



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:56 PM UTC

PDB ID : 5JSM / pdb_00005jsm
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 Full wwPDB X-ray Structure Validation 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

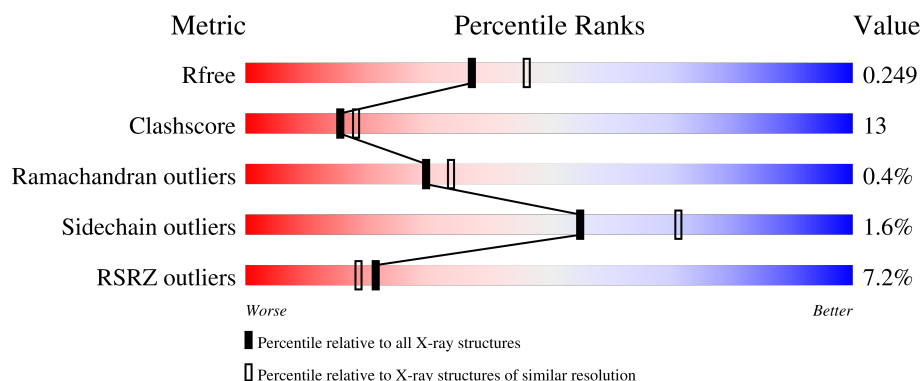
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	280	 3% 67% 26% • 5%
1	B	280	 3% 72% 19% • 6%
1	C	280	 16% 74% 19% • 6%
1	D	280	 5% 71% 20% • 8%

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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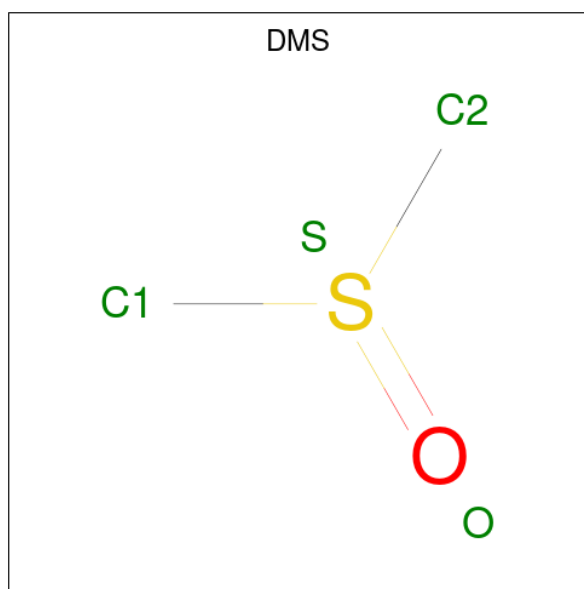
Chain	Residue	Modelled	Actual	Comment	Reference
B	444	GLY	-	expression tag	UNP P15056
B	445	SER	-	expression tag	UNP P15056
B	446	GLU	-	expression tag	UNP P15056
B	447	PHE	-	expression tag	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	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 (CCD ID: DMS) (formula: C₂H₆OS).



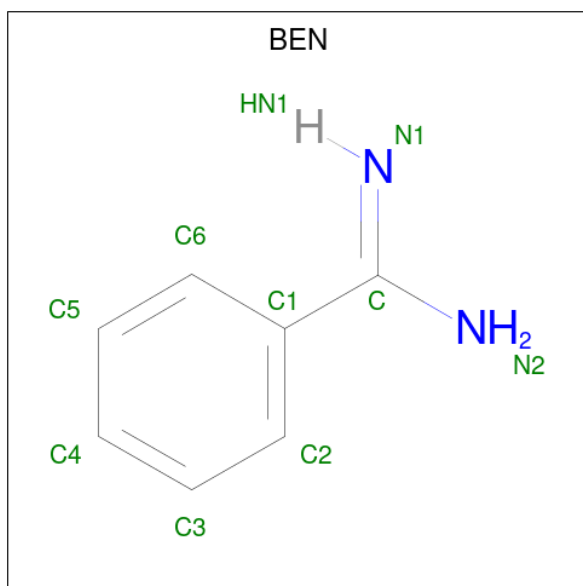
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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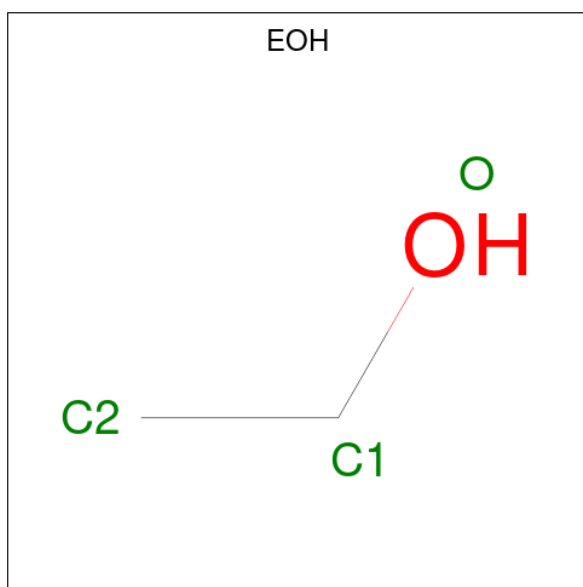
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



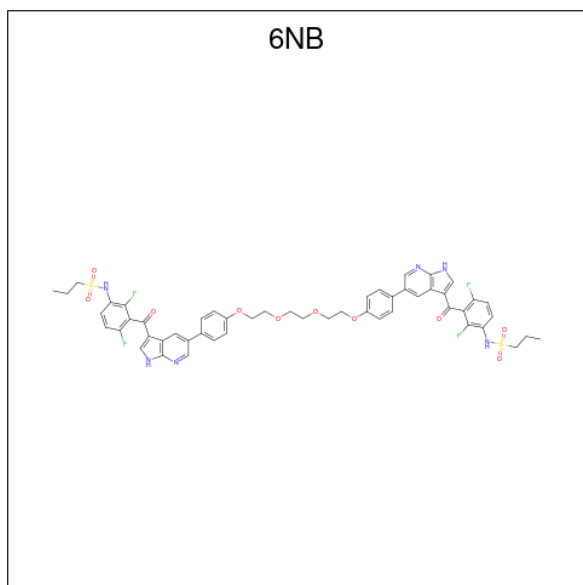
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			17	7	8	2		
3	B	1	Total	C	H	N	0	0
			17	7	8	2		

- Molecule 4 is ETHANOL (CCD ID: 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) (CCD ID: 6NB) (formula: C₅₂H₄₈F₄N₆O₁₀S₂).

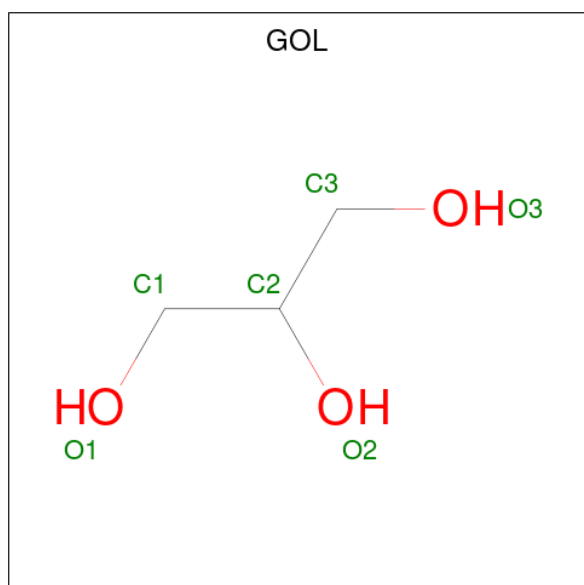


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	S	
			74	52	4	6	10	2	0
5	C	1	Total	C	F	N	O	S	
			74	52	4	6	10	2	0

- Molecule 6 is CHLORIDE ION (CCD ID: 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 (CCD ID: GOL) (formula: C₃H₈O₃).



