



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4MNF / pdb_00004mnf
Title : Crystal structure of BRAF-V600E bound to GDC0879
Authors : Sudhamsu, J.; Haling, J.R.; Morales, T.; Brandhuber, B.; Hymowitz, S.G.
Deposited on : 2013-09-10
Resolution : 2.80 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

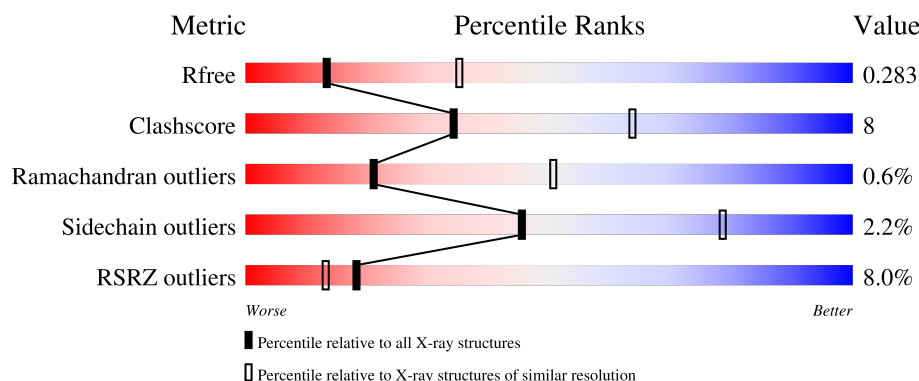
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	5% 63% 15% 22%
1	B	329	8% 61% 16% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4271 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	3	3	0
			2075	1331	359	371	14			
1	B	257	Total	C	N	O	S	1	1	0
			2065	1324	359	369	13			

There are 50 discrepancies between the modelled and reference sequences:

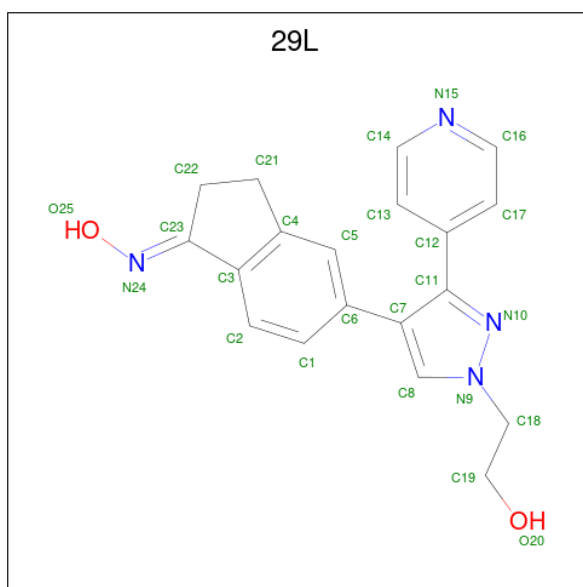
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	MET	-	expression tag	UNP P15056
A	409	SER	-	expression tag	UNP P15056
A	410	GLY	-	expression tag	UNP P15056
A	411	ALA	-	expression tag	UNP P15056
A	412	HIS	-	expression tag	UNP P15056
A	413	HIS	-	expression tag	UNP P15056
A	414	HIS	-	expression tag	UNP P15056
A	415	HIS	-	expression tag	UNP P15056
A	416	HIS	-	expression tag	UNP P15056
A	417	HIS	-	expression tag	UNP P15056
A	418	HIS	-	expression tag	UNP P15056
A	419	HIS	-	expression tag	UNP P15056
A	420	GLY	-	expression tag	UNP P15056
A	421	GLY	-	expression tag	UNP P15056
A	422	GLY	-	expression tag	UNP P15056
A	423	GLY	-	expression tag	UNP P15056
A	424	GLY	-	expression tag	UNP P15056
A	425	LEU	-	expression tag	UNP P15056
A	426	VAL	-	expression tag	UNP P15056
A	427	PRO	-	expression tag	UNP P15056
A	428	ARG	-	expression tag	UNP P15056
A	429	GLY	-	expression tag	UNP P15056
A	430	ALA	-	expression tag	UNP P15056
A	431	MET	-	expression tag	UNP P15056
A	600	GLU	VAL	engineered mutation	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	MET	-	expression tag	UNP P15056
B	409	SER	-	expression tag	UNP P15056
B	410	GLY	-	expression tag	UNP P15056
B	411	ALA	-	expression tag	UNP P15056
B	412	HIS	-	expression tag	UNP P15056
B	413	HIS	-	expression tag	UNP P15056
B	414	HIS	-	expression tag	UNP P15056
B	415	HIS	-	expression tag	UNP P15056
B	416	HIS	-	expression tag	UNP P15056
B	417	HIS	-	expression tag	UNP P15056
B	418	HIS	-	expression tag	UNP P15056
B	419	HIS	-	expression tag	UNP P15056
B	420	GLY	-	expression tag	UNP P15056
B	421	GLY	-	expression tag	UNP P15056
B	422	GLY	-	expression tag	UNP P15056
B	423	GLY	-	expression tag	UNP P15056
B	424	GLY	-	expression tag	UNP P15056
B	425	LEU	-	expression tag	UNP P15056
B	426	VAL	-	expression tag	UNP P15056
B	427	PRO	-	expression tag	UNP P15056
B	428	ARG	-	expression tag	UNP P15056
B	429	GLY	-	expression tag	UNP P15056
B	430	ALA	-	expression tag	UNP P15056
B	431	MET	-	expression tag	UNP P15056
B	600	GLU	VAL	engineered mutation	UNP P15056

