



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 07:03 AM GMT

PDB ID : 3A0M
Title : Structure of (PPG)4-OVG-(PPG)4, monoclinic, twinned crystal
Authors : Okuyama, K.; Morimoto, T.; Mizuno, K.; Bachinger, H.P.
Deposited on : 2009-03-21
Resolution : 1.02 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>

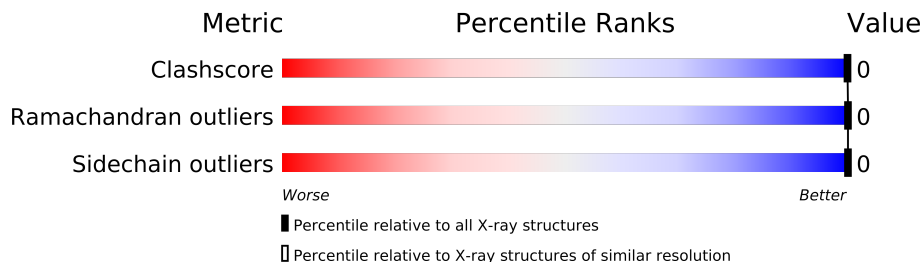
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
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 1.02 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	79885	1070 (1.12-0.92)
Ramachandran outliers	78287	1000 (1.12-0.92)
Sidechain outliers	78261	1222 (1.14-0.90)

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 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	31	
1	B	31	
1	C	31	
1	D	31	
1	E	31	
1	F	31	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1209 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 collagen-like peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	26	Total	C	N	O	0	0	0
			159	106	26	27			
1	B	24	Total	C	N	O	0	0	0
			146	96	24	26			
1	C	25	Total	C	N	O	0	0	0
			149	98	25	26			
1	D	24	Total	C	N	O	0	0	0
			145	96	24	25			
1	E	25	Total	C	N	O	0	0	0
			152	101	25	26			
1	F	24	Total	C	N	O	0	5	0
			178	118	29	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	13	PRO	HYP	MICROHETEROGENEITY	PDB 3A0M
F	14	PRO	VAL	MICROHETEROGENEITY	PDB 3A0M
F	16	HYP	PRO	MICROHETEROGENEITY	PDB 3A0M
F	17	VAL	PRO	MICROHETEROGENEITY	PDB 3A0M

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total	O	0	0
			47	47		
2	B	49	Total	O	0	0
			49	49		
2	C	56	Total	O	0	0
			56	56		
2	D	37	Total	O	0	0
			37	37		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	43	Total 43	O 43	0	0
2	F	48	Total 48	O 48	0	0

3 Residue-property plots

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 failed to run properly.

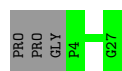
- Molecule 1: collagen-like peptide

Chain A: 



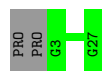
- Molecule 1: collagen-like peptide

Chain B: 



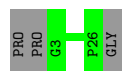
- Molecule 1: collagen-like peptide

Chain C: 



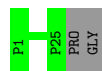
- Molecule 1: collagen-like peptide

Chain D: 



- Molecule 1: collagen-like peptide

Chain E: 



- Molecule 1: collagen-like peptide

Chain F: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	26.12Å 26.37Å 79.94Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	24.80 – 1.02	Depositor
% Data completeness (in resolution range)	92.1 (24.80-1.02)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 0.98Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.116 , 0.143	Depositor
Wilson B-factor (Å ²)	7.7	Xtriage
Anisotropy	0.096	Xtriage
Estimated twinning fraction	0.395 for H,-K,-L 0.079 for -k,-h,-l 0.075 for k,h,-l 0.417 for h,-k,-l	Xtriage
Reported twinning fraction	0.395 for H,-K,-L	Depositor
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	3 of 60013 reflections (0.005%)	Xtriage
Total number of atoms	1209	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.51 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2465e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: HYP

