



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2016 – 01:37 PM EDT

PDB ID : 5JSM  
Title : BRAFV600E Kinase Domain In Complex with Chemically Linked Vemurafenib Inhibitor VEM-3-VEM  
Authors : Grasso, M.J.; Marmorstein, R.  
Deposited on : 2016-05-08  
Resolution : 2.19 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

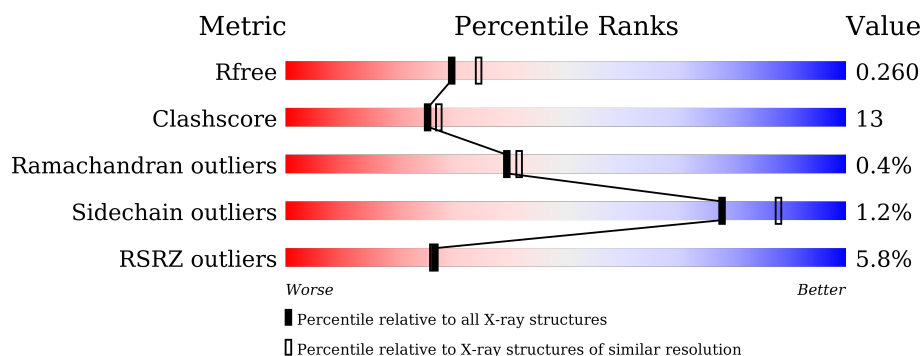
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	280	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	B	280	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div> </div>
1	C	280	<div> <div>14%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div> </div>
1	D	280	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	A	802	-	-	-	X
2	DMS	B	802	-	-	-	X
4	EOH	A	805	-	-	-	X
4	EOH	B	805	-	-	-	X
6	CL	D	802	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8864 atoms, of which 78 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	2	0
			2095	1329	365	388	13			
1	B	263	Total	C	N	O	S	0	5	0
			2128	1350	377	388	13			
1	C	262	Total	C	N	O	S	0	2	0
			2063	1309	361	381	12			
1	D	259	Total	C	N	O	S	0	1	0
			2001	1281	341	366	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	GLY	-	expression tag	UNP P15056
A	445	SER	-	expression tag	UNP P15056
A	446	GLU	-	expression tag	UNP P15056
A	447	PHE	-	expression tag	UNP P15056
A	543	ALA	ILE	engineered mutation	UNP P15056
A	544	SER	ILE	engineered mutation	UNP P15056
A	551	LYS	ILE	engineered mutation	UNP P15056
A	562	ARG	GLN	engineered mutation	UNP P15056
A	588	ASN	LEU	engineered mutation	UNP P15056
A	600	GLU	VAL	engineered mutation	UNP P15056
A	630	SER	LYS	engineered mutation	UNP P15056
A	667	GLU	PHE	engineered mutation	UNP P15056
A	673	SER	TYR	engineered mutation	UNP P15056
A	688	ARG	ALA	engineered mutation	UNP P15056
A	706	SER	LEU	engineered mutation	UNP P15056
A	709	ARG	GLN	engineered mutation	UNP P15056
A	713	GLU	SER	engineered mutation	UNP P15056
A	716	GLU	LEU	engineered mutation	UNP P15056
A	720	GLU	SER	engineered mutation	UNP P15056
A	722	SER	PRO	engineered mutation	UNP P15056
A	723	GLY	LYS	engineered mutation	UNP P15056