- Molecule 2 is 2-{4-[(1E)-1-(hydroxyimino)-2,3-dihydro-1H-inden-5-yl]-3-(pyridin-4-yl)-1H-pyrazol-1-yl}ethanol (CCD ID: 29L) (formula: C₁₉H₁₈N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	19	4	2		
2	B	1	Total	C	N	O	0	0
			25	19	4	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	23	Total	O	0	0
			23	23		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.74Å 99.74Å 159.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.80 49.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.87-2.80) 99.9 (49.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.211 , 0.275 0.232 , 0.283	Depositor DCC
R_{free} test set	1044 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4271	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: CL, 29L

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	0.55	0/2127	0.97	6/2868 (0.2%)
1	B	0.58	0/2112	0.97	4/2850 (0.1%)
All	All	0.56	0/4239	0.97	10/5718 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	GLY	N-CA-C	-8.83	102.64	111.56
1	A	452	ILE	CA-C-N	6.26	126.20	119.76
1	A	452	ILE	C-N-CA	6.26	126.20	119.76
1	B	629	ASP	N-CA-C	5.74	117.33	109.18
1	A	617	ILE	N-CA-C	5.71	115.90	110.42
1	B	631	ASN	CA-C-N	5.45	125.12	119.56
1	B	631	ASN	C-N-CA	5.45	125.12	119.56
1	B	653	GLN	N-CA-C	5.22	116.92	109.14
1	A	631	ASN	CA-C-N	5.13	125.58	120.04
1	A	631	ASN	C-N-CA	5.13	125.58	120.04

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	2075	0	2115	34	1
1	B	2065	0	2102	32	1
2	A	25	0	18	0	0
2	B	25	0	18	0	0
3	B	1	0	0	0	0
4	A	57	0	0	5	0
4	B	23	0	0	1	0
All	All	4271	0	4253	64	1

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 8.

