



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:45 pm BST

PDB ID : 3L54  
Title : Structure of Pi3K gamma with inhibitor  
Authors : Elkins, P.A.; Smallwood, A.M.  
Deposited on : 2009-12-21  
Resolution : 2.30 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](mailto: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.

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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 : 2.11  
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) : 2.11

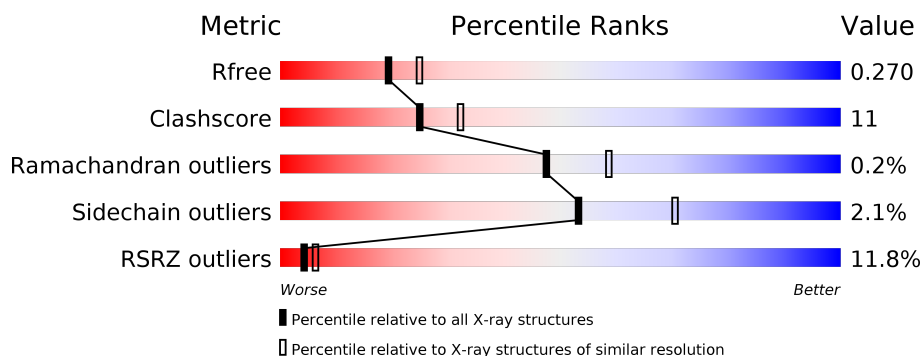
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	966	<div> <div>10%</div> <div>65%</div> <div>21%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6836 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
1	A	837	Total	C	N	O	S	3	0	0
			6779	4363	1153	1228	35			

There are 11 discrepancies between the modelled and reference sequences:

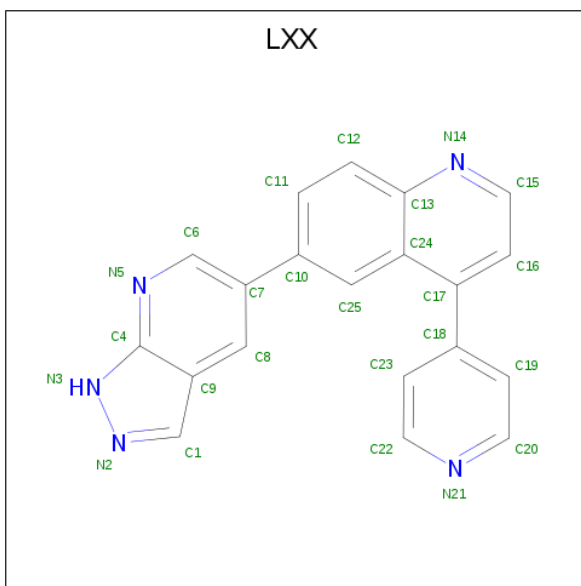
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736
A	295	GLN	HIS	CONFLICT	UNP P48736
A	777	LEU	SER	CONFLICT	UNP P48736
A	778	ASN	GLN	CONFLICT	UNP P48736
A	1012	VAL	ILE	CONFLICT	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP 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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 6-(1H-pyrazolo[3,4-b]pyridin-5-yl)-4-pyridin-4-ylquinoline (three-letter code: LXX) (formula: C<sub>20</sub>H<sub>13</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			25	20	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.26 Å 68.41 Å 106.72 Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	39.43 – 2.30 41.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	81.1 (39.43-2.30) 81.1 (41.05-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.216 , 0.280 0.207 , 0.270	Depositor DCC
$R_{free}$ test set	1895 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, LXX

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	0.27	0/6923	0.43	0/9368

There are no bond length outliers.

There are no bond angle outliers.

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	6779	0	6833	146	0
2	A	5	0	0	0	0
3	A	25	0	13	1	0
4	A	27	0	0	0	0
All	All	6836	0	6846	147	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 11.

