Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:22 PM BST

PDB ID	:	6TZI
Title	:	ADC-7 in complex with boronic acid transition state inhibitor PFC_001
Authors	:	Fish, E.R.; Powers, R.A.; Wallar, B.J.
Deposited on	:	2019-08-12
Resolution	:	1.74 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:

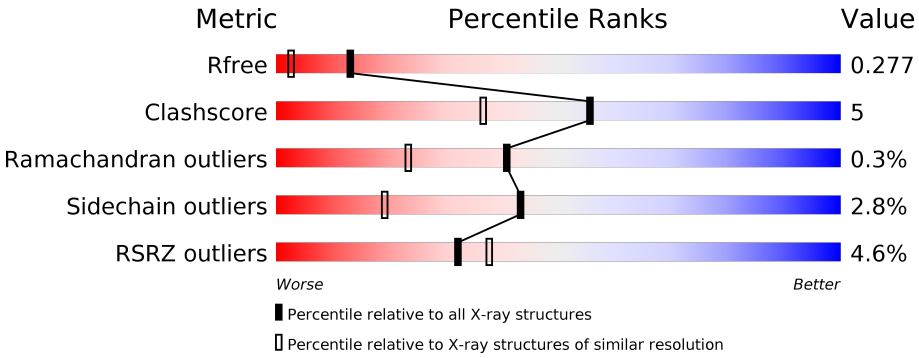
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 <=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	361	2% 86% 12%
1	B	361	91% 8%
1	C	361	10% 86% 12%
1	D	361	6% 82% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12071 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.

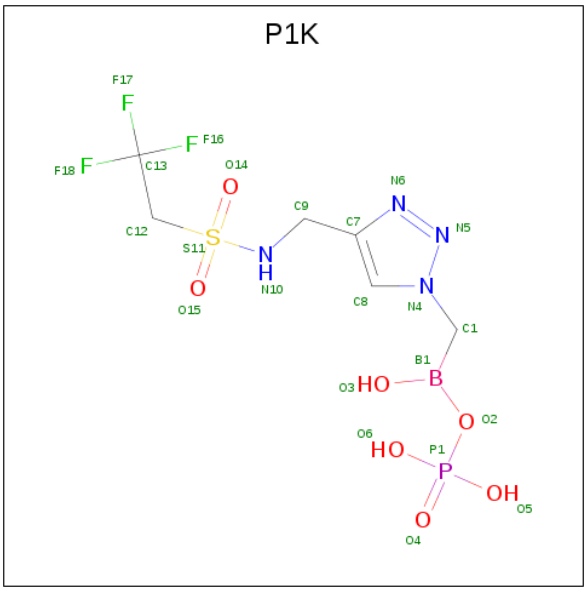
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2753	1773	454	517	9			
1	B	357	Total	C	N	O	S	0	0	0
			2810	1806	466	529	9			
1	C	354	Total	C	N	O	S	0	0	0
			2714	1746	448	511	9			
1	D	357	Total	C	N	O	S	0	0	0
			2784	1789	463	523	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q6DRA1
B	-1	MET	-	expression tag	UNP Q6DRA1
C	-1	MET	-	expression tag	UNP Q6DRA1
D	-1	MET	-	expression tag	UNP Q6DRA1

- Molecule 2 is phosphonooxy-[[4-[[2,2,2-tris(fluoranyl)ethylsulfonylamino]methyl]-1,2,3-triazol-1-yl]methyl]borinic acid (three-letter code: P1K) (formula: $C_6H_{11}BF_3N_4O_7PS$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
2	A	1	Total	B	C	F	N	O	P	S	0	1
			46	2	12	6	8	14	2	2		
2	B	1	Total	B	C	F	N	O	P	S	0	0
			23	1	6	3	4	7	1	1		
2	C	1	Total	B	C	F	N	O	P	S	0	0
			23	1	6	3	4	7	1	1		
2	D	1	Total	B	C	F	N	O	P	S	0	0
			23	1	6	3	4	7	1	1		

- Molecule 3 is water.

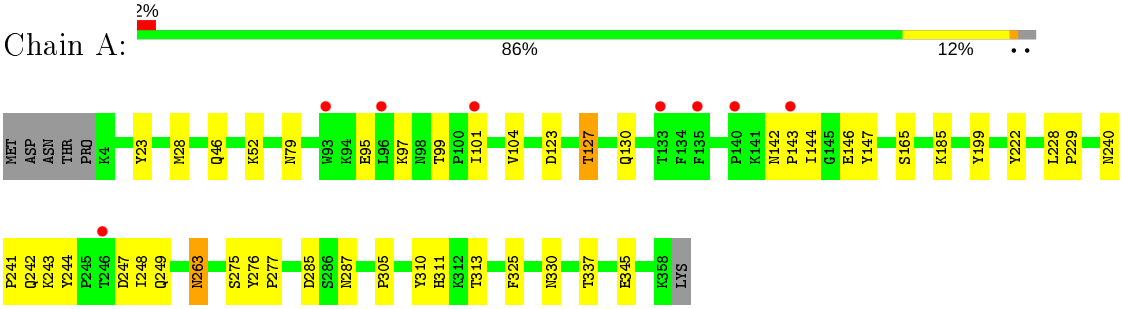
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	3
			217	217		
3	B	353	Total	O	0	9
			362	362		
3	C	124	Total	O	0	5
			129	129		
3	D	180	Total	O	0	7
			187	187		

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.

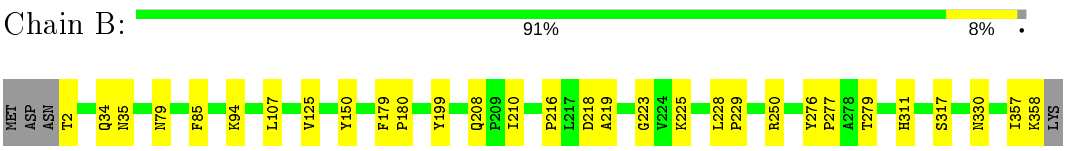
- Molecule 1: Beta-lactamase

Chain A:



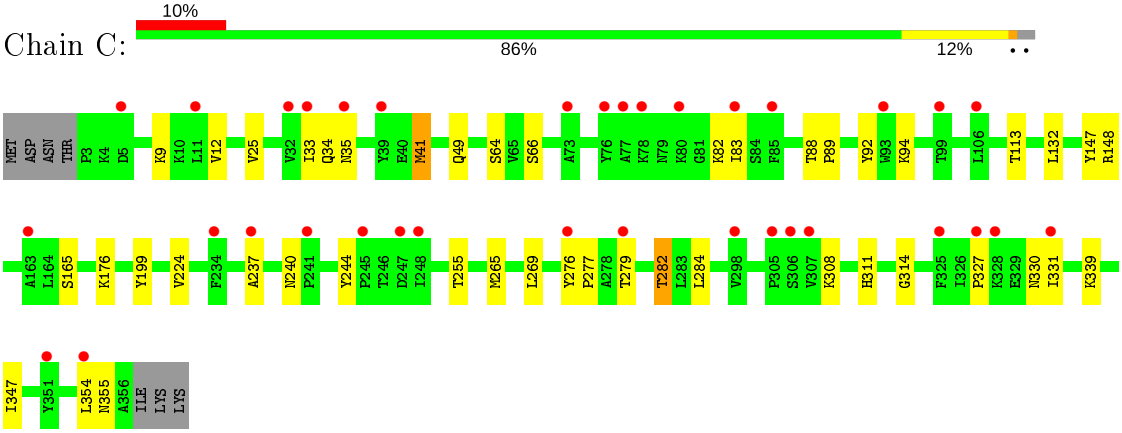
- Molecule 1: Beta-lactamase

Chain B:



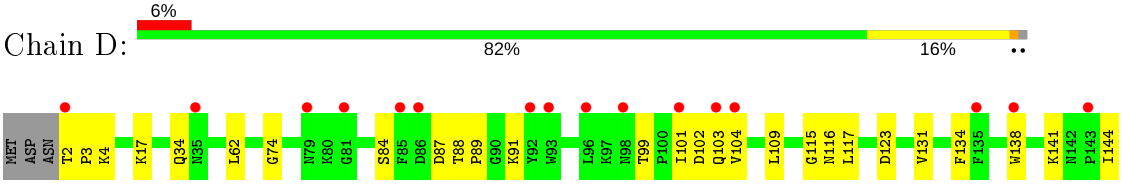
- Molecule 1: Beta-lactamase

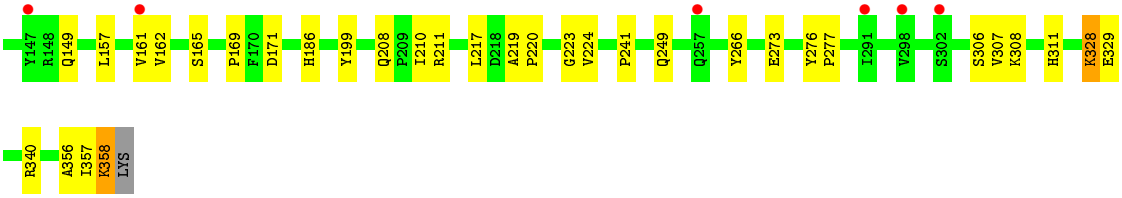
Chain C:



- Molecule 1: Beta-lactamase

Chain D:




Y147
R148
Q149
L157
V161
V162
S165
P169
F170
D171
H186
Y199
Q208
P209
I210
R211
L217
D218
A219
P220
G223
V224
P241
Q249
Q257
Y266
E273
Y276
P277
I291
V298
S302
S306
V307
K308
H311
K328
E329
R340
A356
I357
K358
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.93Å 81.10Å 105.94Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	81.95 – 1.74 81.82 – 1.74	Depositor EDS
% Data completeness (in resolution range)	82.6 (81.95-1.74) 82.6 (81.82-1.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.216 , 0.273 0.220 , 0.277	Depositor DCC
R_{free} test set	5806 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12071	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9562e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: P1K

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	0.39	0/2820	0.77	1/3840 (0.0%)
1	B	0.43	0/2878	0.76	0/3912
1	C	0.32	0/2781	0.66	1/3791 (0.0%)
1	D	0.33	0/2850	0.69	0/3875
All	All	0.37	0/11329	0.72	2/15418 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	355	ASN	CB-CA-C	5.42	121.24	110.40
1	A	79	ASN	CB-CA-C	5.36	121.12	110.40

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	2753	0	2691	25	0
1	B	2810	0	2784	22	0
1	C	2714	0	2614	27	0
1	D	2784	0	2728	37	0
2	A	46	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	0	1	0
2	C	23	0	0	0	0
2	D	23	0	0	1	0
3	A	217	0	0	6	0
3	B	362	0	0	4	0
3	C	129	0	0	4	0
3	D	187	0	0	7	0
All	All	12071	0	10817	111	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 5.

