



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:03 am BST

PDB ID : 4J6I
Title : Discovery of thiazolobenzoxepin PI3-kinase inhibitors that spare the PI3-kinase beta isoform
Authors : Murray, J.M.; Rouge, L.; Wu, P.
Deposited on : 2013-02-11
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

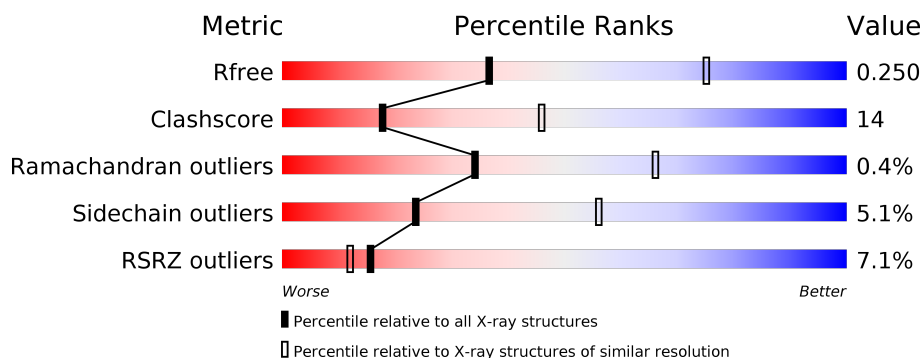
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	<div> <div>6%</div> <div>61%</div> <div>22%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6783 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.

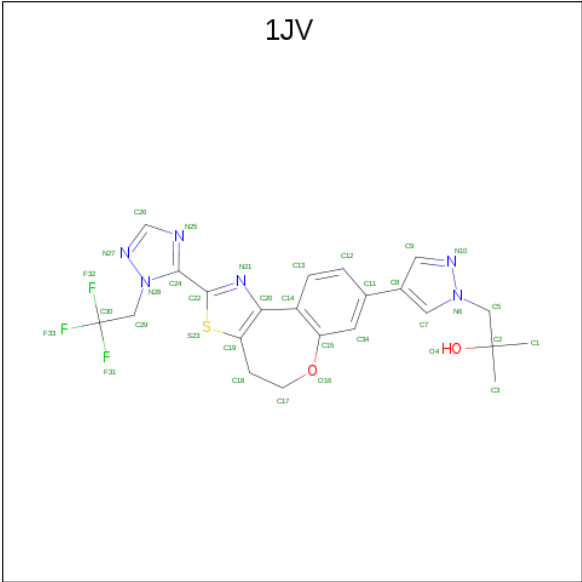
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6749	4331	1150	1234	34			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	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 2-methyl-1-(4-{2-[1-(2,2,2-trifluoroethyl)-1H-1,2,4-triazol-5-yl]-4,5-dihydro[1]benzoxepino[5,4-d][1,3]thiazol-8-yl}-1H-pyrazol-1-yl)propan-2-ol (three-letter code: 1JV) (formula: C₂₂H₂₁F₃N₆O₂S).

