Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2022 – 09:28 pm BST

PDB ID	:	7PG6
Title	:	Crystal Structure of PI3Kalpha in complex with the inhibitor NVP-BYL719
Authors	:	Gong, G.; Pinotsis, N.; Williams, R.L.; Vanhaesebroeck, B.
Deposited on	:	2021-08-13
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

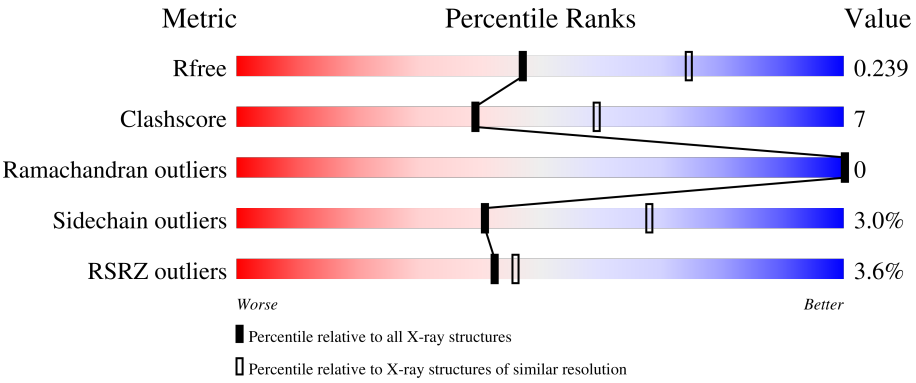
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	1068	2% 77% 18%
2	B	287	9% 70% 21% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10727 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 alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1026	8415	5375	1452	1521	67	0	5	0

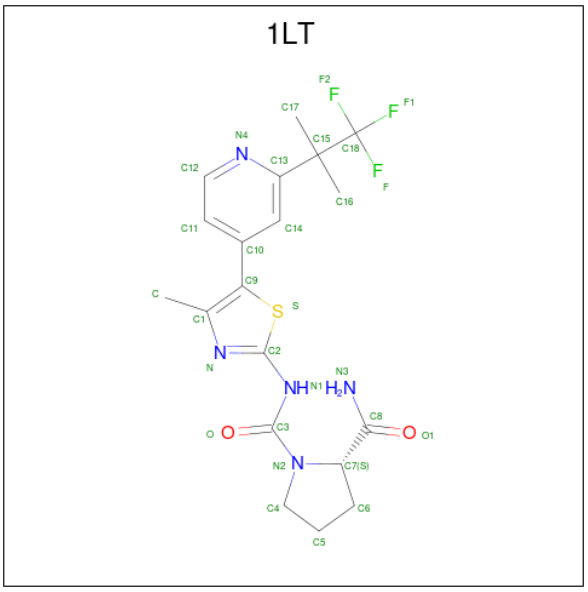
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	LYS	MET	engineered mutation	UNP P42336
A	233	LYS	LEU	engineered mutation	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	266	2222	1391	394	431	6	0	0	0

- Molecule 3 is (2S)-N 1 -{4-methyl-5-[2-(1,1,1-trifluoro-2-methylpropan-2-yl)pyridin-4-yl]-1,3-thiazol-2-yl}pyrrolidine-1,2-dicarboxamide (three-letter code: 1LT) (formula: $C_{19}H_{22}F_3N_5O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O S 30 19 3 5 2 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is water.

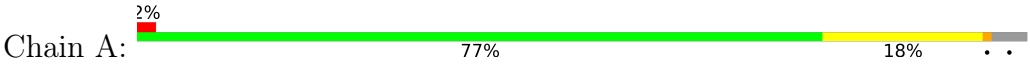
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	B	3	Total O 3 3	0	0

