



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:14 AM UTC

PDB ID : 3MVL / pdb_00003mvl
Title : P38 Alpha Map Kinase complexed with pyrrolotriazine inhibitor 7K
Authors : Sack, J.S.
Deposited on : 2010-05-04
Resolution : 2.80 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

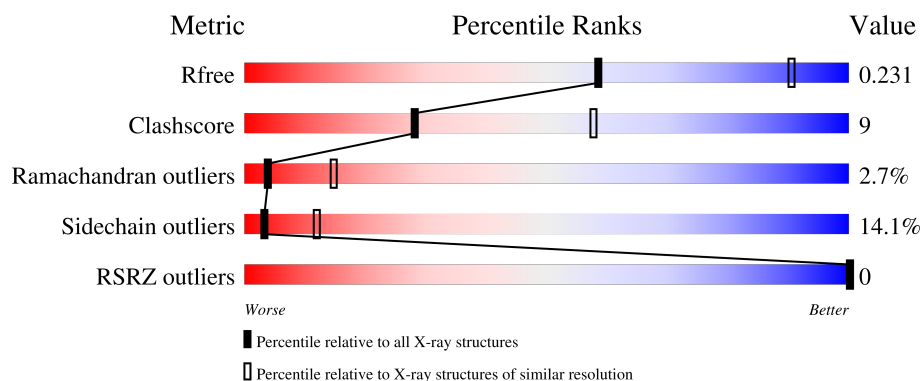
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	366	
1	B	366	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5667 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.

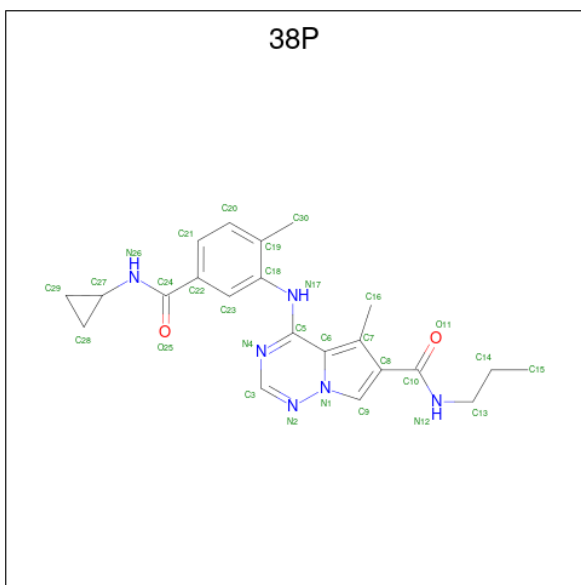
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2741	1759	471	499	12			
1	B	339	Total	C	N	O	S	0	0	0
			2741	1759	471	499	12			

There are 14 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
B	-5	MET	-	expression tag	UNP Q16539
B	-4	ALA	-	expression tag	UNP Q16539
B	-3	HIS	-	expression tag	UNP Q16539
B	-2	HIS	-	expression tag	UNP Q16539
B	-1	HIS	-	expression tag	UNP Q16539
B	0	HIS	-	expression tag	UNP Q16539
B	1	HIS	-	expression tag	UNP Q16539

- Molecule 2 is 4-{{5-(cyclopropylcarbamoyl)-2-methylphenyl}amino}-5-methyl-N-propylpyrrolo[2,1-f][1,2,4]triazine-6-carboxamide (CCD ID: 38P) (formula: C₂₂H₂₆N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	6	2		
2	B	1	Total	C	N	O	0	0
			30	22	6	2		

