



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 4H58 / pdb_00004h58
Title : BRAF in complex with compound 3
Authors : Vasbinder, M.; Aquila, B.; Augustin, M.; Chueng, T.; Cook, D.; Drew, L.; Fauber, B.; Glossop, S.; Godin, R.; Grondine, M.; Hennessy, E.; Johannes, J.; Lee, S.; Lyne, P.; Moertl, M.; Omer, C.; Palakurthi, S.; Pontz, T.; Read, J.; Sha, L.; Shen, M.; Steinbacher, S.; Wang, H.; Wu, A.; Ye, M.; Bagal, B.
Deposited on : 2012-09-18
Resolution : 3.10 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](#) ①) were used in the production of this report:

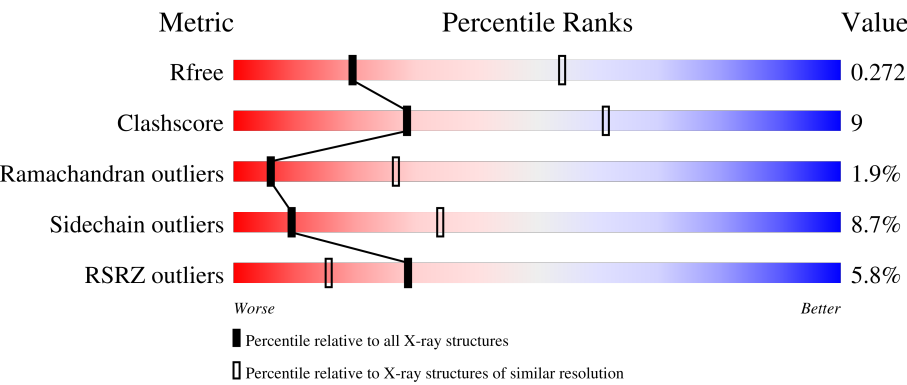
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	275	4% 67%25%... .
1	B	275	4% 65%26%. 5%
1	C	275	9% 77%20%..

2 Entry composition [i](#)

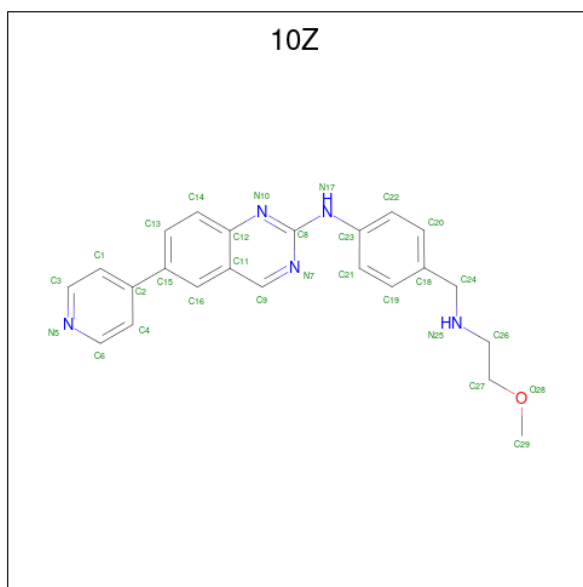
There are 4 unique types of molecules in this entry. The entry contains 6432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	263	Total	C	N	O	S	0	1	0
			2108	1351	366	378	13			
1	B	262	Total	C	N	O	S	0	1	0
			2102	1350	364	375	13			
1	C	272	Total	C	N	O	S	0	0	0
			2177	1396	381	387	13			

- Molecule 2 is N-(4-[(2-methoxyethyl)amino]methyl}phenyl)-6-(pyridin-4-yl)quinazolin-2-amine (CCD ID: 10Z) (formula: C₂₃H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	23	5	1		

