



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:14 AM UTC

PDB ID : 1000 / pdb_000010oo
Title : FGFR2 mutant D650V with compound 4 (AZD3463)
Authors : Hoffman, I.D.; Nelson, K.J.
Deposited on : 2026-01-29
Resolution : 1.85 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

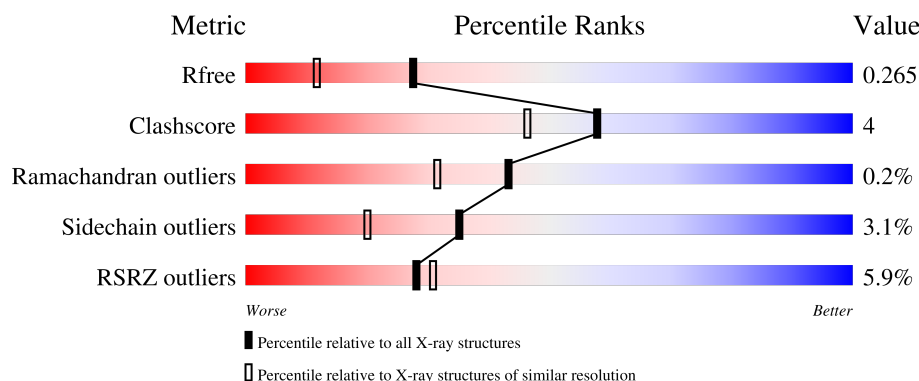
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	324	 5% 71% 14% .. 14%
1	B	324	 5% 71% 14% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4734 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2218	1414	380	403	21			
1	B	283	Total	C	N	O	S	0	0	0
			2269	1449	387	412	21			

There are 28 discrepancies between the modelled and reference sequences:

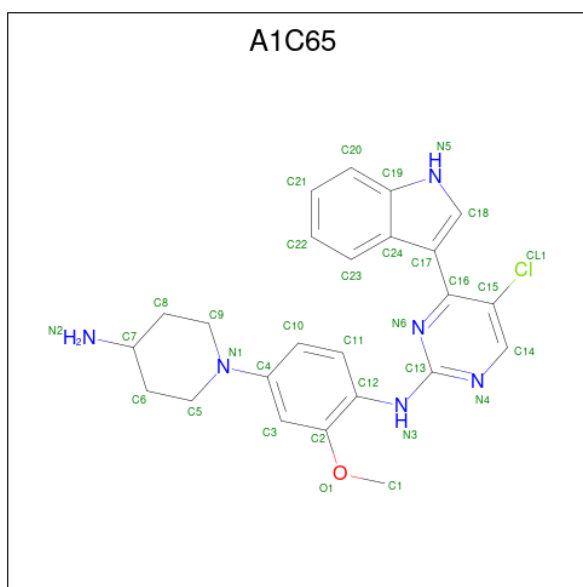
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	UNP P21802
A	452	HIS	-	expression tag	UNP P21802
A	453	HIS	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	SER	-	expression tag	UNP P21802
A	456	GLN	-	expression tag	UNP P21802
A	457	ASP	-	expression tag	UNP P21802
A	650	VAL	ASP	conflict	UNP P21802
B	445	MET	-	initiating methionine	UNP P21802
B	446	GLY	-	expression tag	UNP P21802
B	447	SER	-	expression tag	UNP P21802
B	448	SER	-	expression tag	UNP P21802
B	449	HIS	-	expression tag	UNP P21802
B	450	HIS	-	expression tag	UNP P21802
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	650	VAL	ASP	conflict	UNP P21802

- Molecule 2 is (4P)-N-[4-(4-aminopiperidin-1-yl)-2-methoxyphenyl]-5-chloro-4-(1H-indol-3-yl)pyrimidin-2-amine (CCD ID: A1C65) (formula: C₂₄H₂₅ClN₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			32	24	1	6	1		
2	B	1	Total	C	Cl	N	O	0	0
			32	24	1	6	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	B	86	Total	O	0	0
			86	86		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.93Å 77.98Å 116.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 1.85 39.02 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.02-1.85) 99.1 (39.02-1.85)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.211 , 0.256 0.220 , 0.265	Depositor DCC
R_{free} test set	2617 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4734	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4896e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, A1C65, GOL