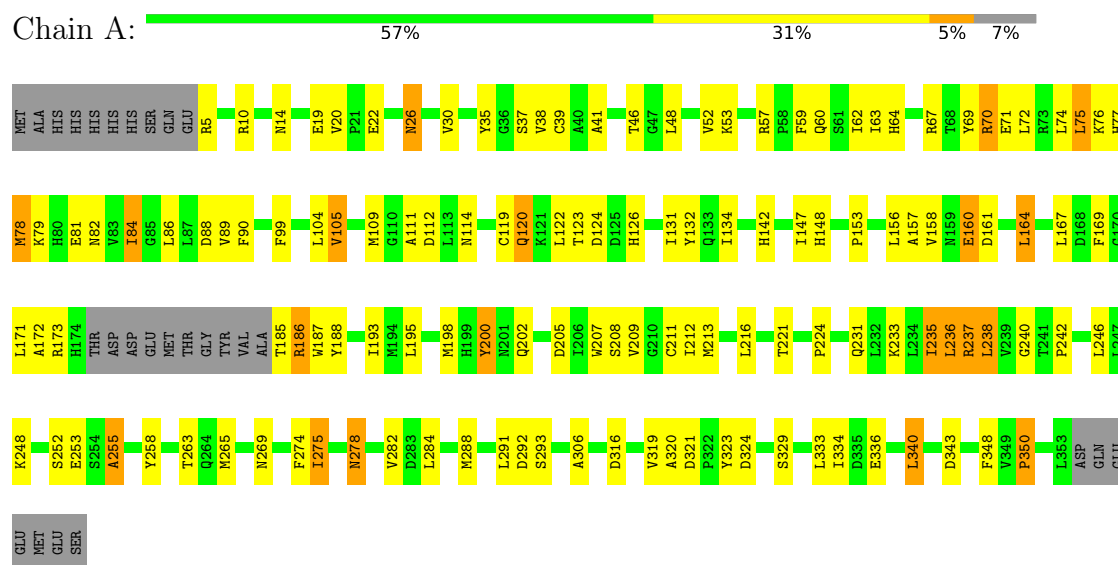
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	67	Total	O	0	0
			67	67		

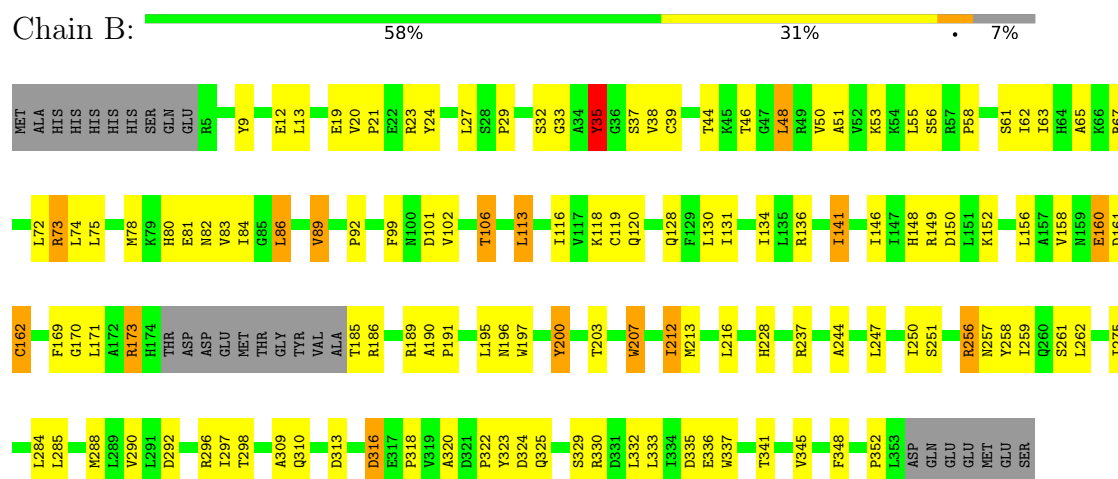
3 Residue-property plots

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 14



- Molecule 1: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.54Å 71.68Å 72.82Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	33.77 – 2.80 33.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.77-2.80) 99.5 (33.77-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.33 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.9.4	Depositor
R, R_{free}	0.227 , 0.335 0.180 , 0.231	Depositor DCC
R_{free} test set	871 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.106 for -h,l,k 0.105 for -h,-l,-k 0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5667	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 38P