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

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

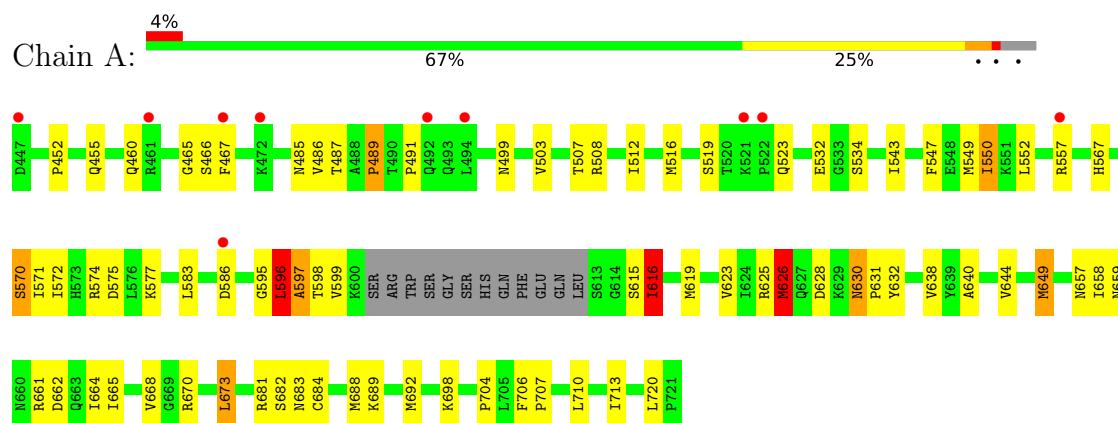
- Molecule 4 is water.

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

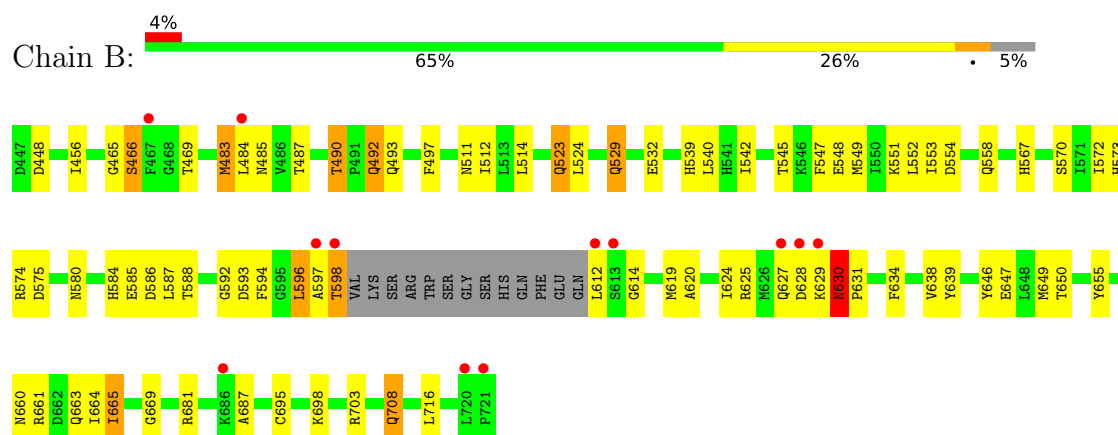
3 Residue-property plots [i](#)

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.

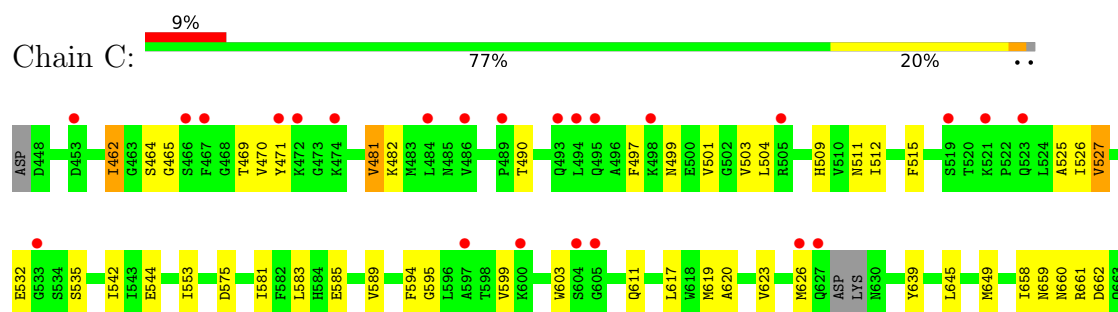
• Molecule 1: Serine/threonine-protein kinase B-raf



