



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:29 PM UTC

PDB ID : 6XAG / pdb_00006xag
Title : Apo BRAF dimer bound to 14-3-3
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Deposited on : 2020-06-04
Resolution : 3.30 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

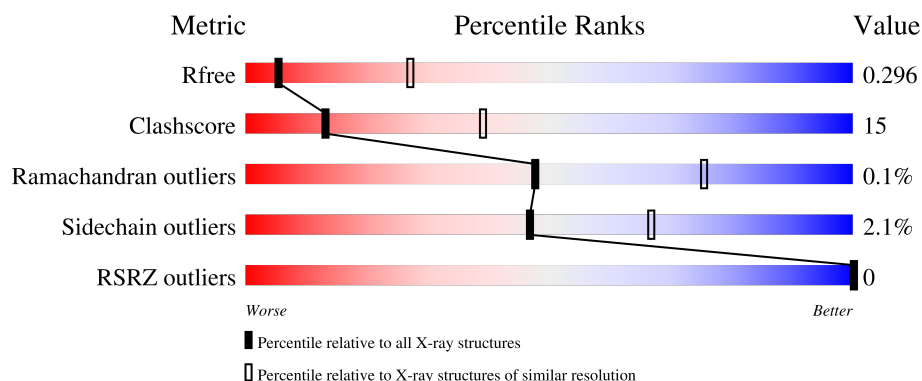
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	232	 74% 25% .
1	B	232	 66% 28% . .
2	C	290	 68% 25% . 5%
2	D	290	 69% 24% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8063 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 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	1	0
			1843	1154	309	370	10			
1	B	223	Total	C	N	O	S	0	0	0
			1787	1121	302	354	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P63104
A	0	SER	-	expression tag	UNP P63104
B	-1	GLY	-	expression tag	UNP P63104
B	0	SER	-	expression tag	UNP P63104

- Molecule 2 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	276	Total	C	N	O	P S	0	0	0
			2202	1388	396	404	1 13			
2	D	278	Total	C	N	O	P S	0	0	0
			2227	1408	398	407	1 13			

There are 30 discrepancies between the modelled and reference sequences:

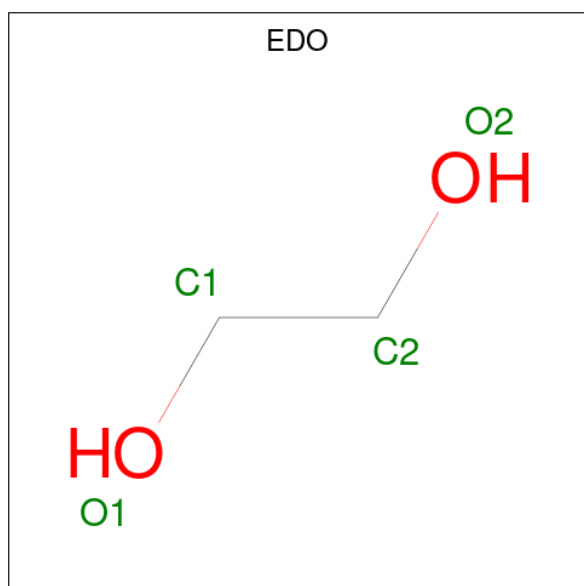
Chain	Residue	Modelled	Actual	Comment	Reference
C	446	GLY	-	expression tag	UNP P15056
C	543	ALA	ILE	conflict	UNP P15056
C	544	SER	ILE	conflict	UNP P15056
C	551	LYS	ILE	conflict	UNP P15056
C	562	ARG	GLN	conflict	UNP P15056
C	588	ASN	LEU	conflict	UNP P15056
C	630	SER	LYS	conflict	UNP P15056
C	667	GLU	PHE	conflict	UNP P15056

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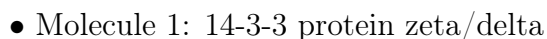
Chain	Residue	Modelled	Actual	Comment	Reference
C	673	SER	TYR	conflict	UNP P15056
C	688	ARG	ALA	conflict	UNP P15056
C	706	SER	LEU	conflict	UNP P15056
C	709	ARG	GLN	conflict	UNP P15056
C	713	GLU	SER	conflict	UNP P15056
C	716	GLU	LEU	conflict	UNP P15056
C	720	GLU	SER	conflict	UNP P15056
D	446	GLY	-	expression tag	UNP P15056
D	543	ALA	ILE	conflict	UNP P15056
D	544	SER	ILE	conflict	UNP P15056
D	551	LYS	ILE	conflict	UNP P15056
D	562	ARG	GLN	conflict	UNP P15056
D	588	ASN	LEU	conflict	UNP P15056
D	630	SER	LYS	conflict	UNP P15056
D	667	GLU	PHE	conflict	UNP P15056
D	673	SER	TYR	conflict	UNP P15056
D	688	ARG	ALA	conflict	UNP P15056
D	706	SER	LEU	conflict	UNP P15056
D	709	ARG	GLN	conflict	UNP P15056
D	713	GLU	SER	conflict	UNP P15056
D	716	GLU	LEU	conflict	UNP P15056
D	720	GLU	SER	conflict	UNP P15056

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 1: 14-3-3 protein zeta/delta