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	1.01	4/2805 (0.1%)	1.60	35/3807 (0.9%)
1	B	0.98	1/2805 (0.0%)	1.52	26/3807 (0.7%)
All	All	1.00	5/5610 (0.1%)	1.56	61/7614 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	GLN	CD-OE1	5.55	1.34	1.23
1	A	20	VAL	CA-C	5.34	1.58	1.52
1	A	172	ALA	C-N	5.31	1.38	1.33
1	A	142	HIS	ND1-CE1	5.22	1.37	1.32
1	A	269	ASN	CG-OD1	5.21	1.33	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ILE	N-CA-C	-10.12	102.04	111.45
1	A	316	ASP	CA-C-N	8.08	129.89	122.37
1	A	316	ASP	C-N-CA	8.08	129.89	122.37
1	A	350	PRO	N-CA-C	8.02	120.48	110.70
1	A	142	HIS	CB-CG-CD2	-7.88	120.95	131.20
1	B	99	PHE	CA-CB-CG	7.37	121.17	113.80
1	A	324	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	132	TYR	CA-C-N	6.77	129.66	120.38
1	A	132	TYR	C-N-CA	6.77	129.66	120.38
1	B	195	LEU	N-CA-C	6.75	120.78	112.54
1	B	118	LYS	N-CA-C	-6.57	105.30	113.38
1	A	320	ALA	N-CA-C	6.51	119.69	110.50
1	A	340	LEU	CA-C-N	6.50	129.28	120.44
1	A	340	LEU	C-N-CA	6.50	129.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	PRO	CA-C-N	6.34	129.87	120.87
1	B	92	PRO	C-N-CA	6.34	129.87	120.87
1	A	248	LYS	CA-C-N	6.29	128.71	120.28
1	A	248	LYS	C-N-CA	6.29	128.71	120.28
1	A	142	HIS	N-CA-C	6.20	117.70	111.07
1	A	343	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	20	VAL	N-CA-C	6.17	115.85	108.45
1	A	198	MET	CA-C-N	6.14	129.34	120.38
1	A	198	MET	C-N-CA	6.14	129.34	120.38
1	B	320	ALA	N-CA-C	6.00	119.35	110.48
1	A	323	TYR	CA-C-N	5.98	129.85	121.24
1	A	323	TYR	C-N-CA	5.98	129.85	121.24
1	A	282	VAL	CA-C-N	5.91	128.13	120.44
1	A	282	VAL	C-N-CA	5.91	128.13	120.44
1	B	330	ARG	N-CA-C	5.86	118.28	108.73
1	A	90	PHE	N-CA-C	5.78	117.96	109.24
1	B	256	ARG	N-CA-C	-5.77	106.78	113.88
1	A	211	CYS	N-CA-C	-5.60	105.18	112.23
1	B	316	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	212	ILE	CA-C-N	5.48	127.88	120.65
1	B	212	ILE	C-N-CA	5.48	127.88	120.65
1	B	50	VAL	N-CA-C	5.44	117.01	109.45
1	A	88	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	171	LEU	CA-C-N	5.38	128.88	120.75
1	A	171	LEU	C-N-CA	5.38	128.88	120.75
1	B	298	THR	CA-C-N	5.38	127.49	120.28
1	B	298	THR	C-N-CA	5.38	127.49	120.28
1	A	173	ARG	N-CA-C	5.38	114.67	108.49
1	B	150	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	207	TRP	CA-C-N	5.35	127.98	120.28
1	B	207	TRP	C-N-CA	5.35	127.98	120.28
1	B	58	PRO	N-CA-C	5.32	123.44	112.47
1	B	32	SER	N-CA-C	5.31	117.18	108.52
1	A	185	THR	CA-C-N	5.30	127.91	120.28
1	A	185	THR	C-N-CA	5.30	127.91	120.28
1	B	297	ILE	N-CA-C	5.23	115.75	108.84
1	A	126	HIS	CA-C-N	5.20	127.12	120.56
1	A	126	HIS	C-N-CA	5.20	127.12	120.56
1	B	119	CYS	CA-C-N	5.18	131.03	121.70
1	B	119	CYS	C-N-CA	5.18	131.03	121.70
1	A	274	PHE	CA-C-N	5.13	128.05	120.91
1	A	274	PHE	C-N-CA	5.13	128.05	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ALA	CA-C-N	5.13	127.67	120.28
1	A	255	ALA	C-N-CA	5.13	127.67	120.28
1	B	74	LEU	CA-C-N	5.13	127.16	120.28
1	B	74	LEU	C-N-CA	5.13	127.16	120.28
1	A	278	ASN	CA-CB-CG	5.02	117.62	112.60

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	2741	0	2747	53	0
1	B	2741	0	2747	47	0
2	A	30	0	26	6	0
2	B	30	0	26	4	0
3	A	58	0	0	2	0
3	B	67	0	0	3	0
All	All	5667	0	5546	99	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 9.

