Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:56 AM UTC

PDB ID	:	1WZY / pdb_00001wzy
Title	:	Crystal structure of human ERK2 complexed with a pyrazolopyridazine derivative
Authors	:	Kinoshita, T.
Deposited on	:	2005-03-10
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

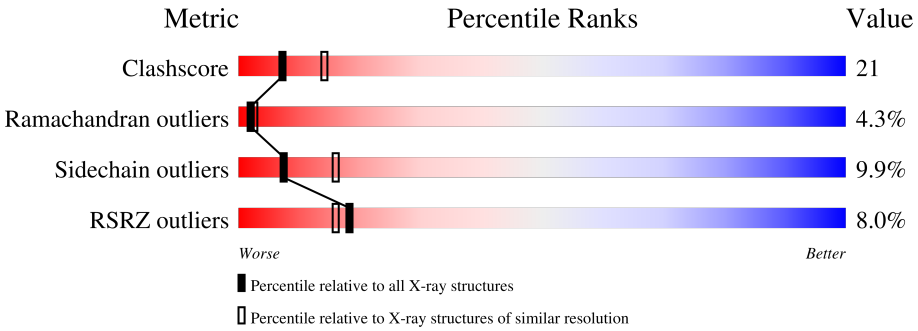
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	368	8% 55% 30% 9% 5%

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
2	F29	A	1001	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3116 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.

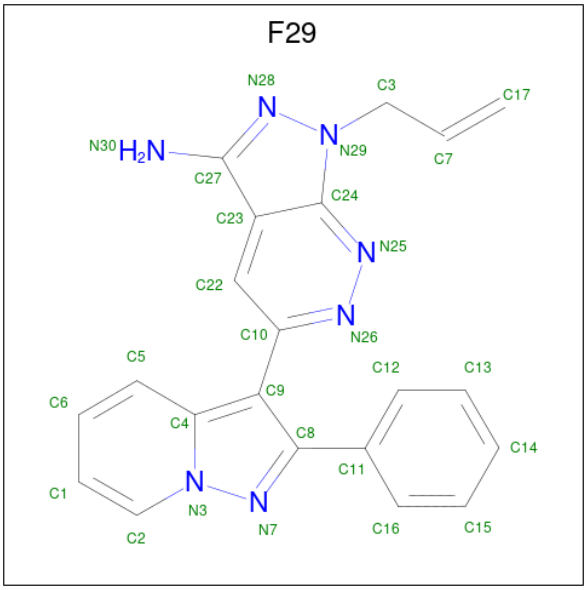
- Molecule 1 is a protein called Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2847	1827	487	518	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	cloning artifact	UNP P28482
A	-6	ASP	-	cloning artifact	UNP P28482
A	-5	LEU	-	cloning artifact	UNP P28482
A	-4	GLY	-	cloning artifact	UNP P28482
A	-3	SER	-	cloning artifact	UNP P28482
A	-2	ASP	-	cloning artifact	UNP P28482
A	-1	GLU	-	cloning artifact	UNP P28482
A	0	LEU	-	cloning artifact	UNP P28482

- Molecule 2 is 1-ALLYL-5-(2-PHENYLPYRAZOLO[1,5-A]PYRIDIN-3-YL)-1H-PYRAZOLO[3,4-C]PYRIDAZIN-3-AMINE (CCD ID: F29) (formula: $C_{21}H_{17}N_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 28 21 7	0	0

- Molecule 3 is water.