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	0.69	0/165	0.92	0/235
1	B	0.82	0/150	1.02	0/211
1	C	0.79	0/153	0.95	0/217
1	D	0.77	0/149	1.13	0/212
1	E	0.79	0/157	0.90	0/223
1	F	1.69	1/173 (0.6%)	1.36	2/239 (0.8%)
All	All	1.01	1/947 (0.1%)	1.06	2/1337 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	14[B]	PRO	C-N	-20.21	0.96	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13[B]	PRO	O-C-N	9.89	138.53	122.70
1	F	13[B]	PRO	CA-C-N	-7.52	100.66	117.20

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	159	0	0	0	0
1	B	146	0	0	0	0
1	C	149	0	2	0	0
1	D	145	0	0	0	0
1	E	152	0	0	0	0
1	F	178	0	0	0	0
2	A	47	0	0	0	0
2	B	49	0	0	0	0
2	C	56	0	0	0	0
2	D	37	0	0	0	0
2	E	43	0	0	0	0
2	F	48	0	0	0	0
All	All	1209	0	2	0	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 0.

There are no clashes within the asymmetric unit.

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	23/31 (74%)	23 (100%)	0	0	100	100
1	B	21/31 (68%)	21 (100%)	0	0	100	100
1	C	22/31 (71%)	22 (100%)	0	0	100	100
1	D	21/31 (68%)	21 (100%)	0	0	100	100
1	E	22/31 (71%)	22 (100%)	0	0	100	100
1	F	19/31 (61%)	19 (100%)	0	0	100	100
All	All	128/186 (69%)	128 (100%)	0	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	17/20 (85%)	17 (100%)	0	100	100
1	B	15/20 (75%)	15 (100%)	0	100	100
1	C	15/20 (75%)	15 (100%)	0	100	100
1	D	15/20 (75%)	15 (100%)	0	100	100
1	E	16/20 (80%)	16 (100%)	0	100	100
1	F	18/20 (90%)	18 (100%)	0	100	100
All	All	96/120 (80%)	96 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

7 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	HYP	A	13	1	8,8,9	6.33	2 (25%)	8,10,12	1.46	1 (12%)
1	HYP	B	13	1	8,8,9	5.02	2 (25%)	8,10,12	1.48	1 (12%)
1	HYP	C	13	1	8,8,9	5.92	2 (25%)	8,10,12	2.57	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	D	13	1	8,8,9	5.73	1 (12%)	8,10,12	1.13	0
1	HYP	E	13	1	8,8,9	6.72	1 (12%)	8,10,12	1.07	0
1	HYP	F	13[A]	1	8,8,9	6.42	2 (25%)	8,10,12	0.70	0
1	HYP	F	16[B]	1	8,8,9	6.32	2 (25%)	8,10,12	1.64	3 (37%)

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
1	HYP	A	13	1	-	0/0/11/13	0/1/1/1
1	HYP	B	13	1	-	0/0/11/13	0/1/1/1
1	HYP	C	13	1	-	0/0/11/13	0/1/1/1
1	HYP	D	13	1	-	0/0/11/13	0/1/1/1
1	HYP	E	13	1	-	0/0/11/13	0/1/1/1
1	HYP	F	13[A]	1	-	0/0/11/13	0/1/1/1
1	HYP	F	16[B]	1	-	0/0/11/13	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	13	HYP	O-C	18.77	1.24	1.11
1	F	13[A]	HYP	O-C	17.78	1.23	1.11
1	A	13	HYP	O-C	17.63	1.23	1.11
1	F	16[B]	HYP	O-C	17.48	1.23	1.11
1	C	13	HYP	O-C	16.33	1.22	1.11

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	HYP	CG-CD-N	-4.49	98.23	105.47
1	C	13	HYP	CB-CG-CD	3.72	108.75	103.46
1	C	13	HYP	CD-N-CA	3.43	114.63	108.15
1	A	13	HYP	CG-CB-CA	3.11	108.76	104.22
1	F	16[B]	HYP	CD-N-CA	2.74	113.32	108.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.