All (99) 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:71:GLU:HG3	2:A:361:38P:H29	1.54	0.87
1:B:75:LEU:HB3	1:B:86:LEU:HB2	1.61	0.82
1:B:213:MET:SD	1:B:288:MET:HE1	2.19	0.81
1:A:22:GLU:HG2	3:A:380:HOH:O	1.86	0.75
1:B:203:THR:HB	1:B:296:ARG:HD2	1.74	0.70
1:A:84:ILE:HG13	1:A:167:LEU:HD23	1.74	0.69
1:B:82:ASN:OD1	1:B:136:ARG:NH1	2.27	0.67
1:A:111:ALA:HA	2:A:361:38P:H14A	1.76	0.67
1:B:67:ARG:HB2	3:B:416:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HB2	2:A:361:38P:H30B	1.82	0.60
1:A:131:ILE:HG13	1:A:213:MET:HG3	1.83	0.60
1:A:213:MET:SD	1:A:288:MET:HE1	2.42	0.59
1:B:55:LEU:HD12	1:B:102:VAL:HB	1.85	0.59
1:A:57:ARG:HB3	1:A:60:GLN:HB2	1.84	0.59
1:A:76:LYS:HE3	1:A:348:PHE:HB2	1.84	0.59
1:A:153:PRO:HD3	1:A:212:ILE:HG12	1.84	0.58
1:A:319:VAL:HG23	1:B:237:ARG:HH12	1.67	0.58
1:A:109:MET:HG3	1:A:157:ALA:HB1	1.85	0.57
1:B:38:VAL:HG22	1:B:53:LYS:HG3	1.86	0.57
1:A:221:THR:HB	1:A:224:PRO:HG3	1.87	0.57
1:B:113:LEU:HD21	1:B:216:LEU:HD21	1.87	0.56
1:B:146:ILE:HD11	1:B:323:TYR:CD2	2.42	0.55
1:A:64:HIS:HA	1:A:67:ARG:HG2	1.89	0.54
1:A:63:ILE:HG22	1:A:67:ARG:HD3	1.90	0.53
1:B:80:HIS:HB3	1:B:83:VAL:HB	1.90	0.53
1:A:187:TRP:HD1	1:A:231:GLN:NE2	2.07	0.53
1:A:147:ILE:HG12	1:A:202:GLN:HA	1.91	0.53
1:A:72:LEU:HD13	1:A:89:VAL:HG21	1.90	0.52
1:B:75:LEU:HD13	1:B:86:LEU:HD23	1.91	0.52
1:A:169:PHE:O	2:A:361:38P:H28	2.08	0.52
1:A:134:ILE:HG12	1:A:156:LEU:HD22	1.92	0.51
1:A:148:HIS:CD2	1:A:169:PHE:HB3	2.45	0.51
1:A:187:TRP:CD1	1:A:231:GLN:HE22	2.29	0.51
1:B:73:ARG:NH2	1:B:324:ASP:O	2.44	0.51
1:B:169:PHE:O	2:B:361:38P:H28	2.12	0.50
1:B:190:ALA:HA	1:B:207:TRP:CD1	2.46	0.50
1:A:52:VAL:HG13	1:A:105:VAL:HG22	1.93	0.50
1:B:13:LEU:HD22	1:B:29:PRO:HD3	1.94	0.50
1:B:244:ALA:HA	1:B:247:LEU:HD12	1.92	0.50
1:B:106:THR:HG21	2:B:361:38P:HN17	1.75	0.50
1:B:316:ASP:C	1:B:318:PRO:HD3	2.37	0.50
1:A:10:ARG:HG3	1:A:19:GLU:HG2	1.95	0.49
1:B:310:GLN:HB3	3:B:426:HOH:O	2.12	0.48
1:B:207:TRP:HB2	1:B:296:ARG:NH1	2.28	0.48
1:A:255:ALA:HA	1:A:258:TYR:HB3	1.95	0.48
1:B:72:LEU:HD11	1:B:89:VAL:HG11	1.95	0.48
1:A:53:LYS:HE3	2:A:361:38P:C20	2.43	0.47
1:A:160:GLU:H	1:A:160:GLU:CD	2.19	0.47
1:B:86:LEU:HD12	1:B:348:PHE:CE1	2.49	0.47
1:B:160:GLU:C	1:B:162:CYS:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:HA	1:A:164:LEU:O	2.15	0.47
1:A:236:LEU:C	1:A:238:LEU:H	2.21	0.47
1:A:69:TYR:CE1	1:A:340:LEU:HB3	2.49	0.47
