Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:06 PM BST

PDB ID	:	5T23
Title	:	PI3Kg IN COMPLEX WITH 5d
Authors	:	Petersen, J.; Terstige, I.; Perry, M.; Svensson, T.; Tyrchan, C.; Lindmark, H.; Oster, L.
Deposited on	:	2016-08-23
Resolution	:	2.78 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 following versions of software and data (see references ⓘ) were used in the production of this report:

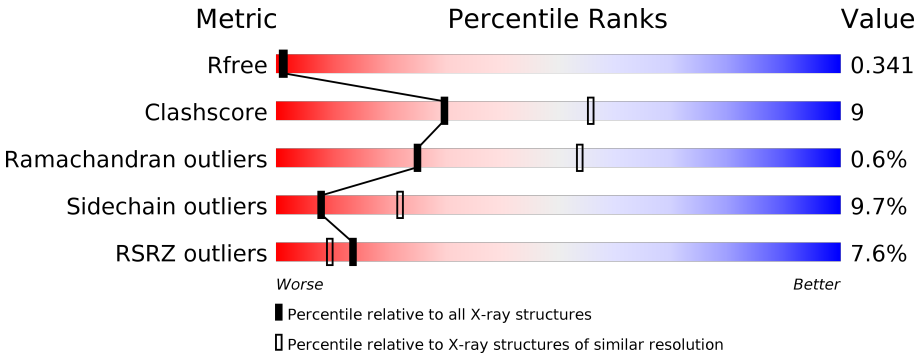
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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% 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	966	6% 61% 19% • 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6581 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.

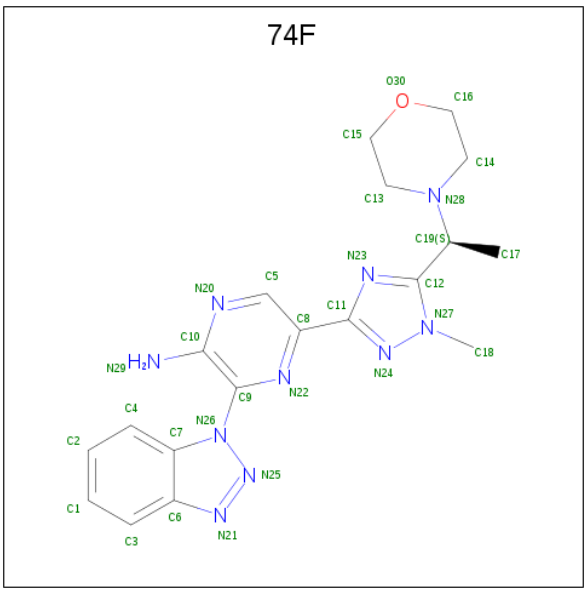
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	804	6534	4201	1115	1183	35	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 3-(benzotriazol-1-yl)-5-[1-methyl-5-[(1 {S})-1-morpholin-4-ylethyl]-1,2,4-triazol-3-yl]pyrazin-2-amine (three-letter code: 74F) (formula: $C_{19}H_{22}N_{10}O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	19	10	1		

- Molecule 3 is water.

