



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:31 PM GMT

PDB ID : 3MJW
Title : PI3 Kinase gamma with a benzofuranone inhibitor
Authors : Bard, J.; Svenson, K.
Deposited on : 2010-04-13
Resolution : 2.87 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

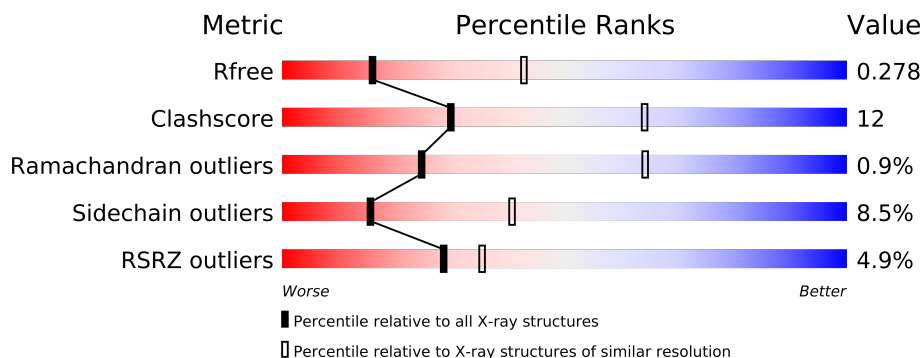
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.87 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}	66092	1360 (2.90-2.86)
Clashscore	79885	1696 (2.90-2.86)
Ramachandran outliers	78287	1647 (2.90-2.86)
Sidechain outliers	78261	1650 (2.90-2.86)
RSRZ outliers	66119	1362 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6472 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

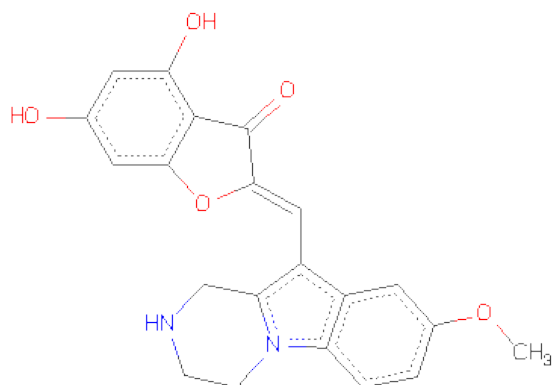
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total	C	N	O	S	0	0	0
			6444	4133	1102	1177	32			

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	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 (2Z)-4,6-DIHYDROXY-2-[(8-METHOXY-1,2,3,4-TETRAHYDROPYRAZINO[1,2-A]INDOL-10-YL)METHYLIDENE]-1-BENZOFURAN-3(2H)-ONE (three-letter code: WYF) (formula: C₂₁H₁₈N₂O₅).