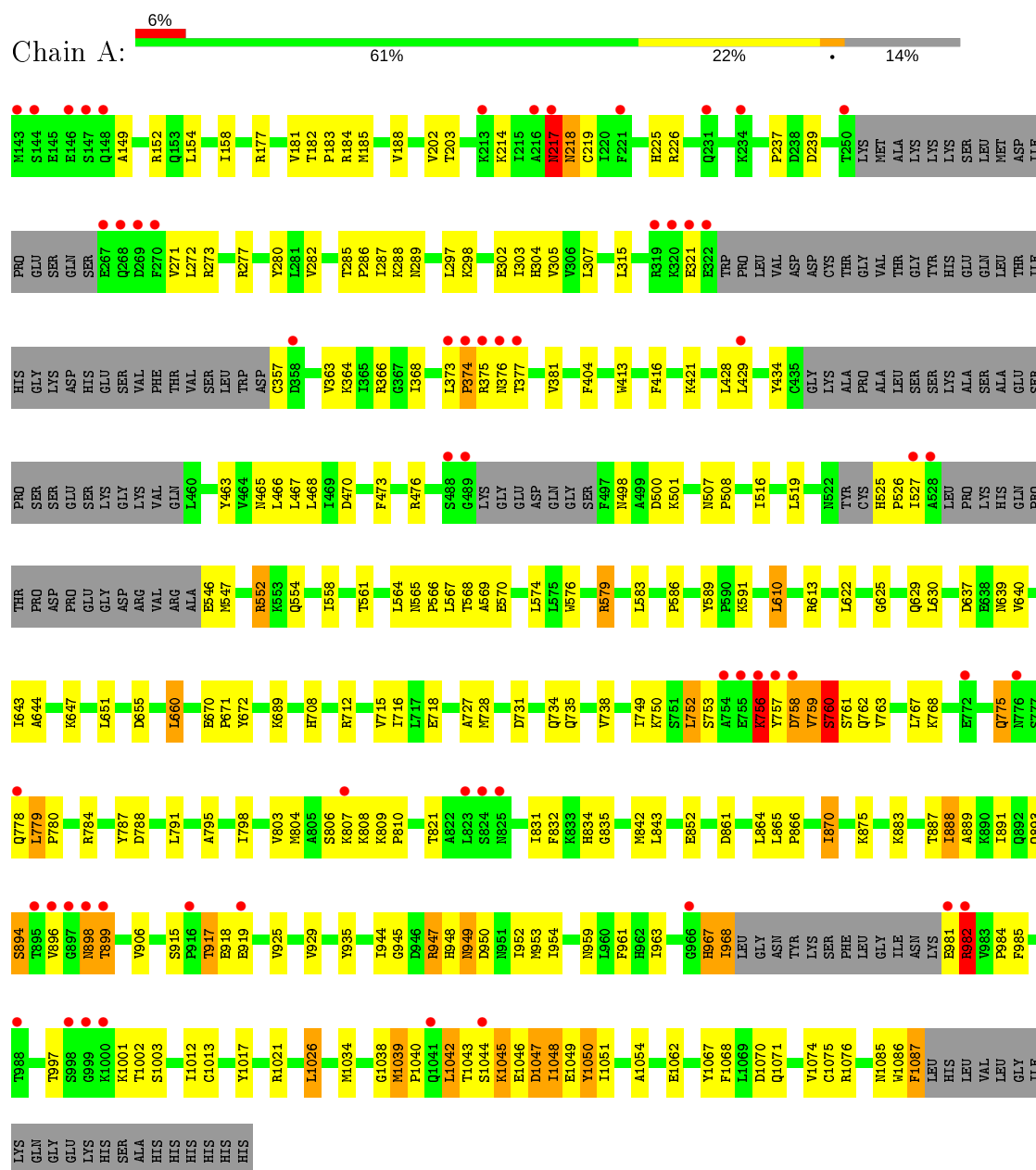


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	34	22	3	6	2	1	0	0

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 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	143.67Å 67.16Å 106.66Å 90.00° 95.43° 90.00°	Depositor
Resolution (Å)	19.85 – 2.90 19.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.85-2.90) 98.3 (19.85-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.88Å)	Xtriage
Refinement program	PHENIX 1.8_1068	Depositor
R, R_{free}	0.205 , 0.251 0.207 , 0.250	Depositor DCC
R_{free} test set	1115 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6783	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1JV

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	0.63	0/6894	0.96	20/9327 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1086	TRP	N-CA-C	-9.46	85.46	111.00
1	A	1026	LEU	CA-CB-CG	8.35	134.50	115.30
1	A	870	ILE	CG1-CB-CG2	-7.30	95.34	111.40
1	A	947	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	760	SER	N-CA-C	7.23	130.52	111.00
1	A	749	ILE	CG1-CB-CG2	-7.22	95.51	111.40
1	A	552	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	217	ASN	N-CA-C	6.32	128.05	111.00
1	A	888	ILE	CG1-CB-CG2	-6.26	97.62	111.40
1	A	779	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	915	SER	C-N-CD	-5.83	107.76	120.60
1	A	947	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	778	GLN	N-CA-C	5.70	126.38	111.00
1	A	303	ILE	CG1-CB-CG2	-5.68	98.91	111.40
1	A	982	ARG	CA-CB-CG	5.46	125.41	113.40
1	A	527	ILE	N-CA-C	-5.27	96.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	A	832	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	A	760	SER	CB-CA-C	-5.15	100.31	110.10
1	A	791	LEU	CB-CG-CD2	-5.11	102.31	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ASN	Peptide
1	A	374	PRO	Peptide
1	A	756	LYS	Peptide
1	A	760	SER	Peptide
1	A	967	HIS	Peptide

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	6749	0	6771	184	0
2	A	34	0	21	3	0
All	All	6783	0	6792	185	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 14.

