



Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 03:28 AM 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 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/ValidationPDFNotes.html>

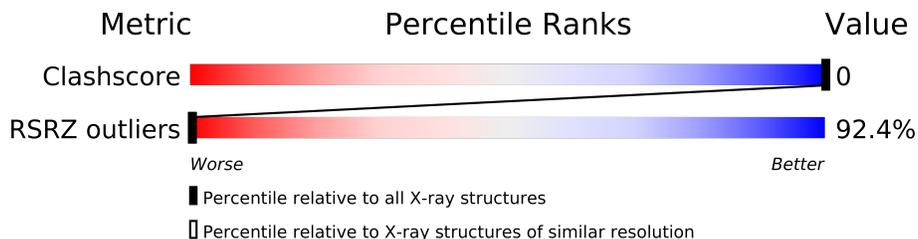
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1039 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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			

4 Data and refinement statistics i

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	1.17 (at 3.48Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.310 , (Not available) 0.740 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	202.7	Xtrriage
Anisotropy	0.719	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.71$, $\langle L^2 \rangle = 0.59$	Xtrriage
Outliers	11 of 2454 reflections (0.448%)	Xtrriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	105	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.62 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4963e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry 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 i

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

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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%)	15.93	97 (92%) 0 0	35, 35, 35, 35	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ILE	53.2
1	A	91	ARG	48.7
1	A	58	GLY	45.3
1	A	34	PHE	43.4
1	A	22	ALA	41.9
1	A	59	ASP	41.5
1	A	25	ASP	40.8
1	A	36	ASP	40.0
1	A	35	THR	39.2
1	A	104	GLY	35.7
1	A	17	ASP	35.3
1	A	24	LYS	34.8
1	A	3	LEU	34.4
1	A	93	ILE	34.4
1	A	28	VAL	31.2
1	A	102	GLU	29.9
1	A	71	ARG	28.4
1	A	105	LYS	27.7
1	A	11	THR	27.4
1	A	70	GLY	26.6
1	A	83	PHE	26.5
1	A	101	GLY	25.2
1	A	106	MET	25.1
1	A	37	LYS	23.8
1	A	92	PHE	23.1
1	A	82	GLU	21.5
1	A	65	LYS	21.4

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Mol	Chain	Res	Type	RSRZ
1	A	94	ASP	21.3
1	A	78	GLN	21.0
1	A	111	LEU	20.7
1	A	100	ASP	20.3
1	A	21	ARG	19.4
1	A	76	MET	19.0
1	A	47	GLY	18.7
1	A	96	GLY	18.3
1	A	57	GLU	18.3
1	A	114	VAL	17.4
1	A	110	ILE	17.4
1	A	84	ASP	17.2
1	A	108	VAL	16.6
1	A	56	GLU	16.5
1	A	113	ALA	15.4
1	A	112	SER	15.3
1	A	81	LYS	15.3
1	A	72	ASP	15.2
1	A	55	VAL	14.9
1	A	54	LYS	14.6
1	A	10	SER	14.3
1	A	87	GLY	14.0
1	A	90	ILE	13.5
1	A	109	THR	13.1
1	A	107	VAL	12.9
1	A	64	LYS	12.3
1	A	29	LYS	12.3
1	A	52	ARG	12.0
1	A	79	LEU	11.4
1	A	115	ALA	10.9
1	A	51	LEU	10.7
1	A	62	LEU	10.5
1	A	80	ILE	10.5
1	A	2	ARG	10.0
1	A	75	ASP	9.9
1	A	30	ALA	9.9
1	A	20	VAL	9.8
1	A	15	SER	9.7
1	A	99	THR	9.6
1	A	50	LEU	9.4
1	A	8	ARG	9.2
1	A	1	MET	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	45	ARG	8.9
1	A	31	ASN	8.8
1	A	60	VAL	8.8
1	A	48	LEU	8.2
1	A	4	PHE	7.9
1	A	63	VAL	7.6
1	A	74	ALA	7.6
1	A	46	LYS	7.3
1	A	95	ASP	7.1
1	A	53	MET	6.9
1	A	77	ILE	6.7
1	A	19	GLN	6.5
1	A	88	VAL	6.3
1	A	26	ALA	6.1
1	A	49	ASP	6.1
1	A	103	MET	5.4
1	A	32	ARG	5.4
1	A	68	ARG	4.7
1	A	61	ILE	4.1
1	A	73	THR	3.7
1	A	23	LEU	3.7
1	A	69	LEU	3.7
1	A	98	SER	3.4
1	A	27	GLY	3.4
1	A	18	ILE	3.0
1	A	89	SER	2.9
1	A	7	ALA	2.3
1	A	5	GLY	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.