wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 07:34 AM EDT

PDB ID	:	5JT2
Title	:	BRAFV600E Kinase Domain In Complex with Chemically Linked Vemurafenib Inhibitor VEM-BISAMIDE
Authors	:	Grasso, M.J.; Marmorstein, R.
Deposited on	:	2016-05-09
Resolution	:	2.70 Å(reported)

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

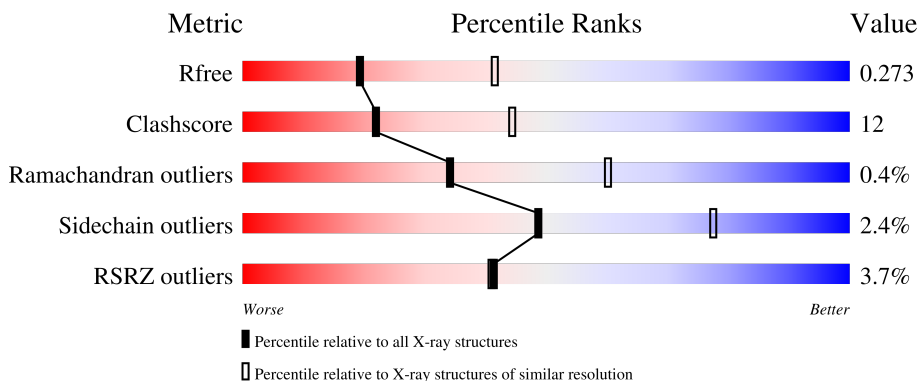|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	Percentile Ranks	Value
Rfree		0.273
Clashscore		12
Ramachandran outliers		0.4%
Sidechain outliers		2.4%
RSRZ outliers		3.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	2% / 71% / 20% / • / 8%
1	B	280	2% / 67% / 21% / • / 10%
1	C	280	5% / 67% / 22% / • / 10%
1	D	280	4% / 65% / 18% / • / 16%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BEN	A	801	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8051 atoms, of which 104 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	257	Total	C	N	O	S	0	0	0
			1958	1249	339	358	12			
1	B	251	Total	C	N	O	S	0	0	0
			1921	1225	331	353	12			
1	C	251	Total	C	N	O	S	0	0	0
			1925	1231	333	349	12			
1	D	234	Total	C	N	O	S	0	0	0
			1801	1152	309	329	11			

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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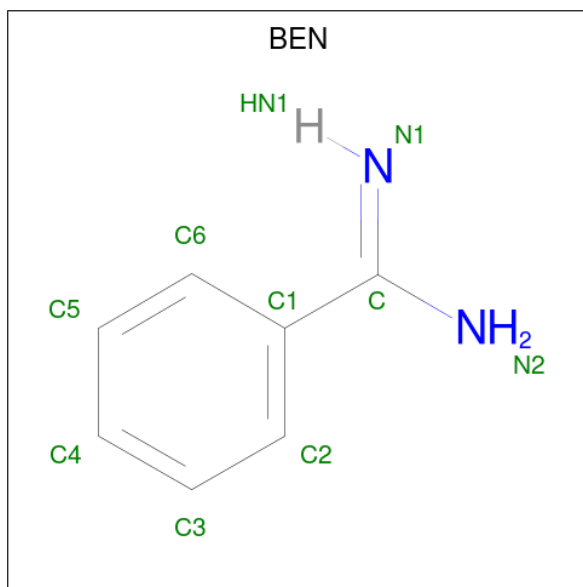
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Chain	Residue	Modelled	Actual	Comment	Reference
B	444	GLY	-	expression tag	UNP P15056
B	445	SER	-	expression tag	UNP P15056
B	446	GLU	-	expression tag	UNP P15056
B	447	PHE	-	expression tag	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	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 BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).

