



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:15 PM UTC

PDB ID : 4FJZ / pdb_00004fjz
Title : Crystal structure of PI3K-gamma in complex with pyrrolo-pyridine inhibitor 63
Authors : Whittington, D.A.; Tang, J.; Yakowec, P.
Deposited on : 2012-06-12
Resolution : 3.00 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

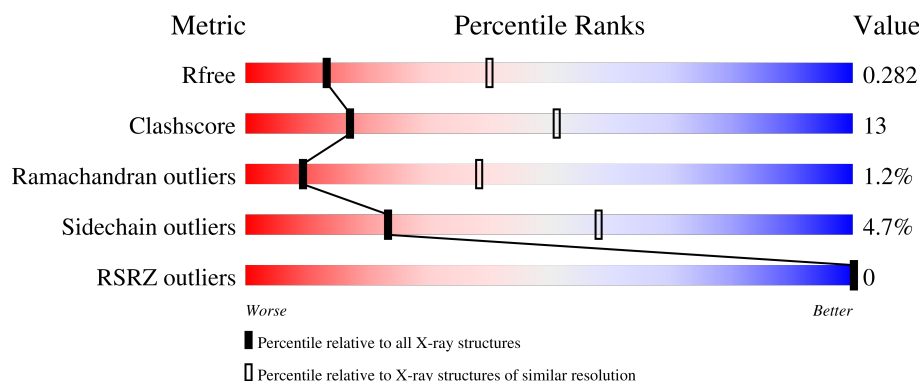
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	960	 61% 22% • 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6726 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 sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6658	4279	1134	1211	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	expression tag	UNP P48736

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



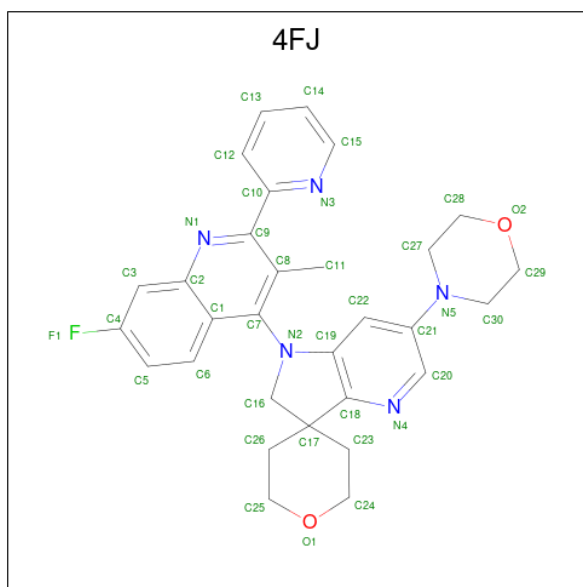
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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 1'-[7-fluoro-3-methyl-2-(pyridin-2-yl)quinolin-4-yl]-6'-(morpholin-4-yl)-1',2,2',3,5,6-hexahydrospiro[pyran-4,3'-pyrrolo[3,2-b]pyridine] (CCD ID: 4FJ) (formula: $C_{30}H_{30}FN_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	30	1	5	2		