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	204.74Å 204.74Å 152.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 3.10 47.25 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.25-3.10) 95.2 (47.25-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.272 0.225 , 0.272	Depositor DCC
R_{free} test set	1412 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: 10Z, CL

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	0.63	0/2153	0.88	2/2906 (0.1%)
1	B	0.70	0/2148	0.90	1/2900 (0.0%)
1	C	0.62	0/2226	0.84	1/3005 (0.0%)
All	All	0.65	0/6527	0.88	4/8811 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	GLY	N-CA-C	7.34	116.89	110.21
1	A	616	ILE	CB-CA-C	-5.75	104.70	111.94
1	C	626	MET	N-CA-C	5.61	118.78	110.48
1	A	596	LEU	N-CA-C	-5.26	101.88	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	MET	Peptide

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	2108	0	2145	39	0
1	B	2102	0	2137	45	0
1	C	2177	0	2209	33	0
2	A	29	0	23	0	0
3	C	1	0	0	0	0
4	A	4	0	0	1	0
4	B	9	0	0	2	0
4	C	2	0	0	0	0
All	All	6432	0	6514	114	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 9.

All (114) 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:B:485:ASN:HD22	1:B:493:GLN:HE22	1.24	0.86
1:A:616:ILE:HG21	1:A:665:ILE:HG12	1.63	0.80
1:B:612:LEU:HD22	1:B:619:MET:HE1	1.69	0.73
1:B:573:HIS:O	1:B:574:ARG:HB2	1.90	0.71
1:B:574:ARG:NE	1:B:598:THR:HG21	2.08	0.68
1:B:575:ASP:O	1:B:580:ASN:ND2	2.27	0.68
1:B:490:THR:OG1	1:B:492:GLN:NE2	2.28	0.65
1:B:551:LYS:NZ	1:B:587:LEU:HA	2.12	0.65
1:A:487:THR:O	1:A:489:PRO:HD3	1.98	0.64
1:C:645:LEU:HB3	1:C:692:MET:HE2	1.83	0.61
1:A:649:MET:HG3	1:A:684:CYS:SG	2.42	0.60
1:A:658:ILE:HD12	1:A:673:LEU:HD11	1.83	0.60
1:B:708:GLN:C	1:B:708:GLN:HE21	2.11	0.59
1:A:508:ARG:HD3	1:C:515:PHE:O	2.03	0.58
1:B:448:ASP:HA	4:B:806:HOH:O	2.04	0.57
1:B:465:GLY:O	1:B:466:SER:C	2.48	0.56
1:A:575:ASP:HB2	1:A:596:LEU:HD23	1.88	0.56
1:B:664:ILE:O	1:B:665:ILE:C	2.49	0.55
1:B:573:HIS:NE2	1:B:593:ASP:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:LEU:HB2	4:B:807:HOH:O	2.06	0.55
