



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:13 PM UTC

PDB ID : 5L72 / pdb_00005l72
Title : PI3 kinase delta in complex with N-[6-(5-methanesulfonamido-6-methoxy-pyridin-3-yl)-1,3-dihydro-2-benzofuran-4-yl]-2-(morpholin-4-yl)acetamide
Authors : Rowland, P.
Deposited on : 2016-06-01
Resolution : 3.06 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

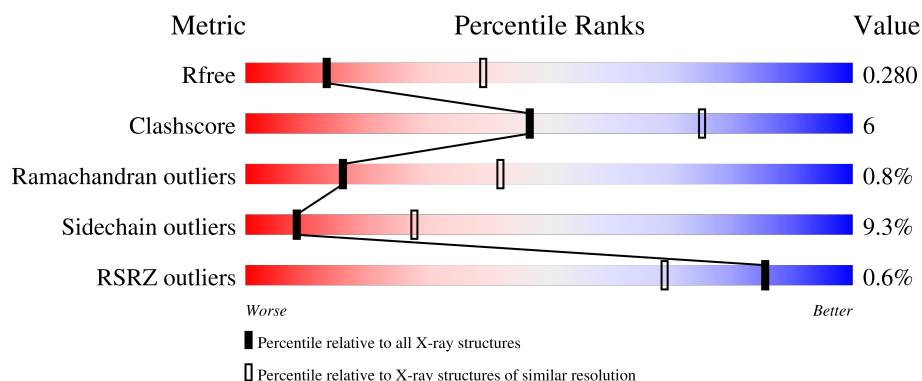
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	940	69% 21% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7225 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.

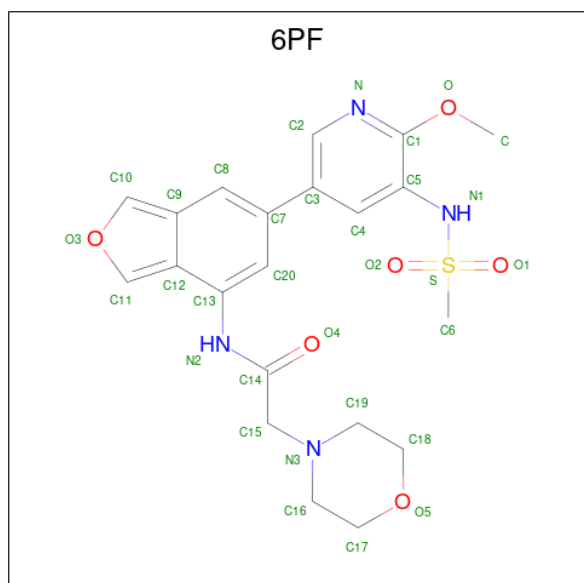
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	858	6925	4424	1189	1258	54	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP O35904
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is N-[6-(5-methanesulfonamido-6-methoxypyridin-3-yl)-1,3-dihydro-2-benzofuran-4-yl]-2-(morpholin-4-yl)acetamide (CCD ID: 6PF) (formula: C₂₁H₂₄N₄O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	32	21	4	6	1	0	0

