



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:14 PM UTC

PDB ID : 4J6I / pdb_00004j6i
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 types of validation reports are described at

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

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

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

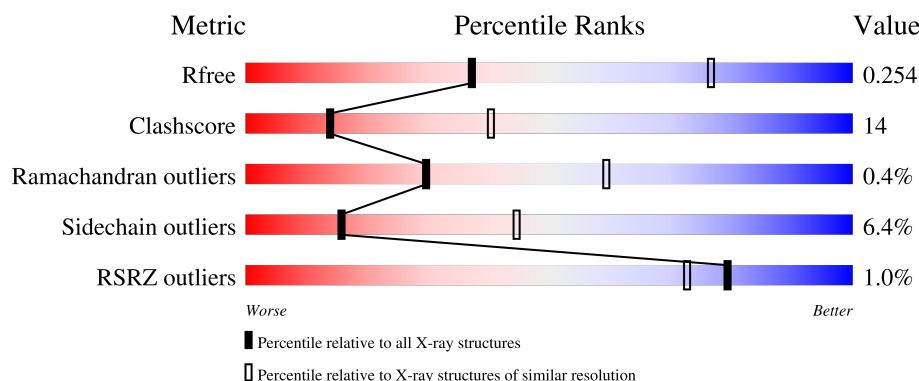
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	58% 23% • • 14%

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.

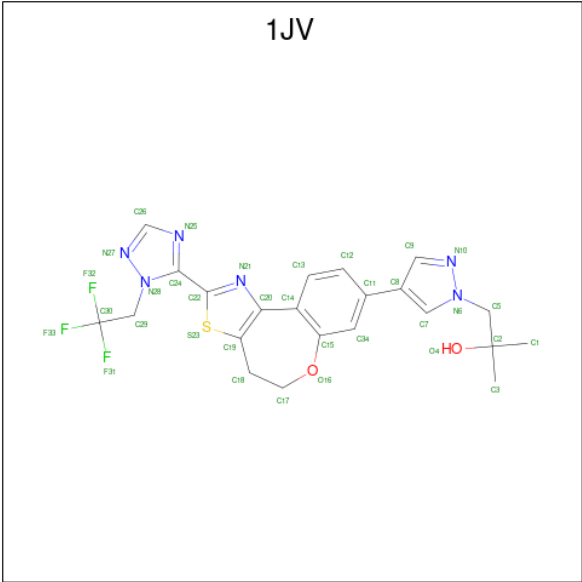
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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 (CCD ID: 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

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) 97.9 (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 0.209 , 0.254	Depositor DCC
R_{free} test set	1115 reflections (4.91%)	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)	0.30 , 60.8	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	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	0.81	0/6894	1.32	78/9327 (0.8%)

