



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:56 AM UTC

PDB ID : 10OQ / pdb_000010oq
Title : FGFR2 mutant D650V with compound 6
Authors : Hoffman, I.D.; Nelson, K.J.; Bensen, D.C.; Rideout, M.; Hudkins, R.L.; Frye, C.; Bailey, J.B.
Deposited on : 2026-01-29
Resolution : 1.98 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

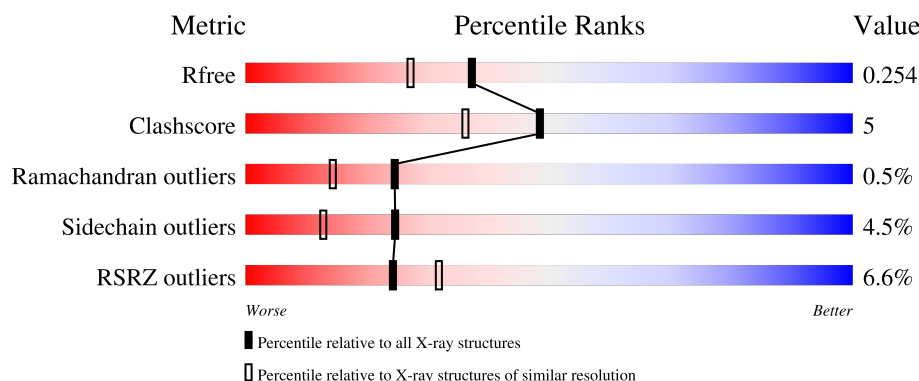
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>6%</div> </div> </div>
1	B	324	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4858 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	304	Total	C	N	O	S	0	1	0
			2428	1547	407	450	24			
1	B	286	Total	C	N	O	S	0	0	0
			2266	1442	384	418	22			

There are 28 discrepancies between the modelled and reference sequences:

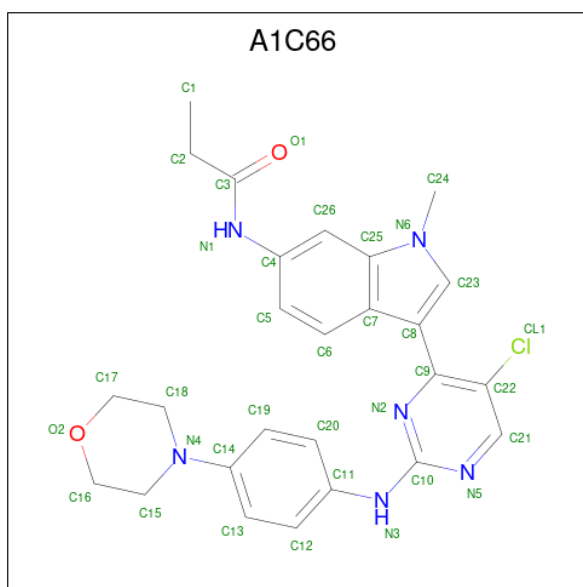
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression 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 N-[(3M)-3-{5-chloro-2-[4-(morpholin-4-yl)anilino]pyrimidin-4-yl}-1-methyl-1H-indol-6-yl]propanamide (CCD ID: A1C66) (formula: C₂₆H₂₇ClN₆O₂).



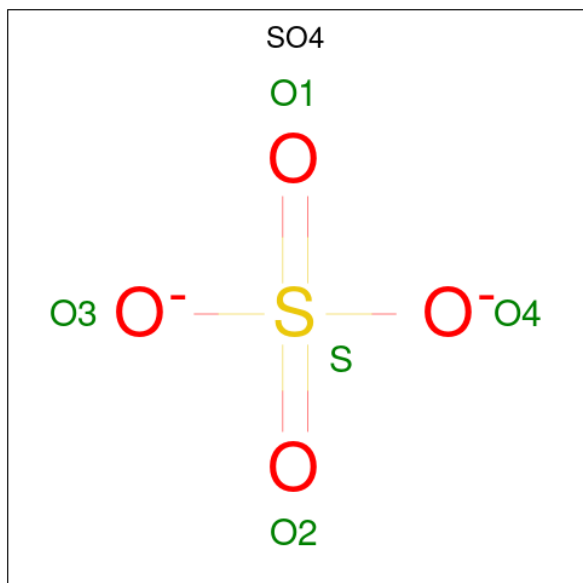
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			35	26	1	6	2		
2	B	1	Total	C	Cl	N	O	0	0
			35	26	1	6	2		