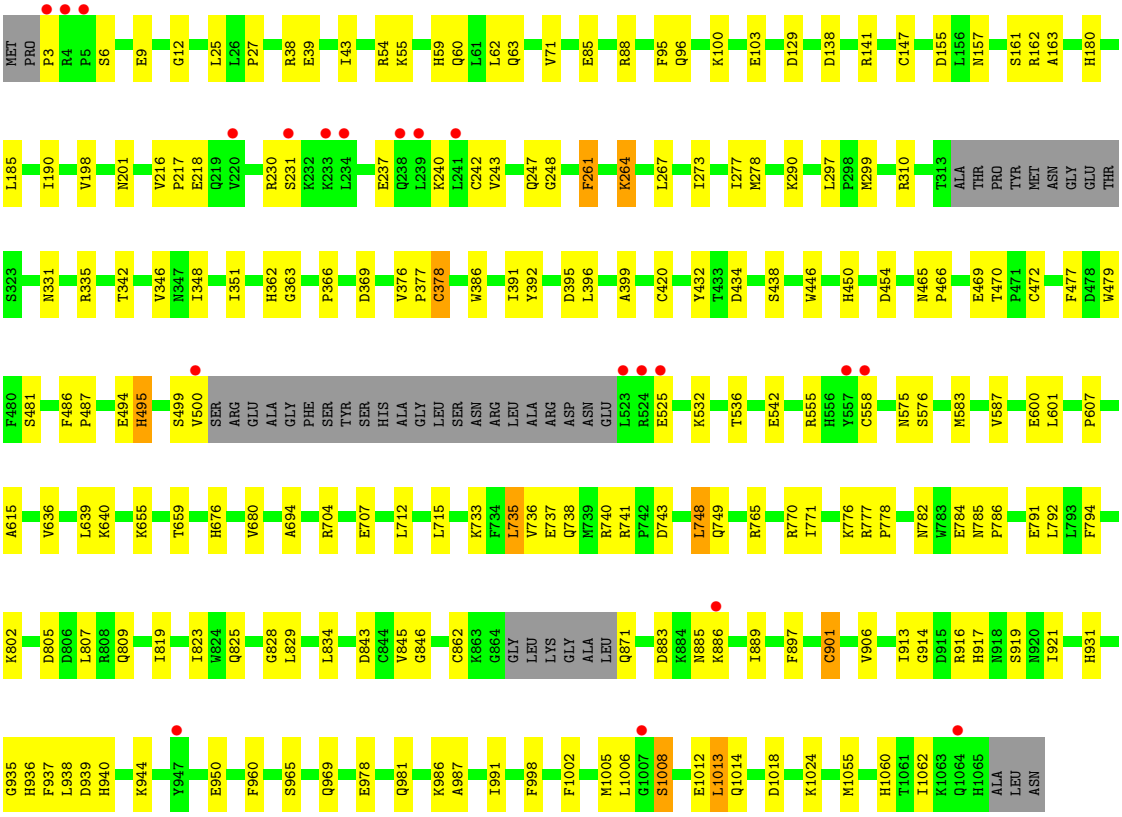
3 Residue-property plots (i)

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 alpha isoform

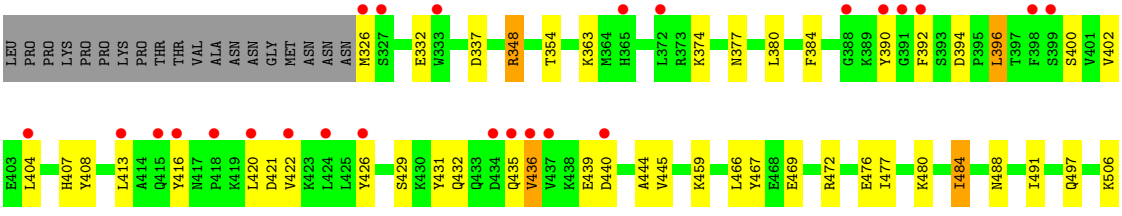
Chain A:

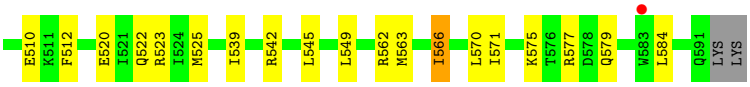




• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B:




E510
K511
F512
E520
I521
Q522
R523
I524
M525
I539
R542
L545
L549
R562
M563
I566
L570
I571
K575
T576
R577
D578
Q579
W583
L584
Q591
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.87Å 105.19Å 135.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.50 49.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.04-2.50) 99.9 (49.04-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.187 , 0.240 0.192 , 0.239	Depositor DCC
R_{free} test set	2632 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10727	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: NA, 1LT

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	0.44	0/8604	0.62	2/11628 (0.0%)
2	B	0.40	0/2260	0.56	0/3036
All	All	0.43	0/10864	0.61	2/14664 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1013	LEU	CA-CB-CG	7.94	133.56	115.30
1	A	748	LEU	CA-CB-CG	-5.16	103.42	115.30

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	8415	0	8395	122	0
2	B	2222	0	2156	44	0
3	A	30	0	21	0	0
4	A	1	0	0	0	0
5	A	56	0	0	5	0
5	B	3	0	0	0	0
All	All	10727	0	10572	157	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 7.

