



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 AM UTC

PDB ID : 3OG7 / pdb_00003og7
Title : B-Raf Kinase V600E oncogenic mutant in complex with PLX4032
Authors : Zhang, Y.; Zhang, K.Y.; Zhang, C.
Deposited on : 2010-08-16
Resolution : 2.45 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

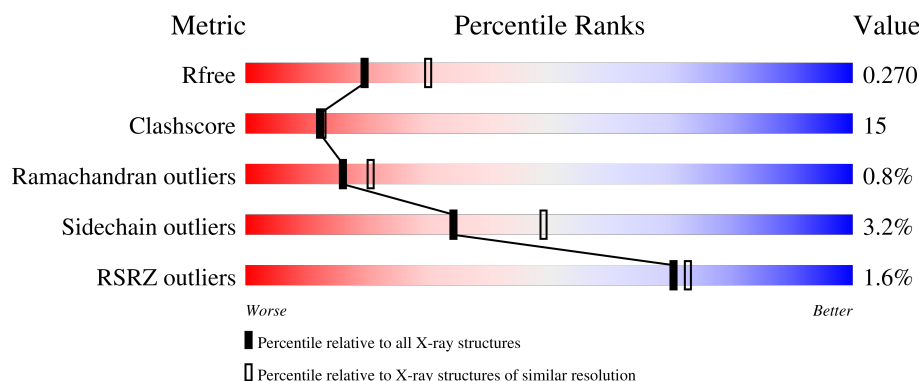
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	289	% 58% 27% • 15%
1	B	289	2% 55% 31% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4100 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 AKAP9-BRAF fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1974	1253	353	356	12			
1	B	254	Total	C	N	O	S	0	0	0
			2028	1286	361	369	12			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	MET	-	expression tag	UNP Q5IBP5
A	433	LYS	-	expression tag	UNP Q5IBP5
A	434	LYS	-	expression tag	UNP Q5IBP5
A	435	GLY	-	expression tag	UNP Q5IBP5
A	436	HIS	-	expression tag	UNP Q5IBP5
A	437	HIS	-	expression tag	UNP Q5IBP5
A	438	HIS	-	expression tag	UNP Q5IBP5
A	439	HIS	-	expression tag	UNP Q5IBP5
A	440	HIS	-	expression tag	UNP Q5IBP5
A	441	HIS	-	expression tag	UNP Q5IBP5
A	442	GLY	-	expression tag	UNP Q5IBP5
A	443	SER	-	expression tag	UNP Q5IBP5
A	444	ARG	-	expression tag	UNP Q5IBP5
A	445	ASP	-	expression tag	UNP Q5IBP5
A	446	ALA	-	expression tag	UNP Q5IBP5
A	447	ALA	-	expression tag	UNP Q5IBP5
A	448	ASP	-	expression tag	UNP Q5IBP5
A	522	ALA	LYS	engineered mutation	UNP Q5IBP5
A	543	ALA	ILE	engineered mutation	UNP Q5IBP5
A	544	SER	ILE	engineered mutation	UNP Q5IBP5
A	551	LYS	ILE	engineered mutation	UNP Q5IBP5
A	562	ARG	GLN	engineered mutation	UNP Q5IBP5
A	588	ASN	LEU	engineered mutation	UNP Q5IBP5
A	600	GLU	VAL	variant	UNP Q5IBP5
A	630	SER	LYS	engineered mutation	UNP Q5IBP5