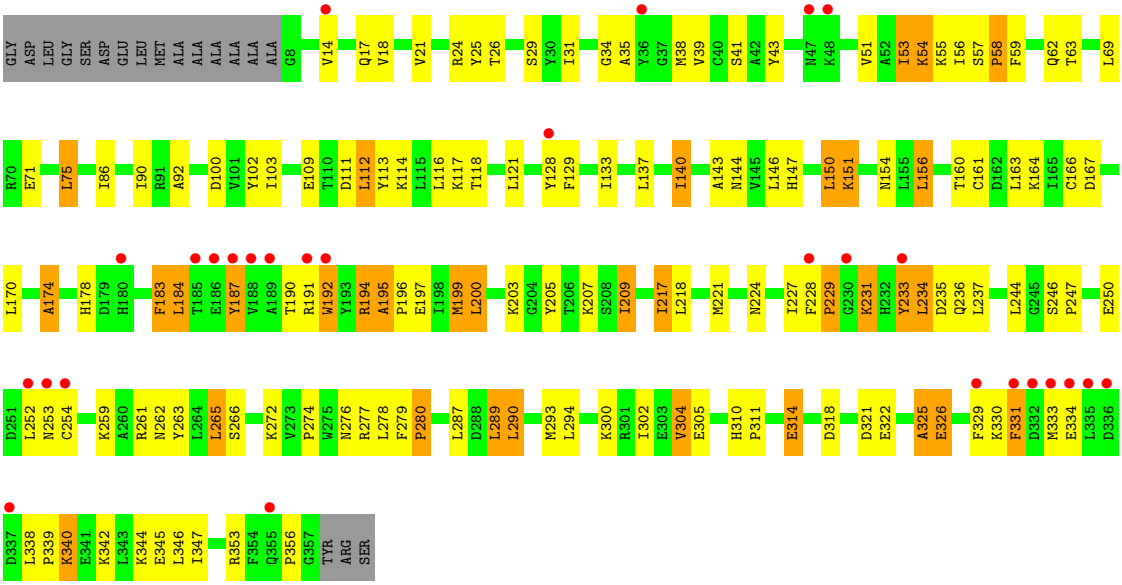
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	241	Total O 241 241	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Mitogen-activated protein kinase 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.60Å 68.54Å 59.83Å 90.00° 110.27° 90.00°	Depositor
Resolution (Å)	11.96 – 2.50 11.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (11.96-2.50) 98.9 (11.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.51Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.249 , 0.292 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3116	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F29

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	0.50	0/2916	1.00	12/3952 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	CYS	N-CA-C	6.34	124.31	110.80
1	A	167	ASP	N-CA-C	6.30	118.44	108.67
1	A	195	ALA	CA-C-N	6.26	126.45	119.32
1	A	195	ALA	C-N-CA	6.26	126.45	119.32
1	A	51	VAL	N-CA-C	6.14	117.00	108.23
1	A	318	ASP	CA-C-N	6.10	127.46	119.84
1	A	318	ASP	C-N-CA	6.10	127.46	119.84
1	A	183	PHE	N-CA-C	5.77	118.72	110.24
1	A	92	ALA	CA-C-N	5.31	125.63	119.47
1	A	92	ALA	C-N-CA	5.31	125.63	119.47
1	A	331	PHE	N-CA-C	5.29	116.92	110.41
1	A	195	ALA	N-CA-C	5.07	115.43	109.60

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	2847	0	2846	119	0
2	A	28	0	17	11	0
3	A	241	0	0	16	0
All	All	3116	0	2863	119	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 21.

