Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2025 – 10:14 AM EDT

PDB ID	:	9D4V
Title	:	Structure of PAK1 in complex with compound 7
Authors	:	Dementiev, A.; Boone, C.D.; Suto, R.K.; Olland, A.M.
Deposited on	:	2024-08-13
Resolution	:	1.84 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 (i) 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 (i)) were used in the production of this report:

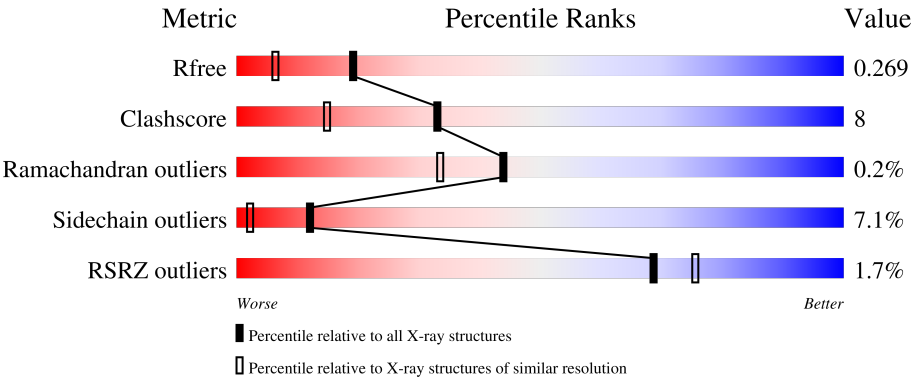
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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

Mol	Chain	Length	Quality of chain
1	A	297	2% 74% 21%
1	B	297	% 77% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4541 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.

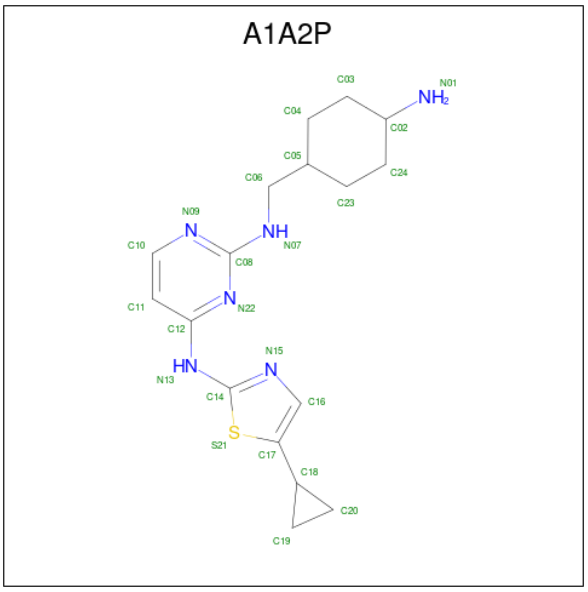
- Molecule 1 is a protein called Serine/threonine-protein kinase PAK 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	1	0
			2247	1428	375	427	17			
1	B	285	Total	C	N	O	S	0	3	0
			2170	1375	366	412	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	ASN	ASP	engineered mutation	UNP Q13153
A	423	GLU	THR	engineered mutation	UNP Q13153
B	389	ASN	ASP	engineered mutation	UNP Q13153
B	423	GLU	THR	engineered mutation	UNP Q13153

- Molecule 2 is N 2 -{[(1s,4s)-4-aminocyclohexyl]methyl}-N 4 -(5-cyclopropyl-1,3-thiazol-2-yl)pyrimidine-2,4-diamine (three-letter code: A1A2P) (formula: $C_{17}H_{24}N_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			24	17	6	1		
2	B	1	Total	C	N	S	0	0
			24	17	6	1		

- Molecule 3 is water.