1:B:51:ALA:HB3	1:B:106:THR:HG22	1.96	0.47
1:B:149:ARG:HD2	1:B:173:ARG:HA	1.97	0.47
1:B:78:MET:HE2	1:B:146:ILE:HD13	1.96	0.46
1:B:148:HIS:HA	1:B:170:GLY:H	1.79	0.46
1:A:284:LEU:HG	1:A:288:MET:HE2	1.97	0.46
1:B:33:GLY:HA3	2:B:361:38P:H3	1.97	0.46
1:A:112:ASP:OD1	1:A:114:ASN:HB3	2.15	0.46
1:B:250:ILE:HB	1:B:256:ARG:HD3	1.97	0.45
1:B:309:ALA:HA	3:B:382:HOH:O	2.17	0.45
1:B:290:VAL:HG12	1:B:292:ASP:H	1.82	0.45
1:A:71:GLU:HG2	1:A:75:LEU:HD11	1.99	0.45
1:B:78:MET:HE3	1:B:141:ILE:HG13	1.99	0.45
1:A:186:ARG:HD3	1:A:186:ARG:H	1.81	0.45
1:A:329:SER:HB3	3:A:375:HOH:O	2.17	0.45
1:B:9:TYR:OH	1:B:27:LEU:HD23	2.17	0.44
1:A:205:ASP:O	1:A:209:VAL:HG23	2.17	0.44
1:A:208:SER:O	1:A:212:ILE:HG13	2.18	0.44
1:A:122:LEU:HD13	1:A:216:LEU:HD22	1.99	0.43
1:A:187:TRP:HD1	1:A:231:GLN:HE22	1.66	0.43
1:B:65:ALA:O	1:B:337:TRP:HB3	2.19	0.43
1:B:258:TYR:CZ	1:B:262:LEU:HD11	2.52	0.43
1:B:75:LEU:HD11	2:B:361:38P:H21	2.01	0.43
1:A:38:VAL:HG22	1:A:53:LYS:HG3	2.01	0.43
1:A:275:ILE:H	1:A:275:ILE:HG13	1.46	0.43
1:A:59:PHE:O	1:A:334:ILE:HG21	2.19	0.42
1:B:21:PRO:HD2	1:B:24:TYR:HD2	1.84	0.42
1:B:131:ILE:HG13	1:B:213:MET:HG3	2.00	0.42
1:A:153:PRO:HA	1:A:156:LEU:HD12	2.02	0.42
1:A:233:LYS:HE2	1:A:237:ARG:HH21	1.85	0.42
1:A:74:LEU:O	1:A:78:MET:HG2	2.19	0.42
1:A:188:TYR:CD2	1:A:188:TYR:N	2.87	0.42
1:A:67:ARG:HA	1:A:70:ARG:HH11	1.85	0.42
1:B:191:PRO:HD3	1:B:207:TRP:CE2	2.55	0.42
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.88	0.42
1:B:341:THR:O	1:B:345:VAL:HG23	2.20	0.42
1:B:23:ARG:HA	1:B:44:THR:OG1	2.20	0.41
1:B:156:LEU:HD11	1:B:212:ILE:HD13	2.02	0.41
1:B:46:THR:OG1	1:B:48:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD11	1:B:130:LEU:HD13	2.01	0.41
1:A:242:PRO:HB3	1:A:246:LEU:HD23	2.02	0.41
1:A:169:PHE:N	2:A:361:38P:H28	2.35	0.41
1:A:26:ASN:O	1:A:41:ALA:HA	2.21	0.41
1:A:207:TRP:HZ2	1:A:235:ILE:HG12	1.86	0.41
1:B:35:TYR:CE2	1:B:171:LEU:HD13	2.56	0.41
1:A:233:LYS:O	1:A:237:ARG:HB2	2.21	0.40
1:A:77:HIS:NE2	1:A:321:ASP:O	2.50	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	335/366 (92%)	283 (84%)	42 (12%)	10 (3%)	3	12
1	B	335/366 (92%)	288 (86%)	39 (12%)	8 (2%)	4	17
All	All	670/732 (92%)	571 (85%)	81 (12%)	18 (3%)	4	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	99	PHE
1	A	252	SER
1	A	306	ALA
1	B	261	SER
1	B	322	PRO
1	A	200	TYR
1	A	237	ARG
1	B	173	ARG
1	B	352	PRO