1:B:660:ASN:HD22	1:B:663:GLN:HB2	1.71	0.55
1:B:594:PHE:HB3	1:B:597:ALA:HB3	1.89	0.54
1:B:551:LYS:HZ1	1:B:587:LEU:HA	1.72	0.54
1:C:462:ILE:HG13	1:C:470:VAL:HG12	1.89	0.54
1:A:557:ARG:HG3	1:A:713:ILE:HG22	1.90	0.54
1:B:598:THR:C	1:C:490:THR:HG22	2.33	0.54
1:A:550:ILE:HD12	1:A:720:LEU:HD23	1.90	0.53
1:A:567:HIS:HD2	1:A:571:ILE:O	1.92	0.53
1:A:625:ARG:O	1:A:626:MET:HB2	2.09	0.52
1:A:649:MET:HE2	1:A:688:MET:HG2	1.91	0.52
1:A:452:PRO:HB2	1:A:455:GLN:HE21	1.73	0.52
1:B:540:LEU:HD23	1:B:647:GLU:HB3	1.91	0.52
1:A:630:ASN:N	1:A:631:PRO:CD	2.72	0.52
1:B:547:PHE:HB2	1:B:552:LEU:HD21	1.93	0.51
1:A:630:ASN:CG	1:A:630:ASN:O	2.52	0.51
1:C:658:ILE:CD1	1:C:673:LEU:HD11	2.40	0.51
1:C:581:ILE:HG23	1:C:589:VAL:HG13	1.93	0.51
1:A:689:LYS:HA	1:A:692:MET:HE3	1.94	0.50
1:A:485:ASN:O	1:A:523:GLN:NE2	2.45	0.49
1:C:603:TRP:HD1	1:C:617:LEU:HD11	1.77	0.49
1:C:482:LYS:O	1:C:525:ALA:HA	2.12	0.49
1:C:603:TRP:HB3	1:C:661:ARG:HD2	1.95	0.49
1:C:619:MET:HE3	1:C:623:VAL:HG12	1.93	0.49
1:C:649:MET:HE3	1:C:688:MET:HE3	1.93	0.49
1:C:501:VAL:HG23	1:C:526:ILE:HD11	1.94	0.49
1:B:620:ALA:HA	1:B:639:TYR:CD2	2.48	0.49
1:B:484:LEU:HD22	1:B:497:PHE:HB2	1.94	0.49
1:A:507:THR:HB	1:A:512:ILE:HG21	1.93	0.49
1:C:532:GLU:O	1:C:585:GLU:N	2.45	0.49
1:B:584:HIS:CD2	1:B:585:GLU:HG3	2.48	0.48
1:A:516:MET:HE3	1:C:509:HIS:HA	1.95	0.48
1:C:504:LEU:HB3	1:C:515:PHE:HB2	1.94	0.48
1:B:695:CYS:O	1:B:703:ARG:HD2	2.13	0.48
1:A:596:LEU:O	1:A:597:ALA:HB2	2.14	0.48
1:C:511:ASN:HA	1:C:589:VAL:O	2.14	0.47
1:B:630:ASN:N	1:B:631:PRO:CD	2.78	0.47
1:B:554:ASP:O	1:B:558:GLN:HG3	2.15	0.47
1:A:616:ILE:HD11	1:A:661:ARG:HD2	1.96	0.46
1:B:511:ASN:O	1:B:512:ILE:HD13	2.16	0.46
1:A:547:PHE:HB2	1:A:552:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:ASN:O	1:C:664:ILE:HG13	2.15	0.46
1:A:662:ASP:HA	1:A:665:ILE:HD12	1.98	0.46
1:B:646:TYR:CE1	1:B:650:THR:HG21	2.51	0.46
1:B:625:ARG:NE	1:B:669:GLY:O	2.49	0.45
1:A:619:MET:HE3	1:A:623:VAL:HG12	1.98	0.45
1:C:481:VAL:HG13	1:C:527:VAL:HG13	1.98	0.45