- 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		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	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	B	1	Total	O	S	0	0
			5	4	1		

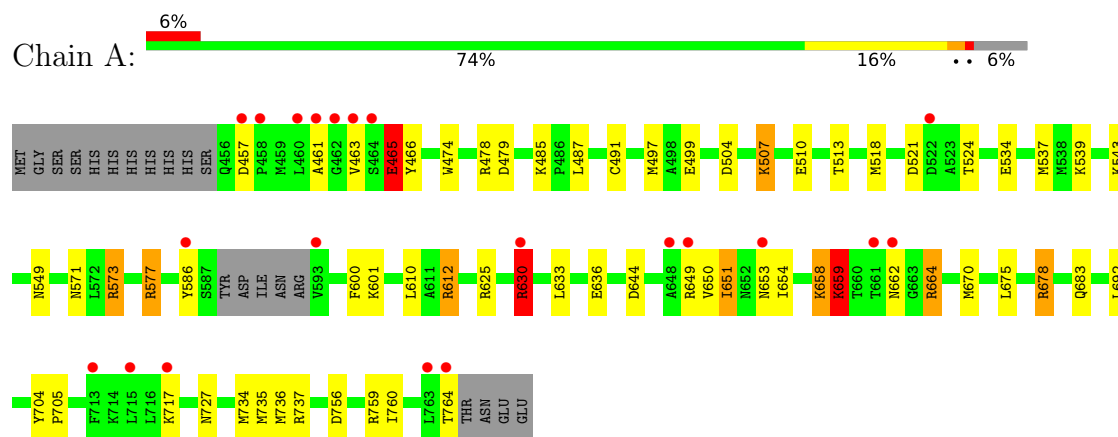
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	29	Total	O	0	0
			29	29		

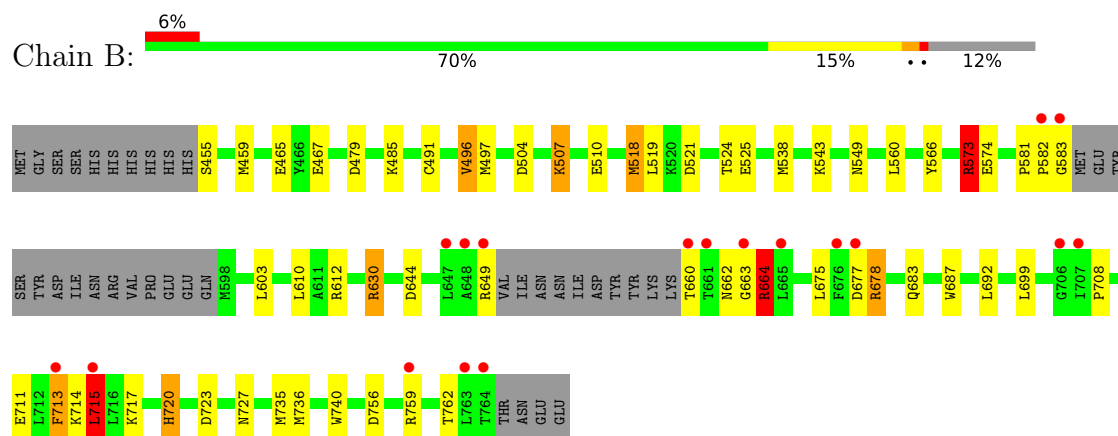
3 Residue-property plots [i](#)

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: Fibroblast growth factor receptor 2



• Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.74Å 96.74Å 145.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.97 – 1.98 54.97 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.97-1.98) 100.0 (54.97-1.98)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.204 , 0.251 0.211 , 0.254	Depositor DCC
R_{free} test set	2768 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: GOL, SO4, A1C66

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	1.00	0/2483	1.63	40/3355 (1.2%)
1	B	0.98	2/2313 (0.1%)	1.61	34/3123 (1.1%)
All	All	0.99	2/4796 (0.0%)	1.62	74/6478 (1.1%)