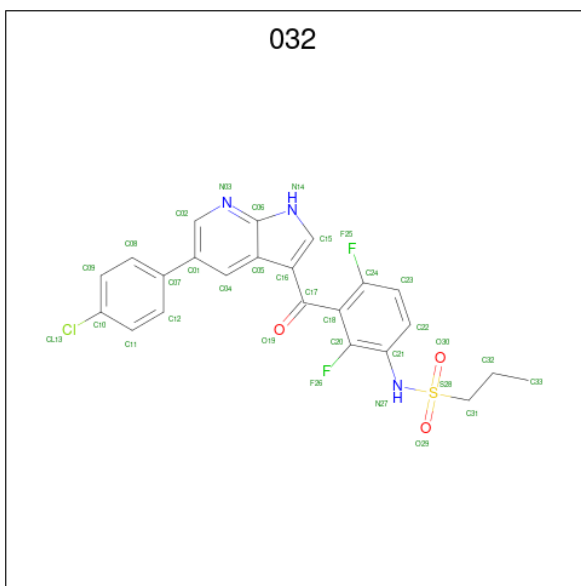
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Chain	Residue	Modelled	Actual	Comment	Reference
A	667	GLU	PHE	engineered mutation	UNP Q5IBP5
A	673	SER	TYR	engineered mutation	UNP Q5IBP5
A	688	ARG	ALA	engineered mutation	UNP Q5IBP5
A	706	SER	LEU	engineered mutation	UNP Q5IBP5
A	709	ARG	GLN	engineered mutation	UNP Q5IBP5
A	713	GLU	SER	engineered mutation	UNP Q5IBP5
A	716	GLU	LEU	engineered mutation	UNP Q5IBP5
A	720	GLU	SER	engineered mutation	UNP Q5IBP5
B	432	MET	-	expression tag	UNP Q5IBP5
B	433	LYS	-	expression tag	UNP Q5IBP5
B	434	LYS	-	expression tag	UNP Q5IBP5
B	435	GLY	-	expression tag	UNP Q5IBP5
B	436	HIS	-	expression tag	UNP Q5IBP5
B	437	HIS	-	expression tag	UNP Q5IBP5
B	438	HIS	-	expression tag	UNP Q5IBP5
B	439	HIS	-	expression tag	UNP Q5IBP5
B	440	HIS	-	expression tag	UNP Q5IBP5
B	441	HIS	-	expression tag	UNP Q5IBP5
B	442	GLY	-	expression tag	UNP Q5IBP5
B	443	SER	-	expression tag	UNP Q5IBP5
B	444	ARG	-	expression tag	UNP Q5IBP5
B	445	ASP	-	expression tag	UNP Q5IBP5
B	446	ALA	-	expression tag	UNP Q5IBP5
B	447	ALA	-	expression tag	UNP Q5IBP5
B	448	ASP	-	expression tag	UNP Q5IBP5
B	522	ALA	LYS	engineered mutation	UNP Q5IBP5
B	543	ALA	ILE	engineered mutation	UNP Q5IBP5
B	544	SER	ILE	engineered mutation	UNP Q5IBP5
B	551	LYS	ILE	engineered mutation	UNP Q5IBP5
B	562	ARG	GLN	engineered mutation	UNP Q5IBP5
B	588	ASN	LEU	engineered mutation	UNP Q5IBP5
B	600	GLU	VAL	variant	UNP Q5IBP5
B	630	SER	LYS	engineered mutation	UNP Q5IBP5
B	667	GLU	PHE	engineered mutation	UNP Q5IBP5
B	673	SER	TYR	engineered mutation	UNP Q5IBP5
B	688	ARG	ALA	engineered mutation	UNP Q5IBP5
B	706	SER	LEU	engineered mutation	UNP Q5IBP5
B	709	ARG	GLN	engineered mutation	UNP Q5IBP5
B	713	GLU	SER	engineered mutation	UNP Q5IBP5
B	716	GLU	LEU	engineered mutation	UNP Q5IBP5
B	720	GLU	SER	engineered mutation	UNP Q5IBP5

- Molecule 2 is N-(3-{[5-(4-chlorophenyl)-1H-pyrrolo[2,3-b]pyridin-3-yl]carbonyl}-2,4-difluoro

phenyl)propane-1-sulfonamide (CCD ID: 032) (formula: $C_{23}H_{18}ClF_2N_3O_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	N	O	S		
2	A	1	33	23	1	2	3	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	24	Total O 24 24	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.77Å 104.42Å 110.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.30 – 2.45 21.30 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (21.30-2.45) 99.3 (21.30-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.212 , 0.258 0.226 , 0.270	Depositor DCC
R_{free} test set	1580 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	0.086 for -h,l,k	Depositor
Outliers	0 of 31341 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4100	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: 032

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	0.28	0/2014	0.71	0/2712
1	B	0.31	0/2069	0.73	1/2788 (0.0%)
All	All	0.30	0/4083	0.72	1/5500 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	594	ASP	N-CA-C	-5.01	104.48	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	522	ALA	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	1974	0	1985	54	0
1	B	2028	0	2041	72	0
2	A	33	0	18	5	0
3	A	41	0	0	1	0
3	B	24	0	0	2	0
All	All	4100	0	4044	125	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 15.

