Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:26 PM GMT

PDB ID	:	1P05
Title	:	STRUCTURE ANALYSIS OF SPECIFICITY. ALPHA-LYTIC PROTEASE COMPLEXES WITH ANALOGUES OF REACTION INTERMEDIATES
Authors	:	Bone, R.; Agard, D.A.
Deposited on	:	1989-04-24
Resolution	:	2.10 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:

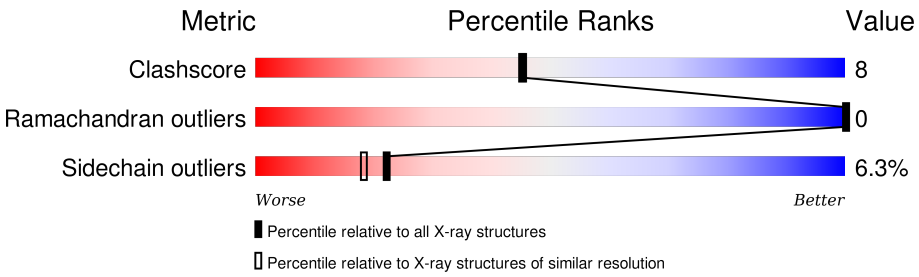
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	198	69% 26% . .
2	P	5	60% 20% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1596 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.

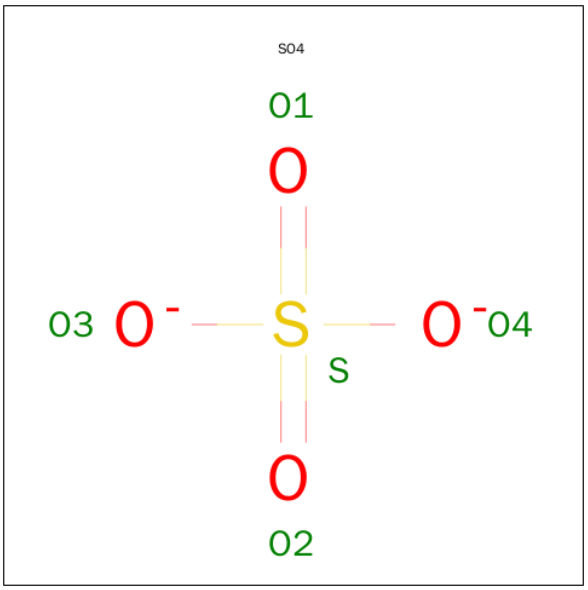
- Molecule 1 is a protein called ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1391	846	262	275	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	B	C	N	O			
2	P	4	26	1	16	4	5	0	0	0

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	171	171	171	0	0
			Total	O		
4	P	3	3	3	0	0

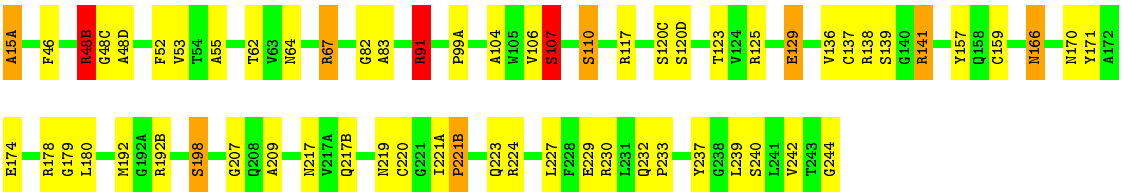
3 Residue-property plots (i)

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: ALPHA-LYTIC PROTEASE

Chain A:



