Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:01 PM GMT

PDB ID	:	1DPE
Title	:	DIPEPTIDE-BINDING PROTEIN
Authors	:	Nickitenko, A.V.; Trakhanov, S.; Quiocho, F.A.
Deposited on	:	1995-07-25
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:

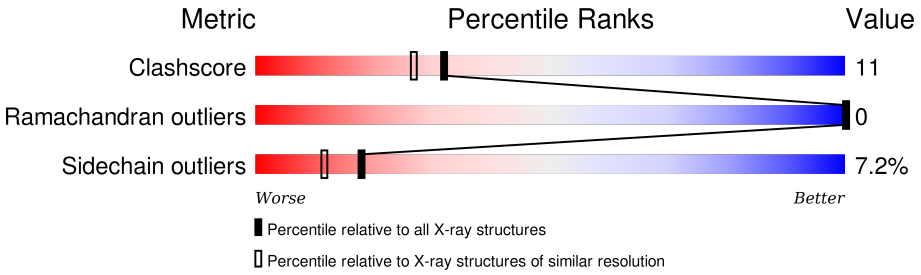
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	507	75% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4539 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 DIPEPTIDE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4046	2583	676	768	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	THR	CONFLICT	UNP P23847
A	419	GLU	LEU	CONFLICT	UNP P23847

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cd	0	0
			5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	488	Total	O	0	0
			488	488		

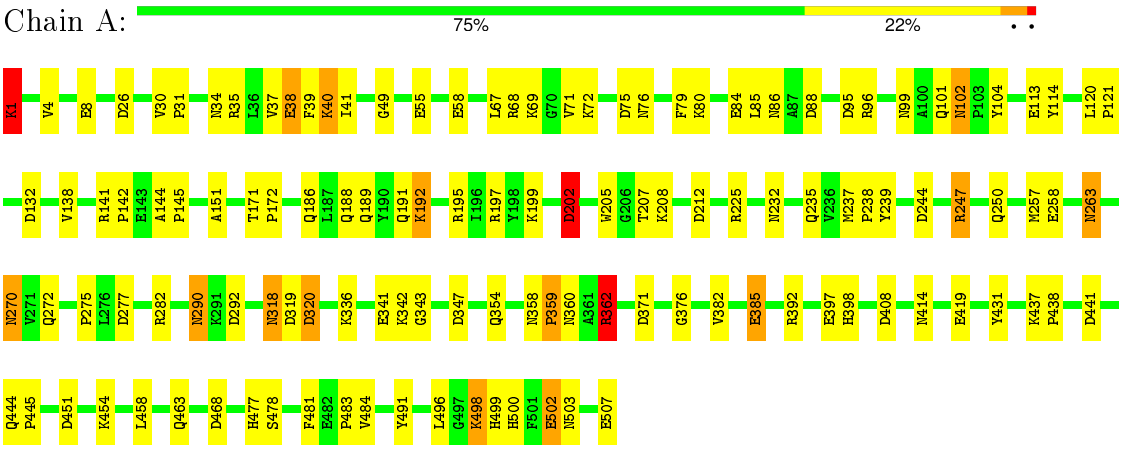
3 Residue-property plots (i)

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: DIPEPTIDE-BINDING PROTEIN

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.27Å 79.78Å 62.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.0 (6.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.70	0/4151	1.44	41/5627 (0.7%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	ASP	CB-CG-OD1	11.60	128.74	118.30
1	A	141	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	A	385	GLU	OE1-CD-OE2	-9.77	111.58	123.30
1	A	132	ASP	CB-CG-OD1	9.66	127.00	118.30
1	A	451	ASP	CB-CG-OD2	-9.35	109.88	118.30
1	A	347	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	362	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	A	68	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	239	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	A	419	GLU	OE1-CD-OE2	-8.04	113.65	123.30
1	A	347	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	239	TYR	CB-CG-CD2	7.78	125.67	121.00
1	A	195	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	451	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	468	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	371	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	88	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	320	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	244	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	397	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	95	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	282	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	392	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	250	GLN	CG-CD-OE1	-5.94	109.72	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	55	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	1	LYS	CB-CG-CD	5.79	126.66	111.60
1	A	502	GLU	OE1-CD-OE2	-5.75	116.39	123.30
1	A	292	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	8	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	502	GLU	CG-CD-OE1	5.51	129.33	118.30
1	A	244	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	277	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	385	GLU	CG-CD-OE1	5.31	128.92	118.30
1	A	282	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	96	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	202	ASP	CA-CB-CG	-5.20	101.96	113.40
1	A	142	PRO	N-CA-CB	5.20	109.54	103.30
1	A	441	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	95	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	225	ARG	NE-CZ-NH1	-5.03	117.79	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	4046	0	3941	84	0
2	A	5	0	0	0	0
3	A	488	0	0	11	0
All	All	4539	0	3941	84	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 11.