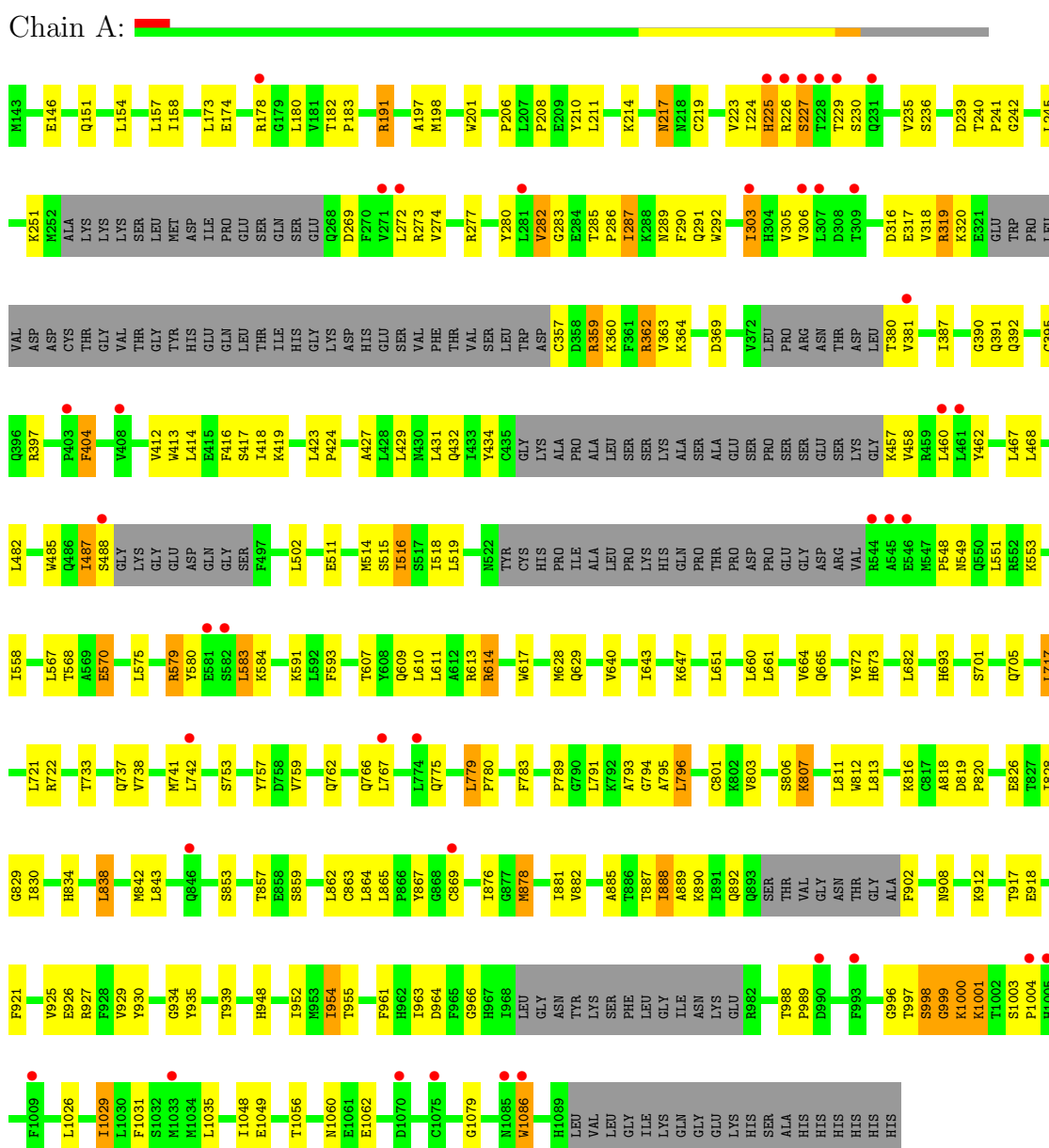


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	28	21	2	5	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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-bisphosphate3-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	145.60Å 68.57Å 107.25Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	36.23 – 2.87 41.24 – 2.86	Depositor EDS
% Data completeness (in resolution range)	86.3 (36.23-2.87) 86.3 (41.24-2.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.281 0.226 , 0.278	Depositor DCC
R_{free} test set	1911 reflections (9.06%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22212 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.22	0/6579	0.40	0/8926