All (125) 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:491:THR:H	1:B:494:GLN:HE21	1.12	0.97
1:B:454:ASP:CG	1:B:523:PRO:HG3	2.02	0.85
1:B:491:THR:H	1:B:494:GLN:NE2	1.77	0.83
1:B:623:GLU:OE1	1:B:701:ARG:HB3	1.79	0.81
1:A:594:ASP:H	2:A:1:032:HN27	1.26	0.80
1:B:468:PHE:HB2	1:B:483:LYS:HD3	1.65	0.78
1:A:706:SER:O	1:A:710:ILE:HG13	1.89	0.72
1:B:491:THR:N	1:B:494:GLN:HE21	1.88	0.70
1:A:620:MET:HE3	1:A:624:VAL:HG12	1.74	0.70
1:B:661:ASN:HD22	1:B:664:GLN:H	1.42	0.68
1:B:688:ARG:HE	1:B:717:LEU:CB	2.08	0.67
1:A:509:ARG:HD3	1:B:516:PHE:O	1.96	0.66
1:A:650:MET:HE3	1:A:689:MET:HG2	1.78	0.66
1:B:688:ARG:HG2	1:B:691:ARG:NH1	2.12	0.65
1:B:661:ASN:HD21	1:B:663:ASP:HB2	1.63	0.64
1:B:537:LEU:HD21	1:B:649:LEU:HD21	1.80	0.64
1:B:688:ARG:HE	1:B:717:LEU:HB2	1.63	0.64
1:A:678:LEU:HB3	1:A:690:LYS:HE3	1.79	0.64
1:A:594:ASP:N	2:A:1:032:HN27	1.93	0.63
1:A:516:PHE:O	1:B:509:ARG:HD3	1.99	0.63
1:A:554:ILE:HD11	1:A:686:PRO:HG2	1.81	0.62
1:B:617:ILE:HA	1:B:620:MET:HG3	1.81	0.62
1:B:560:THR:HG23	1:B:592:ILE:HD11	1.80	0.62
1:A:568:HIS:CG	1:A:635:PHE:HD2	2.18	0.62
1:A:709:ARG:O	1:A:713:GLU:HG2	1.99	0.61
1:A:514:LEU:HD23	2:A:1:032:H33B	1.83	0.60
1:B:548:PHE:CD2	1:B:552:LYS:HD3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD22	2:A:1:032:H32A	1.82	0.60
1:B:468:PHE:CZ	1:B:498:PHE:HA	2.37	0.60
1:A:664:GLN:HG2	1:A:668:MET:HE2	1.84	0.59
1:B:541:LEU:HD21	1:B:649:LEU:HD23	1.84	0.59
1:A:574:HIS:CD2	1:A:595:PHE:HB3	2.37	0.59
1:A:522:ALA:HA	1:A:523:PRO:C	2.27	0.58
1:A:635:PHE:O	1:A:639:VAL:HG23	2.05	0.56
1:B:576:ASP:HB2	1:B:597:LEU:HD12	1.88	0.56
1:B:661:ASN:HB3	1:B:664:GLN:HE21	1.71	0.55
1:A:541:LEU:HD23	1:A:648:GLU:HB3	1.88	0.55
1:B:667:GLU:O	1:B:671:ARG:HB2	2.07	0.54
1:B:625:ILE:HG23	1:B:666:ILE:HG23	1.90	0.54
1:B:651:THR:HG22	1:B:681:VAL:HA	1.88	0.54
1:A:617:ILE:HD13	1:A:662:ARG:HG3	1.90	0.54
1:A:720:GLU:H	1:A:720:GLU:CD	2.16	0.54
1:B:585:HIS:CE1	1:B:586:GLU:HG3	2.43	0.53
