



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 03:03 AM EDT

PDB ID : 5UQD
Title : DPY-21 in complex with Fe(II) and alpha-Ketoglutarate
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Deposited on : 2017-02-07
Resolution : 1.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

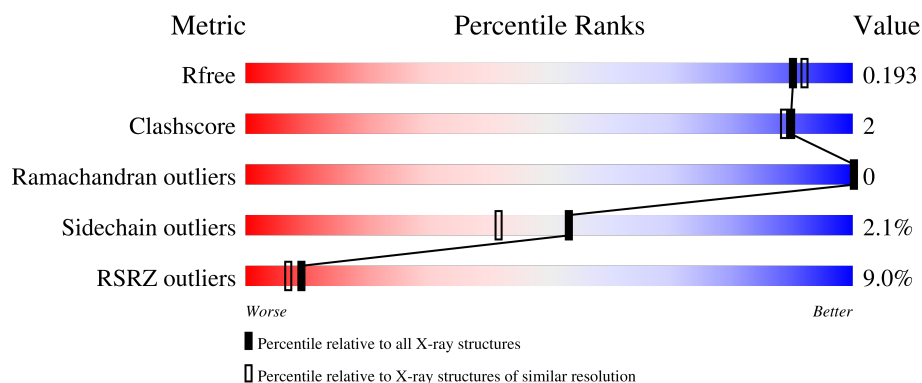
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	442	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2985 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 DumpY: shorter than wild-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2703	1711	490	478	24	0	11	0

There are 34 discrepancies between the modelled and reference sequences:

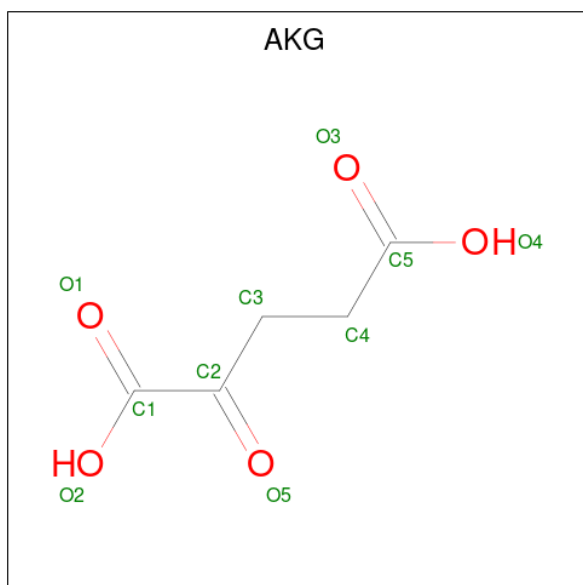
Chain	Residue	Modelled	Actual	Comment	Reference
A	1176	MET	-	initiating methionine	UNP Q9GRZ3
A	1177	LYS	-	expression tag	UNP Q9GRZ3
A	1178	SER	-	expression tag	UNP Q9GRZ3
A	1179	SER	-	expression tag	UNP Q9GRZ3
A	1180	TRP	-	expression tag	UNP Q9GRZ3
A	1181	SER	-	expression tag	UNP Q9GRZ3
A	1182	HIS	-	expression tag	UNP Q9GRZ3
A	1183	PRO	-	expression tag	UNP Q9GRZ3
A	1184	GLN	-	expression tag	UNP Q9GRZ3
A	1185	PHE	-	expression tag	UNP Q9GRZ3
A	1186	GLU	-	expression tag	UNP Q9GRZ3
A	1187	LYS	-	expression tag	UNP Q9GRZ3
A	1188	GLY	-	expression tag	UNP Q9GRZ3
A	1189	ALA	-	expression tag	UNP Q9GRZ3
A	1190	MET	-	expression tag	UNP Q9GRZ3
A	1191	THR	-	expression tag	UNP Q9GRZ3
A	1192	GLY	-	expression tag	UNP Q9GRZ3
A	1193	TRP	-	expression tag	UNP Q9GRZ3
A	1194	SER	-	expression tag	UNP Q9GRZ3
A	1195	HIS	-	expression tag	UNP Q9GRZ3
A	1196	PRO	-	expression tag	UNP Q9GRZ3
A	1197	GLN	-	expression tag	UNP Q9GRZ3
A	1198	PHE	-	expression tag	UNP Q9GRZ3
A	1199	GLU	-	expression tag	UNP Q9GRZ3
A	1200	LYS	-	expression tag	UNP Q9GRZ3
A	1201	GLU	-	expression tag	UNP Q9GRZ3
A	1202	ASN	-	expression tag	UNP Q9GRZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1203	LEU	-	expression tag	UNP Q9GRZ3
A	1204	TYR	-	expression tag	UNP Q9GRZ3
A	1205	PHE	-	expression tag	UNP Q9GRZ3
A	1206	GLN	-	expression tag	UNP Q9GRZ3
A	1207	SER	-	expression tag	UNP Q9GRZ3
A	1208	ASN	-	expression tag	UNP Q9GRZ3
A	1209	ALA	-	expression tag	UNP Q9GRZ3

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).