All (185) 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:759:VAL:HA	1:A:760:SER:CB	1.55	1.34
1:A:759:VAL:CA	1:A:760:SER:HB3	1.75	1.16
1:A:217:ASN:CG	1:A:219:CYS:HB3	1.75	1.05
1:A:1085:ASN:O	1:A:1087:PHE:N	1.89	1.04
1:A:1087:PHE:O	1:A:1087:PHE:HD1	1.38	1.03
1:A:1087:PHE:CD1	1:A:1087:PHE:C	2.30	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:HIS:HB2	1:A:968:ILE:HG22	1.44	0.99
1:A:759:VAL:HA	1:A:760:SER:HB3	0.97	0.96
1:A:1087:PHE:HD1	1:A:1087:PHE:C	1.66	0.96
1:A:759:VAL:CA	1:A:760:SER:CB	2.37	0.94
1:A:1050:TYR:C	1:A:1050:TYR:CD2	2.42	0.93
1:A:889:ALA:O	1:A:893:GLN:HG3	1.71	0.90
1:A:1045:LYS:O	1:A:1048:ILE:HG12	1.71	0.90
1:A:759:VAL:HA	1:A:760:SER:HB2	1.58	0.84
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.57	0.84
1:A:760:SER:OG	1:A:760:SER:O	1.90	0.81
1:A:1045:LYS:O	1:A:1048:ILE:CG1	2.31	0.79
1:A:1048:ILE:O	1:A:1051:ILE:HG22	1.84	0.78
1:A:217:ASN:ND2	1:A:219:CYS:HB3	1.98	0.77
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.65	0.77
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.66	0.76
1:A:1050:TYR:O	1:A:1050:TYR:CD2	2.40	0.74
1:A:1050:TYR:C	1:A:1050:TYR:HD2	1.88	0.73
1:A:947:ARG:NH2	1:A:963:ILE:O	2.21	0.73
1:A:757:TYR:O	1:A:758:ASP:CB	2.37	0.73
1:A:752:LEU:HD12	1:A:752:LEU:O	1.89	0.72
1:A:1087:PHE:O	1:A:1087:PHE:CD1	2.30	0.71
1:A:1043:THR:C	1:A:1045:LYS:H	1.94	0.70
1:A:1085:ASN:C	1:A:1087:PHE:N	2.41	0.70
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.75	0.69
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.24	0.69
1:A:1045:LYS:HG2	1:A:1049:GLU:OE2	1.93	0.69
1:A:756:LYS:NZ	1:A:807:LYS:HE2	2.08	0.68
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.76	0.68
1:A:1002:THR:HG22	1:A:1003:SER:H	1.57	0.68
1:A:758:ASP:CG	1:A:759:VAL:H	1.98	0.66
1:A:1045:LYS:O	1:A:1049:GLU:HG3	1.95	0.66
1:A:758:ASP:O	1:A:760:SER:HB2	1.96	0.66
1:A:757:TYR:O	1:A:758:ASP:HB3	1.97	0.65
1:A:917:THR:OG1	1:A:918:GLU:N	2.24	0.65
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.62	0.65
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.60	0.65
1:A:381:VAL:HG22	1:A:434:TYR:O	1.96	0.65
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.78	0.64
1:A:1040:PRO:O	1:A:1042:LEU:HD13	1.98	0.63
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.80	0.63
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.81	0.62
1:A:567:LEU:HD21	1:A:591:LYS:HD3	1.81	0.62
1:A:217:ASN:OD1	1:A:219:CYS:N	2.28	0.62
1:A:944:ILE:HB	1:A:968:ILE:HD11	1.83	0.61
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.80	0.61
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.83	0.60
1:A:287:ILE:HD12	1:A:288:LYS:N	2.17	0.60
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.37	0.59
1:A:473:PHE:O	1:A:526:PRO:HD2	2.02	0.59
1:A:217:ASN:O	1:A:218:ASN:CB	2.51	0.59
1:A:217:ASN:O	1:A:218:ASN:HB2	2.02	0.58
1:A:981:GLU:O	1:A:982:ARG:HD3	2.03	0.58
1:A:779:LEU:HD23	1:A:780:PRO:O	2.03	0.58
1:A:218:ASN:O	1:A:237:PRO:HD3	2.05	0.57
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.18	0.57