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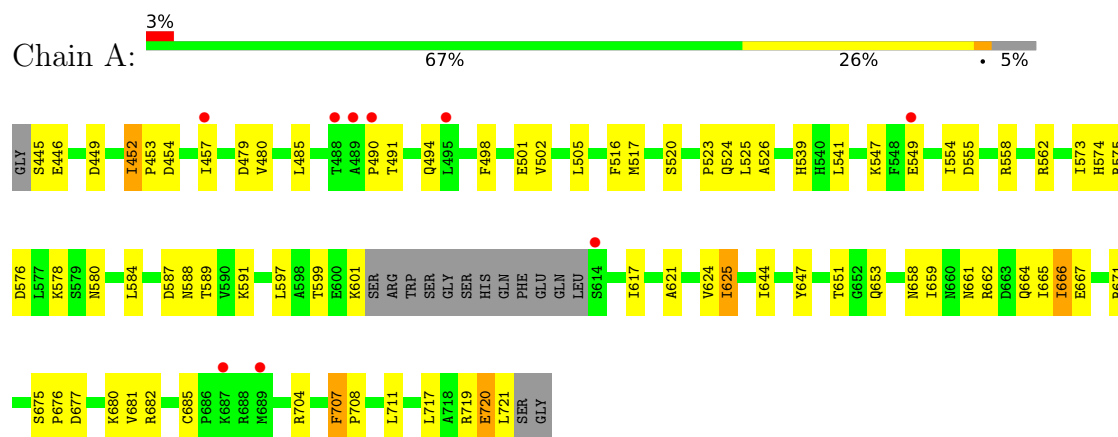
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	53	Total 53	O 53	0	0
8	D	62	Total 62	O 62	0	0

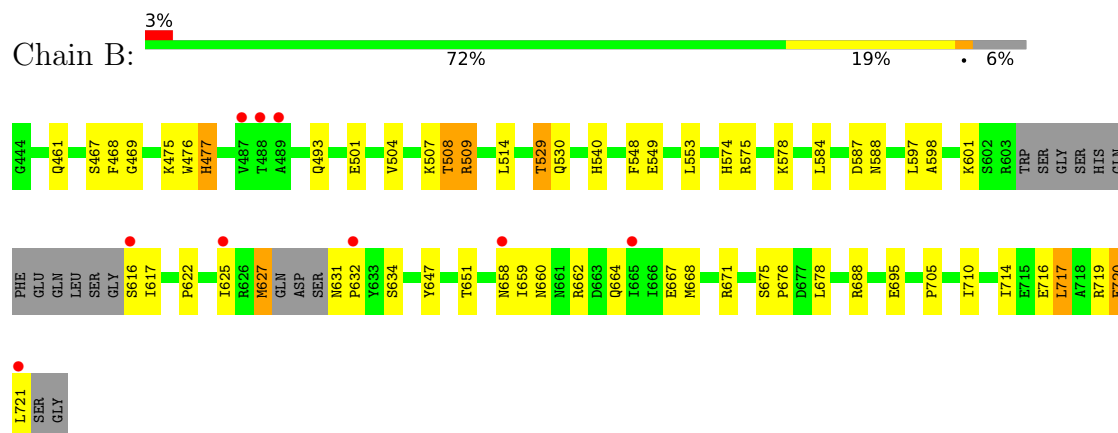
3 Residue-property plots [i](#)

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.

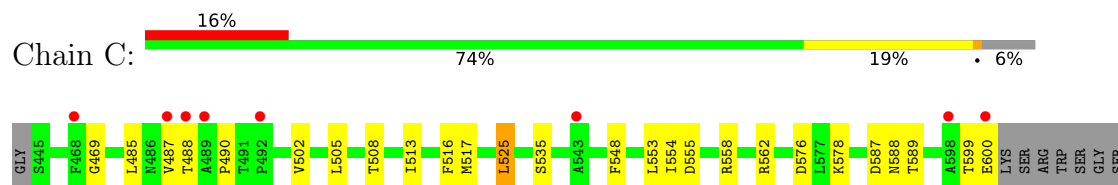
- Molecule 1: Serine/threonine-protein kinase B-raf

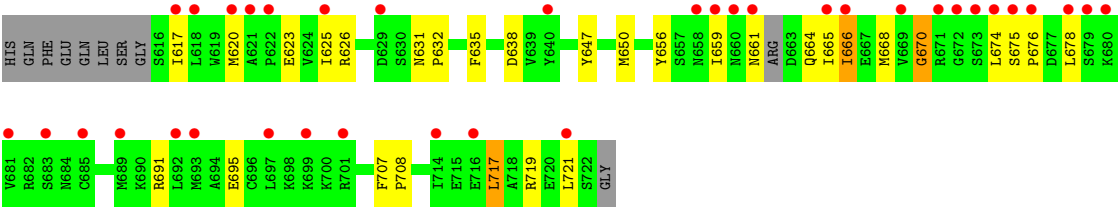


- Molecule 1: Serine/threonine-protein kinase B-raf

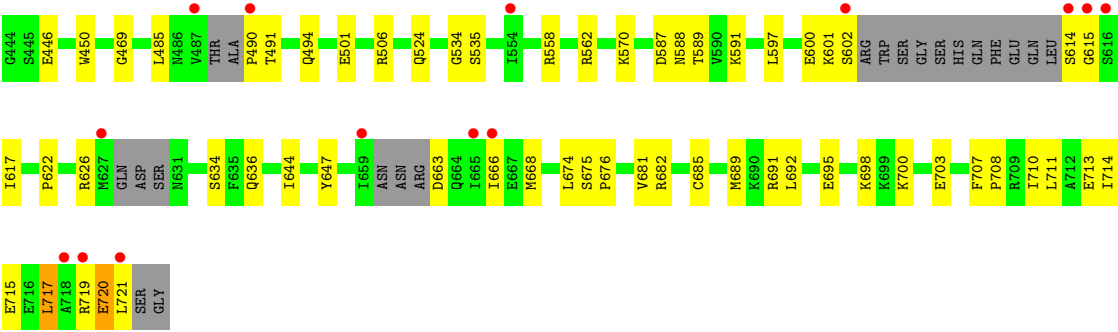


- Molecule 1: Serine/threonine-protein kinase B-raf





● 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, α , β , γ	64.61Å 68.26Å 276.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.91 – 2.19 62.91 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (62.91-2.19) 90.5 (62.91-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.207 , 0.260 (Not available) , 0.249	Depositor DCC
R_{free} test set	2002 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	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	0.95	EDS
Total number of atoms	8864	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEN, DMS, CL, GOL, EOH, 6NB

