



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:56 PM UTC

PDB ID : 6TZI / pdb_00006tzi
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 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

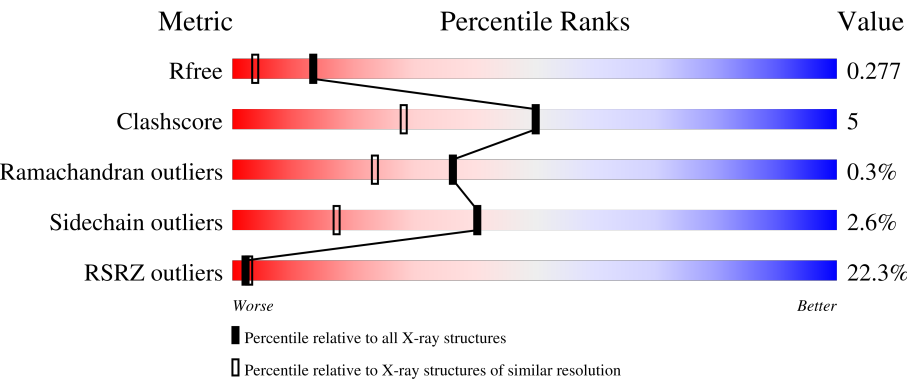
1 Overall quality at a glance i

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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	361	21% 83%14%..
1	B	361	% 90%8%..
1	C	361	37% 86%11%..
1	D	361	29% 81%17%..

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.

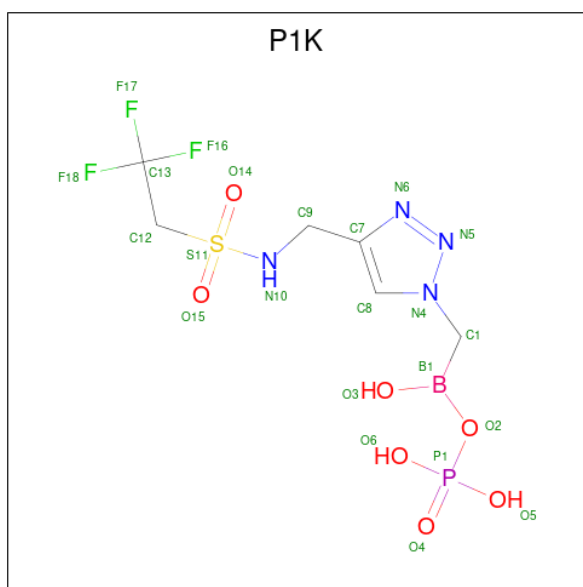
- Molecule 1 is a protein called Beta-lactamase.

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 (CCD ID: P1K) (formula: C₆H₁₁BF₃N₄O₇PS) (labeled as "Ligand of Interest" by depositor).



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		

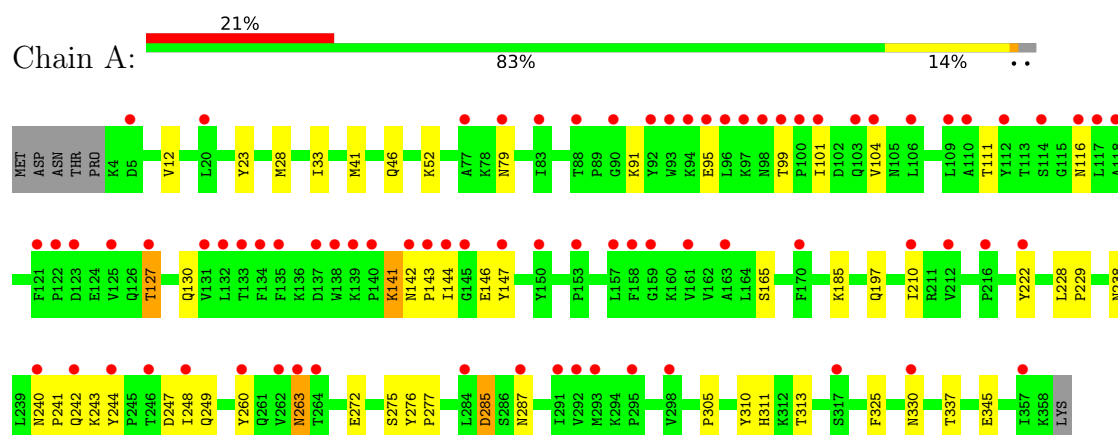
- Molecule 3 is water.

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		

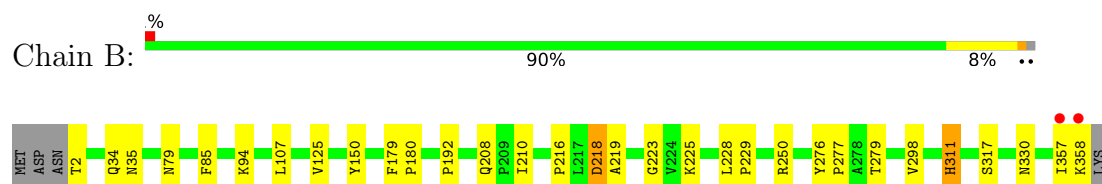
3 Residue-property plots

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.