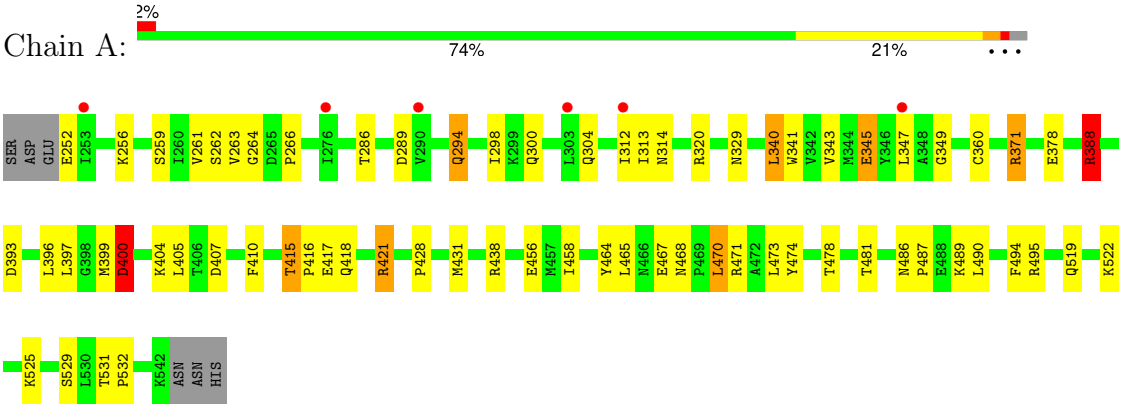
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	31	Total	O	0	0
			31	31		

3 Residue-property plots (i)

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

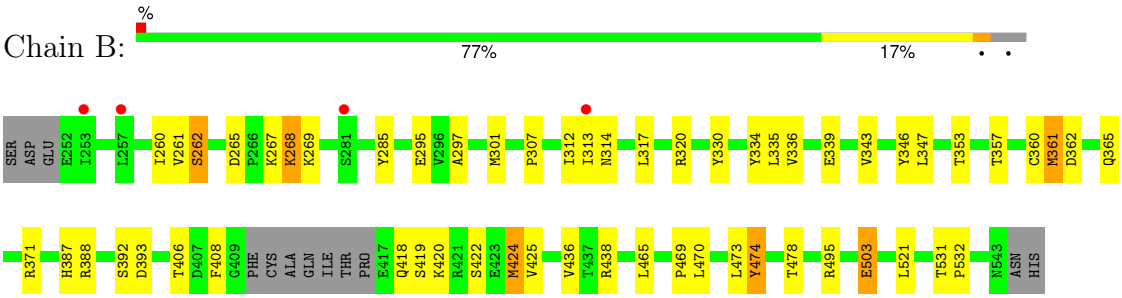
• Molecule 1: Serine/threonine-protein kinase PAK 1

Chain A:



• Molecule 1: Serine/threonine-protein kinase PAK 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.73Å 80.82Å 65.86Å 90.00° 107.27° 90.00°	Depositor
Resolution (Å)	49.63 – 1.84 49.63 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.63-1.84) 99.0 (49.63-1.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.197 , 0.269 0.203 , 0.269	Depositor DCC
R_{free} test set	3893 reflections (7.13%)	wwPDB-VP
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4541	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1A2P

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	0.88	2/2288 (0.1%)	1.31	12/3102 (0.4%)
1	B	0.89	4/2213 (0.2%)	1.23	6/3000 (0.2%)
All	All	0.88	6/4501 (0.1%)	1.27	18/6102 (0.3%)

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	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	GLU	CD-OE1	13.72	1.40	1.25
1	B	393	ASP	CG-OD1	7.29	1.42	1.25
1	A	456	GLU	CD-OE2	-6.94	1.18	1.25
1	B	392	SER	CA-CB	-5.71	1.44	1.52
1	A	388	ARG	CD-NE	-5.22	1.37	1.46
1	B	503	GLU	CD-OE1	5.09	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	ARG	NE-CZ-NH2	-12.91	113.85	120.30
1	B	371	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	A	388	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	B	371	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	B	393	ASP	CB-CG-OD2	-8.26	110.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	464	TYR	CB-CA-C	-6.98	96.44	110.40
1	A	481	THR	CA-CB-OG1	-6.51	95.33	109.00
1	A	371	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	406	THR	CA-CB-OG1	-6.17	96.05	109.00
1	A	431	MET	CG-SD-CE	-6.11	90.42	100.20
1	A	421	ARG	CB-CG-CD	-5.93	96.18	111.60
1	B	474	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	B	269	LYS	CB-CA-C	5.35	121.11	110.40
1	A	438	ARG	CD-NE-CZ	5.13	130.79	123.60
1	A	400	ASP	CB-CA-C	-5.11	100.18	110.40
1	A	314	ASN	CB-CA-C	5.09	120.58	110.40
1	A	388	ARG	CD-NE-CZ	5.06	130.68	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	A	371	ARG	Sidechain
1	A	388	ARG	Sidechain
1	A	471	ARG	Sidechain

5.2 Too-close contacts (i)

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	2247	0	2258	33	0
1	B	2170	0	2139	35	0
2	A	24	0	0	4	0
2	B	24	0	0	2	0
3	A	45	0	0	1	0
3	B	31	0	0	1	0
All	All	4541	0	4397	68	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 8.

