Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PTS
Title	:	CRYSTAL STRUCTURE AND LIGAND BINDING STUDIES OF A SCREENED PEPTIDE COMPLEXED WITH STREPTAVIDIN
Authors	:	Dupont Protein Crystallography Group
Deposited on	:	1992-07-23
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:

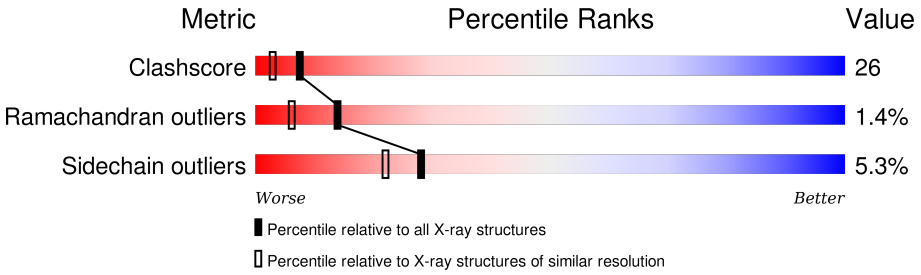
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	A	121	60% 30% 8%
1	B	121	64% 21% 7% 7%
2	P	7	29% 14% 57%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1982 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 protein called STREPTAVIDIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	0	1	0
			888	555	154	179			
1	B	112	Total	C	N	O	0	3	0
			850	534	147	169			

- Molecule 2 is a protein called PEPTIDE (FSHPQNT).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	P	3	Total	C	0	0	3
			3	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	112	Total	O	0	0
			112	112		

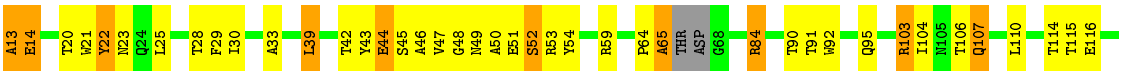
3 Residue-property plots (i)

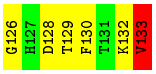
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: STREPTAVIDIN

Chain A:



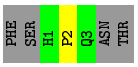


- Molecule 1: STREPTAVIDIN

Chain B:

- Molecule 2: PEPTIDE (FSHPQNT)

Chain P:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	95.20Å 106.50Å 47.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1982	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

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	1.47	2/914 (0.2%)	1.91	18/1250 (1.4%)
1	B	1.45	4/894 (0.4%)	1.83	16/1221 (1.3%)
All	All	1.46	6/1808 (0.3%)	1.87	34/2471 (1.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLY	N-CA	6.65	1.56	1.46
1	B	99	GLY	N-CA	5.51	1.54	1.46
1	A	65	ALA	C-O	5.47	1.33	1.23
1	B	52	SER	CA-CB	-5.43	1.44	1.52
1	B	45	SER	CB-OG	5.25	1.49	1.42
1	B	98	GLY	N-CA	5.12	1.53	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	84	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	B	84	ARG	CD-NE-CZ	11.38	139.53	123.60
1	A	59	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	103	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	59	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	B	31	VAL	CA-CB-CG2	8.04	122.96	110.90
1	A	39	LEU	CA-CB-CG	8.02	133.75	115.30
1	A	22	TYR	CB-CG-CD1	7.93	125.76	121.00
1	A	22	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	B	60	TYR	CB-CG-CD1	7.30	125.38	121.00
1	A	84	ARG	CB-CA-C	-7.06	96.27	110.40
1	B	60	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	B	59	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	B	103	ARG	N-CA-CB	6.56	122.41	110.60
1	A	65	ALA	CA-C-O	-6.53	106.39	120.10
1	A	43	TYR	CB-CG-CD2	-6.51	117.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	GLN	CA-CB-CG	-6.44	99.24	113.40
1	A	133	VAL	CA-C-O	-6.36	106.74	120.10
1	A	84	ARG	CD-NE-CZ	-6.24	114.86	123.60
1	B	52	SER	CB-CA-C	6.24	121.96	110.10
1	A	13	ALA	CB-CA-C	6.17	119.35	110.10
1	B	65	ALA	CA-C-O	-6.07	107.36	120.10
1	B	39	LEU	CB-CG-CD1	5.75	120.78	111.00
1	A	44	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	B	129	THR	CA-CB-CG2	-5.57	104.60	112.40
1	B	53	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	29	PHE	CA-CB-CG	5.49	127.08	113.90
1	A	128	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	92	TRP	O-C-N	5.32	131.21	122.70
1	B	52	SER	N-CA-CB	5.32	118.48	110.50
1	B	31	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	A	49	ASN	N-CA-CB	5.26	120.07	110.60
1	A	64	PRO	N-CD-CG	-5.24	95.34	103.20
1	B	103	ARG	NE-CZ-NH1	5.09	122.85	120.30