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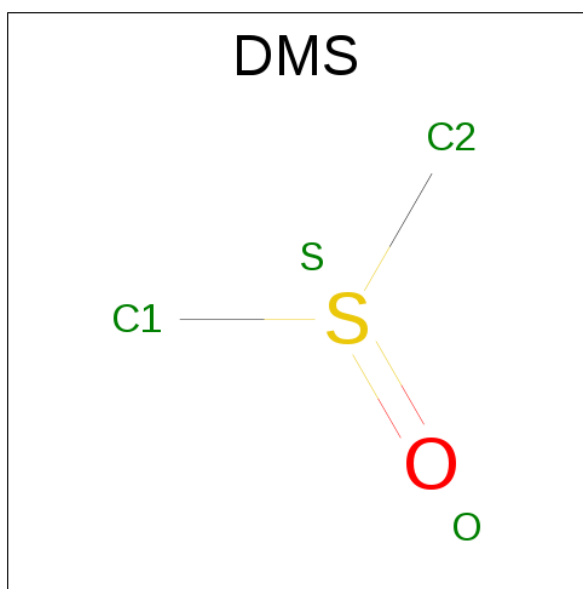
Chain	Residue	Modelled	Actual	Comment	Reference
B	444	GLY	-	expression tag	UNP P15056
B	445	SER	-	expression tag	UNP P15056
B	446	GLU	-	expression tag	UNP P15056
B	447	PHE	-	expression tag	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056
B	588	ASN	LEU	engineered mutation	UNP P15056
B	600	GLU	VAL	engineered mutation	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	667	GLU	PHE	engineered mutation	UNP P15056
B	673	SER	TYR	engineered mutation	UNP P15056
B	688	ARG	ALA	engineered mutation	UNP P15056
B	706	SER	LEU	engineered mutation	UNP P15056
B	709	ARG	GLN	engineered mutation	UNP P15056
B	713	GLU	SER	engineered mutation	UNP P15056
B	716	GLU	LEU	engineered mutation	UNP P15056
B	720	GLU	SER	engineered mutation	UNP P15056
B	722	SER	PRO	engineered mutation	UNP P15056
B	723	GLY	LYS	engineered mutation	UNP P15056
C	444	GLY	-	expression tag	UNP P15056
C	445	SER	-	expression tag	UNP P15056
C	446	GLU	-	expression tag	UNP P15056
C	447	PHE	-	expression tag	UNP P15056
C	543	ALA	ILE	engineered mutation	UNP P15056
C	544	SER	ILE	engineered mutation	UNP P15056
C	551	LYS	ILE	engineered mutation	UNP P15056
C	562	ARG	GLN	engineered mutation	UNP P15056
C	588	ASN	LEU	engineered mutation	UNP P15056
C	600	GLU	VAL	engineered mutation	UNP P15056
C	630	SER	LYS	engineered mutation	UNP P15056
C	667	GLU	PHE	engineered mutation	UNP P15056
C	673	SER	TYR	engineered mutation	UNP P15056
C	688	ARG	ALA	engineered mutation	UNP P15056
C	706	SER	LEU	engineered mutation	UNP P15056
C	709	ARG	GLN	engineered mutation	UNP P15056
C	713	GLU	SER	engineered mutation	UNP P15056
C	716	GLU	LEU	engineered mutation	UNP P15056
C	720	GLU	SER	engineered mutation	UNP P15056
C	722	SER	PRO	engineered mutation	UNP P15056
C	723	GLY	LYS	engineered mutation	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
D	444	GLY	-	expression tag	UNP P15056
D	445	SER	-	expression tag	UNP P15056
D	446	GLU	-	expression tag	UNP P15056
D	447	PHE	-	expression tag	UNP P15056
D	543	ALA	ILE	engineered mutation	UNP P15056
D	544	SER	ILE	engineered mutation	UNP P15056
D	551	LYS	ILE	engineered mutation	UNP P15056
D	562	ARG	GLN	engineered mutation	UNP P15056
D	588	ASN	LEU	engineered mutation	UNP P15056
D	600	GLU	VAL	engineered mutation	UNP P15056
D	630	SER	LYS	engineered mutation	UNP P15056
D	667	GLU	PHE	engineered mutation	UNP P15056
D	673	SER	TYR	engineered mutation	UNP P15056
D	688	ARG	ALA	engineered mutation	UNP P15056
D	706	SER	LEU	engineered mutation	UNP P15056
D	709	ARG	GLN	engineered mutation	UNP P15056
D	713	GLU	SER	engineered mutation	UNP P15056
D	716	GLU	LEU	engineered mutation	UNP P15056
D	720	GLU	SER	engineered mutation	UNP P15056
D	722	SER	PRO	engineered mutation	UNP P15056
D	723	GLY	LYS	engineered mutation	UNP P15056