1:C:649:MET:HE3	1:C:688:MET:HG2	1.96	0.45
1:A:625:ARG:O	1:A:626:MET:CB	2.65	0.45
1:A:572:ILE:HG22	1:A:574:ARG:HG3	1.98	0.45
1:B:567:HIS:O	1:B:570:SER:N	2.47	0.45
1:A:638:VAL:HG21	1:A:704:PRO:O	2.17	0.44
1:A:626:MET:HE2	1:A:631:PRO:HG3	1.99	0.44
1:C:649:MET:CG	1:C:692:MET:HE1	2.48	0.44
1:B:634:PHE:O	1:B:638:VAL:HG23	2.17	0.44
1:C:658:ILE:HD12	1:C:673:LEU:HD11	2.00	0.43
1:C:664:ILE:O	1:C:668:VAL:HG23	2.19	0.43
1:C:497:PHE:C	1:C:499:ASN:N	2.77	0.43
1:B:523:GLN:HA	1:B:523:GLN:HE21	1.83	0.43
1:A:664:ILE:O	1:A:668:VAL:HG23	2.19	0.43
1:B:529:GLN:HE21	1:B:529:GLN:HB2	1.68	0.43
1:B:548:GLU:O	1:B:551:LYS:N	2.52	0.43
1:C:465:GLY:HA3	1:C:470:VAL:HG23	2.00	0.43
1:B:574:ARG:HD2	1:B:596:LEU:O	2.19	0.43
1:A:706:PHE:N	1:A:707:PRO:HD2	2.34	0.43
1:C:499:ASN:O	1:C:503:VAL:HG23	2.19	0.43
1:B:619:MET:HE2	1:B:624:ILE:HG12	2.01	0.42
1:A:574:ARG:HG2	1:A:632:TYR:CD1	2.54	0.42
1:A:659:ASN:OD1	1:A:659:ASN:C	2.63	0.42
1:B:629:LYS:C	1:B:631:PRO:CD	2.92	0.42
1:A:549:MET:HB2	1:A:683:ASN:HD21	1.84	0.42
1:A:570:SER:O	1:A:599:VAL:HG13	2.19	0.42
1:B:539:HIS:O	1:B:545:THR:N	2.53	0.42
1:B:514:LEU:HB3	1:B:529:GLN:HG2	2.01	0.42
1:C:620:ALA:HA	1:C:639:TYR:CE1	2.55	0.42
1:C:617:LEU:HD12	1:C:617:LEU:H	1.84	0.42
1:B:483:MET:HE2	1:B:483:MET:HB3	1.89	0.42
1:B:629:LYS:C	1:B:631:PRO:HD2	2.45	0.41
1:C:659:ASN:OD1	1:C:659:ASN:C	2.63	0.41
1:B:614:GLY:H	1:B:661:ARG:HH22	1.69	0.41
1:C:542:ILE:CD1	1:C:599:VAL:HG21	2.49	0.41
1:C:542:ILE:HD11	1:C:599:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:PHE:O	1:C:595:GLY:C	2.63	0.41
1:C:662:ASP:HA	1:C:665:ILE:HD12	2.01	0.41
1:A:574:ARG:HD3	1:A:598:THR:HG22	2.03	0.41
1:B:574:ARG:HE	1:B:598:THR:HG21	1.83	0.41
1:A:465:GLY:O	1:A:466:SER:C	2.63	0.41
1:A:499:ASN:O	1:A:503:VAL:HG23	2.21	0.41
1:B:586:ASP:O	1:B:587:LEU:HD12	2.21	0.41
1:A:640:ALA:O	1:A:644:VAL:HG23	2.21	0.40
1:A:657:ASN:OD1	1:A:657:ASN:N	2.54	0.40
1:B:614:GLY:N	1:B:661:ARG:HH22	2.19	0.40
1:B:687:ALA:HB3	1:B:716:LEU:HD22	2.03	0.40
1:A:616:ILE:HD12	4:A:902:HOH:O	2.22	0.40
1:C:470:VAL:HA	1:C:481:VAL:O	2.22	0.40