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	A	888	0	830	61	2
1	B	850	0	790	30	0
2	P	3	0	0	2	0
3	A	129	0	0	16	0
3	B	112	0	0	9	1
All	All	1982	0	1620	86	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 26.

All (86) 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:14:GLU:HB2	3:B:808:HOH:O	1.59	1.03
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.30	0.97
1:A:42[B]:THR:HG21	1:A:53:ARG:HH11	1.29	0.94
1:A:95:GLN:HE22	1:B:114:THR:H	1.07	0.92
1:A:114:THR:H	1:B:95:GLN:HE22	1.20	0.89
1:A:42[B]:THR:HG22	3:A:673:HOH:O	1.72	0.88
1:A:25:LEU:HD12	3:A:834:HOH:O	1.74	0.86
1:A:13:ALA:N	3:A:873:HOH:O	2.11	0.84
1:A:51:GLU:O	1:A:52:SER:HB3	1.76	0.84
1:B:45:SER:HB3	2:P:2:PRO:CA	2.10	0.81
1:B:69:SER:N	3:B:829:HOH:O	2.13	0.80
1:A:13:ALA:HA	3:A:856:HOH:O	1.85	0.75
1:A:42[B]:THR:HG23	1:A:53:ARG:HG3	1.69	0.75
1:A:42[A]:THR:OG1	1:A:53:ARG:HG2	1.87	0.74
1:A:42[A]:THR:OG1	1:A:53:ARG:CG	2.36	0.73
1:A:103:ARG:NH1	1:A:103:ARG:HG2	2.05	0.72
1:A:42[B]:THR:CG2	1:A:53:ARG:HH11	2.02	0.71
1:A:51:GLU:HB3	1:A:84:ARG:CG	2.22	0.70
1:A:42[B]:THR:HG23	1:A:53:ARG:CG	2.22	0.70
1:B:24:GLN:HG2	1:B:25:LEU:HG	1.74	0.68
1:A:44:GLU:HG3	3:A:673:HOH:O	1.96	0.66
1:B:45:SER:CB	2:P:2:PRO:CA	2.75	0.64
1:A:51:GLU:OE1	1:A:84:ARG:NH1	2.28	0.64
1:A:107:GLN:NE2	3:A:682:HOH:O	2.22	0.64
1:A:51:GLU:HB2	1:A:84:ARG:NH1	2.14	0.63
1:A:115:THR:HG23	3:A:837:HOH:O	1.99	0.62
1:A:90:THR:OG1	1:A:110:LEU:HD13	1.99	0.62
1:A:95:GLN:NE2	1:B:114:THR:H	1.89	0.62
1:A:51:GLU:O	1:A:52:SER:CB	2.46	0.60
1:A:48:GLY:HA2	3:A:815:HOH:O	2.02	0.59
1:A:51:GLU:OE1	1:A:84:ARG:HD3	2.03	0.58
1:B:13:ALA:HB3	1:B:16:GLY:HA3	1.84	0.58
1:A:30:ILE:HB	1:A:42[A]:THR:HG22	1.84	0.58
1:A:22:TYR:CE2	1:A:133:VAL:HG21	2.39	0.58
1:A:51:GLU:HB3	1:A:84:ARG:HG2	1.86	0.57
1:A:116:GLU:HB2	3:B:632:HOH:O	2.03	0.57
1:A:14:GLU:HA	1:A:33:ALA:HB3	1.85	0.57
1:A:50:ALA:HA	1:A:54:TYR:OH	2.06	0.56
1:A:48:GLY:CA	3:A:815:HOH:O	2.54	0.55
1:A:103:ARG:HD2	1:A:129:THR:CG2	2.36	0.55
1:B:13:ALA:N	3:B:696:HOH:O	2.40	0.54
1:B:53:ARG:NH1	3:B:754:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42[B]:THR:HG21	1:A:53:ARG:HD3	1.91	0.53
1:B:13:ALA:O	1:B:16:GLY:N	2.39	0.53
1:A:42[B]:THR:CG2	3:A:673:HOH:O	2.45	0.53
1:B:44:GLU:HG2	3:B:631:HOH:O	2.08	0.53
1:A:42[B]:THR:HG21	1:A:53:ARG:NH1	2.13	0.51
1:A:42[A]:THR:HG23	3:A:673:HOH:O	2.10	0.51
1:A:30:ILE:HG22	3:A:865:HOH:O	2.09	0.50