1:A:546:GLU:HA	1:A:546:GLU:OE1	2.04	0.56
1:A:1050:TYR:HD2	1:A:1051:ILE:N	2.03	0.56
1:A:758:ASP:CG	1:A:759:VAL:N	2.58	0.56
1:A:768:LYS:HD3	1:A:798:ILE:HG22	1.88	0.56
1:A:154:LEU:O	1:A:158:ILE:HG13	2.05	0.56
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.42	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.05	0.55
1:A:750:LYS:HE3	1:A:808:LYS:HA	1.88	0.55
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.88	0.55
1:A:271:VAL:HG23	1:A:282:VAL:HG22	1.89	0.54
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.43	0.54
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.07	0.54
1:A:843:LEU:HD13	1:A:1034:MET:HG3	1.90	0.54
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.42	0.54
1:A:760:SER:O	1:A:763:VAL:HG23	2.07	0.54
1:A:1046:GLU:O	1:A:1049:GLU:HB2	2.08	0.53
1:A:734:GLN:CD	1:A:780:PRO:HB3	2.30	0.52
1:A:756:LYS:HZ1	1:A:807:LYS:HE2	1.75	0.52
1:A:953:MET:SD	1:A:963:ILE:HD13	2.50	0.52
1:A:177:ARG:HG2	1:A:715:VAL:HG13	1.92	0.52
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.36	0.52
1:A:184:ARG:O	1:A:188:VAL:HG23	2.10	0.51
1:A:917:THR:OG1	1:A:919:GLU:N	2.44	0.51
1:A:888:ILE:HD13	1:A:952:ILE:O	2.11	0.51
1:A:1047:ASP:N	1:A:1047:ASP:OD2	2.40	0.51
1:A:883:LYS:NZ	2:A:1201:1JV:H6	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.76	0.50
1:A:787:TYR:HB3	1:A:870:ILE:HD12	1.94	0.50
1:A:366:ARG:HH12	1:A:519:LEU:HD22	1.76	0.50
1:A:738:VAL:HG23	1:A:780:PRO:HG2	1.94	0.50
1:A:373:LEU:HD12	1:A:374:PRO:N	2.27	0.50
1:A:997:THR:HG21	1:A:1076:ARG:HH12	1.76	0.50
1:A:1050:TYR:CE2	1:A:1054:ALA:HB2	2.47	0.49
1:A:149:ALA:O	1:A:152:ARG:HG2	2.12	0.49
1:A:277:ARG:NH2	1:A:788:ASP:OD2	2.31	0.49
1:A:804:MET:HE1	1:A:831:ILE:CG2	2.38	0.49
1:A:891:ILE:O	1:A:894:SER:OG	2.32	0.48
1:A:280:TYR:HB3	1:A:282:VAL:CG2	2.44	0.48
1:A:1038:GLY:C	1:A:1039:MET:HG2	2.33	0.48
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.95	0.48
1:A:945:GLY:O	1:A:985:PHE:HA	2.14	0.48
1:A:273:ARG:NH2	1:A:821:THR:OG1	2.47	0.48
1:A:759:VAL:CG1	1:A:760:SER:HB3	2.43	0.48
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.14	0.48
1:A:759:VAL:HG12	1:A:760:SER:HB3	1.96	0.48
1:A:864:LEU:C	1:A:866:PRO:HD3	2.34	0.48
1:A:364:LYS:HE3	1:A:413:TRP:CE2	2.49	0.48
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.49	0.48
2:A:1201:1JV:N21	2:A:1201:1JV:H20	2.29	0.47
1:A:1043:THR:C	1:A:1045:LYS:N	2.65	0.47
1:A:181:VAL:O	1:A:185:MET:HG3	2.15	0.47
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.45	0.47
1:A:182:THR:HB	1:A:183:PRO:HD3	1.97	0.46
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.97	0.46
1:A:376:ASN:HB3	1:A:377:THR:H	1.40	0.46
1:A:887:THR:HG22	1:A:889:ALA:H	1.80	0.46
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.98	0.46
1:A:898:ASN:C	1:A:899:THR:OG1	2.54	0.46
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.97	0.46
1:A:887:THR:CG2	1:A:950:ASP:HA	2.46	0.46
1:A:731:ASP:O	1:A:735:GLN:HG3	2.15	0.45
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.43	0.45
1:A:968:ILE:HG21	1:A:968:ILE:HD13	1.56	0.45
