



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 12:25 AM EDT

PDB ID : 6VID
Title : The Crystal Structure of Aps Domain-Swapped Trimer Q108K:K40D:T53A:
R58L:Q38F:Q4F Variant of HCRBPII
Authors : Ghanbarpour, A.; Geiger, J.
Deposited on : 2020-01-12
Resolution : 2.89 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 2.89 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6167 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 Retinol-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	1063	674	176	208	5	0	0	0
1	B	133	1045	663	173	204	5	0	0	0
1	C	133	964	610	158	191	5	0	0	0
1	D	133	1077	684	179	209	5	0	0	0
1	E	133	1002	638	169	190	5	0	0	0
1	F	131	954	602	155	192	5	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	PHE	GLN	engineered mutation	UNP P50120
A	38	PHE	GLN	engineered mutation	UNP P50120
A	40	ASP	LYS	engineered mutation	UNP P50120
A	53	ALA	THR	engineered mutation	UNP P50120
A	58	LEU	ARG	engineered mutation	UNP P50120
A	108	LYS	GLN	engineered mutation	UNP P50120
B	4	PHE	GLN	engineered mutation	UNP P50120
B	38	PHE	GLN	engineered mutation	UNP P50120
B	40	ASP	LYS	engineered mutation	UNP P50120
B	53	ALA	THR	engineered mutation	UNP P50120
B	58	LEU	ARG	engineered mutation	UNP P50120
B	108	LYS	GLN	engineered mutation	UNP P50120
C	4	PHE	GLN	engineered mutation	UNP P50120
C	38	PHE	GLN	engineered mutation	UNP P50120
C	40	ASP	LYS	engineered mutation	UNP P50120
C	53	ALA	THR	engineered mutation	UNP P50120
C	58	LEU	ARG	engineered mutation	UNP P50120

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Chain	Residue	Modelled	Actual	Comment	Reference
C	108	LYS	GLN	engineered mutation	UNP P50120
D	4	PHE	GLN	engineered mutation	UNP P50120
D	38	PHE	GLN	engineered mutation	UNP P50120
D	40	ASP	LYS	engineered mutation	UNP P50120
D	53	ALA	THR	engineered mutation	UNP P50120
D	58	LEU	ARG	engineered mutation	UNP P50120
D	108	LYS	GLN	engineered mutation	UNP P50120
E	4	PHE	GLN	engineered mutation	UNP P50120
E	38	PHE	GLN	engineered mutation	UNP P50120
E	40	ASP	LYS	engineered mutation	UNP P50120
E	53	ALA	THR	engineered mutation	UNP P50120
E	58	LEU	ARG	engineered mutation	UNP P50120
E	108	LYS	GLN	engineered mutation	UNP P50120
F	4	PHE	GLN	engineered mutation	UNP P50120
F	38	PHE	GLN	engineered mutation	UNP P50120
F	40	ASP	LYS	engineered mutation	UNP P50120
F	53	ALA	THR	engineered mutation	UNP P50120
F	58	LEU	ARG	engineered mutation	UNP P50120
F	108	LYS	GLN	engineered mutation	UNP P50120

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



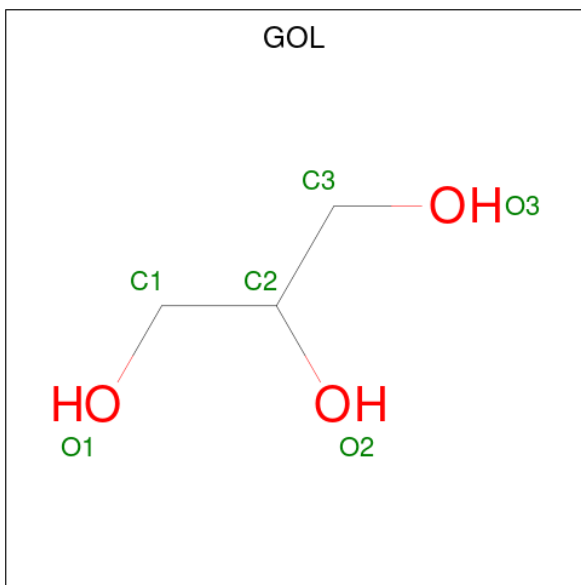
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	D	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total O 2 2	0	0
4	F	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.05Å 72.68Å 164.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.89	Depositor
% Data completeness (in resolution range)	99.5 (49.28-2.89)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.245 , 0.308	Depositor
Wilson B-factor (Å ²)	61.5	Xtrriage
Anisotropy	0.216	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6167	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

9 ligands 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
3	GOL	A	205	-	5,5,5	0.90	0	5,5,5	1.00	0
2	ACT	B	201	-	3,3,3	1.31	0	3,3,3	1.53	0
3	GOL	D	201	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	A	204	-	5,5,5	0.90	0	5,5,5	1.00	0
3	GOL	B	202	-	5,5,5	0.90	0	5,5,5	0.99	0
2	ACT	E	201	-	3,3,3	1.31	0	3,3,3	1.52	0
2	ACT	A	201	-	3,3,3	1.29	0	3,3,3	1.38	0
2	ACT	A	202	-	3,3,3	1.30	0	3,3,3	1.53	0
3	GOL	A	203	-	5,5,5	0.91	0	5,5,5	1.00	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	GOL	A	205	-	-	3/4/4/4	-
3	GOL	D	201	-	-	2/4/4/4	-
3	GOL	A	204	-	-	0/4/4/4	-
3	GOL	B	202	-	-	4/4/4/4	-
3	GOL	A	203	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	GOL	O1-C1-C2-C3
3	B	202	GOL	C1-C2-C3-O3
3	D	201	GOL	O1-C1-C2-C3
3	B	202	GOL	O2-C2-C3-O3
3	B	202	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.