



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:54 AM UTC

PDB ID : 3LJ3 / pdb_00003lj3
Title : PI3-kinase-gamma with a pyrrolopyridine-benzofuran inhibitor
Authors : Bard, J.; Svenson, K.
Deposited on : 2010-01-25
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

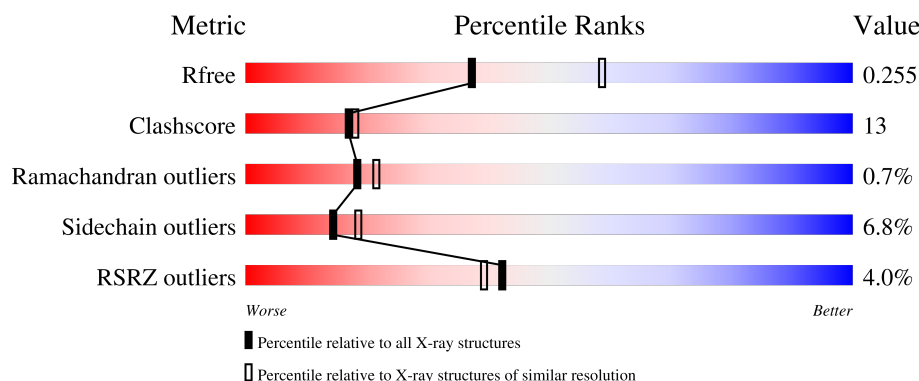
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

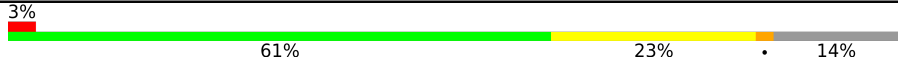
The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	WYE	A	1109	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6592 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	829	Total	C	N	O	S	0	0	0
			6463	4150	1096	1183	34			

There are 8 discrepancies between the modelled and reference sequences:

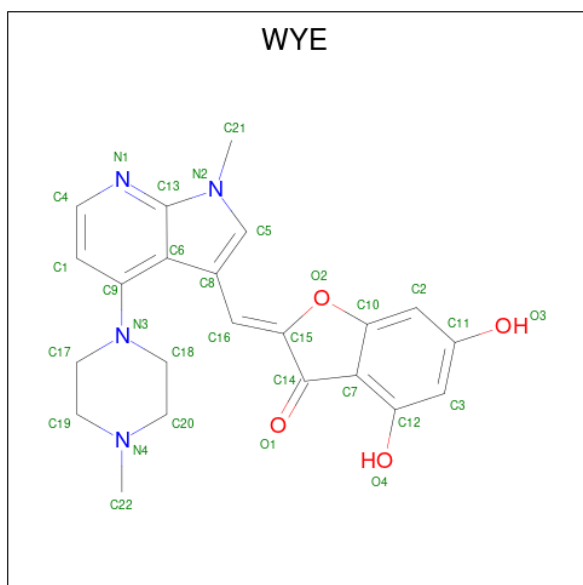
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	459	ARG	GLN	variant	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is (2Z)-4,6-dihydroxy-2-[[1-methyl-4-(4-methylpiperazin-1-yl)-1H-pyrrolo[2,3-b]pyridin-3-yl]methylidene]-1-benzofuran-3(2H)-one (CCD ID: WYE) (formula: C₂₂H₂₂N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	22	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.07Å 68.51Å 106.69Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	62.17 – 2.43 62.17 – 2.43	Depositor EDS
% Data completeness (in resolution range)	83.0 (62.17-2.43) 89.3 (62.17-2.43)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.42Å)	Xtriage
Refinement program	PHENIX dev_256	Depositor
R, R_{free}	0.222 , 0.261 (Not available) , 0.255	Depositor DCC
R_{free} test set	1769 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6592	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WYE, SO4

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	0.28	0/6605	0.70	6/8973 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	788	ASP	CA-C-N	5.49	125.32	119.28
1	A	788	ASP	C-N-CA	5.49	125.32	119.28
1	A	915	SER	CA-C-N	5.08	124.58	119.19
1	A	915	SER	C-N-CA	5.08	124.58	119.19
1	A	819	ASP	CA-C-N	5.06	124.84	119.28
1	A	819	ASP	C-N-CA	5.06	124.84	119.28

There are no chirality outliers.

There are no planarity outliers.

