Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:19 PM GMT

PDB ID	:	1T4U
Title	:	Crystal Structure Analysis of a novel Oxyguanidine bound to Thrombin
Authors	:	Spurlino, J.
Deposited on	:	2004-04-30
Resolution	:	2.00 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 (i) symbol.

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

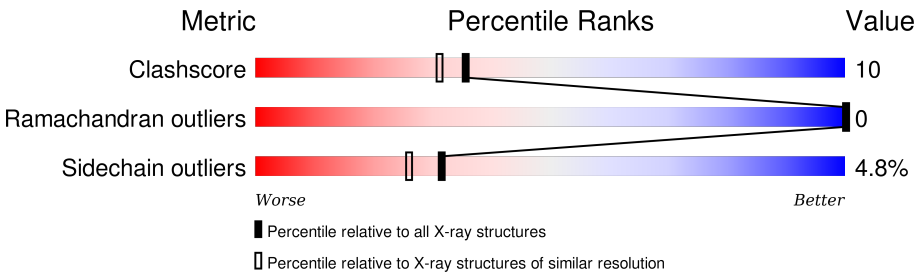
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. 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% 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	26	92% 8%
2	H	259	72% 22% • •
3	I	11	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3258 atoms, of which 772 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 Prothrombin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	L	26	265	134	50	35	45	1	9	0	0

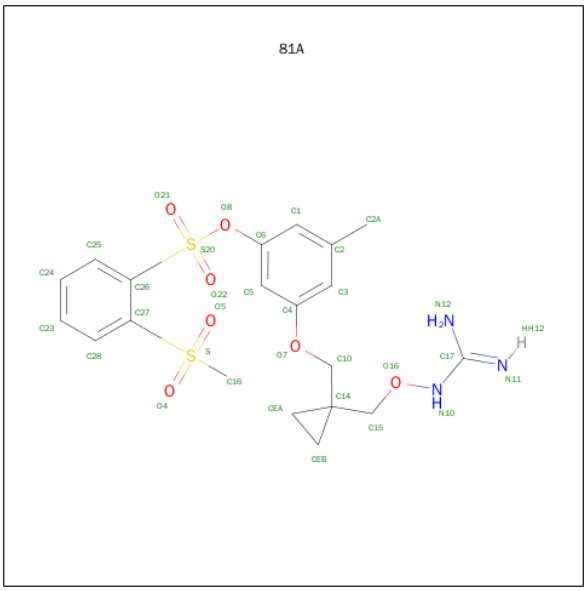
- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	249	2473	1285	461	354	359	14	18	0	0

- Molecule 3 is a protein called Hirudin IIIA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	I	11	119	64	15	12	27	1	13	0	0

- Molecule 4 is 2-METHANESULFONYL-BENZENESULFONIC ACID 3-METHYL-5-((1-AMIDINOAMINOOXYMETHYL-CYCLOPROPYL)METHYLOXY)-PHENYLESTER (three-letter code: 81A) (formula: $C_{20}H_{25}N_3O_7S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	H	1	32	20	3	7	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
5	H	110	330	220	110	0	0
			Total	H	O		
5	L	13	39	26	13	0	0

3 Residue-property plots (i)

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.

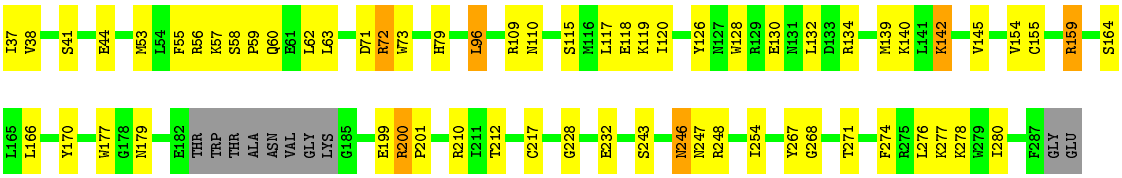
Note EDS was not executed.

• Molecule 1: Prothrombin

Chain L: 92% 8%

• Molecule 2: Prothrombin

Chain H: 72% 22%



• Molecule 3: Hirudin IIIA

Chain I: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	70.71Å 72.23Å 72.68Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.211 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3258	wwPDB-VP
Average B, all atoms ($Å^2$)	16.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 81A, TYS

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	L	0.62	0/217	0.68	0/287
2	H	0.55	0/2064	0.65	0/2789
3	I	0.51	0/88	0.45	0/115
All	All	0.56	0/2369	0.64	0/3191

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	267	TYR	Sidechain

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	L	215	50	211	1	0
2	H	2012	461	1983	43	1
3	I	104	15	82	0	0
4	H	32	0	24	3	0
5	H	110	220	0	2	1
5	L	13	26	0	0	0
All	All	2486	772	2300	43	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 10.