All (119) 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:54:LYS:HE2	2:A:1001:F29:C11	1.84	1.06
1:A:54:LYS:CE	2:A:1001:F29:C12	2.48	0.91
1:A:227:ILE:O	1:A:229:PRO:HD3	1.78	0.83
1:A:151:LYS:HE3	1:A:191:ARG:HD2	1.61	0.82
1:A:199:MET:HE3	1:A:234:LEU:HD13	1.62	0.80
1:A:54:LYS:CE	2:A:1001:F29:C11	2.62	0.77
1:A:325:ALA:O	1:A:326:GLU:HB3	1.85	0.75
1:A:231:LYS:HB2	3:A:1033:HOH:O	1.90	0.71
1:A:117:LYS:HG3	1:A:118:THR:HG23	1.71	0.71
1:A:54:LYS:HE2	2:A:1001:F29:C12	2.18	0.70
1:A:151:LYS:HD3	1:A:154:ASN:OD1	1.92	0.70
1:A:21:VAL:HG21	1:A:53:ILE:HD12	1.75	0.69
1:A:218:LEU:HD12	1:A:290:LEU:HG	1.73	0.69
1:A:54:LYS:HE2	2:A:1001:F29:C8	2.23	0.69
1:A:190:THR:O	1:A:191:ARG:HG2	1.91	0.68
1:A:114:LYS:HG3	1:A:117:LYS:HE2	1.76	0.68
1:A:217:ILE:HD11	1:A:221:MET:HE2	1.77	0.67
1:A:244:LEU:O	1:A:272:LYS:HG3	1.94	0.67
1:A:325:ALA:O	1:A:326:GLU:CB	2.44	0.66
1:A:274:PRO:HB2	1:A:277:ARG:HD2	1.77	0.66
1:A:338:LEU:HD12	1:A:339:PRO:HD2	1.80	0.63
1:A:54:LYS:HE3	2:A:1001:F29:C12	2.27	0.63
1:A:217:ILE:CD1	1:A:221:MET:HE2	2.27	0.63
1:A:121:LEU:H	1:A:224:ASN:HD21	1.47	0.63
1:A:342:LYS:HD3	1:A:345:GLU:OE2	1.97	0.63
1:A:146:LEU:HD22	1:A:207:LYS:HA	1.80	0.63
1:A:184:LEU:HD23	1:A:199:MET:O	1.99	0.62
1:A:209:ILE:HG23	3:A:1041:HOH:O	1.99	0.61
1:A:59:PHE:O	1:A:340:LYS:HE3	2.00	0.60
1:A:253:ASN:HB2	3:A:1007:HOH:O	1.99	0.60
1:A:311:PRO:HA	1:A:314:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:HB2	3:A:1022:HOH:O	2.02	0.59
1:A:90:ILE:HB	1:A:102:TYR:HB2	1.85	0.59
1:A:55:LYS:HG3	3:A:1131:HOH:O	2.02	0.58
1:A:227:ILE:C	1:A:229:PRO:HD3	2.29	0.58
1:A:111:ASP:OD1	1:A:114:LYS:HD3	2.04	0.57
1:A:311:PRO:O	1:A:314:GLU:HB2	2.04	0.57
1:A:146:LEU:HD21	1:A:207:LYS:HD3	1.86	0.56
1:A:26:THR:HA	3:A:1110:HOH:O	2.05	0.55
1:A:71:GLU:O	1:A:75:LEU:HB2	2.07	0.54
1:A:233:TYR:HB2	3:A:1206:HOH:O	2.06	0.54
1:A:207:LYS:HG2	3:A:1028:HOH:O	2.08	0.54
