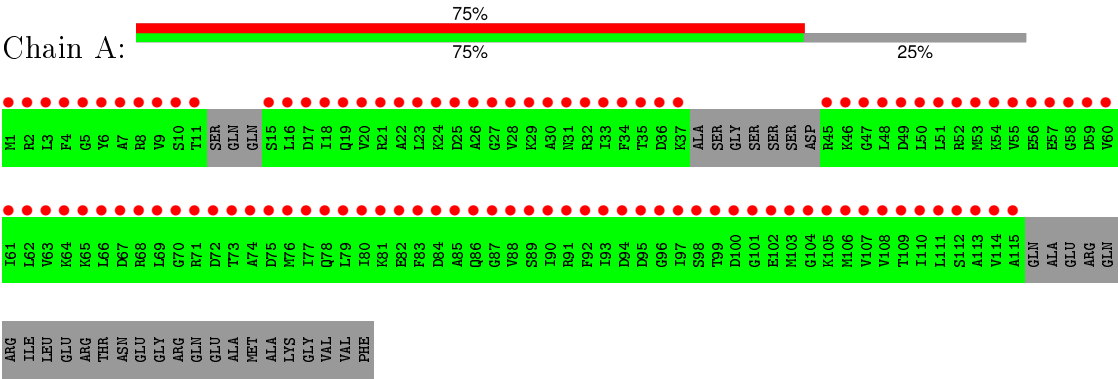
- Molecule 1 is a protein called GAMMA DELTA-RESOLVASE.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	105	Total	C	0	0	105
			105	105			

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.

- Molecule 1: GAMMA DELTA-RESOLVASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	60.20Å 60.20Å 170.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.50 49.85 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50) 86.1 (49.85-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.48Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.310 , (Not available) 0.434 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	113.7	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 2454 reflections	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	105	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

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	105	0	0	0	0
All	All	105	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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	A	105/140 (75%)	21.11	105 (100%) 0 0	35, 35, 35, 35	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	GLU	54.9
1	A	94	ASP	53.3
1	A	78	GLN	52.1
1	A	96	GLY	49.4
1	A	75	ASP	44.1
1	A	100	ASP	42.9
1	A	28	VAL	41.0
1	A	95	ASP	40.9
1	A	59	ASP	39.6
1	A	37	LYS	38.2
1	A	15	SER	36.3
1	A	36	ASP	34.9
1	A	82	GLU	34.8
1	A	10	SER	34.7
1	A	70	GLY	32.8
1	A	58	GLY	32.7
1	A	93	ILE	32.2
1	A	112	SER	32.0
1	A	55	VAL	31.9
1	A	29	LYS	30.0
1	A	47	GLY	29.6
1	A	72	ASP	29.4
1	A	62	LEU	28.8
1	A	104	GLY	28.2
1	A	103	MET	27.6
1	A	35	THR	27.4
1	A	24	LYS	26.4

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Mol	Chain	Res	Type	RSRZ
1	A	65	LYS	25.8
1	A	52	ARG	25.6
1	A	45	ARG	25.3
1	A	76	MET	25.3
1	A	92	PHE	25.3
1	A	101	GLY	24.9
1	A	2	ARG	24.8
1	A	83	PHE	24.6
1	A	17	ASP	24.6
1	A	111	LEU	24.4
1	A	84	ASP	24.1
1	A	63	VAL	23.8
1	A	105	LYS	23.2
1	A	109	THR	22.7
1	A	114	VAL	22.5
1	A	3	LEU	22.4
1	A	66	LEU	22.2
1	A	25	ASP	21.5
1	A	11	THR	21.5
1	A	67	ASP	21.1
1	A	51	LEU	20.8
1	A	71	ARG	20.1
1	A	97	ILE	19.9
1	A	21	ARG	19.4
1	A	113	ALA	19.4
1	A	53	MET	18.8
1	A	50	LEU	18.7
1	A	49	ASP	18.2
1	A	106	MET	17.6
1	A	19	GLN	17.3
1	A	33	ILE	17.3
1	A	60	VAL	17.2
1	A	80	ILE	17.2
1	A	115	ALA	17.0
1	A	81	LYS	17.0
1	A	85	ALA	17.0
1	A	87	GLY	17.0
1	A	34	PHE	16.9
1	A	54	LYS	16.9
1	A	98	SER	16.8
1	A	110	ILE	16.5
1	A	86	GLN	16.2

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Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	16.0
1	A	6	TYR	15.6
1	A	48	LEU	15.0
1	A	91	ARG	14.9
1	A	89	SER	14.6
1	A	108	VAL	14.5
1	A	26	ALA	13.7
1	A	56	GLU	13.5
1	A	31	ASN	13.3
1	A	20	VAL	13.1
1	A	30	ALA	12.3
1	A	107	VAL	12.3
1	A	22	ALA	12.0
1	A	68	ARG	10.8
1	A	4	PHE	10.8
1	A	1	MET	10.1
1	A	77	ILE	9.9
1	A	88	VAL	9.7
1	A	18	ILE	9.6
1	A	8	ARG	9.3
1	A	74	ALA	8.9
1	A	99	THR	8.7
1	A	32	ARG	8.3
1	A	61	ILE	8.3
1	A	64	LYS	8.1
1	A	16	LEU	8.0
1	A	46	LYS	7.9
1	A	73	THR	7.7
1	A	7	ALA	7.6
1	A	9	VAL	6.7
1	A	27	GLY	6.5
1	A	69	LEU	6.3
1	A	5	GLY	5.1
1	A	90	ILE	4.8
1	A	23	LEU	4.1
1	A	57	GLU	3.1

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.