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	0.88	0/2264	1.45	20/3056 (0.7%)
1	B	0.90	3/2316 (0.1%)	1.46	21/3124 (0.7%)
All	All	0.89	3/4580 (0.1%)	1.45	41/6180 (0.7%)

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
1	B	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	684	SER	CA-CB	-6.85	1.42	1.53
1	B	688	SER	CA-CB	5.34	1.61	1.53
1	B	547	ILE	CB-CG1	-5.32	1.42	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	TYR	CB-CA-C	8.42	117.18	111.20
1	B	704	TYR	CB-CA-C	8.38	117.15	111.20
1	B	655	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	478	ARG	N-CA-CB	8.20	122.98	110.28
1	A	736	MET	CB-CA-C	-7.62	98.91	110.88
1	A	530	ASP	CA-CB-CG	7.43	120.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	GLU	CB-CA-C	-7.29	99.38	110.90
1	A	470	GLU	CB-CG-CD	6.82	124.20	112.60
1	B	755	GLU	CB-CA-C	-6.77	100.25	110.88
1	A	478	ARG	CB-CA-C	-6.69	97.83	110.67
1	A	678	ARG	CA-CB-CG	6.68	127.47	114.10
1	A	478	ARG	CG-CD-NE	-6.58	97.52	112.00
1	B	736	MET	CB-CA-C	-6.40	100.83	110.88
1	A	727	ASN	CA-CB-CG	-6.37	106.23	112.60
1	B	738	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	598	MET	CG-SD-CE	6.21	114.56	100.90
1	B	685	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	727	ASN	CA-CB-CG	-6.08	106.52	112.60
1	B	530	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	527	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	606	CYS	CB-CA-C	6.00	120.41	110.81
1	A	685	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	478	ARG	CG-CD-NE	-5.85	99.13	112.00
1	B	697	PHE	CA-CB-CG	-5.76	108.04	113.80
1	B	679	VAL	N-CA-CB	-5.67	100.17	111.91
1	B	723	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	504	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	686	VAL	N-CA-CB	5.48	120.68	110.77
1	A	527	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	738	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	595	GLU	CB-CG-CD	5.32	121.65	112.60
1	A	702	SER	O-C-N	-5.30	116.47	121.35
1	A	617	LEU	N-CA-CB	5.28	117.67	110.01
1	A	697	PHE	CA-CB-CG	-5.28	108.52	113.80
1	B	497	MET	CG-SD-CE	-5.24	89.38	100.90
1	B	469	PRO	CB-CA-C	5.19	117.19	111.11
1	B	537	MET	CG-SD-CE	5.14	112.20	100.90
1	B	637	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	543	LYS	CB-CG-CD	5.01	122.82	111.30
1	B	490	GLY	CA-C-N	5.01	127.30	120.54
1	B	490	GLY	C-N-CA	5.01	127.30	120.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	ARG	Sidechain
1	B	580	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	664	ARG	Sidechain
1	B	759	ARG	Sidechain

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	2218	0	2241	22	0
1	B	2269	0	2293	20	0
2	A	32	0	0	1	0
2	B	32	0	0	2	0
3	A	6	0	8	3	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
5	A	66	0	0	3	0
5	B	86	0	0	1	0
All	All	4734	0	4542	41	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 4.