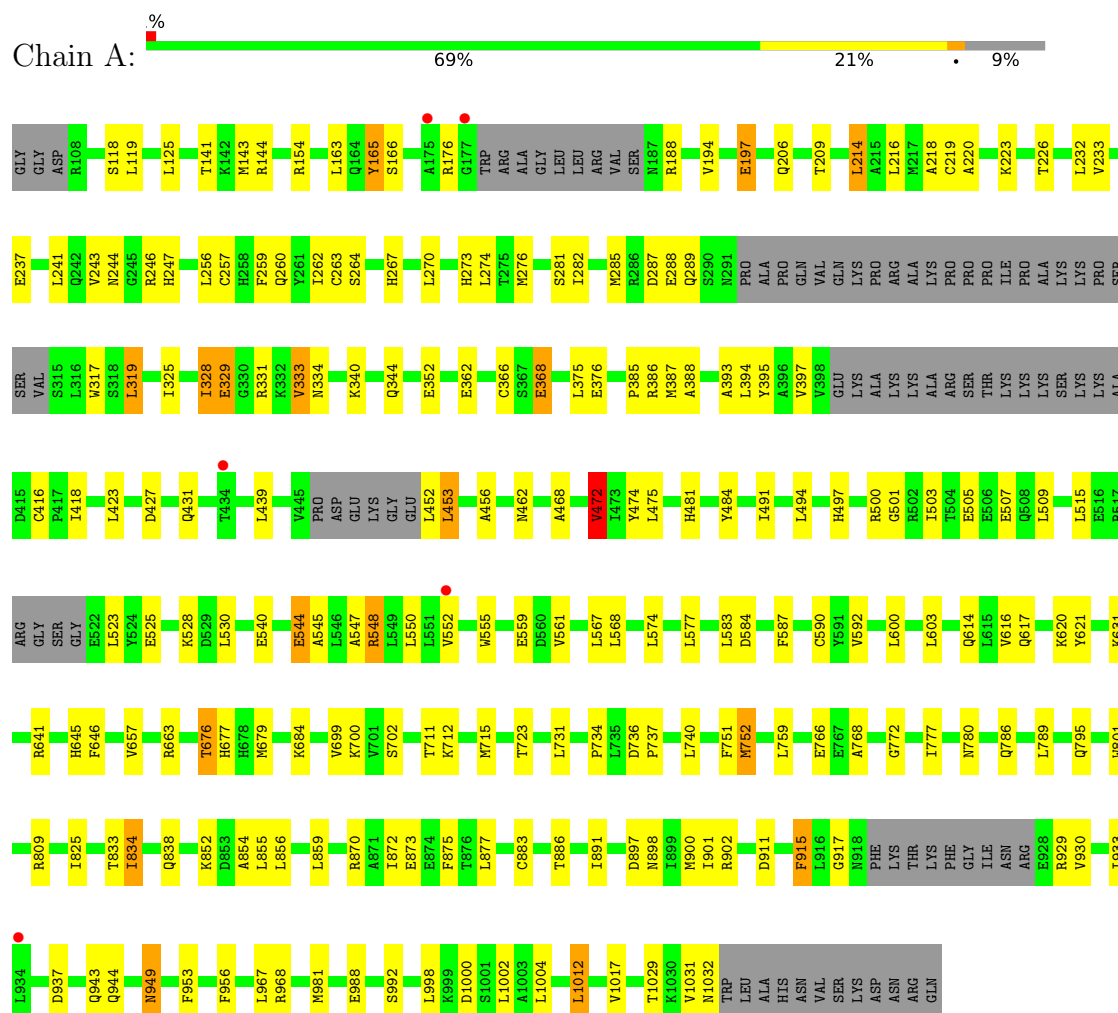
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total 268	O 268	0	0

3 Residue-property plots

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.40Å 64.36Å 115.83Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	112.92 – 3.06 112.92 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.4 (112.92-3.06) 97.4 (112.92-3.06)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.172 , 0.277 0.177 , 0.280	Depositor DCC
R_{free} test set	967 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 102.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.17% 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: 6PF