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	260/275 (94%)	229 (88%)	23 (9%)	8 (3%)	3	18
1	B	259/275 (94%)	229 (88%)	25 (10%)	5 (2%)	6	27
1	C	268/275 (98%)	240 (90%)	26 (10%)	2 (1%)	18	49
All	All	787/825 (95%)	698 (89%)	74 (9%)	15 (2%)	6	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	MET
1	A	628	ASP
1	B	466	SER
1	A	489	PRO

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Mol	Chain	Res	Type
1	A	586	ASP
1	A	491	PRO
1	A	597	ALA
1	B	549	MET
1	B	628	ASP
1	C	611	GLN
1	A	577	LYS
1	B	665	ILE
1	C	575	ASP
1	A	595	GLY
1	B	630	ASN

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	232/242 (96%)	211 (91%)	21 (9%)	9	32
1	B	231/242 (96%)	208 (90%)	23 (10%)	7	29
1	C	239/242 (99%)	222 (93%)	17 (7%)	13	41
All	All	702/726 (97%)	641 (91%)	61 (9%)	9	34

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	GLN
1	A	467	PHE
1	A	486	VAL
1	A	519	SER
1	A	532	GLU
1	A	534	SER
1	A	543	ILE
1	A	550	ILE
1	A	570	SER
1	A	583	LEU
1	A	596	LEU

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Mol	Chain	Res	Type
1	A	615	SER
1	A	616	ILE
1	A	630	ASN
1	A	649	MET
1	A	670	ARG
1	A	673	LEU
1	A	681	ARG
1	A	682	SER
1	A	698	LYS
1	A	710	LEU
1	B	456	ILE
1	B	469	THR
1	B	483	MET
1	B	487	THR
1	B	490	THR
1	B	492	GLN
1	B	523	GLN
1	B	524	LEU
1	B	529	GLN
1	B	532	GLU
1	B	542	ILE
1	B	553	ILE
1	B	572	ILE
1	B	588	THR
1	B	596	LEU
1	B	598	THR
1	B	627	GLN
1	B	630	ASN
1	B	649	MET
1	B	655	TYR
1	B	681	ARG
1	B	698	LYS
1	B	708	GLN
1	C	462	ILE
1	C	464	SER
1	C	469	THR
1	C	471	TYR
1	C	481	VAL
1	C	512	ILE
1	C	527	VAL
1	C	535	SER
1	C	544	GLU

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Mol	Chain	Res	Type
1	C	553	ILE
1	C	583	LEU
1	C	664	ILE
1	C	673	LEU
1	C	681	ARG
1	C	682	SER
1	C	715	LEU
1	C	720	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	A	460	GLN
1	A	485	ASN
1	A	523	GLN
1	A	579	ASN
1	A	580	ASN
1	A	627	GLN
1	B	455	GLN
1	B	492	GLN
1	B	493	GLN
1	B	511	ASN
1	B	529	GLN
1	B	652	GLN
1	B	657	ASN
1	B	660	ASN
1	B	663	GLN
1	B	708	GLN
1	C	485	ASN
1	C	492	GLN
1	C	538	HIS
1	C	567	HIS
1	C	652	GLN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	10Z	A	801	-	32,32,32	1.46	5 (15%)	42,42,42	1.96	9 (21%)

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	10Z	A	801	-	-	2/14/14/14	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	10Z	C9-N7	4.19	1.39	1.32
2	A	801	10Z	C8-N7	3.21	1.39	1.34
2	A	801	10Z	C8-N17	3.10	1.43	1.36
2	A	801	10Z	C14-C12	-2.06	1.38	1.41
2	A	801	10Z	C6-N5	2.03	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	10Z	N7-C8-N10	-9.01	117.62	126.41
2	A	801	10Z	C9-N7-C8	4.46	121.82	115.81
2	A	801	10Z	C8-N10-C12	3.21	120.62	115.54
2	A	801	10Z	C11-C9-N7	-2.41	120.37	124.25
2	A	801	10Z	C1-C3-N5	-2.31	119.65	123.60
2	A	801	10Z	C23-N17-C8	2.22	135.38	129.38
2	A	801	10Z	C16-C11-C12	2.09	120.98	118.31
2	A	801	10Z	C21-C23-N17	-2.03	113.75	120.61
2	A	801	10Z	C22-C23-N17	2.00	127.40	120.61

There are no chirality outliers.