All (41) 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:548:ILE:HD12	1:B:641:LYS:HB3	1.50	0.92
1:A:675:LEU:O	1:A:678:ARG:NH1	2.18	0.77
3:A:802:GOL:H11	5:A:911:HOH:O	1.85	0.76
1:B:548:ILE:HD12	1:B:641:LYS:CB	2.20	0.70
1:B:592:ARG:HB3	1:B:594:PRO:HD3	1.74	0.69
1:A:714:LYS:HE3	1:A:718:GLU:OE1	1.94	0.68
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.34	0.62
1:A:702:SER:OG	1:B:521:ASP:OD2	2.16	0.61
1:B:714:LYS:HE3	1:B:718:GLU:OE1	2.00	0.61
1:A:468:LEU:HD23	1:A:469:PRO:CD	2.32	0.60
1:B:680:TYR:CE1	1:B:684:SER:HB2	2.38	0.58
3:A:802:GOL:H32	5:A:911:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:CYS:HB3	1:B:491:CYS:SG	2.44	0.56
1:A:468:LEU:HD23	1:A:469:PRO:HD2	1.90	0.53
1:A:662:ASN:O	1:A:664:ARG:N	2.33	0.53
2:B:801:A1C65:C11	2:B:801:A1C65:N6	2.71	0.52
1:A:490:GLY:HA3	1:A:492:PHE:CE1	2.47	0.50
1:A:739:CYS:O	1:A:747:ARG:HD3	2.12	0.49
2:A:801:A1C65:C11	2:A:801:A1C65:N6	2.74	0.49
1:B:490:GLY:HA3	1:B:492:PHE:CE1	2.48	0.48
1:B:581:PRO:HA	1:B:597:GLN:OE1	2.13	0.48
1:A:559:PRO:HD3	1:B:708:PRO:HG3	1.96	0.47
1:A:683:GLN:NE2	1:A:747:ARG:HB2	2.31	0.46
1:A:549:ASN:ND2	1:A:565:GLU:OE2	2.49	0.45
1:A:491:CYS:HB3	1:B:491:CYS:HB3	1.99	0.45
1:B:548:ILE:HD11	1:B:633:LEU:HB2	1.98	0.45
1:A:478:ARG:HD3	5:A:939:HOH:O	2.17	0.45
1:A:495:VAL:HG22	1:A:517:LYS:HG2	1.98	0.44
1:B:580:ARG:HG2	1:B:699:LEU:HD23	2.00	0.44
1:B:592:ARG:C	1:B:594:PRO:HD3	2.42	0.44
1:A:733:TYR:CZ	1:A:737:ARG:HD3	2.54	0.43
1:A:549:ASN:HD22	1:A:565:GLU:CD	2.26	0.43
1:A:571:ASN:HB3	3:A:802:GOL:H12	2.00	0.42
1:A:708:PRO:HG3	1:B:559:PRO:HD3	2.00	0.42
1:A:662:ASN:OD1	1:A:664:ARG:NH1	2.44	0.42
1:B:733:TYR:CZ	1:B:737:ARG:HD3	2.55	0.42
1:B:592:ARG:CB	1:B:594:PRO:HD3	2.46	0.42
1:B:564:VAL:HG21	2:B:801:A1C65:CL1	2.57	0.41
1:B:482:THR:HG23	5:B:959:HOH:O	2.19	0.41
1:B:549:ASN:HD22	1:B:565:GLU:CD	2.28	0.41
1:A:683:GLN:HA	1:A:686:VAL:HG13	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	272/324 (84%)	266 (98%)	5 (2%)	1 (0%)	30	17
1	B	277/324 (86%)	269 (97%)	8 (3%)	0	100	100
All	All	549/648 (85%)	535 (97%)	13 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	GLY

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	243/285 (85%)	235 (97%)	8 (3%)	33	18
1	B	248/285 (87%)	241 (97%)	7 (3%)	38	23
All	All	491/570 (86%)	476 (97%)	15 (3%)	35	20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	VAL
1	A	650	VAL
1	A	651	ILE
1	A	675	LEU
1	A	678	ARG
1	A	686	VAL
1	A	709	VAL
1	A	717	LYS
1	B	468	LEU
1	B	496	VAL
1	B	548	ILE
1	B	595	GLU
1	B	652	ASN
1	B	679	VAL
1	B	709	VAL