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	0.89	1/7075 (0.0%)	1.42	42/9549 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	HIS	CA-C	5.69	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	9.94	123.74	113.80
1	A	427	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	472	VAL	N-CA-CB	6.99	118.34	110.72
1	A	243	VAL	N-CA-C	-6.64	100.12	108.89
1	A	259	PHE	CA-C-N	6.42	129.18	120.38
1	A	259	PHE	C-N-CA	6.42	129.18	120.38
1	A	736	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	877	LEU	CA-C-N	6.14	128.50	120.28
1	A	877	LEU	C-N-CA	6.14	128.50	120.28
1	A	1012	LEU	CA-C-N	5.89	128.09	120.44
1	A	1012	LEU	C-N-CA	5.89	128.09	120.44
1	A	144	ARG	CA-C-N	5.84	128.43	120.54
1	A	144	ARG	C-N-CA	5.84	128.43	120.54
1	A	584	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	646	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	663	ARG	CA-C-N	5.69	128.22	120.54
1	A	663	ARG	C-N-CA	5.69	128.22	120.54
1	A	873	GLU	CA-C-N	5.65	127.85	120.28
1	A	873	GLU	C-N-CA	5.65	127.85	120.28
1	A	949	ASN	CA-C-N	5.59	127.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	949	ASN	C-N-CA	5.59	127.77	120.28
1	A	897	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	505	GLU	CA-C-N	5.37	127.75	120.44
1	A	505	GLU	C-N-CA	5.37	127.75	120.44
1	A	834	ILE	CA-C-N	5.36	128.86	120.82
1	A	834	ILE	C-N-CA	5.36	128.86	120.82
1	A	329	GLU	CA-C-N	5.35	126.18	121.58
1	A	329	GLU	C-N-CA	5.35	126.18	121.58
1	A	232	LEU	CA-C-N	5.30	128.84	120.47
1	A	232	LEU	C-N-CA	5.30	128.84	120.47
1	A	218	ALA	CA-C-N	5.28	127.31	120.44
1	A	218	ALA	C-N-CA	5.28	127.31	120.44
1	A	875	PHE	CA-C-N	5.21	127.57	120.54
1	A	875	PHE	C-N-CA	5.21	127.57	120.54
1	A	592	VAL	CA-C-N	5.14	125.65	119.94
1	A	592	VAL	C-N-CA	5.14	125.65	119.94
1	A	456	ALA	CA-C-N	5.07	124.91	120.10
1	A	456	ALA	C-N-CA	5.07	124.91	120.10
1	A	883	CYS	CA-C-N	5.01	127.33	120.46
1	A	883	CYS	C-N-CA	5.01	127.33	120.46
1	A	165	TYR	CA-C-N	5.01	126.99	120.28
1	A	165	TYR	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6925	0	6910	79	0
2	A	32	0	0	0	0
3	A	268	0	0	2	0
All	All	7225	0	6910	79	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 6.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HG2	1:A:677:HIS:CG	2.27	0.70
1:A:329:GLU:HG2	1:A:472:VAL:HG22	1.74	0.68
1:A:194:VAL:HG22	1:A:274:LEU:HB2	1.76	0.67
1:A:385:PRO:HD2	1:A:388:ALA:HB2	1.81	0.63
1:A:331:ARG:HA	1:A:368:GLU:HG3	1.83	0.61
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.82	0.60
1:A:340:LYS:HE3	1:A:362:GLU:HB3	1.84	0.60
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.84	0.60
1:A:462:ASN:HD22	1:A:468:ALA:HB2	1.67	0.58
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.86	0.57
1:A:917:GLY:HA2	1:A:930:VAL:HG23	1.87	0.57
1:A:209:THR:HB	1:A:257:CYS:HB3	1.87	0.57
1:A:702:SER:HB3	1:A:711:THR:HG23	1.87	0.56
1:A:786:GLN:HE22	1:A:988:GLU:HB2	1.72	0.55
1:A:247:HIS:CE1	1:A:740:LEU:HD21	2.43	0.54
1:A:953:PHE:O	1:A:956:PHE:HB3	2.08	0.53
1:A:621:TYR:HE2	3:A:4111:HOH:O	1.90	0.53
1:A:555:TRP:CE3	1:A:561:VAL:HG22	2.44	0.52