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	7
1	B	0	4
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	573	ARG	NE-CZ	6.74	1.40	1.33
1	B	467	GLU	CD-OE2	5.27	1.35	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	ASN	CB-CA-C	-12.61	90.87	110.92
1	A	465	GLU	CB-CG-CD	11.85	132.74	112.60
1	B	736	MET	CG-SD-CE	-10.16	78.54	100.90
1	A	537	MET	CG-SD-CE	-9.76	79.42	100.90
1	A	465	GLU	CB-CA-C	9.49	126.98	110.85
1	B	713	PHE	CA-CB-CG	9.23	123.03	113.80
1	A	664	ARG	NE-CZ-NH2	8.70	127.03	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	CYS	CB-CA-C	-8.40	96.85	110.79
1	B	736	MET	CB-CA-C	-8.01	97.50	110.79
1	B	491	CYS	CB-CA-C	-7.98	97.12	110.68
1	A	518	MET	CG-SD-CE	-7.36	84.70	100.90
1	A	521	ASP	CB-CA-C	-7.25	97.22	110.63
1	A	736	MET	CB-CA-C	-7.02	99.86	110.88
1	A	465	GLU	N-CA-CB	-7.01	99.78	110.16
1	B	467	GLU	CB-CA-C	-6.98	98.23	109.75
1	B	521	ASP	CB-CA-C	-6.97	97.73	110.63
1	B	573	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	B	762	THR	CA-CB-OG1	-6.73	99.50	109.60
1	A	478	ARG	CB-CA-C	-6.65	98.33	110.63
1	B	467	GLU	CB-CG-CD	6.61	123.84	112.60
1	B	524	THR	CA-CB-OG1	-6.58	99.72	109.60
1	A	658	LYS	CB-CA-C	-6.48	99.05	109.75
1	B	727	ASN	CA-CB-CG	-6.48	106.12	112.60
1	B	683	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	B	723	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	683	GLN	CB-CA-C	6.26	122.69	110.67
1	B	630	ARG	N-CA-CB	6.24	119.83	110.22
1	A	683	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	A	678	ARG	CG-CD-NE	-6.19	98.38	112.00
1	A	644	ASP	CB-CA-C	-6.16	101.19	111.23
1	B	518	MET	CG-SD-CE	-6.11	87.47	100.90
1	A	664	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	B	715	LEU	N-CA-CB	-6.07	101.18	110.16
1	A	659	LYS	CB-CA-C	6.04	120.66	109.54
1	B	678	ARG	CG-CD-NE	-6.03	98.73	112.00
1	B	644	ASP	CB-CA-C	-5.96	101.64	111.36
1	A	612	ARG	CB-CA-C	-5.86	101.69	110.88
1	B	612	ARG	CB-CA-C	-5.83	101.11	110.79
1	A	649	ARG	CA-CB-CG	-5.82	102.45	114.10
1	B	677	ASP	CA-CB-CG	-5.81	106.79	112.60
1	B	736	MET	N-CA-CB	5.80	118.65	110.12
1	A	636	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	513	THR	CA-CB-OG1	-5.65	101.12	109.60
1	A	457	ASP	CB-CA-C	5.64	118.44	109.52
1	A	465	GLU	CA-C-N	5.64	131.12	121.87
1	A	465	GLU	C-N-CA	5.64	131.12	121.87
1	A	625	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	B	574	GLU	N-CA-CB	5.52	118.33	110.16
1	B	525	GLU	CB-CA-C	-5.50	101.34	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	734	MET	CG-SD-CE	-5.44	88.93	100.90
1	A	659	LYS	CB-CG-CD	5.43	123.79	111.30
1	A	756	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	496	VAL	N-CA-CB	-5.38	102.62	111.45
1	A	717	LYS	CB-CG-CD	5.35	123.60	111.30
1	A	504	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	479	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	504	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	683	GLN	CB-CA-C	5.32	119.89	110.85
1	A	649	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	B	720	HIS	CB-CA-C	5.29	118.25	109.53
1	A	658	LYS	N-CA-CB	5.28	119.04	110.43
1	B	465	GLU	CB-CG-CD	-5.28	103.62	112.60
1	B	662	ASN	N-CA-CB	5.25	117.80	109.82
1	A	573	ARG	CG-CD-NE	-5.24	100.46	112.00
1	B	538	MET	CG-SD-CE	5.24	112.42	100.90
1	A	534	GLU	CB-CA-C	-5.17	102.77	110.88
1	A	479	ASP	CB-CA-C	5.16	119.91	110.11
1	A	650	VAL	N-CA-CB	-5.15	105.79	111.66
1	A	600	PHE	CA-C-N	5.07	127.39	120.54
1	A	600	PHE	C-N-CA	5.07	127.39	120.54
1	A	524	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	478	ARG	CG-CD-NE	-5.05	100.89	112.00
1	B	675	LEU	N-CA-CB	-5.02	102.73	110.01
1	B	524	THR	OG1-CB-CG2	5.00	119.31	109.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	577	ARG	Sidechain
1	A	612	ARG	Sidechain
1	A	630	ARG	Sidechain
1	A	664	ARG	Sidechain
1	A	678	ARG	Sidechain
1	A	737	ARG	Sidechain
1	A	759	ARG	Sidechain
1	B	573	ARG	Sidechain
1	B	649	ARG	Sidechain
1	B	664	ARG	Sidechain
1	B	678	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	2428	0	2433	29	1
1	B	2266	0	2276	22	0
2	A	35	0	0	1	0
2	B	35	0	0	0	0
3	A	18	0	24	2	0
3	B	6	0	8	3	0
4	B	5	0	0	0	0
5	A	36	0	0	0	0
5	B	29	0	0	0	0
All	All	4858	0	4741	52	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 5.

