wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 06:57 AM EDT

PDB ID	:	1GDT
Title	:	CRYSTAL STRUCTURE OF A SITE-SPECIFIC RECOMBINASE, GAMMA-DELTA RESOLVASE COMPLEXED WITH A 34 BP CLEAVAGE SITE
Authors	:	Yang, W.; Steitz, T.A.
Deposited on	:	1995-04-11
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

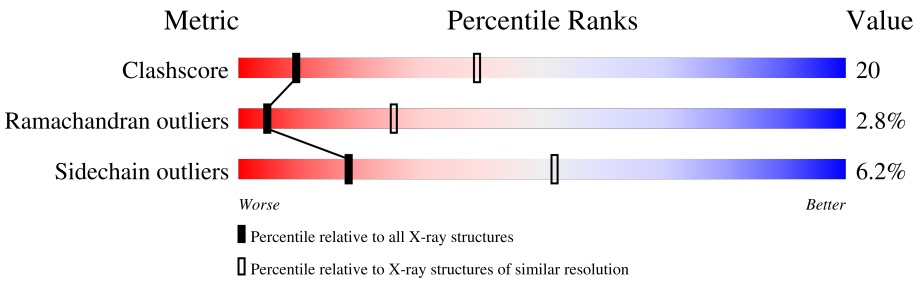
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	22	9% 59% 32%
2	D	13	8% 62% 31%
2	F	13	15% 62% 23%
3	E	21	24% 62% 14%
4	A	183	59% 37% • •
4	B	183	64% 32% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4284 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 DNA chain called SITE I OF RES DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	22	450	217	83	129	21	0	0	0

- Molecule 2 is a DNA chain called SITE I OF RES DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	13	263	127	47	77	12	0	0	0
2	F	13	263	127	47	77	12	0	0	0

- Molecule 3 is a DNA chain called SITE I OF RES DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	21	431	207	78	125	21	0	0	0

- Molecule 4 is a protein called PROTEIN (GAMMA DELTA RESOLVASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	183	1424	877	267	272	8	0	0	0
4	B	183	1424	877	267	272	8	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	4	4	4	0	0
5	E	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	F	2	2	2	0	0
			Total	O		
5	A	9	9	9	0	0
			Total	O		
5	B	12	12	12	0	0

3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: SITE I OF RES DNA

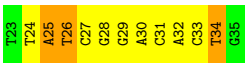
Chain C: 9% 59% 32%

• Molecule 2: SITE I OF RES DNA

Chain D: 8% 62% 31%

• Molecule 2: SITE I OF RES DNA

Chain F: 15% 62% 23%

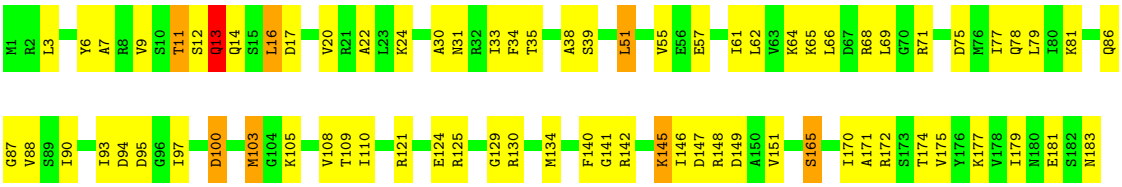


• Molecule 3: SITE I OF RES DNA

Chain E: 24% 62% 14%

• Molecule 4: PROTEIN (GAMMA DELTA RESOLVASE)

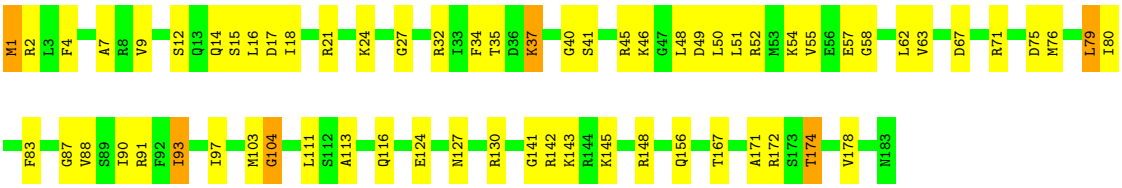
Chain A: 59% 37%



• Molecule 4: PROTEIN (GAMMA DELTA RESOLVASE)