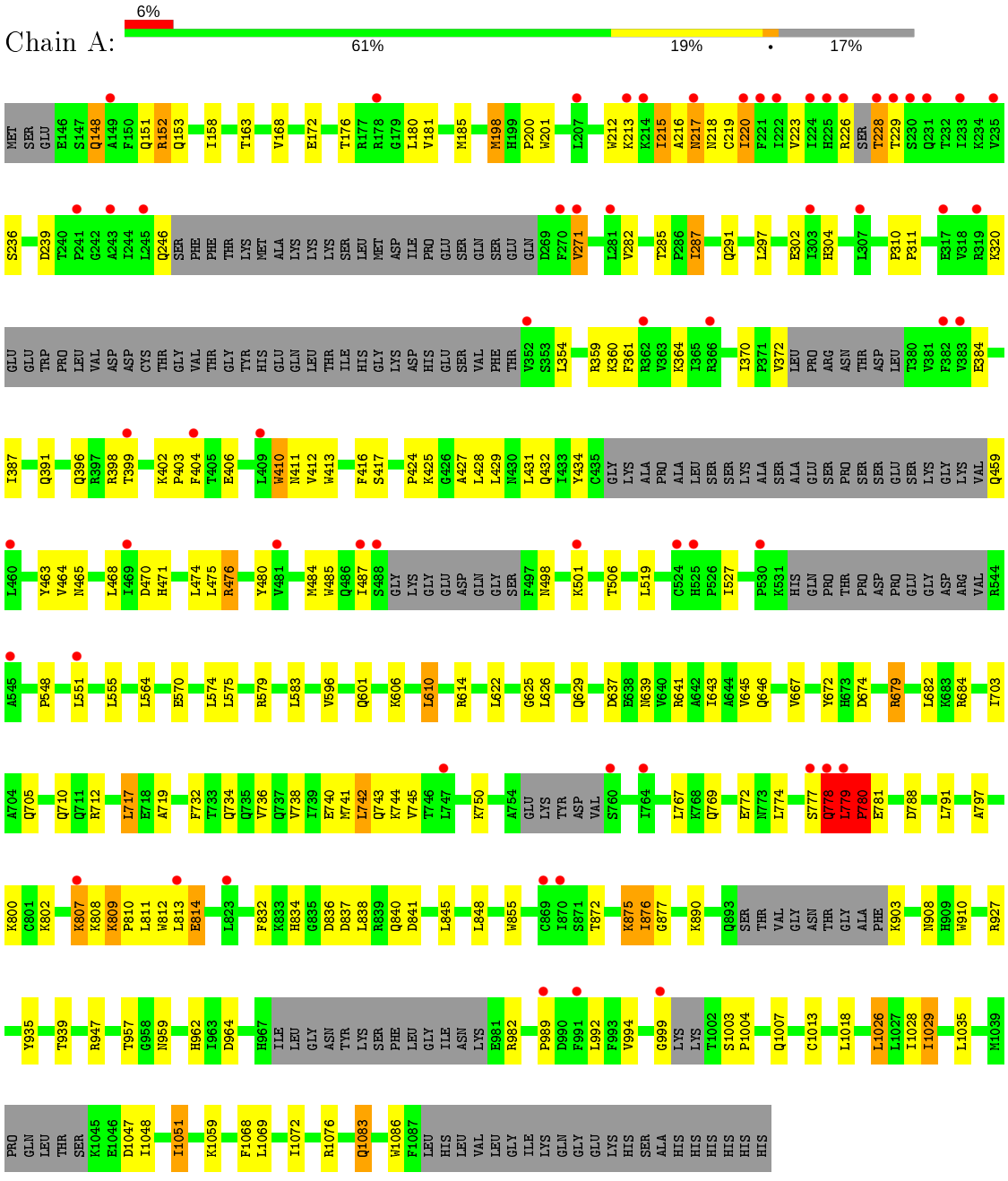
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		

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: 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	144.15Å 68.21Å 106.81Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	41.06 – 2.78 40.98 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.06-2.78) 98.6 (40.98-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.77Å)	Xtriage
Refinement program	BUSTER-TNT 5.6.0117, REFMAC 5.6.0117	Depositor
R, R_{free}	0.255 , 0.339 0.257 , 0.341	Depositor DCC
R_{free} test set	1317 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	78.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6581	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: 74F

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	0.50	6/6671 (0.1%)	0.56	1/9019 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	TRP	CD2-CE2	5.33	1.47	1.41
1	A	1086	TRP	CD2-CE2	5.33	1.47	1.41
1	A	485	TRP	CD2-CE2	5.31	1.47	1.41
1	A	413	TRP	CD2-CE2	5.22	1.47	1.41
1	A	855	TRP	CD2-CE2	5.20	1.47	1.41
1	A	910	TRP	CD2-CE2	5.12	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	779	LEU	N-CA-C	6.00	127.19	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ASN	Peptide
1	A	778	GLN	Peptide
1	A	779	LEU	Peptide

5.2 Too-close contacts (i)

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	6534	0	6570	123	0
2	A	30	0	0	1	0
3	A	17	0	0	2	0
All	All	6581	0	6570	124	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 9.