1:A:31:ILE:HD11	1:A:41:SER:HB3	1.89	0.54
1:A:54:LYS:NZ	2:A:1001:F29:C12	2.70	0.53
1:A:304:VAL:HG22	3:A:1011:HOH:O	2.07	0.53
1:A:254:CYS:HB2	3:A:1024:HOH:O	2.09	0.53
1:A:147:HIS:HB3	1:A:150:LEU:HD22	1.91	0.53
1:A:18:VAL:O	1:A:18:VAL:HG23	2.09	0.53
1:A:114:LYS:HA	1:A:117:LYS:HE2	1.91	0.53
1:A:262:ASN:HA	1:A:265:LEU:HD23	1.91	0.53
1:A:192:TRP:HB3	1:A:236:GLN:OE1	2.09	0.52
1:A:300:LYS:HD2	3:A:1201:HOH:O	2.09	0.52
1:A:195:ALA:HB1	1:A:197:GLU:OE1	2.11	0.51
1:A:71:GLU:HB2	3:A:1145:HOH:O	2.10	0.51
1:A:274:PRO:HB2	1:A:277:ARG:CD	2.41	0.51
1:A:290:LEU:CD2	1:A:294:LEU:HD12	2.41	0.51
1:A:69:LEU:HD23	1:A:347:ILE:HG12	1.93	0.50
1:A:194:ARG:HB3	3:A:1202:HOH:O	2.12	0.49
1:A:21:VAL:HG13	1:A:25:TYR:HB2	1.94	0.49
1:A:289:LEU:HG	1:A:310:HIS:CG	2.47	0.49
1:A:183:PHE:HA	1:A:200:LEU:O	2.12	0.49
1:A:146:LEU:CD2	1:A:207:LYS:HD3	2.43	0.48
1:A:293:MET:HA	1:A:302:ILE:HG22	1.94	0.48
1:A:259:LYS:HE3	1:A:259:LYS:H	1.79	0.48
1:A:331:PHE:CD2	1:A:333:MET:HB3	2.48	0.48
1:A:54:LYS:HE3	2:A:1001:F29:C13	2.44	0.48
1:A:156:LEU:HG	2:A:1001:F29:H171	1.96	0.48
1:A:195:ALA:HA	1:A:196:PRO:HD3	1.78	0.47
1:A:191:ARG:C	1:A:194:ARG:HE	2.22	0.47
1:A:261:ARG:O	1:A:265:LEU:HD22	2.14	0.47
1:A:86:ILE:HD12	1:A:103:ILE:CG2	2.44	0.47
1:A:192:TRP:CB	1:A:228:PHE:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:HA	1:A:43:TYR:O	2.16	0.46
1:A:129:PHE:O	1:A:133:ILE:HG13	2.14	0.46
1:A:54:LYS:HE2	2:A:1001:F29:N7	2.30	0.46
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.69	0.46
1:A:263:TYR:O	1:A:266:SER:HB2	2.15	0.45
1:A:231:LYS:HB3	1:A:235:ASP:OD1	2.17	0.45
1:A:54:LYS:NZ	2:A:1001:F29:H12	2.32	0.45
1:A:53:ILE:HD11	1:A:102:TYR:HB3	1.98	0.45
1:A:321:ASP:C	1:A:322:GLU:HG3	2.42	0.45
1:A:14:VAL:HB	3:A:1147:HOH:O	2.16	0.44
1:A:57:SER:OG	1:A:100:ASP:HB3	2.17	0.44
1:A:58:PRO:O	1:A:59:PHE:HB2	2.16	0.44
1:A:237:LEU:C	1:A:237:LEU:HD23	2.43	0.44