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

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

- Molecule 3 is 2,2'-oxybis(N-{[4-(3-{2,6-difluoro-3-[(propane-1-sulfonyl)amino]benzoyl}-1H-pyrrolo[2,3-b]pyridin-5-yl)phenyl]methyl}acetamide) (three-letter code: 6NC) (formula: $C_{52}H_{46}F_4N_8O_9S_2$).
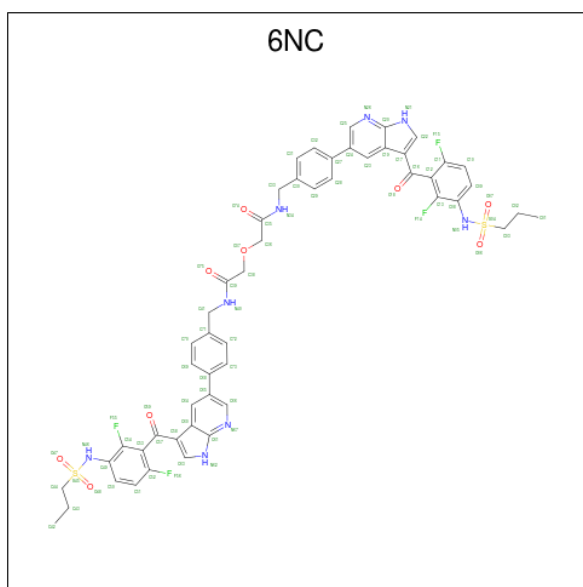
6NC

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total 119	C 52	F 4	H 44	N 8	O 9	S 2	0	0
3	C	1	Total 119	C 52	F 4	H 44	N 8	O 9	S 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total 49	O 49	0	0
4	B	63	Total 63	O 63	0	0
4	C	26	Total 26	O 26	0	0
4	D	36	Total 36	O 36	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

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E667 M668 V669 G670 R671 G672 SER LEU S675 K680 V681 R688 L692 S706 F707 P708 R709 I710 E713 E716 L717 A718 R719 GLU LEU SER GLY

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

Chain D:

GLY SER E446 F447 D448 D449 W450 E451 I452 P453 D454 G455 Q456 I457 Q461 R462 G469 Y472 W476 H477 M484 L485 N486 V487 THR ALA P490 T491 P492 Q493 Q494 V502 I513 F516 M517 G518 Q524 I527 S544 F548 K552 L553 R558 R562

H574 R575 D587 N588 F595 G596 L597 E600 LYS SER ARG TRP SER GLY SER HIS GLN PHE GLU GLN LEU SER GLY S616 I617 M620 A621 P622 E623 V624 I625 R626 MET GLN ASP SER N631 Q636 M650 Y656 S657 ASN ILE ASN ASN ARG ASP GLN ILE ILE GLU MET VAL

GLY ARG GLY SER LEU S675 R682 SER N684 M689 A694 K699 K700 E703 S706 F707 I710 E715 E716 L717 A718 ARG GLU LEU SER GLY

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.10Å 68.44Å 275.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.70 29.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.59-2.70) 96.1 (29.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.212 , 0.273 0.213 , 0.273	Depositor DCC
R_{free} test set	2001 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8051	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6NC, BEN

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	0.48	0/1999	0.64	0/2705
1	B	0.48	0/1960	0.66	1/2652 (0.0%)
1	C	0.44	0/1962	0.60	0/2647
1	D	0.44	0/1839	0.62	0/2489
All	All	0.46	0/7760	0.63	1/10493 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	ASP	CB-CA-C	-5.23	99.94	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1958	0	1864	43	0
1	B	1921	0	1828	50	0
1	C	1925	0	1846	54	0
1	D	1801	0	1705	39	0
2	A	9	8	7	0	0
2	B	9	8	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	75	44	0	1	0
3	C	75	44	0	2	0
4	A	49	0	0	8	0
4	B	63	0	0	9	0
4	C	26	0	0	2	0
4	D	36	0	0	5	0
All	All	7947	104	7257	177	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 12.