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6444	0	6306	153	0
2	A	28	0	17	3	0
All	All	6472	0	6323	155	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:ASN:HD22	1:A:219:CYS:HB3	1.52	0.75
1:A:887:THR:HG22	1:A:889:ALA:H	1.54	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:PHE:N	1:A:404:PHE:CD1	2.55	0.72
1:A:487:ILE:HG22	1:A:488:SER:H	1.59	0.67
1:A:613:ARG:HA	1:A:614:ARG:CB	2.26	0.65
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.80	0.64
1:A:793:ALA:HB2	1:A:828:ILE:HD12	1.80	0.63
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.82	0.62
1:A:219:CYS:HA	1:A:235:VAL:O	2.00	0.62
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.82	0.61
1:A:404:PHE:N	1:A:404:PHE:HD1	1.97	0.61
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.82	0.61
1:A:303:ILE:H	1:A:303:ILE:HD12	1.66	0.60
1:A:174:GLU:O	1:A:178:ARG:HD2	2.01	0.60
1:A:613:ARG:HA	1:A:614:ARG:HB3	1.83	0.60
1:A:182:THR:HB	1:A:183:PRO:HD3	1.84	0.60
1:A:998:SER:H	1:A:1001:LYS:HG3	1.66	0.59
1:A:240:THR:HG22	1:A:242:GLY:H	1.68	0.58
1:A:239:ASP:O	1:A:286:PRO:HA	2.04	0.57
1:A:380:THR:HA	1:A:404:PHE:CD1	2.39	0.57
1:A:568:THR:HG22	1:A:570:GLU:H	1.69	0.56
1:A:482:LEU:HB2	1:A:516:ILE:HG22	1.87	0.56
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.88	0.56
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.41	0.56
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.55
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.87	0.55
1:A:998:SER:H	1:A:1001:LYS:CG	2.19	0.55
1:A:660:LEU:O	1:A:664:VAL:HG23	2.06	0.55
1:A:273:ARG:HG2	1:A:274:VAL:N	2.22	0.54
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.88	0.54
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.89	0.54
1:A:225:HIS:N	1:A:225:HIS:ND1	2.55	0.54
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.43	0.54
1:A:737:GLN:O	1:A:741:MET:HG3	2.08	0.53
1:A:434:TYR:CZ	1:A:460:LEU:HD13	2.44	0.53
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.89	0.53
1:A:362:ARG:HG3	1:A:413:TRP:CE3	2.45	0.52
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.44	0.52
1:A:811:LEU:HB3	1:A:813:LEU:CD1	2.40	0.52
1:A:779:LEU:HD12	1:A:796:LEU:HD12	1.92	0.52
1:A:948:HIS:HB2	1:A:1086:TRP:HD1	1.75	0.52
1:A:794:GLY:HA3	1:A:818:ALA:HB2	1.92	0.51
1:A:224:ILE:HD12	1:A:224:ILE:N	2.25	0.51
1:A:842:MET:HG2	1:A:869:CYS:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:583:LEU:HD21	1:A:614:ARG:H	1.75	0.51
1:A:229:THR:HG22	1:A:230:SER:N	2.26	0.51
1:A:395:CYS:SG	1:A:417:SER:HB2	2.50	0.51
1:A:753:SER:HB2	1:A:757:TYR:CB	2.40	0.51
1:A:701:SER:O	1:A:705:GLN:HG2	2.11	0.50
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.94	0.50
1:A:303:ILE:HD12	1:A:303:ILE:N	2.26	0.50
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.47	0.50
1:A:549:ASN:O	1:A:553:LYS:HG2	2.12	0.50
1:A:795:ALA:HB3	1:A:816:LYS:HE3	1.95	0.49
1:A:210:TYR:HE2	1:A:859:SER:C	2.16	0.49
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.53	0.49
1:A:567:LEU:HD21	1:A:591:LYS:HD2	1.95	0.49
1:A:807:LYS:H	1:A:807:LYS:CD	2.25	0.49
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.28	0.49
1:A:882:VAL:HG12	1:A:885:ALA:HB2	1.95	0.49
1:A:359:ARG:HG3	1:A:360:LYS:N	2.28	0.49
1:A:277:ARG:NH1	1:A:791:LEU:HG	2.28	0.48
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.96	0.48
1:A:198:MET:HE2	1:A:282:VAL:HG21	1.94	0.48
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.96	0.48
1:A:779:LEU:HD22	1:A:780:PRO:O	2.14	0.48
1:A:853:SER:O	1:A:857:THR:HG23	2.13	0.48
2:A:1:WYF:O3	2:A:1:WYF:H7	2.14	0.47
1:A:282:VAL:HG23	1:A:283:GLY:N	2.28	0.47
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.47
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.97	0.47
1:A:210:TYR:CD1	1:A:211:LEU:HG	2.50	0.47
1:A:1060:ASN:C	1:A:1062:GLU:H	2.18	0.47
1:A:997:THR:HA	1:A:1001:LYS:HD2	1.96	0.47
1:A:807:LYS:HD2	1:A:807:LYS:N	2.30	0.46
1:A:912:LYS:HE2	1:A:918:GLU:OE2	2.15	0.46