All (111) 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:79:ASN:HB3	1:B:250:ARG:NH2	1.56	1.19
1:C:132:LEU:HA	3:C:529:HOH:O	1.42	1.14
1:A:242:GLN:HA	1:A:249:GLN:NE2	1.84	0.92
1:D:186:HIS:HD2	3:D:599:HOH:O	1.52	0.92
1:D:307:VAL:HG11	1:D:328:LYS:HD3	1.61	0.81
1:B:2:THR:HG23	3:B:532:HOH:O	1.81	0.80
1:D:17:LYS:HE3	3:D:657:HOH:O	1.84	0.76
1:D:356:ALA:HB2	3:D:615[B]:HOH:O	1.87	0.75
2:A:401[B]:P1K:F16	2:A:401[B]:P1K:N6	2.10	0.74
1:D:340:ARG:HD3	3:D:562:HOH:O	1.89	0.71
1:B:79:ASN:CB	1:B:250:ARG:NH2	2.46	0.70
1:D:89:PRO:HD3	1:D:104:VAL:O	1.92	0.69
1:D:4:LYS:HE2	1:D:34:GLN:OE1	1.93	0.69
1:A:99:THR:OG1	1:A:101:ILE:HG22	1.94	0.67
1:D:116:ASN:HB2	1:D:141:LYS:HB3	1.78	0.65
1:B:357:ILE:O	1:B:358:LYS:HB2	1.95	0.65
1:D:88:THR:OG1	1:D:102:ASP:O	2.15	0.64
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.32	0.64
1:B:79:ASN:HB3	1:B:250:ARG:CZ	2.26	0.64
1:D:149:GLN:HB3	3:D:653[B]:HOH:O	1.99	0.62
1:A:263:ASN:CB	3:C:565:HOH:O	2.48	0.62
1:B:208:GLN:HG3	3:B:666:HOH:O	2.01	0.61
1:B:79:ASN:HB3	1:B:250:ARG:HH22	1.59	0.60
1:C:282:THR:HG21	3:C:597:HOH:O	2.01	0.60
1:A:127:THR:HG23	1:A:130:GLN:H	1.66	0.59
1:C:66:SER:HB3	1:C:224:VAL:HG23	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HB3	3:A:699:HOH:O	2.03	0.57
1:B:34:GLN:HE22	1:B:358:LYS:HG3	1.69	0.57
1:A:247:ASP:HA	3:A:631:HOH:O	2.04	0.56
1:C:9:LYS:CD	1:C:41:MET:HE2	2.36	0.56
1:C:279:THR:HG23	1:C:282:THR:H	1.70	0.56
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.41	0.55
1:D:117:LEU:O	1:D:149:GLN:HG2	2.07	0.55
1:B:225:LYS:HE3	3:B:770:HOH:O	2.06	0.54
1:A:242:GLN:HA	1:A:249:GLN:CD	2.28	0.52
1:B:225:LYS:HE2	3:B:596:HOH:O	2.10	0.52
1:C:9:LYS:HD3	1:C:41:MET:CE	2.39	0.52
1:D:62:LEU:HD12	1:D:224:VAL:HG12	1.92	0.51
1:C:9:LYS:HD3	1:C:41:MET:HE2	1.92	0.51
1:D:307:VAL:CG1	1:D:328:LYS:HD3	2.38	0.51
1:A:285:ASP:OD2	3:A:501:HOH:O	2.19	0.51
1:C:255:THR:HA	1:C:269:LEU:HB2	1.93	0.51
1:C:237:ALA:HA	1:C:244:TYR:CE1	2.46	0.51
1:C:34:GLN:HB2	1:C:331:ILE:HG13	1.93	0.51
1:C:12:VAL:HG11	1:C:41:MET:HG3	1.92	0.50
1:D:101:ILE:C	1:D:103:GLN:H	2.14	0.49
1:D:357:ILE:O	1:D:358:LYS:HB2	2.12	0.49
1:D:199:TYR:CZ	1:D:211:ARG:HD3	2.47	0.49
1:A:28:MET:HG3	1:A:337:THR:HG22	1.95	0.49
1:D:157:LEU:O	1:D:161:VAL:HG23	2.12	0.49
1:A:287:ASN:ND2	1:A:313:THR:HG21	2.27	0.49
1:D:109:LEU:HD13	1:D:157:LEU:HD23	1.95	0.48
1:A:143:PRO:O	1:A:146:GLU:HB2	2.14	0.47
1:C:64:SER:HB2	1:C:314:GLY:HA2	1.95	0.47
1:B:210:ILE:HD12	1:B:317:SER:OG	2.15	0.47
1:A:101:ILE:O	1:A:104:VAL:HG23	2.14	0.47
1:A:241:PRO:O	1:A:249:GLN:HG2	2.15	0.47
1:A:142:ASN:HB3	1:A:147:TYR:CD1	2.51	0.46
1:C:113:THR:HA	1:C:147:TYR:O	2.15	0.46
1:D:219:ALA:HB3	1:D:220:PRO:HD3	1.97	0.46
1:D:115:GLY:HA2	3:D:624:HOH:O	2.16	0.46
1:B:279:THR:H	1:D:208:GLN:NE2	2.14	0.46
1:A:23:TYR:OH	1:A:345:GLU:OE2	2.20	0.46
1:C:284:LEU:HD23	1:C:347:ILE:HG21	1.98	0.46
1:C:9:LYS:HD2	1:C:41:MET:HE2	1.98	0.46
1:B:219:ALA:HA	1:B:223:GLY:HA3	1.98	0.46
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LYS:HA	1:C:176:LYS:HD3	1.73	0.45
1:B:125:VAL:O	1:B:216:PRO:HG3	2.15	0.45
1:C:88:THR:HB	1:C:89:PRO:HD2	1.99	0.45
1:C:35:ASN:HA	1:C:330:ASN:ND2	2.31	0.45
1:C:83:ILE:HG22	1:C:92:TYR:CZ	2.52	0.45
1:D:2:THR:N	1:D:3:PRO:HD2	2.31	0.45
1:B:35:ASN:HA	1:B:330:ASN:ND2	2.32	0.44
1:D:186:HIS:CD2	3:D:599:HOH:O	2.41	0.44
1:D:217:LEU:O	1:D:220:PRO:HD2	2.17	0.44
1:B:79:ASN:C	1:B:250:ARG:HH22	2.19	0.44
1:D:74:GLY:HA2	1:D:162:VAL:HG21	2.00	0.44
1:A:244:TYR:HB3	1:A:248:ILE:CG2	2.47	0.44
1:B:150:TYR:OH	2:B:401:P1K:O4	2.29	0.44
1:A:104:VAL:HG22	1:A:144:ILE:HD13	2.00	0.44
1:D:357:ILE:HG22	1:D:358:LYS:N	2.32	0.44
1:A:275:SER:HB2	1:A:305:PRO:HB3	2.00	0.43
1:B:228:LEU:N	1:B:229:PRO:CD	2.81	0.43
1:D:88:THR:O	1:D:91:LYS:HB3	2.18	0.43
1:B:276:TYR:CD1	1:B:277:PRO:HA	2.53	0.43
1:D:340:ARG:NH2	2:D:401:P1K:O14	2.52	0.43
1:B:179:PHE:N	1:B:180:PRO:CD	2.81	0.43
1:A:127:THR:HG22	1:A:130:GLN:OE1	2.19	0.42
1:A:228:LEU:N	1:A:229:PRO:CD	2.82	0.42
1:C:308:LYS:O	1:C:327:PRO:HD2	2.20	0.42
1:D:169:PRO:HB2	1:D:171:ASP:OD1	2.20	0.42
1:D:276:TYR:CD1	1:D:277:PRO:HA	2.54	0.42
1:B:179:PHE:HB2	1:B:180:PRO:HD3	2.01	0.42
1:D:241:PRO:O	1:D:249:GLN:HG3	2.20	0.42
1:A:46:GLN:NE2	1:A:52:LYS:HD2	2.35	0.41
3:A:651:HOH:O	1:C:49:GLN:HG2	2.20	0.41
1:D:131:VAL:O	1:D:134:PHE:HB3	2.19	0.41
1:D:99:THR:CG2	1:D:101:ILE:HG22	2.49	0.41
1:D:101:ILE:HB	1:D:138:TRP:CE3	2.55	0.41
1:A:127:THR:HG22	1:A:130:GLN:CD	2.41	0.41
1:C:148:ARG:HD3	3:C:545:HOH:O	2.21	0.41
1:D:266:TYR:HB2	1:D:273:GLU:HB3	2.01	0.41
1:D:328:LYS:NZ	1:D:329:GLU:OE2	2.54	0.41
1:C:83:ILE:HA	1:C:92:TYR:OH	2.21	0.41
1:C:33:ILE:O	1:C:331:ILE:HA	2.21	0.40
1:A:287:ASN:CG	3:A:506:HOH:O	2.60	0.40
3:A:651:HOH:O	1:C:49:GLN:CG	2.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TYR:HB2	1:A:325:PHE:CE1	2.56	0.40
1:C:25:VAL:HG22	1:C:339:LYS:HB3	2.03	0.40
1:D:219:ALA:HA	1:D:223:GLY:HA3	2.03	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	353/361 (98%)	336 (95%)	14 (4%)	3 (1%)	19 6
1	B	355/361 (98%)	346 (98%)	9 (2%)	0	100 100
1	C	352/361 (98%)	336 (96%)	16 (4%)	0	100 100
1	D	355/361 (98%)	333 (94%)	21 (6%)	1 (0%)	41 23
All	All	1415/1444 (98%)	1351 (96%)	60 (4%)	4 (0%)	41 23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	263	ASN
1	D	87	ASP
1	A	222	TYR

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	294/319 (92%)	285 (97%)	9 (3%)	40 16
1	B	307/319 (96%)	303 (99%)	4 (1%)	69 52
1	C	284/319 (89%)	274 (96%)	10 (4%)	36 12
1	D	298/319 (93%)	288 (97%)	10 (3%)	37 13
All	All	1183/1276 (93%)	1150 (97%)	33 (3%)	43 19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	123	ASP
1	A	127	THR
1	A	165	SER
1	A	199	TYR
1	A	240	ASN
1	A	243	LYS
1	A	311	HIS
1	A	330	ASN
1	B	94	LYS
1	B	199	TYR
1	B	218	ASP
1	B	311	HIS
1	C	41	MET
1	C	82	LYS
1	C	94	LYS
1	C	165	SER
1	C	199	TYR
1	C	240	ASN
1	C	265	MET
1	C	282	THR
1	C	311	HIS
1	C	354	LEU
1	D	84	SER
1	D	123	ASP
1	D	144	ILE
1	D	165	SER
1	D	210	ILE
1	D	306	SER
1	D	308	LYS
1	D	311	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	328	LYS
1	D	358	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	287	ASN
1	C	15	ASN
1	C	49	GLN
1	C	213	ASN
1	C	249	GLN
1	D	142	ASN
1	D	208	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	P1K	B	401	1	21,23,23	2.31	8 (38%)	18,35,35	3.84	6 (33%)
2	P1K	C	401	1	21,23,23	2.38	8 (38%)	18,35,35	2.49	3 (16%)
2	P1K	D	401	1	21,23,23	2.45	8 (38%)	18,35,35	3.04	4 (22%)
2	P1K	A	401[B]	1	21,23,23	2.74	7 (33%)	18,35,35	1.95	3 (16%)
2	P1K	A	401[A]	1	21,23,23	2.45	7 (33%)	18,35,35	2.91	4 (22%)