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	0.57	0/2143	0.89	5/2890 (0.2%)
1	B	0.53	0/2185	0.88	3/2940 (0.1%)
1	C	0.50	0/2110	0.90	2/2848 (0.1%)
1	D	0.52	0/2044	0.86	1/2755 (0.0%)
All	All	0.53	0/8482	0.88	11/11433 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	GLY	N-CA-C	7.11	120.83	110.80
1	D	469	GLY	N-CA-C	6.54	120.03	110.80
1	C	469	GLY	N-CA-C	6.31	119.70	110.80
1	B	477	HIS	N-CA-C	-6.24	105.49	113.23
1	C	670	GLY	N-CA-C	-6.21	105.30	112.50
1	A	707	PHE	CA-C-N	-5.57	113.15	119.28
1	A	707	PHE	C-N-CA	-5.57	113.15	119.28
1	A	452	ILE	CA-C-N	5.24	125.18	119.78
1	A	452	ILE	C-N-CA	5.24	125.18	119.78
1	A	653	GLN	N-CA-C	5.15	117.24	109.41
1	B	476	TRP	N-CA-C	-5.11	99.92	110.80

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	2095	0	2081	66	0
1	B	2128	0	2143	55	0
1	C	2063	0	2037	55	0
1	D	2001	0	1968	49	0
2	A	12	18	18	1	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	225	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.