1:A:547:MET:HE2	1:A:552:ARG:N	2.32	0.45
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.51	0.45
1:A:1045:LYS:O	1:A:1048:ILE:HG13	2.13	0.45
1:A:759:VAL:CB	1:A:760:SER:HB3	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ARG:O	1:A:716:ILE:HG13	2.17	0.45
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.52	0.45
1:A:1085:ASN:O	1:A:1087:PHE:HB3	2.17	0.45
1:A:568:THR:HG22	1:A:569:ALA:N	2.31	0.45
1:A:286:PRO:HD2	1:A:289:ASN:HD22	1.81	0.44
1:A:381:VAL:HG21	1:A:404:PHE:CD1	2.52	0.44
1:A:576:TRP:O	1:A:579:ARG:NH1	2.50	0.44
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.52	0.44
1:A:507:ASN:HA	1:A:508:PRO:HD2	1.88	0.44
1:A:887:THR:HG22	1:A:889:ALA:N	2.33	0.44
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.51	0.44
1:A:660:LEU:HD12	1:A:660:LEU:HA	1.70	0.44
1:A:954:ILE:HA	1:A:959:ASN:O	2.18	0.44
1:A:1043:THR:O	1:A:1045:LYS:N	2.49	0.43
1:A:368:ILE:HG22	1:A:516:ILE:HG13	1.99	0.43
1:A:558:ILE:HD12	1:A:574:LEU:HD23	2.00	0.43
1:A:568:THR:HG22	1:A:570:GLU:H	1.82	0.43
1:A:554:GLN:O	1:A:558:ILE:HG13	2.19	0.43
1:A:835:GLY:HA2	1:A:875:LYS:O	2.19	0.43
1:A:298:LYS:HE3	1:A:861:ASP:OD2	2.19	0.43
1:A:564:LEU:O	1:A:566:PRO:HD3	2.19	0.43
1:A:630:LEU:HB2	1:A:644:ALA:HB2	2.00	0.42
1:A:756:LYS:HE2	1:A:756:LYS:HB3	1.40	0.42
1:A:214:LYS:HD2	1:A:297:LEU:O	2.19	0.42
1:A:239:ASP:O	1:A:287:ILE:HG23	2.19	0.42
1:A:997:THR:HG21	1:A:1076:ARG:NH1	2.34	0.42
1:A:149:ALA:C	1:A:152:ARG:HG2	2.40	0.42
1:A:177:ARG:NH2	1:A:718:GLU:OE2	2.53	0.42
1:A:757:TYR:O	1:A:758:ASP:HB2	2.17	0.42
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	0.42
1:A:984:PRO:HG2	1:A:1075:CYS:SG	2.60	0.42
1:A:315:LEU:O	1:A:727:ALA:HB2	2.20	0.42
1:A:271:VAL:CG2	1:A:272:LEU:N	2.83	0.41
1:A:888:ILE:HB	1:A:949:ASN:HB2	2.01	0.41
1:A:891:ILE:HG22	1:A:906:VAL:HG12	2.01	0.41
1:A:898:ASN:O	1:A:899:THR:OG1	2.34	0.41
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.48	0.41
1:A:561:THR:OG1	1:A:591:LYS:HE2	2.20	0.41
1:A:852:GLU:HG3	1:A:864:LEU:HD12	2.01	0.41
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.20	0.41
1:A:202:VAL:CG1	1:A:203:THR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:ILE:HD13	1:A:1012:ILE:HG21	1.93	0.41
1:A:670:GLU:HA	1:A:671:PRO:HD3	1.88	0.41
1:A:217:ASN:CB	1:A:219:CYS:HB3	2.49	0.41
1:A:565:ASN:HA	1:A:566:PRO:HD2	1.72	0.41
1:A:625:GLY:O	1:A:629:GLN:HG3	2.21	0.41
1:A:637:ASP:OD1	1:A:639:ASN:HB2	2.21	0.41
1:A:689:LYS:HG2	1:A:728:MET:SD	2.61	0.41
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.87	0.40
1:A:760:SER:O	1:A:763:VAL:CG2	2.69	0.40
1:A:834:HIS:HA	1:A:835:GLY:HA2	1.92	0.40
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.22	0.40
1:A:883:LYS:HZ2	2:A:1201:1JV:H6	1.87	0.40
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.04	0.40
1:A:760:SER:OG	1:A:763:VAL:CG2	2.70	0.40
1:A:809:LYS:N	1:A:810:PRO:HD3	2.37	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	817/966 (85%)	772 (94%)	42 (5%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	ASP
1	A	760	SER
1	A	1044	SER

