



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:17 PM GMT

PDB ID : 1G3S
Title : CYS102SER DTXR
Authors : Pohl, E.; Goranson-Siekierke, J.; Holmes, R.K.; Hol, W.G.J.
Deposited on : 2000-10-25
Resolution : 2.40 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>

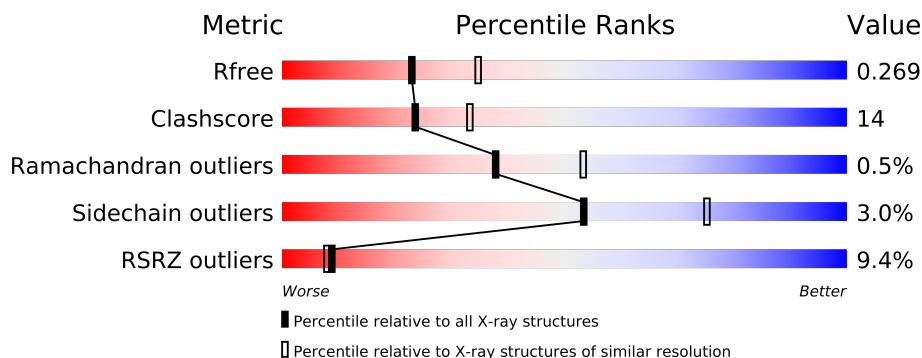
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. 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	226	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1670 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 DIPHTHERIA TOXIN REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1590	987	284	314	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	SER	CYS	ENGINEERED	UNP P33120

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 63.60Å 110.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.40 31.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 94.9 (31.80-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.185 , 0.271 0.194 , 0.269	Depositor DCC
R_{free} test set	529 reflections (5.60%)	DCC
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 147.2	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 9980 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1670	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/1606	0.73	1/2183 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	PRO	N-CA-CB	6.08	110.60	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1590	0	1542	45	0
2	A	80	0	0	4	0
All	All	1670	0	1542	45	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 14.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:LEU:HD22	1:A:213:LEU:HG	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.60	0.66
1:A:160:PRO:HG3	1:A:196:VAL:HG22	1.76	0.66
1:A:151:ARG:HH12	1:A:222:ARG:NH2	1.97	0.63
1:A:115:ARG:NH1	1:A:118:LYS:HD2	2.13	0.62
1:A:5:VAL:HA	1:A:106:HIS:HB3	1.80	0.62
1:A:151:ARG:HD3	1:A:153:ILE:HG22	1.82	0.62
1:A:160:PRO:HA	1:A:195:ILE:O	2.02	0.60
1:A:5:VAL:HA	1:A:106:HIS:CB	2.31	0.60
1:A:162:LYS:HA	1:A:193:VAL:O	2.02	0.60
1:A:193:VAL:HG13	1:A:205:SER:O	2.06	0.56
1:A:117:VAL:HG11	1:A:140:VAL:HG21	1.87	0.55
1:A:151:ARG:N	1:A:222:ARG:HH11	2.07	0.53
1:A:37:SER:HB2	1:A:39:PRO:HD2	1.91	0.53
1:A:151:ARG:HH12	1:A:222:ARG:HH22	1.57	0.53
1:A:151:ARG:HD3	1:A:153:ILE:CG2	2.40	0.51
1:A:178:GLN:O	1:A:182:LEU:HG	2.11	0.51
1:A:14:THR:OG1	1:A:34:LEU:HD21	2.11	0.50
1:A:136:ASP:HA	1:A:140:VAL:O	2.11	0.50
1:A:26:LEU:O	1:A:30:ILE:HD12	2.12	0.49
1:A:13:ARG:HG3	1:A:76:MET:HG2	1.95	0.49
1:A:160:PRO:HG3	1:A:196:VAL:CG2	2.40	0.49
1:A:38:GLY:N	1:A:39:PRO:CD	2.76	0.48
1:A:165:ILE:HG21	1:A:168:ILE:HD11	1.97	0.47
1:A:151:ARG:NH1	1:A:222:ARG:NH2	2.64	0.46
1:A:14:THR:HG23	1:A:33:ARG:HD2	1.97	0.46
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.68	0.46
1:A:7:THR:HG22	2:A:320:HOH:O	2.14	0.46
1:A:87:THR:CG2	1:A:97:VAL:HG21	2.46	0.46
1:A:204:LEU:CD2	1:A:213:LEU:HG	2.43	0.46
1:A:169:ASN:HB3	1:A:172:PHE:HD2	1.81	0.45
1:A:191:SER:O	1:A:193:VAL:HG23	2.16	0.45
1:A:148:PRO:O	1:A:222:ARG:HB3	2.17	0.45
1:A:86:LEU:HD23	1:A:90:ILE:HD12	1.98	0.44
1:A:193:VAL:HG12	1:A:194:GLU:N	2.32	0.44
1:A:4:LEU:O	1:A:6:ASP:N	2.51	0.43
1:A:165:ILE:HB	1:A:188:ARG:O	2.19	0.42
1:A:150:THR:CG2	1:A:155:ALA:HB2	2.48	0.42
1:A:180:THR:HB	2:A:363:HOH:O	2.18	0.42
1:A:130:ASN:HB2	2:A:341:HOH:O	2.20	0.42
1:A:30:ILE:HD13	1:A:62:LEU:HD12	2.02	0.42
1:A:71:LEU:O	1:A:75:VAL:HG23	2.20	0.41
1:A:5:VAL:HG13	1:A:106:HIS:HD2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:LEU:HD23	1:A:211:VAL:HB	2.02	0.41
1:A:4:LEU:N	2:A:356:HOH:O	2.53	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	206/226 (91%)	202 (98%)	3 (2%)	1 (0%)	38 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL

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	167/198 (84%)	162 (97%)	5 (3%)	53 75

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

Mol	Chain	Res	Type
1	A	47	ARG
1	A	54	VAL
1	A	76	MET
1	A	110	ASP
1	A	151	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	173	GLN

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 ⓘ

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	212/226 (93%)	0.12	20 (9%) 9 8	22, 48, 94, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	5.3
1	A	211	VAL	4.4
1	A	156	ALA	3.4
1	A	203	THR	3.4
1	A	157	THR	3.2
1	A	5	VAL	3.2
1	A	158	SER	3.0
1	A	206	HIS	3.0
1	A	202	ILE	3.0
1	A	208	GLY	3.0
1	A	196	VAL	2.7
1	A	185	ALA	2.6
1	A	195	ILE	2.5
1	A	154	ASP	2.3
1	A	204	LEU	2.2
1	A	152	VAL	2.2
1	A	160	PRO	2.2
1	A	207	ASN	2.2
1	A	165	ILE	2.1
1	A	148	PRO	2.0

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.