1:B:36:ASP:HA	3:B:759:HOH:O	2.11	0.49
1:A:42[B]:THR:CG2	1:A:53:ARG:CG	2.90	0.49
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.73	0.49
1:B:22:TYR:O	1:B:130:PHE:HA	2.13	0.49
1:A:42[B]:THR:CG2	1:A:53:ARG:HG3	2.40	0.48
1:A:22:TYR:HE1	1:A:28:THR:HG1	1.62	0.47
1:A:30:ILE:HB	1:A:42[A]:THR:CG2	2.43	0.47
1:B:13:ALA:N	1:B:96:TYR:CE2	2.83	0.47
1:B:42:THR:HB	1:B:53:ARG:HG2	1.95	0.47
1:B:13:ALA:HB2	3:B:700:HOH:O	2.14	0.47
1:A:46:ALA:C	1:A:47:VAL:HG13	2.36	0.45
1:A:84:ARG:HD2	3:A:845:HOH:O	2.15	0.45
1:A:20:THR:OG1	3:A:804:HOH:O	2.21	0.45
1:B:100:ALA:N	3:B:866:HOH:O	2.49	0.45
1:A:22:TYR:CD2	1:A:133:VAL:HG21	2.53	0.44
1:A:13:ALA:O	1:A:14:GLU:C	2.55	0.44
1:A:54:TYR:HE2	3:A:640:HOH:O	2.01	0.44
1:A:23:ASN:HB3	1:A:130:PHE:CE2	2.52	0.44
1:A:21:TRP:CZ3	1:A:132:LYS:HB2	2.53	0.44
1:A:42[A]:THR:HG1	1:A:53:ARG:HG2	1.84	0.43
1:A:95:GLN:HE22	1:B:114:THR:N	1.91	0.43
1:A:91:THR:HB	1:B:91:THR:HB	2.00	0.42
1:A:104:ILE:HG22	1:A:106:THR:HG23	2.00	0.42
1:B:23:ASN:HB3	1:B:130:PHE:CE1	2.55	0.42
1:A:84:ARG:HD3	1:A:84:ARG:HH11	1.64	0.42
1:A:84:ARG:HA	1:A:84:ARG:HD2	2.00	0.41
1:A:22:TYR:HE2	1:A:133:VAL:HG21	1.81	0.41
1:B:127:HIS:CD2	1:B:127:HIS:N	2.89	0.41
1:A:13:ALA:CB	3:A:856:HOH:O	2.69	0.41
1:B:13:ALA:C	1:B:16:GLY:H	2.23	0.41
1:A:45:SER:OG	1:A:47:VAL:O	2.39	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)
1:A:22:TYR:OH	1:A:22:TYR:OH[3_655]	1.98	0.22
1:A:65:ALA:O	3:B:751:HOH:O[4_556]	2.08	0.12

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	A	116/121 (96%)	111 (96%)	3 (3%)	2 (2%)	11 4
1	B	109/121 (90%)	106 (97%)	2 (2%)	1 (1%)	21 13
All	All	225/242 (93%)	217 (96%)	5 (2%)	3 (1%)	14 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	52	SER
1	B	14	GLU

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	A	87/88 (99%)	84 (97%)	3 (3%)	44 41
1	B	86/88 (98%)	78 (91%)	8 (9%)	11 6
All	All	173/176 (98%)	162 (94%)	11 (6%)	28 15

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	103	ARG
1	A	133	VAL
1	B	31	VAL
1	B	36	ASP
1	B	39	LEU
1	B	103	ARG
1	B	107[A]	GLN
1	B	107[B]	GLN
1	B	110[A]	LEU
1	B	110[B]	LEU

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

Mol	Chain	Res	Type
1	A	82	ASN
1	A	95	GLN
1	B	95	GLN

5.3.3 RNA

There are no RNA molecules 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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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