



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:33 am BST

PDB ID : 3BV3
Title : Morpholino pyrrolotriazine P38 Alpha Map Kinase inhibitor compound 2
Authors : Sack, J.S.
Deposited on : 2008-01-04
Resolution : 2.59 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

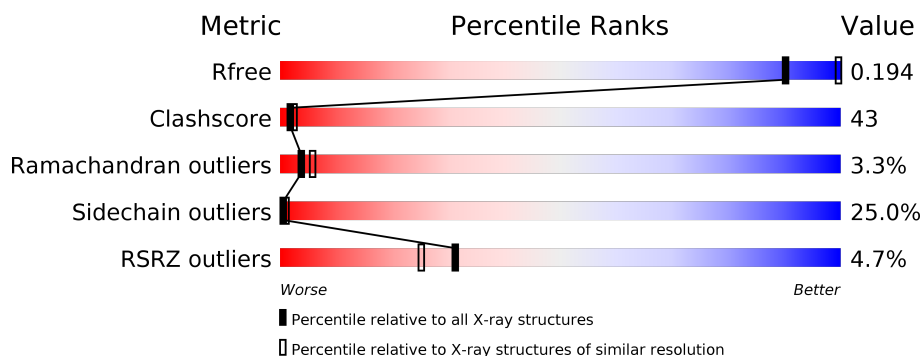
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	366	<div> <div>4%</div> <div>34%</div> <div>41%</div> <div>16%</div> <div>• 8%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2869 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.

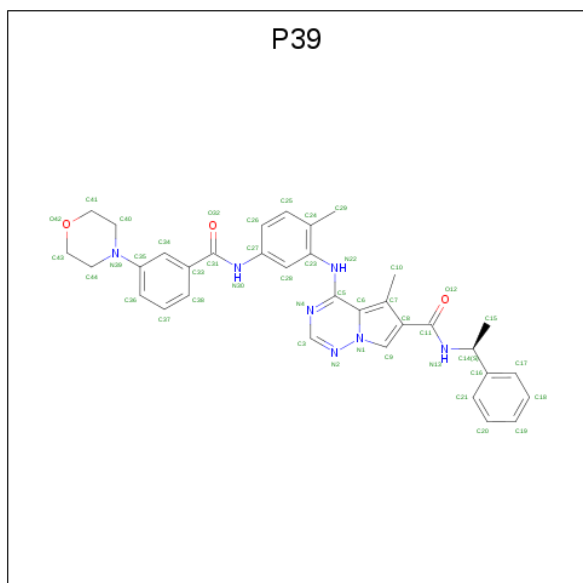
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2731	1755	465	499	12	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q16539
A	-4	ALA	-	EXPRESSION TAG	UNP Q16539
A	-3	HIS	-	EXPRESSION TAG	UNP Q16539
A	-2	HIS	-	EXPRESSION TAG	UNP Q16539
A	-1	HIS	-	EXPRESSION TAG	UNP Q16539
A	0	HIS	-	EXPRESSION TAG	UNP Q16539
A	1	HIS	-	EXPRESSION TAG	UNP Q16539

- Molecule 2 is 5-methyl-4-[(2-methyl-5-[(3-morpholin-4-ylphenyl)carbonyl]amino}phenyl)amino]-N-[(1S)-1-phenylethyl]pyrrolo[2,1-f][1,2,4]triazine-6-carboxamide (three-letter code: P39) (formula: C₃₄H₃₅N₇O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	34	7	3		

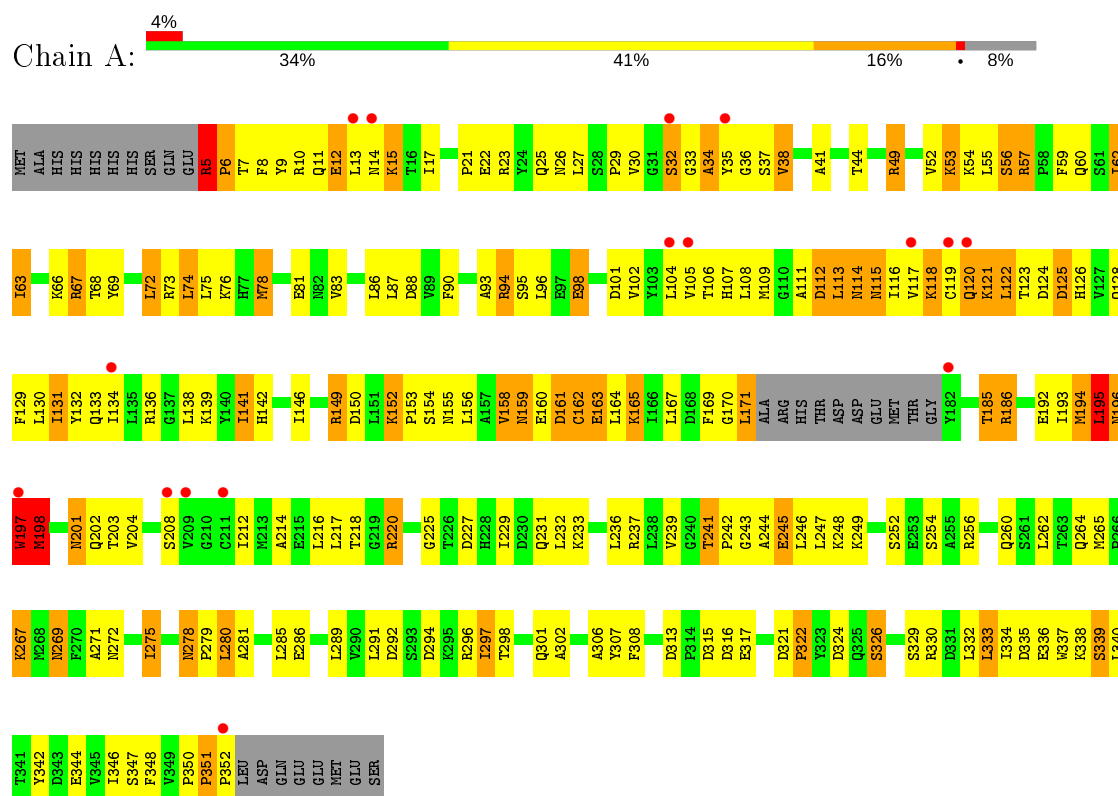
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		