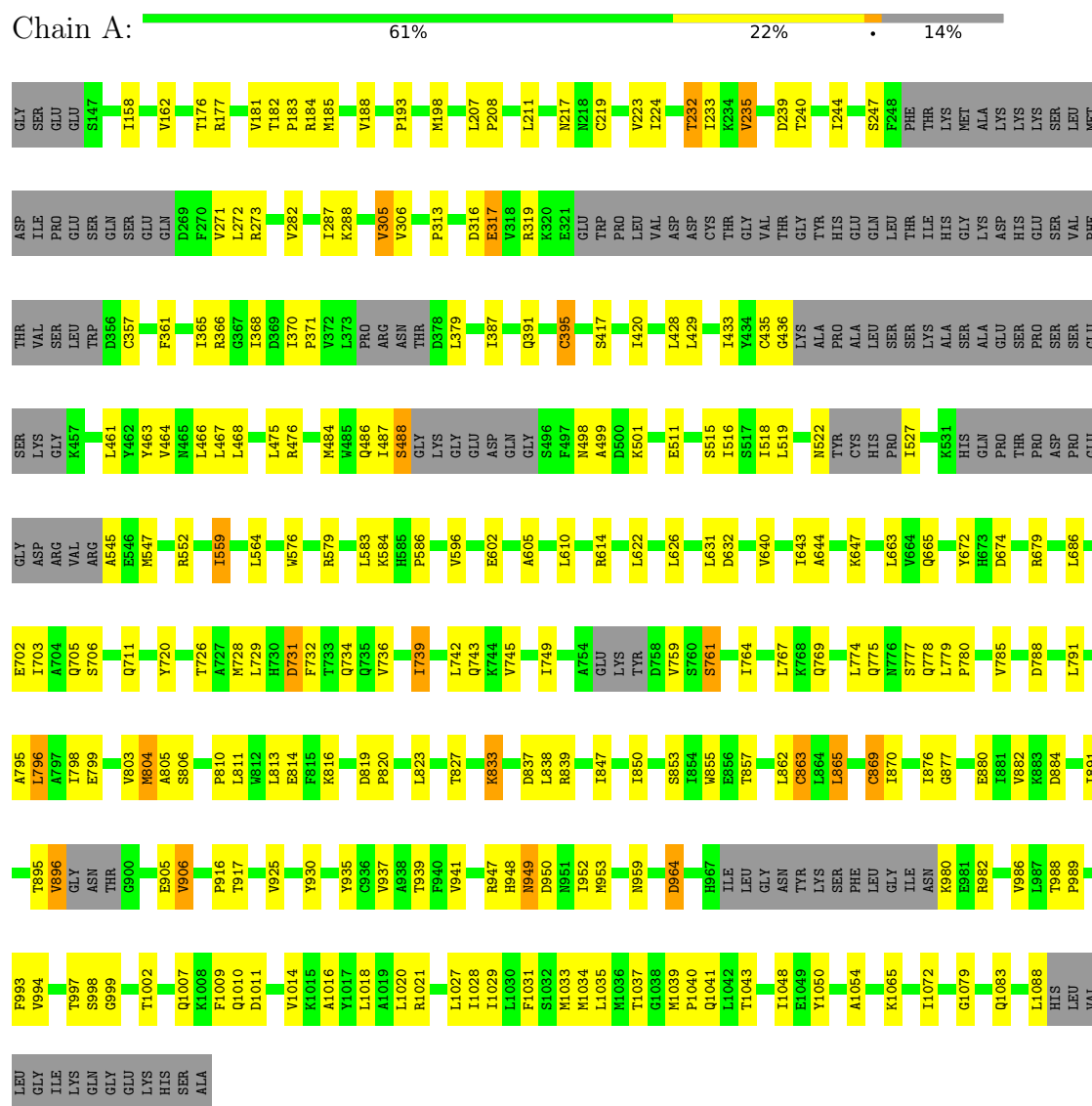
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.31Å 67.90Å 106.31Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-3.00) 97.5 (30.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.280 0.204 , 0.282	Depositor DCC
R_{free} test set	1242 reflections (5.98%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6726	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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: SO4, 4FJ

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	0.70	0/6796	0.81	1/9187 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	ILE	CB-CA-C	-6.21	102.99	112.05