All (157) 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)
2:B:488:ASN:OD1	2:B:542:ARG:NH1	2.16	0.78
2:B:396:LEU:HD12	2:B:396:LEU:H	1.53	0.73
1:A:157:ASN:HB2	1:A:161:SER:HB3	1.71	0.72
1:A:162:ARG:NH1	1:A:299:MET:SD	2.63	0.72
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.74	0.70
1:A:55:LYS:O	2:B:523:ARG:NH2	2.26	0.68
1:A:1005:MET:O	1:A:1008:SER:HB3	1.94	0.68
1:A:771:ILE:HG21	1:A:777:ARG:HD3	1.76	0.66
1:A:776:LYS:NZ	1:A:805:ASP:OD1	2.28	0.66
1:A:871:GLN:N	5:A:1203:HOH:O	2.29	0.65
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.81	0.63
1:A:71:VAL:HG13	1:A:100:LYS:HB3	1.79	0.63
1:A:138:ASP:OD2	1:A:432:TYR:OH	2.06	0.63
1:A:346:VAL:HG21	1:A:378:CYS:HB3	1.80	0.63
1:A:712:LEU:HD21	1:A:748:LEU:HD21	1.81	0.62
1:A:935:GLY:O	1:A:936:HIS:ND1	2.33	0.61
1:A:829:LEU:HD11	1:A:986:LYS:HB3	1.82	0.61
1:A:978:GLU:HA	1:A:981:GLN:HE21	1.66	0.60
1:A:1006:LEU:HD23	1:A:1013:LEU:HD23	1.84	0.60
2:B:413:LEU:H	2:B:421:ASP:HA	1.65	0.60
1:A:335:ARG:HG2	1:A:386:TRP:CE3	2.37	0.59
1:A:25:LEU:HD13	2:B:497:GLN:HG3	1.84	0.59
2:B:374:LYS:HD3	2:B:422:VAL:HG21	1.83	0.59
1:A:95:PHE:CD2	1:A:96:GLN:HG2	2.37	0.59
2:B:407:HIS:O	2:B:407:HIS:ND1	2.36	0.58
1:A:348:ILE:HD12	1:A:348:ILE:H	1.69	0.58
1:A:9:GLU:OE2	1:A:38:ARG:NH2	2.35	0.58
1:A:454:ASP:HA	2:B:348:ARG:HH11	1.69	0.57
1:A:1055:MET:HB3	1:A:1060:HIS:HA	1.87	0.56
2:B:392:PHE:HD2	2:B:416:TYR:HB2	1.71	0.56
1:A:267:LEU:HG	1:A:273:ILE:HG13	1.87	0.56
1:A:216:VAL:HG22	1:A:264:LYS:O	2.06	0.55
2:B:522:GLN:HA	2:B:525:MET:HE2	1.87	0.55
1:A:495:HIS:O	1:A:495:HIS:ND1	2.37	0.55
1:A:138:ASP:OD1	1:A:141:ARG:NH2	2.39	0.55
2:B:562:ARG:O	2:B:566:ILE:HD13	2.07	0.54
1:A:1002:PHE:HD1	1:A:1013:LEU:HD11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:NE2	1:A:103:GLU:OE1	2.37	0.54
1:A:450:HIS:HB2	2:B:467:TYR:CZ	2.42	0.54
2:B:354:THR:HA	2:B:426:TYR:O	2.08	0.54
2:B:469:GLU:OE1	2:B:472:ARG:NH2	2.38	0.54
1:A:240:LYS:HA	1:A:243:VAL:HB	1.90	0.54
1:A:791:GLU:H	1:A:791:GLU:CD	2.10	0.54
2:B:459:LYS:HG2	2:B:570:LEU:HD13	1.89	0.54
1:A:190:ILE:HD12	1:A:277:ILE:HG12	1.89	0.54
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.90	0.54
1:A:1014:GLN:N	1:A:1018:ASP:OD2	2.32	0.52
1:A:897:PHE:O	1:A:901:CYS:HB2	2.09	0.52
2:B:436:VAL:HG21	2:B:579:GLN:NE2	2.23	0.52
1:A:885:ASN:HB3	1:A:889:ILE:HG13	1.91	0.52
1:A:180:HIS:HD1	1:A:828:GLY:HA2	1.75	0.52
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.91	0.52
1:A:765:ARG:NH2	1:A:784:GLU:HG2	2.25	0.52
1:A:147:CYS:HB3	1:A:694:ALA:HB2	1.92	0.52