All (68) 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:B:336:VAL:HG12	1:B:336:VAL:O	1.88	0.73
1:A:286:THR:HG23	3:A:707:HOH:O	1.90	0.71
1:B:353:THR:O	1:B:357:THR:HG23	1.91	0.70
1:B:313:ILE:O	1:B:317:LEU:HD12	1.91	0.69
1:B:474:TYR:O	1:B:478:THR:HG23	1.94	0.68
1:A:388:ARG:HD3	1:A:410:PHE:O	1.94	0.67
1:A:417:GLU:OE1	1:A:418:GLN:HG2	1.95	0.67
1:A:525:LYS:HB3	1:A:529:SER:OG	1.93	0.67
1:B:387:HIS:O	1:B:388:ARG:HB2	1.95	0.66
1:B:424:MET:CE	1:B:470:LEU:HD23	2.26	0.65
1:B:301:MET:O	1:B:339:GLU:HA	1.97	0.64
1:B:261:VAL:HG12	1:B:262:SER:O	2.00	0.61
1:B:474:TYR:CE1	1:B:478:THR:HG21	2.38	0.59
1:B:347:LEU:O	2:B:601:A1A2P:N13	2.37	0.58
1:B:260:ILE:HD12	1:B:320:ARG:HD2	1.86	0.57
1:A:487:PRO:HB2	1:A:495:ARG:CZ	2.36	0.55
1:B:424:MET:HE2	1:B:470:LEU:HD23	1.89	0.54
1:A:349:GLY:HA3	1:A:397:LEU:O	2.07	0.53
1:A:465:LEU:HG	1:A:465:LEU:O	2.09	0.52
1:A:256:LYS:HD3	1:A:313:ILE:HD13	1.93	0.51
1:B:474:TYR:CZ	1:B:478:THR:HG21	2.46	0.51
1:B:362:ASP:HB2	3:B:716:HOH:O	2.11	0.50
1:A:415:THR:OG1	1:A:416:PRO:HD2	2.11	0.50
1:B:260:ILE:CD1	1:B:320:ARG:HD2	2.40	0.50
1:B:261:VAL:HG13	1:B:334:TYR:HA	1.94	0.49
1:A:458:ILE:HD11	1:A:494:PHE:CZ	2.47	0.49
1:A:400:ASP:N	1:A:400:ASP:OD1	2.44	0.49
1:A:470:LEU:HD12	1:A:473:LEU:HD12	1.94	0.49
2:A:601:A1A2P:N22	2:A:601:A1A2P:S21	2.86	0.47
1:A:531:THR:N	1:A:532:PRO:CD	2.77	0.47
1:A:347:LEU:O	2:A:601:A1A2P:N13	2.47	0.47
1:B:261:VAL:HG11	1:B:335:LEU:H	1.78	0.47
1:B:424:MET:HE1	1:B:473:LEU:HG	1.97	0.47
1:B:336:VAL:O	1:B:336:VAL:CG1	2.57	0.46
1:B:265:ASP:HB3	1:B:268:LYS:HD3	1.98	0.46
1:A:264:GLY:O	1:A:266:PRO:HD3	2.16	0.46
1:A:519:GLN:O	1:A:522:LYS:HB2	2.16	0.45
1:A:298:ILE:HG12	1:A:343:VAL:HG22	1.98	0.45
1:A:458:ILE:HD13	1:A:490:LEU:HD11	1.98	0.45
1:B:469:PRO:O	1:B:473:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HG13	1:A:262:SER:O	2.16	0.44