All (64) 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:623:GLU:OE1	4:A:955:HOH:O	2.04	0.75
1:B:698:LYS:O	1:B:704:ARG:NH1	2.24	0.70
1:A:458:THR:HB	1:A:475:LYS:HB2	1.79	0.65
1:B:650:MET:HE3	1:B:689:MET:HG2	1.78	0.64
1:A:700:LYS:NZ	1:A:702:ASP:OD1	2.31	0.63
1:B:623:GLU:OE2	1:B:704:ARG:NH2	2.34	0.61
1:B:564:MET:SD	1:B:592:ILE:HD13	2.43	0.58
1:A:650:MET:HE3	1:A:689:MET:HG2	1.86	0.57
1:A:659:ILE:HG22	1:A:661:ASN:H	1.69	0.57
1:B:522:LYS:HA	1:B:523:PRO:C	2.29	0.57
1:A:502:VAL:O	1:A:506:ARG:HG3	2.03	0.57
1:B:617:ILE:HA	1:B:620:MET:HE3	1.87	0.56
1:B:710:ILE:O	1:B:714:ILE:HG13	2.07	0.55
1:B:586:GLU:O	1:B:588:LEU:N	2.40	0.54
1:B:560:THR:O	1:B:564:MET:HG2	2.08	0.54
1:B:634:SER:O	1:B:637:SER:OG	2.22	0.53
1:B:591:LYS:NZ	4:B:901:HOH:O	2.41	0.53
1:B:484:MET:HG3	1:B:526:ALA:HB2	1.92	0.52
1:B:573:ILE:HG22	1:B:575:ARG:HG2	1.91	0.51
1:A:654:LEU:HD21	4:A:920:HOH:O	2.10	0.51
1:A:642:PHE:CZ	1:A:646:LEU:HD21	2.45	0.51
1:A:623:GLU:OE2	1:A:704:ARG:NH2	2.43	0.51
1:B:599:THR:OG1	1:B:600:GLU:N	2.45	0.50
1:B:586:GLU:C	1:B:588:LEU:H	2.20	0.50
1:B:650:MET:O	1:B:682:ARG:HG2	2.11	0.50
1:B:575:ARG:HD2	1:B:633:TYR:CG	2.49	0.47
1:A:512:ASN:HA	1:A:590:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:GLY:O	1:A:699:LYS:NZ	2.46	0.47
1:A:689:MET:HB2	1:A:717:LEU:HD11	1.96	0.47
1:A:698:LYS:O	1:A:704:ARG:NH1	2.43	0.46
1:A:617:ILE:HG13	1:A:666:ILE:HD11	1.98	0.46
1:A:626:ARG:NH1	4:A:949:HOH:O	2.39	0.46
1:A:644:ILE:O	1:A:648:GLU:HG3	2.15	0.46
1:A:537:LEU:HD21	1:A:649:LEU:HD21	1.98	0.46
1:A:617:ILE:HG12	1:A:662:ARG:NH1	2.30	0.46
1:B:620:MET:HG2	1:B:624:VAL:HB	1.98	0.45
1:A:550:MET:HE1	1:A:650:MET:SD	2.57	0.45
1:A:537:LEU:HD12	1:A:537:LEU:HA	1.82	0.45
1:A:654:LEU:HD12	1:A:654:LEU:HA	1.68	0.44
1:A:704:ARG:O	4:A:948:HOH:O	2.20	0.43
1:B:576:ASP:HB2	1:B:597:LEU:HD12	2.00	0.43
1:A:516:PHE:O	1:B:509:ARG:HD3	2.19	0.43
1:A:509:ARG:HD3	1:B:516:PHE:O	2.18	0.43
1:B:491:THR:O	1:B:494:GLN:N	2.51	0.43
1:B:631:ASN:HA	1:B:632:PRO:HD2	1.83	0.43
1:B:550:MET:O	1:B:554:ILE:HG13	2.19	0.43
1:A:677:ASP:HB3	1:A:680:LYS:HD3	2.01	0.43
1:B:586:GLU:O	1:B:588:LEU:HG	2.19	0.43
1:A:626:ARG:HB3	1:A:628:GLN:HG3	2.01	0.42
1:B:463:ILE:HD13	1:B:473:LYS:H	1.84	0.42
1:B:682:ARG:HB3	1:B:684:ASN:OD1	2.19	0.42
1:A:690:LYS:HE2	1:A:690:LYS:HB3	1.85	0.42
1:B:578:LYS:HB3	1:B:619:TRP:CD2	2.54	0.42
1:A:674:LEU:O	4:A:905:HOH:O	2.21	0.42
1:B:505:LEU:HA	1:B:505:LEU:HD23	1.83	0.42
1:A:454:ASP:OD1	1:A:454:ASP:N	2.53	0.41
1:A:681:VAL:HG21	1:A:690:LYS:HD2	2.02	0.41
1:B:635:PHE:O	1:B:639:VAL:HG23	2.19	0.41
1:B:701:ARG:HA	1:B:704:ARG:HG3	2.02	0.41
1:B:489:ALA:HA	1:B:490:PRO:HD3	1.84	0.41
1:A:550:MET:HA	1:A:553:LEU:HD12	2.02	0.41
1:A:564:MET:SD	1:A:592:ILE:HD13	2.61	0.41
1:A:686:PRO:HG2	1:A:717:LEU:HD21	2.03	0.40