All (147) 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:798:ILE:H	1:A:798:ILE:HD12	1.35	0.91
1:A:1041:GLN:HG2	1:A:1042:LEU:HD13	1.50	0.89
1:A:955:THR:HG22	1:A:957:THR:H	1.39	0.86
1:A:896:VAL:HG11	1:A:901:ALA:HB3	1.60	0.83
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.63	0.80
1:A:181:VAL:O	1:A:185:MET:HG3	1.85	0.76
1:A:355:TRP:HA	1:A:421:LYS:HB2	1.67	0.75
1:A:887:THR:HG22	1:A:889:ALA:H	1.51	0.75
1:A:775:GLN:OE1	1:A:798:ILE:HD11	1.91	0.71
1:A:739:ILE:HG23	1:A:832:PHE:HZ	1.56	0.71
1:A:935:TYR:O	1:A:939:THR:HB	1.93	0.69
1:A:219:CYS:SG	1:A:234:LYS:HG3	2.33	0.68
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.29	0.68
1:A:738:VAL:HA	1:A:741:MET:HE2	1.77	0.67
1:A:947:ARG:HD3	1:A:968:ILE:HD12	1.78	0.66
1:A:498:ASN:ND2	1:A:1040:PRO:HB3	2.10	0.65
1:A:424:PRO:HG3	1:A:598:TRP:O	1.96	0.65
1:A:917:THR:OG1	1:A:919:GLU:HG2	1.95	0.65
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.80	0.63
1:A:800:LYS:CB	1:A:814:GLU:HG3	2.30	0.61
1:A:1092:LEU:HD12	1:A:1093:GLY:N	2.15	0.61
1:A:1092:LEU:HD11	1:A:1094:ILE:HG13	1.83	0.60
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.83	0.60
1:A:625:GLY:O	1:A:629:GLN:HG3	2.02	0.60
1:A:798:ILE:CD1	1:A:798:ILE:H	2.12	0.60
1:A:887:THR:HG22	1:A:889:ALA:N	2.16	0.59
1:A:896:VAL:HG21	1:A:901:ALA:O	2.02	0.59
1:A:242:GLY:HA2	1:A:245:LEU:HD12	1.85	0.58
1:A:1087:PHE:CD2	1:A:1091:VAL:HG21	2.37	0.58
1:A:768:LYS:O	1:A:772:GLU:HG3	2.04	0.57
1:A:779:LEU:HD12	1:A:780:PRO:HD2	1.87	0.57
1:A:939:THR:HG23	1:A:945:GLY:CA	2.35	0.57
1:A:382:PHE:CE2	1:A:398:ARG:HD3	2.40	0.56
1:A:498:ASN:HD21	1:A:1040:PRO:HB3	1.70	0.56
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.40	0.56
1:A:889:ALA:O	1:A:893:GLN:HG3	2.05	0.56
1:A:387:ILE:HD13	1:A:468:LEU:HD12	1.88	0.56
1:A:748:ASP:O	1:A:752:LEU:HD23	2.05	0.55
1:A:509:ASP:OD2	1:A:512:ASN:HB2	2.06	0.55
1:A:1092:LEU:CD1	1:A:1094:ILE:HG13	2.36	0.55
1:A:182:THR:HB	1:A:183:PRO:HD3	1.88	0.55
1:A:800:LYS:HB2	1:A:814:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:LYS:HB3	1:A:814:GLU:HG3	1.90	0.54
1:A:726:THR:HA	1:A:729:LEU:HD12	1.90	0.54
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.37	0.54
1:A:739:ILE:O	1:A:743:GLN:HG3	2.08	0.54
1:A:957:THR:HG22	1:A:957:THR:O	2.08	0.53
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.89	0.53
1:A:580:TYR:HE2	1:A:613:ARG:HD2	1.72	0.53
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.22	0.53
1:A:775:GLN:HE21	1:A:795:ALA:HB1	1.74	0.52
1:A:996:GLY:O	1:A:1003:SER:HB2	2.09	0.52
3:A:1:LXX:C23	3:A:1:LXX:H25	2.37	0.52
1:A:357:CYS:SG	1:A:527:ILE:HD13	2.49	0.52
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.91	0.52
1:A:387:ILE:HD11	1:A:427:ALA:HB1	1.91	0.52
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.45	0.52
1:A:387:ILE:HD13	1:A:468:LEU:CD1	2.40	0.51
1:A:425:LYS:HD2	1:A:672:TYR:OH	2.09	0.51