The worst 5 of 177 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:C:491:THR:HG23	1:C:494:GLN:HE21	1.29	0.95
1:C:665:ILE:HG22	1:C:666:ILE:H	1.39	0.87
1:A:668:MET:HB3	1:A:674:LEU:HB2	1.59	0.84
1:B:502:VAL:HG13	1:B:516:PHE:CE2	2.17	0.79
1:C:546:THR:HA	4:C:926:HOH:O	1.84	0.77

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	249/280 (89%)	240 (96%)	9 (4%)	0	100	100
1	B	243/280 (87%)	233 (96%)	8 (3%)	2 (1%)	19	43
1	C	237/280 (85%)	227 (96%)	9 (4%)	1 (0%)	34	60
1	D	222/280 (79%)	214 (96%)	7 (3%)	1 (0%)	29	54
All	All	951/1120 (85%)	914 (96%)	33 (4%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	PRO
1	B	493	GLN
1	C	666	ILE
1	D	492	PRO

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	196/245 (80%)	191 (97%)	5 (3%)	46	75
1	B	195/245 (80%)	189 (97%)	6 (3%)	40	69
1	C	193/245 (79%)	191 (99%)	2 (1%)	76	91
1	D	181/245 (74%)	176 (97%)	5 (3%)	43	73
All	All	765/980 (78%)	747 (98%)	18 (2%)	49	77

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

Mol	Chain	Res	Type
1	D	454	ASP
1	D	616	SER
1	D	552	LYS
1	B	636	GLN
1	D	450	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	GLN
1	C	494	GLN
1	C	539	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	6NC	A	802	-	80,82,82	1.85	17 (21%)	99,119,119	2.63	33 (33%)
2	BEN	B	801	-	9,9,9	4.62	8 (88%)	7,11,11	0.83	0
3	6NC	C	801	-	80,82,82	1.85	17 (21%)	99,119,119	2.67	32 (32%)
2	BEN	A	801	-	9,9,9	4.79	8 (88%)	7,11,11	0.77	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	6NC	A	802	-	-	8/50/58/58	0/8/8/8
2	BEN	B	801	-	-	0/4/4/4	0/1/1/1
3	6NC	C	801	-	-	4/50/58/58	0/8/8/8
2	BEN	A	801	-	-	2/4/4/4	0/1/1/1

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	BEN	C6-C1	7.63	1.52	1.39
2	B	801	BEN	C6-C1	7.12	1.51	1.39
2	A	801	BEN	C3-C2	6.96	1.53	1.38
2	B	801	BEN	C3-C2	6.93	1.53	1.38
3	C	801	6NC	C58-C57	6.81	1.57	1.50

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	6NC	O07-S04-O06	-11.48	102.72	119.35
3	C	801	6NC	O48-S45-O47	-10.73	103.81	119.35
3	C	801	6NC	O07-S04-O06	-10.68	103.88	119.35
3	A	802	6NC	O48-S45-O47	-10.40	104.28	119.35
3	C	801	6NC	O07-S04-C03	7.37	119.62	107.86

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	6NC	C02-C03-S04-N05
3	A	802	6NC	C02-C03-S04-O06
3	A	802	6NC	C02-C03-S04-O07
3	A	802	6NC	C43-C44-S45-O47
3	C	801	6NC	C43-C44-S45-O48

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	6NC	1	0
3	C	801	6NC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 6NC A 802