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 (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	217	ASN	N-CA-C	15.31	128.05	111.36
1	A	1086	TRP	N-CA-C	-13.25	85.46	108.52
1	A	298	LYS	N-CA-C	10.33	122.12	111.07
1	A	565	ASN	CA-C-N	9.80	129.85	119.76
1	A	565	ASN	C-N-CA	9.80	129.85	119.76
1	A	779	LEU	N-CA-C	-9.80	97.78	109.93
1	A	547	MET	N-CA-C	9.70	121.96	109.93
1	A	757	TYR	N-CA-C	8.91	121.08	111.36
1	A	775	GLN	N-CA-C	8.55	120.22	111.07
1	A	248	PHE	N-CA-C	-8.50	102.84	113.55
1	A	615	GLU	N-CA-C	8.45	121.25	111.11
1	A	904	ASP	N-CA-C	8.32	121.47	111.82
1	A	1000	LYS	N-CA-C	7.98	122.40	111.39
1	A	738	VAL	N-CA-C	7.69	118.48	110.72
1	A	1048	ILE	N-CA-C	-7.55	102.92	110.62
1	A	906	VAL	N-CA-C	7.50	119.17	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1046	GLU	N-CA-C	7.28	119.22	111.28
1	A	918	GLU	N-CA-C	-7.22	105.00	113.88
1	A	833	LYS	N-CA-C	7.21	121.33	109.06
1	A	761	SER	N-CA-C	7.19	119.12	111.28
1	A	317	GLU	CA-C-N	-6.98	114.10	123.10
1	A	317	GLU	C-N-CA	-6.98	114.10	123.10
1	A	760	SER	N-CA-C	6.97	130.52	111.00
1	A	762	GLN	N-CA-C	-6.79	103.88	111.28
1	A	478	GLY	N-CA-C	6.69	121.33	111.76
1	A	763	VAL	CB-CA-C	-6.58	103.54	111.97
1	A	219	CYS	N-CA-C	6.54	120.62	107.41
1	A	894	SER	N-CA-C	-6.48	104.95	112.92
1	A	1051	ILE	CA-C-N	6.38	129.15	120.54
1	A	1051	ILE	C-N-CA	6.38	129.15	120.54
1	A	760	SER	CA-C-N	6.37	128.81	120.28
1	A	760	SER	C-N-CA	6.37	128.81	120.28
1	A	374	PRO	N-CA-C	6.22	120.98	111.15
1	A	207	LEU	CA-C-N	6.22	127.62	119.84
1	A	207	LEU	C-N-CA	6.22	127.62	119.84
1	A	836	ASP	N-CA-C	-6.22	100.50	110.14
1	A	376	ASN	CB-CA-C	-6.18	109.46	116.63
1	A	869	CYS	N-CA-C	6.15	118.31	107.61
1	A	547	MET	CA-C-N	-6.10	113.47	119.76
1	A	547	MET	C-N-CA	-6.10	113.47	119.76
1	A	527	ILE	N-CA-C	-6.04	96.77	109.34
1	A	1051	ILE	N-CA-C	6.02	116.76	110.62
1	A	216	ALA	CA-C-N	5.82	128.56	120.29
1	A	216	ALA	C-N-CA	5.82	128.56	120.29
1	A	376	ASN	N-CA-C	5.78	117.85	108.08
1	A	780	PRO	N-CA-C	-5.76	102.16	111.14
1	A	983	VAL	CA-C-N	5.71	124.90	118.97
1	A	983	VAL	C-N-CA	5.71	124.90	118.97
1	A	310	PRO	CA-C-N	5.67	125.62	119.78
1	A	310	PRO	C-N-CA	5.67	125.62	119.78
1	A	982	ARG	CA-CB-CG	5.65	125.41	114.10
1	A	507	ASN	CA-C-N	5.59	125.25	119.05
1	A	507	ASN	C-N-CA	5.59	125.25	119.05
1	A	309	THR	N-CA-C	5.57	117.09	110.07
1	A	756	LYS	CA-C-N	5.51	128.12	120.29
1	A	756	LYS	C-N-CA	5.51	128.12	120.29
1	A	211	LEU	N-CA-C	-5.50	106.74	113.50
1	A	778	GLN	N-CA-C	5.49	126.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ALA	N-CA-C	5.44	116.89	111.07
1	A	220	ILE	N-CA-C	5.38	116.32	108.58
1	A	569	ALA	N-CA-C	-5.35	105.44	111.28
1	A	759	VAL	CB-CA-C	-5.35	102.86	110.83
1	A	968	ILE	CA-CB-CG1	5.25	119.33	110.40
1	A	832	PHE	CA-C-N	-5.22	113.39	122.37
1	A	832	PHE	C-N-CA	-5.22	113.39	122.37
1	A	1026	LEU	CA-CB-CG	5.20	134.50	116.30
1	A	152	ARG	N-CA-C	-5.19	105.70	111.36
1	A	760	SER	CB-CA-C	-5.15	100.31	110.10
1	A	1008	LYS	N-CA-C	-5.15	105.56	111.07
1	A	373	LEU	N-CA-C	5.12	121.13	109.81
1	A	870	ILE	CG1-CB-CG2	-5.12	95.34	110.70
1	A	897	GLY	N-CA-C	5.10	118.41	112.50
1	A	205	LYS	CA-C-N	5.08	124.99	119.76
1	A	205	LYS	C-N-CA	5.08	124.99	119.76
1	A	749	ILE	CG1-CB-CG2	-5.06	95.51	110.70
1	A	950	ASP	N-CA-C	-5.05	105.87	112.23
1	A	214	LYS	N-CA-C	-5.03	107.10	113.18
1	A	378	ASP	N-CA-C	5.02	116.59	108.41