3 Residue-property plots [i](#)

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: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.31Å 74.94Å 78.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.42 – 2.59 24.42 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.42-2.59) 91.5 (24.42-2.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.33Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.193 , 0.284 0.207 , 0.194	Depositor DCC
R_{free} test set	781 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2869	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P39

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	0.38	0/2795	0.60	0/3795

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PRO	Peptide
1	A	5	ARG	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	2731	0	2734	235	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	35	9	0
3	A	94	0	0	7	0
All	All	2869	0	2769	237	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 43.

All (237) 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:7:THR:CG2	1:A:22:GLU:HG3	1.94	0.97
1:A:233:LYS:HE2	1:A:237:ARG:HH22	1.26	0.96
1:A:87:LEU:HD21	1:A:107:HIS:CD2	2.02	0.95
1:A:111:ALA:HA	2:A:501:P39:H15A	1.49	0.92
1:A:233:LYS:HE2	1:A:237:ARG:NH2	1.85	0.92
1:A:297:ILE:HD13	1:A:302:ALA:HB2	1.52	0.91
1:A:32:SER:CB	1:A:171:LEU:HG	2.05	0.86
1:A:195:LEU:HD13	1:A:197:TRP:CD1	2.13	0.83
1:A:333:LEU:HD23	1:A:336:GLU:OE1	1.82	0.80
1:A:159:ASN:CB	1:A:163:GLU:HB3	2.12	0.80
1:A:111:ALA:HA	2:A:501:P39:C15	2.11	0.79
1:A:138:LEU:HA	1:A:141:ILE:HG22	1.64	0.78
1:A:112:ASP:OD2	1:A:114:ASN:HB3	1.84	0.78
1:A:281:ALA:HB2	1:A:307:TYR:CE1	2.18	0.78
1:A:159:ASN:CG	1:A:163:GLU:HB3	2.03	0.77
1:A:32:SER:HB2	1:A:171:LEU:HG	1.67	0.77
1:A:94:ARG:CZ	1:A:94:ARG:HB3	2.14	0.77
1:A:159:ASN:HB2	1:A:163:GLU:HB3	1.66	0.76
1:A:159:ASN:ND2	1:A:163:GLU:HB3	2.00	0.76
1:A:7:THR:CB	1:A:22:GLU:HG3	2.15	0.75
1:A:7:THR:HB	1:A:22:GLU:HG3	1.68	0.75
1:A:13:LEU:HD12	1:A:29:PRO:HG3	1.67	0.75
1:A:32:SER:HB3	1:A:171:LEU:HG	1.67	0.74
1:A:298:THR:H	1:A:301:GLN:HE21	1.34	0.74
1:A:96:LEU:HB2	1:A:342:TYR:CD2	2.23	0.73
1:A:7:THR:HG22	1:A:22:GLU:HG3	1.72	0.72
1:A:163:GLU:HG2	1:A:165:LYS:HE2	1.71	0.72
1:A:5:ARG:O	1:A:5:ARG:HG2	1.89	0.72
1:A:125:ASP:HA	1:A:128:GLN:NE2	2.06	0.71
1:A:5:ARG:O	1:A:5:ARG:CG	2.38	0.70
1:A:201:ASN:HD22	1:A:203:THR:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:ND2	1:A:280:LEU:H	1.90	0.70
1:A:269:ASN:HD21	1:A:271:ALA:HB3	1.58	0.69
1:A:33:GLY:HA2	1:A:36:GLY:O	1.92	0.69
1:A:113:LEU:HD21	1:A:216:LEU:HD11	1.75	0.69
1:A:11:GLN:HG2	1:A:13:LEU:HD22	1.76	0.67
1:A:201:ASN:ND2	1:A:203:THR:H	1.93	0.67
1:A:292:ASP:OD1	1:A:294:ASP:HB2	1.95	0.67
1:A:262:LEU:O	1:A:264:GLN:NE2	2.28	0.67
1:A:159:ASN:HB2	1:A:163:GLU:H	1.59	0.67
1:A:275:ILE:HG12	1:A:275:ILE:O	1.94	0.66
1:A:242:PRO:HB2	1:A:247:LEU:HD11	1.76	0.66