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.77	0.44
1:A:396:LEU:HD21	2:A:601:A1A2P:S21	2.57	0.44
1:A:396:LEU:HD11	2:A:601:A1A2P:C03	2.47	0.44
1:A:474:TYR:CZ	1:A:478:THR:HG21	2.52	0.44
1:A:415:THR:HG23	1:A:418:GLN:H	1.83	0.44
1:A:467:GLU:O	1:B:420:LYS:HE2	2.18	0.43
1:A:312:ILE:CG2	1:A:340:LEU:HD22	2.49	0.43
1:B:418:GLN:O	1:B:418:GLN:HG3	2.17	0.43
1:B:436:VAL:C	1:B:438:ARG:H	2.22	0.43
1:B:314:ASN:O	1:B:317:LEU:HB2	2.19	0.43
1:A:300:GLN:HG2	1:A:341:TRP:CD1	2.54	0.43
1:B:531:THR:N	1:B:532:PRO:CD	2.81	0.42
1:A:486:ASN:HB3	1:A:489:LYS:HG3	2.01	0.42
1:B:346:TYR:HA	2:B:601:A1A2P:C16	2.49	0.42
1:B:436:VAL:O	1:B:438:ARG:N	2.53	0.42
1:A:329:ASN:HB3	1:A:345:GLU:HB3	2.02	0.42
1:B:285:TYR:O	1:B:297:ALA:HA	2.20	0.42
1:B:465:LEU:HD23	1:B:465:LEU:HA	1.78	0.42
1:A:347:LEU:HD22	1:A:404:LYS:HD2	2.02	0.41
1:A:421:ARG:HD3	1:A:421:ARG:HA	1.60	0.41
1:B:261:VAL:CG1	1:B:262:SER:N	2.84	0.41
1:B:265:ASP:OD1	1:B:267:LYS:HB2	2.21	0.41
1:B:261:VAL:HG11	1:B:335:LEU:N	2.37	0.40
1:B:361[A]:MET:HG2	1:B:365:GLN:HB2	2.02	0.40
1:A:289:ASP:OD2	1:A:294:GLN:NE2	2.49	0.40
1:A:519:GLN:HA	1:A:522:LYS:HD3	2.03	0.40
1:A:487:PRO:HB2	1:A:495:ARG:NH2	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	290/297 (98%)	273 (94%)	17 (6%)	0	100 100
1	B	284/297 (96%)	257 (90%)	26 (9%)	1 (0%)	30 18
All	All	574/594 (97%)	530 (92%)	43 (8%)	1 (0%)	44 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	244/258 (95%)	225 (92%)	19 (8%)	10 2
1	B	228/258 (88%)	210 (92%)	18 (8%)	10 2
All	All	472/516 (92%)	435 (92%)	37 (8%)	12 2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	GLU
1	A	259	SER
1	A	263	VAL
1	A	294	GLN
1	A	304	GLN
1	A	340	LEU
1	A	345	GLU
1	A	360[A]	CYS
1	A	360[B]	CYS
1	A	378	GLU
1	A	393	ASP
1	A	399	MET
1	A	400	ASP
1	A	405	LEU
1	A	407	ASP