1:A:578:LYS:HD2	1:A:580:ASN:HD21	1.74	0.52
1:B:707:PHE:HA	1:B:710:ILE:HB	1.91	0.52
1:A:617:ILE:CD1	1:A:662:ARG:HG3	2.39	0.52
1:B:700:LYS:HD2	1:B:703:GLU:OE1	2.10	0.52
1:A:668:MET:HE3	1:A:674:LEU:HD22	1.92	0.52
1:B:558:ARG:HD2	1:B:715:GLU:OE2	2.10	0.52
1:B:471:VAL:HA	1:B:482:VAL:O	2.11	0.51
1:B:684:ASN:H	1:B:684:ASN:ND2	2.08	0.51
1:B:681:VAL:HG21	1:B:690:LYS:HD2	1.95	0.49
1:B:684:ASN:ND2	1:B:684:ASN:N	2.60	0.49
1:A:664:GLN:O	1:A:668:MET:HG3	2.13	0.49
1:B:688:ARG:HE	1:B:717:LEU:HB3	1.78	0.49
1:A:451:GLU:HB2	1:A:519:TYR:CZ	2.48	0.49
1:A:619:TRP:HA	1:A:644:ILE:HG13	1.94	0.49
1:B:507:LYS:O	1:B:570:LYS:HE2	2.12	0.49
1:B:550:MET:HE3	1:B:685:CYS:HA	1.95	0.49
1:B:585:HIS:ND1	1:B:586:GLU:HG3	2.28	0.48
1:B:623:GLU:OE1	1:B:704:ARG:NH2	2.46	0.48
1:A:641:ALA:O	1:A:645:VAL:HG23	2.13	0.48
1:B:688:ARG:HG2	1:B:691:ARG:HH12	1.78	0.48
1:B:650:MET:O	1:B:682:ARG:HG3	2.13	0.48
1:B:586:GLU:O	1:B:587:ASP:HB2	2.13	0.48
1:B:520:SER:HB3	1:B:526:ALA:HB3	1.95	0.48
1:B:550:MET:O	1:B:554:ILE:HG12	2.14	0.48
1:B:661:ASN:HB3	1:B:664:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:LYS:O	1:B:691:ARG:HB2	2.14	0.47
1:A:574:HIS:O	1:A:575:ARG:HB2	2.14	0.47
1:B:490:PRO:HA	1:B:494:GLN:NE2	2.29	0.47
1:B:623:GLU:HG2	3:B:25:HOH:O	2.15	0.47
1:B:661:ASN:HD22	1:B:664:GLN:HG3	1.79	0.47
1:B:578:LYS:HD2	1:B:580:ASN:HB3	1.96	0.46
1:B:501:GLU:HA	1:B:504:VAL:HG12	1.96	0.46
1:A:540:HIS:CD2	1:A:584:LEU:HD12	2.50	0.46
1:A:704:ARG:HA	1:A:705:PRO:HD3	1.80	0.46
1:B:550:MET:HE1	1:B:650:MET:SD	2.56	0.46
1:B:573:ILE:HG22	1:B:575:ARG:HG3	1.97	0.46
1:A:568:HIS:CD2	1:A:635:PHE:HD2	2.32	0.46
1:A:476:TRP:HB3	1:A:480:VAL:HG11	1.97	0.46
1:A:714:ILE:HA	1:A:717:LEU:HG	1.99	0.45
1:A:541:LEU:HD21	1:A:649:LEU:HD23	1.98	0.45
1:A:459:VAL:HG21	1:A:484:MET:HE1	1.99	0.45
1:B:465:SER:HA	1:B:469:GLY:O	2.17	0.44
1:A:539:HIS:O	1:A:543:ALA:HB3	2.17	0.44
1:B:495:LEU:HG	1:B:499:LYS:HE2	2.00	0.44