1:A:759:VAL:HG12	1:A:764:ILE:HG12	1.92	0.51
1:A:393:VAL:O	1:A:393:VAL:HG23	2.11	0.51
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.46	0.51
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.46	0.50
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.27	0.50
1:A:280:TYR:HB3	1:A:282:VAL:CG2	2.42	0.50
1:A:293:VAL:HG13	1:A:303:ILE:HD11	1.94	0.50
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.94	0.49
1:A:1035:LEU:CD2	1:A:1039:MET:HG3	2.42	0.49
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.46	0.49
1:A:149:ALA:HA	1:A:152:ARG:HD2	1.94	0.49
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.94	0.49
1:A:607:THR:O	1:A:610:LEU:HB2	2.13	0.49
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.42	0.49
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.96	0.48
1:A:683:LYS:HE3	1:A:687:ARG:NH2	2.28	0.48
1:A:953:MET:SD	1:A:963:ILE:HD13	2.54	0.48
1:A:377:THR:HG23	1:A:378:ASP:HB3	1.96	0.48
1:A:173:LEU:O	1:A:177:ARG:HG3	2.14	0.48
1:A:148:GLN:O	1:A:152:ARG:HG3	2.14	0.48
1:A:705:GLN:HG3	1:A:839:ARG:CZ	2.44	0.48
1:A:774:LEU:HA	1:A:778:ASN:HB3	1.97	0.47
1:A:373:LEU:HD12	1:A:374:PRO:O	2.14	0.47
1:A:354:LEU:HA	1:A:527:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:THR:HG23	1:A:945:GLY:HA3	1.97	0.47
1:A:207:LEU:HD23	1:A:212:TRP:CD2	2.50	0.47
1:A:988:THR:HB	1:A:989:PRO:HD2	1.97	0.46
1:A:1042:LEU:HA	1:A:1047:ASP:OD2	2.16	0.45
1:A:377:THR:HA	1:A:378:ASP:HA	1.59	0.45
1:A:224:ILE:HD12	1:A:248:PHE:CD1	2.51	0.45
1:A:1087:PHE:O	1:A:1091:VAL:HB	2.17	0.45
1:A:624:VAL:O	1:A:628:MET:HG2	2.16	0.45
1:A:965:PHE:O	1:A:969:LEU:HG	2.17	0.45
1:A:898:ASN:O	1:A:1087:PHE:HZ	2.00	0.44
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.98	0.44
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.99	0.44
1:A:1071:GLN:OE1	1:A:1071:GLN:HA	2.17	0.44
1:A:589:TYR:O	1:A:593:PHE:HD1	2.00	0.44
1:A:389:HIS:O	1:A:392:GLN:HB3	2.17	0.44
1:A:387:ILE:CG2	1:A:395:CYS:HB3	2.47	0.44
1:A:410:TRP:O	1:A:412:VAL:HG23	2.18	0.44
1:A:779:LEU:HD12	1:A:780:PRO:CD	2.48	0.44
1:A:375:ARG:HD2	1:A:375:ARG:C	2.39	0.43
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.46	0.43
1:A:774:LEU:O	1:A:778:ASN:HB3	2.18	0.43
1:A:915:SER:OG	1:A:921:PHE:HB2	2.18	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.19	0.43
1:A:555:LEU:O	1:A:559:ILE:HG13	2.18	0.43
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.99	0.43
1:A:366:ARG:NH1	1:A:479:GLU:OE2	2.52	0.43
1:A:282:VAL:HG12	1:A:283:GLY:H	1.84	0.43
1:A:731:ASP:O	1:A:735:GLN:HG3	2.18	0.43
1:A:933:ALA:O	1:A:937:VAL:HG23	2.19	0.43
1:A:380:THR:O	1:A:435:CYS:HA	2.19	0.43
1:A:291:GLN:OE1	1:A:291:GLN:HA	2.19	0.42
1:A:378:ASP:O	1:A:379:LEU:HB2	2.19	0.42
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.91	0.42
1:A:809:LYS:N	1:A:810:PRO:HD3	2.34	0.42
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.54	0.42