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Mol	Chain	Res	Type
1	A	415	THR
1	A	428	PRO
1	A	468	ASN
1	A	470	LEU
1	B	262	SER
1	B	268	LYS
1	B	312	ILE
1	B	330	TYR
1	B	343	VAL
1	B	360[A]	CYS
1	B	360[B]	CYS
1	B	361[A]	MET
1	B	361[B]	MET
1	B	408	PHE
1	B	419	SER
1	B	422	SER
1	B	424	MET
1	B	425	VAL
1	B	495[A]	ARG
1	B	495[B]	ARG
1	B	503	GLU
1	B	521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	304	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)

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	A1A2P	A	601	-	25,27,27	2.28	10 (40%)	27,37,37	5.35	14 (51%)
2	A1A2P	B	601	-	25,27,27	3.37	12 (48%)	27,37,37	5.79	15 (55%)

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	A1A2P	A	601	-	-	2/9/25/25	0/4/4/4
2	A1A2P	B	601	-	-	2/9/25/25	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	A1A2P	C08-N07	10.86	1.51	1.34
2	B	601	A1A2P	C14-N13	7.81	1.50	1.36
2	A	601	A1A2P	C08-N07	4.94	1.42	1.34
2	A	601	A1A2P	C14-N13	4.50	1.44	1.36
2	B	601	A1A2P	C12-N13	4.23	1.46	1.38
2	B	601	A1A2P	C17-S21	4.01	1.81	1.74
2	A	601	A1A2P	C16-N15	-3.63	1.30	1.36
2	B	601	A1A2P	C06-C05	3.59	1.58	1.52
2	B	601	A1A2P	C24-C02	3.23	1.60	1.51
2	A	601	A1A2P	C06-C05	3.11	1.57	1.52
2	A	601	A1A2P	C24-C23	2.98	1.60	1.52
2	A	601	A1A2P	C17-S21	-2.96	1.68	1.74
2	B	601	A1A2P	C06-N07	2.85	1.50	1.45
2	B	601	A1A2P	C24-C23	2.37	1.58	1.52
2	B	601	A1A2P	C23-C05	2.34	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1A2P	C08-N09	-2.26	1.31	1.34
2	A	601	A1A2P	C12-N22	-2.26	1.29	1.34
2	B	601	A1A2P	C17-C18	2.25	1.54	1.51
2	A	601	A1A2P	C02-N01	-2.23	1.39	1.46
2	B	601	A1A2P	C03-C02	2.19	1.58	1.51
2	B	601	A1A2P	C04-C05	2.14	1.58	1.52
2	A	601	A1A2P	C23-C05	2.13	1.58	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	A1A2P	C19-C18-C17	20.23	143.42	120.30
2	A	601	A1A2P	C23-C24-C02	-19.70	88.95	111.53
2	B	601	A1A2P	C10-N09-C08	11.02	124.62	115.42
2	A	601	A1A2P	C19-C18-C17	10.87	132.72	120.30
2	B	601	A1A2P	C24-C02-C03	10.19	120.65	110.29
2	B	601	A1A2P	N09-C08-N22	-8.41	118.29	126.42
2	A	601	A1A2P	C16-C17-S21	-7.19	104.85	112.00
2	A	601	A1A2P	C10-N09-C08	6.92	121.20	115.42
2	B	601	A1A2P	C16-C17-S21	-6.91	105.13	112.00
2	B	601	A1A2P	C05-C06-N07	-6.45	102.39	112.83
2	A	601	A1A2P	C17-C16-N15	6.08	120.39	108.79
2	B	601	A1A2P	C11-C10-N09	-5.27	117.51	123.97
2	A	601	A1A2P	C11-C10-N09	-4.58	118.36	123.97
2	A	601	A1A2P	C05-C06-N07	-4.20	106.03	112.83
2	A	601	A1A2P	C04-C03-C02	-4.18	106.74	111.53
2	A	601	A1A2P	N09-C08-N22	-3.91	122.64	126.42
2	A	601	A1A2P	C03-C02-N01	-3.75	100.03	111.17
2	B	601	A1A2P	C04-C05-C23	3.63	118.17	109.29
2	B	601	A1A2P	N07-C08-N09	3.58	122.03	117.21
2	B	601	A1A2P	C06-N07-C08	3.41	129.44	123.94
2	A	601	A1A2P	C24-C02-C03	3.40	113.74	110.29
2	A	601	A1A2P	C24-C23-C05	-3.05	106.60	112.36
2	B	601	A1A2P	C04-C03-C02	2.65	114.57	111.53
2	B	601	A1A2P	C20-C18-C19	2.24	61.63	58.97
2	B	601	A1A2P	C17-C16-N15	2.24	113.06	108.79
2	B	601	A1A2P	C20-C18-C17	-2.23	117.75	120.30
2	A	601	A1A2P	C19-C20-C18	-2.22	58.44	60.51
2	B	601	A1A2P	C03-C02-N01	-2.17	104.71	111.17
2	A	601	A1A2P	N07-C08-N22	2.08	120.75	117.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1A2P	C16-C17-C18-C19
2	A	601	A1A2P	C16-C17-C18-C20
2	B	601	A1A2P	C16-C17-C18-C19
2	B	601	A1A2P	C16-C17-C18-C20

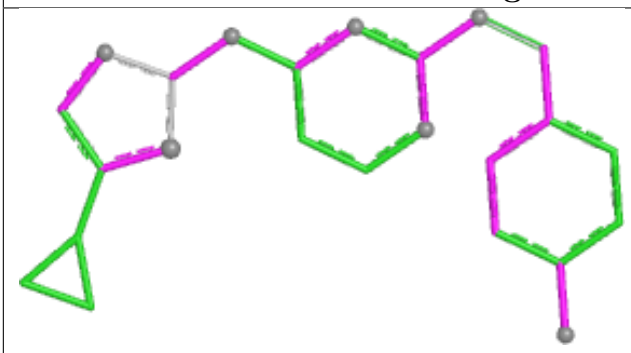
There are no ring outliers.