All (52) 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:715:LEU:HD13	1:B:720:HIS:HB2	1.45	0.96
1:B:715:LEU:CD1	1:B:720:HIS:HB2	2.13	0.79
1:B:581:PRO:O	1:B:583:GLY:N	2.18	0.75
1:A:670:MET:HE1	1:A:675:LEU:HA	1.69	0.75
1:A:659:LYS:HE3	1:A:659:LYS:H	1.58	0.69
1:A:670:MET:HE2	1:A:675:LEU:HB2	1.77	0.67
1:A:662:ASN:OD1	3:A:802:GOL:H2	1.97	0.64
1:A:659:LYS:H	1:A:659:LYS:CE	2.14	0.59
1:A:507:LYS:HD2	1:A:510:GLU:OE2	2.03	0.59
1:A:659:LYS:H	1:A:659:LYS:CD	2.17	0.58
1:A:662:ASN:HB2	3:A:802:GOL:H11	1.86	0.58
1:A:573:ARG:NH1	1:A:577:ARG:HH12	2.05	0.54
1:B:663:GLY:O	1:B:664:ARG:HB2	2.06	0.54
1:A:760:ILE:O	1:A:764:THR:HG23	2.08	0.53
1:A:670:MET:CE	1:A:675:LEU:HA	2.39	0.52
1:A:573:ARG:NH1	1:A:577:ARG:NH1	2.58	0.52
1:A:465:GLU:HG2	1:A:466:TYR:CE1	2.46	0.51
1:B:630:ARG:HD3	1:B:664:ARG:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:MET:CE	1:A:675:LEU:CA	2.92	0.48
1:A:474:TRP:CD1	1:A:539:LYS:HE2	2.48	0.48
1:A:704:TYR:N	1:A:705:PRO:CD	2.77	0.48
1:A:573:ARG:HH12	1:A:577:ARG:HH12	1.62	0.47
1:B:560:LEU:CB	3:B:802:GOL:H32	2.45	0.47
1:B:543:LYS:HA	1:B:549:ASN:OD1	2.15	0.47
1:A:487:LEU:HD21	1:A:497:MET:HE2	1.97	0.47
1:A:543:LYS:HA	1:A:549:ASN:OD1	2.14	0.46
1:B:630:ARG:HD3	1:B:664:ARG:HD2	1.96	0.46
1:A:651:ILE:CG1	1:A:654:ILE:HD11	2.46	0.46
1:B:507:LYS:HB2	1:B:510:GLU:HB2	1.97	0.46
1:A:465:GLU:H	1:A:465:GLU:CD	2.24	0.46
1:B:560:LEU:H	3:B:802:GOL:H32	1.81	0.46
1:B:663:GLY:O	1:B:664:ARG:CB	2.64	0.46
1:B:708:PRO:HD2	1:B:711:GLU:OE1	2.16	0.45
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.98	0.45
1:B:715:LEU:CD1	1:B:720:HIS:CB	2.92	0.45
1:A:670:MET:HE1	1:A:675:LEU:CA	2.45	0.45
1:A:573:ARG:HH11	1:A:573:ARG:HD2	1.63	0.43
1:B:518:MET:HE2	1:B:518:MET:HB3	1.74	0.42
1:A:659:LYS:CD	1:A:659:LYS:N	2.81	0.42
1:A:610:LEU:HD13	1:A:692:LEU:HD21	2.00	0.42
2:A:801:A1C66:CL1	2:A:801:A1C66:C6	3.04	0.42
1:B:687:TRP:CE3	1:B:740:TRP:HA	2.54	0.42
1:A:571:ASN:HA	1:A:633:LEU:HD23	2.01	0.41
1:B:603:LEU:HD11	1:B:699:LEU:CD2	2.51	0.41
1:A:630:ARG:NH2	1:A:630:ARG:CG	2.84	0.41
1:A:659:LYS:N	1:A:659:LYS:HD3	2.36	0.41
1:B:459:MET:HB3	1:B:459:MET:HE3	1.75	0.41
1:B:519:LEU:HD12	3:B:802:GOL:H31	2.03	0.41
1:A:735:MET:HE3	1:A:735:MET:HB2	1.84	0.41
1:B:497:MET:HE3	1:B:566:TYR:CZ	2.56	0.41
1:B:735:MET:HE2	1:B:756:ASP:HB3	2.02	0.41
1:B:603:LEU:HD11	1:B:699: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:653:ASN:OD1	1:A:653:ASN:OD1[4_555]	1.92	0.28