1:A:819:ILE:O	1:A:823:ILE:HG12	2.10	0.51
1:A:542:GLU:HB3	2:B:380:LEU:HD13	1.92	0.51
1:A:738:GLN:OE1	1:A:741:ARG:NH1	2.43	0.51
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.46	0.51
2:B:512:PHE:CZ	2:B:520:GLU:HG2	2.46	0.51
1:A:937:PHE:CD1	1:A:938:LEU:HG	2.45	0.50
1:A:331:ASN:OD1	1:A:392:TYR:OH	2.25	0.50
1:A:809:GLN:HE22	1:A:1012:GLU:HG3	1.77	0.49
1:A:261:PHE:N	1:A:261:PHE:CD1	2.81	0.49
2:B:512:PHE:CE1	2:B:520:GLU:HG2	2.47	0.49
1:A:1062:ILE:H	1:A:1062:ILE:HD12	1.78	0.48
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.94	0.48
1:A:438:SER:HA	1:A:477:PHE:HB2	1.95	0.48
2:B:332:GLU:OE2	2:B:429:SER:HB2	2.13	0.48
1:A:897:PHE:HZ	1:A:960:PHE:HD1	1.61	0.48
1:A:243:VAL:O	1:A:247:GLN:HB2	2.12	0.48
1:A:39:GLU:HB2	1:A:88:ARG:HH11	1.78	0.48
1:A:479:TRP:CZ2	1:A:481:SER:HA	2.48	0.48
2:B:326:MET:N	2:B:402:VAL:HG11	2.29	0.48
1:A:366:PRO:HD2	2:B:377:ASN:OD1	2.13	0.48
2:B:390:TYR:CE2	2:B:400:SER:HA	2.49	0.48
1:A:583:MET:O	1:A:587:VAL:HG23	2.14	0.48
1:A:937:PHE:HD1	1:A:938:LEU:HG	1.78	0.48
1:A:991:ILE:HG23	1:A:998:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:LYS:HE2	1:A:737:GLU:OE2	2.14	0.47
2:B:392:PHE:CZ	2:B:404:LEU:HD21	2.49	0.47
1:A:917:HIS:CE1	1:A:919:SER:HB2	2.48	0.47
1:A:555:ARG:O	1:A:558:CYS:HB2	2.14	0.47
1:A:944:LYS:O	2:B:577:ARG:NH1	2.45	0.47
1:A:499:SER:OG	1:A:500:VAL:N	2.48	0.47
1:A:655:LYS:O	1:A:659:THR:HG23	2.14	0.47
2:B:484:ILE:HG13	2:B:545:LEU:HD23	1.97	0.47
1:A:479:TRP:CE2	1:A:481:SER:HA	2.50	0.47
1:A:770[B]:ARG:NH2	5:A:1201:HOH:O	2.12	0.47
1:A:3:PRO:HB3	2:B:472:ARG:NH1	2.30	0.47
2:B:337:ASP:HB2	2:B:363:LYS:NZ	2.30	0.46
1:A:765:ARG:HD2	1:A:782:ASN:ND2	2.30	0.46
1:A:216:VAL:HG13	1:A:217:PRO:HD2	1.98	0.46
1:A:777:ARG:N	1:A:778:PRO:HD3	2.30	0.46
2:B:440:ASP:OD1	2:B:440:ASP:N	2.42	0.46
1:A:335:ARG:HG2	1:A:386:TRP:HE3	1.81	0.46
1:A:362:HIS:CD2	1:A:399:ALA:HB3	2.50	0.46
1:A:771:ILE:HG21	1:A:777:ARG:HH21	1.81	0.45
1:A:60:GLN:CD	1:A:60:GLN:H	2.20	0.45
2:B:491:ILE:HD13	2:B:539:ILE:HG12	1.98	0.45
2:B:477:ILE:HG23	2:B:549:LEU:HD11	1.99	0.45
1:A:601:LEU:HB2	1:A:615:ALA:HB2	1.99	0.45
1:A:936:HIS:HB3	1:A:940[A]:HIS:CD2	2.52	0.45
1:A:486:PHE:CG	1:A:487:PRO:HD2	2.52	0.45
1:A:676:HIS:CG	1:A:843:ASP:HB2	2.53	0.44
2:B:394:ASP:OD1	2:B:394:ASP:N	2.46	0.44
1:A:978:GLU:HA	1:A:981:GLN:NE2	2.31	0.44
2:B:439:GLU:HG2	2:B:444:ALA:HB1	2.00	0.44
1:A:395:ASP:HB3	1:A:575:ASN:O	2.17	0.44
1:A:376:VAL:HB	1:A:377:PRO:HD2	1.98	0.44
2:B:467:TYR:HD1	2:B:563:MET:HE1	1.83	0.44
2:B:432:GLN:HA	2:B:435:GLN:HG2	2.00	0.44