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	6658	0	6715	168	0
2	A	20	0	0	0	0
3	A	38	0	30	5	0
4	A	10	0	0	1	0
All	All	6726	0	6745	169	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 (169) 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:767:LEU:HD22	1:A:803:VAL:HG23	1.64	0.77
1:A:370:ILE:HD12	1:A:371:PRO:HD2	1.68	0.75
1:A:428:LEU:HD23	1:A:467:LEU:HD23	1.68	0.75
1:A:198:MET:HE3	1:A:282:VAL:HG21	1.69	0.74
1:A:895:THR:HG22	1:A:896:VAL:HG23	1.69	0.73
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.19	0.73
1:A:576:TRP:O	1:A:579:ARG:HD3	1.89	0.72
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.72	0.71
1:A:726:THR:HA	1:A:729:LEU:HD12	1.73	0.70
1:A:941:VAL:HG21	1:A:1020:LEU:HD13	1.71	0.70
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.73	0.70
1:A:272:LEU:HD22	1:A:305:VAL:HG21	1.73	0.69
1:A:880:GLU:O	3:A:1205:4FJ:H17	1.94	0.68
1:A:198:MET:CE	1:A:282:VAL:HG21	2.25	0.66
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.31	0.65
1:A:464:VAL:HG12	1:A:484:MET:HE3	1.78	0.64
1:A:953:MET:SD	3:A:1205:4FJ:H20	2.38	0.62
1:A:365:ILE:HD13	1:A:518:ILE:HG22	1.81	0.62
1:A:547:MET:HE2	1:A:552:ARG:N	2.15	0.61
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.81	0.61
1:A:223:VAL:HG22	1:A:232:THR:HG23	1.82	0.61
1:A:547:MET:HE2	1:A:552:ARG:CA	2.31	0.61
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.66	0.60
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.83	0.60
1:A:804:MET:HE3	1:A:806:SER:HB3	1.84	0.59
1:A:937:VAL:O	1:A:941:VAL:HG23	2.01	0.59
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.86	0.58
1:A:952:ILE:CD1	1:A:986:VAL:HG11	2.34	0.58
1:A:745:VAL:O	1:A:749:ILE:HD13	2.04	0.58
1:A:395:CYS:SG	1:A:417:SER:OG	2.61	0.58
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.85	0.58
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.85	0.58
1:A:798:ILE:HD12	1:A:798:ILE:H	1.69	0.57
1:A:779:LEU:HD23	1:A:780:PRO:O	2.04	0.57
1:A:379:LEU:HD22	1:A:436:GLY:O	2.04	0.57
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.86	0.57
1:A:162:VAL:CG1	1:A:177:ARG:HD2	2.34	0.57
1:A:869:CYS:O	1:A:870:ILE:HD13	2.04	0.57
1:A:895:THR:HG22	1:A:896:VAL:CG2	2.36	0.56
1:A:925:VAL:HG13	1:A:994:VAL:HG12	1.87	0.56
1:A:475:LEU:HD23	1:A:476:ARG:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:LYS:HE3	1:A:1088:LEU:HD11	1.87	0.56
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.87	0.55
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.88	0.55
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.88	0.55
1:A:937:VAL:HG21	1:A:1016:ALA:HB3	1.89	0.55
1:A:1007:GLN:O	1:A:1011:ASP:N	2.38	0.55
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.46	0.54
1:A:732:PHE:O	1:A:736:VAL:HG23	2.07	0.54
1:A:833:LYS:HG3	3:A:1205:4FJ:H12	1.88	0.54
1:A:742:LEU:HD22	1:A:813:LEU:CD1	2.38	0.54
1:A:705:GLN:NE2	1:A:837:ASP:OD1	2.41	0.54
1:A:665:GLN:NE2	1:A:702:GLU:OE2	2.32	0.53