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



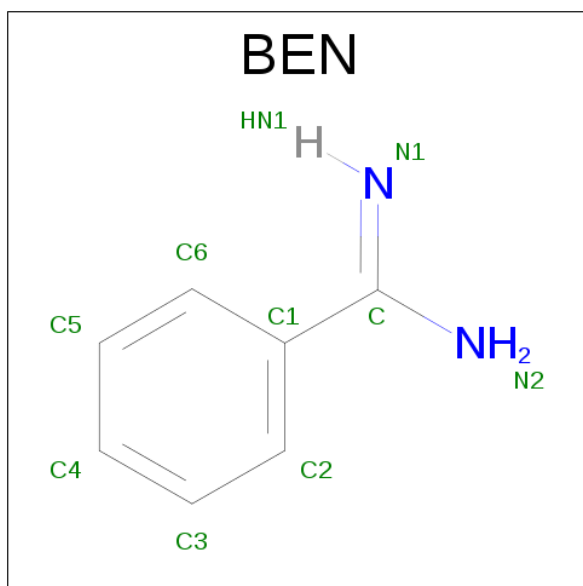
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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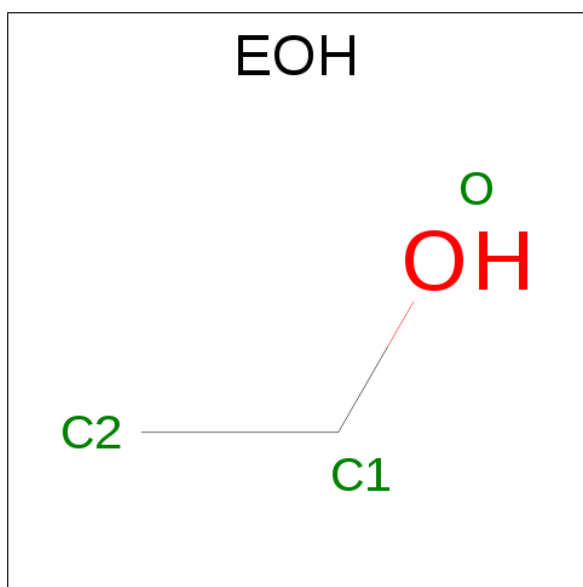
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula:  $C_7H_8N_2$ ).



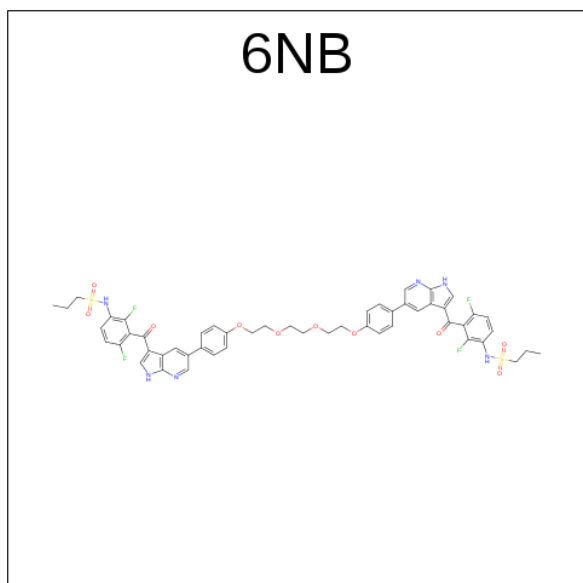
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			17	7	8	2		
3	B	1	Total	C	H	N	0	0
			17	7	8	2		

- Molecule 4 is ETHANOL (three-letter code: EOH) (formula:  $C_2H_6O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			9	2	6	1		
4	B	1	Total	C	H	O	0	0
			9	2	6	1		
4	B	1	Total	C	H	O	0	0
			9	2	6	1		

- Molecule 5 is N,N'-{ethane-1,2-diylbis[oxyethane-2,1-diyl-oxy-4,1-phenylene-1H-pyrrolo[2,3-b]pyridine-5,3-diylcarbonyl(2,4-difluoro-3,1-phenylene)]}di(propane-1-sulfonamide) (three-letter code: 6NB) (formula: C<sub>52</sub>H<sub>48</sub>F<sub>4</sub>N<sub>6</sub>O<sub>10</sub>S<sub>2</sub>).