1:A:1090:LEU:HD12	1:A:1090:LEU:N	2.34	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.00	0.42
1:A:280:TYR:OH	1:A:311:PRO:HG3	2.19	0.42
1:A:899:THR:C	1:A:901:ALA:H	2.23	0.42
1:A:235:VAL:HG21	1:A:244:ILE:HD13	2.02	0.42
1:A:745:VAL:HG12	1:A:811:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:PHE:CD1	1:A:717:LEU:HD11	2.55	0.41
1:A:358:ASP:O	1:A:419:LYS:HG3	2.19	0.41
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	2.01	0.41
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.02	0.41
1:A:422:ASP:HB3	1:A:599:GLY:O	2.21	0.41
1:A:640:VAL:O	1:A:643:ILE:HG12	2.21	0.41
1:A:862:LEU:N	1:A:862:LEU:HD22	2.36	0.41
1:A:953:MET:HG3	1:A:963:ILE:HD13	2.01	0.41
1:A:1008:LYS:O	1:A:1012:VAL:HG23	2.20	0.41
1:A:1086:TRP:HE3	1:A:1090:LEU:HD13	1.85	0.41
1:A:233:ILE:HD12	1:A:248:PHE:HD1	1.86	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.89	0.41
1:A:557:ALA:O	1:A:561:THR:HG23	2.21	0.41
1:A:762:GLN:O	1:A:766:GLN:HG2	2.21	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.21	0.41
1:A:1035:LEU:HD12	1:A:1048:ILE:HA	2.04	0.40
1:A:605:ALA:O	1:A:609:GLN:HG3	2.21	0.40
1:A:802:LYS:HG3	1:A:812:TRP:HB3	2.03	0.40
1:A:892:GLN:HE22	1:A:1080:TRP:HH2	1.69	0.40
1:A:915:SER:HA	1:A:916:PRO:HD3	1.89	0.40
1:A:914:LYS:HA	1:A:914:LYS:HD3	1.95	0.40
1:A:1041:GLN:O	1:A:1042:LEU:HD12	2.21	0.40
1:A:783:PHE:CE1	1:A:793:ALA:HB3	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	818/966 (85%)	777 (95%)	39 (5%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	896	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	751/864 (87%)	735 (98%)	16 (2%)	53 70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	A	271	VAL
1	A	380	THR
1	A	601	GLN
1	A	763	VAL
1	A	779	LEU
1	A	791	LEU
1	A	832	PHE
1	A	907	LEU
1	A	939	THR
1	A	959	ASN
1	A	983	VAL
1	A	1026	LEU
1	A	1027	LEU
1	A	1039	MET
1	A	1076	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	834	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	LXX	A	1	-	29,29,29	1.40	8 (27%)	35,41,41	2.41	7 (20%)
2	SO4	A	2	-	4,4,4	0.13	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LXX	A	1	-	-	0/8/8/8	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	LXX	C17-C18	-2.84	1.44	1.49
3	A	1	LXX	C24-C13	-2.43	1.38	1.42
3	A	1	LXX	C12-C13	-2.30	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	LXX	C25-C24	-2.10	1.38	1.42
3	A	1	LXX	C10-C7	-2.08	1.43	1.49
3	A	1	LXX	C4-N5	-2.08	1.34	1.37
3	A	1	LXX	C17-C24	-2.02	1.38	1.42
3	A	1	LXX	C13-N14	-2.01	1.33	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	LXX	C7-C8-C9	-8.10	107.51	121.53
3	A	1	LXX	C6-N5-C4	-6.59	110.08	116.69
3	A	1	LXX	C7-C6-N5	5.09	130.26	125.55
3	A	1	LXX	C17-C24-C13	3.75	119.46	117.44
3	A	1	LXX	C8-C7-C6	3.65	121.35	116.24
3	A	1	LXX	C8-C9-C4	3.60	130.14	118.16
3	A	1	LXX	C9-C1-N2	-2.88	103.93	111.30