1:B:574:HIS:O	1:B:575:ARG:HB2	2.17	0.44
1:B:637:SER:HB2	3:B:49:HOH:O	2.17	0.44
1:A:710:ILE:O	1:A:714:ILE:HG13	2.17	0.44
1:A:714:ILE:O	1:A:718:ALA:HB2	2.17	0.44
1:B:463:ILE:HD12	1:B:463:ILE:N	2.32	0.44
1:B:690:LYS:HA	1:B:693:MET:HE3	2.00	0.44
1:B:707:PHE:N	1:B:708:PRO:CD	2.81	0.44
1:A:582:ILE:HG23	1:A:590:VAL:HG13	1.98	0.43
1:B:468:PHE:CD1	1:B:483:LYS:HD3	2.53	0.43
1:A:506:ARG:NH2	3:A:60:HOH:O	2.42	0.43
1:B:705:PRO:HB3	1:B:709:ARG:HH11	1.83	0.43
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.88	0.43
1:B:550:MET:HE3	1:B:685:CYS:CA	2.49	0.43
1:A:642:PHE:CE2	1:A:646:LEU:HD21	2.53	0.43
1:B:661:ASN:ND2	1:B:664:GLN:H	2.15	0.43
1:B:468:PHE:HZ	1:B:497:ALA:C	2.28	0.42
1:A:707:PHE:N	1:A:708:PRO:CD	2.83	0.42
1:B:664:GLN:O	1:B:668:MET:HG3	2.20	0.42
1:B:623:GLU:H	1:B:623:GLU:HG3	1.40	0.42
1:B:578:LYS:HB2	1:B:619:TRP:CE2	2.55	0.42
1:B:698:LYS:O	1:B:704:ARG:NH1	2.50	0.42
1:B:717:LEU:HD12	1:B:717:LEU:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:032:O30	2:A:1:032:H22	2.20	0.41
1:A:631:ASN:N	1:A:632:PRO:HD3	2.35	0.41
1:A:512:ASN:HA	1:A:590:VAL:O	2.21	0.41
1:B:486:ASN:HA	1:B:524:GLN:NE2	2.35	0.41
1:A:462:ARG:NH1	1:A:465:SER:OG	2.48	0.41
1:A:700:LYS:HD2	1:A:703:GLU:OE1	2.19	0.41
1:A:718:ALA:O	1:A:719:ARG:C	2.63	0.41
1:A:489:ALA:HA	1:A:490:PRO:HD3	1.73	0.41
1:A:622:PRO:O	1:A:626:ARG:HG2	2.21	0.41
1:B:624:VAL:HA	1:B:632:PRO:HB2	2.03	0.41
1:A:619:TRP:CD1	1:A:644:ILE:HB	2.56	0.41
1:A:459:VAL:HG21	1:A:484:MET:CE	2.51	0.40
1:A:513:ILE:O	1:A:514:LEU:C	2.65	0.40
1:A:662:ARG:O	1:A:666:ILE:HG13	2.21	0.40
1:B:635:PHE:O	1:B:639:VAL:HG23	2.21	0.40
1:B:510:HIS:HB3	1:B:513:ILE:HG12	2.03	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	239/289 (83%)	225 (94%)	13 (5%)	1 (0%)	30	37
1	B	248/289 (86%)	234 (94%)	11 (4%)	3 (1%)	10	11
All	All	487/578 (84%)	459 (94%)	24 (5%)	4 (1%)	16	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	522	ALA
1	B	523	PRO