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

Mol	Chain	Res	Type
1	B	638	ASN
1	B	653	ASN
1	B	730	ASN

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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	803	-	4,4,4	0.27	0	6,6,6	0.12	0
4	SO4	B	803	-	4,4,4	0.15	0	6,6,6	0.29	0
4	SO4	B	804	-	4,4,4	0.33	0	6,6,6	0.13	0
4	SO4	B	802	-	4,4,4	0.31	0	6,6,6	0.21	0
2	A1C65	B	801	-	35,36,36	0.94	3 (8%)	48,51,51	1.48	7 (14%)
4	SO4	A	804	-	4,4,4	0.22	0	6,6,6	0.12	0
2	A1C65	A	801	-	35,36,36	1.00	2 (5%)	48,51,51	1.38	6 (12%)
3	GOL	A	802	-	5,5,5	0.25	0	5,5,5	0.59	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
2	A1C65	A	801	-	-	0/14/24/24	0/5/5/5
2	A1C65	B	801	-	-	0/14/24/24	0/5/5/5
3	GOL	A	802	-	-	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	A1C65	C18-C17	3.16	1.40	1.37
2	B	801	A1C65	C18-C17	2.65	1.40	1.37
2	B	801	A1C65	C16-C17	2.29	1.49	1.46
2	A	801	A1C65	C4-N1	2.27	1.45	1.38
2	B	801	A1C65	C4-N1	2.09	1.44	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1C65	C9-N1-C5	5.42	123.75	111.57
2	A	801	A1C65	C9-N1-C5	5.18	123.23	111.57
2	B	801	A1C65	C17-C16-N6	-3.64	112.60	115.17
2	B	801	A1C65	C11-C12-N3	3.52	128.37	121.32
2	A	801	A1C65	C9-C8-C7	3.49	117.15	110.79
2	B	801	A1C65	C14-C15-C16	-3.38	118.68	120.43
2	A	801	A1C65	C15-C14-N4	-3.36	120.20	122.78
2	A	801	A1C65	C17-C16-N6	-3.12	112.97	115.17
2	A	801	A1C65	C14-C15-C16	-2.45	119.16	120.43
2	B	801	A1C65	C2-C12-N3	-2.42	112.69	118.10
2	B	801	A1C65	C12-N3-C13	-2.25	122.36	129.22
2	A	801	A1C65	C8-C9-N1	2.22	115.97	110.92
2	B	801	A1C65	C8-C7-C6	-2.18	108.07	110.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

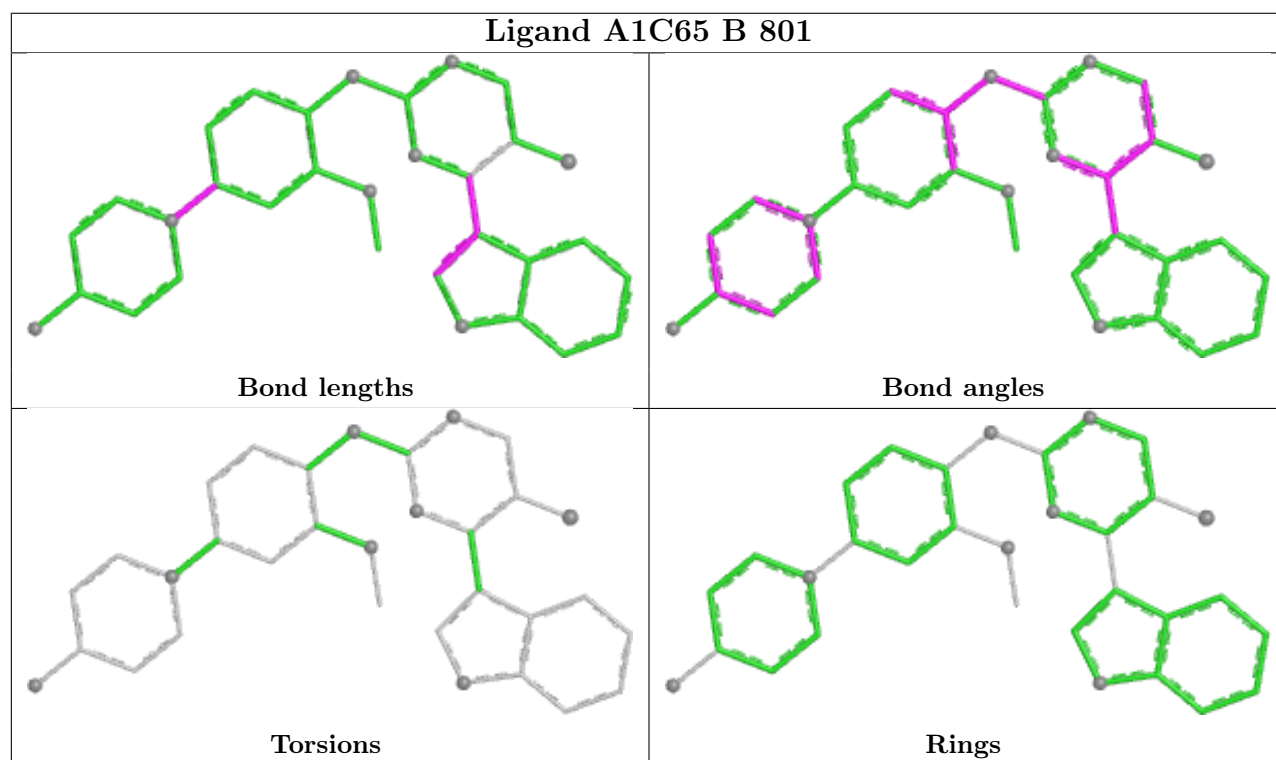
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	A1C65	2	0