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	P1K	B	401	1	-	5/10/21/21	0/1/1/1
2	P1K	C	401	1	-	6/10/21/21	0/1/1/1
2	P1K	D	401	1	-	5/10/21/21	0/1/1/1
2	P1K	A	401[B]	1	-	6/10/21/21	0/1/1/1
2	P1K	A	401[A]	1	-	6/10/21/21	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	P1K	P1-O2	7.75	1.64	1.56
2	A	401[A]	P1K	P1-O2	5.87	1.62	1.56
2	D	401	P1K	C12-S11	-5.69	1.69	1.78
2	C	401	P1K	P1-O2	5.43	1.62	1.56
2	C	401	P1K	C12-S11	-5.39	1.69	1.78
2	A	401[B]	P1K	C12-S11	-5.35	1.69	1.78
2	B	401	P1K	C12-C13	4.94	1.58	1.48
2	D	401	P1K	P1-O2	4.84	1.61	1.56
2	A	401[A]	P1K	C12-S11	-4.66	1.71	1.78
2	B	401	P1K	C12-S11	-4.49	1.71	1.78
2	B	401	P1K	N6-N5	4.32	1.42	1.34
2	A	401[A]	P1K	C12-C13	4.30	1.57	1.48
2	A	401[B]	P1K	B1-C1	4.13	1.62	1.56
2	D	401	P1K	N6-N5	4.13	1.41	1.34
2	D	401	P1K	C12-C13	4.07	1.56	1.48
2	A	401[A]	P1K	N6-N5	3.88	1.41	1.34
2	A	401[B]	P1K	N6-N5	3.84	1.41	1.34
2	C	401	P1K	C12-C13	3.81	1.56	1.48
2	A	401[B]	P1K	C12-C13	3.67	1.55	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	P1K	N5-N4	3.42	1.41	1.34
2	B	401	P1K	P1-O2	3.22	1.59	1.56
2	C	401	P1K	N5-N4	3.18	1.40	1.34
2	C	401	P1K	N6-N5	3.13	1.40	1.34
2	D	401	P1K	C7-N6	2.97	1.38	1.34
2	A	401[B]	P1K	N5-N4	2.96	1.40	1.34
2	B	401	P1K	N5-N4	2.94	1.40	1.34
2	A	401[A]	P1K	C8-C7	2.85	1.40	1.36
2	D	401	P1K	N5-N4	2.78	1.39	1.34
2	C	401	P1K	B1-C1	2.77	1.60	1.56
2	B	401	P1K	C8-C7	2.73	1.40	1.36
2	A	401[A]	P1K	B1-C1	2.64	1.60	1.56
2	B	401	P1K	C7-N6	2.51	1.37	1.34
2	D	401	P1K	B1-C1	2.39	1.59	1.56
2	A	401[B]	P1K	C8-C7	2.39	1.39	1.36
2	D	401	P1K	C8-C7	2.30	1.39	1.36
2	C	401	P1K	C8-N4	-2.26	1.33	1.35
2	B	401	P1K	C1-N4	-2.13	1.42	1.47
2	C	401	P1K	C7-N6	2.06	1.36	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	P1K	O15-S11-O14	-13.05	100.44	119.35
2	D	401	P1K	O15-S11-O14	-10.11	104.71	119.35
2	A	401[A]	P1K	O15-S11-O14	-9.44	105.67	119.35
2	C	401	P1K	O15-S11-O14	-8.20	107.47	119.35
2	A	401[B]	P1K	O15-S11-O14	-7.10	109.06	119.35
2	D	401	P1K	N6-N5-N4	-5.72	103.00	107.31
2	A	401[A]	P1K	N6-N5-N4	-5.06	103.50	107.31
2	B	401	P1K	C7-C9-N10	-4.62	102.71	112.71
2	B	401	P1K	O14-S11-C12	4.60	116.53	108.04
2	C	401	P1K	N6-N5-N4	-4.52	103.91	107.31
2	B	401	P1K	O15-S11-N10	4.29	116.73	106.97
2	B	401	P1K	N6-N5-N4	-4.12	104.21	107.31
2	A	401[A]	P1K	C7-C9-N10	-3.86	104.36	112.71
2	A	401[A]	P1K	O15-S11-C12	3.20	113.94	108.04
2	C	401	P1K	O14-S11-N10	3.10	114.02	106.97
2	B	401	P1K	O15-S11-C12	2.56	112.77	108.04
2	A	401[B]	P1K	N6-N5-N4	-2.44	105.47	107.31
2	A	401[B]	P1K	C8-C7-N6	-2.43	107.72	111.34
2	D	401	P1K	O14-S11-C12	2.21	112.12	108.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	P1K	C8-C7-N6	-2.17	108.11	111.34

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	P1K	S11-C12-C13-F18
2	B	401	P1K	S11-C12-C13-F16
2	B	401	P1K	S11-C12-C13-F17
2	B	401	P1K	C9-N10-S11-C12
2	B	401	P1K	C9-N10-S11-O14
2	C	401	P1K	S11-C12-C13-F18
2	C	401	P1K	S11-C12-C13-F16
2	C	401	P1K	S11-C12-C13-F17
2	C	401	P1K	C9-N10-S11-O14
2	D	401	P1K	S11-C12-C13-F18
2	D	401	P1K	S11-C12-C13-F16
2	D	401	P1K	S11-C12-C13-F17
2	D	401	P1K	C9-N10-S11-C12
2	D	401	P1K	C9-N10-S11-O14
2	A	401[B]	P1K	C13-C12-S11-N10
2	A	401[B]	P1K	C9-N10-S11-O14
2	A	401[A]	P1K	C13-C12-S11-O14
2	A	401[A]	P1K	C13-C12-S11-O15
2	A	401[A]	P1K	C13-C12-S11-N10
2	A	401[A]	P1K	C9-N10-S11-C12
2	A	401[A]	P1K	C9-N10-S11-O14
2	A	401[A]	P1K	C9-N10-S11-O15
2	A	401[B]	P1K	C13-C12-S11-O14
2	A	401[B]	P1K	C13-C12-S11-O15
2	A	401[B]	P1K	C9-N10-S11-C12
2	A	401[B]	P1K	S11-C12-C13-F16
2	C	401	P1K	C9-N10-S11-C12
2	C	401	P1K	C13-C12-S11-O15