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

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	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	66.32Å 66.32Å 80.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.139 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1596	wwPDB-VP
Average B, all atoms ($Å^2$)	9.0	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: BNO, 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	1.39	3/1409 (0.2%)	2.67	65/1909 (3.4%)
2	P	1.02	0/17	2.79	1/23 (4.3%)
All	All	1.39	3/1426 (0.2%)	2.67	66/1932 (3.4%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLU	CD-OE1	-6.02	1.19	1.25
1	A	240	SER	CB-OG	5.42	1.49	1.42
1	A	178	ARG	NE-CZ	5.37	1.40	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48(B)	ARG	CD-NE-CZ	38.01	176.81	123.60
1	A	91	ARG	NE-CZ-NH2	24.57	132.58	120.30
1	A	48(B)	ARG	NE-CZ-NH1	-23.27	108.66	120.30
1	A	230	ARG	NE-CZ-NH1	17.29	128.94	120.30
1	A	67	ARG	NE-CZ-NH1	17.04	128.82	120.30
1	A	125	ARG	NE-CZ-NH1	-13.71	113.44	120.30
1	A	178	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	171	TYR	CB-CG-CD1	-11.35	114.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120(D)	SER	N-CA-CB	-11.27	93.60	110.50
1	A	125	ARG	NH1-CZ-NH2	11.24	131.77	119.40
1	A	91	ARG	NH1-CZ-NH2	-11.09	107.20	119.40
1	A	125	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	230	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	A	171	TYR	CB-CG-CD2	9.98	126.99	121.00
1	A	48(B)	ARG	NH1-CZ-NH2	9.58	129.94	119.40
1	A	139	SER	N-CA-CB	-9.15	96.77	110.50
1	A	117	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	A	174	GLU	CG-CD-OE2	-8.64	101.01	118.30
2	P	4	ALA	N-CA-CB	8.64	122.20	110.10
1	A	91	ARG	CD-NE-CZ	8.62	135.67	123.60
1	A	224	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	192(B)	ARG	CD-NE-CZ	-8.28	112.00	123.60
1	A	224	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	125	ARG	CD-NE-CZ	7.66	134.32	123.60
1	A	110	SER	CA-CB-OG	-7.59	90.71	111.20
1	A	67	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	209	ALA	N-CA-CB	-7.05	100.23	110.10
1	A	242	VAL	N-CA-CB	-6.95	96.22	111.50
1	A	110	SER	CB-CA-C	-6.92	96.95	110.10
1	A	48(B)	ARG	CB-CG-CD	-6.55	94.57	111.60
1	A	192(B)	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	A	129	GLU	OE1-CD-OE2	6.46	131.05	123.30
1	A	107	SER	CA-CB-OG	-6.34	94.09	111.20
1	A	178	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	139	SER	CA-CB-OG	-6.22	94.41	111.20
1	A	192(B)	ARG	CG-CD-NE	-6.17	98.83	111.80
1	A	178	ARG	CD-NE-CZ	-6.09	115.08	123.60
1	A	120(C)	SER	CB-CA-C	-6.06	98.58	110.10
1	A	129	GLU	CG-CD-OE2	-6.02	106.25	118.30
1	A	230	ARG	CD-NE-CZ	-6.02	115.17	123.60
1	A	106	VAL	CA-C-O	-5.99	107.52	120.10
1	A	141	ARG	CA-CB-CG	5.92	126.44	113.40
1	A	180	LEU	O-C-N	5.91	132.16	122.70
1	A	174	GLU	CG-CD-OE1	5.90	130.10	118.30
1	A	136	VAL	N-CA-CB	-5.83	98.68	111.50
1	A	48(D)	ALA	N-CA-CB	-5.82	101.96	110.10
1	A	82	GLY	CA-C-O	-5.81	110.14	120.60
1	A	157	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	141	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	229	GLU	CG-CD-OE2	-5.62	107.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ALA	N-CA-CB	5.57	117.90	110.10
1	A	48(C)	GLY	N-CA-C	-5.57	99.17	113.10
1	A	157	TYR	N-CA-CB	-5.52	100.67	110.60
1	A	120(D)	SER	CA-CB-OG	-5.48	96.39	111.20
1	A	15(A)	ALA	O-C-N	5.48	131.47	122.70
1	A	170	ASN	CA-CB-CG	-5.48	101.34	113.40
1	A	227	LEU	CB-CG-CD2	5.47	120.29	111.00
1	A	53	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	A	220	CYS	CA-C-N	5.34	126.89	116.20
1	A	237	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	A	62	THR	CA-CB-CG2	-5.22	105.09	112.40
1	A	110	SER	N-CA-CB	-5.22	102.67	110.50
1	A	123	THR	CA-CB-OG1	-5.11	98.27	109.00
1	A	221(B)	PRO	O-C-N	5.10	130.85	122.70
1	A	207	GLY	O-C-N	5.07	130.82	122.70
1	A	64	ASN	CB-CG-ND2	5.05	128.82	116.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ARG	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	A	1391	0	1360	22	0
2	P	26	0	28	0	0
3	A	5	0	0	1	0
4	A	171	0	0	9	0
4	P	3	0	0	0	0
All	All	1596	0	1388	22	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 8.