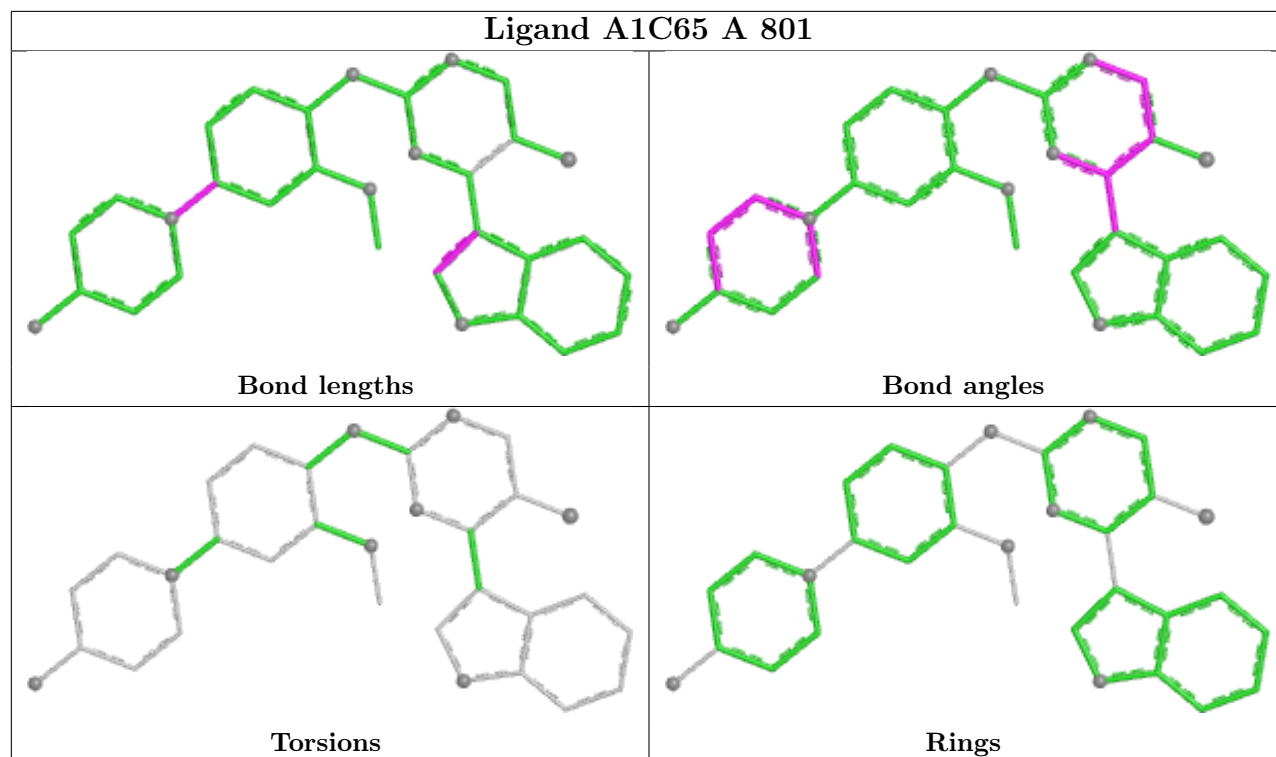
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	A1C65	1	0
3	A	802	GOL	3	0