All (124) 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:215:ILE:HD12	1:A:215:ILE:H	1.20	1.07
1:A:216:ALA:O	1:A:219:CYS:N	1.91	1.01
1:A:181:VAL:O	1:A:185:MET:HG2	1.62	1.00
1:A:947:ARG:HG2	1:A:947:ARG:HH11	1.42	0.85
1:A:614:ARG:HH22	1:A:643:ILE:HG22	1.45	0.81
1:A:732:PHE:O	1:A:736:VAL:HG23	1.83	0.78
1:A:198:MET:HG2	1:A:282:VAL:HG21	1.64	0.78
1:A:548:PRO:HG2	1:A:551:LEU:HD13	1.69	0.72
2:A:1201:74F:N25	2:A:1201:74F:N29	2.37	0.72
1:A:744:LYS:HD2	1:A:744:LYS:H	1.54	0.72
1:A:777:SER:O	1:A:778:GLN:O	2.08	0.71
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.57	0.70
1:A:148:GLN:O	1:A:152:ARG:NH2	2.25	0.70
1:A:198:MET:HG2	1:A:282:VAL:CG2	2.23	0.69
1:A:506:THR:HG21	3:A:1309:HOH:O	1.92	0.69
1:A:152:ARG:CZ	1:A:152:ARG:H	2.08	0.67
1:A:774:LEU:O	1:A:778:GLN:O	2.13	0.67
1:A:740:GLU:O	1:A:744:LYS:HD3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:HG2	1:A:947:ARG:NH1	2.12	0.65
1:A:215:ILE:CD1	1:A:215:ILE:H	1.98	0.65
1:A:215:ILE:HD12	1:A:215:ILE:N	2.04	0.65
1:A:872:THR:OG1	1:A:877:GLY:HA2	1.97	0.64
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.80	0.64
1:A:1028:ILE:HD13	1:A:1051:ILE:HG23	1.79	0.64
1:A:999:GLY:HA2	1:A:1076:ARG:HE	1.63	0.63
1:A:808:LYS:O	1:A:810:PRO:HD3	1.97	0.63
1:A:198:MET:CE	1:A:311:PRO:HD2	2.29	0.63
1:A:836:ASP:C	1:A:875:LYS:HZ1	2.02	0.62
1:A:463:TYR:HD2	1:A:487:ILE:HD11	1.63	0.62
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.82	0.62
1:A:744:LYS:N	1:A:744:LYS:HD2	2.15	0.60
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.37	0.59
1:A:471:HIS:H	1:A:471:HIS:CD2	2.20	0.59
1:A:625:GLY:O	1:A:629:GLN:HG3	2.03	0.58
1:A:807:LYS:HD2	1:A:807:LYS:H	1.68	0.57
1:A:402:LYS:HB3	1:A:403:PRO:HD2	1.87	0.57
1:A:498:ASN:HB3	1:A:501:LYS:HD3	1.85	0.57
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.87	0.57
1:A:239:ASP:HB2	1:A:287:ILE:HD11	1.88	0.56
1:A:198:MET:HE1	1:A:311:PRO:HD2	1.88	0.56
1:A:387:ILE:N	1:A:387:ILE:HD12	2.21	0.56
1:A:1035:LEU:HD12	1:A:1048:ILE:HG13	1.88	0.56
1:A:1083:GLN:HA	1:A:1083:GLN:HE21	1.70	0.55
1:A:750:LYS:HD2	1:A:809:LYS:H	1.73	0.53
1:A:667:VAL:HG12	1:A:712:ARG:HD3	1.90	0.53
1:A:151:GLN:H	1:A:152:ARG:HH22	1.55	0.52
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.91	0.52
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.25	0.52
1:A:750:LYS:HE2	1:A:834:HIS:HB3	1.92	0.52
1:A:750:LYS:HE2	1:A:834:HIS:CD2	2.44	0.52
1:A:641:ARG:O	1:A:645:VAL:HG23	2.10	0.52
1:A:779:LEU:CD2	1:A:779:LEU:N	2.73	0.52
1:A:734:GLN:O	1:A:738:VAL:HG23	2.09	0.51
1:A:464:VAL:HB	1:A:484:MET:HG2	1.92	0.51
1:A:198:MET:HB3	1:A:200:PRO:HD3	1.92	0.51
1:A:779:LEU:HD23	1:A:780:PRO:N	2.26	0.50
1:A:836:ASP:C	1:A:875:LYS:NZ	2.65	0.50
1:A:360:LYS:HE3	1:A:417:SER:HA	1.93	0.50
1:A:402:LYS:HB3	1:A:403:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ASP:OD2	1:A:679:ARG:NH2	2.47	0.48
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.96	0.48
1:A:425:LYS:HE2	1:A:672:TYR:CE2	2.49	0.48
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.96	0.47
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.44	0.47