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Mol	Chain	Res	Type
1	A	35	TYR
1	A	120	GLN
1	B	200	TYR
1	B	35	TYR
1	B	196	ASN
1	A	350	PRO
1	B	313	ASP
1	A	240	GLY

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	301/325 (93%)	259 (86%)	42 (14%)	3	12
1	B	301/325 (93%)	258 (86%)	43 (14%)	3	11
All	All	602/650 (93%)	517 (86%)	85 (14%)	3	12

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	14	ASN
1	A	30	VAL
1	A	37	SER
1	A	39	CYS
1	A	46	THR
1	A	48	LEU
1	A	62	ILE
1	A	70	ARG
1	A	75	LEU
1	A	78	MET
1	A	79	LYS
1	A	81	GLU
1	A	84	ILE
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	104	LEU
1	A	105	VAL
1	A	119	CYS
1	A	120	GLN
1	A	123	THR
1	A	124	ASP
1	A	158	VAL
1	A	160	GLU
1	A	161	ASP
1	A	164	LEU
1	A	186	ARG
1	A	193	ILE
1	A	195	LEU
1	A	200	TYR
1	A	235	ILE
1	A	236	LEU
1	A	238	LEU
1	A	253	GLU
1	A	263	THR
1	A	265	MET
1	A	275	ILE
1	A	278	ASN
1	A	291	LEU
1	A	292	ASP
1	A	293	SER
1	A	333	LEU
1	A	336	GLU
1	B	12	GLU
1	B	19	GLU
1	B	35	TYR
1	B	37	SER
1	B	39	CYS
1	B	48	LEU
1	B	56	SER
1	B	61	SER
1	B	62	ILE
1	B	63	ILE
1	B	73	ARG
1	B	81	GLU
1	B	84	ILE
1	B	86	LEU
1	B	89	VAL

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Mol	Chain	Res	Type
1	B	101	ASP
1	B	106	THR
1	B	113	LEU
1	B	116	ILE
1	B	120	GLN
1	B	128	GLN
1	B	141	ILE
1	B	152	LYS
1	B	158	VAL
1	B	160	GLU
1	B	161	ASP
1	B	162	CYS
1	B	185	THR
1	B	186	ARG
1	B	189	ARG
1	B	197	TRP
1	B	200	TYR
1	B	228	HIS
1	B	251	SER
1	B	257	ASN
1	B	259	ILE
1	B	275	ILE
1	B	285	LEU
1	B	329	SER
1	B	332	LEU
1	B	333	LEU
1	B	335	ASP
1	B	336	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	257	ASN
1	A	264	GLN
1	A	305	HIS
1	A	325	GLN
1	B	26	ASN
1	B	128	GLN
1	B	196	ASN
1	B	231	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	38P	B	361	-	32,33,33	2.08	9 (28%)	38,47,47	3.46	8 (21%)
2	38P	A	361	-	32,33,33	2.09	8 (25%)	38,47,47	3.48	8 (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	38P	B	361	-	-	6/20/22/22	0/4/4/4
2	38P	A	361	-	-	5/20/22/22	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	38P	C6-N1	5.91	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	361	38P	C6-N1	5.84	1.46	1.38
2	A	361	38P	C9-N1	5.51	1.45	1.36
2	B	361	38P	C9-N1	5.42	1.45	1.36
2	B	361	38P	C6-C7	-2.98	1.34	1.43
2	A	361	38P	C6-C7	-2.92	1.35	1.43
2	A	361	38P	C8-C7	2.77	1.50	1.41
2	B	361	38P	C8-C7	2.69	1.50	1.41
2	B	361	38P	C21-C20	2.61	1.43	1.38
2	A	361	38P	C21-C20	2.48	1.42	1.38
2	A	361	38P	C21-C22	2.46	1.43	1.39
2	B	361	38P	C6-C5	2.43	1.50	1.43
2	A	361	38P	C6-C5	2.43	1.50	1.43
2	B	361	38P	C23-C18	2.37	1.43	1.39
2	B	361	38P	C21-C22	2.29	1.42	1.39
2	A	361	38P	C23-C18	2.23	1.43	1.39
2	B	361	38P	C18-N17	-2.05	1.37	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	38P	C28-C27-N26	-19.62	92.78	118.52
2	B	361	38P	C28-C27-N26	-19.54	92.88	118.52
2	A	361	38P	C9-C8-C7	3.30	109.75	107.47
2	B	361	38P	C9-C8-C7	3.18	109.66	107.47
2	A	361	38P	C29-C28-C27	-2.76	57.40	59.80
2	B	361	38P	C29-C28-C27	-2.76	57.40	59.80
2	B	361	38P	C28-C29-C27	2.67	62.12	59.80
2	A	361	38P	C28-C29-C27	2.62	62.08	59.80
2	B	361	38P	C27-N26-C24	-2.41	118.00	122.56
2	A	361	38P	C3-N2-N1	2.34	121.25	113.72
2	B	361	38P	C3-N2-N1	2.32	121.18	113.72
2	A	361	38P	C27-N26-C24	-2.31	118.18	122.56
2	A	361	38P	C18-N17-C5	-2.28	121.40	128.45
2	B	361	38P	C18-N17-C5	-2.26	121.48	128.45
2	A	361	38P	N17-C5-N4	-2.22	116.19	121.73
2	B	361	38P	N17-C5-N4	-2.13	116.41	121.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	361	38P	C22-C24-N26-C27