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	301/324 (93%)	293 (97%)	7 (2%)	1 (0%)	36	27
1	B	280/324 (86%)	274 (98%)	4 (1%)	2 (1%)	18	9
All	All	581/648 (90%)	567 (98%)	11 (2%)	3 (0%)	24	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	664	ARG
1	A	461	ALA
1	B	582	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	267/285 (94%)	255 (96%)	12 (4%)	24	13
1	B	248/285 (87%)	237 (96%)	11 (4%)	25	14
All	All	515/570 (90%)	492 (96%)	23 (4%)	24	13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	VAL
1	A	465	GLU
1	A	485	LYS

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Mol	Chain	Res	Type
1	A	499	GLU
1	A	507	LYS
1	A	586	TYR
1	A	601	LYS
1	A	630	ARG
1	A	651	ILE
1	A	658	LYS
1	A	659	LYS
1	A	727	ASN
1	B	455	SER
1	B	485	LYS
1	B	496	VAL
1	B	507	LYS
1	B	573	ARG
1	B	660	THR
1	B	713	PHE
1	B	714	LYS
1	B	715	LEU
1	B	717	LYS
1	B	759	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	662	ASN
1	B	682	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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
2	A1C66	B	801	1	38,39,39	0.86	2 (5%)	51,55,55	1.74	9 (17%)
3	GOL	A	802	-	5,5,5	0.24	0	5,5,5	0.50	0
3	GOL	A	803	-	5,5,5	0.14	0	5,5,5	0.34	0
4	SO4	B	803	-	4,4,4	0.30	0	6,6,6	0.31	0
3	GOL	A	804	-	5,5,5	0.27	0	5,5,5	0.73	0
2	A1C66	A	801	1	38,39,39	0.83	0	51,55,55	1.45	9 (17%)
3	GOL	B	802	-	5,5,5	0.26	0	5,5,5	0.79	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	A1C66	B	801	1	-	4/18/26/26	0/5/5/5
3	GOL	A	802	-	-	3/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
2	A1C66	A	801	1	-	5/18/26/26	0/5/5/5
3	GOL	B	802	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1C66	C9-C8	2.45	1.49	1.46
2	B	801	A1C66	C7-C8	-2.07	1.42	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1C66	C8-C9-N2	-6.09	110.87	115.17
2	B	801	A1C66	C5-C4-C26	4.46	125.05	119.66
2	A	801	A1C66	C8-C9-N2	-4.39	112.07	115.17
2	B	801	A1C66	C21-C22-C9	-3.77	118.48	120.43
2	B	801	A1C66	C25-N6-C23	-3.24	106.19	108.54
2	A	801	A1C66	C18-N4-C14	3.07	126.49	118.11
2	B	801	A1C66	C8-C23-N6	2.95	113.09	110.95
2	A	801	A1C66	C7-C8-C23	-2.82	104.55	106.02
2	A	801	A1C66	C5-C4-C26	2.76	122.99	119.66
2	A	801	A1C66	C18-N4-C15	2.50	117.19	111.57
2	B	801	A1C66	C17-C18-N4	-2.47	105.25	109.93
2	B	801	A1C66	C7-C8-C23	-2.41	104.77	106.02
2	B	801	A1C66	C7-C25-N6	2.31	109.32	107.91
2	B	801	A1C66	C4-C26-C25	-2.26	115.65	119.48
2	A	801	A1C66	C24-N6-C23	2.18	127.99	125.70
2	A	801	A1C66	C12-C11-N3	-2.16	113.29	120.61
2	A	801	A1C66	C21-C22-C9	-2.08	119.35	120.43
2	A	801	A1C66	C4-C26-C25	-2.08	115.95	119.48