1:A:26:ASN:O	1:A:26:ASN:ND2	2.28	0.66
1:A:186:ARG:NH1	1:A:225:GLY:O	2.29	0.66
1:A:201:ASN:ND2	1:A:203:THR:OG1	2.28	0.65
1:A:76:LYS:NZ	1:A:344:GLU:O	2.28	0.65
1:A:7:THR:O	1:A:22:GLU:N	2.30	0.64
1:A:194:MET:O	1:A:195:LEU:HG	1.98	0.63
1:A:62:ILE:HG13	1:A:334:ILE:HG12	1.79	0.63
1:A:138:LEU:HA	1:A:141:ILE:CG2	2.27	0.63
1:A:53:LYS:HD3	1:A:55:LEU:HD23	1.81	0.63
1:A:109:MET:O	2:A:501:P39:H17	1.99	0.63
1:A:38:VAL:HG13	1:A:171:LEU:HD22	1.79	0.63
1:A:129:PHE:O	1:A:133:GLN:HG3	1.98	0.63
1:A:196:ASN:O	1:A:198:MET:N	2.31	0.63
1:A:23:ARG:HA	1:A:44:THR:HB	1.80	0.63
1:A:66:LYS:HD2	1:A:337:TRP:CZ2	2.34	0.62
1:A:155:ASN:HD21	1:A:170:GLY:H	1.46	0.62
1:A:141:ILE:HG23	1:A:142:HIS:N	2.14	0.62
1:A:93:ALA:HB2	3:A:545:HOH:O	1.98	0.62
1:A:112:ASP:O	1:A:116:ILE:HG13	2.00	0.62
1:A:134:ILE:CD1	1:A:156:LEU:HD13	2.29	0.62
1:A:298:THR:H	1:A:301:GLN:NE2	1.97	0.61
1:A:117:VAL:HA	1:A:120:GLN:O	2.01	0.61
1:A:74:LEU:HD11	1:A:146:ILE:HD13	1.82	0.61
1:A:155:ASN:ND2	1:A:170:GLY:H	1.98	0.61
1:A:195:LEU:HD13	1:A:197:TRP:HD1	1.64	0.61
1:A:244:ALA:O	1:A:248:LYS:HG3	2.00	0.61
1:A:195:LEU:C	1:A:197:TRP:H	2.04	0.61
1:A:90:PHE:HA	3:A:525:HOH:O	2.01	0.60
1:A:278:ASN:HD22	1:A:279:PRO:N	2.00	0.60
1:A:120:GLN:HG3	1:A:121:LYS:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASN:HB2	1:A:163:GLU:N	2.16	0.59
1:A:322:PRO:HA	3:A:538:HOH:O	2.01	0.59
1:A:124:ASP:OD2	1:A:278:ASN:HB2	2.03	0.59
1:A:13:LEU:CD1	1:A:29:PRO:HD3	2.33	0.58
1:A:134:ILE:HD11	1:A:156:LEU:HD13	1.86	0.58
1:A:297:ILE:HD13	1:A:302:ALA:CB	2.28	0.58
1:A:159:ASN:CB	1:A:163:GLU:H	2.17	0.58
1:A:87:LEU:HD21	1:A:107:HIS:NE2	2.18	0.58
1:A:152:LYS:HD2	1:A:185:THR:HB	1.85	0.57
1:A:76:LYS:HD3	1:A:344:GLU:HG3	1.86	0.57
1:A:72:LEU:O	1:A:76:LYS:HG3	2.03	0.57
1:A:13:LEU:HD12	1:A:29:PRO:CG	2.32	0.57
1:A:195:LEU:N	1:A:195:LEU:HD12	2.19	0.57
1:A:119:CYS:O	1:A:120:GLN:HB3	2.03	0.57
1:A:197:TRP:O	1:A:198:MET:HB3	2.03	0.57
1:A:278:ASN:HD22	1:A:280:LEU:H	1.51	0.57
1:A:201:ASN:HD22	1:A:201:ASN:C	2.08	0.57
1:A:8:PHE:O	1:A:9:TYR:HB3	2.05	0.56
1:A:269:ASN:HD21	1:A:271:ALA:CB	2.18	0.56
1:A:88:ASP:O	1:A:105:VAL:HG23	2.06	0.56
1:A:239:VAL:O	1:A:267:LYS:HG3	2.06	0.55
1:A:243:GLY:O	1:A:247:LEU:HD13	2.07	0.55
1:A:13:LEU:O	1:A:14:ASN:HB2	2.06	0.55
1:A:26:ASN:ND2	1:A:49:ARG:HH12	2.05	0.55
1:A:350:PRO:O	1:A:352:PRO:HD2	2.06	0.55
1:A:78:MET:HG2	1:A:83:VAL:CG1	2.38	0.54
1:A:11:GLN:HG2	1:A:13:LEU:CD2	2.38	0.54
1:A:192:GLU:HA	1:A:197:TRP:CE3	2.43	0.54
1:A:59:PHE:CD2	1:A:338:LYS:HE2	2.43	0.54
1:A:141:ILE:HG12	1:A:146:ILE:HB	1.90	0.53
1:A:278:ASN:C	1:A:278:ASN:HD22	2.11	0.53
1:A:233:LYS:CE	1:A:237:ARG:HH22	2.11	0.53
1:A:159:ASN:HB2	1:A:163:GLU:CB	2.34	0.53
1:A:52:VAL:HG22	1:A:105:VAL:HG13	1.89	0.53
1:A:149:ARG:HE	1:A:193:ILE:HD12	1.74	0.53
1:A:272:ASN:O	1:A:275:ILE:HG23	2.08	0.53
1:A:13:LEU:HD12	1:A:29:PRO:HD3	1.89	0.53
1:A:27:LEU:HD23	1:A:41:ALA:HB2	1.91	0.52