1:A:25:LEU:HB3	2:B:497:GLN:CD	2.38	0.44
1:A:342:THR:CG2	1:A:472:CYS:HB3	2.48	0.43
1:A:446:TRP:CH2	1:A:466:PRO:HD2	2.53	0.43
1:A:636:VAL:O	1:A:639:LEU:HB2	2.17	0.43
1:A:600:GLU:HB2	5:A:1211:HOH:O	2.18	0.43
2:B:476:GLU:O	2:B:480:LYS:HG3	2.19	0.43
2:B:506:LYS:O	2:B:510:GLU:HG3	2.18	0.43
1:A:216:VAL:HG12	1:A:218:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:LEU:HB3	2:B:420:LEU:HD23	1.99	0.43
1:A:785:ASN:HA	1:A:786:PRO:HD2	1.84	0.43
2:B:408:TYR:CD1	2:B:413:LEU:HD23	2.53	0.43
1:A:278:MET:SD	1:A:825:GLN:NE2	2.91	0.43
1:A:342:THR:HG23	1:A:472:CYS:HB3	2.01	0.43
1:A:27:PRO:HD2	1:A:62:LEU:CD2	2.48	0.42
1:A:54:ARG:HA	1:A:59:HIS:CD2	2.53	0.42
1:A:129:ASP:CG	1:A:310:ARG:HH22	2.21	0.42
1:A:363:GLY:N	1:A:607:PRO:HG3	2.33	0.42
1:A:738:GLN:O	1:A:741:ARG:HB2	2.19	0.42
1:A:906:VAL:HG21	1:A:987:ALA:HB3	2.01	0.42
1:A:180:HIS:ND1	1:A:828:GLY:HA2	2.34	0.42
1:A:542:GLU:HG3	5:A:1215:HOH:O	2.18	0.42
1:A:883:ASP:O	1:A:886:LYS:HE3	2.20	0.42
1:A:950:GLU:OE2	1:A:1024:LYS:HG2	2.19	0.42
1:A:465:ASN:ND2	1:A:470:THR:HG21	2.34	0.42
1:A:43:ILE:HG13	1:A:85:GLU:O	2.18	0.42
2:B:407:HIS:O	2:B:407:HIS:CG	2.72	0.42
1:A:6:SER:HB2	1:A:12:GLY:C	2.40	0.42
1:A:39:GLU:HB2	1:A:88:ARG:NH1	2.35	0.41
1:A:185:LEU:HD21	1:A:277:ILE:HD13	2.01	0.41
1:A:391:ILE:HD13	1:A:396:LEU:HD23	2.02	0.41
1:A:704[A]:ARG:O	1:A:707:GLU:HG2	2.20	0.41
1:A:1024:LYS:HE2	1:A:1024:LYS:HB2	1.97	0.41
1:A:201:ASN:HB2	5:A:1243:HOH:O	2.20	0.41
1:A:399:ALA:HB1	1:A:607:PRO:HB2	2.03	0.41
1:A:913:ILE:HG22	1:A:914:GLY:O	2.20	0.41
2:B:571:ILE:HG22	2:B:575:LYS:HD2	2.03	0.41
1:A:736:VAL:O	1:A:740:ARG:HG3	2.21	0.41
1:A:741:ARG:NH2	1:A:743:ASP:OD2	2.45	0.41
1:A:802:LYS:HE2	1:A:805:ASP:OD2	2.21	0.41
2:B:445:VAL:HG12	2:B:584:LEU:HD13	2.03	0.41
1:A:916:ARG:HD2	1:A:931:HIS:ND1	2.36	0.41
2:B:431:TYR:O	2:B:435:GLN:HG2	2.21	0.41
1:A:248:GLY:O	1:A:290:LYS:HE3	2.21	0.40
1:A:532:LYS:O	1:A:536:THR:HG23	2.22	0.40
1:A:792:LEU:HD23	1:A:792:LEU:HA	1.83	0.40
1:A:704[A]:ARG:NH2	1:A:749:GLN:O	2.54	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	1023/1068 (96%)	1011 (99%)	12 (1%)	0	100	100
2	B	264/287 (92%)	254 (96%)	10 (4%)	0	100	100
All	All	1287/1355 (95%)	1265 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	938/974 (96%)	910 (97%)	28 (3%)	41	68
2	B	238/266 (90%)	231 (97%)	7 (3%)	42	69
All	All	1176/1240 (95%)	1141 (97%)	35 (3%)	41	68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	A	198	VAL
1	A	230	ARG
1	A	231	SER
1	A	237	GLU
1	A	242	CYS
1	A	261	PHE
1	A	264	LYS

