Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:50 pm BST

PDB ID	:	1P10
Title	:	STRUCTURAL PLASTICITY AS A DETERMINANT OF ENZYME SPECIFICITY. CREATING BROADLY SPECIFIC PROTEASES
Authors	:	Bone, R.; Agard, D.A.
Deposited on	:	1989-04-24
Resolution	:	2.25 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:

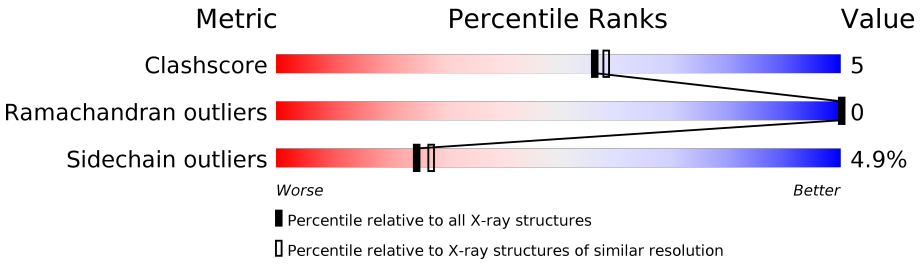
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	198	74% 21%
2	P	5	40% 40% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1566 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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1388	844	262	275	7			

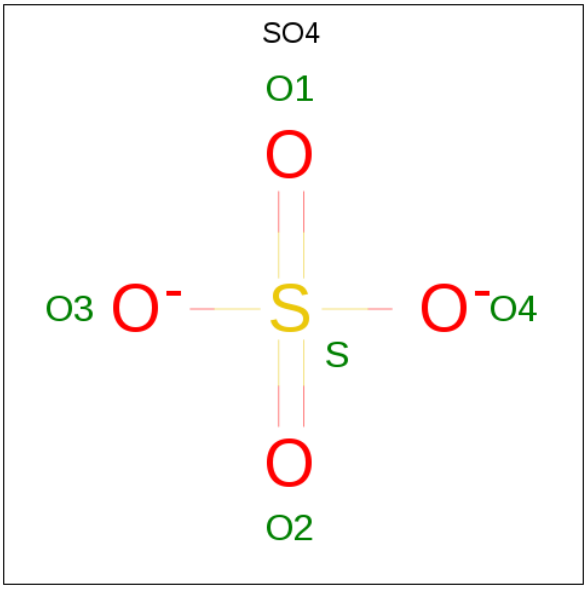
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	MET	CONFLICT	UNP P00778

- Molecule 2 is a protein called METHOXYSUCCINYL-ALA-ALA-PRO-VALINE BORONIC ACID INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total	B	C	N	O	0	0	0
			25	1	15	4	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	144	Total O 144 144	0	0
4	P	4	Total O 4 4	0	0

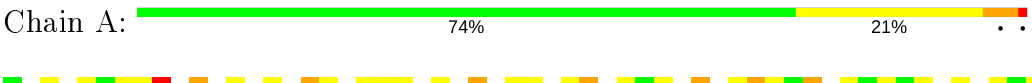
3 Residue-property plots (i)

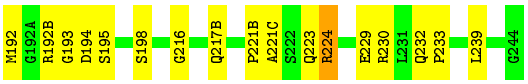
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: ALPHA-LYTIC PROTEASE

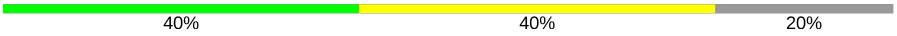
Chain A:





• Molecule 2: METHOXYSUCCINYL-ALA-ALA-PRO-VALINE BORONIC ACID INHIBITOR

Chain P:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	66.30Å 66.30Å 80.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.144 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1566	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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: B2V, SO4