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	748/864 (87%)	710 (95%)	38 (5%)	24 56

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	225	HIS
1	A	226	ARG
1	A	307	LEU
1	A	357	CYS
1	A	375	ARG
1	A	421	LYS
1	A	498	ASN
1	A	579	ARG
1	A	610	LEU
1	A	613	ARG
1	A	752	LEU
1	A	753	SER
1	A	756	LYS
1	A	759	VAL
1	A	761	SER
1	A	762	GLN
1	A	775	GLN
1	A	806	SER
1	A	842	MET
1	A	865	LEU
1	A	894	SER
1	A	896	VAL
1	A	898	ASN
1	A	899	THR
1	A	917	THR
1	A	949	ASN
1	A	968	ILE
1	A	982	ARG
1	A	1026	LEU

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Mol	Chain	Res	Type
1	A	1039	MET
1	A	1042	LEU
1	A	1045	LYS
1	A	1047	ASP
1	A	1048	ILE
1	A	1050	TYR
1	A	1062	GLU
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	304	HIS
1	A	554	GLN
1	A	708	HIS
1	A	775	GLN
1	A	948	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1JV	A	1201	-	32,38,38	1.37	5 (15%)	32,58,58	2.02	7 (21%)

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	1JV	A	1201	-	-	3/13/28/28	0/4/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	1JV	N10-N6	3.99	1.41	1.35
2	A	1201	1JV	C14-C20	2.46	1.52	1.49
2	A	1201	1JV	O16-C15	-2.31	1.34	1.38
2	A	1201	1JV	O16-C17	-2.28	1.40	1.44
2	A	1201	1JV	F31-C30	2.04	1.41	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	1JV	C29-N28-N27	5.37	127.16	117.08
2	A	1201	1JV	C7-N6-N10	-4.95	107.25	111.56
2	A	1201	1JV	C9-N10-N6	4.14	108.54	104.23
2	A	1201	1JV	F32-C30-C29	-3.78	105.94	112.12
2	A	1201	1JV	C7-C8-C11	-3.08	123.71	127.74
2	A	1201	1JV	O16-C15-C34	2.22	120.16	116.95
2	A	1201	1JV	F33-C30-C29	-2.20	108.52	112.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

