Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2022 – 04:24 pm BST

PDB ID	:	7Z61
Title	:	Crystal structure of PI3Kgamma with a dihydropurinone inhibitor (compound 18)
Authors	:	Goldberg, F.W.; Ting, A.K.T.; Schimpl, M.
Deposited on	:	2022-03-10
Resolution	:	2.74 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:

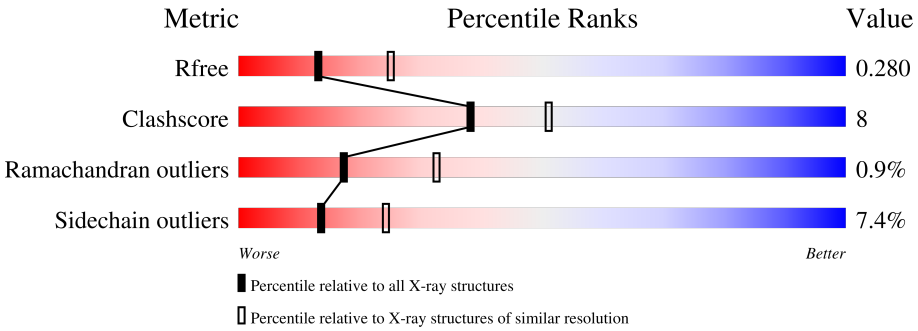
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	966	67% 17% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6778 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.

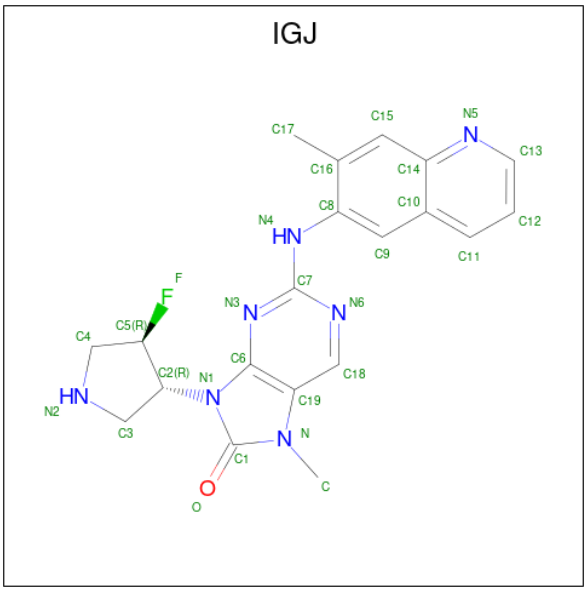
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	834	6749	4333	1148	1234	34	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 9-[(3 {R},4 {R})-4-fluoranylpyrrolidin-3-yl]-7-methyl-2-[(7-methylquinolin-6-yl)amino]purin-8-one (three-letter code: IGJ) (formula: $C_{20}H_{20}FN_7O$) (labeled as "Ligand of Interest" by depositor).



