



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:38 AM GMT

PDB ID : 3L24
Title : Crystal Structure of the Nerve Agent Degrading Organophosphate Anhydrolase/Prolidasein Complex with Inhibitors
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Deposited on : 2009-12-14
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

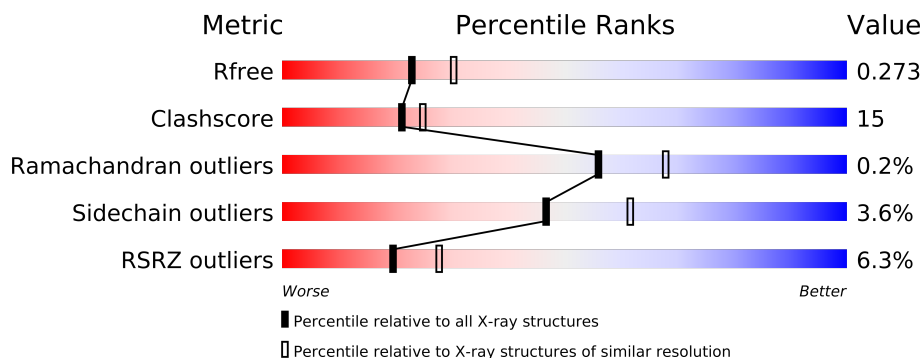
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	517	
1	B	517	
1	C	517	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MN	B	518	-	X
2	MN	B	519	-	X
3	GOA	B	522	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10683 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3443	2208	589	632	14			
1	B	417	Total	C	N	O	S	0	0	0
			3392	2175	581	624	12			
1	C	417	Total	C	N	O	S	0	0	0
			3392	2175	581	624	12			

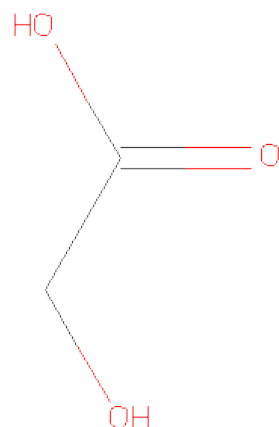
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	PRO	ALA	SEE REMARK 999	UNP Q44238
A	283	MET	CYS	SEE REMARK 999	UNP Q44238
A	439	LEU	ALA	SEE REMARK 999	UNP Q44238
B	211	PRO	ALA	SEE REMARK 999	UNP Q44238
B	283	MET	CYS	SEE REMARK 999	UNP Q44238
B	439	LEU	ALA	SEE REMARK 999	UNP Q44238
C	211	PRO	ALA	SEE REMARK 999	UNP Q44238
C	283	MET	CYS	SEE REMARK 999	UNP Q44238
C	439	LEU	ALA	SEE REMARK 999	UNP Q44238

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Mn	0	0
			4	4		
2	A	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		

- Molecule 3 is GLYCOLIC ACID (three-letter code: GOA) (formula: C₂H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	2	3		
3	B	1	Total	C	O	0	0
			5	2	3		
3	C	1	Total	C	O	0	0
			5	2	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	134	Total	O	0	0
			134	134		
4	C	110	Total	O	0	0
			110	110		

SER	H402	T326	L218	H1
TRP	I403	S327	Y103	N3
PRO	K407	S328	H226	L4
SER	D406	F329	R232	A5
GLU	V403	L340	K111	V6
PRO	A409	V345	T237	L7
LEU	E410	GLY	H238	Y8
TRP	L411	GLY	R239	A9
GLU	P413	PHE	S240	I12
GLU	P413	MET	F241	A13
GLU	F414	ALA	L242	T14
ILE	G415	ASP	I243	L15
LVS	G416	GLU	D244	Q16
LVS		GLN	A247	K17
SER	E420	GLN	A247	K17
THR	D421	GLY	R125	X18
PHE	N422	ALA	Y252	T19
ILE	I423	HIS	T129	I22
VAL	L424	GLN	T257	I23
HIS	V425	GLU	Q137	I23
VAL	H426	PRO	Y260	D29
ARG		PRO	M144	D29
THR	S429	GLU	K276	F33
ARG	L430	GLY	Q277	F33
ARG	E431	HIS	H278	Q37
ILE	N432	PRO	Y153	Q37
LEU	M433	PHE	H154	R40
VAL	T434	LEU	Y155	R40
ARG	R435	ARG	H156	F50
ARG	E436	CYS	Q285	X51
ARG	L437	T369	K160	V52
THR	R438	R370	T161	N53
THR	L439	K371	Q162	X54
SER	R440	L372	Y292	Q55
PRO	LEU	E373	G293	Q55
ILE	THR	A374	E294	A58
ILE	THR		M168	X59
ILE	HIS	V377	L297	L60
SER	SER	F378	D298	P66
VAL	LEU	T379	N172	W69
THR	ARG	S380	Q301	I70
PRO	GLY	E381	R302	V71
MET	LEU		F186	A72
PRO	SER	L384	Q305	K77
ALA	ALA	Y385	G189	P78
PRO	PRO	F386	N311	A72
ILE	GLN	L387	I312	K77
THR	PHE		V313	P78
THR	SER	L391	D314	V71
GLY	ILE	G392	L315	A72
LEU	ASN	R393	S316	K79
MET	ASP	L394	E319	I81
	PRO	A395	X319	D209
	ALA	A396	T320	N210
	VAL	V397	V321	V86
	MET	R398	A322	D87
	SER	N399	K323	F88
	GLU	N400	G324	W89
	THR	V403	T235	I215