1:A:632:ASP:C	1:A:632:ASP:OD1	2.52	0.53
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.38	0.53
1:A:475:LEU:HD23	1:A:476:ARG:N	2.24	0.53
1:A:498:ASN:HD22	1:A:499:ALA:N	2.07	0.53
1:A:941:VAL:HG21	1:A:1020:LEU:CD1	2.39	0.53
1:A:370:ILE:HD12	1:A:371:PRO:CD	2.38	0.52
1:A:631:LEU:HD21	1:A:644:ALA:HB3	1.90	0.52
1:A:162:VAL:HG13	1:A:177:ARG:HD2	1.91	0.52
1:A:208:PRO:HG2	1:A:211:LEU:HD12	1.90	0.52
1:A:665:GLN:HE22	1:A:702:GLU:CD	2.15	0.52
1:A:804:MET:CE	1:A:806:SER:HB3	2.39	0.52
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.91	0.51
1:A:176:THR:HG23	1:A:674:ASP:CB	2.39	0.51
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.93	0.51
1:A:586:PRO:O	1:A:626:LEU:HD21	2.11	0.51
1:A:785:VAL:HG23	1:A:791:LEU:O	2.11	0.51
1:A:181:VAL:HG13	1:A:185:MET:HE2	1.92	0.51
1:A:583:LEU:HD13	1:A:610:LEU:HG	1.93	0.51
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.93	0.50
1:A:804:MET:HE2	1:A:810:PRO:HG2	1.92	0.50
1:A:602:GLU:O	1:A:605:ALA:HB3	2.12	0.50
1:A:952:ILE:HD12	1:A:986:VAL:HG11	1.94	0.50
1:A:761:SER:HA	1:A:764:ILE:HD12	1.93	0.50
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.11	0.50
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.93	0.50
1:A:880:GLU:O	3:A:1205:4FJ:C28	2.59	0.49
1:A:1031:PHE:CE2	1:A:1035:LEU:HD11	2.48	0.49
1:A:579:ARG:HG2	1:A:610:LEU:HD22	1.96	0.48
1:A:559:ILE:HG22	1:A:559:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:CYS:HA	1:A:235:VAL:O	2.14	0.48
1:A:989:PRO:O	1:A:993:PHE:N	2.41	0.48
1:A:545:ALA:HB1	1:A:584:LYS:HZ1	1.79	0.48
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.28	0.48
1:A:855:TRP:CD2	1:A:862:LEU:HD13	2.48	0.48
1:A:184:ARG:O	1:A:188:VAL:HG23	2.14	0.48
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.96	0.48
1:A:387:ILE:HD12	1:A:468:LEU:HD11	1.96	0.48
1:A:947:ARG:NH2	1:A:964:ASP:O	2.47	0.48
1:A:1033:MET:O	1:A:1037:THR:HG23	2.14	0.48
1:A:1007:GLN:HA	1:A:1010:GLN:HE21	1.79	0.47
1:A:863:CYS:SG	1:A:930:TYR:HB3	2.54	0.47
1:A:739:ILE:HD12	1:A:739:ILE:C	2.39	0.47
1:A:1034:MET:HG2	1:A:1039:MET:HE3	1.97	0.47
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.29	0.47
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.41	0.47
1:A:1050:TYR:CE2	1:A:1054:ALA:HB2	2.50	0.47
1:A:357:CYS:H	1:A:527:ILE:HD11	1.80	0.47
1:A:387:ILE:HD12	1:A:468:LEU:CD1	2.44	0.47
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.96	0.47
1:A:686:LEU:HD23	1:A:720:TYR:CE1	2.50	0.46
1:A:545:ALA:HB1	1:A:584:LYS:NZ	2.31	0.46
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.97	0.46
1:A:233:ILE:HD13	1:A:247:SER:OG	2.15	0.46
1:A:804:MET:HE2	1:A:810:PRO:CG	2.46	0.46
1:A:182:THR:HB	1:A:183:PRO:CD	2.45	0.46
1:A:876:ILE:HG23	1:A:876:ILE:O	2.16	0.46
1:A:805:ALA:HB3	4:A:1307:HOH:O	2.16	0.45
1:A:487:ILE:HG22	1:A:488:SER:H	1.81	0.45
1:A:997:THR:HG22	1:A:998:SER:N	2.32	0.45
1:A:1034:MET:CG	1:A:1039:MET:HE3	2.46	0.45
1:A:235:VAL:HG12	1:A:239:ASP:HB2	1.98	0.45