2 monomers are involved in 6 short contacts:

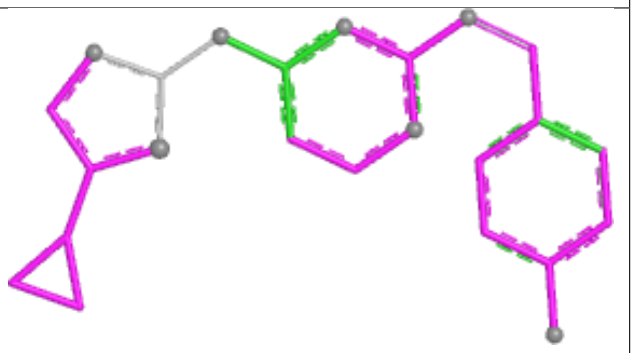
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	A1A2P	4	0
2	B	601	A1A2P	2	0

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

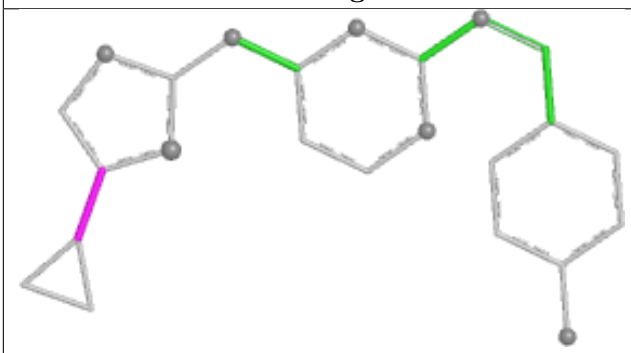
Ligand A1A2P A 601



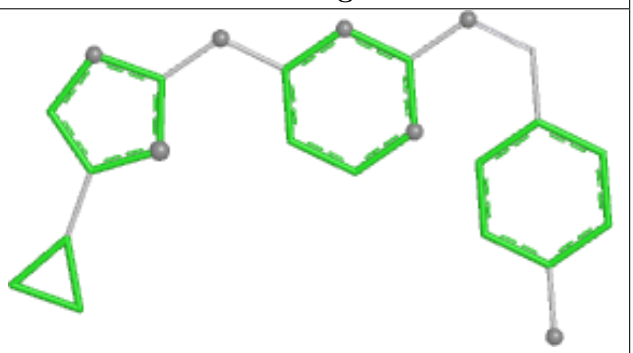
Bond lengths



Bond angles

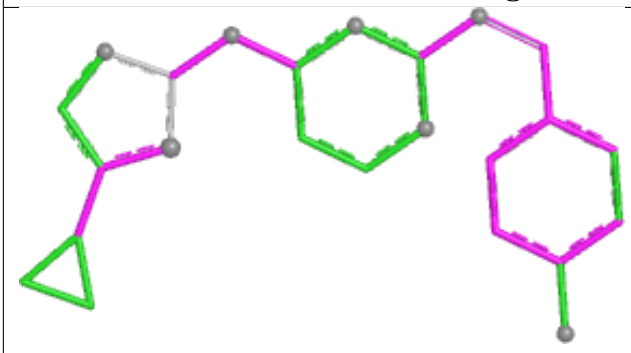


Torsions

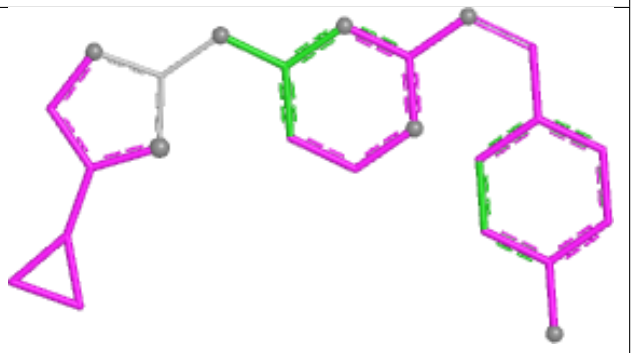


Rings

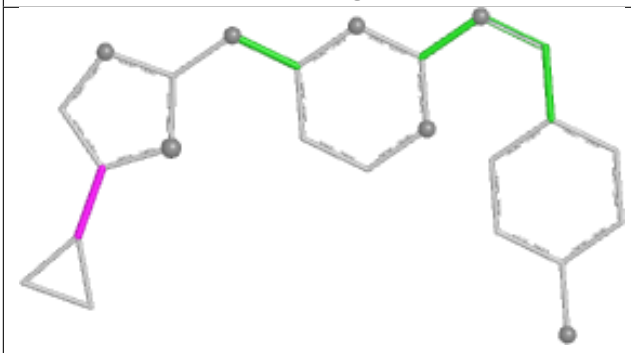
Ligand A1A2P B 601



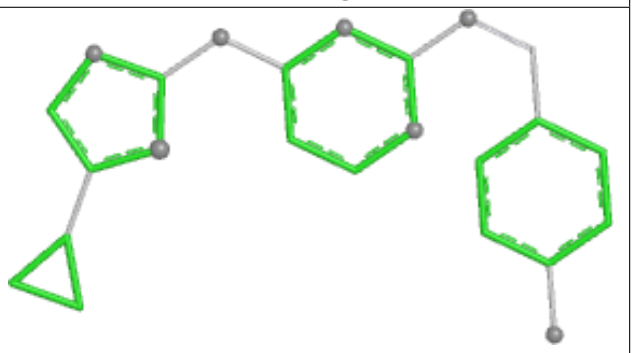
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	291/297 (97%)	0.07	6 (2%)	63	69	40, 64, 105, 132	1 (0%)