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NC C 801

Bond lengths

Bond angles

Torsions

Rings
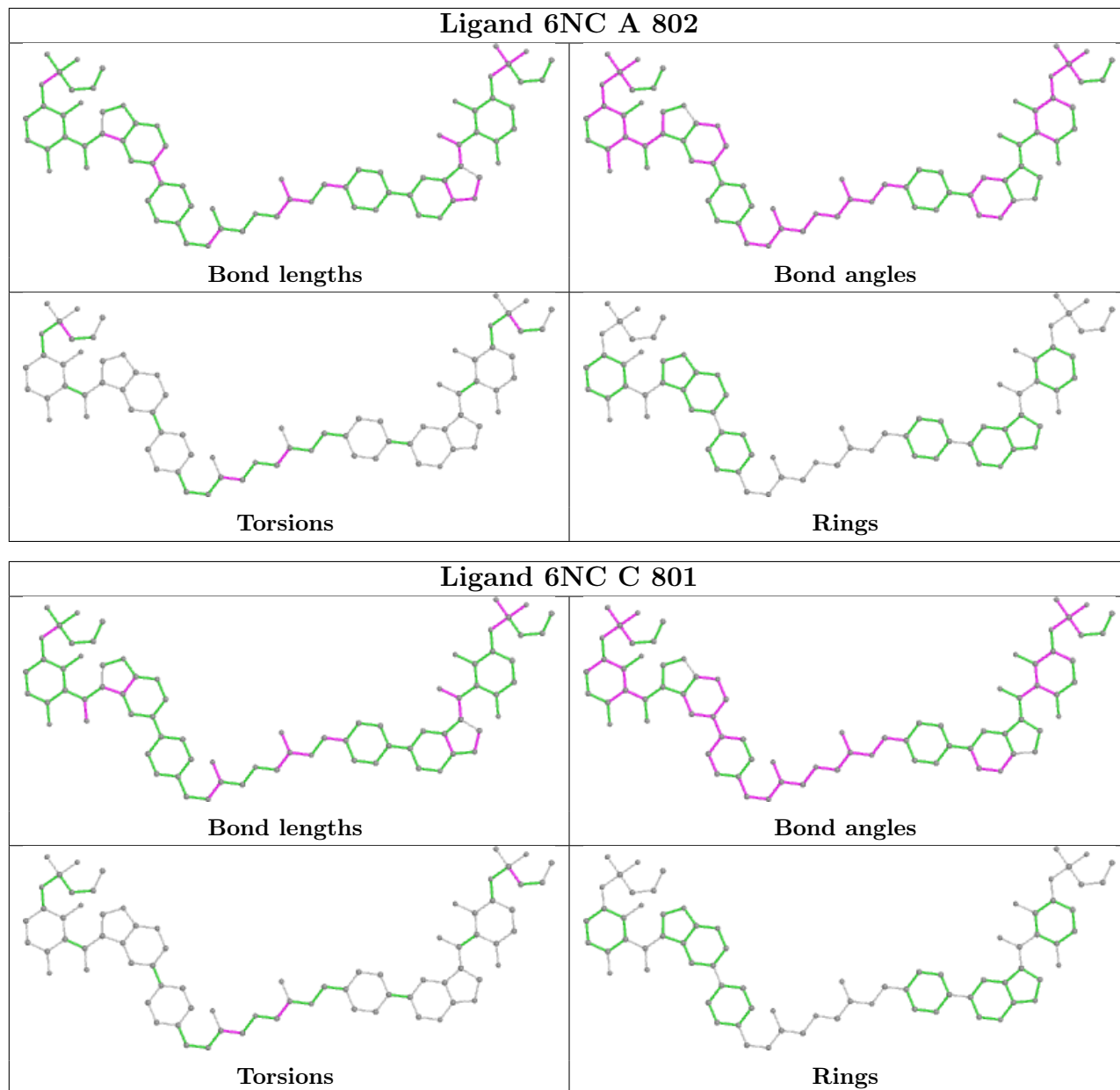
5.7 Other polymers ⓘ

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 ⓘ

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	257/280 (91%)	-0.10	5 (1%)	66	69	21, 35, 56, 69	0
1	B	251/280 (89%)	-0.13	7 (2%)	53	54	19, 35, 53, 71	0
1	C	251/280 (89%)	0.21	15 (5%)	21	20	21, 48, 69, 85	0
1	D	234/280 (83%)	0.09	10 (4%)	35	33	24, 44, 70, 84	0
All	All	993/1120 (88%)	0.02	37 (3%)	41	41	19, 39, 65, 85	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	660	ASN	6.1
1	C	656	TYR	4.5
1	A	604	TRP	4.3
1	C	661	ASN	3.9
1	C	671	ARG	3.7