All (225) 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
1:A:549:GLU:OE2	1:A:549:GLU:N	2.13	0.80
1:B:549:GLU:OE1	1:B:549:GLU:N	2.09	0.79
1:D:450:TRP:NE1	1:D:506:ARG:HD3	1.98	0.79
1:D:490:PRO:HA	1:D:494:GLN:HE21	1.49	0.77
1:B:631:ASN:HB3	1:B:632:PRO:CD	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461[B]:GLN:NE2	8:B:901:HOH:O	2.17	0.75
1:D:668:MET:HB3	1:D:674:LEU:HB2	1.68	0.74
1:D:450:TRP:CE2	1:D:506:ARG:HD3	2.23	0.73
1:B:504:VAL:O	1:B:508:THR:HG23	1.87	0.72
1:C:625:ILE:HG21	1:C:670:GLY:HA2	1.71	0.72
1:A:555:ASP:OD1	1:A:558:ARG:NH2	2.25	0.69
1:C:691:ARG:O	1:C:695:GLU:HG2	1.92	0.69
1:D:485:LEU:O	1:D:524:GLN:NE2	2.14	0.68
1:C:675:SER:HB3	1:C:676:PRO:HD2	1.76	0.68
1:A:498:PHE:CZ	1:A:525[B]:LEU:HD11	2.30	0.67
1:C:508:THR:HG22	1:C:513:ILE:CD1	2.24	0.67
1:A:562:ARG:HG3	1:A:711:LEU:HD11	1.76	0.66
1:A:490:PRO:CA	1:A:494:GLN:HE21	2.03	0.66
1:C:626:ARG:NH1	1:C:670:GLY:O	2.28	0.65
1:D:490:PRO:HA	1:D:494:GLN:NE2	2.12	0.65
1:A:479:ASP:OD1	8:A:901:HOH:O	2.14	0.64
1:A:549:GLU:H	1:A:549:GLU:CD	2.05	0.64
1:B:548:PHE:HB2	1:B:553:LEU:HD21	1.78	0.64
1:B:508:THR:HG22	8:B:965:HOH:O	1.97	0.64
1:A:524:GLN:HG3	8:A:907:HOH:O	1.97	0.63
1:B:501:GLU:CB	1:B:597:LEU:HD23	2.29	0.62
1:B:716:GLU:HA	1:B:719:ARG:NH1	2.15	0.62
1:A:558:ARG:HE	1:A:562:ARG:NH1	1.98	0.61
1:B:514:LEU:HD13	1:B:529:THR:HG21	1.82	0.61
1:B:507:LYS:HE2	8:B:969:HOH:O	1.99	0.61
1:B:617:ILE:HD11	1:B:662:ARG:HG2	1.81	0.60
1:D:717:LEU:C	1:D:717:LEU:HD12	2.26	0.60
1:A:449:ASP:OD1	1:D:506:ARG:HD2	2.01	0.60
1:A:485:LEU:HD12	1:A:525[B]:LEU:CD1	2.30	0.60
1:A:662:ARG:O	1:A:666:ILE:HD12	2.00	0.60
1:C:647:TYR:CE1	1:C:676:PRO:HB2	2.37	0.60
1:C:617:ILE:HA	1:C:620:MET:HG3	1.84	0.60
1:B:664:GLN:HG3	1:B:668:MET:HE3	1.83	0.60
1:A:452:ILE:HG21	1:A:457:ILE:HG13	1.84	0.59
1:A:651:THR:HG22	1:A:681:VAL:HA	1.83	0.59
1:A:587:ASP:O	1:A:588:ASN:HB2	2.01	0.58
1:C:548:PHE:HB2	1:C:553:LEU:HD21	1.85	0.58
1:B:501:GLU:HB3	1:B:597:LEU:HD23	1.85	0.58
1:A:720:GLU:C	1:A:721:LEU:HD12	2.29	0.58
1:D:491:THR:H	1:D:494:GLN:HE21	1.52	0.58
1:C:617:ILE:HG22	1:C:620:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:PHE:HB2	1:C:553:LEU:CD2	2.34	0.57
1:D:501:GLU:HG3	1:D:597:LEU:HD23	1.86	0.57
1:A:681:VAL:CG1	1:A:685:CYS:HB3	2.33	0.57
1:B:508:THR:O	1:B:508:THR:OG1	2.22	0.57
1:D:446:GLU:OE2	8:D:901:HOH:O	2.17	0.57
1:A:677:ASP:HB3	1:A:680:LYS:HE3	1.88	0.56
1:D:617:ILE:HD13	1:D:666:ILE:HD11	1.86	0.56
1:A:597:LEU:O	1:A:601:LYS:HG3	2.06	0.55
1:B:676:PRO:O	1:B:678:LEU:HD12	2.07	0.55
3:B:807:BEN:N1	6:B:808:CL:CL	2.76	0.55
1:A:454:ASP:OD1	1:A:523:PRO:HD3	2.07	0.54
1:B:587:ASP:O	1:B:588:ASN:HB2	2.08	0.54
1:B:508:THR:C	1:B:509:ARG:HG2	2.33	0.54
1:C:617:ILE:HA	1:C:620:MET:CG	2.37	0.54
1:C:587:ASP:OD1	1:C:589:THR:HG23	2.08	0.54
1:A:661:ASN:HB3	1:A:664:GLN:HB2	1.90	0.54
1:D:589:THR:OG1	1:D:591:LYS:HE2	2.08	0.54
1:D:719:ARG:C	1:D:721:LEU:H	2.16	0.53
1:C:668:MET:HB3	1:C:674:LEU:HB2	1.91	0.53
1:D:491:THR:N	1:D:494:GLN:HE21	2.06	0.53
1:C:558:ARG:HH11	1:C:562:ARG:HH12	1.56	0.52
1:B:710:ILE:O	1:B:714:ILE:HG13	2.10	0.52
1:C:508:THR:HG22	1:C:513:ILE:HD11	1.92	0.52
1:C:623:GLU:OE1	1:C:623:GLU:N	2.34	0.52
1:B:616:SER:N	8:B:913:HOH:O	2.42	0.52
1:D:534:GLY:O	1:D:535:SER:OG	2.27	0.52
1:C:554:ILE:HD13	1:C:717:LEU:HD11	1.92	0.51
1:D:600:GLU:C	1:D:602:SER:H	2.18	0.51
1:A:719:ARG:C	1:A:721:LEU:H	2.18	0.51
1:B:720:GLU:O	1:B:721:LEU:CD2	2.58	0.51
3:A:804:BEN:N1	6:D:802:CL:CL	2.80	0.51
1:C:717:LEU:C	1:C:717:LEU:HD12	2.35	0.51
1:D:491:THR:H	1:D:494:GLN:NE2	2.08	0.51
1:D:681:VAL:HG11	1:D:685:CYS:SG	2.51	0.51
1:A:720:GLU:O	1:A:721:LEU:HD12	2.11	0.51
1:B:529:THR:CG2	1:B:530:GLN:N	2.74	0.51
1:C:664:GLN:HG3	1:C:668:MET:HE3	1.93	0.51
1:D:490:PRO:CA	1:D:494:GLN:HE21	2.20	0.51
1:D:695:GLU:O	1:D:698:LYS:HG2	2.12	0.50
1:B:529:THR:HG23	1:B:530:GLN:N	2.25	0.50
1:A:485:LEU:HD12	1:A:525[B]:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520[B]:SER:OG	1:A:526:ALA:HB3	2.12	0.50
1:D:668:MET:HB3	1:D:674:LEU:CB	2.38	0.50
1:A:498:PHE:CE1	1:A:525[B]:LEU:HD11	2.46	0.49
1:A:576:ASP:OD2	1:A:578:LYS:HE2	2.12	0.49
1:D:587:ASP:OD1	1:D:589:THR:HG23	2.12	0.49
1:A:580:ASN:O	2:A:802:DMS:H13	2.11	0.49
1:A:445:SER:O	1:A:446:GLU:HB2	2.12	0.49
1:A:717:LEU:C	1:A:717:LEU:HD12	2.37	0.49
1:C:617:ILE:O	1:C:620:MET:HB2	2.13	0.49
1:D:691:ARG:O	1:D:695:GLU:HG2	2.12	0.49
1:B:477:HIS:CE1	1:C:517:MET:HE1	2.48	0.49
1:A:501:GLU:OE2	1:A:599:THR:HB	2.12	0.49
1:A:558:ARG:HH11	1:A:562:ARG:HH12	1.59	0.49
1:A:562:ARG:HG3	1:A:711:LEU:CD1	2.43	0.48
1:A:491:THR:H	1:A:494:GLN:NE2	2.12	0.48
1:A:682:ARG:NH1	8:A:909:HOH:O	2.42	0.48
1:B:617:ILE:CD1	1:B:662:ARG:HG2	2.43	0.48
1:C:535:SER:HB2	5:C:801:6NB:C30	2.43	0.48
1:C:617:ILE:HA	1:C:620:MET:SD	2.54	0.48
1:A:589:THR:OG1	1:A:591:LYS:HE2	2.13	0.48
1:B:501:GLU:HG3	1:B:597:LEU:CD2	2.43	0.48
1:C:661:ASN:O	1:C:664:GLN:HB3	2.13	0.48