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

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	278/324 (85%)	0.35	17 (6%) 27 29	17, 32, 61, 83	0
1	B	283/324 (87%)	0.33	16 (5%) 29 32	17, 31, 59, 124	0
All	All	561/648 (86%)	0.34	33 (5%) 28 31	17, 31, 60, 124	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	651	ILE	5.1
1	A	763	LEU	4.5
1	B	468	LEU	4.4
1	B	594	PRO	4.3
1	B	492	PHE	4.0
1	A	492	PHE	4.0
1	B	593	VAL	3.6
1	A	662	ASN	3.5
1	B	763	LEU	3.5
1	A	491	CYS	3.4
1	B	581	PRO	3.4
1	B	595	GLU	3.3
1	A	582	PRO	3.1
1	B	659	LYS	3.1
1	A	713	PHE	3.0
1	A	468	LEU	2.9
1	B	491	CYS	2.8
1	A	663	GLY	2.8
1	A	675	LEU	2.6
1	A	542	GLY	2.6
1	B	592	ARG	2.5
1	A	717	LYS	2.5
1	A	469	PRO	2.4
1	B	663	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	650	VAL	2.4
1	A	680	TYR	2.3
1	B	493	GLY	2.3
1	A	678	ARG	2.3
1	B	658	LYS	2.3
1	B	541	ILE	2.1
1	A	541	ILE	2.1
1	B	727	ASN	2.1
1	B	652	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](#)

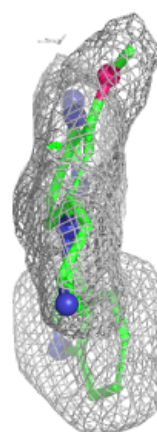
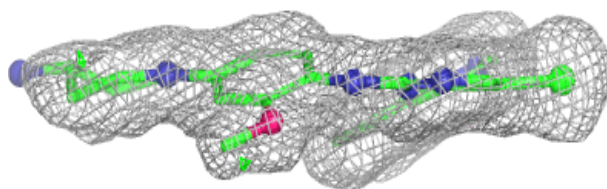
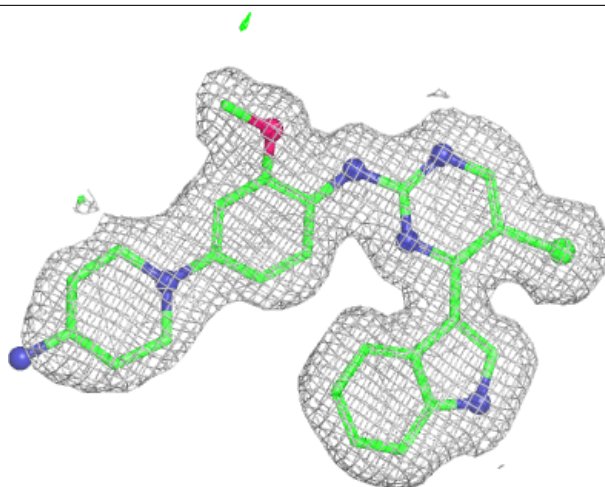
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