All (84) 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:A:342:LYS:HE3	1:A:342:LYS:HA	1.55	0.88
1:A:1:LYS:HG2	1:A:212:ASP:HB2	1.56	0.88
1:A:1:LYS:HB3	1:A:1:LYS:HZ2	1.38	0.87
1:A:385:GLU:CD	1:A:385:GLU:H	1.77	0.84
1:A:102:ASN:HD22	1:A:104:TYR:H	1.23	0.81
1:A:263:ASN:HD21	1:A:478:SER:H	1.31	0.75
1:A:26:ASP:OD2	1:A:499:HIS:HD2	1.70	0.73
1:A:507:GLU:O	1:A:507:GLU:HG2	1.91	0.70
1:A:188:GLN:NE2	3:A:788:HOH:O	2.11	0.70
1:A:257:MET:HE1	1:A:491:TYR:CD1	2.28	0.69
1:A:102:ASN:ND2	1:A:104:TYR:H	1.95	0.65
1:A:4:VAL:H	1:A:235:GLN:NE2	1.95	0.65
1:A:257:MET:HE1	1:A:484:VAL:HG21	1.80	0.64
1:A:342:LYS:HE3	1:A:342:LYS:CA	2.27	0.63
1:A:186:GLN:HE21	1:A:188:GLN:NE2	1.96	0.63
1:A:318:ASN:HD21	1:A:320:ASP:HB2	1.65	0.61
1:A:192:LYS:HB3	3:A:561:HOH:O	2.00	0.61
1:A:40:LYS:C	1:A:40:LYS:HD3	2.19	0.61
1:A:398:HIS:H	1:A:398:HIS:CD2	2.16	0.61
1:A:40:LYS:HD3	1:A:41:ILE:N	2.15	0.60
1:A:197:ARG:HH11	1:A:197:ARG:HG2	1.67	0.59
1:A:318:ASN:H	1:A:463:GLN:HE22	1.50	0.58
1:A:30:VAL:HB	1:A:31:PRO:HD3	1.86	0.57
1:A:186:GLN:HE21	1:A:188:GLN:HE22	1.51	0.57
1:A:257:MET:HE1	1:A:491:TYR:HD1	1.70	0.56
1:A:30:VAL:HG21	1:A:498:LYS:HG3	1.88	0.56
1:A:342:LYS:CA	1:A:342:LYS:CE	2.85	0.54
1:A:102:ASN:HD22	1:A:104:TYR:N	2.02	0.54
1:A:40:LYS:CD	1:A:40:LYS:C	2.76	0.54
1:A:336:LYS:HA	1:A:341:GLU:HG2	1.91	0.53
1:A:263:ASN:O	1:A:477:HIS:HD2	1.92	0.52
1:A:113:GLU:OE2	3:A:723:HOH:O	2.19	0.52
1:A:398:HIS:HE1	1:A:431:TYR:O	1.91	0.52
1:A:503:ASN:HB2	3:A:993:HOH:O	2.09	0.52
1:A:202:ASP:OD1	1:A:208:LYS:NZ	2.34	0.52
1:A:318:ASN:H	1:A:463:GLN:NE2	2.08	0.52
1:A:270:ASN:HD21	1:A:272:GLN:HB2	1.77	0.50
1:A:186:GLN:HG3	1:A:188:GLN:NE2	2.25	0.50
1:A:76:ASN:OD1	1:A:79:PHE:N	2.44	0.50
1:A:120:LEU:N	1:A:121:PRO:CD	2.76	0.49
1:A:500:HIS:ND1	3:A:896:HOH:O	2.33	0.49
1:A:354:GLN:HG3	1:A:359:PRO:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:OE2	3:A:896:HOH:O	2.20	0.48
1:A:408:ASP:H	1:A:414:ASN:ND2	2.11	0.48
1:A:75:ASP:HB2	1:A:79:PHE:O	2.13	0.48
1:A:197:ARG:NH1	1:A:197:ARG:HG2	2.29	0.48
1:A:34:ASN:ND2	1:A:205:TRP:HE1	2.13	0.47
1:A:290:ASN:HD22	1:A:290:ASN:C	2.17	0.47
1:A:1:LYS:HB3	1:A:1:LYS:NZ	2.19	0.47
1:A:171:THR:N	1:A:172:PRO:CD	2.77	0.47
1:A:237:MET:O	1:A:483:PRO:HD2	2.14	0.47
1:A:4:VAL:H	1:A:235:GLN:HE22	1.61	0.46
1:A:270:ASN:HD22	1:A:272:GLN:H	1.64	0.46
1:A:444:GLN:N	1:A:445:PRO:HD2	2.31	0.46
1:A:247:ARG:NH2	3:A:809:HOH:O	2.48	0.46
1:A:1:LYS:CG	1:A:212:ASP:HB2	2.37	0.46
1:A:71:VAL:O	1:A:84:GLU:HB3	2.16	0.45
1:A:362:ARG:HA	1:A:362:ARG:HD3	1.41	0.44
1:A:290:ASN:ND2	3:A:848:HOH:O	2.50	0.44
1:A:343:GLY:HA3	1:A:376:GLY:O	2.17	0.44
1:A:454:LYS:HE2	1:A:458:LEU:HD11	2.00	0.44
1:A:477:HIS:HE1	3:A:577:HOH:O	1.99	0.43
1:A:189:GLN:HE21	1:A:189:GLN:HB3	1.61	0.43
1:A:37:VAL:HG23	1:A:151:ALA:HB2	2.00	0.43
1:A:258:GLU:HG2	1:A:481:PHE:CD1	2.54	0.43
1:A:186:GLN:NE2	1:A:199:LYS:HD3	2.35	0.42
1:A:342:LYS:HA	1:A:342:LYS:CE	2.27	0.42
1:A:318:ASN:HD22	1:A:320:ASP:H	1.66	0.42
1:A:71:VAL:HB	1:A:85:LEU:HB3	2.00	0.42
1:A:408:ASP:H	1:A:414:ASN:HD21	1.67	0.42
1:A:99:ASN:OD1	1:A:101:GLN:HB2	2.20	0.42
1:A:39:PHE:CD2	1:A:496:LEU:HD13	2.55	0.42
1:A:341:GLU:H	1:A:341:GLU:HG3	1.39	0.42
1:A:38:GLU:OE1	1:A:49:GLY:HA3	2.20	0.42
1:A:499:HIS:HE1	3:A:565:HOH:O	2.03	0.41
1:A:498:LYS:HA	1:A:498:LYS:HD3	1.87	0.41
1:A:270:ASN:C	1:A:270:ASN:HD22	2.23	0.41
1:A:186:GLN:CG	1:A:199:LYS:HG2	2.50	0.41
1:A:270:ASN:ND2	1:A:272:GLN:HB2	2.35	0.41
1:A:30:VAL:CG2	1:A:498:LYS:HG3	2.49	0.41
1:A:437:LYS:HB3	1:A:438:PRO:HD3	2.02	0.41
1:A:144:ALA:N	1:A:145:PRO:CD	2.84	0.40
1:A:342:LYS:HD3	3:A:998:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:C	1:A:263:ASN:HD22	2.25	0.40