1:B:688:ARG:HG3	8:B:978:HOH:O	2.13	0.48
1:A:658:ASN:OD1	1:A:659:ILE:HG13	2.14	0.48
1:C:576:ASP:OD2	1:C:578:LYS:HE2	2.14	0.48
1:C:599:THR:O	1:C:600:GLU:HB3	2.14	0.48
1:A:491:THR:H	1:A:494:GLN:HE21	1.62	0.48
1:B:634:SER:OG	8:B:903:HOH:O	2.19	0.48
1:D:720:GLU:O	1:D:721:LEU:HD12	2.14	0.47
1:A:574:HIS:O	1:A:575:ARG:HB2	2.15	0.47
1:C:599:THR:O	1:C:600:GLU:CB	2.62	0.47
1:C:647:TYR:CD1	1:C:676:PRO:HB2	2.50	0.47
1:C:664:GLN:HE21	1:C:668:MET:HE1	1.80	0.47
1:A:558:ARG:HE	1:A:562:ARG:CZ	2.28	0.47
1:A:625:ILE:HD13	1:A:666:ILE:HA	1.97	0.47
1:A:661:ASN:O	1:A:665:ILE:HG13	2.15	0.47
1:C:554:ILE:HD13	1:C:717:LEU:CD1	2.45	0.47
1:C:502:VAL:HG13	1:C:516:PHE:HE2	1.79	0.47
1:D:491:THR:OG1	1:D:494:GLN:HG2	2.15	0.47
1:D:689:MET:HE2	1:D:717:LEU:HD21	1.96	0.47
1:D:700:LYS:O	1:D:703:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:614:SER:OG	1:D:615:GLY:N	2.48	0.46
1:B:461[A]:GLN:NE2	8:B:904:HOH:O	2.24	0.46
1:A:644:ILE:O	1:A:647:TYR:HB3	2.16	0.46
1:B:501:GLU:HG3	1:B:597:LEU:HD23	1.97	0.46
1:D:663:ASP:HA	1:D:666:ILE:HD13	1.96	0.46
1:D:675:SER:HB2	1:D:676:PRO:HD2	1.98	0.46
1:D:570:LYS:NZ	8:D:904:HOH:O	2.35	0.46
1:A:491:THR:OG1	1:A:494:GLN:HG2	2.15	0.46
1:A:502:VAL:HG13	1:A:516:PHE:HE2	1.81	0.46
1:A:485:LEU:HD12	1:A:525[B]:LEU:HD12	1.98	0.45
1:C:656:TYR:CE1	1:C:674:LEU:CD1	3.00	0.45
1:D:587:ASP:O	1:D:588:ASN:HB2	2.17	0.45
1:B:501:GLU:CG	1:B:597:LEU:HD23	2.47	0.45
1:C:587:ASP:O	1:C:588:ASN:HB2	2.16	0.45
1:B:664:GLN:HG3	1:B:668:MET:CE	2.45	0.45
1:B:695[B]:GLU:HB3	1:B:705:PRO:HD3	1.99	0.45
1:A:539:HIS:HD2	8:A:986:HOH:O	1.99	0.44
1:C:635:PHE:O	1:C:638:ASP:HB2	2.17	0.44
1:B:667:GLU:HB3	1:B:671:ARG:HH21	1.83	0.44
1:D:617:ILE:CD1	1:D:666:ILE:HD11	2.46	0.44
1:B:627:MET:HE3	1:B:627:MET:HB3	1.88	0.44
1:C:488:THR:O	1:C:490:PRO:HD3	2.18	0.44
1:C:666:ILE:O	8:C:901:HOH:O	2.21	0.44
1:A:675:SER:HB2	1:A:676:PRO:HD2	2.00	0.44
1:B:529:THR:HG21	5:B:801:6NB:C13	2.48	0.44
1:C:625:ILE:CG2	1:C:670:GLY:HA2	2.45	0.44
1:D:622:PRO:O	1:D:626:ARG:HG2	2.17	0.44
1:A:505:LEU:HD23	1:A:505:LEU:HA	1.84	0.44
1:C:555:ASP:OD1	1:C:558:ARG:NH1	2.51	0.44
1:C:555:ASP:OD1	1:C:558:ARG:NH2	2.51	0.44
1:D:558:ARG:HD2	1:D:715:GLU:OE1	2.18	0.44
1:C:502:VAL:HG13	1:C:516:PHE:CE2	2.52	0.44
1:C:650:MET:HE2	1:C:650:MET:HA	1.98	0.44
1:B:467:SER:O	1:B:468:PHE:HB2	2.18	0.43
1:B:540:HIS:CD2	1:B:584:LEU:HD22	2.52	0.43
1:C:719:ARG:C	1:C:721:LEU:H	2.26	0.43
1:B:716:GLU:HA	1:B:719:ARG:HH11	1.84	0.43
1:C:661:ASN:O	1:C:665:ILE:HG13	2.18	0.43
1:B:548:PHE:HB2	1:B:553:LEU:CD2	2.48	0.43
1:C:554:ILE:HD12	1:C:721:LEU:HD22	2.01	0.43
1:B:717:LEU:O	1:B:717:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:LEU:HD22	1:C:525:LEU:HD12	2.01	0.43
1:B:717:LEU:HD23	1:B:717:LEU:C	2.44	0.43
1:A:704:ARG:O	8:A:902:HOH:O	2.21	0.42
1:D:692:LEU:HD22	1:D:713:GLU:HG2	2.01	0.42
1:A:485:LEU:HB2	1:A:525[B]:LEU:HB3	2.02	0.42
1:A:621:ALA:HB3	1:A:624:VAL:HG23	2.02	0.42
1:A:562:ARG:HD3	8:A:980:HOH:O	2.19	0.42
1:B:598:ALA:O	1:B:601:LYS:HB2	2.19	0.42
1:B:622:PRO:O	1:B:625:ILE:HG22	2.19	0.42
1:C:631:ASN:N	1:C:632:PRO:HD3	2.34	0.42
1:C:676:PRO:O	1:C:678:LEU:HD22	2.20	0.42
1:A:525[A]:LEU:HD23	1:A:525[A]:LEU:HA	1.86	0.42
1:B:475:LYS:HG2	8:B:919:HOH:O	2.20	0.42
1:B:675:SER:HB2	1:B:676:PRO:CD	2.50	0.42
1:D:644:ILE:O	1:D:647:TYR:HB3	2.20	0.42
1:A:681:VAL:CG1	1:A:685:CYS:CB	2.96	0.42
1:B:578:LYS:HE2	1:B:616:SER:HB3	2.01	0.42
1:B:658:ASN:OD1	1:B:659:ILE:HD12	2.19	0.42
1:C:707:PHE:N	1:C:708:PRO:CD	2.83	0.42
1:B:647:TYR:O	1:B:651:THR:HG23	2.19	0.42
1:D:682:ARG:O	1:D:685:CYS:HB3	2.19	0.42
1:A:617:ILE:HD13	1:A:666:ILE:HD11	2.02	0.41
1:C:647:TYR:CD2	1:C:647:TYR:C	2.98	0.41
1:C:674:LEU:C	1:C:674:LEU:HD13	2.45	0.41
1:D:707:PHE:N	1:D:708:PRO:CD	2.83	0.41
1:D:719:ARG:O	1:D:721:LEU:N	2.49	0.41
1:A:667:GLU:O	1:A:671:ARG:HG3	2.21	0.41
1:B:529:THR:HG22	1:B:530:GLN:O	2.20	0.41
1:B:660:ASN:HB2	8:B:967:HOH:O	2.20	0.41
1:C:664:GLN:CG	1:C:668:MET:HE3	2.50	0.41
1:D:634:SER:OG	1:D:636:GLN:HB2	2.21	0.41
1:D:710:ILE:O	1:D:714:ILE:HG13	2.20	0.41
1:B:622:PRO:HA	1:B:625:ILE:HG22	2.02	0.41
1:C:485:LEU:N	1:C:485:LEU:HD12	2.35	0.41
1:B:574:HIS:O	1:B:575:ARG:HB2	2.21	0.41
1:C:487:VAL:O	1:C:487:VAL:HG23	2.21	0.41
1:A:480:VAL:HG12	1:A:517:MET:HE1	2.03	0.41
1:A:707:PHE:N	1:A:708:PRO:CD	2.84	0.41
1:B:493[B]:GLN:H	1:B:493[B]:GLN:HG3	1.62	0.40
1:B:667:GLU:HB3	1:B:671:ARG:NH2	2.37	0.40
1:D:692:LEU:HD22	1:D:713:GLU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ILE:HG22	1:A:575:ARG:HG3	2.03	0.40
1:C:505:LEU:HD23	1:C:505:LEU:HA	1.83	0.40
1:D:719:ARG:C	1:D:721:LEU:N	2.79	0.40
1:A:485:LEU:HD12	1:A:525[B]:LEU:CG	2.50	0.40
1:A:491:THR:N	1:A:494:GLN:HE21	2.20	0.40
1:D:681:VAL:CG1	1:D:685:CYS:SG	3.10	0.40
1:A:541:LEU:HA	1:A:541:LEU:HD23	1.85	0.40
1:D:717:LEU:O	1:D:721:LEU:HD13	2.22	0.40
1:A:452:ILE:HA	1:A:453:PRO:HD3	1.89	0.40
1:D:562:ARG:HG3	1:D:711:LEU:HD11	2.04	0.40