1:A:112:LEU:O	1:A:116:LEU:HG	2.17	0.43
1:A:217:ILE:O	1:A:221:MET:HG3	2.18	0.43
1:A:246:SER:HA	1:A:247:PRO:HD3	1.84	0.43
1:A:39:VAL:CG2	1:A:54:LYS:HD3	2.48	0.43
1:A:59:PHE:O	1:A:340:LYS:HG3	2.17	0.43
1:A:178:HIS:O	1:A:203:LYS:HD3	2.18	0.43
1:A:116:LEU:HD23	1:A:121:LEU:HD11	2.00	0.43
1:A:56:ILE:HG22	1:A:58:PRO:HD3	2.00	0.43
1:A:163:LEU:C	1:A:164:LYS:HG3	2.44	0.43
1:A:17:GLN:HB2	1:A:38:MET:HE1	1.99	0.43
1:A:192:TRP:HB2	1:A:228:PHE:HB3	2.00	0.43
1:A:34:GLY:O	1:A:35:ALA:HB3	2.18	0.43
1:A:21:VAL:HG22	1:A:25:TYR:HD1	1.84	0.42
1:A:160:THR:O	1:A:161:CYS:HB2	2.18	0.42
1:A:321:ASP:O	1:A:322:GLU:HG3	2.19	0.42
1:A:21:VAL:HG21	1:A:53:ILE:CD1	2.46	0.42
1:A:137:LEU:HA	1:A:140:ILE:HG23	2.01	0.42
1:A:56:ILE:O	1:A:100:ASP:HB2	2.18	0.42
1:A:59:PHE:CE1	1:A:344:LYS:HG3	2.55	0.42
1:A:331:PHE:CE2	1:A:333:MET:HB3	2.54	0.42
1:A:279:PHE:HA	1:A:280:PRO:HD2	1.83	0.42
1:A:276:ASN:HB3	3:A:1048:HOH:O	2.20	0.41
1:A:146:LEU:CD1	1:A:174:ALA:HA	2.50	0.41
1:A:203:LYS:HG3	1:A:205:TYR:CZ	2.55	0.41
1:A:143:ALA:O	1:A:144:ASN:HB2	2.19	0.41
1:A:289:LEU:HD22	1:A:293:MET:HE2	2.02	0.41
1:A:29:SER:HB2	1:A:41:SER:OG	2.21	0.41
1:A:113:TYR:HA	1:A:116:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:CD2	1:A:207:LYS:HA	2.50	0.41
1:A:111:ASP:CG	1:A:114:LYS:HD3	2.45	0.41
1:A:199:MET:CE	1:A:234:LEU:HD13	2.44	0.40
1:A:305:GLU:HA	1:A:305:GLU:OE1	2.22	0.40
1:A:187:TYR:HB3	3:A:1127:HOH:O	2.20	0.40
1:A:163:LEU:C	1:A:163:LEU:HD23	2.47	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	348/368 (95%)	301 (86%)	32 (9%)	15 (4%)	2 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ALA
1	A	229	PRO
1	A	233	TYR
1	A	325	ALA
1	A	326	GLU
1	A	334	GLU
1	A	58	PRO
1	A	109	GLU
1	A	184	LEU
1	A	187	TYR
1	A	231	LYS
1	A	330	LYS
1	A	356	PRO
1	A	200	LEU
1	A	280	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	314/324 (97%)	283 (90%)	31 (10%)	7 16