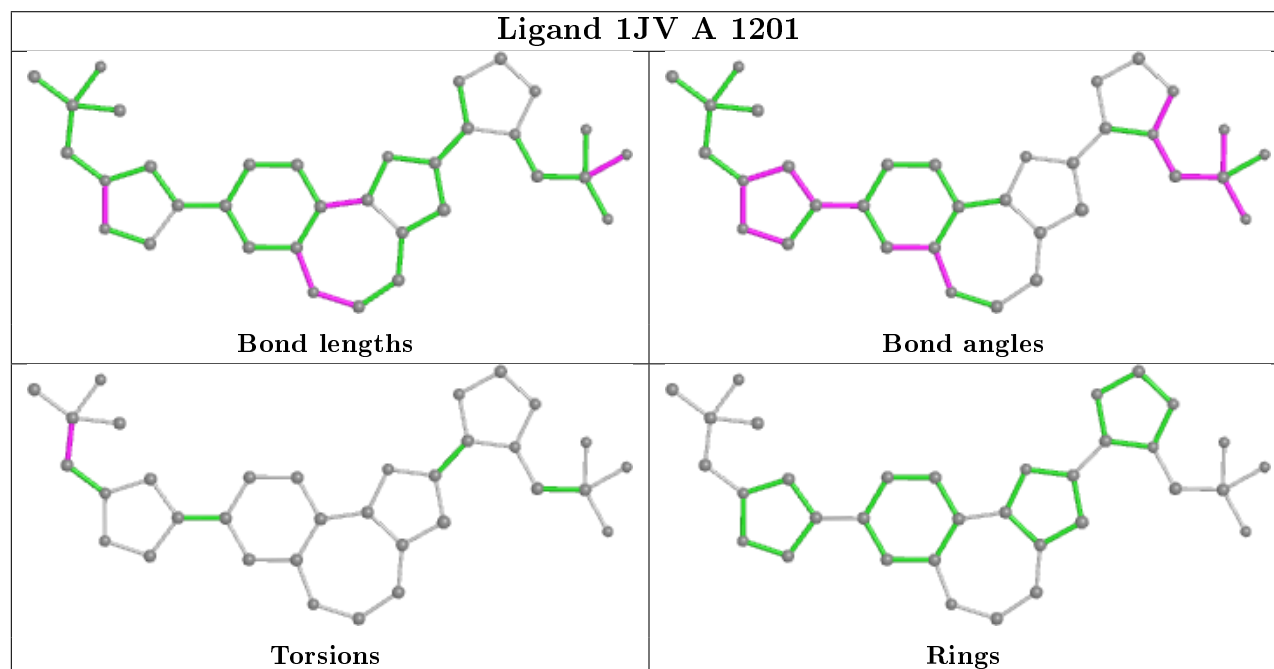
Mol	Chain	Res	Type	Atoms
2	A	1201	1JV	C1-C2-C5-N6
2	A	1201	1JV	O4-C2-C5-N6
2	A	1201	1JV	C3-C2-C5-N6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	1JV	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	833/966 (86%)	0.21	59 (7%) 16 12	42, 88, 157, 213	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	GLY	16.8
1	A	1044	SER	16.4
1	A	528	ALA	10.2
1	A	896	VAL	9.7
1	A	899	THR	9.6
1	A	143	MET	8.6
1	A	375	ARG	7.4
1	A	757	TYR	6.7
1	A	376	ASN	5.7
1	A	216	ALA	5.2
1	A	320	LYS	5.1
1	A	999	GLY	5.1
1	A	998	SER	5.0
1	A	234	LYS	4.9
1	A	377	THR	4.4
1	A	981	GLU	4.1
1	A	823	LEU	4.1
1	A	756	LYS	4.1
1	A	898	ASN	3.9
1	A	148	GLN	3.6
1	A	489	GLY	3.6
1	A	824	SER	3.5
1	A	321	GLU	3.4
1	A	825	ASN	3.4
1	A	1000	LYS	3.3
1	A	322	GLU	3.2
1	A	778	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	147	SER	3.1
1	A	527	ILE	3.1
1	A	250	THR	3.1
1	A	374	PRO	3.1
1	A	1041	GLN	2.9
1	A	213	LYS	2.9
1	A	916	PRO	2.8
1	A	758	ASP	2.6
1	A	988	THR	2.6
1	A	267	GLU	2.6
1	A	268	GLN	2.5
1	A	755	GLU	2.5
1	A	895	THR	2.5
1	A	217	ASN	2.4
1	A	772	GLU	2.3
1	A	269	ASP	2.3
1	A	146	GLU	2.3
1	A	488	SER	2.3
1	A	358	ASP	2.3
1	A	807	LYS	2.2
1	A	319	ARG	2.2
1	A	270	PHE	2.2
1	A	754	ALA	2.2
1	A	373	LEU	2.2
1	A	982	ARG	2.1
1	A	144	SER	2.1
1	A	221	PHE	2.1
1	A	776	ASN	2.1
1	A	231	GLN	2.1
1	A	919	GLU	2.0
1	A	966	GLY	2.0
1	A	429	LEU	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](#)