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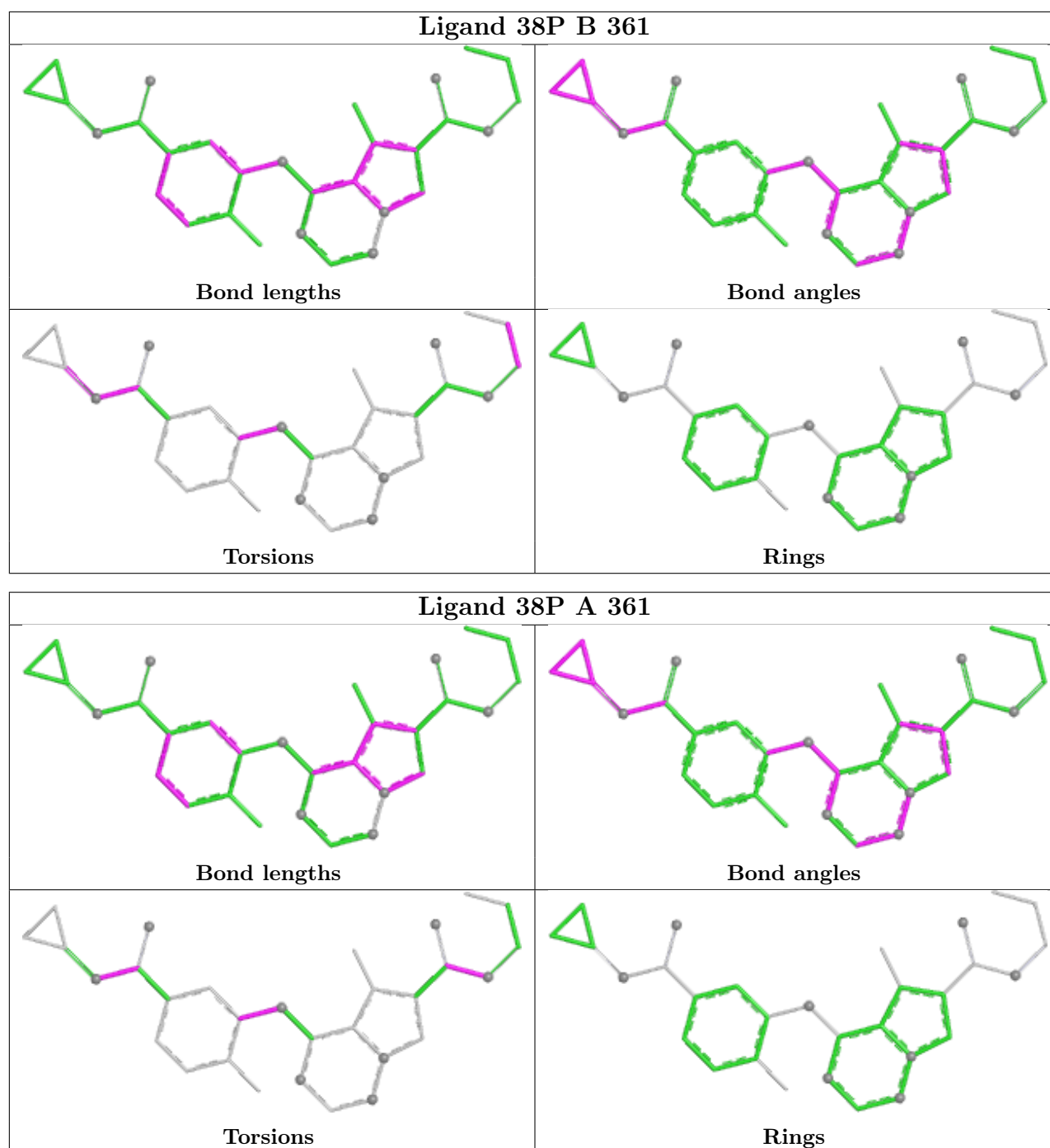
Mol	Chain	Res	Type	Atoms
2	A	361	38P	O11-C10-N12-C13
2	A	361	38P	O25-C24-N26-C27
2	A	361	38P	C8-C10-N12-C13
2	B	361	38P	C23-C18-N17-C5
2	B	361	38P	C22-C24-N26-C27
2	B	361	38P	C28-C27-N26-C24
2	B	361	38P	O25-C24-N26-C27
2	B	361	38P	C19-C18-N17-C5
2	B	361	38P	N12-C13-C14-C15
2	A	361	38P	C23-C18-N17-C5