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	195	0
2	A	34	0	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6783	0	6792	196	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 (196) 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	1.10
1:A:1087:PHE:C	1:A:1087:PHE:CD1	2.30	1.04
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:C	1:A:1087:PHE:HD1	1.66	1.00
1:A:967:HIS:HB2	1:A:968:ILE:HG22	1.44	0.99
1:A:1050:TYR:CD2	1:A:1050:TYR:C	2.42	0.98
1:A:759:VAL:HA	1:A:760:SER:HB3	0.97	0.96
1:A:759:VAL:CA	1:A:760:SER:CB	2.37	0.94
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:O	1:A:760:SER:OG	1.90	0.81
1:A:1045:LYS:O	1:A:1048:ILE:CG1	2.31	0.79
1:A:1050:TYR:C	1:A:1050:TYR:HD2	1.88	0.78
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:1043:THR:C	1:A:1045:LYS:H	1.94	0.75
1:A:1085:ASN:C	1:A:1087:PHE:N	2.41	0.75
1:A:1050:TYR:CD2	1:A:1050:TYR:O	2.40	0.74
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:CD1	1:A:1087:PHE:O	2.30	0.71
1:A:758:ASP:CG	1:A:759:VAL:H	1.98	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:760:SER:HB2	1.96	0.66
1:A:1045:LYS:O	1:A:1049:GLU:HG3	1.95	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:804:MET:HE3	1:A:810:PRO:HB2	1.78	0.64
1:A:1040:PRO:O	1:A:1042:LEU:HD13	1.98	0.63
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.80	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
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:758:ASP:CG	1:A:759:VAL:N	2.58	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:734:GLN:CD	1:A:780:PRO:HB3	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:883:LYS:HZ2	2:A:1201:1JV:H6	1.73	0.54
1:A:1046:GLU:O	1:A:1049:GLU:HB2	2.08	0.53
1:A:1038:GLY:C	1:A:1039:MET:HG2	2.33	0.53
1:A:864:LEU:C	1:A:866:PRO:HD3	2.34	0.53
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:804:MET:HE1	1:A:831:ILE:HG12	1.91	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:181:VAL:HG12	1:A:185:MET:HE2	1.91	0.51
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:883:LYS:NZ	2:A:1201:1JV:H6	2.26	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:149:ALA:O	1:A:152:ARG:HG2	2.12	0.49
1:A:1050:TYR:CE2	1:A:1054:ALA:HB2	2.47	0.49
1:A:277:ARG:NH2	1:A:788:ASP:OD2	2.31	0.49
1:A:898:ASN:C	1:A:899:THR:OG1	2.54	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: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:734:GLN:OE1	1:A:780:PRO:HB3	2.14	0.48
1:A:759:VAL:CG1	1:A:760:SER:HB3	2.43	0.48
1:A:759:VAL:HG12	1:A:760:SER:HB3	1.96	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
1:A:217:ASN:CG	1:A:219:CYS:CB	2.68	0.47
2:A:1201:1JV:N21	2:A:1201:1JV:H20	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:MET:HE1	1:A:831:ILE:CG2	2.42	0.47
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.97	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:149:ALA:C	1:A:152:ARG:HG2	2.40	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: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:HD13	1:A:968:ILE:HG21	1.56	0.45
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.51	0.45
1:A:759:VAL:CB	1:A:760:SER:HB3	2.40	0.45
1:A:1045:LYS:O	1:A:1048:ILE:HG13	2.13	0.45
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:568:THR:HG22	1:A:569:ALA:N	2.31	0.45
1:A:1085:ASN:O	1:A:1087:PHE:HB3	2.17	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:184:ARG:HH21	1:A:321:GLU:CD	2.24	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: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:1043:THR:O	1:A:1045:LYS:N	2.49	0.43
1:A:180:LEU:C	1:A:183:PRO:HD2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:LEU:HB2	1:A:644:ALA:HB2	2.00	0.42
1:A:756:LYS:HB3	1:A:756:LYS:HE2	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: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:928:PHE:HE2	1:A:995:MET:HE3	1.85	0.42
1:A:804:MET:HE1	1:A:831:ILE:CG1	2.48	0.42
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	0.42
1:A:315:LEU:O	1:A:727:ALA:HB2	2.20	0.42
1:A:984:PRO:HG2	1:A:1075:CYS:SG	2.60	0.42
1:A:946:ASP:C	1:A:947:ARG:HG2	2.43	0.41
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: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:914:LYS:HD2	1:A:956:GLU:CD	2.44	0.41
1:A:547:MET:HE2	1:A:547:MET:HB3	1.82	0.41
1:A:202:VAL:CG1	1:A:203:THR:N	2.83	0.41
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.20	0.41
1:A:1012:ILE:HD13	1:A:1012:ILE:HG21	1.93	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:670:GLU:HA	1:A:671:PRO:HD3	1.88	0.41
1:A:755:GLU:C	1:A:756:LYS:CG	2.93	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:217:ASN:CG	1:A:219:CYS:H	2.21	0.40
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.22	0.40
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.04	0.40
1:A:752:LEU:HD12	1:A:752:LEU:C	2.41	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