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	P1K	1	0
2	D	401	P1K	1	0

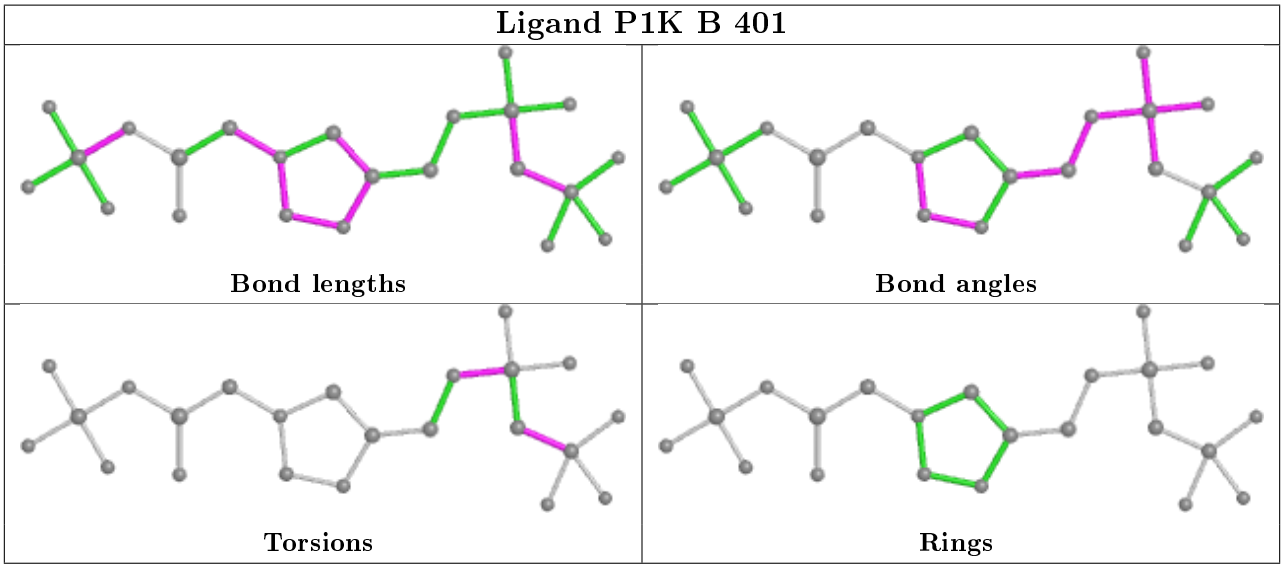
Continued on next page...

Continued from previous page...

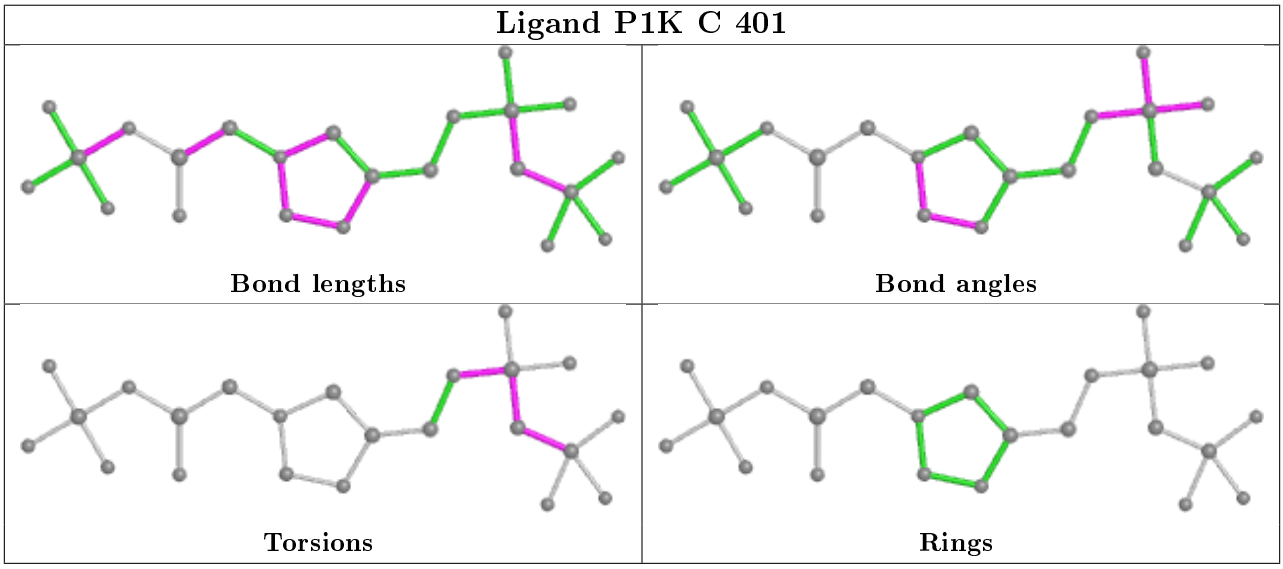
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[B]	P1K	1	0

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.

