



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:50 PM UTC

PDB ID : 1P12 / pdb_00001p12
Title : CRYSTAL STRUCTURES OF ALPHA-LYTIC PROTEASE COMPLEXES
WITH IRREVERSIBLY BOUND PHOSPHONATE ESTERS
Authors : Bone, R.; Agard, D.A.
Deposited on : 1990-10-26
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

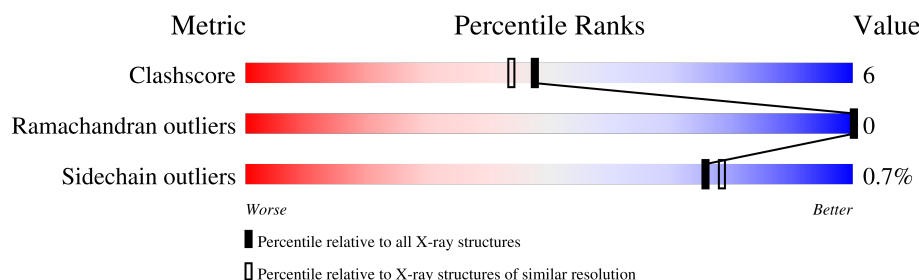
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	198	
2	I	7	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1644 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	E	198	Total	C	N	O	S	0	3	0
			1414	858	268	280	8			

- Molecule 2 is a protein called PHOSPHONATE ESTER INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	7	Total	C	N	O	P	0	0	0
			42	26	5	10	1			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

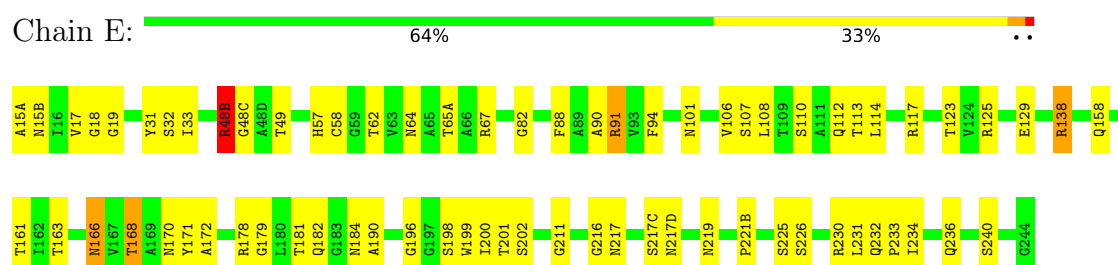
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	179	Total 179	O 179	0	0
4	I	4	Total 4	O 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



• Molecule 2: PHOSPHONATE ESTER INHIBITOR



4 Data and refinement statistics

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	66.79Å 66.79Å 79.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.124 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1644	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: BOC, PVA, SO4, LAC

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	E	1.41	3/1432 (0.2%)	2.38	72/1939 (3.7%)
2	I	1.88	0/22	4.28	5/27 (18.5%)
All	All	1.42	3/1454 (0.2%)	2.42	77/1966 (3.9%)