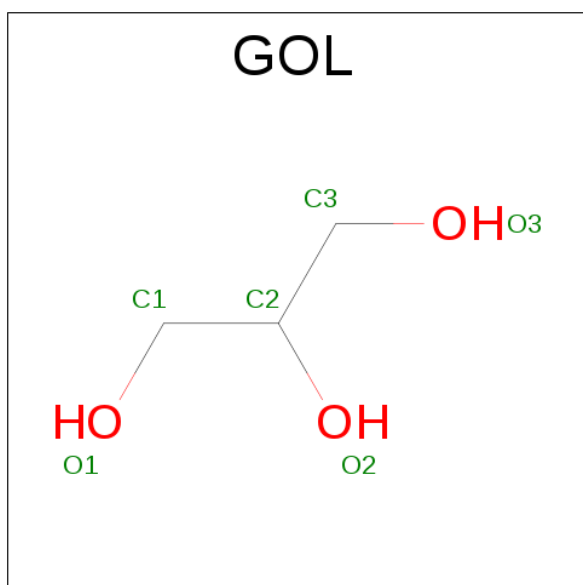


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	S	
			74	52	4	6	10	2	0
5	C	1	Total	C	F	N	O	S	
			74	52	4	6	10	2	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cl		
			2	2	0	0
6	D	1	Total	Cl		
			1	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O		
			14	3	8	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	90	Total	O		
			90	90	0	0
8	B	86	Total	O		
			86	86	0	0

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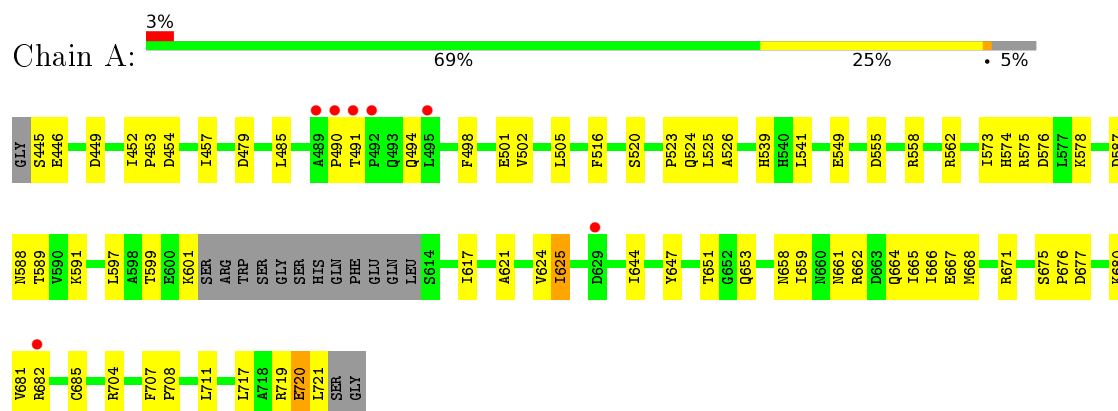
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	53	Total	O	0	0
			53	53		
8	D	62	Total	O	0	0
			62	62		

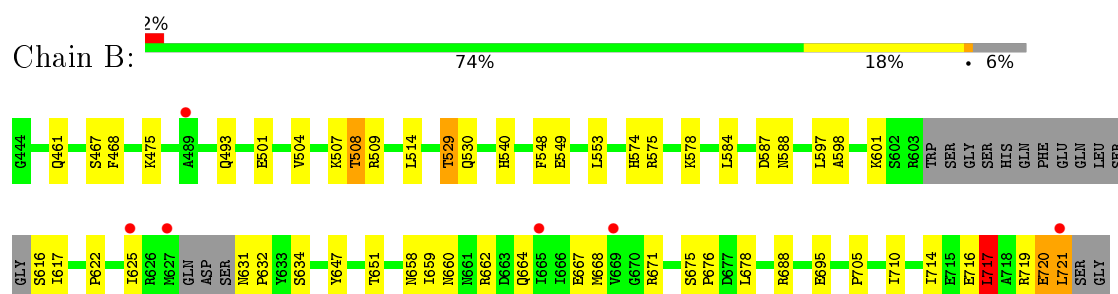
### 3 Residue-property plots [i](#)

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.