1:A:641:ARG:HH12	1:A:737:PRO:HB2	1.74	0.52
1:A:751:PHE:HB3	1:A:759:LEU:HD23	1.92	0.51
1:A:614:GLN:HG3	1:A:981:MET:HG2	1.93	0.50
1:A:194:VAL:HG21	1:A:216:LEU:CD2	2.42	0.50
1:A:256:LEU:HB3	1:A:262:ILE:HG21	1.94	0.50
1:A:700:LYS:HE3	1:A:780:ASN:HD22	1.77	0.49
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.46	0.49
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.95	0.48
1:A:759:LEU:O	1:A:777:ILE:HA	2.14	0.48
1:A:943:GLN:HB3	1:A:949:ASN:HB3	1.95	0.48
1:A:684:LYS:HE2	1:A:731:LEU:HB3	1.97	0.47
1:A:163:LEU:HD21	1:A:282:ILE:HG12	1.97	0.47
1:A:325:ILE:HD11	1:A:375:LEU:HD12	1.97	0.46
1:A:752:MET:H	1:A:752:MET:HG2	1.51	0.46
1:A:998:LEU:C	1:A:1000:ASP:H	2.24	0.46
1:A:834:ILE:HD12	1:A:855:LEU:HD11	1.97	0.46
1:A:333:VAL:HG22	1:A:366:CYS:O	2.16	0.45
1:A:423:LEU:HD22	1:A:439:LEU:HD21	1.98	0.45
1:A:387:MET:HE3	1:A:590:CYS:SG	2.57	0.45
1:A:968:ARG:HG2	1:A:1002:LEU:O	2.16	0.45
1:A:768:ALA:HB3	1:A:772:GLY:HA3	1.99	0.44
1:A:431:GLN:HB2	1:A:484:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ALA:HA	1:A:550:LEU:HD12	1.99	0.44
1:A:118:SER:OG	1:A:125:LEU:HG	2.18	0.44
1:A:699:VAL:HG21	1:A:759:LEU:HD21	2.00	0.44
1:A:194:VAL:HG21	1:A:216:LEU:HD22	2.00	0.44
1:A:497:HIS:HD2	3:A:4327:HOH:O	2.00	0.44
1:A:523:LEU:HD22	1:A:548:ARG:HD3	1.99	0.44
1:A:789:LEU:HD13	1:A:981:MET:HG3	2.00	0.44
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.16	0.44
1:A:143:MET:HA	1:A:143:MET:HE2	2.01	0.43
1:A:886:THR:HA	1:A:891:ILE:HD12	2.01	0.43
1:A:838:GLN:HE22	1:A:937:ASP:CG	2.26	0.43
1:A:328:ILE:HB	1:A:472:VAL:HG23	2.01	0.43
1:A:544:GLU:HA	1:A:574:LEU:HD22	2.01	0.43
1:A:645:HIS:CE1	1:A:734:PRO:HA	2.54	0.42
1:A:801:TRP:HE1	1:A:967:LEU:HG	1.84	0.42
1:A:859:LEU:HD21	1:A:901:ILE:HD11	2.00	0.42
1:A:547:ALA:HB1	1:A:587:PHE:CZ	2.54	0.42
1:A:600:LEU:HD22	1:A:603:LEU:HD11	2.01	0.42
1:A:241:LEU:HD13	1:A:274:LEU:HD13	2.02	0.42
1:A:676:THR:O	1:A:679:MET:HB3	2.19	0.41
1:A:393:ALA:HB2	1:A:453:LEU:HD13	2.02	0.41
1:A:752:MET:HE2	1:A:777:ILE:HG12	2.01	0.41
1:A:281:SER:O	1:A:285:MET:HG3	2.21	0.41
1:A:515:LEU:HD22	1:A:545:ALA:HB1	2.01	0.41
1:A:287:ASP:C	1:A:289:GLN:H	2.27	0.41
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.36	0.41
1:A:220:ALA:HB3	1:A:276:MET:HE2	2.02	0.41
1:A:789:LEU:CD1	1:A:981:MET:HG3	2.51	0.41
1:A:285:MET:HA	1:A:288:GLU:HG2	2.03	0.41
1:A:325:ILE:HG13	1:A:375:LEU:HB2	2.02	0.41
1:A:387:MET:HE3	1:A:590:CYS:CB	2.51	0.41
1:A:833:THR:HG22	1:A:900:MET:HG2	2.04	0.40
1:A:214:LEU:HD21	1:A:237:GLU:OE2	2.20	0.40
1:A:317:TRP:HH2	1:A:491:ILE:HA	1.85	0.40
1:A:528:LYS:HG2	1:A:552:VAL:HG12	2.04	0.40
1:A:344:GLN:HB2	1:A:395:TYR:CE2	2.56	0.40
1:A:494:LEU:HD21	1:A:559:GLU:HG3	2.03	0.40
1:A:777:ILE:HB	1:A:825:ILE:HB	2.03	0.40
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	844/940 (90%)	783 (93%)	54 (6%)	7 (1%)	16	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	ARG
1	A	197	GLU
1	A	319	LEU
1	A	911	ASP
1	A	854	ALA
1	A	328	ILE
1	A	501	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	760/827 (92%)	689 (91%)	71 (9%)	8	28