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	E	0	2
2	I	1	0
All	All	1	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	65(A)	THR	CA-CB	5.64	1.60	1.53
1	E	163	THR	CA-CB	5.46	1.61	1.54
1	E	18	GLY	N-CA	5.21	1.51	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48(B)	ARG	NE-CZ-NH1	19.73	141.22	121.50
1	E	48(B)	ARG	NE-CZ-NH2	-16.36	104.47	119.20
2	I	2	PRO	N-CA-CB	-11.55	90.29	103.00
2	I	2	PRO	CA-CB-CG	10.35	124.16	104.50
1	E	88	PHE	CA-C-O	-8.90	110.26	120.58
1	E	64	ASN	O-C-N	8.66	130.96	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ARG	NE-CZ-NH1	8.38	129.88	121.50
1	E	200	ILE	CA-C-O	-8.17	113.28	121.45
1	E	64	ASN	CB-CG-ND2	8.10	128.55	116.40
2	I	3	ALA	O-C-N	8.09	127.62	121.88
1	E	33	ILE	CA-C-O	-7.64	112.44	120.39
1	E	202	SER	CA-CB-OG	-7.44	96.22	111.10
1	E	82	GLY	CA-C-O	-7.34	111.26	119.04
1	E	216	GLY	O-C-N	7.31	132.34	124.15
1	E	113	THR	CA-CB-OG1	-7.21	98.78	109.60
1	E	64	ASN	CA-C-O	-7.08	109.74	119.16
1	E	91	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	E	101	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	E	107	SER	CA-CB-OG	-6.98	97.14	111.10
1	E	221(B)	PRO	CB-CA-C	6.90	120.07	111.23
1	E	166	ASN	CA-CB-CG	-6.90	105.70	112.60
1	E	112	GLN	OE1-CD-NE2	-6.89	115.70	122.60
1	E	216	GLY	CA-C-O	-6.83	114.90	121.05
1	E	182	GLN	CB-CG-CD	-6.82	101.01	112.60
1	E	31	TYR	CA-C-O	-6.62	113.92	121.40
1	E	110	SER	CA-CB-OG	-6.53	98.03	111.10
1	E	219	ASN	N-CA-C	-6.53	103.93	112.41
1	E	217	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	E	58	CYS	CA-C-O	-6.45	112.81	120.10
1	E	91	ARG	NH1-CZ-NH2	6.45	127.69	119.30
1	E	196	GLY	CA-C-O	-6.44	112.57	119.27
1	E	240	SER	CA-CB-OG	-6.30	98.50	111.10
1	E	107	SER	N-CA-CB	6.28	120.52	110.16
1	E	200	ILE	O-C-N	6.24	129.62	122.82
2	I	2	PRO	N-CD-CG	6.23	112.55	103.20
1	E	19	GLY	CA-C-O	-6.22	112.10	119.07
1	E	49	THR	CA-CB-OG1	-6.16	100.36	109.60
1	E	33	ILE	O-C-N	6.12	129.68	123.20
1	E	217(C)	SER	CA-C-O	-6.09	112.12	119.49
1	E	158	GLN	CG-CD-NE2	6.06	125.49	116.40
1	E	171	TYR	O-C-N	6.00	129.69	122.85
1	E	108	LEU	N-CA-CB	-5.99	101.18	110.46
1	E	65(A)	THR	CA-CB-OG1	-5.88	100.78	109.60
1	E	166	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	E	129	GLU	CA-C-O	-5.60	114.30	120.69
1	E	211	GLY	O-C-N	5.59	129.50	123.96
1	E	94	PHE	O-C-N	5.58	127.73	121.32
1	E	94	PHE	CA-C-O	-5.58	112.52	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	32	SER	CA-C-O	-5.57	114.94	121.46
1	E	190	ALA	N-CA-C	-5.57	102.04	110.28
1	E	106	VAL	CA-C-O	-5.57	114.58	120.48
1	E	113	THR	O-C-N	5.47	129.72	123.27
1	E	226	SER	CA-C-O	-5.47	114.66	120.40
1	E	90	ALA	CA-C-O	-5.46	115.38	121.23
1	E	231	LEU	N-CA-CB	-5.46	102.06	110.20
2	I	3	ALA	CA-C-O	-5.44	114.68	120.28
1	E	236	GLN	CA-C-O	-5.41	114.82	120.55
1	E	225	SER	CA-C-O	-5.41	114.72	120.40
1	E	114	LEU	CA-C-O	-5.35	114.76	120.92
1	E	199	TRP	N-CA-C	-5.31	100.24	108.90
1	E	170	ASN	CA-CB-CG	-5.30	107.30	112.60
1	E	15(B)	ASN	CB-CG-ND2	5.29	124.33	116.40
1	E	161	THR	CA-CB-OG1	-5.26	101.70	109.60
1	E	234	ILE	N-CA-C	-5.24	105.42	110.72
1	E	184	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	E	123	THR	CA-CB-OG1	-5.22	101.76	109.60
1	E	181	THR	CA-CB-OG1	-5.20	101.81	109.60
1	E	230	ARG	CA-C-O	-5.17	115.50	121.19
1	E	211	GLY	CA-C-N	-5.15	115.95	123.06
1	E	211	GLY	C-N-CA	-5.15	115.95	123.06
1	E	168	THR	CA-CB-OG1	-5.14	101.88	109.60
1	E	236	GLN	CA-CB-CG	-5.14	103.81	114.10
1	E	17	VAL	N-CA-CB	-5.08	103.10	111.44
1	E	217(D)	ASN	CB-CG-ND2	-5.08	108.78	116.40
1	E	172	ALA	N-CA-CB	-5.04	102.70	110.12
1	E	48(C)	GLY	N-CA-C	-5.04	102.81	111.47
1	E	62	THR	CA-CB-OG1	-5.01	102.09	109.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	-1	LAC	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	138	ARG	Sidechain
1	E	48(B)	ARG	Sidechain

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	E	1414	0	1381	14	0
2	I	42	0	31	2	0
3	E	5	0	0	0	0
4	E	179	0	0	8	0
4	I	4	0	0	1	0
All	All	1644	0	1412	16	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 6.

All (16) 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:E:166:ASN:HD22	1:E:179:GLY:HA2	1.63	0.63
4:E:340:HOH:O	2:I:5:BOC:H22	2.03	0.58
1:E:57:HIS:HE1	4:I:144:HOH:O	1.87	0.58
1:E:232:GLN:HG2	4:E:419:HOH:O	2.04	0.58
1:E:48(B):ARG:HD2	4:E:351:HOH:O	2.06	0.55
1:E:168:THR:HG23	1:E:178[A]:ARG:HG2	1.95	0.48
1:E:178[A]:ARG:HG3	1:E:178[A]:ARG:HH11	1.81	0.46
1:E:15(A):ALA:N	4:E:343:HOH:O	2.51	0.44
1:E:232:GLN:N	1:E:233:PRO:HD2	2.32	0.43
2:I:5:BOC:O1	2:I:5:BOC:H23	2.18	0.43
1:E:125:ARG:NH1	4:E:415:HOH:O	2.51	0.42
1:E:138:ARG:HA	1:E:198:SER:O	2.19	0.41
1:E:48(B):ARG:NE	4:E:376:HOH:O	2.53	0.41
1:E:166:ASN:HD22	1:E:166:ASN:HA	1.73	0.41
1:E:117:ARG:HD3	4:E:269:HOH:O	2.22	0.40
1:E:201:THR:HB	4:E:386:HOH:O	2.20	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	E	199/198 (100%)	191 (96%)	8 (4%)	0	100	100
2	I	3/7 (43%)	3 (100%)	0	0	100	100
All	All	202/205 (98%)	194 (96%)	8 (4%)	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	E	145/142 (102%)	144 (99%)	1 (1%)	76	78
2	I	1/1 (100%)	1 (100%)	0	100	100
All	All	146/143 (102%)	145 (99%)	1 (1%)	76	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	57	HIS
1	E	101	ASN

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Mol	Chain	Res	Type
1	E	166	ASN
1	E	170	ASN
1	E	182	GLN
1	E	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	E	1	-	4,4,4	0.68	0	6,6,6	1.09	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.