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	817/966 (85%)	772 (94%)	42 (5%)	3 (0%)	30	59

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%)	700 (94%)	48 (6%)	16	44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	225	HIS
1	A	268	GLN
1	A	271	VAL
1	A	282	VAL
1	A	305	VAL
1	A	307	LEU
1	A	357	CYS

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	381	VAL
1	A	393	VAL
1	A	402	LYS
1	A	421	LYS
1	A	498	ASN
1	A	579	ARG
1	A	610	LEU
1	A	613	ARG
1	A	707	ARG
1	A	739	ILE
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	806	SER
1	A	842	MET
1	A	865	LEU
1	A	870	ILE
1	A	893	GLN
1	A	894	SER
1	A	896	VAL
1	A	899	THR
1	A	917	THR
1	A	939	THR
1	A	949	ASN
1	A	968	ILE
1	A	982	ARG
1	A	1026	LEU
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	1051	ILE
1	A	1062	GLU
1	A	1087	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	304	HIS
1	A	483	HIS
1	A	554	GLN
1	A	634	ASN
1	A	708	HIS
1	A	775	GLN
1	A	948	HIS
1	A	959	ASN
1	A	1041	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	1JV	A	1201	-	37,38,38	1.40	7 (18%)	48,58,58	2.87	15 (31%)