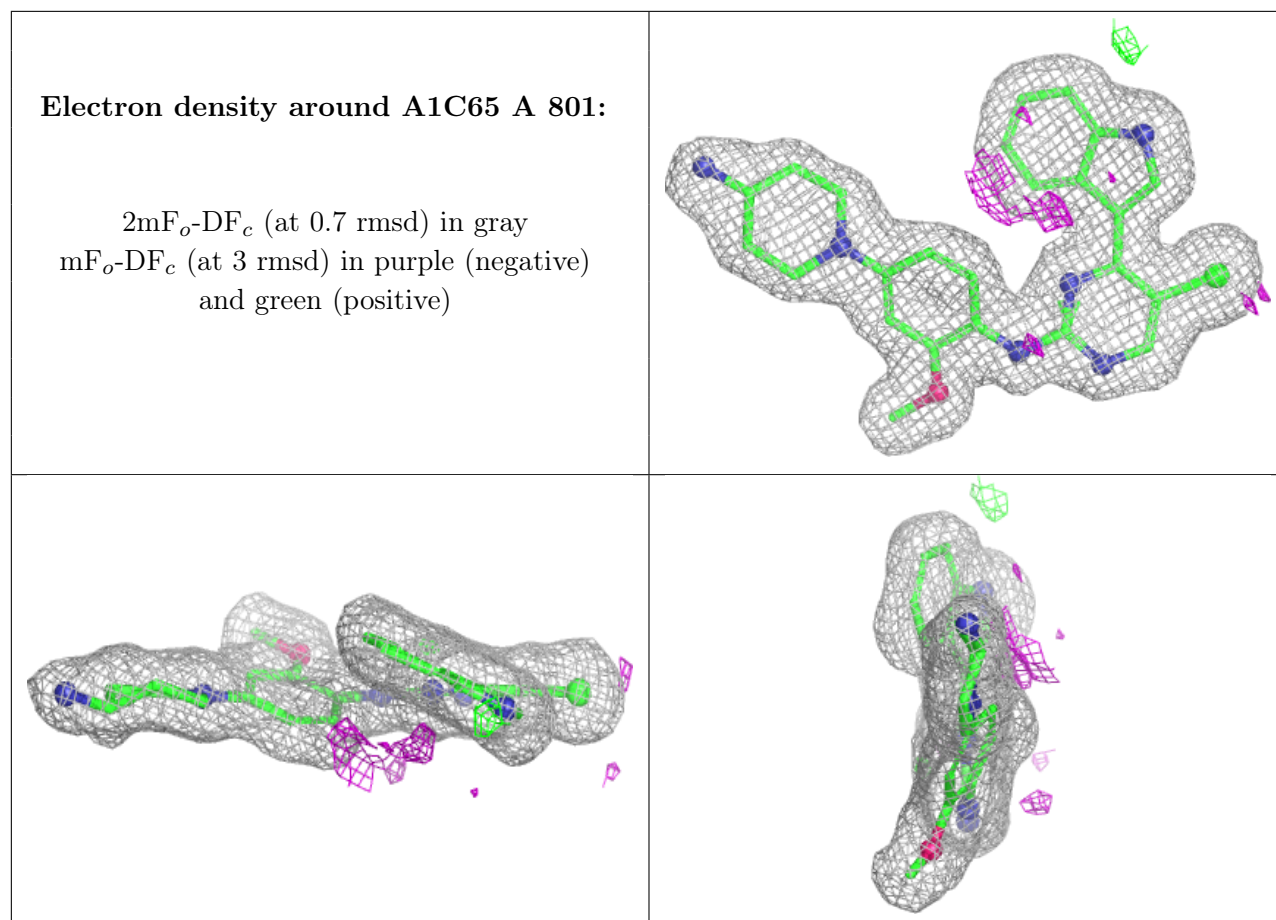
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	803	5/5	0.33	0.20	89,105,130,132	0
4	SO4	A	804	5/5	0.56	0.16	72,87,118,128	0
4	SO4	B	804	5/5	0.72	0.13	68,85,104,109	0
4	SO4	B	803	5/5	0.75	0.11	58,65,83,85	0
4	SO4	B	802	5/5	0.85	0.11	53,60,73,89	0
3	GOL	A	802	6/6	0.86	0.15	36,41,51,62	0
2	A1C65	B	801	32/32	0.95	0.09	20,28,50,58	0
2	A1C65	A	801	32/32	0.96	0.07	17,24,37,43	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 A1C65 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 ⓘ

There are no such residues in this entry.