1:A:67:ARG:HH11	1:A:67:ARG:CG	2.22	0.52
1:A:25:GLN:O	1:A:26:ASN:HB3	2.10	0.52
1:A:236:LEU:CD2	1:A:291:LEU:HD11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:HB	1:A:265:MET:H	1.73	0.52
1:A:280:LEU:HD13	1:A:306:ALA:HB3	1.90	0.52
1:A:169:PHE:O	1:A:171:LEU:HD13	2.10	0.52
1:A:269:ASN:ND2	1:A:271:ALA:H	2.07	0.52
1:A:159:ASN:HB2	1:A:163:GLU:CA	2.39	0.52
1:A:121:LYS:HD3	1:A:217:LEU:O	2.10	0.52
1:A:87:LEU:HD21	1:A:107:HIS:HD2	1.63	0.51
1:A:35:TYR:CD1	1:A:67:ARG:NE	2.79	0.51
1:A:35:TYR:CD2	1:A:67:ARG:NH2	2.78	0.51
1:A:131:ILE:HG22	1:A:308:PHE:CZ	2.45	0.51
1:A:225:GLY:HA3	1:A:231:GLN:OE1	2.10	0.51
1:A:5:ARG:O	1:A:5:ARG:NE	2.44	0.51
1:A:5:ARG:O	1:A:5:ARG:CD	2.59	0.50
1:A:122:LEU:HD11	1:A:216:LEU:HB3	1.93	0.50
1:A:14:ASN:O	1:A:15:LYS:HB2	2.12	0.50
1:A:333:LEU:CD2	1:A:333:LEU:N	2.75	0.50
1:A:12:GLU:O	1:A:12:GLU:OE1	2.30	0.49
1:A:134:ILE:HD13	1:A:156:LEU:CD1	2.42	0.49
1:A:220:ARG:CG	1:A:220:ARG:HH11	2.25	0.49
1:A:195:LEU:O	1:A:196:ASN:HB2	2.12	0.49
1:A:96:LEU:HB2	1:A:342:TYR:CE2	2.48	0.49
1:A:7:THR:HG21	1:A:22:GLU:HG3	1.91	0.49
1:A:54:LYS:NZ	1:A:101:ASP:OD2	2.38	0.49
1:A:113:LEU:O	1:A:117:VAL:HG23	2.13	0.49
1:A:241:THR:HG21	1:A:264:GLN:OE1	2.13	0.49
1:A:197:TRP:CE3	1:A:198:MET:CE	2.96	0.49
1:A:55:LEU:CD1	1:A:68:THR:HG23	2.43	0.49
1:A:94:ARG:N	1:A:98:GLU:OE2	2.40	0.49
1:A:88:ASP:HA	1:A:348:PHE:CE2	2.47	0.48
1:A:57:ARG:HE	1:A:60:GLN:NE2	2.11	0.48
1:A:194:MET:C	1:A:195:LEU:HG	2.33	0.48
1:A:78:MET:CG	1:A:83:VAL:HG11	2.44	0.48
1:A:78:MET:HE2	1:A:78:MET:HA	1.96	0.48
1:A:236:LEU:HD22	1:A:242:PRO:HD3	1.96	0.48
1:A:30:VAL:HB	1:A:38:VAL:HG23	1.96	0.48
1:A:242:PRO:HB2	1:A:247:LEU:CD1	2.43	0.47
1:A:75:LEU:HB3	1:A:86:LEU:HB2	1.96	0.47
1:A:106:THR:OG1	2:A:501:P39:H29B	2.13	0.47
1:A:141:ILE:HG23	1:A:142:HIS:H	1.76	0.47
1:A:321:ASP:HB2	1:A:322:PRO:HD2	1.96	0.47
1:A:66:LYS:HE2	3:A:594:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASN:HB2	1:A:163:GLU:O	2.14	0.47
1:A:141:ILE:CG2	1:A:142:HIS:N	2.78	0.47
1:A:232:LEU:O	1:A:232:LEU:HD12	2.14	0.47
1:A:324:ASP:OD1	1:A:326:SER:OG	2.27	0.47
2:A:501:P39:O32	2:A:501:P39:H28	2.14	0.47
1:A:7:THR:HG22	1:A:22:GLU:CG	2.42	0.46
1:A:11:GLN:CG	1:A:13:LEU:HD22	2.44	0.46
1:A:33:GLY:O	1:A:34:ALA:HB3	2.16	0.46
1:A:75:LEU:HD12	1:A:104:LEU:HD22	1.97	0.46
1:A:83:VAL:HG13	2:A:501:P39:H41	1.98	0.46
1:A:8:PHE:CE1	1:A:21:PRO:HD3	2.50	0.46
1:A:186:ARG:HG2	1:A:186:ARG:O	2.15	0.46
1:A:13:LEU:HD12	1:A:29:PRO:CD	2.45	0.46
1:A:115:ASN:HA	1:A:118:LYS:HB2	1.97	0.45
1:A:30:VAL:HB	1:A:38:VAL:CG2	2.46	0.45
1:A:53:LYS:HD3	1:A:55:LEU:CD2	2.45	0.45
1:A:131:ILE:HD13	1:A:131:ILE:N	2.32	0.45
1:A:171:LEU:CD1	1:A:171:LEU:N	2.78	0.45
1:A:132:TYR:HB2	1:A:308:PHE:CD1	2.52	0.45
1:A:26:ASN:ND2	1:A:49:ARG:NH1	2.65	0.45
1:A:78:MET:HG2	1:A:83:VAL:HG11	1.98	0.45
1:A:154:SER:HB2	3:A:593:HOH:O	2.16	0.45
1:A:138:LEU:CA	1:A:141:ILE:HG22	2.40	0.45