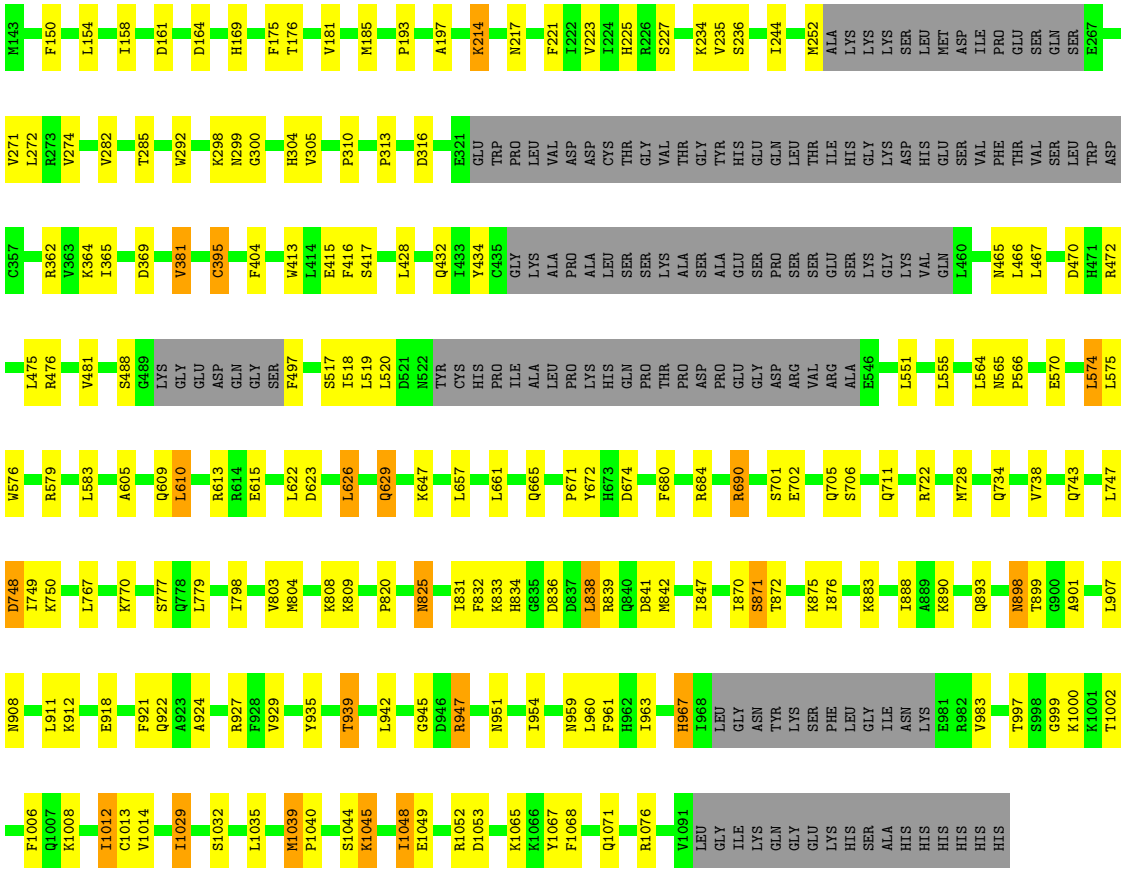
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	20	1	7	1		

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. 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. 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 gamma isoform

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.89Å 67.95Å 107.46Å 90.00° 95.92° 90.00°	Depositor
Resolution (Å)	62.21 – 2.74 62.21 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.9 (62.21-2.74) 98.8 (62.21-2.74)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.8 (24-FEB-2021)	Depositor
R, R_{free}	0.217 , 0.276 0.216 , 0.280	Depositor DCC
R_{free} test set	1317 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	111.9	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6778	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IGJ

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	0.42	0/6894	0.61	1/9328 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	898	ASN	C-N-CA	5.16	134.60	121.70

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	6749	0	6765	103	0
2	A	29	0	0	0	0
All	All	6778	0	6765	103	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 8.