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%)	30	34
1	B	262/280 (94%)	254 (97%)	7 (3%)	1 (0%)	30	34
1	C	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	D	250/280 (89%)	239 (96%)	9 (4%)	2 (1%)	16	16
All	All	1033/1120 (92%)	988 (96%)	41 (4%)	4 (0%)	30	34

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%)	221 (98%)	5 (2%)	45	61
1	B	233/245 (95%)	228 (98%)	5 (2%)	47	63
1	C	221/245 (90%)	218 (99%)	3 (1%)	59	75
1	D	211/245 (86%)	210 (100%)	1 (0%)	81	90
All	All	891/980 (91%)	877 (98%)	14 (2%)	55	71

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	LYS
1	A	554	ILE
1	A	584	LEU
1	A	625	ILE
1	A	666	ILE
1	B	508	THR
1	B	509	ARG
1	B	529	THR
1	B	627	MET
1	B	717	LEU
1	C	525	LEU
1	C	666	ILE
1	C	717	LEU
1	D	717	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	B	512	ASN
1	B	539	HIS
1	C	494	GLN
1	C	512	ASN
1	D	494	GLN
1	D	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	802	-	3,3,3	0.61	0	3,3,3	1.02	0
5	6NB	B	801	-	81,81,81	1.49	13 (16%)	106,116,116	2.40	35 (33%)
7	GOL	B	806	-	5,5,5	0.39	0	5,5,5	0.16	0
2	DMS	C	802	-	3,3,3	0.65	0	3,3,3	0.72	0
5	6NB	C	801	-	81,81,81	1.50	15 (18%)	106,116,116	2.46	23 (21%)
3	BEN	B	807	-	9,9,9	4.23	5 (55%)	7,11,11	1.17	1 (14%)
4	EOH	A	805	-	2,2,2	0.47	0	1,1,1	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	A	801	-	3,3,3	0.57	0	3,3,3	0.87	0
3	BEN	A	804	-	9,9,9	4.14	6 (66%)	7,11,11	0.59	0
4	EOH	B	805	-	2,2,2	0.49	0	1,1,1	0.13	0
2	DMS	D	801	-	3,3,3	0.67	0	3,3,3	0.55	0
2	DMS	A	803	-	3,3,3	0.70	0	3,3,3	0.67	0
4	EOH	B	804	-	2,2,2	0.46	0	1,1,1	0.23	0
2	DMS	B	802	-	3,3,3	0.64	0	3,3,3	0.80	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
5	6NB	B	801	-	-	8/55/64/64	0/8/8/8
7	GOL	B	806	-	-	4/4/4/4	-
5	6NB	C	801	-	-	8/55/64/64	0/8/8/8
3	BEN	B	807	-	-	2/4/4/4	0/1/1/1
3	BEN	A	804	-	-	0/4/4/4	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	BEN	C6-C1	7.28	1.50	1.39
3	B	807	BEN	C6-C1	7.26	1.50	1.39
3	A	804	BEN	C3-C2	6.68	1.50	1.38
3	B	807	BEN	C3-C2	6.62	1.50	1.38
3	B	807	BEN	C5-C4	6.14	1.51	1.38
3	A	804	BEN	C5-C4	5.21	1.49	1.38
5	C	801	6NB	C38-C39	-4.29	1.36	1.41
5	B	801	6NB	O04-C01	4.08	1.46	1.37
5	C	801	6NB	O04-C01	4.04	1.46	1.37
5	B	801	6NB	C13-N02	-3.71	1.31	1.37
5	C	801	6NB	C13-N02	-3.63	1.31	1.37
5	B	801	6NB	C38-C39	-3.60	1.37	1.41
3	A	804	BEN	C2-C1	-3.55	1.34	1.39
3	B	807	BEN	C2-C1	-3.44	1.34	1.39
5	B	801	6NB	C09-C10	-3.23	1.38	1.41
5	C	801	6NB	C08-C09	3.14	1.44	1.39
5	B	801	6NB	C08-C09	2.88	1.44	1.39
5	B	801	6NB	C44-C43	2.88	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	801	6NB	C09-C10	-2.84	1.38	1.41
3	A	804	BEN	C5-C6	-2.79	1.34	1.38
5	C	801	6NB	C13-C12	2.78	1.42	1.38
5	B	801	6NB	C35-C30	2.60	1.43	1.38
3	B	807	BEN	C5-C6	-2.60	1.34	1.38
5	C	801	6NB	C44-C43	2.58	1.56	1.51
5	C	801	6NB	O07-C30	2.51	1.43	1.37
5	C	801	6NB	C08-C07	2.50	1.44	1.39
5	C	801	6NB	C18-C17	2.49	1.42	1.38
5	B	801	6NB	C18-C17	2.48	1.42	1.38
5	B	801	6NB	C13-C12	2.46	1.41	1.38
5	B	801	6NB	C08-C07	2.41	1.43	1.39
5	B	801	6NB	C40-N04	-2.27	1.29	1.34
5	B	801	6NB	O07-C30	2.25	1.42	1.37
5	C	801	6NB	C03-C02	2.24	1.42	1.38
5	C	801	6NB	F03-C49	-2.23	1.31	1.34
5	C	801	6NB	C07-C04	2.18	1.54	1.49
5	C	801	6NB	C35-C30	2.16	1.42	1.38
5	C	801	6NB	C40-N04	-2.10	1.30	1.34
5	B	801	6NB	S-N	2.10	1.67	1.62
3	A	804	BEN	C1-C	2.01	1.51	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	801	6NB	O-S-O09	-11.49	103.27	119.34
5	C	801	6NB	O03-S01-O02	-10.38	104.82	119.34
5	B	801	6NB	O-S-O09	-9.85	105.57	119.34
5	B	801	6NB	C21-S01-N03	7.62	117.55	106.72
5	C	801	6NB	C21-S01-N03	7.02	116.70	106.72
5	B	801	6NB	O03-S01-O02	-6.99	109.56	119.34
5	C	801	6NB	C09-C10-N02	6.04	110.63	108.42
5	B	801	6NB	O09-S-C50	5.75	117.00	107.86
5	B	801	6NB	C45-C44-C49	5.34	120.91	115.66
5	C	801	6NB	C09-C10-N01	-5.08	120.15	126.31
5	C	801	6NB	O09-S-C50	4.88	115.61	107.86
5	B	801	6NB	C39-N05-C42	4.74	110.72	108.48
5	C	801	6NB	C45-C44-C49	4.72	120.31	115.66
5	C	801	6NB	C39-N05-C42	4.65	110.67	108.48
5	C	801	6NB	C16-C15-C20	4.58	120.17	115.66
5	B	801	6NB	C09-C10-N01	-4.48	120.88	126.31
5	B	801	6NB	C16-C15-C20	4.47	120.05	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	801	6NB	C38-C39-N04	-4.03	121.43	126.31
5	B	801	6NB	C37-C36-C40	3.89	121.27	117.10
5	B	801	6NB	O03-S01-C21	3.83	113.94	107.86
5	B	801	6NB	C20-C19-N03	-3.71	116.44	120.73
5	B	801	6NB	C50-S-N	3.69	111.97	106.72
5	B	801	6NB	C10-N02-C13	3.67	110.21	108.48
5	C	801	6NB	C49-C48-N	-3.54	116.64	120.73
5	C	801	6NB	C08-C09-C10	3.29	120.07	117.64
5	B	801	6NB	C49-C48-N	-3.29	116.93	120.73
5	C	801	6NB	C41-C42-N05	-3.06	108.14	110.22
5	B	801	6NB	C09-C10-N02	3.04	109.53	108.42
5	B	801	6NB	C38-C39-N04	-2.91	122.78	126.31
5	B	801	6NB	C11-N01-C10	2.90	121.88	116.19
5	C	801	6NB	C29-O07-C30	-2.88	110.46	117.93
3	B	807	BEN	C1-C-N2	2.84	122.32	118.01
5	C	801	6NB	C11-N01-C10	2.81	121.70	116.19
5	C	801	6NB	C40-N04-C39	2.79	121.66	116.19
5	C	801	6NB	C38-C39-N05	2.75	109.43	108.42
5	B	801	6NB	C41-C42-N05	-2.75	108.36	110.22
5	B	801	6NB	C08-C07-C11	2.72	120.01	117.10
5	B	801	6NB	C08-C09-C10	2.67	119.61	117.64
5	B	801	6NB	C29-O07-C30	-2.62	111.11	117.93
5	B	801	6NB	C36-C40-N04	-2.58	120.18	124.28
5	B	801	6NB	C34-C33-C32	2.56	122.26	117.68
5	B	801	6NB	C49-C44-C43	-2.51	116.91	121.62
5	B	801	6NB	C38-C37-C36	-2.49	116.20	120.82
5	B	801	6NB	O02-S01-C21	-2.46	103.94	107.86
5	C	801	6NB	O03-S01-C21	2.43	111.71	107.86
5	B	801	6NB	C31-C32-C33	-2.40	118.05	121.12
5	C	801	6NB	C37-C38-C39	2.36	119.39	117.64
5	B	801	6NB	C18-C19-C20	2.35	120.99	117.72
5	B	801	6NB	C40-N04-C39	2.33	120.75	116.19
5	B	801	6NB	C09-C08-C07	-2.28	116.58	120.82
5	B	801	6NB	C47-C48-C49	2.25	120.84	117.72
5	C	801	6NB	C09-C08-C07	-2.21	116.72	120.82
5	C	801	6NB	C20-C19-N03	-2.14	118.25	120.73
5	C	801	6NB	C34-C33-C36	-2.12	117.60	121.25
5	B	801	6NB	C40-C36-C33	-2.12	118.05	121.62
5	B	801	6NB	F03-C49-C48	2.11	121.63	118.28
5	C	801	6NB	C36-C40-N04	-2.07	121.00	124.28
5	B	801	6NB	F01-C20-C19	2.06	121.56	118.28
5	B	801	6NB	C07-C11-N01	-2.04	121.04	124.28