1:A:197:TRP:O	1:A:198:MET:HE2	2.17	0.45
1:A:269:ASN:ND2	1:A:271:ALA:HB3	2.29	0.45
1:A:126:HIS:O	1:A:130:LEU:HG	2.16	0.44
1:A:78:MET:CE	1:A:78:MET:HA	2.48	0.44
1:A:232:LEU:HD12	1:A:236:LEU:HG	1.99	0.44
1:A:56:SER:C	1:A:57:ARG:HG2	2.37	0.44
1:A:256:ARG:O	1:A:260:GLN:HG3	2.17	0.44
1:A:67:ARG:CG	1:A:67:ARG:NH1	2.78	0.44
1:A:141:ILE:HG23	1:A:142:HIS:CD2	2.53	0.44
1:A:164:LEU:O	1:A:165:LYS:HD2	2.18	0.44
1:A:116:ILE:HG22	1:A:122:LEU:CD2	2.47	0.44
1:A:117:VAL:O	1:A:120:GLN:N	2.50	0.44
1:A:78:MET:HG2	1:A:83:VAL:HG12	2.00	0.44
1:A:197:TRP:C	1:A:198:MET:HE3	2.38	0.44
1:A:131:ILE:HG22	1:A:308:PHE:HZ	1.81	0.44
1:A:214:ALA:O	1:A:218:THR:HG23	2.18	0.44
1:A:69:TYR:CE1	1:A:340:LEU:HB3	2.54	0.43
1:A:220:ARG:NH1	1:A:220:ARG:CG	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:O	1:A:67:ARG:HB2	2.18	0.43
1:A:38:VAL:HG13	1:A:171:LEU:CD2	2.46	0.43
1:A:208:SER:O	1:A:212:ILE:HD12	2.18	0.43
1:A:313:ASP:O	1:A:316:ASP:N	2.46	0.43
1:A:7:THR:HB	1:A:22:GLU:CG	2.45	0.43
1:A:245:GLU:HG3	1:A:246:LEU:N	2.31	0.42
1:A:332:LEU:HB3	1:A:336:GLU:HB2	2.01	0.42
1:A:204:VAL:HG13	3:A:524:HOH:O	2.18	0.42
1:A:281:ALA:HB2	1:A:307:TYR:CZ	2.53	0.42
1:A:33:GLY:O	1:A:34:ALA:CB	2.67	0.42
1:A:171:LEU:HD13	1:A:171:LEU:N	2.35	0.42
1:A:5:ARG:N	1:A:6:PRO:CD	2.83	0.42
1:A:161:ASP:CG	1:A:162:CYS:H	2.20	0.42
1:A:159:ASN:ND2	1:A:163:GLU:CB	2.78	0.42
1:A:326:SER:HB2	1:A:330:ARG:NH1	2.34	0.42
1:A:116:ILE:HD11	1:A:158:VAL:HG21	2.01	0.42
1:A:203:THR:HB	1:A:296:ARG:HD2	2.02	0.42
2:A:501:P39:H36	2:A:501:P39:H44A	1.77	0.41
1:A:192:GLU:O	1:A:197:TRP:HB3	2.20	0.41
1:A:196:ASN:HA	3:A:568:HOH:O	2.20	0.41
1:A:32:SER:HB3	1:A:171:LEU:CG	2.43	0.41
1:A:333:LEU:N	1:A:333:LEU:HD22	2.35	0.41
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.79	0.41
1:A:116:ILE:CG2	1:A:122:LEU:CD2	2.98	0.41
1:A:141:ILE:CG2	1:A:142:HIS:H	2.32	0.41
1:A:152:LYS:HB2	1:A:153:PRO:CD	2.50	0.41
1:A:232:LEU:CD1	1:A:236:LEU:HG	2.51	0.41
1:A:139:LYS:NZ	1:A:317:GLU:O	2.42	0.41
1:A:38:VAL:HG11	2:A:501:P39:C3	2.51	0.41
1:A:95:SER:OG	1:A:98:GLU:HG3	2.21	0.41
1:A:342:TYR:O	1:A:346:ILE:HG12	2.21	0.41
1:A:116:ILE:HG22	1:A:122:LEU:HD21	2.03	0.41
1:A:201:ASN:HD21	1:A:203:THR:HG1	1.60	0.41
1:A:130:LEU:O	1:A:134:ILE:HG13	2.20	0.41
1:A:333:LEU:HB2	1:A:336:GLU:HG3	2.02	0.41
1:A:351:PRO:O	1:A:352:PRO:C	2.59	0.41
1:A:313:ASP:O	1:A:315:ASP:N	2.54	0.41
1:A:335:ASP:O	1:A:339:SER:HB2	2.20	0.41
1:A:117:VAL:CG2	1:A:216:LEU:CD2	2.99	0.40
1:A:194:MET:C	1:A:195:LEU:CG	2.90	0.40
1:A:109:MET:HG2	2:A:501:P39:H10	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TRP:CE3	1:A:198:MET:HE1	2.56	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	334/366 (91%)	294 (88%)	29 (9%)	11 (3%)	4 6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	159	ASN
1	A	197	TRP
1	A	6	PRO
1	A	34	ALA
1	A	120	GLN
1	A	195	LEU
1	A	198	MET
1	A	322	PRO
1	A	347	SER
1	A	162	CYS