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

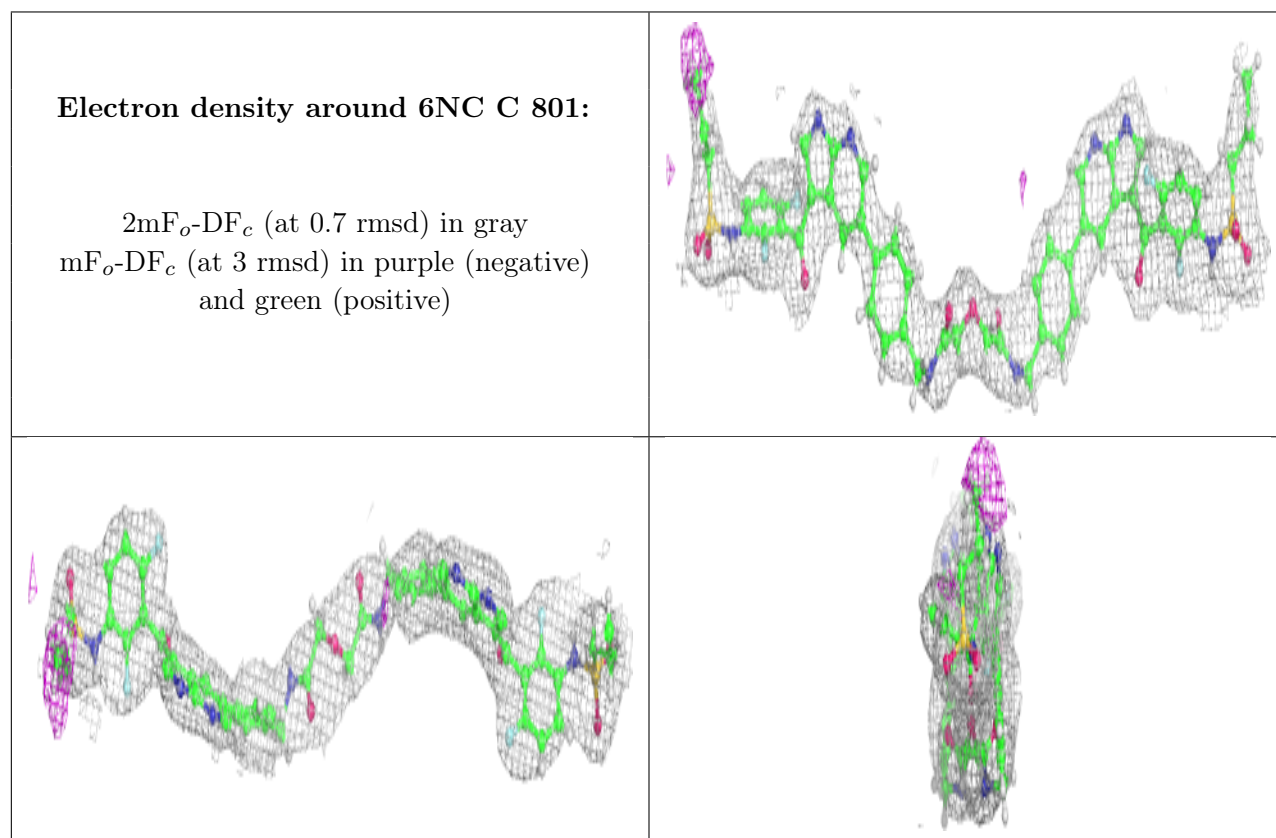There are no non-standard protein/DNA/RNA residues in this entry.