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	53	ILE
1	A	54	LYS
1	A	62	GLN
1	A	63	THR
1	A	75	LEU
1	A	112	LEU
1	A	128	TYR
1	A	140	ILE
1	A	150	LEU
1	A	151	LYS
1	A	156	LEU
1	A	170	LEU
1	A	192	TRP
1	A	194	ARG
1	A	199	MET
1	A	209	ILE
1	A	217	ILE
1	A	234	LEU
1	A	250	GLU
1	A	252	LEU
1	A	265	LEU
1	A	278	LEU
1	A	287	LEU
1	A	289	LEU
1	A	290	LEU
1	A	304	VAL
1	A	314	GLU
1	A	340	LYS
1	A	346	LEU

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Mol	Chain	Res	Type
1	A	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	120	HIS
1	A	144	ASN
1	A	178	HIS
1	A	224	ASN
1	A	238	ASN
1	A	239	HIS
1	A	249	GLN
1	A	262	ASN
1	A	271	ASN
1	A	299	HIS
1	A	355	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)

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	F29	A	1001	-	32,32,32	4.45	27 (84%)	39,46,46	4.52	21 (53%)

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	F29	A	1001	-	-	0/11/11/11	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	F29	N26-N25	10.61	1.60	1.34
2	A	1001	F29	N3-N7	8.39	1.46	1.37
2	A	1001	F29	C24-N29	7.49	1.42	1.35
2	A	1001	F29	C24-N25	6.99	1.42	1.33
2	A	1001	F29	N29-N28	6.31	1.49	1.36
2	A	1001	F29	C8-N7	5.29	1.41	1.33
2	A	1001	F29	C2-C1	4.99	1.45	1.35
2	A	1001	F29	C16-C11	4.96	1.46	1.39
2	A	1001	F29	C12-C11	4.92	1.46	1.39
2	A	1001	F29	C27-N28	4.76	1.41	1.33
2	A	1001	F29	C22-C23	4.19	1.46	1.39
2	A	1001	F29	C13-C12	4.11	1.45	1.38
2	A	1001	F29	C6-C5	4.00	1.46	1.37
2	A	1001	F29	C15-C16	3.92	1.45	1.38
2	A	1001	F29	C27-N30	3.90	1.41	1.34
2	A	1001	F29	C3-N29	-3.65	1.42	1.46
2	A	1001	F29	C15-C14	3.30	1.45	1.38
2	A	1001	F29	C14-C13	3.29	1.45	1.38
2	A	1001	F29	C5-C4	3.15	1.47	1.41
2	A	1001	F29	C23-C24	2.85	1.45	1.41
2	A	1001	F29	C17-C7	2.60	1.45	1.29
2	A	1001	F29	C22-C10	2.49	1.46	1.40
2	A	1001	F29	C9-C4	2.45	1.46	1.40
2	A	1001	F29	C10-N26	2.44	1.42	1.35
2	A	1001	F29	C2-N3	2.24	1.41	1.37
2	A	1001	F29	C23-C27	-2.22	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	F29	C6-C1	2.21	1.46	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	F29	C23-C24-N25	-12.61	113.94	127.03
2	A	1001	F29	C22-C10-N26	-11.83	112.68	121.63
2	A	1001	F29	C24-N29-N28	-10.62	105.08	111.05
2	A	1001	F29	C3-N29-C24	9.36	133.74	127.81
2	A	1001	F29	C9-C10-N26	7.20	124.28	116.81
2	A	1001	F29	C22-C23-C24	6.77	124.48	117.67
2	A	1001	F29	N25-C24-N29	6.00	135.40	126.24
2	A	1001	F29	C23-C22-C10	5.70	124.61	119.93
2	A	1001	F29	C4-N3-N7	-4.28	109.46	112.94
2	A	1001	F29	C23-C24-N29	3.91	109.60	107.18
2	A	1001	F29	C16-C11-C12	-3.18	114.52	118.57
2	A	1001	F29	C16-C11-C8	2.97	125.60	120.74
2	A	1001	F29	C22-C23-C27	-2.94	126.87	130.79
2	A	1001	F29	C15-C16-C11	2.93	123.24	120.36
2	A	1001	F29	C13-C12-C11	2.87	123.18	120.36
2	A	1001	F29	C5-C4-N3	-2.67	115.50	118.15
2	A	1001	F29	C10-N26-N25	2.51	122.76	119.20
2	A	1001	F29	C23-C27-N30	2.44	127.87	124.28
2	A	1001	F29	C11-C8-N7	-2.30	115.55	118.99
2	A	1001	F29	C11-C8-C9	2.22	133.80	129.22
2	A	1001	F29	C2-C1-C6	-2.13	117.01	120.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