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	505/507 (100%)	491 (97%)	14 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	433/434 (100%)	402 (93%)	31 (7%)	18 12

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	35	ARG
1	A	38	GLU
1	A	40	LYS
1	A	58	GLU

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Mol	Chain	Res	Type
1	A	67	LEU
1	A	69	LYS
1	A	72	LYS
1	A	80	LYS
1	A	86	ASN
1	A	102	ASN
1	A	114	TYR
1	A	138	VAL
1	A	191	GLN
1	A	192	LYS
1	A	202	ASP
1	A	207	THR
1	A	232	ASN
1	A	238	PRO
1	A	247	ARG
1	A	263	ASN
1	A	270	ASN
1	A	275	PRO
1	A	290	ASN
1	A	318	ASN
1	A	358	ASN
1	A	359	PRO
1	A	360	ASN
1	A	362	ARG
1	A	382	VAL
1	A	498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	34	ASN
1	A	86	ASN
1	A	97	GLN
1	A	101	GLN
1	A	102	ASN
1	A	136	GLN
1	A	188	GLN
1	A	189	GLN
1	A	191	GLN
1	A	232	ASN
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	263	ASN
1	A	270	ASN
1	A	290	ASN
1	A	318	ASN
1	A	354	GLN
1	A	358	ASN
1	A	360	ASN
1	A	378	GLN
1	A	398	HIS
1	A	414	ASN
1	A	463	GLN
1	A	477	HIS
1	A	499	HIS

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)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.