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	-	-	3/17/28/28	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	1JV	C20-N21	-3.40	1.33	1.38
2	A	1201	1JV	C14-C20	3.00	1.52	1.48
2	A	1201	1JV	N6-N10	2.63	1.41	1.36
2	A	1201	1JV	N28-N27	2.58	1.40	1.37
2	A	1201	1JV	O16-C15	-2.50	1.34	1.38
2	A	1201	1JV	C19-C20	2.41	1.39	1.36
2	A	1201	1JV	F31-C30	2.14	1.41	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	1JV	C26-N25-C24	7.91	108.89	101.80
2	A	1201	1JV	C20-N21-C22	7.06	120.24	111.03
2	A	1201	1JV	C29-N28-N27	6.73	127.16	119.31
2	A	1201	1JV	C24-N28-N27	-6.52	105.67	111.00
2	A	1201	1JV	S23-C22-N21	-5.53	109.41	115.56
2	A	1201	1JV	C19-C20-N21	-5.33	110.08	116.06
2	A	1201	1JV	N27-C26-N25	-4.63	109.43	116.78
2	A	1201	1JV	C2-C5-N6	4.52	119.86	113.32
2	A	1201	1JV	C5-N6-N10	3.97	127.03	121.25
2	A	1201	1JV	F32-C30-C29	-3.24	105.94	112.04
2	A	1201	1JV	C7-N6-N10	-2.90	107.25	112.01
2	A	1201	1JV	C9-N10-N6	2.53	108.54	104.68
2	A	1201	1JV	C5-N6-C7	-2.12	125.67	128.60
2	A	1201	1JV	C26-N27-N28	2.11	107.53	102.85
2	A	1201	1JV	O16-C15-C34	2.05	120.16	116.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

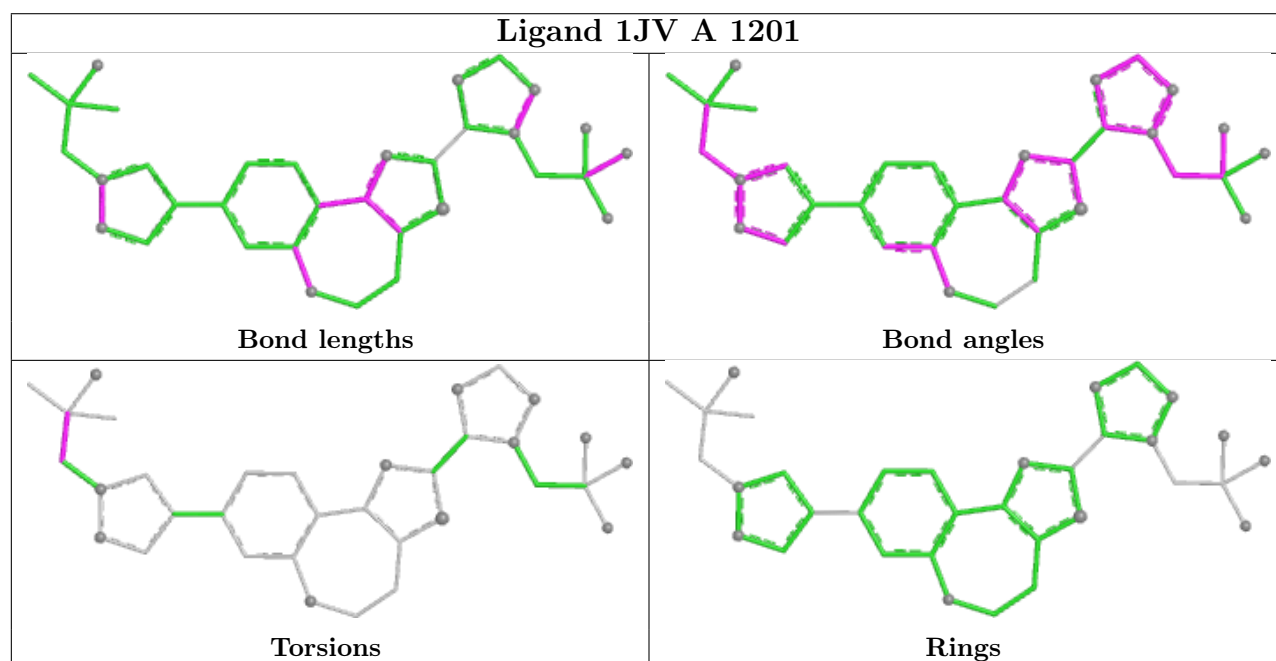
Mol	Chain	Res	Type	Atoms
2	A	1201	1JV	C1-C2-C5-N6
2	A	1201	1JV	O4-C2-C5-N6
2	A	1201	1JV	C3-C2-C5-N6