1:A:379:LEU:HD22	1:A:436:GLY:C	2.42	0.45
1:A:814:GLU:OE2	1:A:827:THR:OG1	2.32	0.45
1:A:272:LEU:CD2	1:A:305:VAL:HG11	2.47	0.45
1:A:935:TYR:O	1:A:939:THR:HG23	2.16	0.45
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.99	0.44
1:A:576:TRP:CZ3	1:A:596:VAL:HG22	2.52	0.44
1:A:948:HIS:ND1	1:A:950:ASP:OD1	2.50	0.44
3:A:1205:4FJ:H8	3:A:1205:4FJ:H19	1.82	0.44
1:A:316:ASP:O	1:A:317:GLU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:SER:O	1:A:857:THR:HG23	2.18	0.44
1:A:1035:LEU:O	1:A:1043:THR:HG22	2.18	0.44
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.52	0.44
1:A:305:VAL:HG22	1:A:306:VAL:H	1.84	0.43
1:A:803:VAL:HG22	1:A:811:LEU:HD23	1.99	0.43
1:A:905:GLU:HA	1:A:993:PHE:CE2	2.53	0.43
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.49	0.43
1:A:949:ASN:H	1:A:949:ASN:HD22	1.66	0.43
1:A:891:ILE:O	1:A:906:VAL:HG11	2.19	0.43
1:A:182:THR:HB	1:A:183:PRO:HD3	2.01	0.43
1:A:162:VAL:HG12	1:A:177:ARG:NH1	2.33	0.43
1:A:365:ILE:HD12	1:A:516:ILE:HD11	2.00	0.43
1:A:366:ARG:NH1	1:A:519:LEU:HD22	2.33	0.43
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.91	0.43
1:A:305:VAL:HG13	1:A:306:VAL:N	2.34	0.42
1:A:467:LEU:O	1:A:476:ARG:HD2	2.19	0.42
1:A:208:PRO:CG	1:A:211:LEU:HD12	2.50	0.42
1:A:287:ILE:HD12	1:A:288:LYS:N	2.34	0.42
1:A:811:LEU:HB3	1:A:813:LEU:CD2	2.48	0.42
1:A:862:LEU:N	1:A:862:LEU:HD12	2.34	0.42
1:A:640:VAL:O	1:A:643:ILE:HG12	2.19	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.94	0.42
1:A:997:THR:HG22	1:A:998:SER:H	1.83	0.42
1:A:273:ARG:H	1:A:305:VAL:HG22	1.85	0.42
1:A:371:PRO:HG2	1:A:511:GLU:O	2.19	0.42
1:A:224:ILE:HA	1:A:305:VAL:HG12	2.02	0.41
1:A:745:VAL:CG2	1:A:774:LEU:HD12	2.50	0.41
1:A:788:ASP:OD2	1:A:791:LEU:HD12	2.20	0.41
1:A:702:GLU:O	1:A:706:SER:HB3	2.20	0.41
1:A:759:VAL:HG12	1:A:764:ILE:HG13	2.01	0.41
1:A:271:VAL:HG13	1:A:282:VAL:CG1	2.50	0.41
1:A:865:LEU:HD22	1:A:882:VAL:HG21	2.03	0.41
1:A:547:MET:HE2	1:A:552:ARG:HA	2.01	0.41
1:A:702:GLU:OE1	1:A:839:ARG:NH2	2.54	0.41
1:A:775:GLN:HE22	1:A:796:LEU:H	1.68	0.41
1:A:1039:MET:C	1:A:1041:GLN:H	2.29	0.41
1:A:795:ALA:HB3	1:A:816:LYS:HB2	2.03	0.41
1:A:1014:VAL:HG11	1:A:1065:LYS:CG	2.51	0.41
1:A:368:ILE:HG21	1:A:433:ILE:HD11	2.03	0.40
1:A:728:MET:HA	1:A:731:ASP:HB2	2.03	0.40
1:A:862:LEU:O	1:A:863:CYS:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:CZ	1:A:643:ILE:HG22	2.52	0.40
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.54	0.40
1:A:181:VAL:CG1	1:A:185:MET:HE2	2.52	0.40
1:A:775:GLN:OE1	1:A:798:ILE:HD11	2.21	0.40
1:A:937:VAL:HG12	1:A:1020:LEU:HD12	2.04	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	800/960 (83%)	724 (90%)	66 (8%)	10 (1%)	9 38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	916	PRO
1	A	1079	GLY
1	A	217	ASN
1	A	778	GLN
1	A	761	SER
1	A	777	SER
1	A	964	ASP
1	A	319	ARG
1	A	999	GLY
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	739/857 (86%)	704 (95%)	35 (5%)	23	58