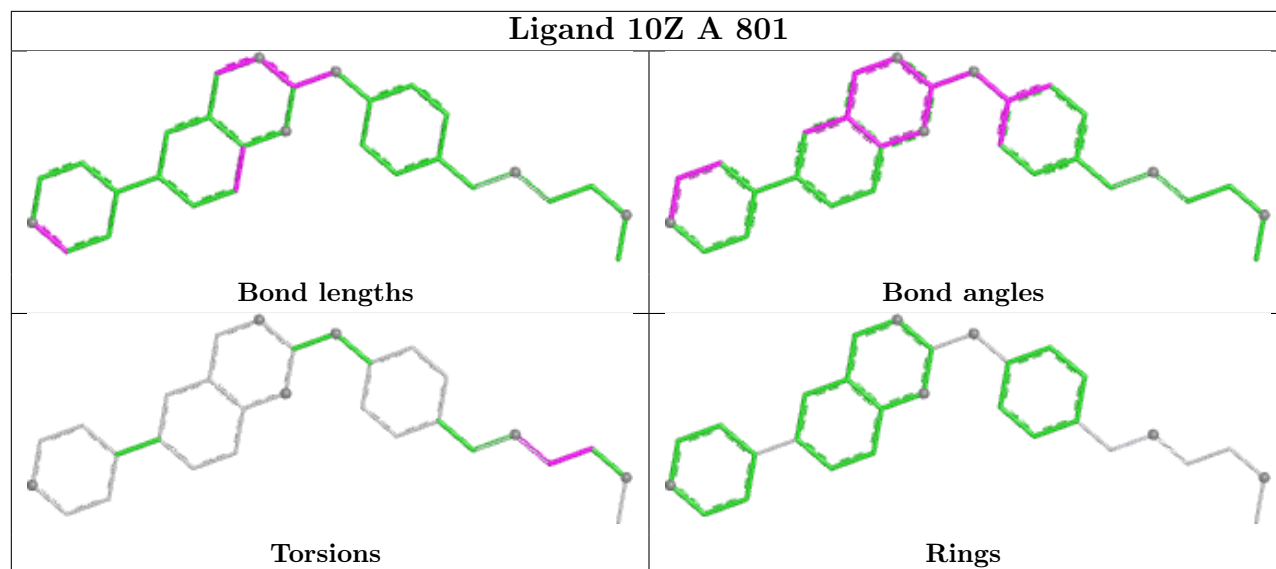
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	10Z	N25-C26-C27-O28
2	A	801	10Z	C27-C26-N25-C24

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 [i](#)

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	263/275 (95%)	0.19	10 (3%)	44 25	32, 69, 106, 117	19 (7%)
1	B	262/275 (95%)	0.07	12 (4%)	37 20	21, 58, 81, 95	14 (5%)
1	C	272/275 (98%)	0.50	24 (8%)	15 9	44, 76, 106, 111	23 (8%)
All	All	797/825 (96%)	0.26	46 (5%)	29 16	21, 68, 101, 117	56 (7%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	626	MET	5.7
1	C	484	LEU	5.5
1	C	494	LEU	4.7
1	C	519	SER	4.4
1	C	597	ALA	4.0
1	C	521	LYS	3.9
1	A	467	PHE	3.7
1	B	629	LYS	3.6
1	C	600	LYS	3.6
1	C	523	GLN	3.5
1	B	627	GLN	3.5
1	C	472	LYS	3.4
1	A	461	ARG	3.3
1	C	467	PHE	3.3
1	A	521	LYS	3.1
1	B	467	PHE	2.9
1	C	495	GLN	2.9
1	B	613	SER	2.8
1	C	471	TYR	2.6
1	A	494	LEU	2.5
1	C	605	GLY	2.5
1	C	604	SER	2.5
1	B	597	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	466	SER	2.4
1	B	612	LEU	2.3
1	A	557	ARG	2.3
1	A	586	ASP	2.3
1	C	486	VAL	2.3
1	C	505	ARG	2.3
1	B	598	THR	2.3
1	B	721	PRO	2.2
1	B	484	LEU	2.2
1	A	522	PRO	2.2
1	B	720	LEU	2.2
1	C	489	PRO	2.2
1	B	628	ASP	2.2
1	C	474	LYS	2.2
1	A	447	ASP	2.2
1	C	453	ASP	2.1
1	A	492	GLN	2.1
1	C	627	GLN	2.1
1	A	472	LYS	2.1
1	C	533	GLY	2.1
1	C	493	GLN	2.0
1	B	686	LYS	2.0
1	C	498	LYS	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](#)