There are no chirality outliers.

All (20) torsion outliers are listed below:

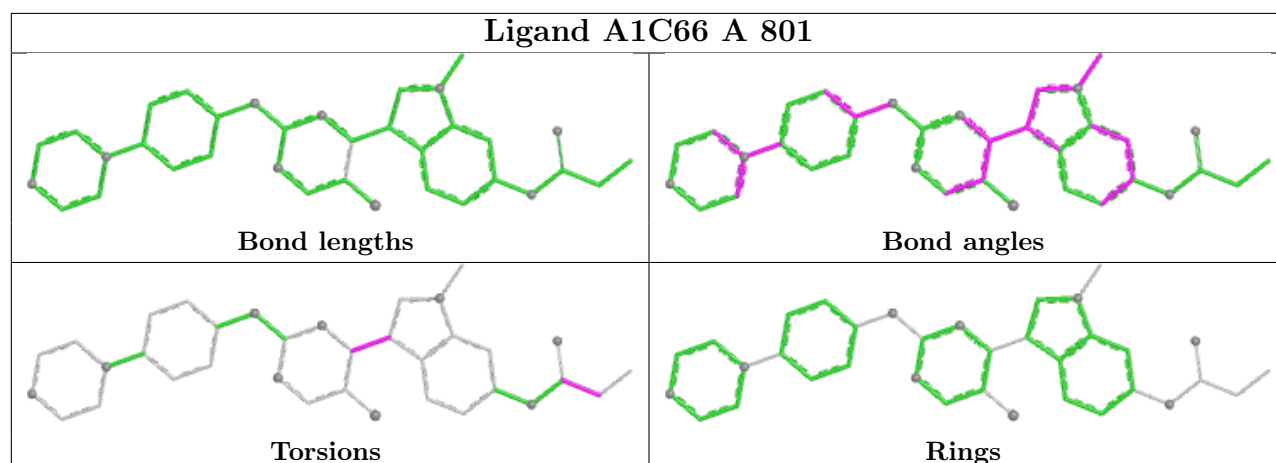
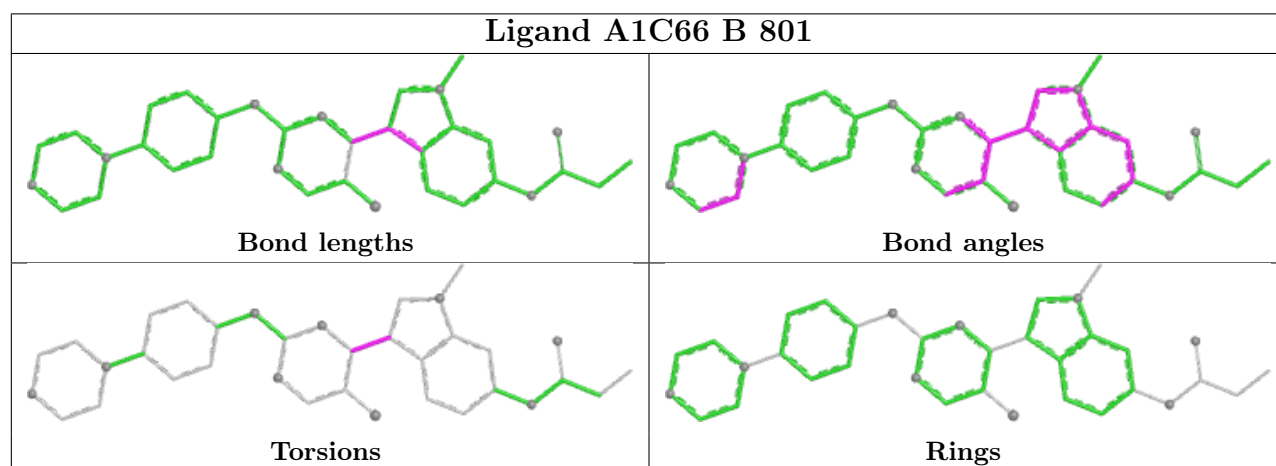
Mol	Chain	Res	Type	Atoms
2	A	801	A1C66	C7-C8-C9-C22
2	A	801	A1C66	C7-C8-C9-N2
2	A	801	A1C66	C23-C8-C9-C22
2	B	801	A1C66	C7-C8-C9-C22
2	B	801	A1C66	C7-C8-C9-N2
2	B	801	A1C66	C23-C8-C9-C22
3	A	802	GOL	C1-C2-C3-O3
3	A	802	GOL	O2-C2-C3-O3
3	B	802	GOL	O1-C1-C2-C3
3	B	802	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-C3
3	A	803	GOL	O1-C1-C2-C3
3	A	804	GOL	C1-C2-C3-O3
3	B	802	GOL	O1-C1-C2-O2
3	B	802	GOL	O2-C2-C3-O3
2	B	801	A1C66	C23-C8-C9-N2
3	A	803	GOL	O1-C1-C2-O2
3	A	804	GOL	O2-C2-C3-O3
2	A	801	A1C66	C23-C8-C9-N2
2	A	801	A1C66	C1-C2-C3-O1