All (103) 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:899:THR:HB	1:A:901:ALA:H	1.19	1.03
1:A:1000:LYS:H	1:A:1076:ARG:HH12	1.11	0.99
1:A:214:LYS:NZ	1:A:300:GLY:HA2	1.83	0.92
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.53	0.89
1:A:899:THR:HB	1:A:901:ALA:N	1.96	0.81
1:A:175:PHE:HD1	1:A:472:ARG:HH21	1.29	0.80
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.63	0.80
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.47	0.78
1:A:181:VAL:O	1:A:185:MET:HG3	1.84	0.77
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.67	0.76
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.03	0.76
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.54	0.72
1:A:497:PHE:HE1	1:A:1045:LYS:HZ3	1.38	0.72
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.55	0.72
1:A:497:PHE:HE1	1:A:1045:LYS:NZ	1.90	0.70
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.28	0.69
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.75	0.69
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.40	0.67
1:A:150:PHE:HE2	1:A:722:ARG:NH1	1.93	0.66
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.78	0.65
1:A:629:GLN:HG3	1:A:1029:ILE:HG13	1.78	0.65
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.97	0.65
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.81	0.63
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.34	0.63
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.81	0.61
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.37	0.60
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.84	0.59
1:A:432:GLN:NE2	1:A:434:TYR:OH	2.35	0.59
1:A:750:LYS:NZ	1:A:808:LYS:HE3	2.17	0.59
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.85	0.59
1:A:750:LYS:HE3	1:A:808:LYS:HA	1.86	0.57
1:A:888:ILE:HD12	1:A:907:LEU:HD11	1.85	0.57
1:A:748:ASP:HB3	1:A:770:LYS:NZ	2.19	0.57
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.87	0.57
1:A:481:VAL:HG22	1:A:517:SER:HB3	1.86	0.56
1:A:657:LEU:HD11	1:A:690:ARG:HG2	1.86	0.56
1:A:750:LYS:HZ1	1:A:808:LYS:HE3	1.71	0.56
1:A:890:LYS:HA	1:A:893:GLN:HG2	1.89	0.54
1:A:274:VAL:HG11	1:A:292:TRP:NE1	2.23	0.54
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.89	0.53
1:A:381:VAL:HB	1:A:404:PHE:HB2	1.90	0.53
1:A:833:LYS:HZ1	1:A:836:ASP:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:NH2	1:A:963:ILE:O	2.43	0.52
1:A:576:TRP:O	1:A:579:ARG:HB2	2.10	0.51
1:A:702:GLU:O	1:A:706:SER:HB3	2.11	0.51
1:A:274:VAL:CG2	1:A:292:TRP:CD1	2.94	0.51
1:A:362:ARG:NH2	1:A:413:TRP:CD1	2.79	0.51
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.93	0.50
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.24	0.50
1:A:235:VAL:HG13	1:A:244:ILE:HG21	1.93	0.50
1:A:929:VAL:HG11	1:A:1008:LYS:HD3	1.94	0.49
1:A:838:LEU:O	1:A:842:MET:HG3	2.12	0.49
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.48	0.49
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.76	0.49
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.46	0.49
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.12	0.48
1:A:825:ASN:ND2	1:A:825:ASN:H	2.11	0.48
1:A:833:LYS:NZ	1:A:836:ASP:HB2	2.29	0.48
1:A:834:HIS:HD2	1:A:876:ILE:HB	1.78	0.47
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.97	0.47
1:A:701:SER:HB2	1:A:871:SER:HB3	1.97	0.46
1:A:362:ARG:NH2	1:A:413:TRP:CG	2.83	0.46
1:A:169:HIS:CE1	1:A:466:LEU:HD12	2.50	0.46
1:A:274:VAL:CG1	1:A:292:TRP:NE1	2.79	0.46
1:A:623:ASP:HB3	1:A:626:LEU:HB2	1.98	0.46
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.97	0.46
1:A:912:LYS:NZ	1:A:921:PHE:CE2	2.79	0.46
1:A:395:CYS:SG	1:A:417:SER:OG	2.71	0.46
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.98	0.46
1:A:193:PRO:HB2	1:A:313:PRO:CB	2.40	0.45
1:A:235:VAL:HG11	1:A:244:ILE:HD13	1.98	0.45
1:A:734:GLN:O	1:A:738:VAL:HG23	2.17	0.45
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.99	0.44
1:A:1002:THR:HG23	1:A:1006:PHE:HD2	1.82	0.44
1:A:551:LEU:HD22	1:A:574:LEU:HD21	1.99	0.44
1:A:605:ALA:O	1:A:609:GLN:HG3	2.17	0.44
1:A:748:ASP:CB	1:A:770:LYS:NZ	2.80	0.43
1:A:661:LEU:O	1:A:665:GLN:HG2	2.19	0.43
1:A:298:LYS:NZ	1:A:299:ASN:HD21	2.16	0.43
1:A:583:LEU:HD13	1:A:610:LEU:HD13	2.00	0.43
1:A:671:PRO:HB2	1:A:672:TYR:CD1	2.54	0.43
1:A:747:LEU:CD2	1:A:834:HIS:CG	3.02	0.43
1:A:161:ASP:O	1:A:164:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:LEU:HD21	1:A:834:HIS:CG	2.53	0.43
1:A:911:LEU:HD22	1:A:924:ALA:HB1	2.00	0.43
1:A:176:THR:HG23	1:A:674:ASP:HB2	2.01	0.42
1:A:918:GLU:O	1:A:922:GLN:HG2	2.20	0.42
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.93	0.42
1:A:225:HIS:CE1	1:A:304:HIS:CD2	2.93	0.42
1:A:705:GLN:HG3	1:A:839:ARG:CZ	2.49	0.42
1:A:154:LEU:O	1:A:158:ILE:HG13	2.19	0.42
1:A:365:ILE:HD13	1:A:518:ILE:HG22	2.02	0.42
1:A:221:PHE:HE1	1:A:234:LYS:HG2	1.86	0.41
1:A:680:PHE:O	1:A:684:ARG:HG2	2.20	0.41
1:A:935:TYR:O	1:A:939:THR:HB	2.20	0.41
1:A:555:LEU:HD11	1:A:575:LEU:HD23	2.02	0.41
1:A:235:VAL:HG12	1:A:236:SER:N	2.35	0.41
1:A:272:LEU:HB3	1:A:305:VAL:HG11	2.03	0.41
1:A:169:HIS:CE1	1:A:466:LEU:CD1	3.04	0.41
1:A:467:LEU:O	1:A:476:ARG:HD2	2.21	0.41
1:A:747:LEU:HD21	1:A:834:HIS:CD2	2.56	0.41
1:A:197:ALA:HB2	1:A:316:ASP:OD2	2.21	0.41
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.55	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	820/966 (85%)	764 (93%)	49 (6%)	7 (1%)	17 32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	777	SER