All (1) 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)
1:A:677:ASP:OD2	1:B:680:LYS:NZ[3_545]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/329 (78%)	238 (93%)	17 (7%)	0	100	100
1	B	254/329 (77%)	236 (93%)	15 (6%)	3 (1%)	10	34
All	All	509/658 (77%)	474 (93%)	32 (6%)	3 (1%)	21	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	587	ASP
1	B	630	LYS
1	B	523	PRO

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	229/284 (81%)	225 (98%)	4 (2%)	53	83
1	B	227/284 (80%)	221 (97%)	6 (3%)	40	75
All	All	456/568 (80%)	446 (98%)	10 (2%)	45	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	487	VAL
1	A	617	ILE
1	A	629	ASP
1	A	693	MET
1	B	463	ILE
1	B	488	THR
1	B	524	GLN
1	B	544	ILE
1	B	578	LYS
1	B	630	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	29L	B	801	-	27,28,28	0.79	1 (3%)	34,39,39	2.64	15 (44%)
2	29L	A	801	-	27,28,28	0.87	1 (3%)	34,39,39	2.64	9 (26%)

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	29L	B	801	-	-	1/13/22/22	0/4/4/4
2	29L	A	801	-	-	1/13/22/22	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	29L	N9-N10	3.38	1.40	1.35
2	B	801	29L	N9-N10	3.21	1.39	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	29L	C11-N10-N9	7.99	110.25	103.72
2	B	801	29L	C18-N9-N10	6.89	126.53	119.56
2	A	801	29L	C8-C7-C11	6.33	108.36	104.71
2	A	801	29L	O25-N24-C23	5.86	120.38	112.52
2	B	801	29L	O25-N24-C23	5.18	119.47	112.52
2	B	801	29L	C11-N10-N9	5.15	107.93	103.72
2	A	801	29L	C8-N9-N10	-5.12	107.29	113.56
2	B	801	29L	C21-C4-C3	-4.87	108.09	111.16
2	A	801	29L	C18-N9-N10	4.69	124.31	119.56
2	B	801	29L	C8-N9-N10	-4.08	108.57	113.56
2	B	801	29L	C1-C6-C7	-3.83	115.49	120.98
2	B	801	29L	C22-C21-C4	3.71	107.04	104.30
2	B	801	29L	C5-C6-C7	3.11	125.40	120.65
2	B	801	29L	C8-C7-C11	3.05	106.47	104.71
2	A	801	29L	C7-C11-N10	-2.68	106.32	111.21
2	B	801	29L	C7-C8-N9	2.47	108.75	106.83
2	B	801	29L	C21-C22-C23	-2.45	104.24	105.42
2	B	801	29L	C12-C11-N10	2.33	122.47	118.99
2	B	801	29L	C16-N15-C14	2.27	122.05	116.86
2	A	801	29L	C12-C11-N10	2.21	122.29	118.99
2	A	801	29L	C16-N15-C14	2.13	121.73	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	29L	C18-N9-C8	-2.11	124.88	128.83
2	B	801	29L	C4-C3-C23	2.09	111.45	108.98
2	A	801	29L	C22-C21-C4	2.07	105.83	104.30

There are no chirality outliers.