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GOL	2	0
2	A	801	A1C66	1	0
3	B	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	304/324 (93%)	0.36	21 (6%) 23 30	25, 45, 84, 108	1 (0%)
1	B	286/324 (88%)	0.41	18 (6%) 26 34	32, 46, 90, 134	0
All	All	590/648 (91%)	0.38	39 (6%) 24 32	25, 45, 88, 134	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	583	GLY	7.8
1	A	586	TYR	6.7
1	A	463	VAL	6.1
1	B	649	ARG	4.0
1	B	713	PHE	4.0
1	A	717	LYS	3.9
1	B	706	GLY	3.8
1	B	764	THR	3.7
1	A	649	ARG	3.6
1	A	715	LEU	3.6
1	B	715	LEU	3.6
1	B	665	LEU	3.4
1	B	661	THR	3.4
1	A	764	THR	3.3
1	A	458	PRO	3.1
1	A	653	ASN	2.8
1	A	457	ASP	2.7
1	A	593	VAL	2.7
1	A	648	ALA	2.6
1	B	660	THR	2.6
1	A	462	GLY	2.6
1	B	676	PHE	2.6
1	B	763	LEU	2.6
1	A	662	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	582	PRO	2.6
1	B	759	ARG	2.5
1	A	713	PHE	2.5
1	A	461	ALA	2.5
1	B	677	ASP	2.4
1	B	647	LEU	2.3
1	A	460	LEU	2.3
1	A	661	THR	2.3
1	A	763	LEU	2.3
1	B	648	ALA	2.2
1	A	522	ASP	2.2
1	A	464	SER	2.2
1	B	707	ILE	2.0
1	B	663	GLY	2.0
1	A	630	ARG	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](#)

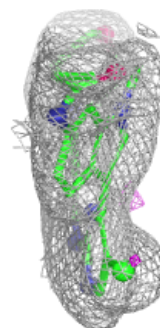
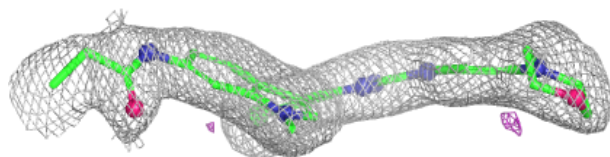
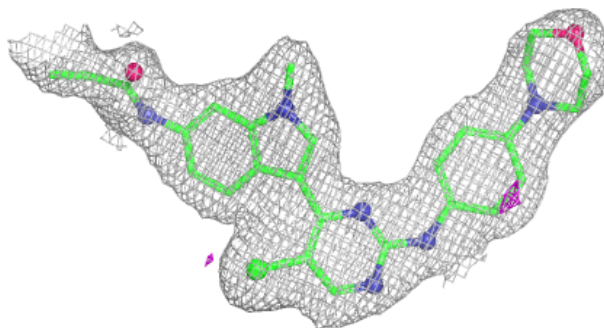
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