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Mol	Chain	Res	Type
1	A	967	HIS
1	A	1044	SER
1	A	227	SER
1	A	999	GLY
1	A	798	ILE
1	A	809	LYS

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	746/864 (86%)	691 (93%)	55 (7%)	13 24

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	LYS
1	A	217	ASN
1	A	252	MET
1	A	282	VAL
1	A	285	THR
1	A	369	ASP
1	A	381	VAL
1	A	395	CYS
1	A	415	GLU
1	A	470	ASP
1	A	475	LEU
1	A	488	SER
1	A	520	LEU
1	A	570	GLU
1	A	574	LEU
1	A	610	LEU
1	A	613	ARG
1	A	615	GLU
1	A	626	LEU
1	A	629	GLN

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Mol	Chain	Res	Type
1	A	690	ARG
1	A	711	GLN
1	A	728	MET
1	A	748	ASP
1	A	749	ILE
1	A	779	LEU
1	A	820	PRO
1	A	825	ASN
1	A	832	PHE
1	A	838	LEU
1	A	841	ASP
1	A	870	ILE
1	A	871	SER
1	A	875	LYS
1	A	883	LYS
1	A	898	ASN
1	A	908	ASN
1	A	927	ARG
1	A	939	THR
1	A	947	ARG
1	A	951	ASN
1	A	954	ILE
1	A	959	ASN
1	A	960	LEU
1	A	967	HIS
1	A	983	VAL
1	A	997	THR
1	A	1012	ILE
1	A	1029	ILE
1	A	1032	SER
1	A	1039	MET
1	A	1045	LYS
1	A	1048	ILE
1	A	1049	GLU
1	A	1053	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	225	HIS
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	299	ASN
1	A	304	HIS
1	A	432	GLN
1	A	550	GLN
1	A	743	GLN
1	A	825	ASN
1	A	834	HIS
1	A	846	GLN
1	A	908	ASN

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 monosaccharides 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	IGJ	A	1201	-	31,33,33	0.26	0	39,49,49	1.46	3 (7%)

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	IGJ	A	1201	-	-	3/8/18/18	0/5/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	IGJ	C19-C6-N3	-5.88	122.20	126.51
2	A	1201	IGJ	C3-C2-N1	-4.12	106.94	113.55
2	A	1201	IGJ	C18-C19-N	3.76	137.36	131.37

There are no chirality outliers.

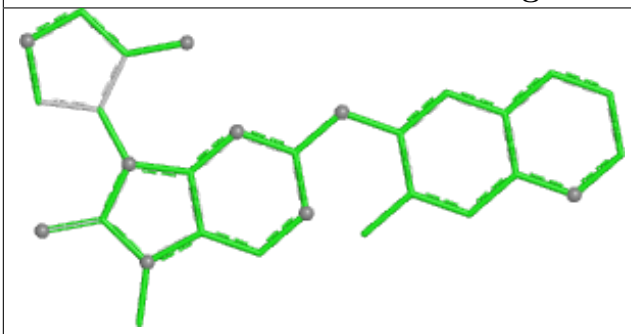
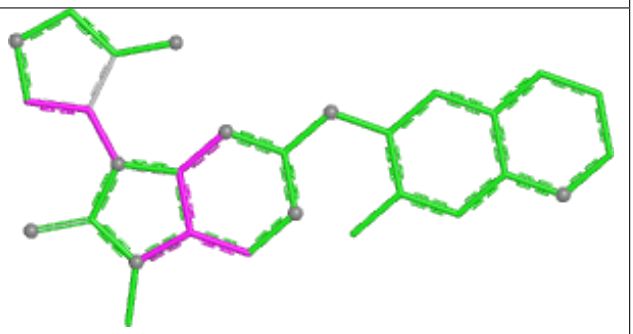
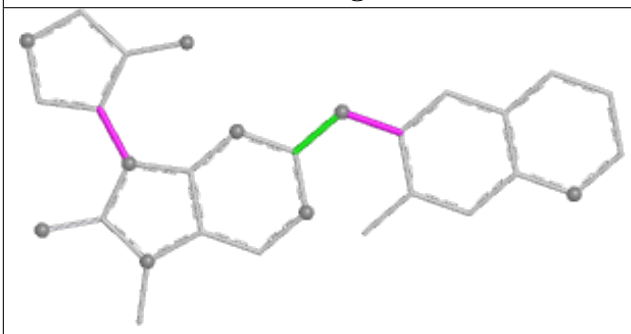
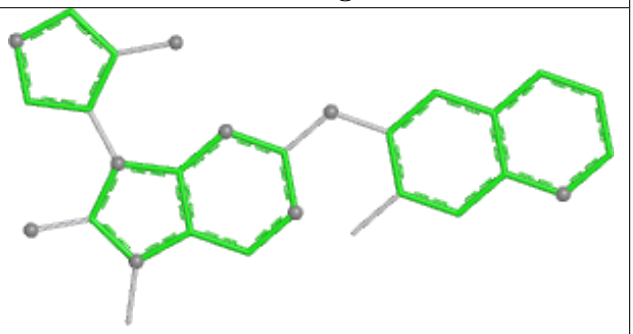
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	IGJ	C3-C2-N1-C1
2	A	1201	IGJ	C5-C2-N1-C6
2	A	1201	IGJ	C9-C8-N4-C7