1:A:398:ARG:HG2	1:A:399:THR:N	2.29	0.47
1:A:354:LEU:HD11	1:A:475:LEU:HD13	1.96	0.47
1:A:476:ARG:HG2	1:A:480:TYR:OH	2.13	0.47
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.96	0.47
1:A:927:ARG:HH11	1:A:959:ASN:ND2	2.11	0.47
1:A:875:LYS:NZ	1:A:875:LYS:HA	2.30	0.47
1:A:172:GLU:O	1:A:176:THR:HG22	2.15	0.47
1:A:811:LEU:HD23	1:A:813:LEU:HD11	1.97	0.47
1:A:738:VAL:HG12	1:A:742:LEU:HD22	1.97	0.46
1:A:152:ARG:NH1	1:A:153:GLN:H	2.14	0.46
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.80	0.46
1:A:387:ILE:HD11	1:A:416:PHE:CD1	2.51	0.46
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.50	0.46
1:A:779:LEU:HD23	1:A:779:LEU:N	2.31	0.46
1:A:219:CYS:SG	1:A:220:ILE:N	2.89	0.45
1:A:927:ARG:HH11	1:A:959:ASN:HD22	1.63	0.45
1:A:947:ARG:NH2	1:A:964:ASP:O	2.50	0.45
1:A:216:ALA:O	1:A:218:ASN:N	2.49	0.45
1:A:158:ILE:HG12	1:A:717:LEU:HD13	1.97	0.45
1:A:779:LEU:H	1:A:779:LEU:HD23	1.81	0.45
1:A:1003:SER:HB3	1:A:1004:PRO:HD2	1.99	0.45
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.52	0.45
1:A:470:ASP:HA	1:A:476:ARG:HH12	1.81	0.45
1:A:639:ASN:H	1:A:639:ASN:HD22	1.64	0.44
1:A:935:TYR:O	1:A:939:THR:OG1	2.28	0.44
1:A:387:ILE:HD11	1:A:416:PHE:CE1	2.52	0.44
1:A:639:ASN:ND2	1:A:639:ASN:H	2.16	0.44
1:A:198:MET:HE3	1:A:311:PRO:HD2	1.98	0.44
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.98	0.44
1:A:474:LEU:HB2	3:A:1311:HOH:O	2.18	0.44
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.99	0.44
1:A:361:PHE:CD2	1:A:416:PHE:HD2	2.36	0.44
1:A:742:LEU:HD23	1:A:832:PHE:CE2	2.53	0.43
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.18	0.43
1:A:606:LYS:O	1:A:610:LEU:HB2	2.18	0.43
1:A:788:ASP:OD2	1:A:791:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:ILE:HG13	1:A:877:GLY:N	2.33	0.43
1:A:703:ILE:HG23	1:A:710:GLN:HB2	2.01	0.43
1:A:228:THR:HG23	1:A:229:THR:H	1.84	0.42
1:A:682:LEU:HD11	1:A:719:ALA:HB1	2.01	0.42
1:A:750:LYS:HG3	1:A:809:LYS:HB2	2.01	0.42
1:A:777:SER:O	1:A:778:GLN:HB2	2.19	0.42
1:A:947:ARG:HD3	1:A:962:HIS:ND1	2.34	0.42
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.20	0.42
1:A:370:ILE:O	1:A:406:GLU:HB2	2.20	0.41
1:A:370:ILE:HG13	1:A:372:VAL:H	1.84	0.41
1:A:797:ALA:HB3	1:A:814:GLU:HB3	2.00	0.41
1:A:434:TYR:HA	1:A:459:GLN:O	2.20	0.41
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.84	0.41
1:A:198:MET:SD	1:A:282:VAL:HG11	2.59	0.41
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	2.01	0.41
1:A:637:ASP:O	1:A:641:ARG:HG3	2.20	0.41
1:A:152:ARG:CZ	1:A:152:ARG:N	2.81	0.41
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.02	0.41
1:A:212:TRP:HA	1:A:215:ILE:HD11	1.20	0.41
1:A:741:MET:O	1:A:745:VAL:HG23	2.21	0.41
1:A:501:LYS:HD2	1:A:501:LYS:N	2.36	0.40
1:A:837:ASP:HB3	1:A:840:GLN:NE2	2.36	0.40
1:A:802:LYS:HG3	1:A:812:TRP:HB3	2.03	0.40
1:A:684:ARG:HA	1:A:684:ARG:HD2	1.86	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	778/966 (80%)	721 (93%)	52 (7%)	5 (1%)	25 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	779	LEU
1	A	778	GLN
1	A	217	ASN
1	A	780	PRO
1	A	957	THR