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Mol	Chain	Res	Type
1	A	351	ILE
1	A	369	ASP
1	A	378	CYS
1	A	420	CYS
1	A	434	ASP
1	A	469	GLU
1	A	494	GLU
1	A	495	HIS
1	A	525	GLU
1	A	576	SER
1	A	735	LEU
1	A	794	PHE
1	A	834	LEU
1	A	845	VAL
1	A	862	CYS
1	A	901	CYS
1	A	939	ASP
1	A	965	SER
1	A	969	GLN
1	A	1008	SER
2	B	348	ARG
2	B	384	PHE
2	B	396	LEU
2	B	436	VAL
2	B	466	LEU
2	B	484	ILE
2	B	566	ILE

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

Mol	Chain	Res	Type
1	A	809	GLN
1	A	825	GLN

5.3.3 RNA

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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	1LT	A	1101	-	26,32,32	3.77	9 (34%)	29,49,49	2.04	9 (31%)

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
3	1LT	A	1101	-	-	5/27/41/41	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	1LT	C6-C7	-10.67	1.28	1.53
3	A	1101	1LT	C4-N2	-10.20	1.28	1.47
3	A	1101	1LT	C7-N2	7.48	1.62	1.47
3	A	1101	1LT	C10-C9	5.25	1.53	1.48
3	A	1101	1LT	C2-N1	4.82	1.45	1.36
3	A	1101	1LT	C8-N3	3.51	1.41	1.32
3	A	1101	1LT	C14-C10	2.75	1.44	1.39
3	A	1101	1LT	C3-N1	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	1LT	O-C3	-2.20	1.19	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	1LT	C12-N4-C13	5.20	124.60	117.49
3	A	1101	1LT	C11-C12-N4	-4.55	118.31	123.96
3	A	1101	1LT	C8-C7-N2	-3.48	106.69	112.29
3	A	1101	1LT	C6-C7-N2	2.65	106.96	103.03
3	A	1101	1LT	O1-C8-N3	-2.57	118.54	123.00
3	A	1101	1LT	C17-C15-C13	-2.45	104.95	109.76
3	A	1101	1LT	F2-C18-C15	-2.43	107.24	112.33
3	A	1101	1LT	C10-C14-C13	-2.33	116.97	119.73
3	A	1101	1LT	F-C18-C15	-2.17	107.79	112.33

There are no chirality outliers.