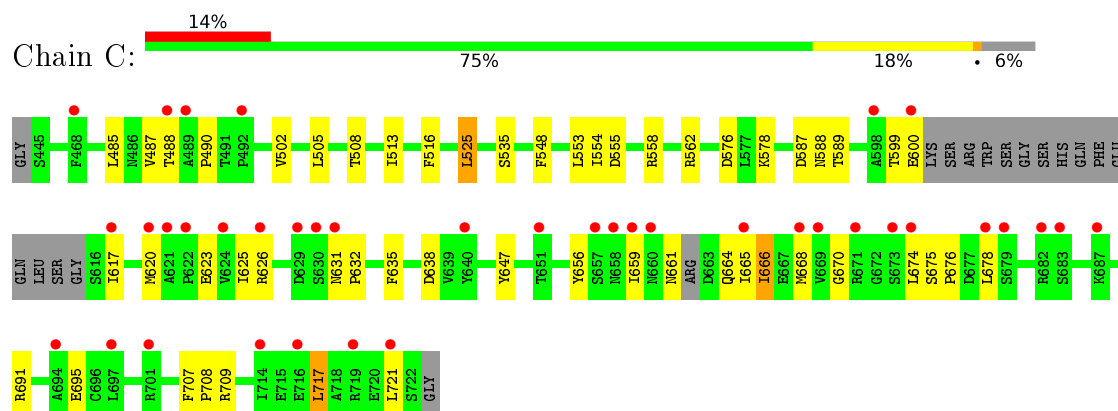
- Molecule 1: Serine/threonine-protein kinase B-raf



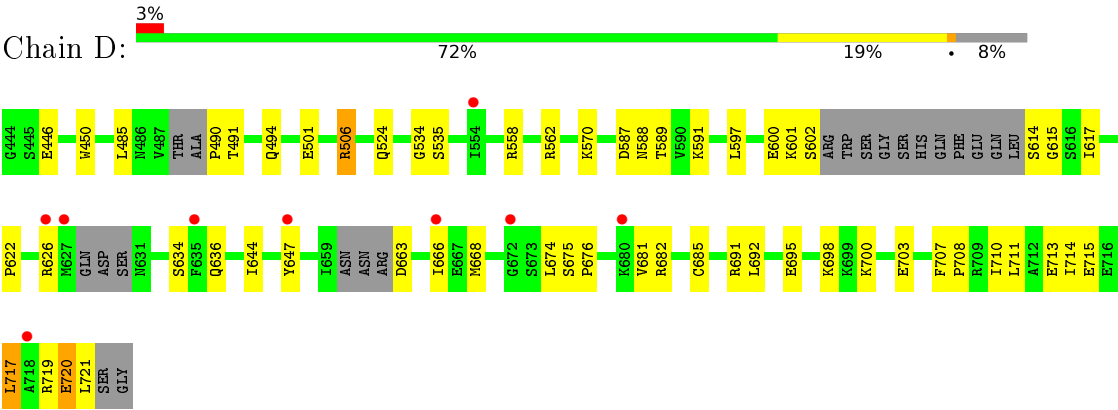
- Molecule 1: Serine/threonine-protein kinase B-raf



- Molecule 1: Serine/threonine-protein kinase B-raf



● Molecule 1: Serine/threonine-protein kinase B-raf



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.61Å 68.26Å 276.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.91 – 2.19 69.00 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (62.91-2.19) 90.5 (69.00-2.19)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.260 0.205 , 0.260	Depositor DCC
$R_{free}$ test set	1833 reflections (3.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, BEN, 6NB, CL, EOH, DMS