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	723/864 (84%)	653 (90%)	70 (10%)	8 22

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	152	ARG
1	A	163	THR
1	A	168	VAL
1	A	180	LEU
1	A	198	MET
1	A	213	LYS
1	A	215	ILE
1	A	220	ILE
1	A	223	VAL
1	A	226	ARG
1	A	228	THR
1	A	246	GLN
1	A	271	VAL
1	A	285	THR
1	A	287	ILE
1	A	297	LEU
1	A	320	LYS
1	A	359	ARG
1	A	384	GLU

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	396	GLN
1	A	404	PHE
1	A	411	ASN
1	A	431	LEU
1	A	432	GLN
1	A	476	ARG
1	A	527	ILE
1	A	555	LEU
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	583	LEU
1	A	596	VAL
1	A	601	GLN
1	A	610	LEU
1	A	622	LEU
1	A	626	LEU
1	A	646	GLN
1	A	679	ARG
1	A	705	GLN
1	A	717	LEU
1	A	742	LEU
1	A	767	LEU
1	A	769	GLN
1	A	772	GLU
1	A	779	LEU
1	A	780	PRO
1	A	781	GLU
1	A	800	LYS
1	A	807	LYS
1	A	809	LYS
1	A	814	GLU
1	A	838	LEU
1	A	841	ASP
1	A	845	LEU
1	A	848	LEU
1	A	875	LYS
1	A	876	ILE
1	A	890	LYS
1	A	903	LYS
1	A	982	ARG

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Mol	Chain	Res	Type
1	A	1007	GLN
1	A	1018	LEU
1	A	1026	LEU
1	A	1029	ILE
1	A	1047	ASP
1	A	1051	ILE
1	A	1059	LYS
1	A	1083	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	153	GLN
1	A	218	ASN
1	A	246	GLN
1	A	291	GLN
1	A	299	ASN
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	392	GLN
1	A	471	HIS
1	A	498	ASN
1	A	512	ASN
1	A	554	GLN
1	A	601	GLN
1	A	639	ASN
1	A	646	GLN
1	A	662	GLN
1	A	743	GLN
1	A	769	GLN
1	A	776	ASN
1	A	834	HIS
1	A	909	HIS
1	A	951	ASN
1	A	959	ASN
1	A	1023	HIS
1	A	1083	GLN
1	A	1085	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 monosaccharides 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	74F	A	1201	-	29,34,34	1.11	2 (6%)	33,49,49	1.59	7 (21%)

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	74F	A	1201	-	-	4/9/24/24	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	74F	C10-N29	2.38	1.40	1.34
2	A	1201	74F	C12-N23	-2.04	1.31	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	74F	C5-N20-C10	-3.78	114.84	118.70
2	A	1201	74F	C8-N22-C9	-3.08	113.92	117.45
2	A	1201	74F	C1-C3-C6	-2.96	115.82	120.08
2	A	1201	74F	C2-C4-C7	-2.49	114.67	119.44
2	A	1201	74F	N21-N25-N26	2.41	109.05	106.37
2	A	1201	74F	C5-C8-N22	2.34	122.81	119.82
2	A	1201	74F	C16-C14-N28	-2.21	107.55	109.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	74F	C12-C19-N28-C13
2	A	1201	74F	C12-C19-N28-C14
2	A	1201	74F	C17-C19-N28-C13
2	A	1201	74F	C17-C19-N28-C14