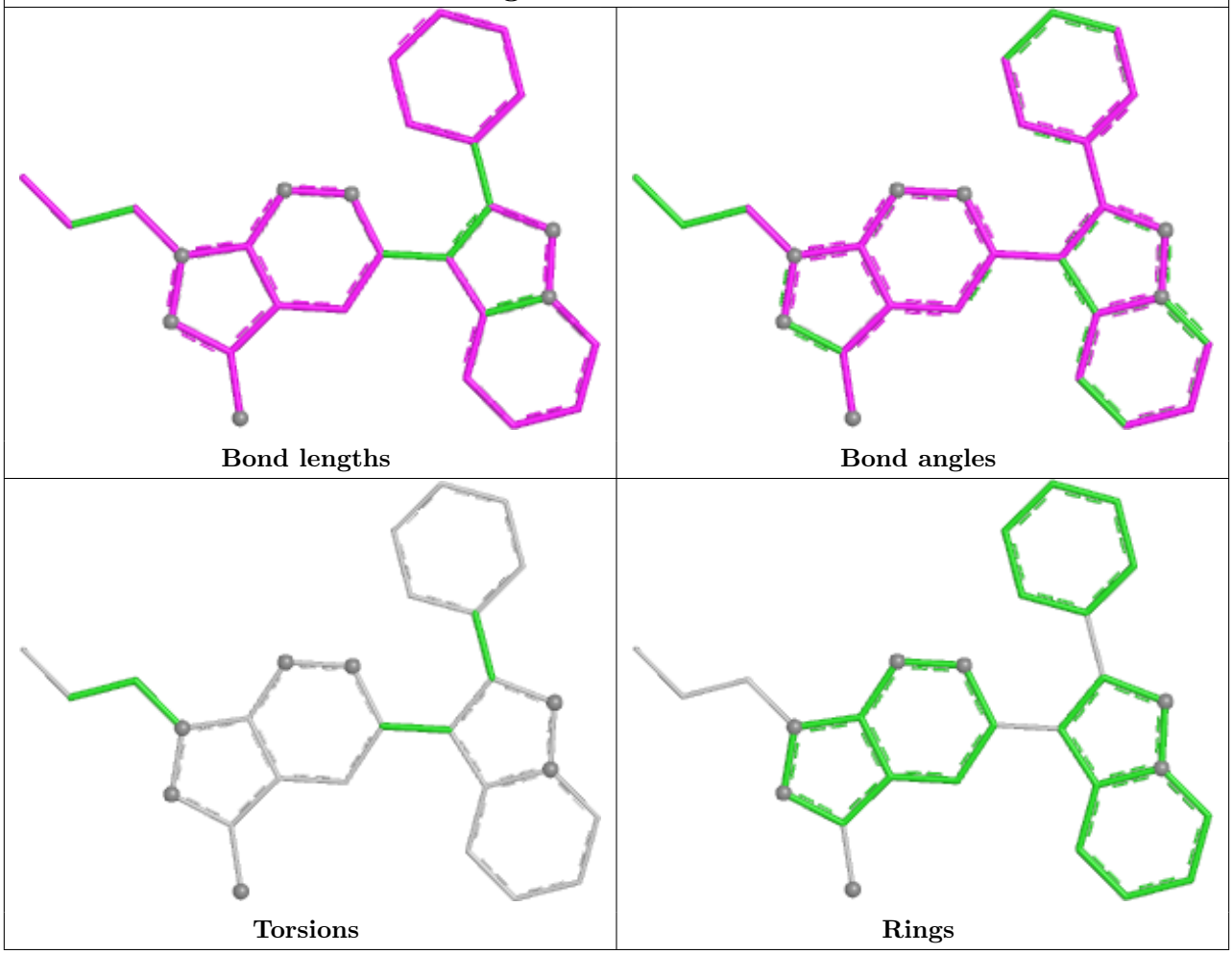
1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	F29	11	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand F29 A 1001



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	350/368 (95%)	0.33	28 (8%)	18	16	3, 20, 51, 63	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	PHE	4.5
1	A	192	TRP	4.4
1	A	335	LEU	4.4
1	A	253	ASN	4.1
1	A	233	TYR	4.0
1	A	14	VAL	3.5
1	A	187	TYR	3.5
1	A	332	ASP	3.2
1	A	188	VAL	3.2
1	A	252	LEU	3.1
1	A	180	HIS	2.8
1	A	337	ASP	2.8
1	A	329	PHE	2.7
1	A	36	TYR	2.7
1	A	336	ASP	2.6
1	A	185	THR	2.6
1	A	334	GLU	2.6
1	A	128	TYR	2.6
1	A	331	PHE	2.5
1	A	254	CYS	2.4
1	A	186	GLU	2.3
1	A	333	MET	2.3
1	A	48	LYS	2.3
1	A	355	GLN	2.2
1	A	230	GLY	2.2
1	A	191	ARG	2.2
1	A	189	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	47	ASN	2.1

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)