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 then 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.

Ligand IGJ A 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

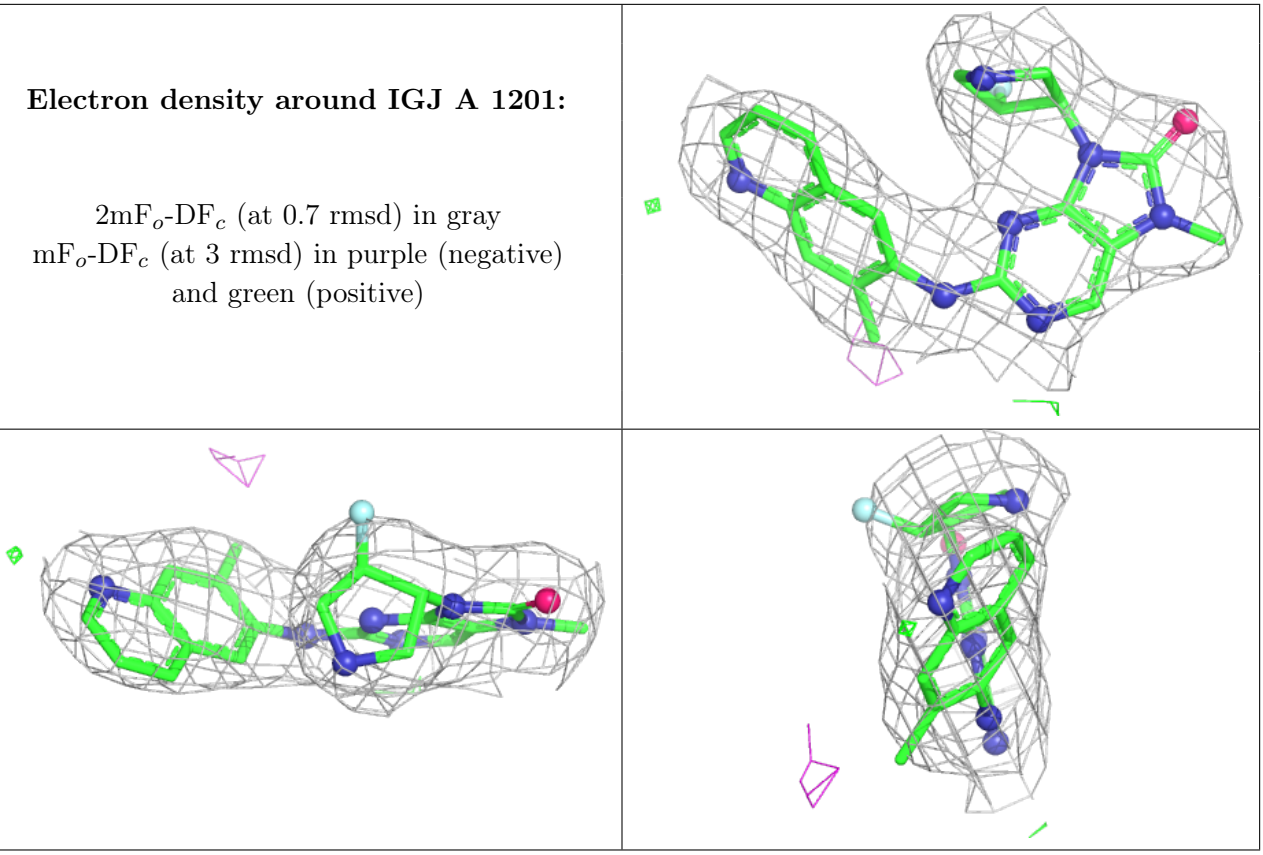
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 IGJ A 1201:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.