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	1.12	0/1406	2.42	55/1906 (2.9%)
2	P	1.02	0/17	2.43	1/23 (4.3%)
All	All	1.11	0/1423	2.42	56/1929 (2.9%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48(B)	ARG	NE-CZ-NH1	-22.57	109.01	120.30
1	A	125	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	A	91	ARG	NE-CZ-NH2	20.18	130.39	120.30
1	A	48(B)	ARG	NH1-CZ-NH2	17.77	138.94	119.40
1	A	48(B)	ARG	NE-CZ-NH2	-16.55	112.02	120.30
1	A	91	ARG	NH1-CZ-NH2	-14.36	103.60	119.40
1	A	67	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	A	230	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	A	125	ARG	NH1-CZ-NH2	12.14	132.75	119.40
1	A	91	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	A	192(B)	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	A	141	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	141	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	192(B)	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	A	230	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	139	SER	N-CA-CB	-8.85	97.22	110.50
1	A	178	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	117	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	103	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	178	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	120(D)	SER	N-CA-CB	-7.56	99.16	110.50
1	A	31	TYR	CB-CG-CD1	7.40	125.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	SER	CA-CB-OG	-7.39	91.24	111.20
1	A	157	TYR	CB-CG-CD1	6.96	125.17	121.00
1	A	194	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	129	GLU	OE1-CD-OE2	6.81	131.47	123.30
1	A	102	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	125	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	A	161	THR	CA-CB-CG2	6.57	121.60	112.40
1	A	123	THR	O-C-N	6.57	133.21	122.70
2	P	4	ALA	CB-CA-C	-6.47	100.40	110.10
1	A	217(B)	GLN	CG-CD-NE2	6.41	132.08	116.70
1	A	174	GLU	CG-CD-OE2	-6.33	105.63	118.30
1	A	174	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	A	67	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	48(A)	THR	O-C-N	6.19	132.61	122.70
1	A	48	VAL	CA-CB-CG2	6.17	120.16	110.90
1	A	110	SER	CB-CA-C	-6.12	98.46	110.10
1	A	103	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	217(B)	GLN	CG-CD-OE1	-6.02	109.56	121.60
1	A	224	ARG	CD-NE-CZ	-5.93	115.30	123.60
1	A	157	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	129	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	A	57	HIS	CA-C-O	-5.75	108.03	120.10
1	A	171	TYR	CB-CG-CD2	5.64	124.39	121.00
1	A	178	ARG	N-CA-CB	-5.59	100.54	110.60
1	A	120(C)	SER	CB-CA-C	-5.49	99.67	110.10
1	A	48(B)	ARG	CB-CG-CD	-5.45	97.42	111.60
1	A	138	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	48	VAL	O-C-N	5.36	131.27	122.70
1	A	107	SER	O-C-N	5.36	131.27	122.70
1	A	224	ARG	O-C-N	5.33	131.23	122.70
1	A	117	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	A	216	GLY	O-C-N	5.14	130.92	122.70
1	A	52	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	224	ARG	CA-C-O	-5.02	109.55	120.10

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	1388	0	1356	14	0
2	P	25	0	26	2	0
3	A	5	0	0	0	0
4	A	144	0	0	2	0
4	P	4	0	0	0	0
All	All	1566	0	1382	14	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 5.

All (14) 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:195:SER:OG	2:P:1:B2V:CA	2.46	0.64
1:A:137:CYS:HA	1:A:159:CYS:HA	1.90	0.52
1:A:166:ASN:HD22	1:A:179:GLY:HA2	1.74	0.51
1:A:48(B):ARG:HG3	1:A:239:LEU:HD23	1.92	0.51
1:A:221(C):ALA:HA	1:A:224:ARG:HD2	1.94	0.48
1:A:129:GLU:HG3	4:A:362:HOH:O	2.16	0.45
1:A:46:PHE:O	1:A:52:PHE:HA	2.17	0.45
1:A:232:GLN:N	1:A:233:PRO:HD2	2.31	0.45
1:A:101:ASN:HB3	1:A:229:GLU:OE2	2.18	0.44
1:A:93:VAL:HG11	1:A:101:ASN:HD22	1.85	0.42
1:A:193:GLY:N	2:P:1:B2V:O1	2.44	0.42
1:A:48(B):ARG:HD3	4:A:353:HOH:O	2.20	0.41
1:A:138:ARG:HA	1:A:198:SER:O	2.20	0.40
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

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	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	198/203 (98%)	191 (96%)	7 (4%)	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	A	141/141 (100%)	134 (95%)	7 (5%)	24	26
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	142/142 (100%)	135 (95%)	7 (5%)	25	27

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(B)	ARG
1	A	91	ARG
1	A	110	SER
1	A	116	PRO
1	A	120(D)	SER
1	A	141	ARG
1	A	192	MET

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	101	ASN
1	A	166	ASN
1	A	223	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
2	B2V	P	1	1,2	2,7,7	0.20	0	4,9,9	0.95	0

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	B2V	P	1	1,2	-	0/4/8/8	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	B2V	2	0

5.5 Carbohydrates

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	$\#\|Z\| > 2$
3	SO4	A	1	-	4,4,4	0.61	0	6,6,6	0.56	0

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 (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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.