Chain B:

64%
32%


M1 R2 L3 F4 A7 R8 V9 S12 Q13 Q14 S15 L16 D17 I18 R21 K24 G27 R32 I33 F34 T35 D36 K37 G40 S41 R45 K46 G47 L48 D49 I50 L51 R52 M53 K54 V55 E56 E57 G58 L62 V63 D67 R71 D75 M76 L79 I80
F83 G87 V88 S89 I90 R91 F92 I93 I97 M103 G104 L111 S112 A113 Q116 E124 N127 R130 G141 R142 K143 R144 K145 R148 Q156 T167 A171 R172 S173 T174 V178 N183

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.00Å 157.00Å 37.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	89.5 (10.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.235 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4284	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

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	C	1.79	6/505 (1.2%)	1.66	7/778 (0.9%)
2	D	1.63	2/294 (0.7%)	1.62	2/452 (0.4%)
2	F	1.73	1/294 (0.3%)	1.64	2/452 (0.4%)
3	E	1.70	0/483	1.66	3/743 (0.4%)
4	A	0.37	0/1433	0.62	0/1912
4	B	0.37	0/1433	0.59	0/1912
All	All	1.07	9/4442 (0.2%)	1.13	14/6249 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	DG	P-O5'	-7.50	1.52	1.59
2	F	25	DA	C5-C4	-6.37	1.34	1.38
1	C	17	DT	C3'-C2'	-6.19	1.44	1.52
1	C	6	DG	C5'-C4'	-6.07	1.44	1.51
1	C	5	DT	O3'-P	-5.32	1.54	1.61

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	7	DT	C4-C5-C6	5.72	121.44	118.00
1	C	11	DA	C4'-C3'-C2'	5.63	108.16	103.10
1	C	5	DT	C4-C5-C7	-5.53	115.69	119.00
1	C	7	DT	C4-C5-C6	5.47	121.28	118.00
2	D	26	DT	C4-C5-C6	5.35	121.21	118.00

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	C	450	0	251	15	0
2	D	263	0	149	16	0
2	F	263	0	149	12	0
3	E	431	0	239	22	0
4	A	1424	0	1476	59	0
4	B	1424	0	1476	53	0
5	A	9	0	0	0	0
5	B	12	0	0	0	0
5	C	4	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	4284	0	3740	156	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 20.

The worst 5 of 156 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)
4:A:100:ASP:HB3	4:A:103:MET:SD	2.00	1.01
2:D:28:DG:H2"	2:D:29:DG:H5"	1.53	0.90
4:B:40:GLY:HA2	4:B:71:ARG:HD2	1.59	0.82
1:C:17:DT:O3'	4:A:129:GLY:HA3	1.82	0.79
3:E:6:DG:H2"	3:E:7:DT:OP2	1.81	0.79

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	
4	A	181/183 (99%)	153 (84%)	21 (12%)	7 (4%)	3	17
4	B	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	9	39
All	All	362/366 (99%)	314 (87%)	38 (10%)	10 (3%)	5	25

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	38	ALA
4	B	104	GLY
4	B	93	ILE
4	A	100	ASP
4	B	12	SER

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	
4	A	153/153 (100%)	143 (94%)	10 (6%)	17	50
4	B	153/153 (100%)	144 (94%)	9 (6%)	19	54
All	All	306/306 (100%)	287 (94%)	19 (6%)	18	52

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	116	GLN
4	B	167	THR
4	B	174	THR
4	B	156	GLN
4	A	149	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	156	GLN
4	B	153	ASN

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.