There are no chirality outliers.

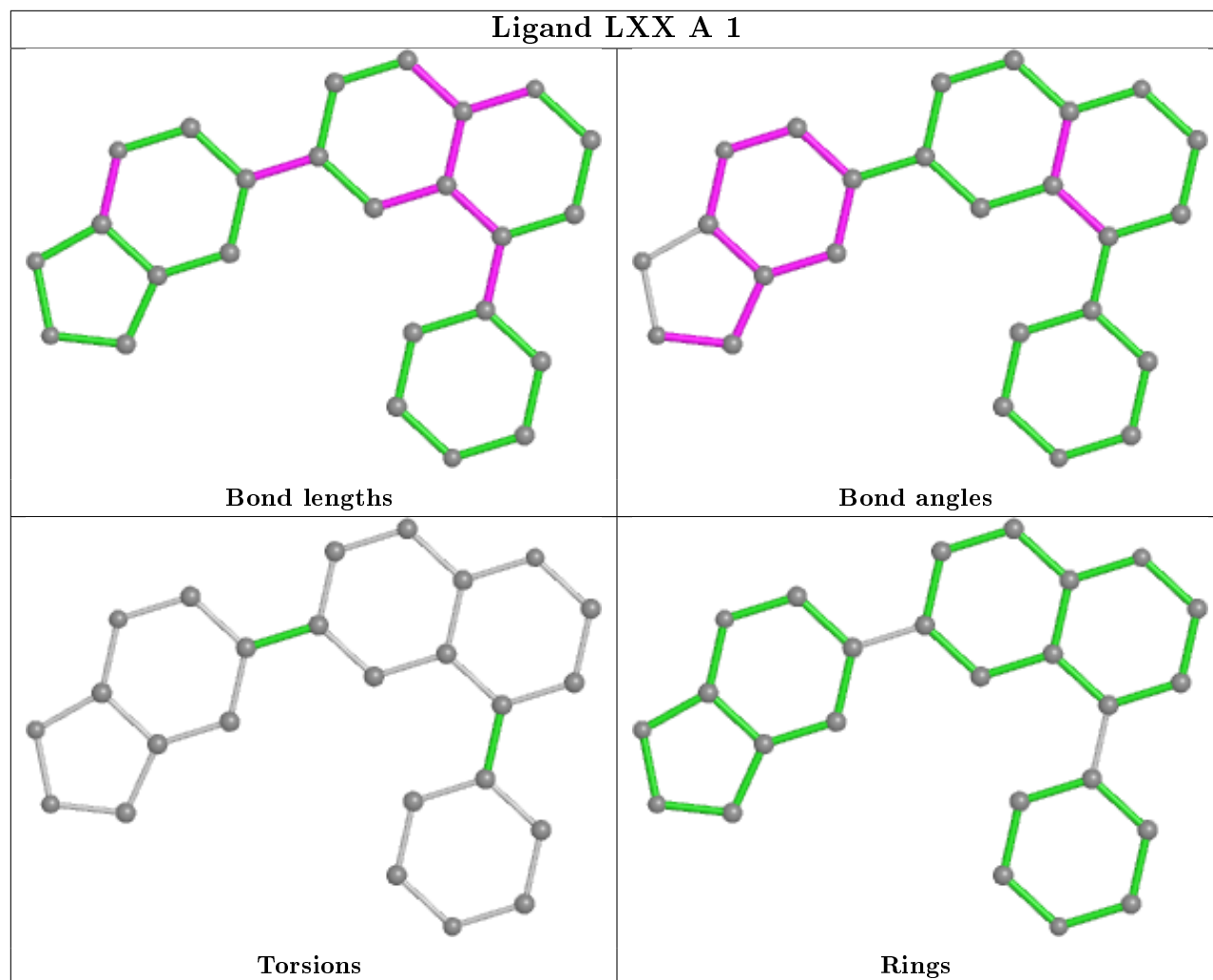
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	LXX	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	837/966 (86%)	0.64	99 (11%) 4 6	25, 56, 110, 174	1 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	777	LEU	13.2
1	A	377	THR	12.6
1	A	378	ASP	8.7
1	A	375	ARG	8.1
1	A	229	THR	7.4
1	A	374	PRO	7.1
1	A	376	ASN	6.9
1	A	143	MET	6.2
1	A	228	THR	6.1
1	A	379	LEU	6.0
1	A	898	ASN	5.9
1	A	895	THR	5.6
1	A	148	GLN	5.5
1	A	270	PHE	5.5
1	A	231	GLN	5.4
1	A	531	LYS	5.0
1	A	778	ASN	4.9
1	A	227	SER	4.9
1	A	234	LYS	4.6
1	A	661	LEU	4.3
1	A	248	PHE	4.2
1	A	1094	ILE	4.1
1	A	657	LEU	4.0
1	A	779	LEU	4.0
1	A	1091	VAL	4.0
1	A	843	LEU	3.8
1	A	230	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	664	VAL	3.8
1	A	353	SER	3.8
1	A	354	LEU	3.7
1	A	758	ASP	3.7
1	A	774	LEU	3.6
1	A	896	VAL	3.6
1	A	999	GLY	3.6
1	A	147	SER	3.5
1	A	694	PHE	3.4
1	A	373	LEU	3.3
1	A	823	LEU	3.2
1	A	250	THR	3.2
1	A	660	LEU	3.2
1	A	216	ALA	3.1