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	300/325 (92%)	225 (75%)	75 (25%)	0 1

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	10	ARG
1	A	12	GLU
1	A	17	ILE
1	A	32	SER
1	A	37	SER
1	A	38	VAL
1	A	49	ARG
1	A	53	LYS
1	A	56	SER
1	A	57	ARG
1	A	62	ILE
1	A	63	ILE
1	A	67	ARG
1	A	72	LEU
1	A	73	ARG
1	A	74	LEU
1	A	78	MET
1	A	81	GLU
1	A	94	ARG
1	A	98	GLU
1	A	102	VAL
1	A	108	LEU
1	A	112	ASP
1	A	113	LEU
1	A	114	ASN
1	A	115	ASN
1	A	118	LYS
1	A	121	LYS
1	A	122	LEU
1	A	123	THR
1	A	125	ASP
1	A	131	ILE
1	A	136	ARG
1	A	141	ILE
1	A	149	ARG
1	A	150	ASP
1	A	152	LYS

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Mol	Chain	Res	Type
1	A	158	VAL
1	A	160	GLU
1	A	161	ASP
1	A	163	GLU
1	A	165	LYS
1	A	167	LEU
1	A	171	LEU
1	A	185	THR
1	A	186	ARG
1	A	194	MET
1	A	195	LEU
1	A	196	ASN
1	A	197	TRP
1	A	198	MET
1	A	201	ASN
1	A	202	GLN
1	A	220	ARG
1	A	227	ASP
1	A	229	ILE
1	A	241	THR
1	A	245	GLU
1	A	249	LYS
1	A	252	SER
1	A	254	SER
1	A	267	LYS
1	A	269	ASN
1	A	275	ILE
1	A	278	ASN
1	A	280	LEU
1	A	285	LEU
1	A	286	GLU
1	A	289	LEU
1	A	297	ILE
1	A	326	SER
1	A	329	SER
1	A	333	LEU
1	A	339	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN

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Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	ASN
1	A	60	GLN
1	A	77	HIS
1	A	107	HIS
1	A	114	ASN
1	A	115	ASN
1	A	128	GLN
1	A	155	ASN
1	A	196	ASN
1	A	199	HIS
1	A	201	ASN
1	A	260	GLN
1	A	269	ASN
1	A	278	ASN
1	A	301	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 carbohydrates 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	P39	A	501	-	45,49,49	2.43	22 (48%)	53,69,69	3.00	22 (41%)