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	801	6NB	C51-C50-S-N
5	C	801	6NB	C51-C50-S-O09
5	C	801	6NB	C51-C50-S-O
7	B	806	GOL	C1-C2-C3-O3
5	B	801	6NB	C29-C28-O06-C27
5	C	801	6NB	C29-C28-O06-C27
7	B	806	GOL	O2-C2-C3-O3
5	B	801	6NB	C31-C30-O07-C29
5	C	801	6NB	O06-C28-C29-O07
5	B	801	6NB	C35-C30-O07-C29
7	B	806	GOL	O1-C1-C2-C3
7	B	806	GOL	O1-C1-C2-O2
5	B	801	6NB	O04-C24-C25-O05
5	B	801	6NB	O05-C26-C27-O06
5	C	801	6NB	O04-C24-C25-O05
5	B	801	6NB	C28-C29-O07-C30
5	C	801	6NB	C25-C24-O04-C01
3	B	807	BEN	N1-C-C1-C6
5	B	801	6NB	C24-C25-O05-C26
5	B	801	6NB	O06-C28-C29-O07
5	C	801	6NB	O05-C26-C27-O06
3	B	807	BEN	N2-C-C1-C2

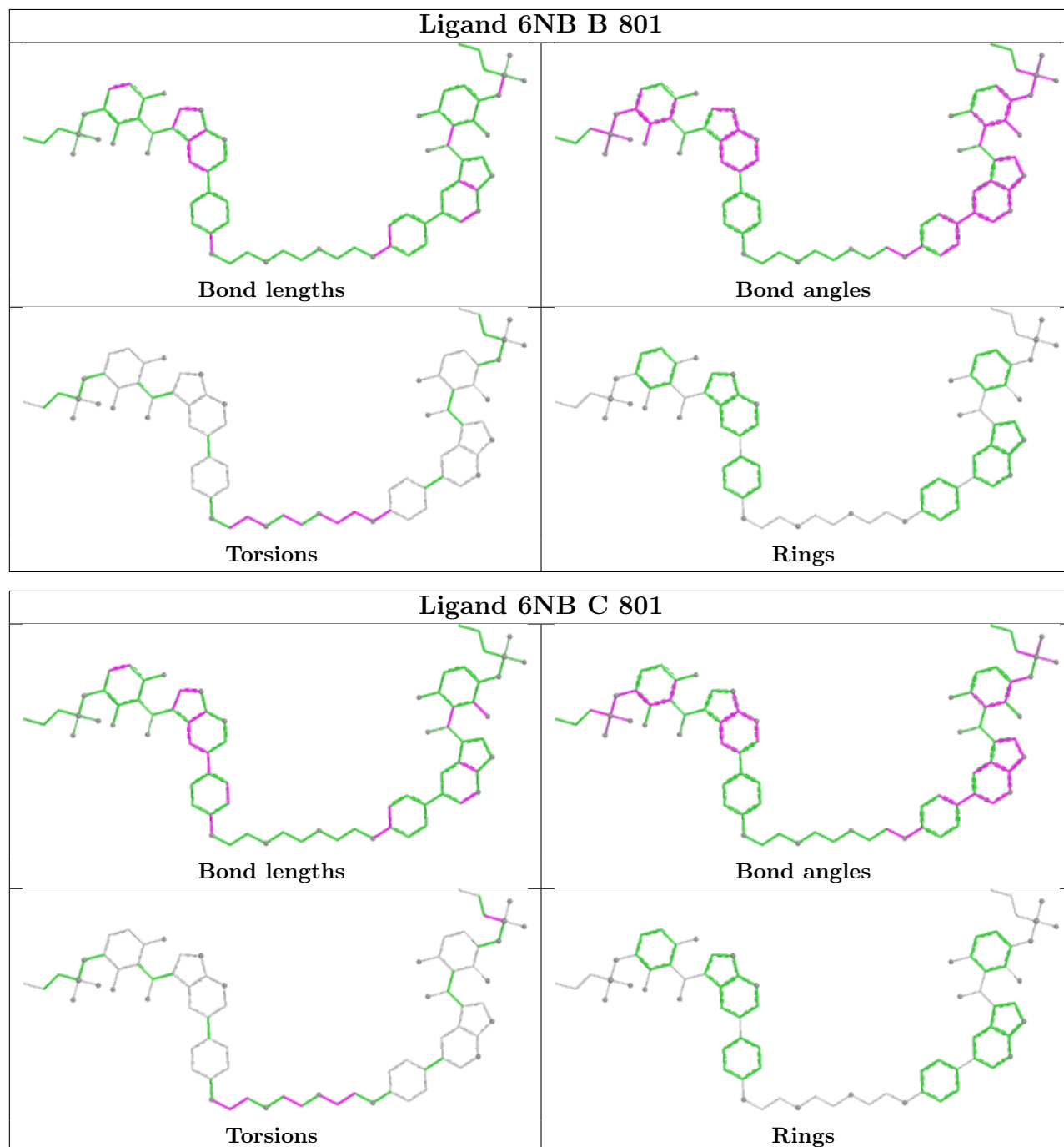
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	DMS	1	0
5	B	801	6NB	1	0
5	C	801	6NB	1	0
3	B	807	BEN	1	0
3	A	804	BEN	1	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 than 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.