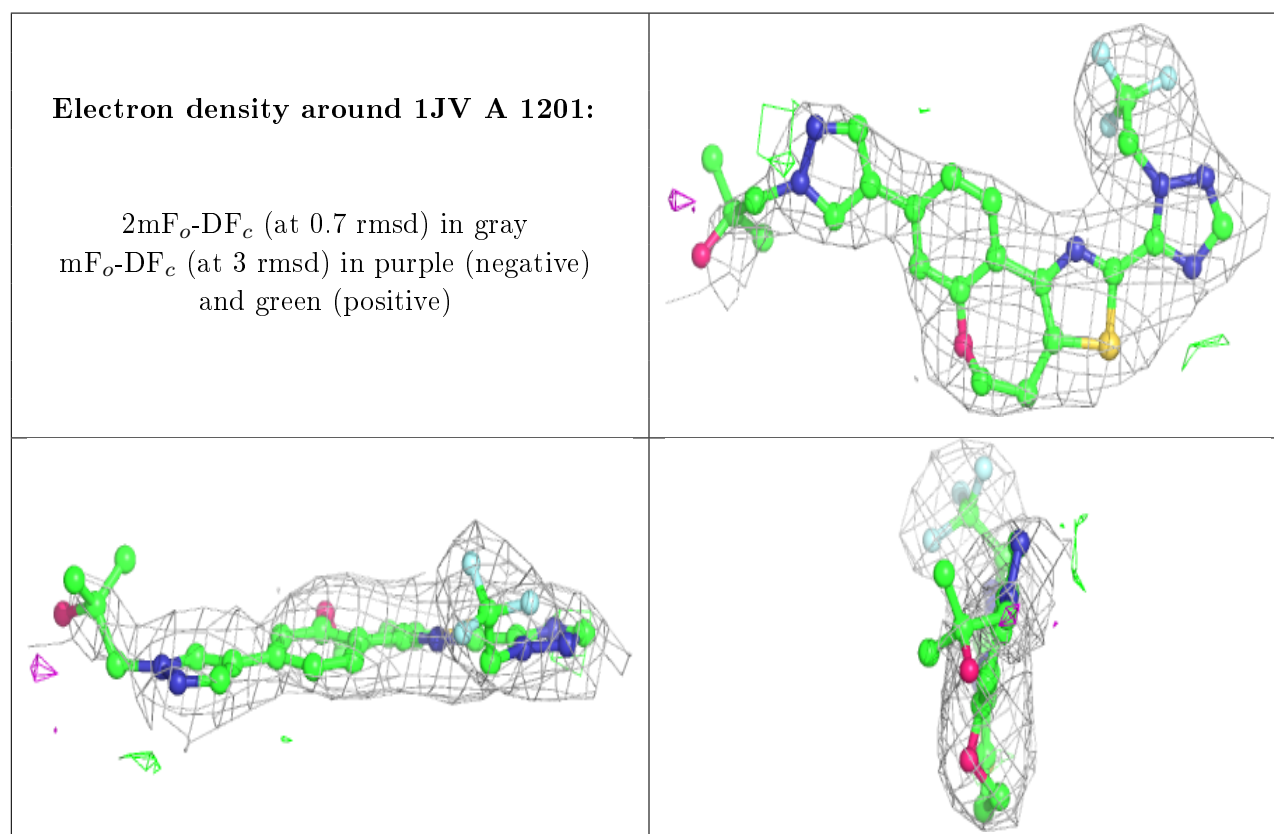
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	1JV	A	1201	34/34	0.91	0.23	64,79,134,135	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.