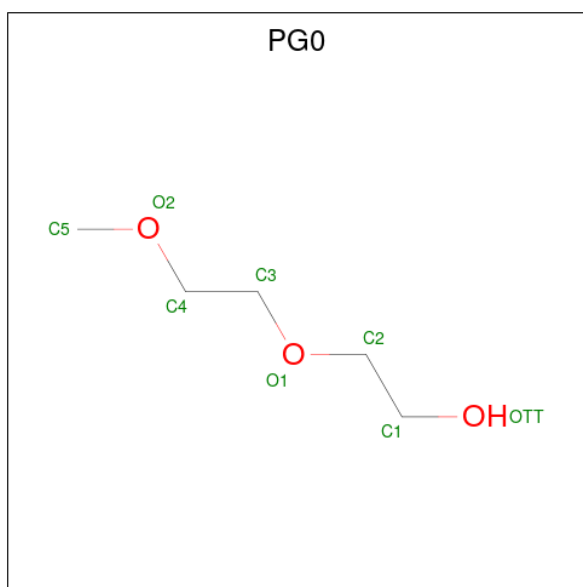


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	5	3		
4	A	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	1
			255	255		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.62Å 97.88Å 98.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 1.80 43.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.86-1.80) 99.4 (43.86-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.163 , 0.193 0.163 , 0.193	Depositor DCC
R_{free} test set	1978 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2985	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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.

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: AKG, PG0, FE2

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	0.68	1/2777 (0.0%)	0.71	1/3743 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1581	GLU	CD-OE1	-5.35	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1302	ASP	CB-CG-OD1	5.45	123.21	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2703	0	2662	10	0
2	A	10	0	4	0	0
3	A	1	0	0	0	0
4	A	16	0	24	1	0
5	A	255	0	0	0	0
All	All	2985	0	2690	10	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 2.

The worst 5 of 10 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:1448[B]:ARG:HG2	1:A:1558:TRP:CH2	2.27	0.70
1:A:1446:ASN:HB3	1:A:1448[B]:ARG:HD3	1.78	0.65
1:A:1358[B]:MET:HE1	1:A:1373:MET:SD	2.51	0.51
1:A:1448[B]:ARG:HG2	1:A:1558:TRP:CZ3	2.49	0.47
1:A:1319:GLY:O	1:A:1351:GLY:HA3	2.17	0.45

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	323/442 (73%)	320 (99%)	3 (1%)	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	294/389 (76%)	288 (98%)	6 (2%)	55	44

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1378	ASN
1	A	1404	ASP
1	A	1454	ASP
1	A	1293	MET
1	A	1267	MET

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	PG0	A	1703	-	7,7,7	0.44	0	6,6,6	0.31	0
2	AKG	A	1701	3	9,9,9	1.97	3 (33%)	11,11,11	2.76	7 (63%)
4	PG0	A	1704	-	7,7,7	0.47	0	6,6,6	0.26	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
4	PG0	A	1703	-	-	0/5/5/5	-
2	AKG	A	1701	3	-	1/9/9/9	-
4	PG0	A	1704	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	AKG	O1-C1	3.17	1.31	1.22
2	A	1701	AKG	O4-C5	-2.85	1.21	1.30
2	A	1701	AKG	C3-C2	2.76	1.54	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	AKG	C4-C3-C2	-4.24	105.04	113.03
2	A	1701	AKG	C3-C4-C5	-4.10	104.78	113.60
2	A	1701	AKG	C3-C2-C1	3.61	122.68	115.97
2	A	1701	AKG	O5-C2-C3	-3.35	113.79	121.20
2	A	1701	AKG	O2-C1-O1	-2.83	117.13	123.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1704	PG0	O1-C3-C4-O2
4	A	1704	PG0	C4-C3-O1-C2
2	A	1701	AKG	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1704	PG0	1	0

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 [i](#)

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

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	324/442 (73%)	0.52	29 (8%) 9 7	13, 24, 50, 66	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1548	TYR	9.0
1	A	1395	VAL	7.3
1	A	1369	ASN	5.3
1	A	1402	THR	5.2
1	A	1403	SER	4.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PG0	A	1704	8/8	0.70	0.25	72,75,76,76	0
2	AKG	A	1701	10/10	0.85	0.15	23,29,32,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PG0	A	1703	8/8	0.91	0.18	45,46,57,59	0
3	FE2	A	1702	1/1	1.00	0.09	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.