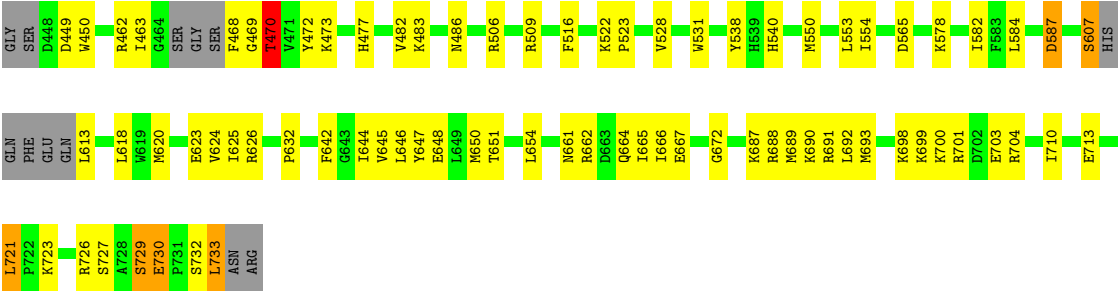
Chain D:

69%

24%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 115.75Å 153.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.33 – 3.30 92.33 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (92.33-3.30) 94.3 (92.33-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660_final	Depositor
R, R_{free}	0.250 , 0.300 0.250 , 0.296	Depositor DCC
R_{free} test set	658 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	109.6	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8063	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: SEP, EDO

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	0.20	0/1868	0.55	1/2510 (0.0%)
1	B	0.36	1/1811 (0.1%)	0.69	5/2432 (0.2%)
2	C	0.35	0/2236	0.73	3/3010 (0.1%)
2	D	0.28	0/2262	0.74	4/3046 (0.1%)
All	All	0.30	1/8177 (0.0%)	0.69	13/10998 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	ARG	CA-C	-5.07	1.46	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	LEU	N-CA-C	-9.53	100.89	111.28
1	B	166	ILE	N-CA-C	8.30	119.09	110.62
1	A	206	LEU	N-CA-C	6.55	119.77	110.14
1	B	168	LEU	N-CA-CB	6.22	119.26	110.12
2	C	626	ARG	CB-CA-C	-5.94	100.93	110.79

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	1843	0	1825	44	0
1	B	1787	0	1782	64	0
2	C	2202	0	2217	78	0
2	D	2227	0	2243	77	0
3	D	4	0	6	2	0
All	All	8063	0	8073	240	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 15.

The worst 5 of 240 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)
2:D:462:ARG:HB2	2:D:472:TYR:CE1	1.85	1.09
2:D:701:ARG:HA	2:D:704:ARG:NH2	1.72	1.04
2:D:462:ARG:HB2	2:D:472:TYR:HE1	1.33	0.92
2:C:625:ILE:HD13	2:C:669:VAL:HG21	1.55	0.88
1:B:66:GLU:OE2	1:B:80:ARG:HA	1.74	0.87

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	228/232 (98%)	224 (98%)	4 (2%)	0	100	100
1	B	219/232 (94%)	208 (95%)	11 (5%)	0	100	100
2	C	269/290 (93%)	256 (95%)	13 (5%)	0	100	100
2	D	271/290 (93%)	257 (95%)	13 (5%)	1 (0%)	30	60
All	All	987/1044 (94%)	945 (96%)	41 (4%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	470	THR

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	200/201 (100%)	200 (100%)	0	100	100
1	B	193/201 (96%)	188 (97%)	5 (3%)	40	64
2	C	241/254 (95%)	235 (98%)	6 (2%)	42	64
2	D	244/254 (96%)	237 (97%)	7 (3%)	37	62
All	All	878/910 (96%)	860 (98%)	18 (2%)	47	67

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	613	LEU
2	D	733	LEU
2	D	727	SER
2	C	721	LEU
2	D	607	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	664	GLN
2	D	540	HIS
2	D	725	HIS
1	B	161	GLN
1	B	50	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	SEP	D	729	2	8,9,10	1.33	2 (25%)	7,12,14	2.49	1 (14%)
2	SEP	C	729	2	8,9,10	0.91	0	7,12,14	1.52	1 (14%)

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
2	SEP	D	729	2	-	0/6/8/10	-
2	SEP	C	729	2	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	729	SEP	P-O2P	-2.28	1.46	1.54
2	D	729	SEP	P-O3P	-2.19	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	729	SEP	OG-CB-CA	6.05	114.04	108.14
2	C	729	SEP	OG-CB-CA	2.57	110.64	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	729	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
2	C	729	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	729	SEP	3	0
2	C	729	SEP	2	0

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	EDO	D	801	-	3,3,3	0.19	0	2,2,2	1.08	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	EDO	D	801	-	-	0/1/1/1	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	EDO	2	0

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 [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	230/232 (99%)	-0.51	0 100 100	69, 111, 168, 244	0
1	B	223/232 (96%)	-0.26	0 100 100	97, 157, 219, 288	0
2	C	275/290 (94%)	-0.26	0 100 100	76, 115, 191, 256	0
2	D	277/290 (95%)	-0.25	0 100 100	76, 128, 199, 266	0
All	All	1005/1044 (96%)	-0.32	0 100 100	69, 126, 204, 288	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	SEP	C	729	10/11	0.91	0.08	136,144,156,158	0
2	SEP	D	729	10/11	0.91	0.07	85,88,90,91	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	EDO	D	801	4/4	0.69	0.27	74,75,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.