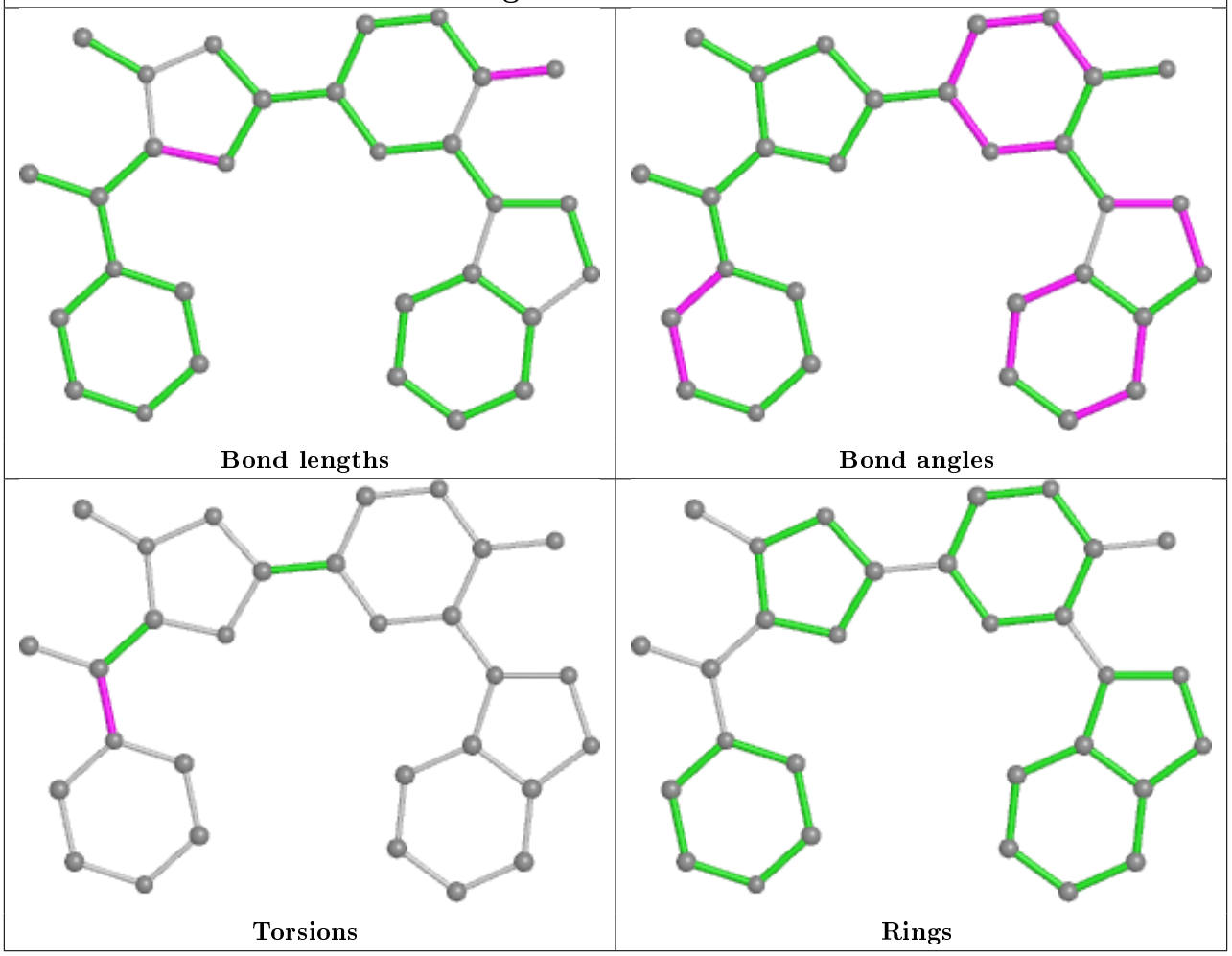
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	74F	1	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 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 74F A 1201