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	0.45	0/2143	0.58	0/2890
1	B	0.44	0/2185	0.61	2/2940 (0.1%)
1	C	0.40	0/2110	0.59	0/2848
1	D	0.44	0/2044	0.59	1/2755 (0.0%)
All	All	0.43	0/8482	0.59	3/11433 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	506	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	721	LEU	CA-CB-CG	6.61	130.51	115.30
1	B	717	LEU	CA-CB-CG	5.31	127.51	115.30

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	2095	0	2081	64	0
1	B	2128	0	2143	51	0
1	C	2063	0	2037	49	0
1	D	2001	0	1968	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	18	18	0	0
2	B	4	6	6	0	0
2	C	4	6	6	0	0
2	D	4	6	6	0	0
3	A	9	8	7	1	0
3	B	9	8	7	1	0
4	A	3	6	6	0	0
4	B	6	12	12	0	0
5	B	74	0	0	1	0
5	C	74	0	0	1	0
6	B	2	0	0	1	0
6	D	1	0	0	1	0
7	B	6	8	8	0	0
8	A	90	0	0	6	1
8	B	86	0	0	9	2
8	C	53	0	0	1	0
8	D	62	0	0	3	1
All	All	8786	78	8305	212	2

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 13.

The worst 5 of 212 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:490:PRO:HA	1:A:494:GLN:HE21	1.16	1.08
1:B:631:ASN:HB3	1:B:632:PRO:HD3	1.50	0.93
1:A:490:PRO:HA	1:A:494:GLN:NE2	1.91	0.84
1:D:490:PRO:HB2	8:D:953:HOH:O	1.79	0.83
1:C:659:ILE:HG22	1:C:661:ASN:H	1.45	0.81

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:902:HOH:O	8:D:901:HOH:O[1_565]	1.78	0.42
8:A:947:HOH:O	8:B:981:HOH:O[1_545]	2.18	0.02

## 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	263/280 (94%)	248 (94%)	14 (5%)	1 (0%)	39	42
1	B	262/280 (94%)	254 (97%)	7 (3%)	1 (0%)	39	42
1	C	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	D	250/280 (89%)	239 (96%)	9 (4%)	2 (1%)	24	22
All	All	1033/1120 (92%)	988 (96%)	41 (4%)	4 (0%)	39	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	720	GLU
1	D	720	GLU
1	A	720	GLU
1	D	601	LYS

### 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	226/245 (92%)	223 (99%)	3 (1%)	76	87
1	B	233/245 (95%)	230 (99%)	3 (1%)	76	87
1	C	221/245 (90%)	217 (98%)	4 (2%)	66	79
1	D	211/245 (86%)	210 (100%)	1 (0%)	92	96
All	All	891/980 (91%)	880 (99%)	11 (1%)	78	88



5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	529	THR
1	B	717	LEU
1	C	709	ARG
1	B	508	THR
1	C	666	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	D	494	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\# Z  > 2$
2	DMS	A	801	-	3,3,3	0.56	0	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DMS	A	802	-	3,3,3	0.61	0	3,3,3	0.92	0
2	DMS	A	803	-	3,3,3	0.69	0	3,3,3	0.60	0
3	BEN	A	804	-	9,9,9	3.78	6 (66%)	9,11,11	0.79	0
4	EOH	A	805	-	2,2,2	0.46	0	1,1,1	0.21	0
5	6NB	B	801	-	77,81,81	1.60	14 (18%)	89,116,116	2.26	27 (30%)
2	DMS	B	802	-	3,3,3	0.63	0	3,3,3	0.70	0
4	EOH	B	804	-	2,2,2	0.45	0	1,1,1	0.25	0
4	EOH	B	805	-	2,2,2	0.48	0	1,1,1	0.15	0
7	GOL	B	806	-	5,5,5	0.33	0	5,5,5	0.25	0
3	BEN	B	807	-	9,9,9	3.85	5 (55%)	9,11,11	1.22	1 (11%)
5	6NB	C	801	-	77,81,81	1.60	15 (19%)	89,116,116	2.19	14 (15%)
2	DMS	C	802	-	3,3,3	0.64	0	3,3,3	0.63	0
2	DMS	D	801	-	3,3,3	0.65	0	3,3,3	0.48	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
2	DMS	A	801	-	-	0/0/0/0	0/0/0/0
2	DMS	A	802	-	-	0/0/0/0	0/0/0/0
2	DMS	A	803	-	-	0/0/0/0	0/0/0/0
3	BEN	A	804	-	-	0/4/4/4	0/1/1/1
4	EOH	A	805	-	-	0/0/0/0	0/0/0/0
5	6NB	B	801	-	-	0/51/64/64	0/8/8/8
2	DMS	B	802	-	-	0/0/0/0	0/0/0/0
4	EOH	B	804	-	-	0/0/0/0	0/0/0/0
4	EOH	B	805	-	-	0/0/0/0	0/0/0/0
7	GOL	B	806	-	-	0/4/4/4	0/0/0/0
3	BEN	B	807	-	-	0/4/4/4	0/1/1/1
5	6NB	C	801	-	-	0/51/64/64	0/8/8/8
2	DMS	C	802	-	-	0/0/0/0	0/0/0/0
2	DMS	D	801	-	-	0/0/0/0	0/0/0/0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	6NB	C13-N02	-5.16	1.31	1.45
5	C	801	6NB	C13-N02	-5.11	1.31	1.45
5	C	801	6NB	C09-C12	-3.65	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	BEN	C2-C1	-3.23	1.34	1.39
3	B	807	BEN	C2-C1	-3.13	1.34	1.39