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.35Å 143.93Å 219.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 2.30 47.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.10-2.30) 99.9 (47.40-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.273 0.235 , 0.273	Depositor DCC
R_{free} test set	8726 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 99543 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10683	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.39	0/3534	0.62	1/4795 (0.0%)
1	B	0.37	0/3482	0.61	1/4726 (0.0%)
1	C	0.36	1/3482 (0.0%)	0.59	2/4726 (0.0%)
All	All	0.37	1/10498 (0.0%)	0.61	4/14247 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	ASP	C-N	-5.47	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	ASN	N-CA-CB	-5.69	100.36	110.60
1	C	209	ASP	O-C-N	5.67	131.76	122.70
1	B	210	ASN	N-CA-CB	5.50	120.51	110.60
1	A	210	ASN	N-CA-CB	5.48	120.47	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3443	0	3318	93	0
1	B	3392	0	3271	98	0
1	C	3392	0	3270	120	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
3	A	5	0	3	0	0
3	B	5	0	3	0	0
3	C	5	0	3	0	0
4	A	187	0	0	6	0
4	B	134	0	0	2	0
4	C	110	0	0	4	0
All	All	10683	0	9868	309	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 309 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:GLN:HG2	1:B:129:ILE:HG21	1.33	1.05
1:A:55:GLN:HG2	1:A:129:ILE:HG21	1.41	1.02
1:A:169:ARG:HA	1:A:433:MET:HE2	1.45	0.97
1:C:3:LYS:HD3	1:C:3:LYS:H	1.30	0.97
1:B:395:ALA:HA	1:B:400:ASN:HD22	1.29	0.97

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	421/517 (81%)	403 (96%)	18 (4%)	0	100	100
1	B	413/517 (80%)	391 (95%)	21 (5%)	1 (0%)	56	68
1	C	413/517 (80%)	389 (94%)	23 (6%)	1 (0%)	56	68
All	All	1247/1551 (80%)	1183 (95%)	62 (5%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	ASP
1	B	96	PRO

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	360/443 (81%)	347 (96%)	13 (4%)	47	61
1	B	356/443 (80%)	342 (96%)	14 (4%)	43	57
1	C	356/443 (80%)	344 (97%)	12 (3%)	49	64
All	All	1072/1329 (81%)	1033 (96%)	39 (4%)	47	61

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	196	GLN
1	B	302	ARG
1	C	406	ASP
1	B	210	ASN
1	B	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	GLN
1	B	284	ASN
1	C	305	GLN
1	B	196	GLN
1	B	214	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 for Mogul analysis.

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	GOA	A	521	2	4,4,4	1.04	0	4,4,4	0.85	0
3	GOA	B	522	2	4,4,4	1.22	0	4,4,4	0.63	0
3	GOA	C	521	2	4,4,4	0.90	0	4,4,4	0.80	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
3	GOA	A	521	2	-	1/2/2/2	0/0/0/0
3	GOA	B	522	2	-	0/2/2/2	0/0/0/0
3	GOA	C	521	2	-	1/2/2/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	521	GOA	O12-C1-C2-O2
3	A	521	GOA	O12-C1-C2-O2

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/517 (82%)	0.12	21 (4%) 28 39	18, 36, 78, 95	0
1	B	417/517 (80%)	0.27	22 (5%) 25 35	20, 43, 78, 92	0
1	C	417/517 (80%)	0.58	37 (8%) 10 16	28, 51, 88, 98	0
All	All	1259/1551 (81%)	0.32	80 (6%) 19 27	18, 44, 82, 98	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	ILE	4.8
1	A	366	LEU	4.6
1	C	124	ALA	4.6
1	C	394	LEU	4.4
1	B	121	TYR	4.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	B	518	1/1	0.15	3.50	32,32,32,32	0
2	MN	B	519	1/1	0.18	3.50	33,33,33,33	0
3	GOA	B	522	5/5	0.16	2.93	43,48,50,51	0
2	MN	A	518	1/1	0.17	0.61	31,31,31,31	0
2	MN	C	519	1/1	0.14	-0.08	39,39,39,39	0
3	GOA	A	521	5/5	0.14	-0.14	34,34,40,41	0
2	MN	C	518	1/1	0.13	-0.46	39,39,39,39	0
2	MN	A	519	1/1	0.13	-0.56	27,27,27,27	0
2	MN	A	520	1/1	0.09	-0.80	36,36,36,36	0
2	MN	B	520	1/1	0.12	-0.88	57,57,57,57	0
3	GOA	C	521	5/5	0.12	-0.96	49,49,51,52	0
2	MN	C	520	1/1	0.07	-4.89	94,94,94,94	0
2	MN	B	521	1/1	0.10	-7.60	75,75,75,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.