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

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, 95^{th} 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	804/966 (83%)	0.56	61 (7%) 13 9	39, 85, 124, 155	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	PHE	5.8
1	A	823	LEU	5.6
1	A	778	GLN	4.7
1	A	747	LEU	4.3
1	A	488	SER	4.0
1	A	999	GLY	3.9
1	A	217	ASN	3.9
1	A	487	ILE	3.7
1	A	869	CYS	3.6
1	A	207	LEU	3.5
1	A	149	ALA	3.3
1	A	307	LEU	3.3
1	A	271	VAL	3.3
1	A	213	LYS	3.3
1	A	525	HIS	3.2
1	A	362	ARG	3.1
1	A	319	ARG	3.1
1	A	220	ILE	3.1
1	A	226	ARG	3.1
1	A	245	LEU	3.1
1	A	989	PRO	3.0
1	A	281	LEU	3.0
1	A	231	GLN	2.9
1	A	235	VAL	2.9
1	A	481	VAL	2.9
1	A	352	VAL	2.8
1	A	779	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	524	CYS	2.7
1	A	870	ILE	2.7
1	A	460	LEU	2.7
1	A	241	PRO	2.6
1	A	303	ILE	2.6
1	A	551	LEU	2.6
1	A	224	ILE	2.5
1	A	383	VAL	2.5
1	A	233	ILE	2.4
1	A	777	SER	2.4
1	A	409	LEU	2.4
1	A	214	LYS	2.4
1	A	225	HIS	2.4
1	A	229	THR	2.4
1	A	382	PHE	2.4
1	A	243	ALA	2.3
1	A	813	LEU	2.3
1	A	230	SER	2.3
1	A	501	LYS	2.3
1	A	317	GLU	2.3
1	A	404	PHE	2.3
1	A	991	PHE	2.3
1	A	545	ALA	2.2
1	A	469	ILE	2.2
1	A	764	ILE	2.2
1	A	399	THR	2.1
1	A	178	ARG	2.1
1	A	222	ILE	2.1
1	A	221	PHE	2.1
1	A	530	PRO	2.1
1	A	228	THR	2.1
1	A	760	SER	2.0
1	A	366	ARG	2.0
1	A	807	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

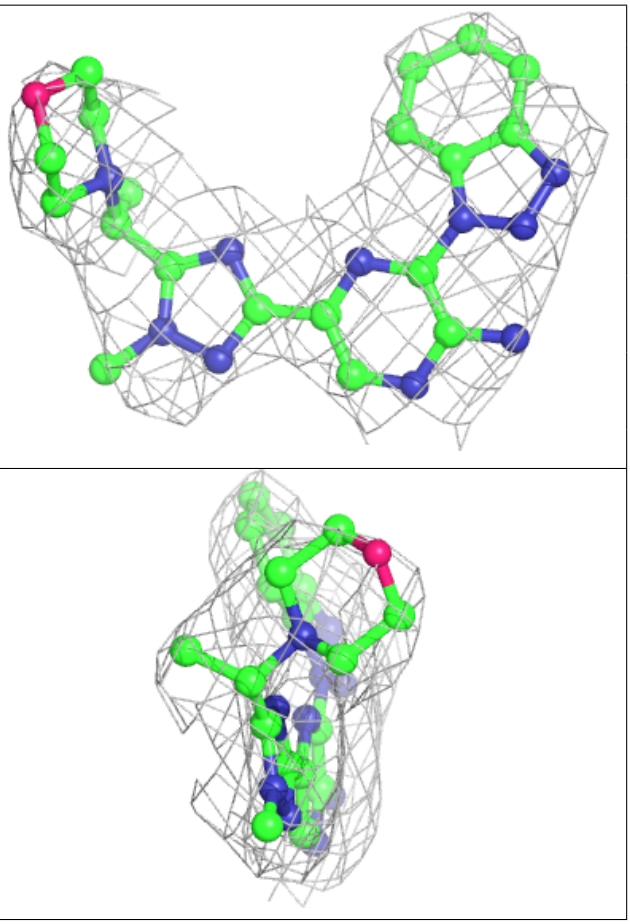
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	74F	A	1201	30/30	0.92	0.20	84,89,103,107	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 74F 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)

There are no such residues in this entry.