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Mol	Chain	Res	Type
1	B	595	PHE
1	A	523	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	215/251 (86%)	210 (98%)	5 (2%)	44	59
1	B	221/251 (88%)	212 (96%)	9 (4%)	27	40
All	All	436/502 (87%)	422 (97%)	14 (3%)	34	49

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

Mol	Chain	Res	Type
1	A	465	SER
1	A	521	THR
1	A	533	GLU
1	A	580	ASN
1	A	681	VAL
1	B	458	THR
1	B	484	MET
1	B	502	VAL
1	B	583	PHE
1	B	623	GLU
1	B	637	SER
1	B	684	ASN
1	B	691	ARG
1	B	699	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	540	HIS

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Mol	Chain	Res	Type
1	A	580	ASN
1	B	477	HIS
1	B	494	GLN
1	B	524	GLN
1	B	581	ASN
1	B	653	GLN
1	B	661	ASN
1	B	664	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](#)

1 ligand is 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	$\# Z > 2$
2	032	A	1	-	36,36,36	1.08	1 (2%)	48,53,53	1.25	4 (8%)

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	032	A	1	-	-	0/21/21/21	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	032	S28-N27	4.70	1.72	1.62

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	032	C24-C18-C20	3.38	118.98	115.66
2	A	1	032	C31-S28-N27	-2.80	102.74	106.72
2	A	1	032	C20-C21-N27	-2.17	118.22	120.73
2	A	1	032	O29-S28-C31	-2.04	104.62	107.86

There are no chirality outliers.

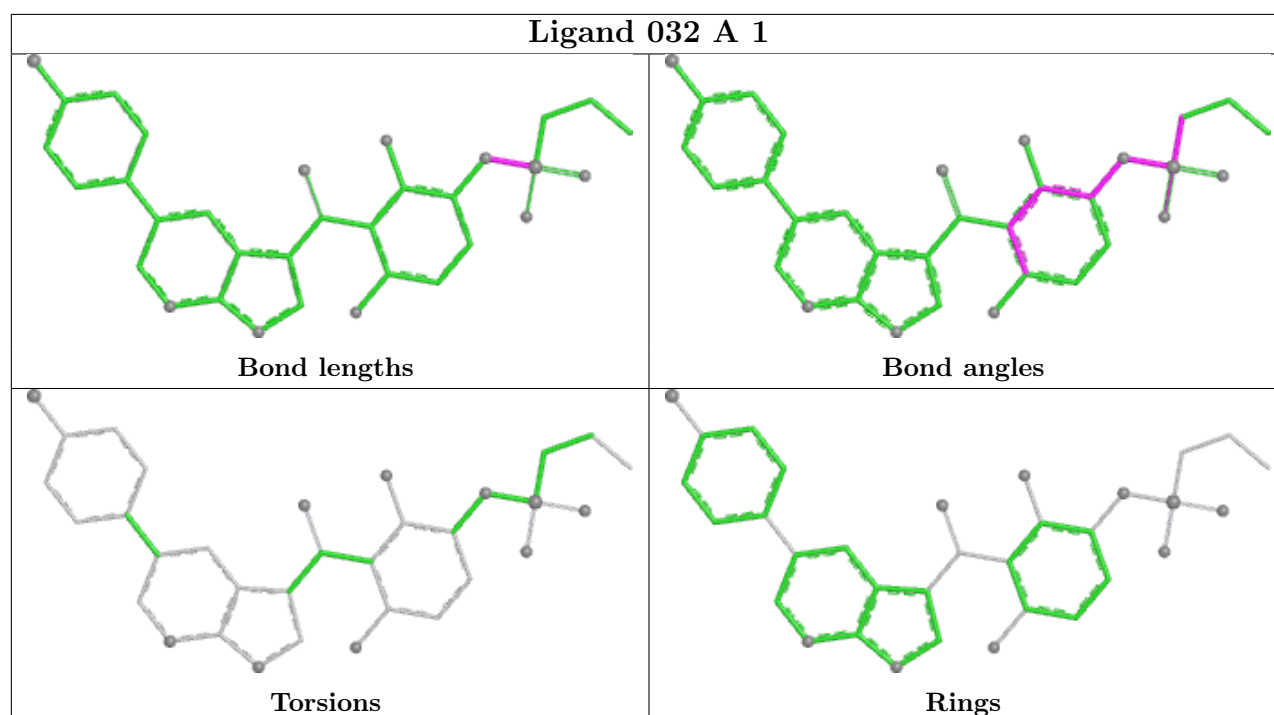
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	032	5	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	247/289 (85%)	0.09	3 (1%) 76 78	28, 58, 105, 156	0
1	B	254/289 (87%)	0.15	5 (1%) 65 66	25, 64, 107, 170	0
All	All	501/578 (86%)	0.12	8 (1%) 70 73	25, 61, 106, 170	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	PHE	3.0
1	B	599	THR	2.7
1	B	688	ARG	2.3
1	A	467	SER	2.3
1	B	583	PHE	2.3
1	B	615	GLY	2.1
1	A	543	ALA	2.1
1	A	544	SER	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.