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

Mol	Chain	Res	Type
1	A	232	THR
1	A	235	VAL
1	A	240	THR
1	A	305	VAL
1	A	317	GLU
1	A	391	GLN
1	A	395	CYS
1	A	486	GLN
1	A	488	SER
1	A	515	SER
1	A	522	ASN
1	A	711	GLN
1	A	731	ASP
1	A	739	ILE
1	A	769	GLN
1	A	796	LEU
1	A	799	GLU
1	A	804	MET
1	A	823	LEU
1	A	833	LYS
1	A	847	ILE
1	A	850	ILE
1	A	863	CYS
1	A	865	LEU
1	A	869	CYS
1	A	884	ASP
1	A	896	VAL
1	A	906	VAL
1	A	917	THR
1	A	949	ASN
1	A	959	ASN
1	A	982	ARG
1	A	1002	THR
1	A	1028	ILE

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Mol	Chain	Res	Type
1	A	1029	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	HIS
1	A	289	ASN
1	A	389	HIS
1	A	391	GLN
1	A	486	GLN
1	A	498	ASN
1	A	554	GLN
1	A	609	GLN
1	A	619	GLN
1	A	629	GLN
1	A	658	HIS
1	A	730	HIS
1	A	734	GLN
1	A	743	GLN
1	A	773	ASN
1	A	840	GLN
1	A	846	GLN
1	A	892	GLN
1	A	922	GLN
1	A	959	ASN
1	A	1010	GLN
1	A	1023	HIS
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	4FJ	A	1205	-	43,44,44	1.80	6 (13%)	50,65,65	1.87	16 (32%)
2	SO4	A	1201	-	4,4,4	0.47	0	6,6,6	0.25	0
2	SO4	A	1204	-	4,4,4	0.51	0	6,6,6	0.16	0
2	SO4	A	1202	-	4,4,4	0.48	0	6,6,6	0.22	0
2	SO4	A	1203	-	4,4,4	0.45	0	6,6,6	0.22	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	4FJ	A	1205	-	-	1/12/45/45	0/7/7/7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	4FJ	C9-C10	-7.18	1.40	1.49
3	A	1205	4FJ	C7-N2	-6.55	1.35	1.44
3	A	1205	4FJ	C19-N2	-2.61	1.34	1.38
3	A	1205	4FJ	C7-C1	-2.36	1.40	1.44
3	A	1205	4FJ	C3-C4	2.17	1.39	1.36
3	A	1205	4FJ	C2-N1	-2.14	1.34	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1205	4FJ	O1-C25-C26	-4.67	106.84	111.50
3	A	1205	4FJ	C16-N2-C19	3.47	111.99	109.27
3	A	1205	4FJ	C9-C10-N3	3.46	121.52	116.35
3	A	1205	4FJ	C20-N4-C18	3.31	121.27	117.50
3	A	1205	4FJ	C5-C4-C3	-3.11	119.70	123.32
3	A	1205	4FJ	C30-N5-C27	3.03	118.39	111.57
3	A	1205	4FJ	C15-N3-C10	2.91	121.31	117.24
3	A	1205	4FJ	C8-C9-N1	-2.71	120.65	123.25
3	A	1205	4FJ	C10-C9-C8	-2.48	121.71	124.11
3	A	1205	4FJ	C7-C1-C2	2.45	120.30	115.74
3	A	1205	4FJ	C8-C7-N2	2.39	121.58	118.67
3	A	1205	4FJ	C1-C7-N2	2.31	120.66	117.32
3	A	1205	4FJ	C8-C7-C1	-2.28	117.76	121.83
3	A	1205	4FJ	C6-C1-C7	-2.23	120.32	124.38
3	A	1205	4FJ	C22-C19-N2	2.21	131.50	128.53
3	A	1205	4FJ	C1-C2-N1	-2.01	120.67	122.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