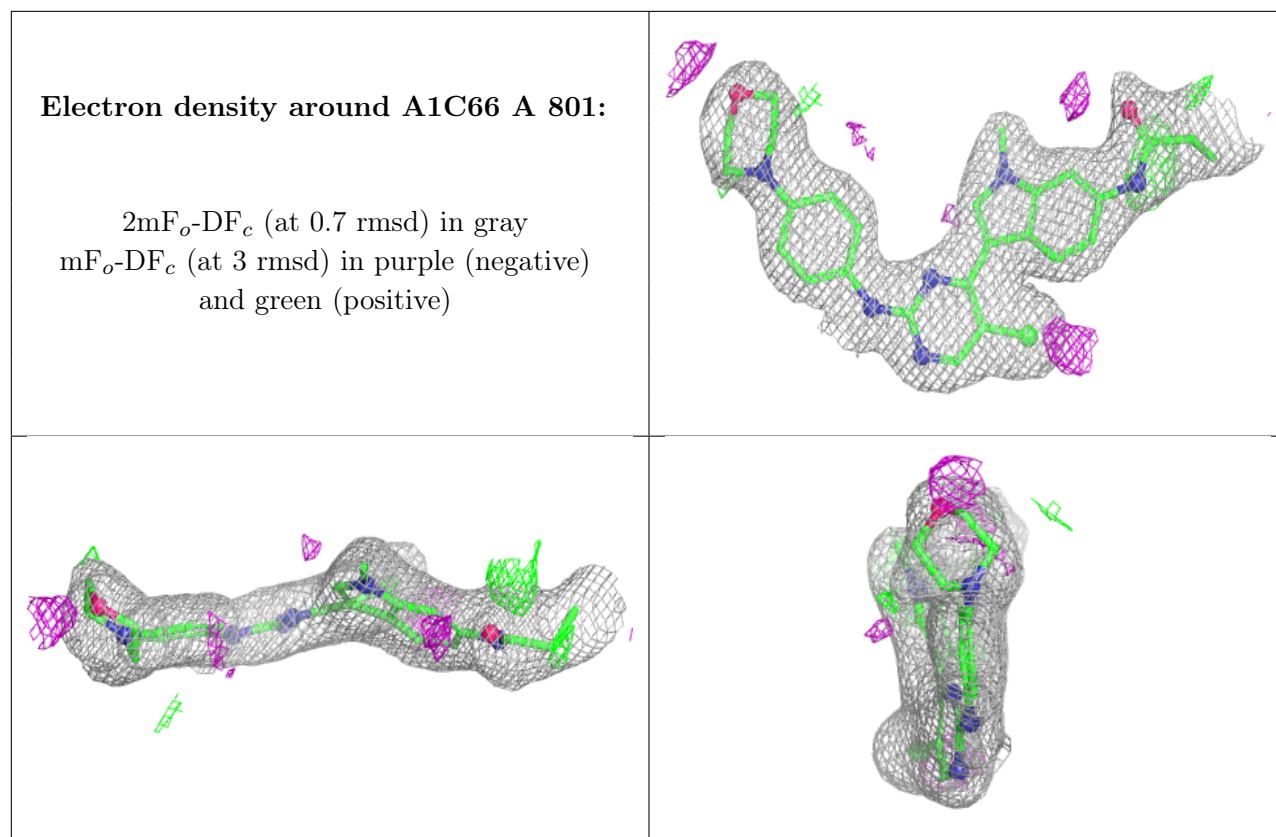
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	803	5/5	0.63	0.15	55,83,117,129	0
3	GOL	A	802	6/6	0.82	0.13	57,67,73,75	0
3	GOL	A	803	6/6	0.83	0.16	57,80,82,90	0
3	GOL	B	802	6/6	0.84	0.17	48,69,75,83	0
3	GOL	A	804	6/6	0.84	0.15	63,76,79,79	0
2	A1C66	B	801	35/35	0.95	0.09	32,44,78,81	0
2	A1C66	A	801	35/35	0.95	0.10	31,45,72,82	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 A1C66 B 801:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.