



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:06 am BST

PDB ID : 2RTR
Title : STREPTAVIDIN-2-IMINOBIOTIN COMPLEX, PH 4.0, SPACE GROUP I222
Authors : Katz, B.A.
Deposited on : 1997-09-11
Resolution : 1.62 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

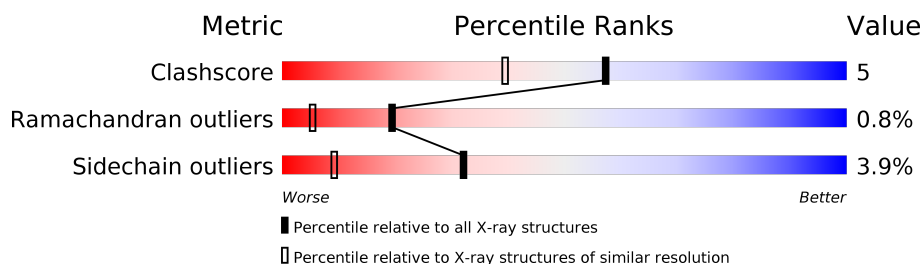
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	135	 73% 15% . . 9%
1	D	135	 70% 16% . . 10%

2 Entry composition [i](#)

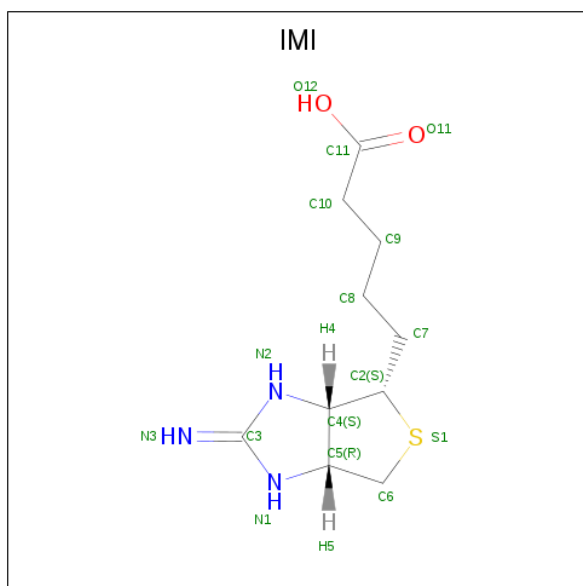
There are 3 unique types of molecules in this entry. The entry contains 2707 atoms, of which 690 are hydrogens and 0 are deuteriums.

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 STREPTAVIDIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	123	Total	C	H	N	O	4	4	0
			1158	595	217	159	187			
1	D	121	Total	C	H	N	O	0	4	0
			1134	577	215	157	185			

- Molecule 2 is 2-IMINOBIOTIN (three-letter code: IMI) (formula: $C_{10}H_{17}N_3O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O S	0	0
			20	10	4	3	2 1		
2	D	1	Total	C	H	N	O S	0	0
			20	10	4	3	2 1		

- Molecule 3 is water.

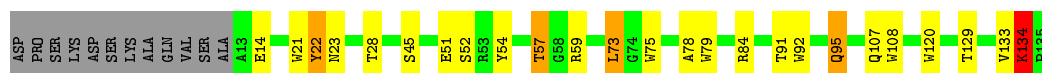
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	54	Total 162	H 108	O 54	0	0
3	D	71	Total 213	H 142	O 71	0	0

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 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.

• Molecule 1: STREPTAVIDIN

Chain B: 



• Molecule 1: STREPTAVIDIN

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.41Å 106.54Å 48.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 1.62 33.51 – 1.64	Depositor EDS
% Data completeness (in resolution range)	91.0 (7.50-1.62) 91.8 (33.51-1.64)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.63Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , 0.234 0.226 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2707	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMI

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	B	0.98	1/982 (0.1%)	1.77	31/1343 (2.3%)
1	D	0.94	0/958	1.80	27/1311 (2.1%)
All	All	0.96	1/1940 (0.1%)	1.78	58/2654 (2.2%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	SER	CA-CB	5.14	1.60	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	TRP	CD1-CG-CD2	9.98	114.28	106.30
1	B	21	TRP	CD1-CG-CD2	9.94	114.25	106.30
1	D	92	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	D	120	TRP	CD1-CG-CD2	8.87	113.39	106.30
1	B	59	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	B	120	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	75	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	D	75	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	B	59	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	107	GLN	CA-CB-CG	-7.85	96.13	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	108	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	D	79	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	D	21	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	B	21	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	B	75	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	D	92	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	D	120	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B	108	TRP	CD1-CG-CD2	7.31	112.14	106.30
1	B	120	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	D	79	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	D	53	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	B	79	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	D	108	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	B	79	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	B	108	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	B	54	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	D	92	TRP	CG-CD1-NE1	-6.67	103.43	110.10
1	B	92	TRP	CD1-CG-CD2	6.67	111.63	106.30
1	D	21	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	D	75	TRP	CG-CD1-NE1	-6.59	103.51	110.10
1	B	57	THR	CA-CB-CG2	6.58	121.61	112.40
1	B	21	TRP	CG-CD1-NE1	-6.44	103.66	110.10
1	B	22[A]	TYR	CB-CG-CD2	-6.39	117.16	121.00
1	B	22[B]	TYR	CB-CG-CD2	-6.39	117.16	121.00
1	D	92	TRP	CB-CG-CD1	-6.34	118.75	127.00
1	D	92	TRP	CG-CD2-CE3	6.27	139.54	133.90
1	B	92	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	D	103	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	84	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	14	GLU	CA-CB-CG	5.87	126.31	113.40
1	B	75	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	B	84	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	120	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	B	134	LYS	CB-CG-CD	-5.53	97.22	111.60
1	D	120	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	B	78	ALA	N-CA-C	-5.42	96.37	111.00
1	D	108	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B	73[A]	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	73[B]	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	120	TRP	CG-CD1-NE1	-5.17	104.92	110.10
1	D	29[A]	PHE	N-CA-CB	-5.17	101.29	110.60
1	D	29[B]	PHE	N-CA-CB	-5.17	101.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	D	21	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	D	84	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	108	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	D	60	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	95	GLN	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	LYS	Peptide