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	6463	0	6201	159	0
2	A	10	0	0	0	0
3	A	30	0	20	12	0
4	A	89	0	0	1	0
All	All	6592	0	6221	161	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 13.

All (161) 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:266:SER:HA	1:A:269:ASP:HB2	1.54	0.88
1:A:887:THR:HG22	1:A:889:ALA:H	1.41	0.85
1:A:576:TRP:O	1:A:579:ARG:HG3	1.82	0.80
1:A:549:ASN:O	1:A:553:LYS:HG2	1.88	0.74
1:A:889:ALA:HB2	1:A:949:ASN:HB3	1.73	0.70
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.74	0.69
1:A:602:GLU:H	1:A:602:GLU:CD	2.01	0.69
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.75	0.68
1:A:887:THR:HG22	1:A:889:ALA:N	2.09	0.68
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.76	0.66
1:A:808:LYS:O	1:A:810:PRO:HD3	1.95	0.66
1:A:245:LEU:HD11	1:A:272:LEU:HG	1.78	0.65
1:A:382:PHE:CE2	1:A:398:ARG:HD3	2.31	0.65
1:A:614:ARG:HB3	1:A:618:ASP:OD2	1.96	0.64
1:A:882:VAL:HG23	3:A:1109:WYE:H21	1.80	0.63
3:A:1109:WYE:H5	3:A:1109:WYE:O2	1.99	0.63
1:A:368:ILE:HG22	1:A:516:ILE:HG12	1.80	0.62
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.81	0.62
1:A:701:SER:O	1:A:705:GLN:HG3	2.00	0.62
1:A:209:GLU:HG3	1:A:859:SER:HB3	1.81	0.61
1:A:424:PRO:HG3	1:A:598:TRP:O	2.01	0.61
1:A:887:THR:CG2	1:A:950:ASP:HA	2.30	0.61
1:A:268:GLN:C	1:A:270:PHE:H	2.07	0.61
1:A:964:ASP:HA	3:A:1109:WYE:C3	2.30	0.61
1:A:191:ARG:HD2	1:A:196:TYR:CD1	2.37	0.60
1:A:266:SER:CA	1:A:269:ASP:HB2	2.28	0.60
1:A:180:LEU:C	1:A:183:PRO:HD2	2.27	0.60
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.84	0.59
1:A:887:THR:HG21	1:A:950:ASP:HA	1.83	0.59
1:A:605:ALA:O	1:A:609:GLN:HG3	2.03	0.58
1:A:997:THR:HG23	1:A:1001:LYS:HD3	1.84	0.58
1:A:1074:VAL:O	1:A:1078:LYS:HG2	2.04	0.57
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.87	0.56
1:A:422:ASP:HB3	1:A:599:GLY:O	2.05	0.56
1:A:356:ASP:O	1:A:421:LYS:HE2	2.06	0.56
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.88	0.56
1:A:947:ARG:NH2	1:A:963:ILE:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:SER:O	1:A:857:THR:HG23	2.06	0.55
1:A:893:GLN:HA	1:A:897:GLY:HA2	1.87	0.55
1:A:191:ARG:HD2	1:A:196:TYR:CG	2.41	0.55
1:A:233:ILE:HD12	1:A:233:ILE:N	2.22	0.54
1:A:812:TRP:CZ3	3:A:1109:WYE:H18	2.42	0.54
1:A:207:LEU:HD21	1:A:211:LEU:HB2	1.88	0.54
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.54
1:A:382:PHE:CZ	1:A:434:TYR:HB2	2.41	0.54
1:A:925:VAL:O	1:A:929:VAL:HG23	2.09	0.53
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.39	0.53
1:A:224:ILE:HD13	1:A:233:ILE:HD13	1.89	0.53
1:A:964:ASP:HA	3:A:1109:WYE:C11	2.39	0.53
1:A:968:ILE:O	1:A:969:LEU:C	2.52	0.52
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.92	0.52