1	A	744	LYS	3.1
1	A	842	MET	3.0
1	A	903	LYS	3.0
1	A	656	VAL	3.0
1	A	226	ARG	3.0
1	A	698	PHE	3.0
1	A	663	LEU	2.9
1	A	245	LEU	2.9
1	A	870	ILE	2.9
1	A	666	ALA	2.9
1	A	846	GLN	2.9
1	A	150	PHE	2.9
1	A	695	LEU	2.8
1	A	869	CYS	2.8
1	A	762	GLN	2.8
1	A	237	PRO	2.8
1	A	899	THR	2.8
1	A	221	PHE	2.7
1	A	529	LEU	2.6
1	A	780	PRO	2.6
1	A	232	THR	2.6
1	A	667	VAL	2.6
1	A	747	LEU	2.6
1	A	845	LEU	2.6
1	A	320	LYS	2.6
1	A	844	ILE	2.5
1	A	307	LEU	2.5
1	A	1037	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1030	LEU	2.5
1	A	355	TRP	2.4
1	A	759	VAL	2.4
1	A	213	LYS	2.4
1	A	244	ILE	2.4
1	A	681	LEU	2.4
1	A	659	TYR	2.4
1	A	850	ILE	2.3
1	A	662	GLN	2.3
1	A	214	LYS	2.3
1	A	658	HIS	2.3
1	A	787	TYR	2.3
1	A	246	GLN	2.2
1	A	217	ASN	2.2
1	A	865	LEU	2.2
1	A	982	ARG	2.2
1	A	665	GLN	2.2
1	A	763	VAL	2.2
1	A	894	SER	2.2
1	A	212	TRP	2.1
1	A	152	ARG	2.1
1	A	847	ILE	2.1
1	A	631	LEU	2.1
1	A	1062	GLU	2.1
1	A	1001	LYS	2.1
1	A	871	SER	2.1
1	A	692	GLY	2.0
1	A	381	VAL	2.0
1	A	867	TYR	2.0
1	A	1034	MET	2.0