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	141	THR
1	A	166	SER
1	A	176	ARG

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Mol	Chain	Res	Type
1	A	188	ARG
1	A	197	GLU
1	A	206	GLN
1	A	214	LEU
1	A	219	CYS
1	A	223	LYS
1	A	226	THR
1	A	233	VAL
1	A	246	ARG
1	A	260	GLN
1	A	263	CYS
1	A	264	SER
1	A	267	HIS
1	A	270	LEU
1	A	319	LEU
1	A	333	VAL
1	A	334	ASN
1	A	352	GLU
1	A	368	GLU
1	A	376	GLU
1	A	394	LEU
1	A	397	VAL
1	A	416	CYS
1	A	418	ILE
1	A	452	LEU
1	A	453	LEU
1	A	472	VAL
1	A	475	LEU
1	A	500	ARG
1	A	503	ILE
1	A	507	GLU
1	A	509	LEU
1	A	525	GLU
1	A	530	LEU
1	A	540	GLU
1	A	544	GLU
1	A	548	ARG
1	A	567	LEU
1	A	568	LEU
1	A	577	LEU
1	A	616	VAL
1	A	631	LYS

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Mol	Chain	Res	Type
1	A	657	VAL
1	A	676	THR
1	A	712	LYS
1	A	715	MET
1	A	723	THR
1	A	752	MET
1	A	766	GLU
1	A	795	GLN
1	A	809	ARG
1	A	852	LYS
1	A	856	LEU
1	A	870	ARG
1	A	872	ILE
1	A	898	ASN
1	A	902	ARG
1	A	915	PHE
1	A	933	ILE
1	A	944	GLN
1	A	992	SER
1	A	1004	LEU
1	A	1012	LEU
1	A	1017	VAL
1	A	1029	THR
1	A	1031	VAL
1	A	1032	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	321	GLN
1	A	334	ASN
1	A	349	HIS
1	A	422	ASN
1	A	454	ASN
1	A	462	ASN
1	A	617	GLN
1	A	704	GLN
1	A	721	GLN
1	A	773	ASN
1	A	786	GLN
1	A	838	GLN

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Mol	Chain	Res	Type
1	A	898	ASN
1	A	940	HIS
1	A	948	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 ⓘ

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	6PF	A	4000	-	33,35,35	1.56	5 (15%)	42,50,50	1.63	5 (11%)

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	6PF	A	4000	-	-	7/19/27/27	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	6PF	C11-C12	5.05	1.50	1.34
2	A	4000	6PF	C10-C9	4.73	1.49	1.34
2	A	4000	6PF	O3-C11	2.97	1.42	1.36
2	A	4000	6PF	O3-C10	2.95	1.42	1.36
2	A	4000	6PF	C5-C1	2.86	1.45	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	6PF	O3-C11-C12	-6.73	104.88	110.89
2	A	4000	6PF	C10-O3-C11	4.68	111.21	106.31
2	A	4000	6PF	O3-C10-C9	-3.52	105.44	110.21
2	A	4000	6PF	C1-C5-N1	3.30	124.31	117.95
2	A	4000	6PF	C12-C13-N2	-2.42	114.64	118.81

There are no chirality outliers.