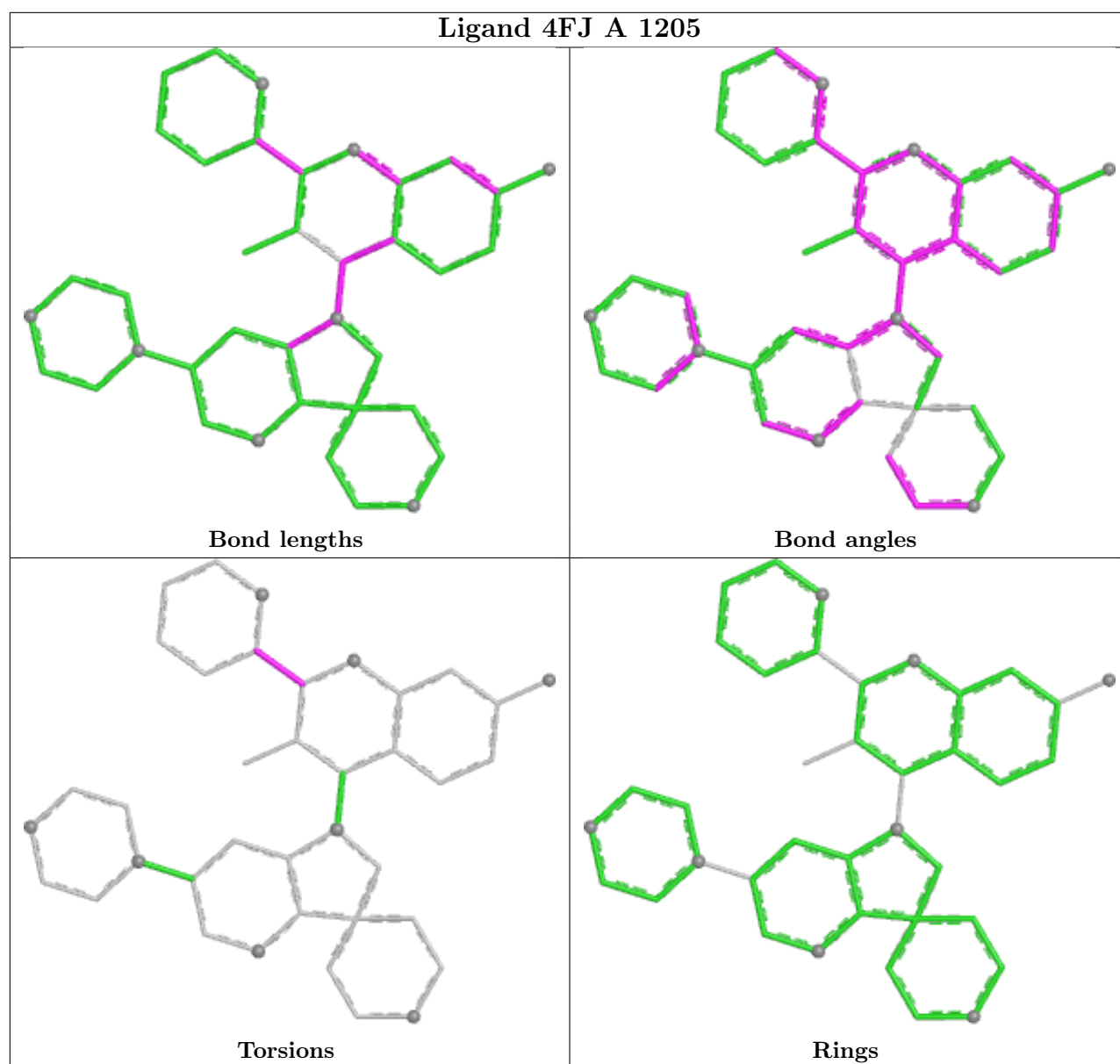
Mol	Chain	Res	Type	Atoms
3	A	1205	4FJ	C12-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1205	4FJ	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	822/960 (85%)	-0.51	0 100 100	48, 85, 133, 155	0

There are no RSRZ outliers to report.