All (22) 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:244:GLY:O	4:A:367:HOH:O	2.15	0.64
1:A:166:ASN:HD22	1:A:179:GLY:HA2	1.61	0.63
1:A:217(B):GLN:HG3	4:A:369:HOH:O	2.00	0.60
1:A:15(A):ALA:N	4:A:346:HOH:O	2.35	0.59
1:A:137:CYS:HA	1:A:159:CYS:HA	1.85	0.58
1:A:217:ASN:HB3	4:A:409:HOH:O	2.05	0.56
1:A:217:ASN:HA	4:A:406:HOH:O	2.08	0.54
1:A:217:ASN:O	1:A:219:ASN:HB3	2.08	0.53
1:A:48(B):ARG:HD2	4:A:354:HOH:O	2.09	0.52
1:A:48(B):ARG:HG3	1:A:239:LEU:HD23	1.93	0.51
1:A:46:PHE:O	1:A:52:PHE:HA	2.12	0.50
1:A:232:GLN:N	1:A:233:PRO:HD2	2.28	0.49
1:A:48(B):ARG:CZ	4:A:379:HOH:O	2.61	0.47
1:A:91:ARG:HB3	1:A:104:ALA:HB2	1.96	0.47
1:A:48(B):ARG:CG	1:A:239:LEU:HD23	2.45	0.46
1:A:129:GLU:HG3	4:A:363:HOH:O	2.15	0.46
1:A:107:SER:HB2	4:A:384:HOH:O	2.16	0.45
1:A:221(A):ILE:HB	1:A:221(B):PRO:HD2	2.00	0.44
1:A:233:PRO:HB3	3:A:1:SO4:O4	2.19	0.43
1:A:138:ARG:HA	1:A:198:SER:O	2.20	0.42
1:A:67:ARG:HA	1:A:83:ALA:O	2.20	0.41
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.35	0.41

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	142/142 (100%)	133 (94%)	9 (6%)	22 18
2	P	1/1 (100%)	1 (100%)	0	100 100
All	All	143/143 (100%)	134 (94%)	9 (6%)	22 18

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

Mol	Chain	Res	Type
1	A	48(B)	ARG
1	A	91	ARG
1	A	99(A)	PRO
1	A	107	SER
1	A	110	SER
1	A	141	ARG
1	A	166	ASN
1	A	192	MET
1	A	198	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	223	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	$\#\|Z\| > 2$
2	BNO	P	1	1,2	7,8,8	0.92	0	4,9,9	1.43	1 (25%)

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	BNO	P	1	1,2	-	0/3/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1	BNO	CG-CB-CA	-2.04	107.53	113.10

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	$\#\|Z\| > 2$
3	SO4	A	1	-	4,4,4	1.11	1 (25%)	6,6,6	1.21	1 (16%)

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	SO4	O4-S	2.12	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	SO4	O4-S-O3	-2.59	98.47	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	SO4	1	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.