1:A:812:TRP:C	1:A:812:TRP:CD1	2.88	0.52
1:A:1060:ASN:CG	1:A:1061:GLU:N	2.67	0.52
1:A:953:MET:O	1:A:960:LEU:HD12	2.10	0.52
1:A:207:LEU:CD2	1:A:211:LEU:HB2	2.40	0.52
1:A:240:THR:O	1:A:244:ILE:HG13	2.10	0.51
1:A:834:HIS:HB2	1:A:876:ILE:HG22	1.92	0.51
1:A:887:THR:CG2	1:A:889:ALA:H	2.18	0.51
1:A:1002:THR:HG22	1:A:1003:SER:N	2.26	0.51
1:A:233:ILE:HD12	1:A:233:ILE:H	1.76	0.51
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.92	0.51
1:A:547:MET:HE2	1:A:551:LEU:C	2.35	0.51
1:A:390:GLY:O	1:A:391:GLN:HB2	2.10	0.50
1:A:808:LYS:C	1:A:810:PRO:HD3	2.35	0.50
1:A:182:THR:HB	1:A:183:PRO:HD3	1.93	0.50
1:A:496:SER:N	1:A:1042:LEU:HB3	2.27	0.50
1:A:576:TRP:CH2	1:A:579:ARG:HD3	2.47	0.49
1:A:268:GLN:C	1:A:270:PHE:N	2.70	0.49
1:A:953:MET:HE1	3:A:1109:WYE:C4	2.43	0.49
1:A:879:ILE:HD13	3:A:1109:WYE:C10	2.43	0.49
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.94	0.49
1:A:966:GLY:HA3	1:A:967:HIS:C	2.38	0.49
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.95	0.49
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.13	0.48
1:A:482:LEU:HB2	1:A:516:ILE:HG22	1.95	0.48
1:A:268:GLN:O	1:A:270:PHE:N	2.47	0.48
1:A:224:ILE:HD12	1:A:224:ILE:N	2.28	0.48
1:A:614:ARG:O	1:A:615:GLU:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:TYR:OH	3:A:1109:WYE:H2	2.13	0.48
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.29	0.47
1:A:497:PHE:HB2	1:A:1043:THR:O	2.15	0.47
1:A:939:THR:HB	1:A:945:GLY:HA2	1.96	0.47
3:A:1109:WYE:O2	3:A:1109:WYE:C5	2.61	0.47
1:A:834:HIS:CG	1:A:835:GLY:N	2.82	0.47
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.50	0.47
1:A:360:LYS:HA	1:A:419:LYS:HA	1.97	0.47
1:A:1060:ASN:CG	1:A:1061:GLU:H	2.23	0.47
1:A:547:MET:HE2	1:A:552:ARG:N	2.31	0.46
1:A:998:SER:H	1:A:1001:LYS:HD2	1.81	0.46
1:A:948:HIS:CE1	1:A:950:ASP:OD1	2.68	0.46
1:A:240:THR:HG22	1:A:242:GLY:H	1.81	0.46
1:A:407:GLU:CD	1:A:409:LEU:HD11	2.40	0.46
1:A:380:THR:O	1:A:435:CYS:HA	2.15	0.46
1:A:240:THR:HG22	1:A:242:GLY:N	2.31	0.45
1:A:841:ASP:CG	3:A:1109:WYE:O3	2.59	0.45
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.97	0.45
1:A:661:LEU:O	1:A:665:GLN:HG2	2.16	0.45
1:A:144:SER:HB2	1:A:145:GLU:H	1.60	0.45
1:A:915:SER:HA	1:A:916:PRO:HD3	1.72	0.45
1:A:202:VAL:CG1	1:A:203:THR:N	2.80	0.45
1:A:321:GLU:OE2	1:A:321:GLU:C	2.60	0.45
1:A:806:SER:O	1:A:807:LYS:C	2.60	0.45
1:A:1001:LYS:HB2	1:A:1002:THR:H	1.55	0.45
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.46	0.45
1:A:614:ARG:HB3	1:A:618:ASP:CG	2.42	0.45
1:A:467:LEU:O	1:A:476:ARG:HD2	2.17	0.44
1:A:850:ILE:O	1:A:854:ILE:HG13	2.17	0.44
1:A:208:PRO:HG2	1:A:211:LEU:HG	1.99	0.44
1:A:786:PRO:HG2	1:A:878:MET:SD	2.57	0.44