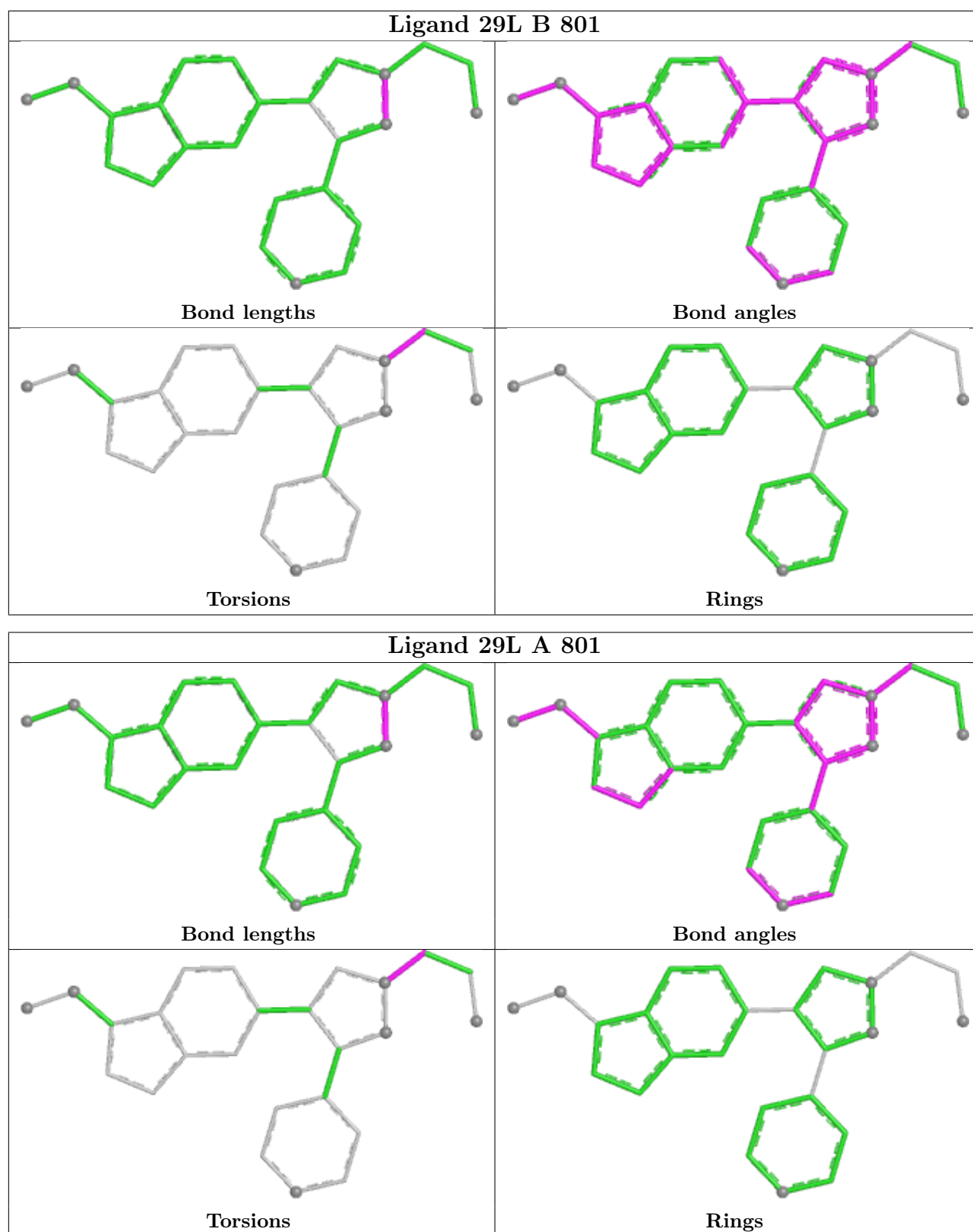
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	29L	C19-C18-N9-N10
2	B	801	29L	C19-C18-N9-N10

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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	257/329 (78%)	0.38	15 (5%) 29 22	17, 40, 74, 137	6 (2%)
1	B	257/329 (78%)	0.64	26 (10%) 12 9	21, 46, 96, 136	2 (0%)
All	All	514/658 (78%)	0.51	41 (7%) 18 13	17, 42, 87, 137	8 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	ASN	5.0
1	B	588	LEU	5.0
1	B	586	GLU	4.5
1	A	719	ARG	3.8
1	B	533	GLU	3.7
1	B	487	VAL	3.3
1	B	616	SER	3.2
1	B	689	MET	3.2
1	A	630	LYS	3.1
1	B	468	PHE	3.0
1	A	488	THR	3.0
1	A	533	GLU	2.9
1	A	571	SER	2.8
1	B	485	LEU	2.8
1	A	489	ALA	2.8
1	B	580	ASN	2.8
1	B	631	ASN	2.8
1	A	696	CYS	2.8
1	B	484	MET	2.7
1	B	467	SER	2.7
1	A	467	SER	2.7
1	B	465	SER	2.5
1	B	685	CYS	2.5
1	B	654	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	454	ASP	2.4
1	A	600[A]	GLU	2.4
1	B	600	GLU	2.4
1	B	628	GLN	2.4
1	B	488	THR	2.3
1	B	696	CYS	2.3
1	B	454	ASP	2.3
1	B	496	GLN	2.3
1	B	462	ARG	2.3
1	B	532	CYS	2.2
1	B	535	SER	2.2
1	A	653	GLN	2.2
1	B	457	ILE	2.2
1	A	620	MET	2.1
1	A	652	GLY	2.1
1	A	689	MET	2.1
1	A	564	MET	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.