1:A:390:GLY:O	1:A:391:GLN:HB2	2.13	0.46
1:A:280:TYR:HB3	1:A:282:VAL:HG13	1.97	0.46
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.50	0.46
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.48	0.46
1:A:457:LYS:HA	1:A:458:VAL:HA	1.79	0.46
1:A:273:ARG:O	1:A:305:VAL:HG13	2.16	0.46
1:A:948:HIS:CB	1:A:1086:TRP:HD1	2.28	0.46
1:A:948:HIS:HB2	1:A:1086:TRP:CD1	2.50	0.46
1:A:387:ILE:HD12	1:A:418:ILE:HD12	1.97	0.46
1:A:888:ILE:HD11	1:A:952:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:964:ASP:HA	2:A:1:WYF:C18	2.46	0.46
1:A:580:TYR:O	1:A:584:LYS:HD3	2.16	0.46
1:A:593:PHE:CE2	1:A:611:LEU:HD21	2.51	0.46
1:A:287:ILE:N	1:A:287:ILE:HD13	2.30	0.46
1:A:413:TRP:CH2	1:A:519:LEU:HD23	2.51	0.45
1:A:762:GLN:O	1:A:766:GLN:HG2	2.17	0.45
1:A:364:LYS:HA	1:A:412:VAL:O	2.16	0.45
1:A:418:ILE:HG22	1:A:419:LYS:O	2.17	0.45
1:A:208:PRO:HB3	1:A:210:TYR:CZ	2.51	0.45
1:A:613:ARG:CA	1:A:614:ARG:CB	2.94	0.45
1:A:287:ILE:HD13	1:A:287:ILE:H	1.82	0.44
1:A:397:ARG:HB3	1:A:414:LEU:HD22	1.99	0.44
1:A:191:ARG:O	1:A:191:ARG:HG3	2.18	0.44
1:A:1003:SER:CB	1:A:1004:PRO:HD2	2.46	0.44
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.53	0.44
1:A:198:MET:CE	1:A:282:VAL:HG21	2.47	0.44
1:A:989:PRO:HD3	1:A:1079:GLY:HA2	1.98	0.44
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.81	0.44
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.47	0.44
1:A:317:GLU:HG2	1:A:318:VAL:N	2.33	0.44
1:A:462:TYR:HA	1:A:485:TRP:O	2.18	0.44
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.52	0.44
1:A:1031:PHE:O	1:A:1035:LEU:HG	2.18	0.44
1:A:157:LEU:HD21	1:A:733:THR:HA	2.00	0.44
1:A:226:ARG:O	1:A:227:SER:HB2	2.18	0.43
1:A:742:LEU:HD22	1:A:813:LEU:HD21	2.01	0.43
1:A:954:ILE:HG13	1:A:955:THR:O	2.19	0.43
1:A:661:LEU:O	1:A:665:GLN:HG2	2.19	0.43
2:A:1:WYF:H7	2:A:1:WYF:H1B	1.78	0.43
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.84	0.43
1:A:838:LEU:O	1:A:842:MET:HG3	2.19	0.43
1:A:717:LEU:HD22	1:A:721:LEU:HG	2.01	0.42
1:A:867:TYR:OH	1:A:963:ILE:HA	2.20	0.42
1:A:926:GLU:O	1:A:929:VAL:HG22	2.20	0.42
1:A:579:ARG:HG3	1:A:579:ARG:H	1.55	0.42
1:A:794:GLY:CA	1:A:818:ALA:HB2	2.48	0.42
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.85	0.42
1:A:197:ALA:HB2	1:A:316:ASP:OD2	2.19	0.42
1:A:434:TYR:HB3	1:A:458:VAL:CG2	2.50	0.42
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.83	0.42
1:A:431:LEU:HD13	1:A:516:ILE:HD12	2.01	0.42
1:A:779:LEU:HD23	1:A:780:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:801:CYS:HA	1:A:812:TRP:O	2.20	0.42
1:A:738:VAL:HG21	1:A:783:PHE:CG	2.55	0.41
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.55	0.41
1:A:360:LYS:HB3	1:A:416:PHE:O	2.19	0.41
1:A:514:MET:HG3	1:A:515:SER:N	2.34	0.41
1:A:767:LEU:HG	1:A:803:VAL:CG2	2.51	0.41
1:A:607:THR:O	1:A:610:LEU:HB2	2.19	0.41
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.56	0.41
1:A:628:MET:HB2	1:A:1029:ILE:HG21	2.02	0.41
1:A:583:LEU:HD12	1:A:610:LEU:HD22	2.03	0.41
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.21	0.41
1:A:999:GLY:O	1:A:1000:LYS:CB	2.68	0.41
1:A:996:GLY:O	1:A:1003:SER:HB3	2.21	0.41
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.03	0.41
1:A:954:ILE:HG13	1:A:955:THR:N	2.33	0.41
1:A:935:TYR:O	1:A:939:THR:HG23	2.21	0.40
1:A:830:ILE:CG2	1:A:878:MET:HB2	2.50	0.40
1:A:921:PHE:O	1:A:925:VAL:HG23	2.19	0.40
1:A:364:LYS:O	1:A:518:ILE:HA	2.21	0.40
1:A:863:CYS:SG	1:A:930:TYR:HB3	2.61	0.40
1:A:154:LEU:O	1:A:158:ILE:HG13	2.20	0.40
1:A:614:ARG:HG2	1:A:617:TRP:HB3	2.03	0.40
1:A:998:SER:O	1:A:999:GLY:C	2.60	0.40
1:A:390:GLY:C	1:A:392:GLN:H	2.25	0.40
1:A:319:ARG:HG3	1:A:320:LYS:N	2.36	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.86	0.40
1:A:807:LYS:N	1:A:807:LYS:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	801/966 (83%)	720 (90%)	74 (9%)	7 (1%)	25 64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	966	GLY
1	A	999	GLY
1	A	206	PRO
1	A	269	ASP
1	A	303	ILE
1	A	227	SER
1	A	1000	LYS