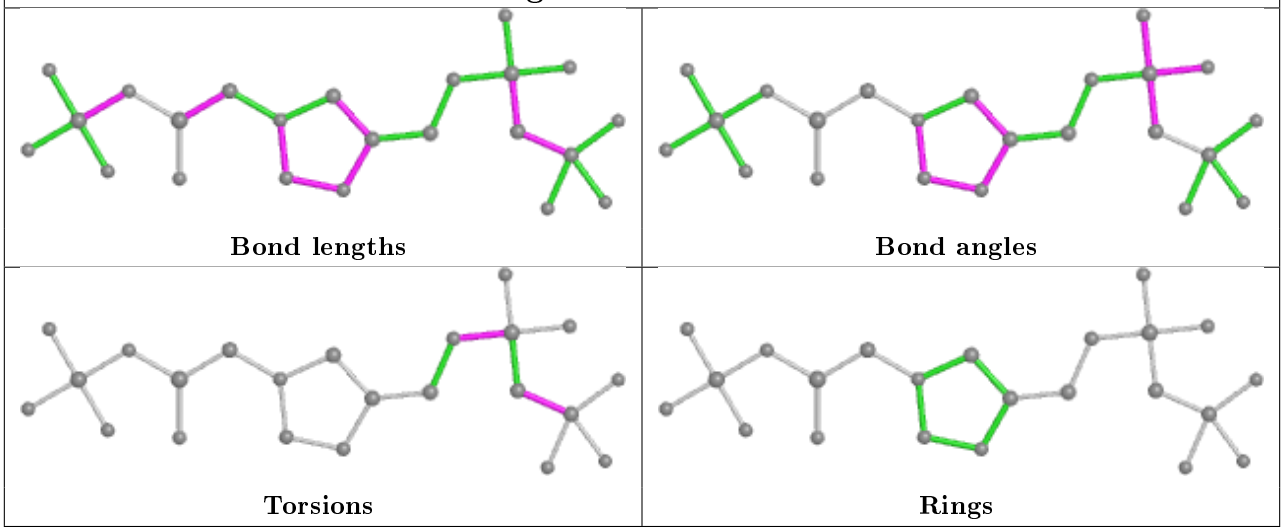
Ligand P1K B 401



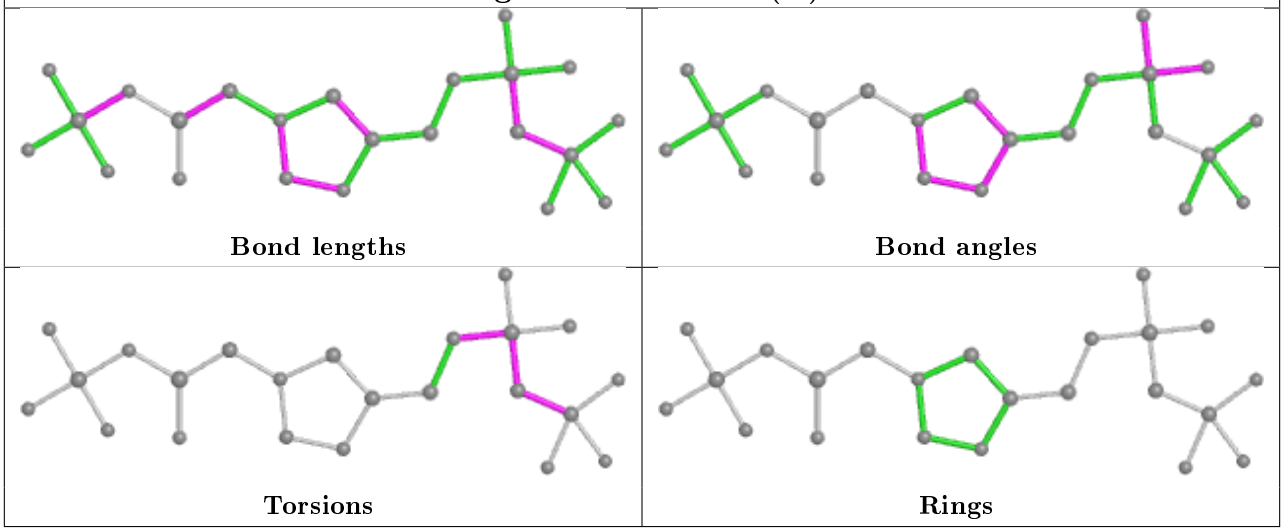
Ligand P1K C 401



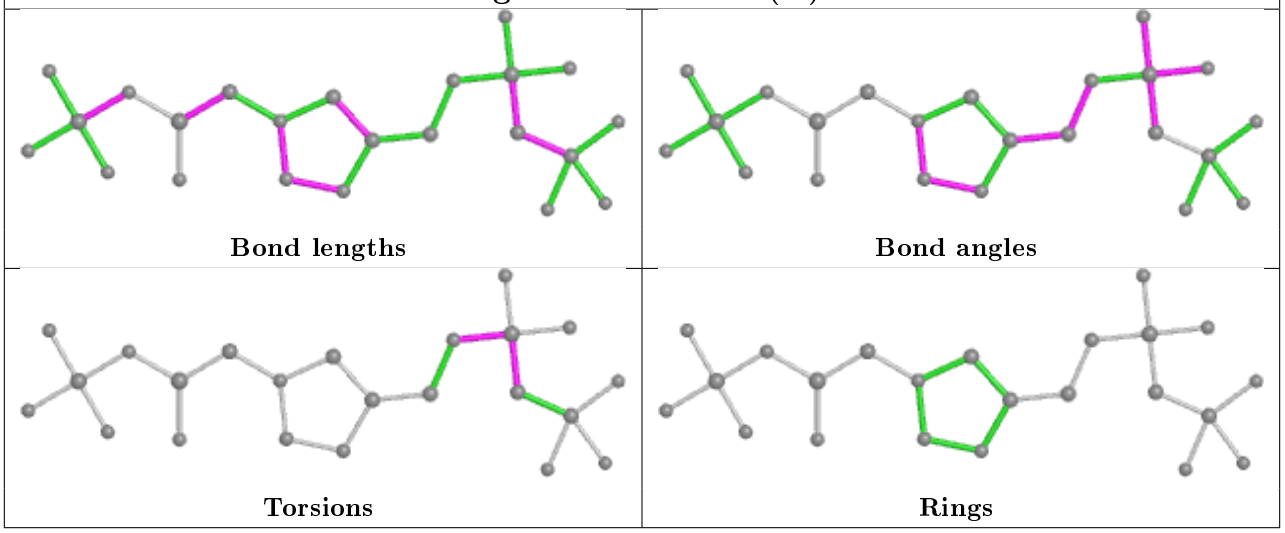
Ligand P1K D 401



Ligand P1K A 401 (B)



Ligand P1K A 401 (A)



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

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	355/361 (98%)	0.32	8 (2%) 60 66	23, 37, 57, 71	0
1	B	357/361 (98%)	0.01	0 100 100	21, 29, 43, 58	0
1	C	354/361 (98%)	0.64	35 (9%) 7 9	26, 48, 65, 89	0
1	D	357/361 (98%)	0.54	22 (6%) 20 25	25, 45, 66, 79	0
All	All	1423/1444 (98%)	0.38	65 (4%) 32 38	21, 38, 62, 89	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	ILE	5.9
1	D	96	LEU	4.6
1	C	306	SER	4.2
1	C	73	ALA	4.1
1	D	86	ASP	3.9
1	D	85	PHE	3.8
1	D	2	THR	3.7
1	D	147	TYR	3.7
1	D	298	VAL	3.7
1	D	138	TRP	3.6
1	D	104	VAL	3.5
1	D	143	PRO	3.4
1	D	135	PHE	3.4
1	D	93	TRP	3.3
1	C	76	TYR	3.2
1	D	103	GLN	3.2
1	C	276	TYR	3.1
1	C	351	TYR	3.1
1	C	33	ILE	3.1
1	C	307	VAL	3.0
1	C	77	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	81	GLY	3.0
1	C	241	PRO	2.9
1	C	93	TRP	2.9
1	D	302	SER	2.8
1	D	79	ASN	2.8
1	D	161	VAL	2.7
1	A	140	PRO	2.6
1	A	93	TRP	2.5
1	A	101	ILE	2.5
1	A	246	THR	2.5
1	C	298	VAL	2.4
1	C	279	THR	2.4
1	A	96	LEU	2.4
1	A	143	PRO	2.4
1	C	305	PRO	2.4
1	C	234	PHE	2.3
1	D	98	ASN	2.3
1	C	39	TYR	2.3
1	D	35	ASN	2.3
1	C	354	LEU	2.3
1	C	245	PRO	2.3
1	C	83	ILE	2.3
1	A	133	THR	2.3
1	C	163	ALA	2.3
1	C	85	PHE	2.3
1	C	331	ILE	2.2
1	D	291	ILE	2.2
1	D	101	ILE	2.2
1	C	327	PRO	2.2
1	C	80	LYS	2.2
1	C	32	VAL	2.1
1	C	99	THR	2.1
1	C	237	ALA	2.1
1	C	106	LEU	2.1
1	C	247	ASP	2.1
1	A	135	PHE	2.1
1	C	35	ASN	2.1
1	C	11	LEU	2.1
1	D	257	GLN	2.1
1	C	78	LYS	2.1
1	C	328	LYS	2.1
1	D	92	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	325	PHE	2.0
1	C	5	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