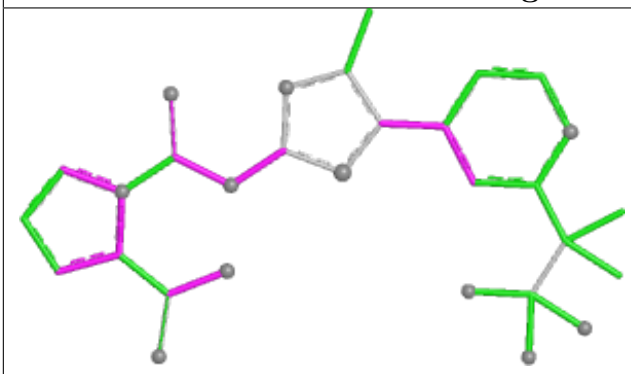
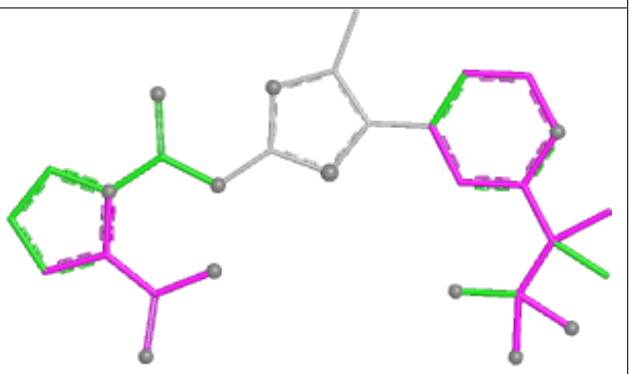
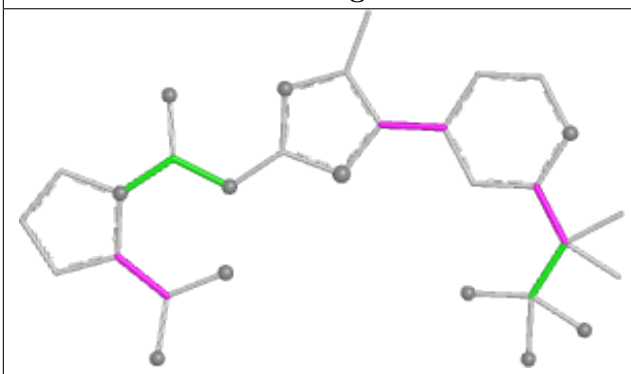
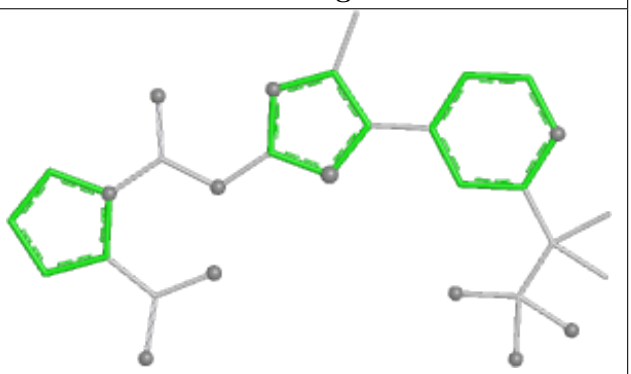
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	1LT	N2-C7-C8-O1
3	A	1101	1LT	C14-C10-C9-C1
3	A	1101	1LT	N2-C7-C8-N3
3	A	1101	1LT	C11-C10-C9-C1
3	A	1101	1LT	C14-C13-C15-C17

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 1LT A 1101	
 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

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	1026/1068 (96%)	-0.12	20 (1%) 66 69	35, 66, 101, 142	0
2	B	266/287 (92%)	0.27	26 (9%) 7 7	50, 87, 139, 152	0
All	All	1292/1355 (95%)	-0.04	46 (3%) 42 46	35, 69, 119, 152	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	418	PRO	6.6
1	A	523	LEU	5.3
2	B	413	LEU	5.0
2	B	416	TYR	5.0
2	B	326	MET	4.6
2	B	365	HIS	4.6
2	B	436	VAL	4.4
2	B	420	LEU	4.3
1	A	557	TYR	4.1
1	A	233	LYS	4.0
2	B	437	VAL	4.0
1	A	231	SER	3.9
2	B	422	VAL	3.7
2	B	327	SER	3.6
2	B	391	GLY	3.5
1	A	4	ARG	3.4
1	A	525	GLU	3.3
2	B	333	TRP	3.1
2	B	388	GLY	3.0
1	A	947	TYR	3.0
2	B	435	GLN	3.0
1	A	500	VAL	2.8
1	A	241	LEU	2.8
2	B	434	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	424	LEU	2.7
2	B	399	SER	2.6
1	A	239	LEU	2.6
1	A	238	GLN	2.6
2	B	415	GLN	2.5
2	B	372	LEU	2.5
2	B	426	TYR	2.4
2	B	398	PHE	2.4
1	A	3	PRO	2.4
1	A	1064	GLN	2.3
1	A	5	PRO	2.3
1	A	220	VAL	2.3
1	A	886	LYS	2.3
1	A	558	CYS	2.2
1	A	234	LEU	2.2
2	B	390	TYR	2.2
1	A	524	ARG	2.2
2	B	392	PHE	2.2
2	B	583	TRP	2.1
1	A	1007	GLY	2.0
2	B	440	ASP	2.0
2	B	404	LEU	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
4	NA	A	1102	1/1	0.81	0.45	70,70,70,70	1