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](#)

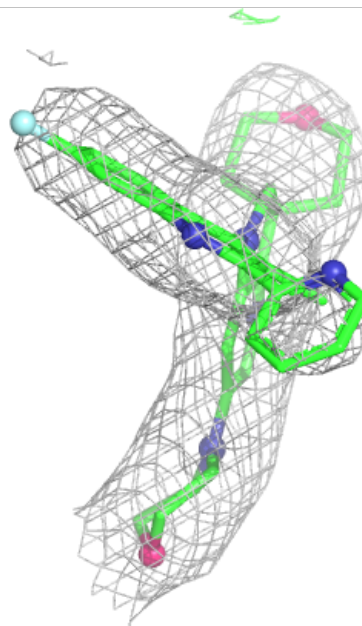
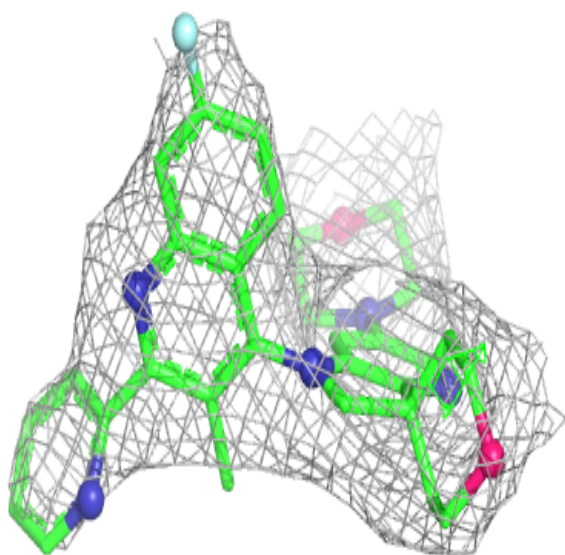
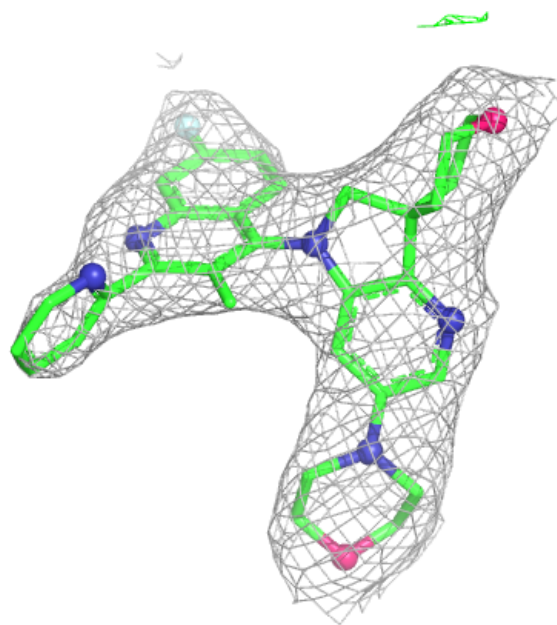
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1202	5/5	0.79	0.14	117,124,128,130	0
2	SO4	A	1203	5/5	0.81	0.11	149,152,155,158	0
2	SO4	A	1204	5/5	0.89	0.12	107,110,116,119	0
2	SO4	A	1201	5/5	0.91	0.08	93,95,101,109	0
3	4FJ	A	1205	38/38	0.92	0.11	77,99,111,114	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 4FJ A 1205:

$2mF_o - DF_c$ (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.