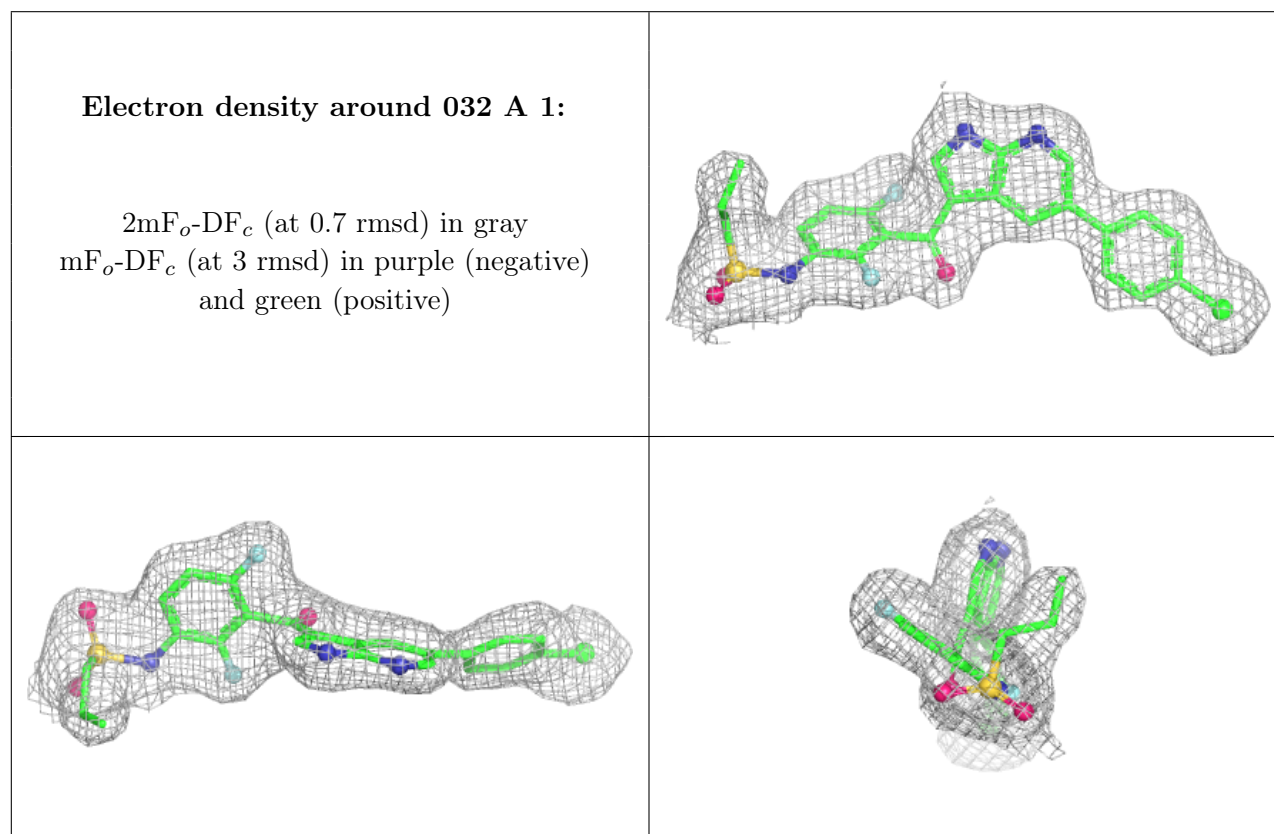
6.4 Ligands [i](#)

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
2	032	A	1	33/33	0.97	0.07	24,42,58,67	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.