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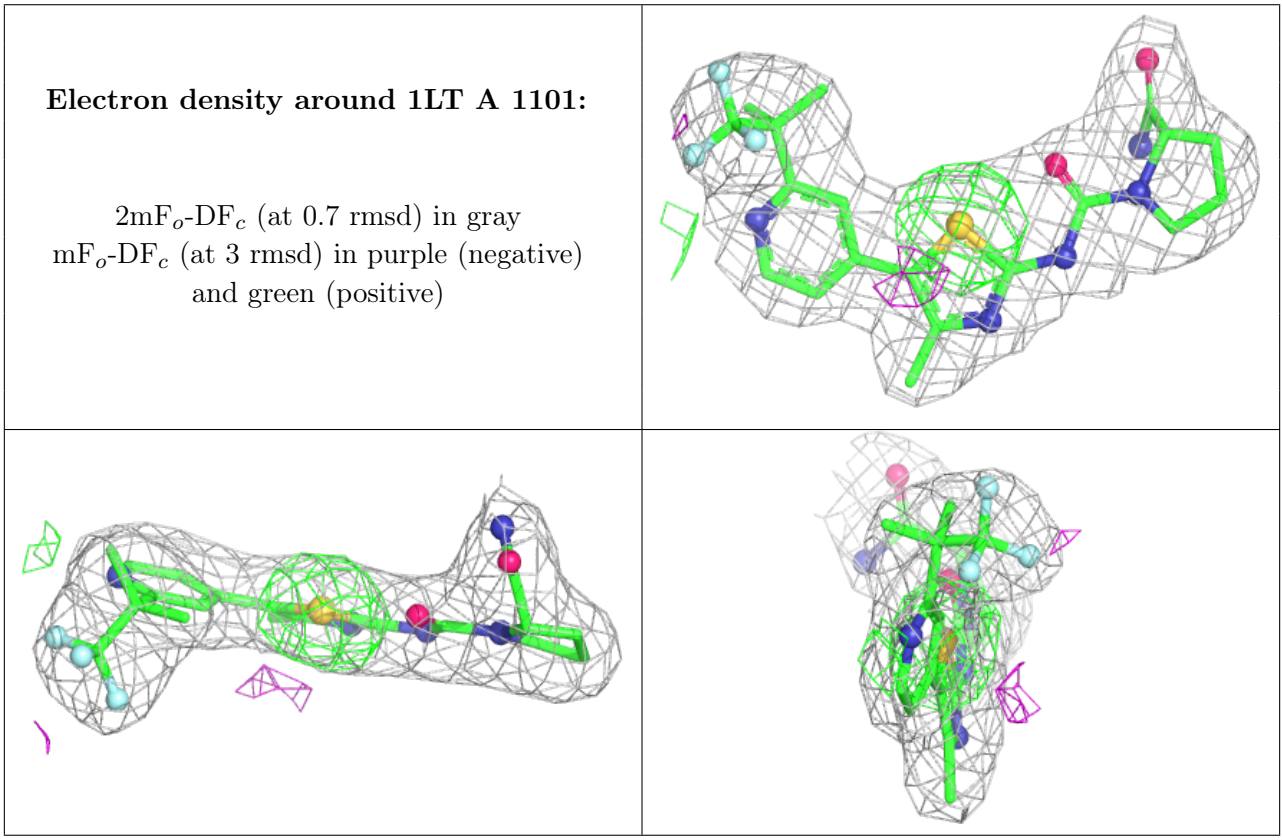
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1LT	A	1101	30/30	0.86	0.17	36,50,68,191	0

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 1LT A 1101:

$2mF_o$-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.