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	685/864 (79%)	627 (92%)	58 (8%)	15	41

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	191	ARG
1	A	214	LYS
1	A	217	ASN
1	A	225	HIS
1	A	245	LEU
1	A	251	LYS
1	A	282	VAL
1	A	287	ILE
1	A	306	VAL
1	A	319	ARG
1	A	357	CYS
1	A	359	ARG
1	A	362	ARG
1	A	369	ASP
1	A	381	VAL
1	A	404	PHE
1	A	487	ILE
1	A	502	LEU
1	A	511	GLU

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Mol	Chain	Res	Type
1	A	516	ILE
1	A	570	GLU
1	A	579	ARG
1	A	583	LEU
1	A	609	GLN
1	A	614	ARG
1	A	647	LYS
1	A	651	LEU
1	A	682	LEU
1	A	717	LEU
1	A	759	VAL
1	A	775	GLN
1	A	779	LEU
1	A	796	LEU
1	A	806	SER
1	A	807	LYS
1	A	826	GLU
1	A	838	LEU
1	A	843	LEU
1	A	864	LEU
1	A	865	LEU
1	A	878	MET
1	A	888	ILE
1	A	890	LYS
1	A	892	GLN
1	A	902	PHE
1	A	908	ASN
1	A	917	THR
1	A	927	ARG
1	A	954	ILE
1	A	988	THR
1	A	998	SER
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1049	GLU
1	A	1056	THR
1	A	1086	TRP

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

Mol	Chain	Res	Type
1	A	217	ASN
1	A	600	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	WYF	A	1	-	32,32,32	1.27	4 (12%)	47,48,48	1.70	13 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WYF	A	1	-	-	1/5/25/25	0/0/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	WYF	C12-N2	3.84	1.51	1.47
2	A	1	WYF	C10-N1	-2.50	1.46	1.48
2	A	1	WYF	C8-C13	-2.46	1.43	1.48
2	A	1	WYF	C7-C2	2.44	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	WYF	C13-C14-C15	-4.27	121.92	126.79
2	A	1	WYF	C12-C9-C8	3.99	132.45	127.67
2	A	1	WYF	O1-C2-C7	-3.82	114.89	124.63
2	A	1	WYF	C11-C10-N1	3.12	113.40	110.34
2	A	1	WYF	O3-C14-C13	2.88	127.61	123.90
2	A	1	WYF	C9-C8-C13	-2.81	121.51	122.88
2	A	1	WYF	C9-N1-C5	2.72	111.04	107.90
2	A	1	WYF	C20-C21-C16	-2.52	121.65	124.79
2	A	1	WYF	O3-C21-C16	2.22	113.18	110.75
2	A	1	WYF	C18-C17-C16	-2.15	118.18	121.01
2	A	1	WYF	C6-C5-N1	-2.12	106.82	108.91
2	A	1	WYF	O2-C15-C14	2.09	128.34	126.20
2	A	1	WYF	C9-C12-N2	2.06	117.06	112.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	WYF	C14-C13-C8-C6

There are no ring outliers.

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, 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	819/966 (84%)	0.24	40 (4%) 28 35	41, 77, 115, 138	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	5.5
1	A	272	LEU	4.8
1	A	1075	CYS	4.3
1	A	1086	TRP	3.9
1	A	403	PRO	3.8
1	A	303	ILE	3.4
1	A	767	LEU	3.3
1	A	1085	ASN	3.3
1	A	460	LEU	3.3
1	A	226	ARG	3.3
1	A	488	SER	3.2
1	A	381	VAL	3.1
1	A	306	VAL	3.0
1	A	1009	PHE	3.0
1	A	581	GLU	2.9
1	A	545	ALA	2.8
1	A	281	LEU	2.8
1	A	846	GLN	2.7
1	A	869	CYS	2.7
1	A	309	THR	2.7
1	A	229	THR	2.7
1	A	231	GLN	2.6
1	A	408	VAL	2.6
1	A	774	LEU	2.4
1	A	544	ARG	2.4
1	A	582	SER	2.3
1	A	271	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	227	SER	2.3
1	A	993	PHE	2.3
1	A	228	THR	2.2
1	A	178	ARG	2.2
1	A	546	GLU	2.2
1	A	1033	MET	2.1
1	A	990	ASP	2.1
1	A	1070	ASP	2.1
1	A	1004	PRO	2.1
1	A	461	LEU	2.1
1	A	225	HIS	2.0
1	A	742	LEU	2.0
1	A	1005	HIS	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	WYF	A	1	28/28	0.18	-0.72	69,85,92,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.