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

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

## 6.3 Carbohydrates ⓘ

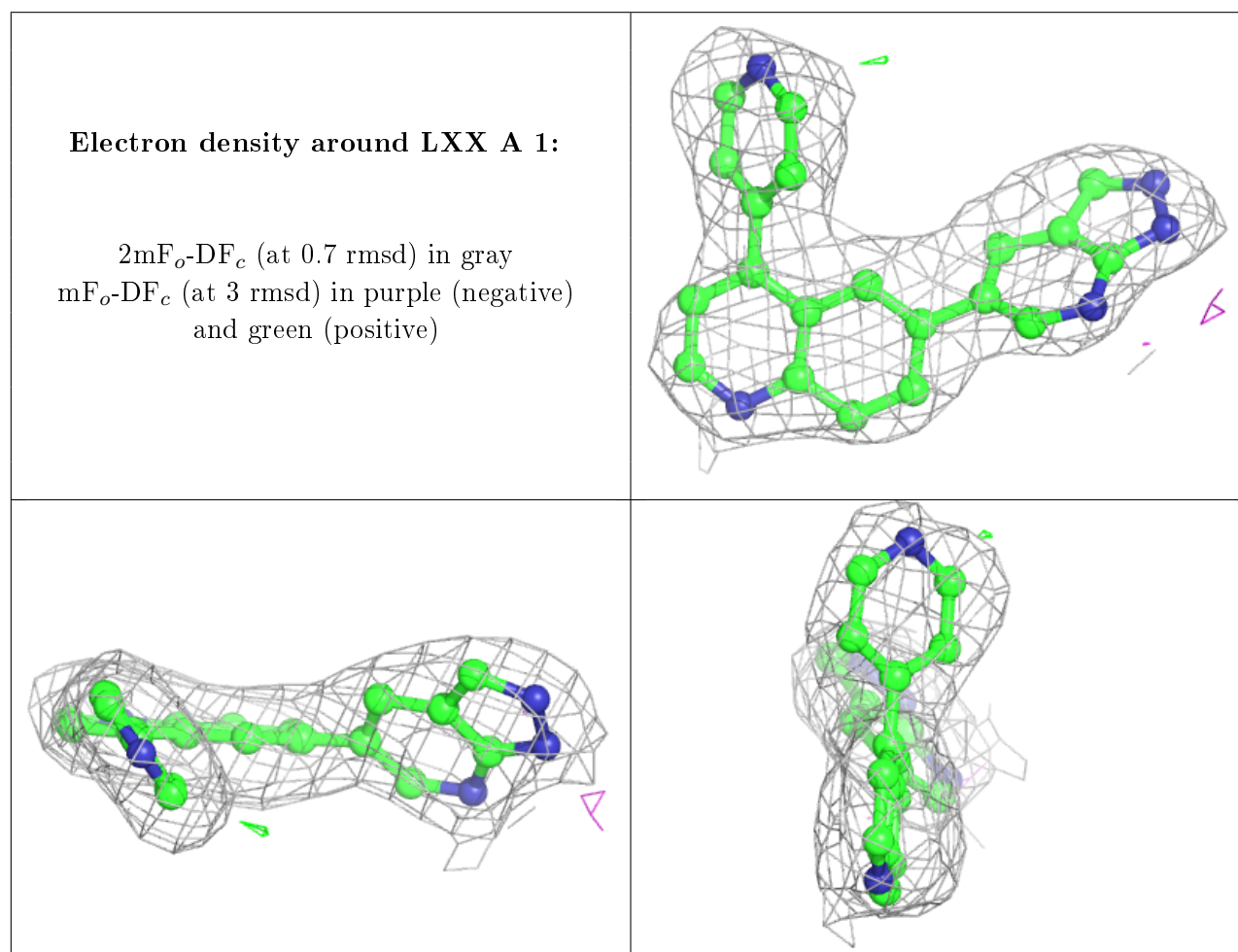
There are no carbohydrates in this entry.

## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	LXX	A	1	25/25	0.90	0.15	46,67,75,76	0
2	SO4	A	2	5/5	0.99	0.14	39,49,56,56	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.