All (7) torsion outliers are listed below:

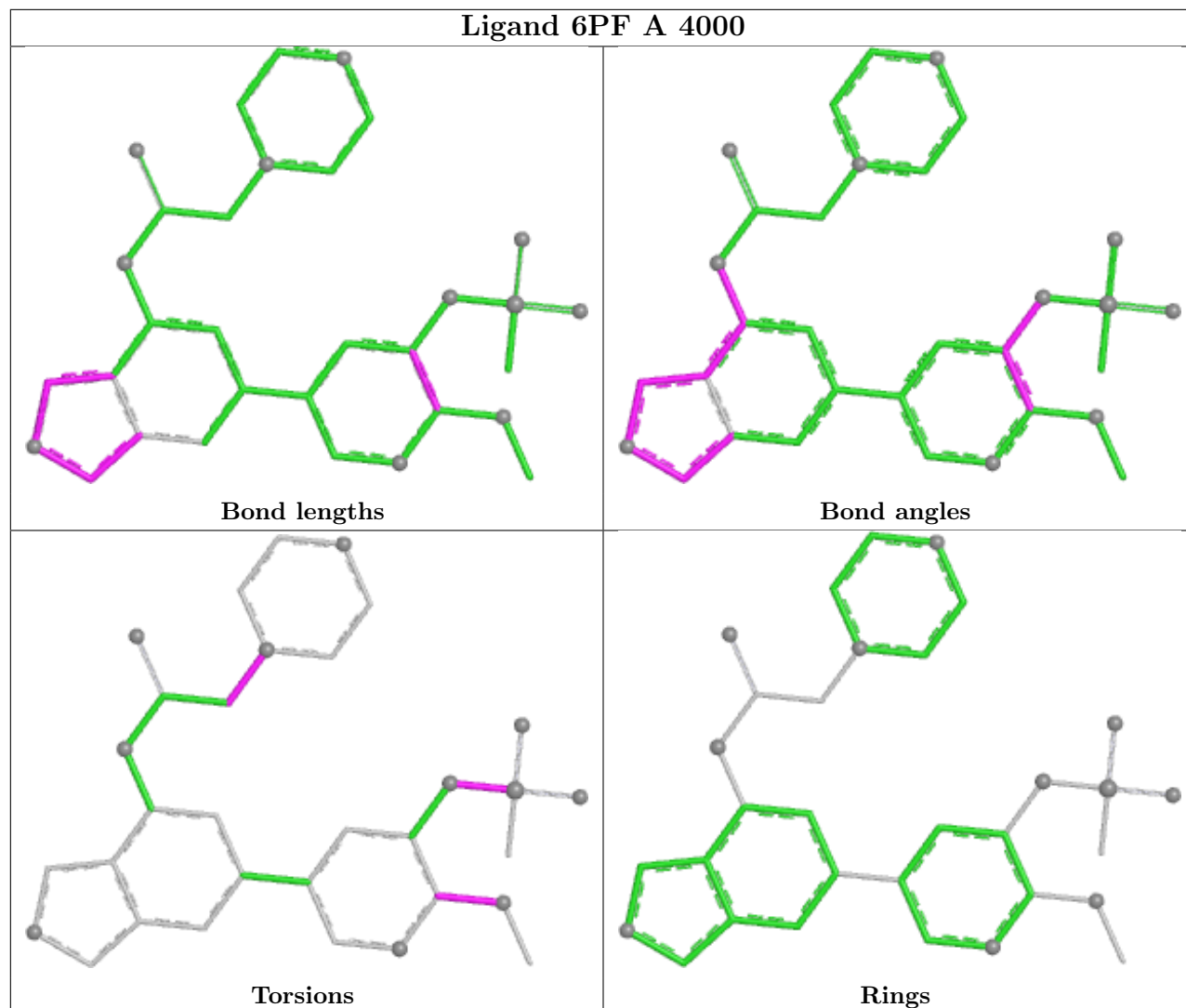
Mol	Chain	Res	Type	Atoms
2	A	4000	6PF	C5-N1-S-C6
2	A	4000	6PF	C5-N1-S-O2
2	A	4000	6PF	C5-C1-O-C
2	A	4000	6PF	C5-N1-S-O1
2	A	4000	6PF	C14-C15-N3-C16
2	A	4000	6PF	C14-C15-N3-C19
2	A	4000	6PF	N-C1-O-C

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 [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	858/940 (91%)	-0.13	5 (0%) 85 69	23, 55, 93, 136	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	934	LEU	2.9
1	A	552	VAL	2.1
1	A	175	ALA	2.0
1	A	434	THR	2.0
1	A	177	GLY	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.