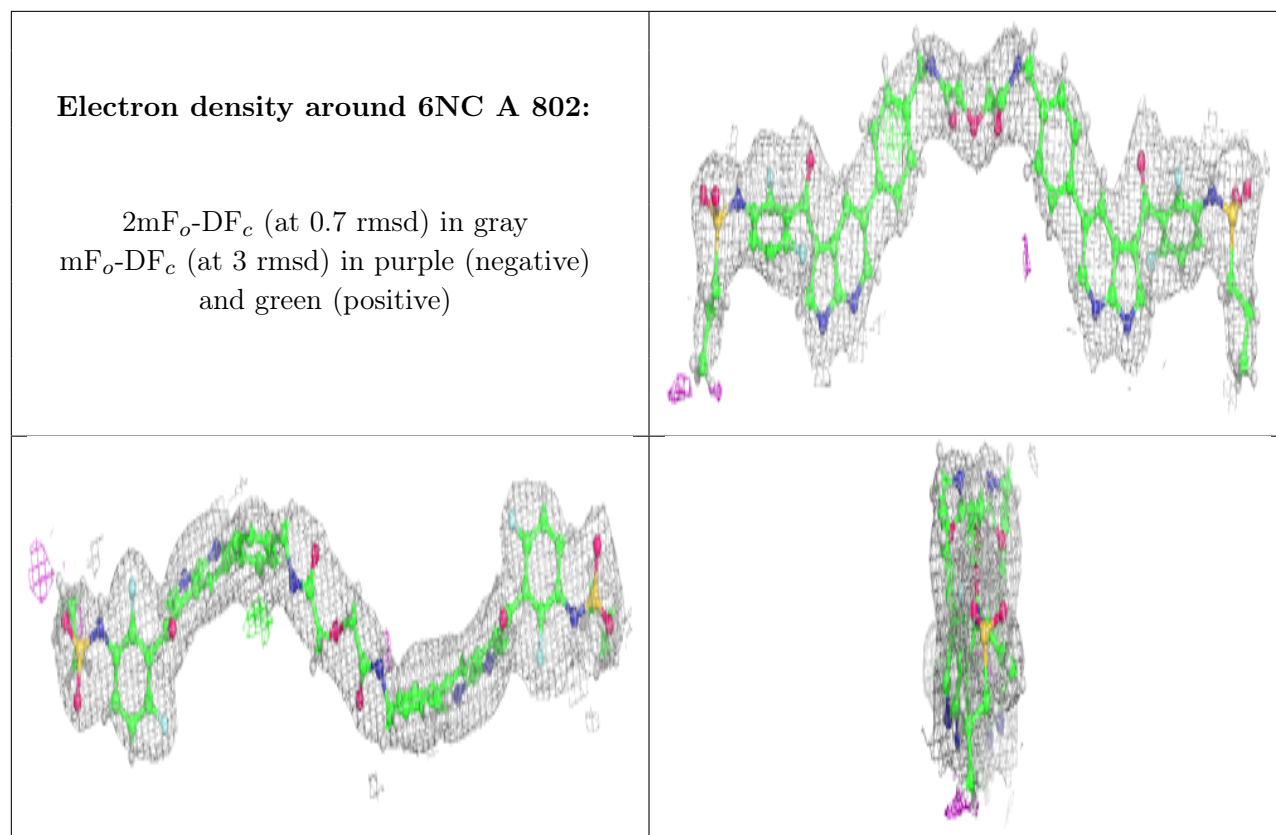## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	6NC	C	801	75/75	0.93	0.18	21,34,52,63	0
3	6NC	A	802	75/75	0.95	0.16	18,28,45,49	0
2	BEN	A	801	9/9	0.97	0.18	21,26,30,32	0
2	BEN	B	801	9/9	0.97	0.12	21,25,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 6NC C 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around 6NC A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.