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	801	6NB	O09-S-O	-9.21	103.27	119.31
5	C	801	6NB	O02-S01-O03	-8.32	104.82	119.31
5	B	801	6NB	O09-S-O	-7.89	105.57	119.31
5	B	801	6NB	C07-C08-C09	-5.91	116.58	122.09
5	C	801	6NB	C07-C08-C09	-5.75	116.72	122.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	BEN	1	0
5	B	801	6NB	1	0
3	B	807	BEN	1	0
5	C	801	6NB	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	265/280 (94%)	0.19	7 (2%) 59 58	26, 42, 69, 81	0
1	B	263/280 (93%)	0.25	6 (2%) 64 63	28, 47, 72, 84	0
1	C	262/280 (93%)	0.78	39 (14%) 3 3	28, 53, 88, 98	0
1	D	259/280 (92%)	0.24	9 (3%) 48 46	25, 50, 83, 93	0
All	All	1049/1120 (93%)	0.36	61 (5%) 26 26	25, 48, 81, 98	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	674	LEU	6.0
1	C	630	SER	5.3
1	C	658	ASN	5.2
1	C	683	SER	5.1
1	C	629	ASP	5.1

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	CL	D	802	1/1	0.98	0.15	6.35	54,54,54,54	0
4	EOH	B	805	3/3	0.72	0.23	6.35	51,62,77,77	0
2	DMS	A	802	4/4	0.91	0.21	2.63	32,49,59,66	0
2	DMS	B	802	4/4	0.91	0.19	2.20	46,64,76,79	0
4	EOH	A	805	3/3	0.87	0.14	2.17	53,63,71,75	0
7	GOL	B	806	6/6	0.59	0.18	1.47	58,75,88,96	0
3	BEN	A	804	9/9	0.95	0.13	1.12	21,28,43,43	0
2	DMS	D	801	4/4	0.90	0.14	0.41	57,68,70,71	0
3	BEN	B	807	9/9	0.97	0.14	0.18	22,29,43,43	0
2	DMS	C	802	4/4	0.88	0.15	0.12	58,70,78,92	0
5	6NB	C	801	74/74	0.97	0.13	0.00	28,36,48,58	0
5	6NB	B	801	74/74	0.97	0.13	-0.48	23,33,48,62	0
6	CL	B	803	1/1	0.94	0.09	-3.80	53,53,53,53	0
6	CL	B	808	1/1	0.97	0.07	-3.93	54,54,54,54	0
2	DMS	A	801	4/4	0.90	0.17	-	43,55,66,83	0
2	DMS	A	803	4/4	0.65	0.18	-	65,79,83,100	0
4	EOH	B	804	3/3	0.78	0.14	-	72,87,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.