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	P39	A	501	-	-	2/26/36/36	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	P39	C34-C33	4.94	1.46	1.39
2	A	501	P39	C10-C7	4.37	1.62	1.51
2	A	501	P39	C8-C7	4.32	1.46	1.40
2	A	501	P39	C17-C16	4.06	1.45	1.39
2	A	501	P39	C9-C8	3.94	1.46	1.39
2	A	501	P39	C5-N4	-3.89	1.28	1.34
2	A	501	P39	C37-C36	-3.67	1.31	1.38
2	A	501	P39	C36-C35	-3.25	1.32	1.39
2	A	501	P39	C40-N39	-3.25	1.41	1.46
2	A	501	P39	C26-C27	3.21	1.44	1.39
2	A	501	P39	C21-C16	2.88	1.43	1.39
2	A	501	P39	C28-C27	2.80	1.44	1.39
2	A	501	P39	C26-C25	2.79	1.43	1.38
2	A	501	P39	C34-C35	-2.71	1.34	1.39
2	A	501	P39	C19-C18	2.59	1.44	1.38
2	A	501	P39	C44-N39	2.59	1.50	1.46
2	A	501	P39	C5-N22	2.57	1.40	1.36
2	A	501	P39	C8-C11	-2.47	1.45	1.50
2	A	501	P39	C16-C14	-2.47	1.45	1.52
2	A	501	P39	C3-N4	2.37	1.38	1.33
2	A	501	P39	C14-N13	-2.30	1.42	1.47
2	A	501	P39	O12-C11	2.08	1.27	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	P39	C37-C36-C35	8.34	130.58	119.68
2	A	501	P39	N22-C5-N4	-6.52	109.98	118.72
2	A	501	P39	N2-C3-N4	-6.37	118.59	128.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	P39	C26-C27-C28	-5.63	112.97	119.65
2	A	501	P39	C18-C17-C16	-5.22	114.19	120.65
2	A	501	P39	C14-N13-C11	-4.86	112.00	122.56
2	A	501	P39	C15-C14-N13	4.85	117.59	109.05
2	A	501	P39	O42-C43-C44	-4.66	101.54	111.80
2	A	501	P39	C44-N39-C40	4.59	121.66	111.52
2	A	501	P39	O42-C41-C40	4.34	121.36	111.80
2	A	501	P39	O32-C31-C33	-4.09	113.64	120.94
2	A	501	P39	C15-C14-C16	-4.05	103.00	112.25
2	A	501	P39	C16-C14-N13	-3.97	102.13	111.31
2	A	501	P39	C21-C16-C17	3.58	122.76	118.29
2	A	501	P39	C27-C28-C23	3.56	127.21	120.17
2	A	501	P39	C27-N30-C31	-3.11	118.51	126.58
2	A	501	P39	C19-C20-C21	-3.07	115.52	120.19
2	A	501	P39	C43-O42-C41	2.88	119.52	109.89
2	A	501	P39	C38-C37-C36	-2.80	116.27	120.25
2	A	501	P39	O12-C11-C8	2.21	125.06	121.01
2	A	501	P39	C28-C27-N30	2.14	127.16	120.18
2	A	501	P39	C33-C31-N30	2.10	120.53	115.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	P39	C24-C23-N22-C5
2	A	501	P39	C28-C23-N22-C5

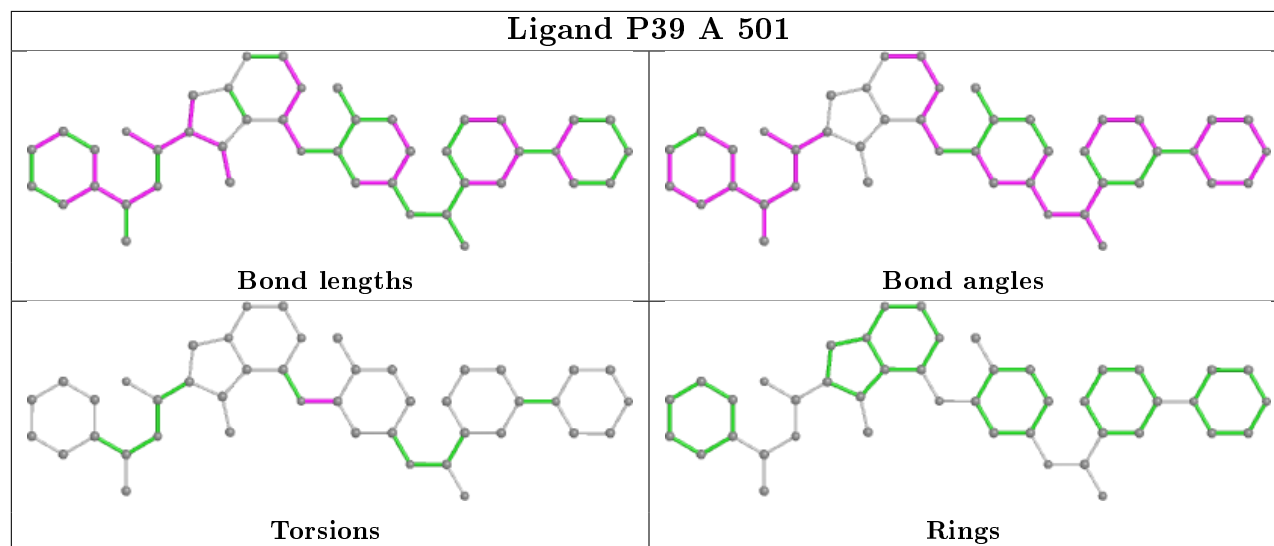
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	P39	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/366 (92%)	-0.00	16 (4%) 31 25	29, 51, 87, 108	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	TYR	6.8
1	A	14	ASN	3.9
1	A	209	VAL	3.9
1	A	197	TRP	3.8
1	A	35	TYR	3.4
1	A	211	CYS	3.1
1	A	352	PRO	2.8
1	A	104	LEU	2.4
1	A	120	GLN	2.4
1	A	117	VAL	2.3
1	A	134	ILE	2.2
1	A	32	SER	2.2
1	A	105	VAL	2.2
1	A	119	CYS	2.2
1	A	13	LEU	2.1
1	A	208	SER	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](#)