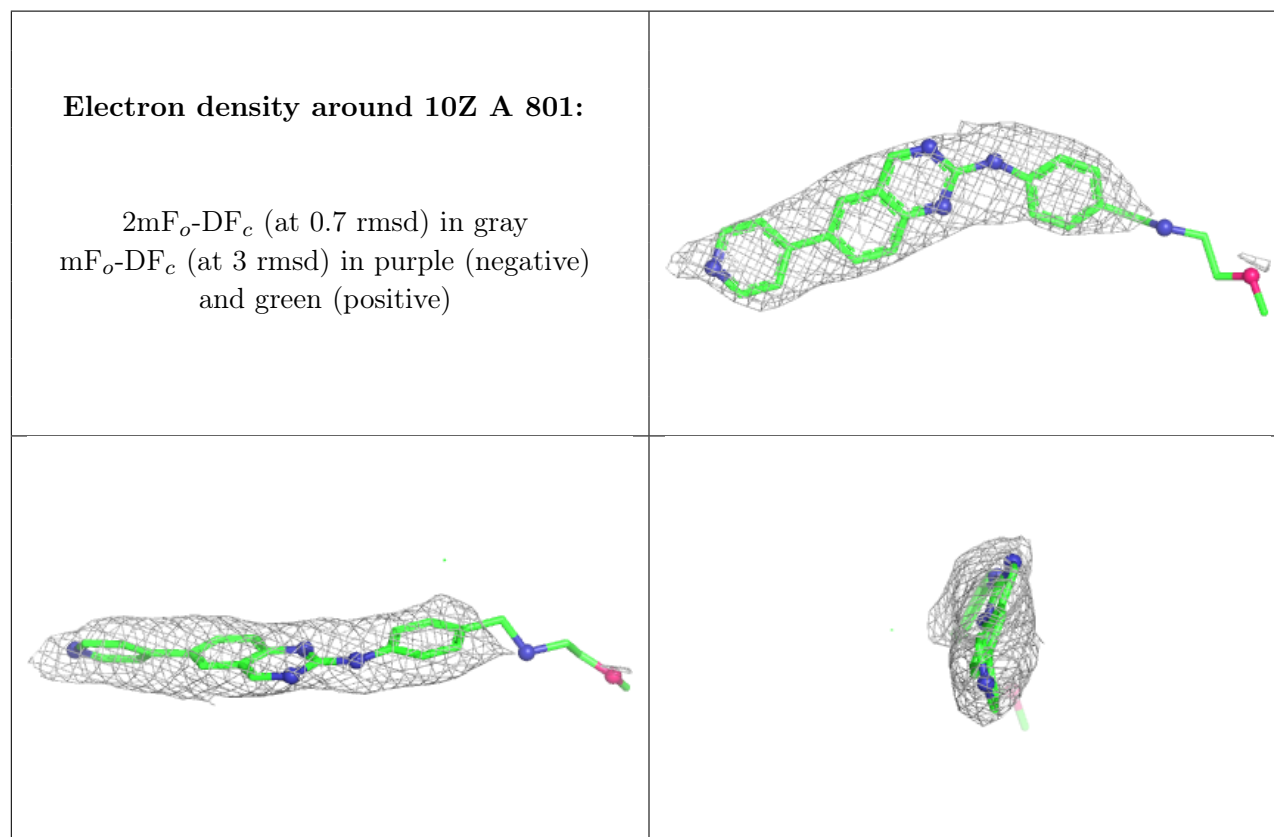
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	10Z	A	801	29/29	0.92	0.16	87,88,97,98	0
3	CL	C	801	1/1	0.94	0.11	72,72,72,72	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.