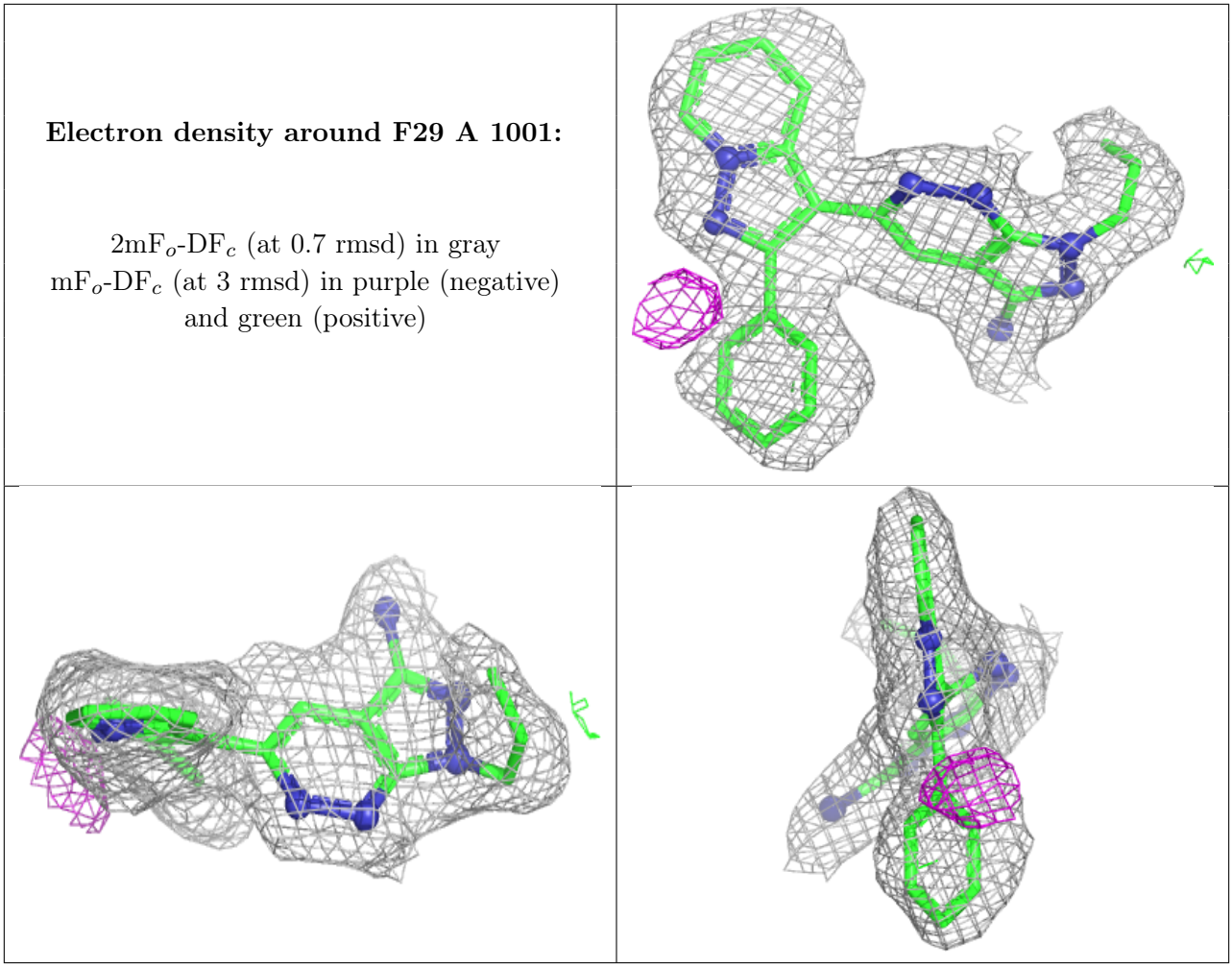
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F29	A	1001	28/28	0.85	0.13	26,29,31,32	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 F29 A 1001:

$2mF_o$-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.