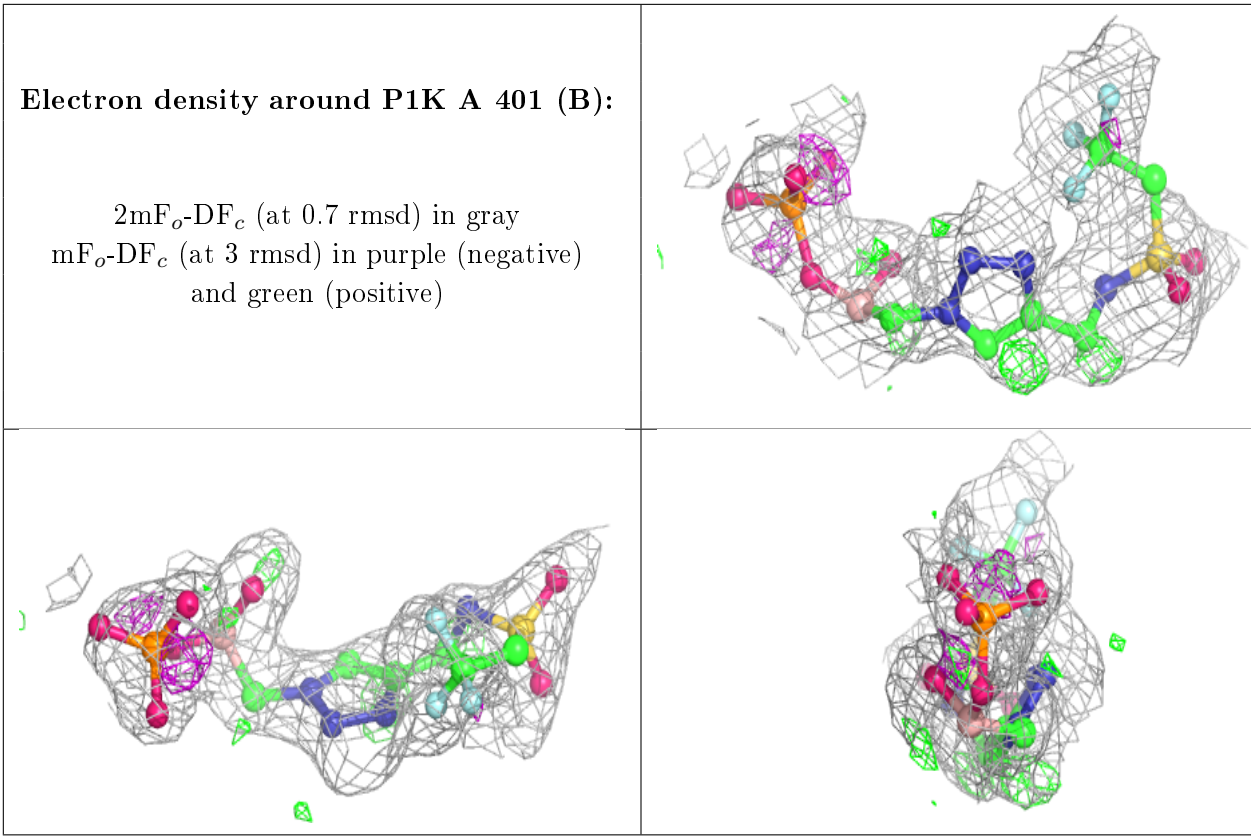
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	P1K	A	401[B]	23/23	0.84	0.18	35,53,75,80	23
2	P1K	A	401[A]	23/23	0.84	0.18	35,45,61,62	23
2	P1K	D	401	23/23	0.86	0.13	46,57,75,80	0
2	P1K	C	401	23/23	0.90	0.14	43,59,81,82	0
2	P1K	B	401	23/23	0.92	0.12	35,42,57,64	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.

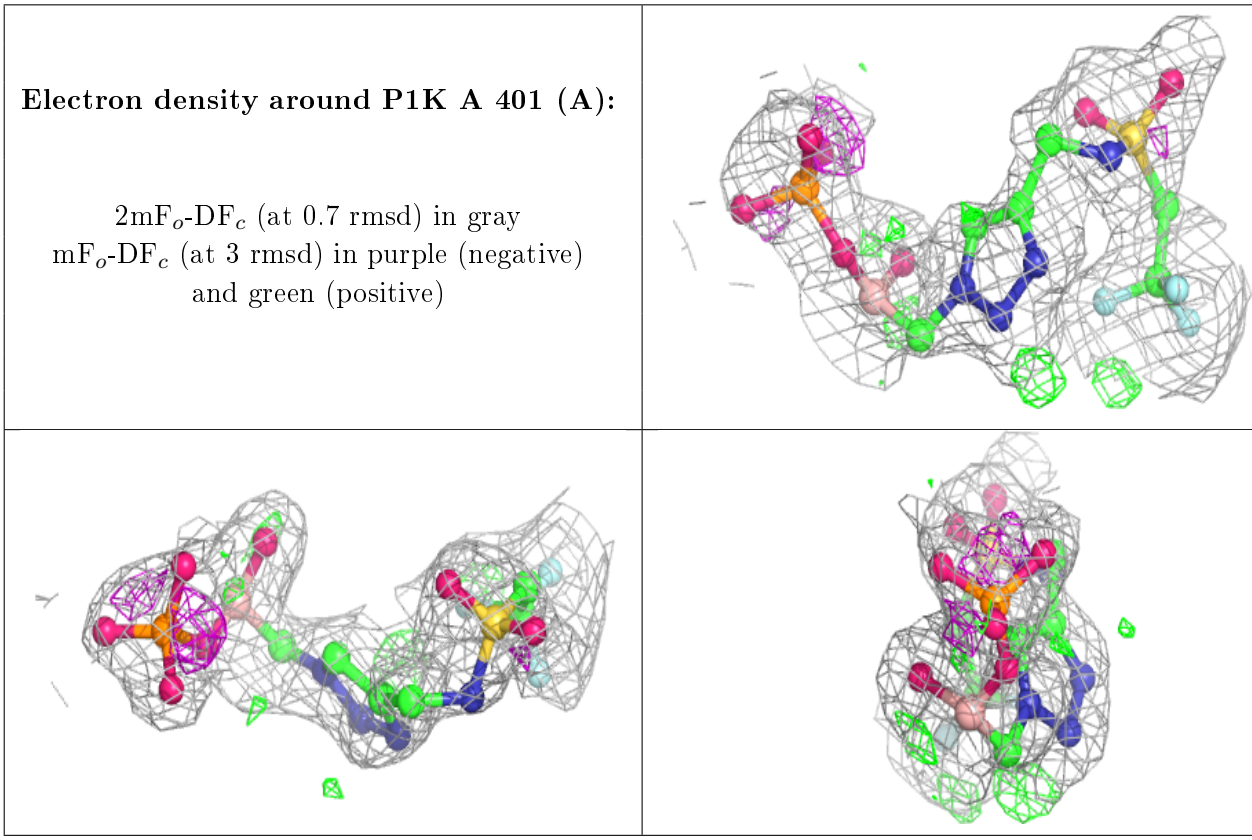
Electron density around P1K A 401 (B):

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



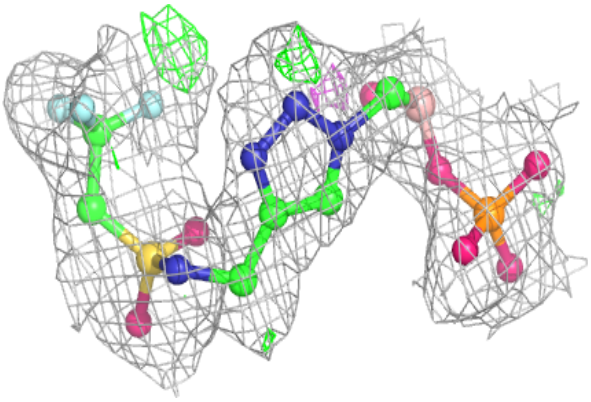
Electron density around P1K A 401 (A):