1:A:209:GLU:HG3	1:A:859:SER:CB	2.47	0.44
1:A:483:HIS:CE1	1:A:510:LYS:HG2	2.52	0.44
1:A:709:TYR:HB3	1:A:713:PHE:CE1	2.52	0.44
1:A:984:PRO:HB2	1:A:985:PHE:CD2	2.52	0.44
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.44	0.44
1:A:172:GLU:HG2	1:A:673:HIS:HD2	1.83	0.43
1:A:224:ILE:HA	1:A:305:VAL:O	2.18	0.43
1:A:198:MET:O	1:A:199:HIS:C	2.60	0.43
1:A:246:GLN:O	1:A:250:THR:HG23	2.17	0.43
1:A:355:TRP:CD1	1:A:355:TRP:C	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:ARG:HD3	1:A:959:ASN:HB2	2.01	0.43
1:A:225:HIS:HA	1:A:229:THR:O	2.19	0.43
1:A:662:GLN:HE21	1:A:1030:LEU:HD22	1.82	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.17	0.42
1:A:355:TRP:HA	1:A:356:ASP:HA	1.85	0.42
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.85	0.42
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	2.01	0.42
1:A:207:LEU:HD12	1:A:288:LYS:HB2	2.01	0.42
1:A:811:LEU:HB3	1:A:813:LEU:CD1	2.50	0.42
1:A:180:LEU:O	1:A:183:PRO:HD2	2.19	0.42
1:A:948:HIS:CD2	1:A:969:LEU:O	2.71	0.42
1:A:948:HIS:ND1	1:A:950:ASP:OD1	2.53	0.42
1:A:990:ASP:CG	1:A:1080:TRP:HH2	2.28	0.42
1:A:999:GLY:HA2	1:A:1000:LYS:HA	1.66	0.42
1:A:830:ILE:HG21	1:A:878:MET:HE2	2.01	0.42
1:A:933:ALA:O	1:A:937:VAL:HG23	2.20	0.42
1:A:407:GLU:HG2	1:A:409:LEU:HD11	2.01	0.42
1:A:840:GLN:OE1	1:A:1040:PRO:HD3	2.19	0.42
1:A:371:PRO:HG2	1:A:511:GLU:O	2.20	0.42
1:A:596:VAL:HG13	1:A:603:ILE:HG22	2.02	0.42
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.20	0.41
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.87	0.41
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.21	0.41
1:A:671:PRO:HD2	4:A:31:HOH:O	2.18	0.41
1:A:731:ASP:O	1:A:735:GLN:HG3	2.20	0.41
1:A:826:GLU:OE2	1:A:826:GLU:HA	2.20	0.41
1:A:288:LYS:HG3	1:A:289:ASN:OD1	2.21	0.41
1:A:918:GLU:O	1:A:922:GLN:HG2	2.20	0.41
1:A:251:LYS:O	1:A:252:MET:CB	2.69	0.41
1:A:207:LEU:HD21	1:A:211:LEU:CB	2.49	0.41
1:A:1085:ASN:O	1:A:1089:HIS:CD2	2.74	0.41
1:A:802:LYS:HG2	1:A:812:TRP:HB3	2.03	0.41
1:A:943:GLY:HA2	1:A:1050:TYR:OH	2.20	0.41
1:A:953:MET:HE1	3:A:1109:WYE:C1	2.51	0.41
1:A:362:ARG:HG3	1:A:413:TRP:CE3	2.56	0.41
1:A:628:MET:HE3	1:A:628:MET:HA	2.03	0.41
1:A:624:VAL:O	1:A:628:MET:HG2	2.21	0.40
1:A:1087:PHE:O	1:A:1088:LEU:C	2.63	0.40
1:A:921:PHE:O	1:A:925:VAL:HG23	2.22	0.40
1:A:547:MET:HB3	1:A:552:ARG:NH2	2.36	0.40
1:A:587:LYS:N	1:A:587:LYS:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:MET:SD	3:A:1109:WYE:H18A	2.61	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	717/966 (74%)	675 (94%)	37 (5%)	5 (1%)	18 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	615	GLU
1	A	949	ASN
1	A	901	ALA
1	A	1001	LYS
1	A	1040	PRO