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	265/280 (94%)	0.19	9 (3%)	48	45	24, 42, 69, 81	2 (0%)
1	B	263/280 (93%)	0.35	9 (3%)	48	45	19, 47, 72, 84	5 (1%)
1	C	262/280 (93%)	0.85	44 (16%)	4	3	23, 53, 88, 98	2 (0%)
1	D	259/280 (92%)	0.46	14 (5%)	31	28	25, 50, 83, 93	1 (0%)
All	All	1049/1120 (93%)	0.46	76 (7%)	21	18	19, 48, 81, 98	10 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	LEU	5.0
1	D	659	ILE	4.9
1	C	674	LEU	4.1
1	C	488	THR	3.6
1	C	658	ASN	3.6
1	B	488	THR	3.5
1	C	721	LEU	3.2
1	C	697	LEU	3.2
1	D	602	SER	3.2
1	C	620	MET	3.1
1	D	487	VAL	3.1
1	C	678	LEU	3.1
1	C	679	SER	3.1
1	A	489	ALA	3.0
1	D	721	LEU	3.0
1	C	672	GLY	3.0
1	C	487	VAL	2.9
1	C	669	VAL	2.9
1	C	671	ARG	2.9
1	C	660	ASN	2.9
1	C	622	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	673	SER	2.8
1	C	683	SER	2.8
1	C	681	VAL	2.8
1	C	659	ILE	2.8
1	C	598	ALA	2.7
1	C	640	TYR	2.7
1	A	490	PRO	2.7
1	A	488	THR	2.7
1	A	614	SER	2.7
1	D	616	SER	2.6
1	C	600	GLU	2.6
1	C	629	ASP	2.6
1	D	614	SER	2.5
1	D	627	MET	2.5
1	C	699	LYS	2.5
1	C	489	ALA	2.5
1	C	693	MET	2.5
1	C	685	CYS	2.4
1	C	543	ALA	2.4
1	B	489	ALA	2.4
1	C	621	ALA	2.4
1	C	618	LEU	2.4
1	C	468	PHE	2.4
1	B	665	ILE	2.4
1	D	615	GLY	2.4
1	D	666	ILE	2.4
1	A	689	MET	2.4
1	C	665	ILE	2.3
1	C	675	SER	2.3
1	C	714	ILE	2.3
1	C	680	LYS	2.3
1	C	492	PRO	2.3
1	D	719	ARG	2.3
1	C	617	ILE	2.3
1	C	692	LEU	2.3
1	D	554	ILE	2.2
1	A	687	LYS	2.2
1	C	625	ILE	2.2
1	D	490	PRO	2.2
1	D	665	ILE	2.1
1	B	616	SER	2.1
1	C	666	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	487	VAL	2.1
1	C	676	PRO	2.1
1	A	495	LEU	2.1
1	B	625	ILE	2.1
1	C	689	MET	2.0
1	C	716	GLU	2.0
1	D	718	ALA	2.1
1	B	658	ASN	2.0
1	C	701	ARG	2.0
1	B	632	PRO	2.0
1	A	457	ILE	2.0
1	A	549	GLU	2.0
1	C	661	ASN	2.0

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 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
4	EOH	B	804	3/3	0.44	0.24	72,87,92,92	0
2	DMS	A	803	4/4	0.52	0.20	65,79,83,100	0
7	GOL	B	806	6/6	0.59	0.17	58,75,88,96	0
4	EOH	B	805	3/3	0.63	0.23	51,62,77,77	0
4	EOH	A	805	3/3	0.72	0.13	53,63,71,75	0
2	DMS	C	802	4/4	0.80	0.14	58,70,78,92	0
2	DMS	A	801	4/4	0.81	0.14	43,55,66,83	0
2	DMS	B	802	4/4	0.86	0.14	46,64,76,79	0
2	DMS	A	802	4/4	0.87	0.16	32,49,59,66	0
2	DMS	D	801	4/4	0.87	0.14	57,68,70,71	0

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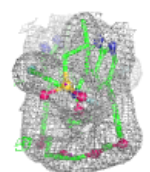
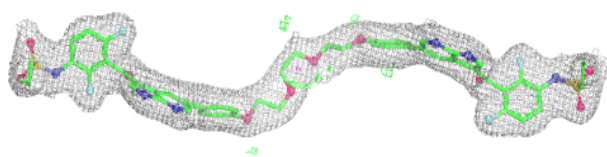
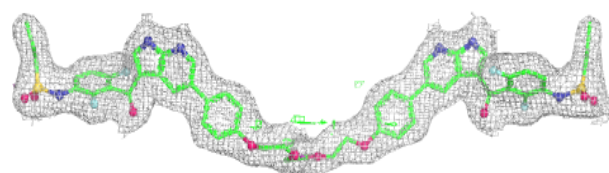
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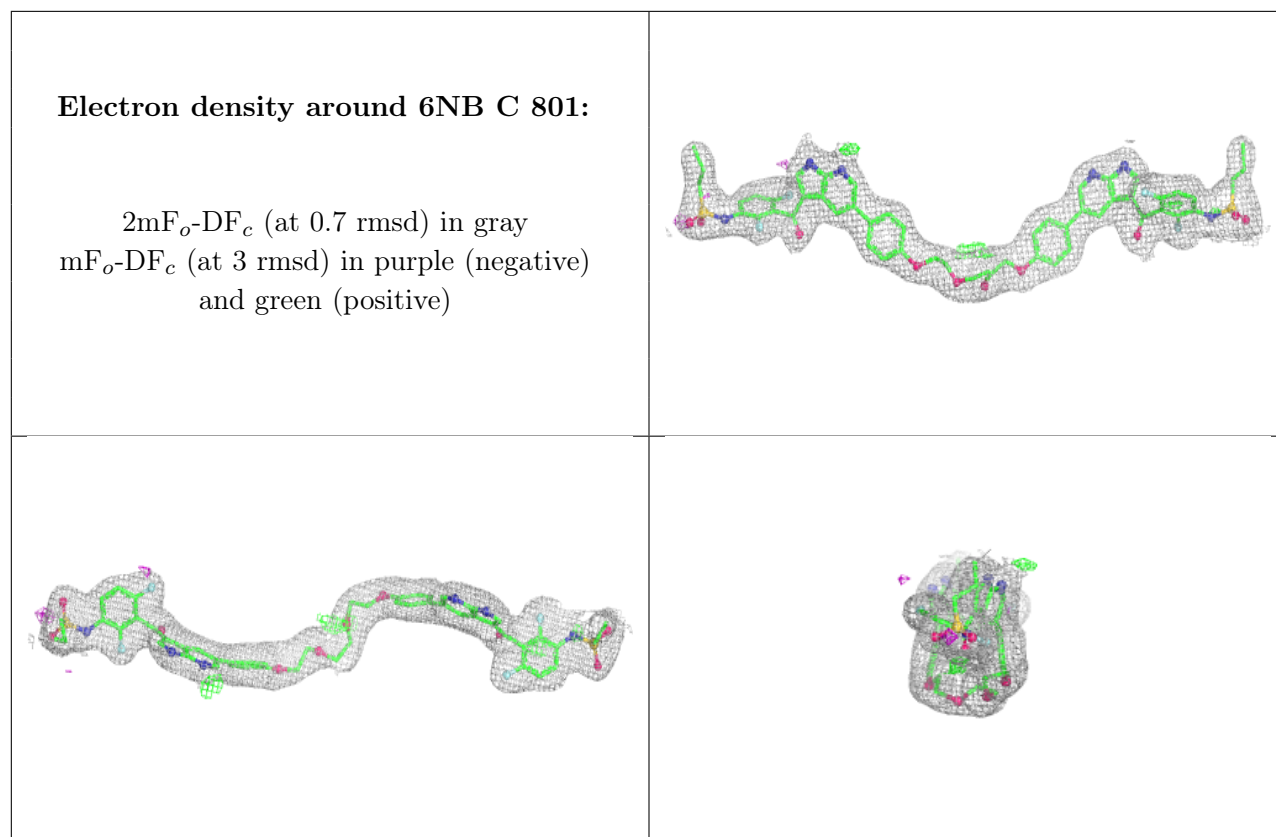
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BEN	A	804	9/9	0.95	0.06	21,28,43,43	0
6	CL	B	803	1/1	0.95	0.19	53,53,53,53	0
3	BEN	B	807	9/9	0.95	0.06	22,29,43,43	0
5	6NB	B	801	74/74	0.96	0.07	23,33,48,62	0
6	CL	B	808	1/1	0.96	0.12	54,54,54,54	0
6	CL	D	802	1/1	0.96	0.26	54,54,54,54	0
5	6NB	C	801	74/74	0.96	0.07	28,36,48,58	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 6NB B 801:

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 [i](#)

There are no such residues in this entry.