1	B	285/297 (95%)	0.16	4 (1%)	73	80	31, 63, 126, 169	3 (1%)
All	All	576/594 (96%)	0.12	10 (1%)	69	75	31, 64, 120, 169	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	LEU	3.0
1	A	253	ILE	2.8
1	B	253	ILE	2.8
1	B	257	LEU	2.4
1	A	312	ILE	2.3
1	A	303	LEU	2.2
1	A	290	VAL	2.2
1	B	313	ILE	2.1
1	B	281	SER	2.0
1	A	276	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

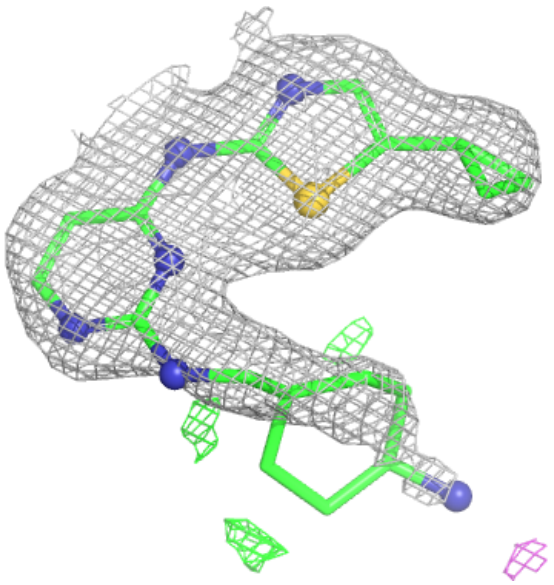
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

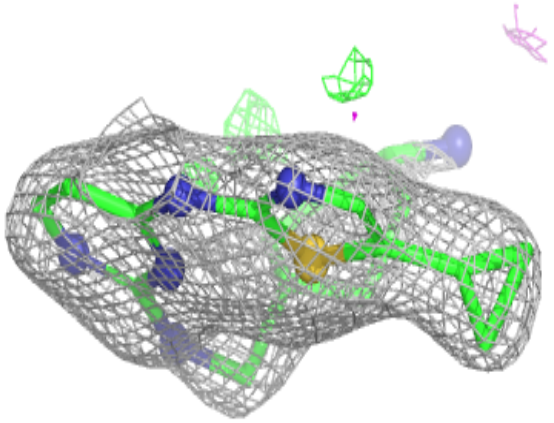
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1A2P	B	601	24/24	0.91	0.11	66,81,115,124	0
2	A1A2P	A	601	24/24	0.95	0.08	55,63,85,89	0