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	674/864 (78%)	628 (93%)	46 (7%)	14 18

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	153	GLN
1	A	209	GLU
1	A	240	THR
1	A	268	GLN
1	A	282	VAL
1	A	321	GLU
1	A	357	CYS
1	A	358	ASP
1	A	366	ARG
1	A	381	VAL
1	A	395	CYS
1	A	498	ASN
1	A	516	ILE
1	A	546	GLU
1	A	549	ASN
1	A	583	LEU
1	A	601	GLN
1	A	602	GLU
1	A	628	MET
1	A	647	LYS
1	A	705	GLN
1	A	799	GLU
1	A	809	LYS
1	A	826	GLU
1	A	832	PHE
1	A	848	LEU
1	A	859	SER
1	A	886	THR
1	A	887	THR
1	A	888	ILE
1	A	906	VAL
1	A	917	THR
1	A	918	GLU
1	A	927	ARG
1	A	949	ASN
1	A	967	HIS
1	A	968	ILE
1	A	1001	LYS
1	A	1015	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1041	GLN

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Mol	Chain	Res	Type
1	A	1049	GLU
1	A	1052	ARG
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	600	GLN
1	A	634	ASN
1	A	646	GLN
1	A	662	GLN
1	A	962	HIS
1	A	967	HIS
1	A	1010	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
2	SO4	A	2	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	A	1	-	4,4,4	0.25	0	6,6,6	0.11	0
3	WYE	A	1109	-	34,34,34	0.89	0	45,51,51	1.98	11 (24%)

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	WYE	A	1109	-	-	0/8/30/30	0/5/5/5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1109	WYE	C13-N2-C5	5.52	109.44	107.52
3	A	1109	WYE	C8-C5-N2	-5.02	108.68	110.73
3	A	1109	WYE	C5-C8-C16	-4.64	122.40	129.52
3	A	1109	WYE	C3-C12-C7	-3.81	116.65	120.92
3	A	1109	WYE	C6-C8-C16	3.16	130.39	124.59
3	A	1109	WYE	O1-C14-C15	3.10	128.96	126.21
3	A	1109	WYE	C7-C14-C15	-3.09	102.73	104.06
3	A	1109	WYE	C8-C16-C15	-2.72	122.42	128.15
3	A	1109	WYE	O2-C10-C7	2.54	113.23	110.69
3	A	1109	WYE	C18-N3-C17	2.46	117.10	111.57
3	A	1109	WYE	O2-C15-C14	2.29	110.94	109.47

There are no chirality outliers.

There are no torsion outliers.

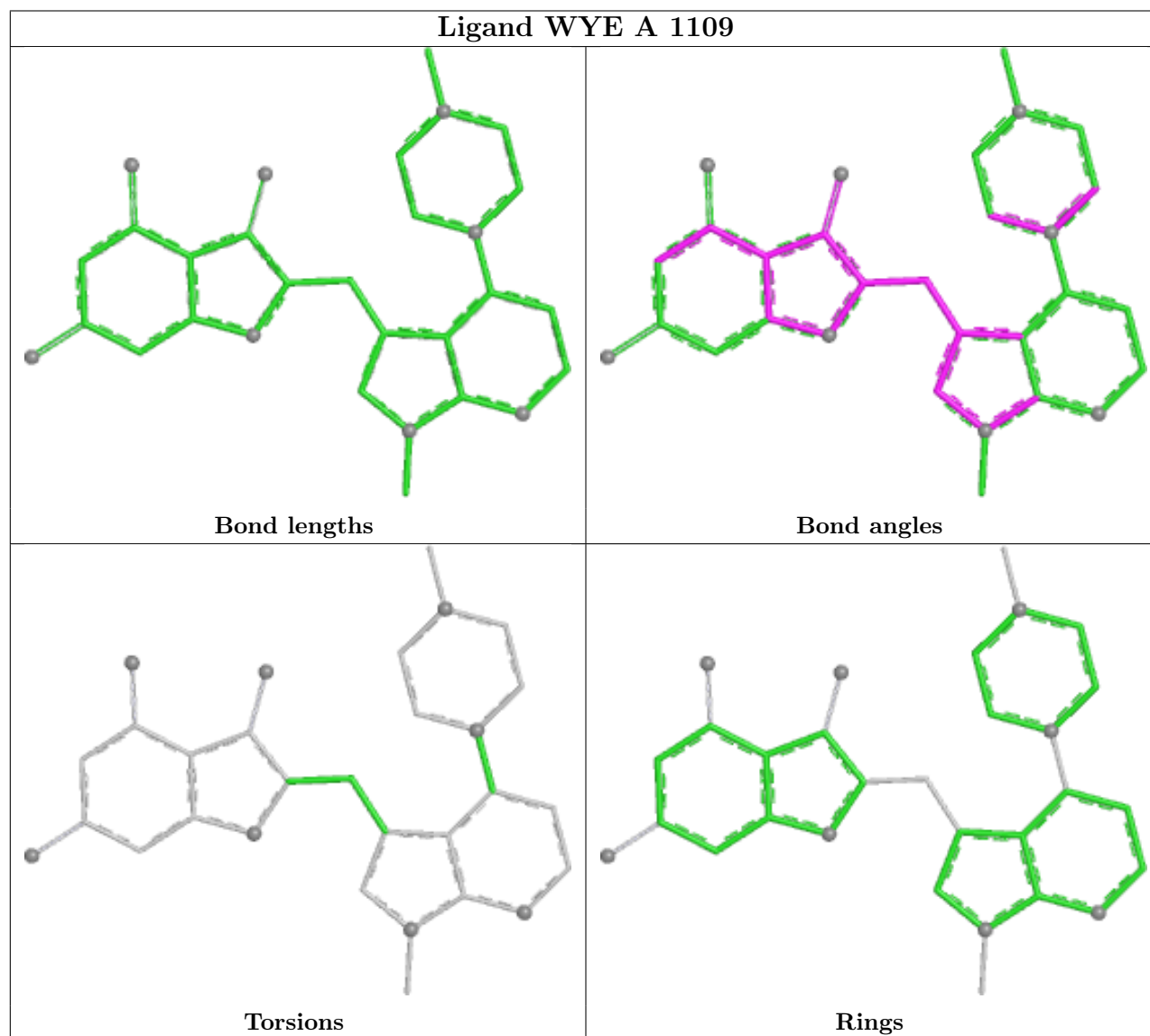
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1109	WYE	12	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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	829/966 (85%)	0.33	33 (3%) 42 39	37, 66, 96, 110	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1090	LEU	4.3
1	A	969	LEU	3.8
1	A	968	ILE	3.6
1	A	896	VAL	3.6
1	A	1042	LEU	3.6
1	A	522	ASN	3.4
1	A	836	ASP	3.2
1	A	248	PHE	3.0
1	A	804	MET	3.0
1	A	355	TRP	2.9
1	A	776	ASN	2.9
1	A	252	MET	2.8
1	A	216	ALA	2.8
1	A	1040	PRO	2.7
1	A	249	PHE	2.7
1	A	876	ILE	2.6
1	A	981	GLU	2.6
1	A	356	ASP	2.5
1	A	221	PHE	2.5
1	A	832	PHE	2.4
1	A	545	ALA	2.4
1	A	762	GLN	2.4
1	A	764	ILE	2.3
1	A	898	ASN	2.2
1	A	749	ILE	2.2
1	A	966	GLY	2.2
1	A	1086	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	497	PHE	2.2
1	A	999	GLY	2.2
1	A	938	ALA	2.1
1	A	1087	PHE	2.0
1	A	893	GLN	2.0
1	A	217	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