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 ⓘ

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 [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	833/966 (86%)	-0.39	8 (0%) 79 73	42, 88, 157, 213	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	GLY	5.6
1	A	899	THR	4.8
1	A	1087	PHE	4.4
1	A	1044	SER	2.8
1	A	896	VAL	2.7
1	A	966	GLY	2.4
1	A	901	ALA	2.4
1	A	757	TYR	2.3

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

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

6.3 Carbohydrates [i](#)

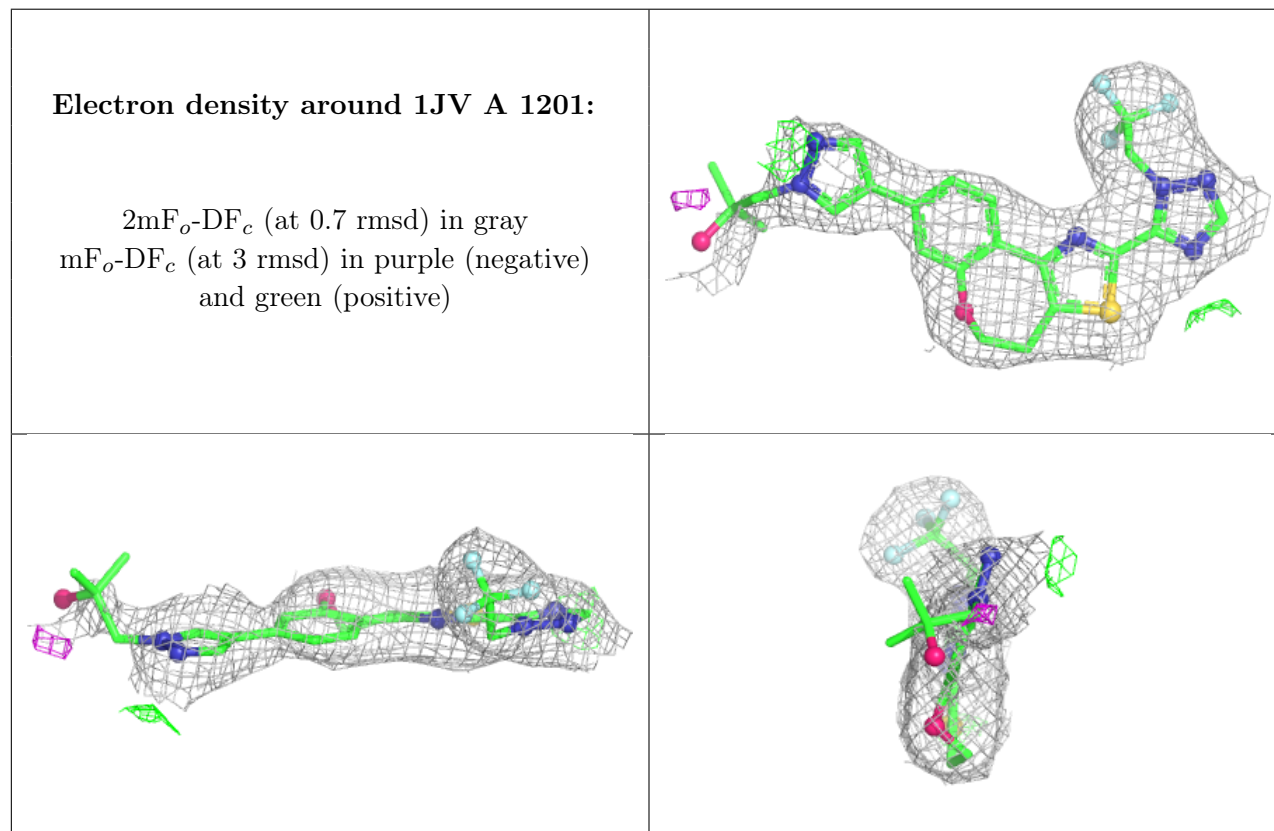
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1JV	A	1201	34/34	0.94	0.08	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.