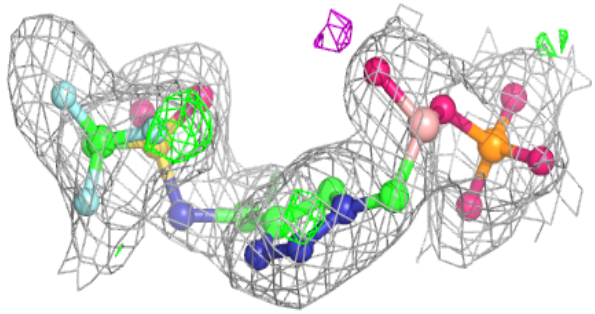
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

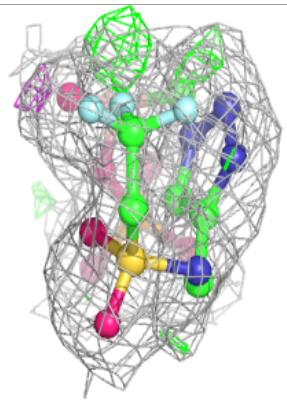


Electron density around P1K D 401:

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

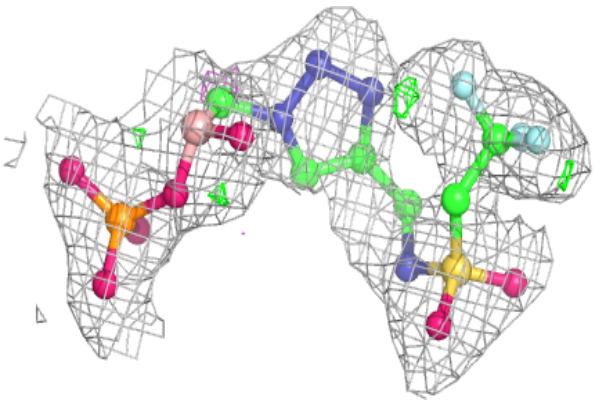


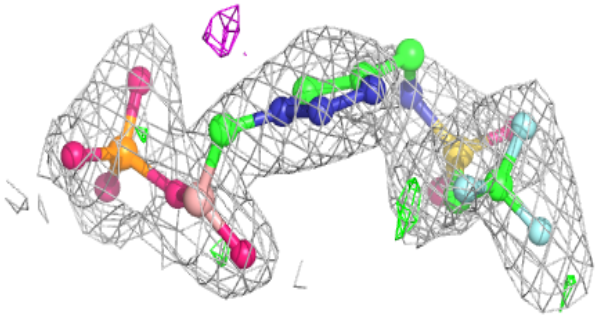


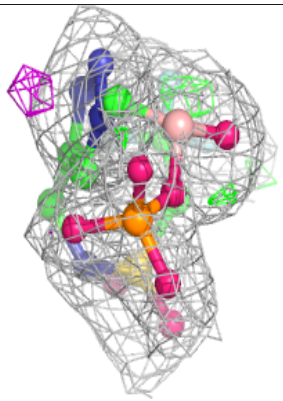


Electron density around P1K C 401:

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

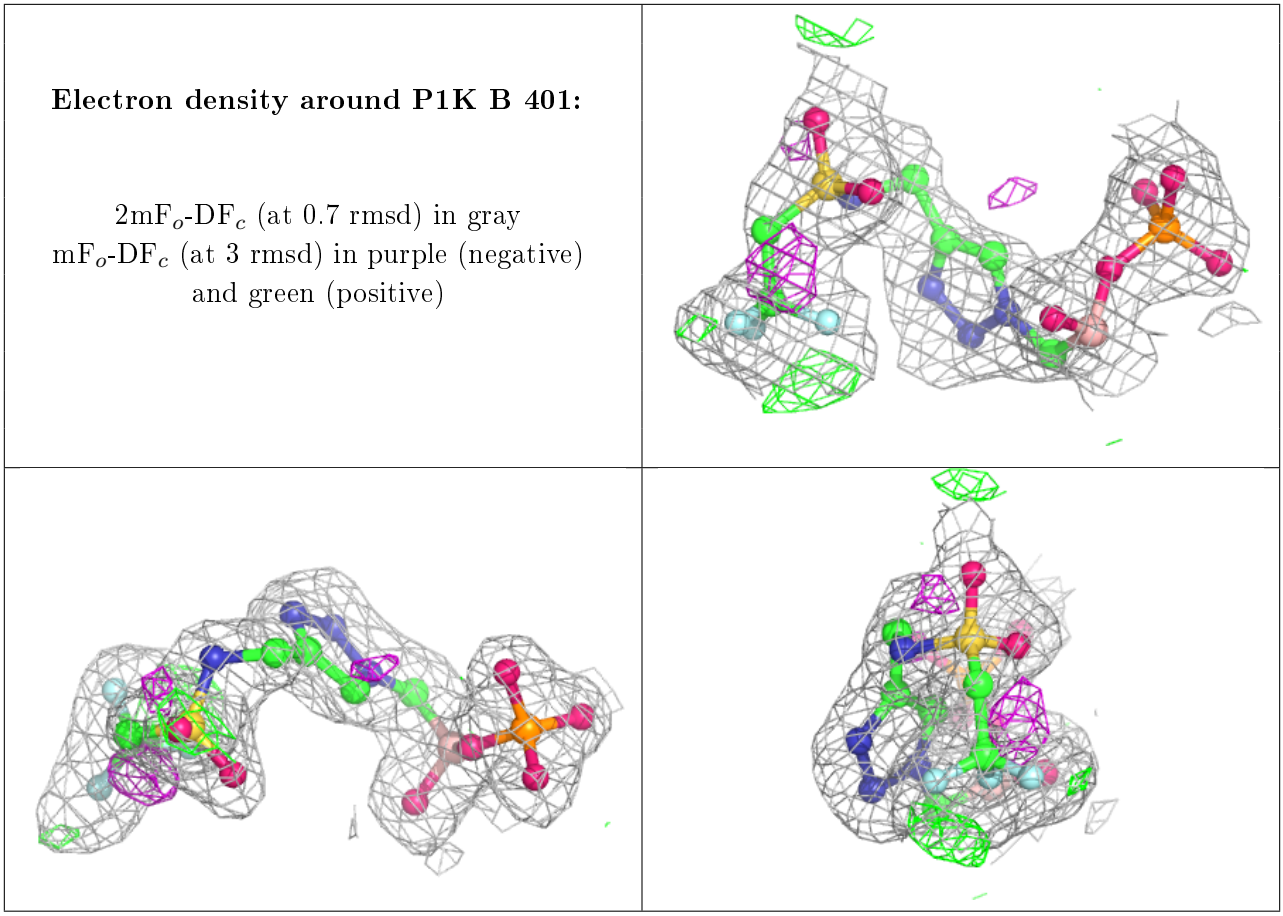






Electron density around P1K B 401:

$2mF_o$-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.