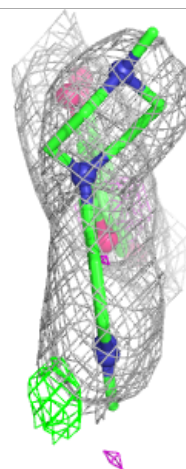
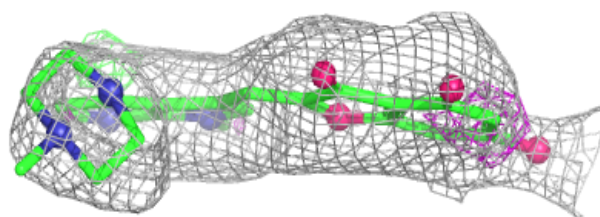
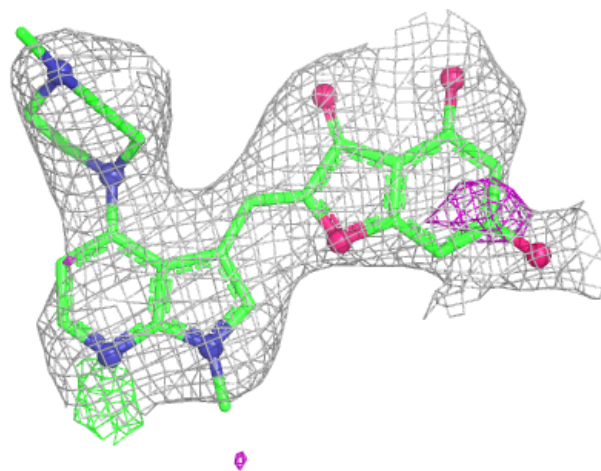
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	2	5/5	0.84	0.15	61,71,85,95	0
3	WYE	A	1109	30/30	0.85	0.15	60,67,81,83	0
2	SO4	A	1	5/5	0.91	0.09	72,73,85,94	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 WYE A 1109:

$2mF_o-DF_c$ (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.