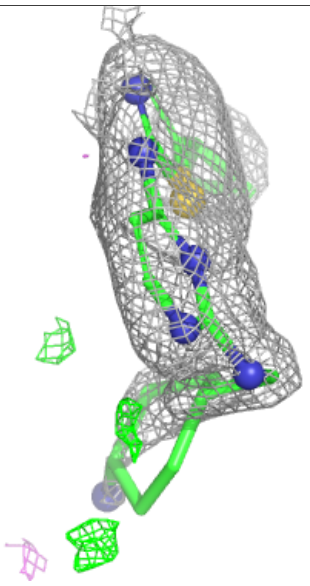
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1A2P B 601:

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

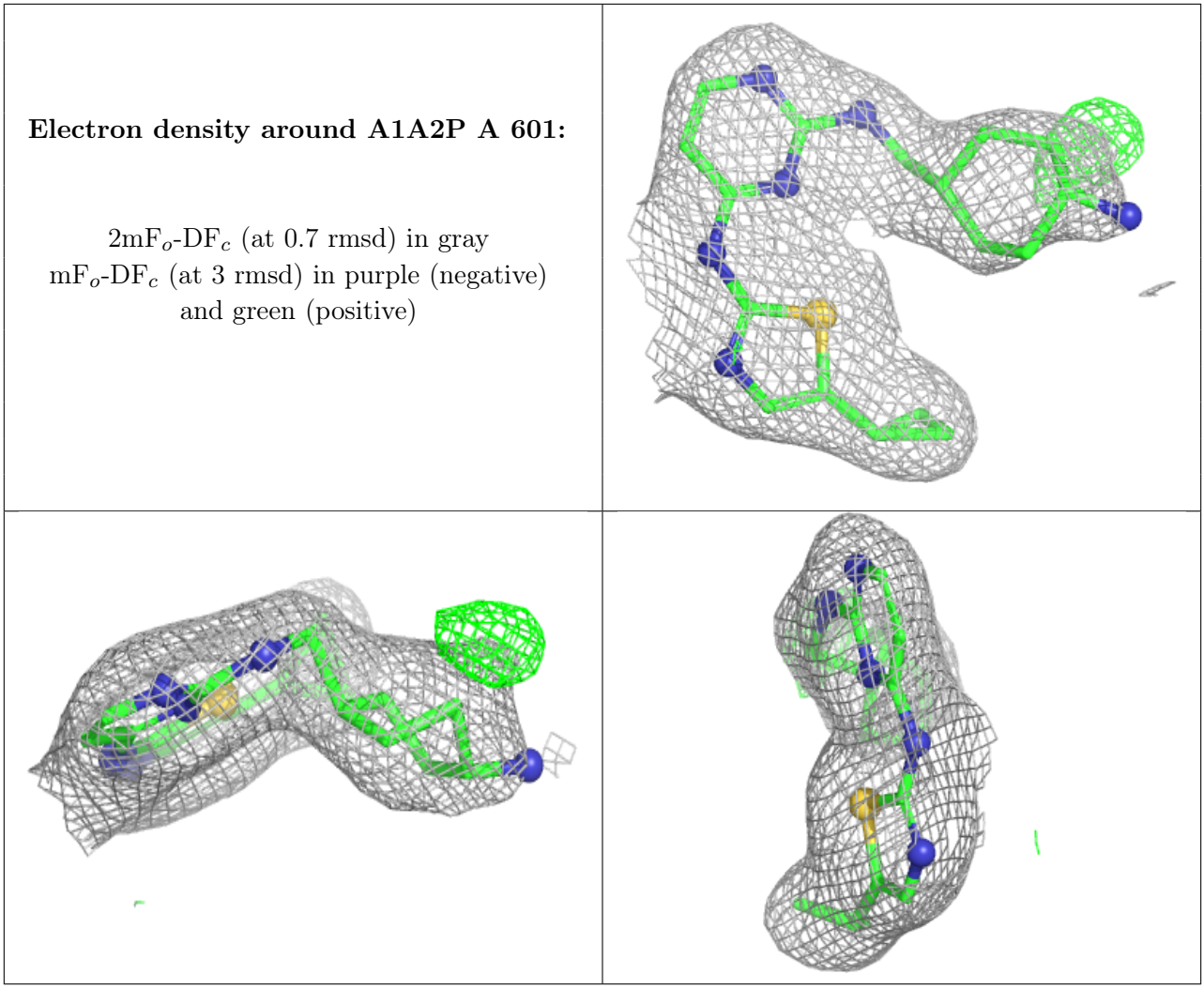






Electron density around A1A2P A 601:

$2mF_o$-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

There are no such residues in this entry.