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	361	38P	4	0
2	A	361	38P	6	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	339/366 (92%)	-1.44	0 100 100	4, 24, 61, 95	0
1	B	339/366 (92%)	-1.35	0 100 100	5, 28, 76, 97	0
All	All	678/732 (92%)	-1.40	0 100 100	4, 26, 67, 97	0

There are no RSRZ outliers to report.

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](#)

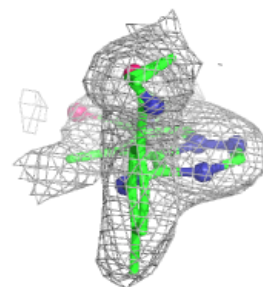
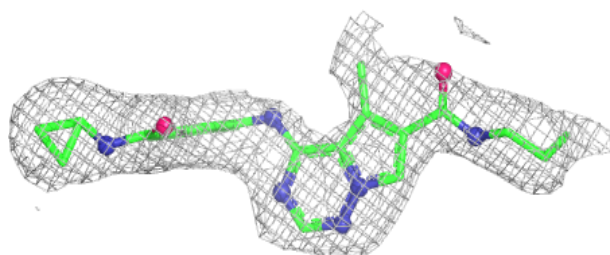
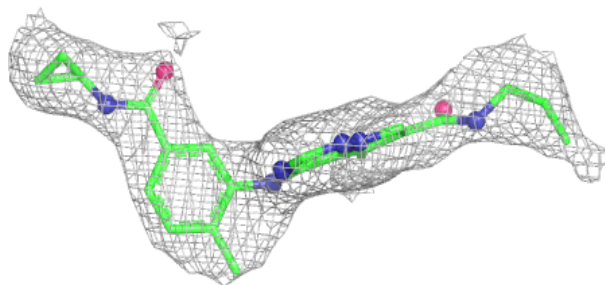
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	38P	A	361	30/30	0.99	0.03	3,19,23,29	0
2	38P	B	361	30/30	0.99	0.03	4,23,30,31	0

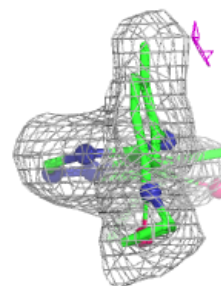
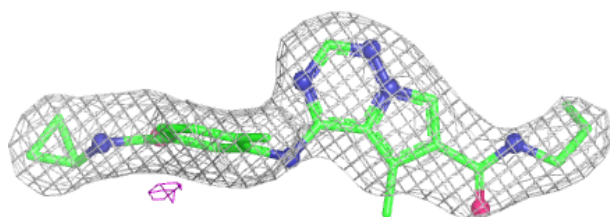
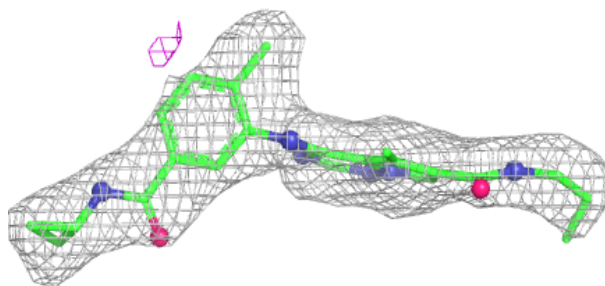
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 38P A 361:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 38P B 361:**

$2mF_o-DF_c$ (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.