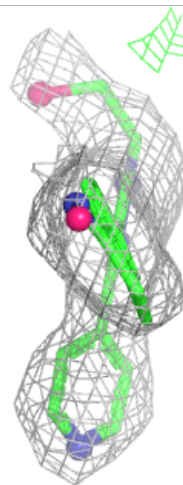
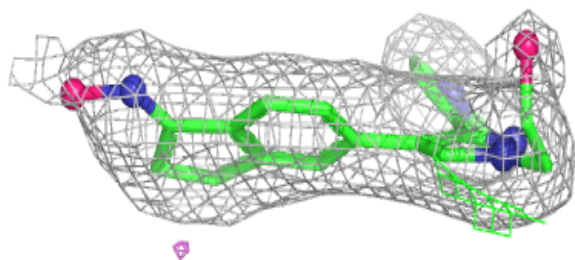
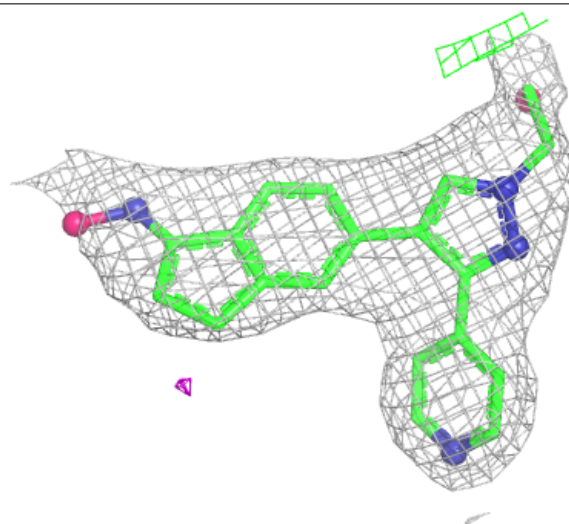
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	B	802	1/1	0.91	0.10	9,9,9,9	0
2	29L	B	801	25/25	0.92	0.13	43,50,59,76	0
2	29L	A	801	25/25	0.92	0.13	39,47,56,62	0

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.

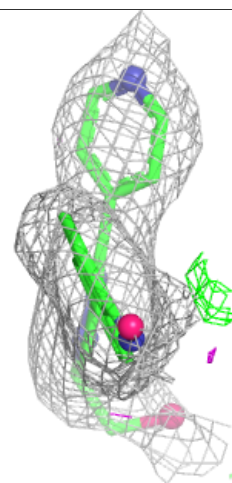
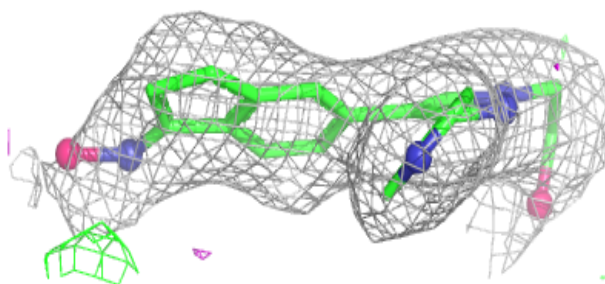
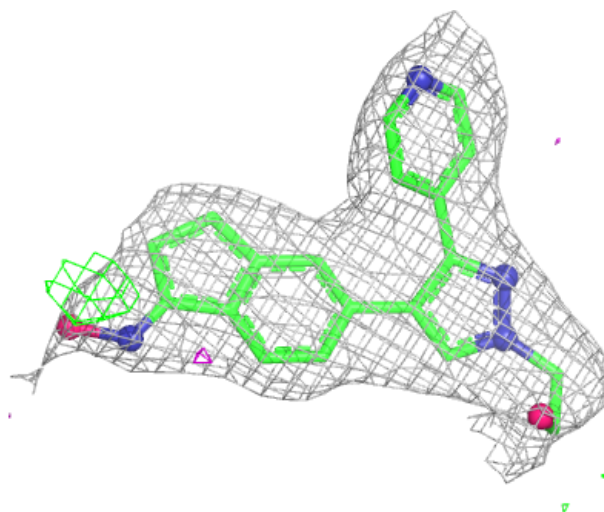
Electron density around 29L B 801:

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



Electron density around 29L A 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.