All (43) 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)
2:H:79:HIS:CD2	4:H:4815:81A:H21A	2.23	0.73
2:H:72:ARG:NH2	2:H:140:LYS:HD3	2.12	0.65
2:H:179:ASN:ND2	2:H:232:GLU:HB3	2.14	0.63
2:H:243:SER:HB3	2:H:246:ASN:ND2	2.16	0.61
2:H:243:SER:HB3	2:H:246:ASN:HD21	1.65	0.60
2:H:132:LEU:HD11	4:H:4815:81A:H23A	1.85	0.57
2:H:38:VAL:O	2:H:228:GLY:HA2	2.07	0.55
2:H:53:MET:HG3	2:H:62:LEU:CD1	2.38	0.54
2:H:159:ARG:HA	2:H:274:PHE:CZ	2.43	0.54
2:H:268:GLY:HA3	5:H:315:HOH:O	2.08	0.53
2:H:117:LEU:HD22	2:H:139:MET:HB3	1.90	0.53
2:H:200:ARG:NH1	2:H:212:THR:O	2.43	0.52
2:H:170:TYR:HD1	2:H:170:TYR:N	2.08	0.51
2:H:126:TYR:CZ	2:H:128:TRP:HB3	2.44	0.51
2:H:130:GLU:OE1	2:H:210:ARG:NH2	2.44	0.51
2:H:246:ASN:HD22	2:H:247:ASN:N	2.08	0.51
2:H:73:TRP:CH2	2:H:140:LYS:HE3	2.45	0.51
2:H:170:TYR:CD1	2:H:170:TYR:N	2.79	0.51
2:H:130:GLU:O	4:H:4815:81A:H23	2.12	0.49
2:H:56:ARG:O	2:H:60:GLN:HA	2.12	0.49
2:H:57:LYS:O	2:H:60:GLN:HG2	2.12	0.49
2:H:71:ASP:O	2:H:145:VAL:HG12	2.12	0.48
2:H:246:ASN:ND2	2:H:248:ARG:H	2.12	0.48
2:H:154:VAL:HG22	2:H:155:CYS:N	2.29	0.48
2:H:37:ILE:N	5:H:312:HOH:O	2.46	0.48
2:H:73:TRP:CZ2	2:H:140:LYS:HE3	2.49	0.47
2:H:254:ILE:HB	2:H:271:THR:HB	1.97	0.47
2:H:134:ARG:HG2	2:H:276:LEU:HD21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:118:GLU:HB2	2:H:142:LYS:HA	1.99	0.45
2:H:200:ARG:HB3	2:H:201:PRO:HD3	1.99	0.44
2:H:277:LYS:HA	2:H:280:ILE:HD12	1.99	0.44
2:H:246:ASN:HD22	2:H:246:ASN:C	2.21	0.44
2:H:110:ASN:HD22	2:H:110:ASN:N	2.16	0.43
2:H:53:MET:HB2	2:H:177:TRP:CZ3	2.54	0.42
2:H:58:SER:HA	2:H:59:PRO:C	2.39	0.42
2:H:63:LEU:HA	2:H:63:LEU:HD12	1.80	0.42
2:H:119:LYS:HD3	2:H:120:ILE:H	1.84	0.42
2:H:166:LEU:HA	2:H:166:LEU:HD23	1.63	0.42
2:H:55:PHE:CZ	2:H:60:GLN:HB3	2.56	0.41
2:H:117:LEU:HD13	2:H:139:MET:HE2	2.03	0.40
2:H:199:GLU:H	2:H:199:GLU:CD	2.24	0.40
2:H:96:LEU:HD12	2:H:96:LEU:HA	1.80	0.40
1:L:22:ASP:HB2	2:H:44:GLU:OE2	2.22	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)
2:H:109:ARG:HH12	5:H:348:HOH:H1[2_555]	1.30	0.30

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	L	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
2	H	245/259 (95%)	230 (94%)	15 (6%)	0	100	100
3	I	8/11 (73%)	8 (100%)	0	0	100	100
All	All	277/296 (94%)	261 (94%)	16 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	L	24/24 (100%)	23 (96%)	1 (4%)	36	31
2	H	217/225 (96%)	206 (95%)	11 (5%)	29	23
3	I	10/10 (100%)	10 (100%)	0	100	100
All	All	251/259 (97%)	239 (95%)	12 (5%)	31	26

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	28	LEU
2	H	41	SER
2	H	72	ARG
2	H	96	LEU
2	H	115	SER
2	H	142	LYS
2	H	159	ARG
2	H	164	SER
2	H	200	ARG
2	H	217	CYS
2	H	246	ASN
2	H	278	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	110	ASN
2	H	246	ASN
2	H	286	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TYS	I	298	3	15,16,17	2.19	5 (33%)	16,22,24	0.69	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	I	298	3	-	0/9/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	298	TYS	OH-S	-4.51	1.55	1.63
3	I	298	TYS	OH-CZ	-3.22	1.37	1.42
3	I	298	TYS	O3-S	3.40	1.68	1.50
3	I	298	TYS	O1-S	3.59	1.58	1.45
3	I	298	TYS	O2-S	3.69	1.58	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	298	TYS	O-C-CA	-2.07	120.08	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	81A	H	4815	-	30,34,34	2.99	5 (16%)	39,51,51	2.16	9 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	81A	H	4815	-	-	0/28/34/34	0/2/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	4815	81A	O16-N10	-14.49	1.28	1.45
4	H	4815	81A	O8-C6	-2.09	1.39	1.42
4	H	4815	81A	C27-C26	2.12	1.43	1.41
4	H	4815	81A	CEA-C14	2.20	1.55	1.50
4	H	4815	81A	C26-S20	4.69	1.86	1.78

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	4815	81A	C27-C26-S20	-6.97	121.25	125.59
4	H	4815	81A	C16-S-C27	-3.62	100.64	105.68
4	H	4815	81A	O22-S20-O21	-2.39	107.77	117.14
4	H	4815	81A	O4-S-C27	-2.12	105.45	108.14
4	H	4815	81A	O22-S20-C26	-2.05	103.61	107.50
4	H	4815	81A	C28-C27-C26	2.13	120.59	119.24
4	H	4815	81A	O8-S20-C26	3.27	108.84	103.95
4	H	4815	81A	O21-S20-C26	5.02	117.05	107.50
4	H	4815	81A	O5-S-C27	6.48	116.35	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	4815	81A	3	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.