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	B	941	217	883	10	0
1	D	919	215	856	12	0
2	B	16	4	15	0	0
2	D	16	4	15	0	0
3	B	54	108	0	0	2
3	D	71	142	0	0	0
All	All	2017	690	1769	18	2

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 5.

All (18) 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)
1:B:22[A]:TYR:HE2	1:B:133:VAL:HG11	1.50	0.75
1:D:51:GLU:HB3	1:D:84:ARG:HG3	1.72	0.71
1:B:133:VAL:HG13	1:B:134:LYS:H	1.62	0.65
1:D:13:ALA:N	1:D:96:TYR:HH	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:HB	1:D:91:THR:HB	1.82	0.62
1:B:22[A]:TYR:CE2	1:B:133:VAL:HG11	2.34	0.61
1:D:23:ASN:HB3	1:D:130:PHE:CE1	2.40	0.56
1:B:95:GLN:NE2	1:D:114:THR:H	2.04	0.54
1:D:21:TRP:CZ2	1:D:132:LYS:HE3	2.42	0.54
1:D:51:GLU:O	1:D:52:SER:HB2	2.08	0.53
1:D:51:GLU:HB3	1:D:84:ARG:CG	2.39	0.53
1:B:22[A]:TYR:HE1	1:B:28:THR:HG1	1.62	0.47
1:B:95:GLN:HE22	1:D:114:THR:H	1.61	0.47
1:D:30:ILE:O	1:D:41:GLY:HA3	2.16	0.45
1:B:133:VAL:HG13	1:B:134:LYS:N	2.32	0.41
1:D:13:ALA:O	1:D:14:GLU:HB2	2.21	0.41
1:B:23:ASN:HA	1:B:129:THR:O	2.21	0.40
1:B:57:THR:HG22	1:D:59:ARG:HG2	2.02	0.40

All (2) 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)
3:B:972:HOH:H2	3:B:1462:HOH:O[6_555]	1.47	0.13
3:B:625:HOH:O	3:B:1082:HOH:H1[4_555]	1.59	0.01

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	B	125/135 (93%)	120 (96%)	4 (3%)	1 (1%)	19	5
1	D	123/135 (91%)	118 (96%)	4 (3%)	1 (1%)	19	5
All	All	248/270 (92%)	238 (96%)	8 (3%)	2 (1%)	19	5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	52	SER
1	B	52	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	
1	B	94/100 (94%)	91 (97%)	3 (3%)	39	14
1	D	92/100 (92%)	86 (94%)	6 (6%)	17	3
All	All	186/200 (93%)	177 (95%)	9 (5%)	32	6

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	GLU
1	B	73[A]	LEU
1	B	73[B]	LEU
1	D	14	GLU
1	D	29[A]	PHE
1	D	29[B]	PHE
1	D	52	SER
1	D	73	LEU
1	D	101	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	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](#)

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](#)

2 ligands are 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	$\# Z > 2$
2	IMI	D	300	-	14,17,17	0.80	0	16,23,23	1.81	4 (25%)
2	IMI	B	300	-	14,17,17	0.71	0	16,23,23	3.57	8 (50%)

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
2	IMI	D	300	-	-	2/5/28/28	0/2/2/2
2	IMI	B	300	-	-	1/5/28/28	0/2/2/2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	IMI	C4-C2-S1	9.46	114.22	105.20
2	B	300	IMI	C5-C6-S1	6.41	111.79	106.31
2	B	300	IMI	C2-C4-N2	-4.28	109.29	113.13
2	D	300	IMI	C2-C4-N2	-4.23	109.34	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	IMI	C6-C5-N1	-4.05	107.89	113.03
2	B	300	IMI	C7-C2-S1	3.73	122.96	112.64
2	B	300	IMI	C6-C5-C4	3.22	111.45	108.66
2	B	300	IMI	C9-C8-C7	-3.16	102.44	113.62
2	B	300	IMI	N2-C3-N1	3.11	112.39	109.20
2	D	300	IMI	N2-C3-N1	2.34	111.60	109.20
2	B	300	IMI	C6-C5-N1	-2.15	110.30	113.03
2	D	300	IMI	C5-C6-S1	2.09	108.10	106.31

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	300	IMI	S1-C2-C7-C8
2	D	300	IMI	C4-C2-C7-C8
2	B	300	IMI	C4-C2-C7-C8

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.