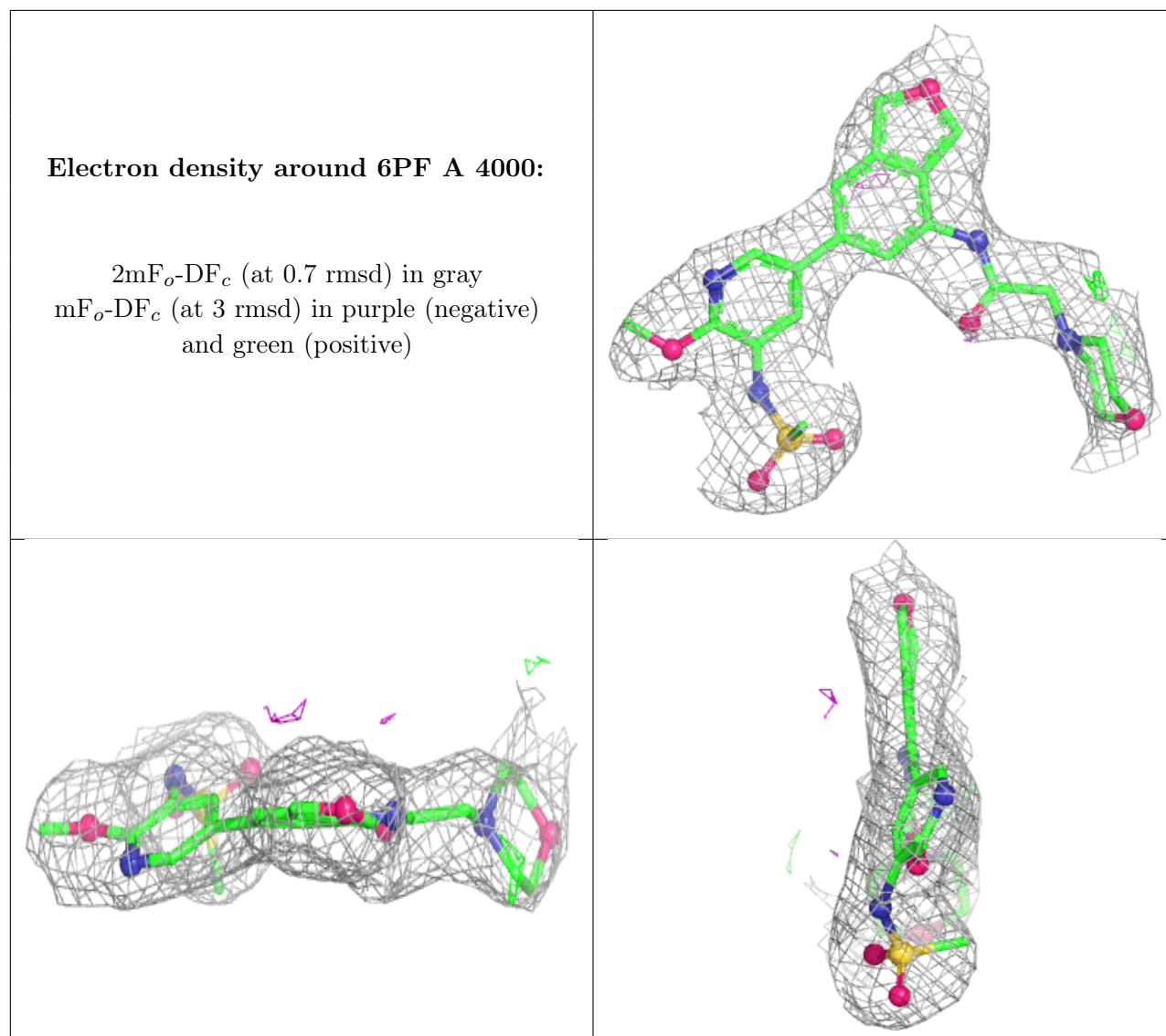
6.4 Ligands [i](#)

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	6PF	A	4000	32/32	0.92	0.12	34,44,81,83	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.