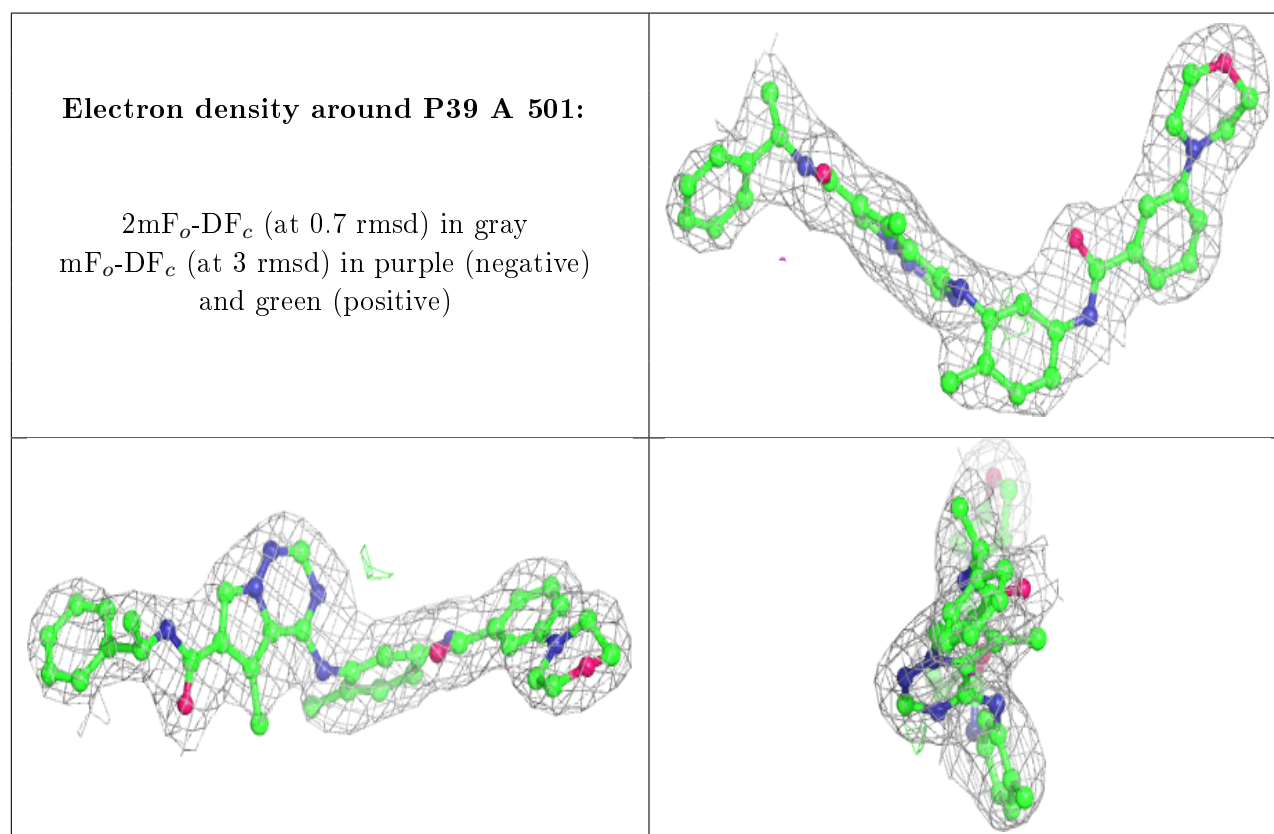
There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
2	P39	A	501	44/44	0.91	0.16	31,40,55,57	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.