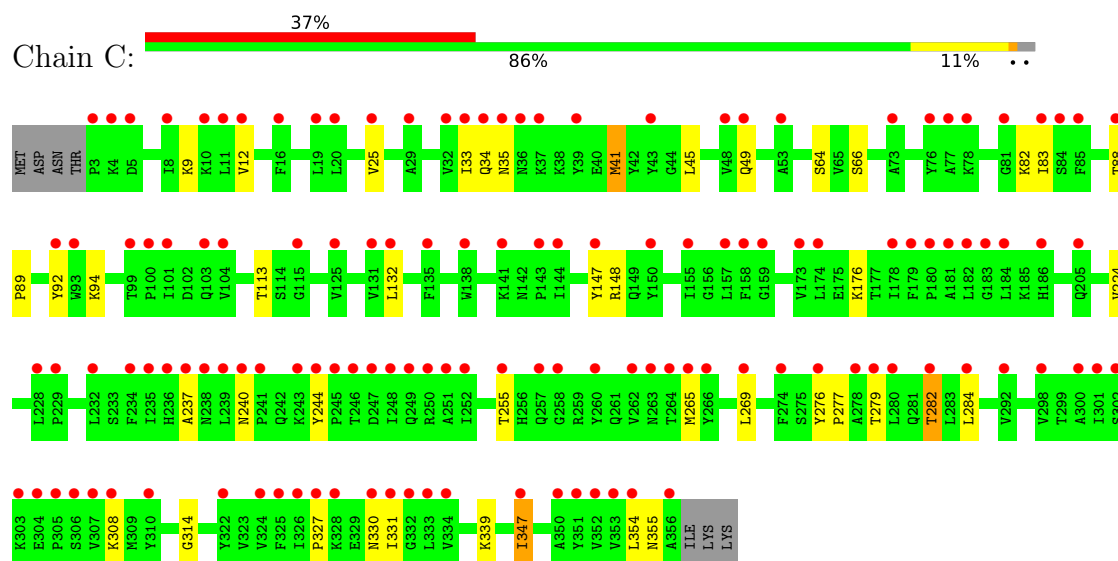
• Molecule 1: Beta-lactamase



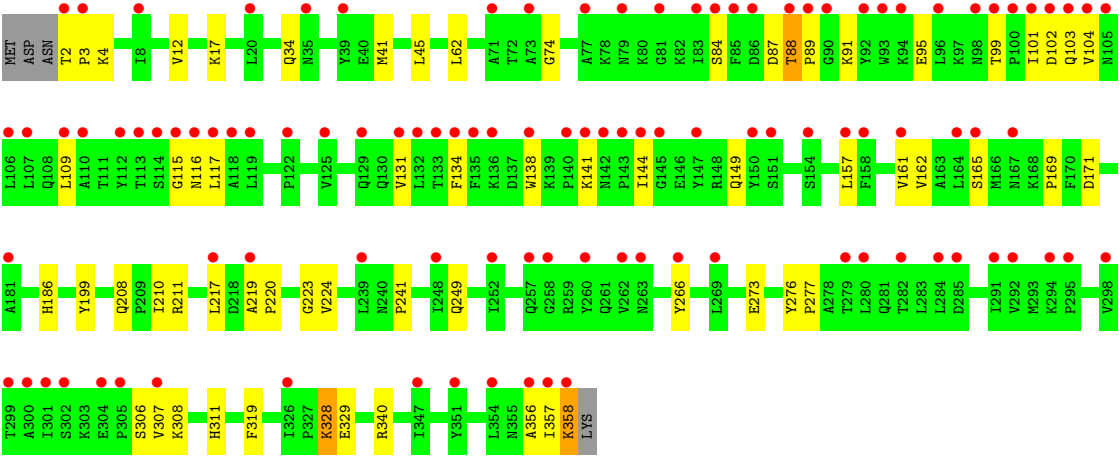
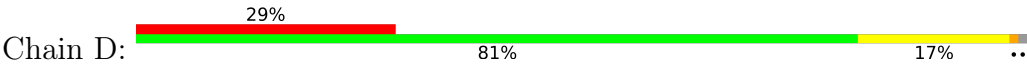
• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase



● Molecule 1: Beta-lactamase



4 Data and refinement statistics

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 81.95 – 1.74	Depositor EDS
% Data completeness (in resolution range)	82.6 (81.95-1.74) 82.6 (81.95-1.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.12%)	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)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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: 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	0.57	0/2820	1.09	5/3840 (0.1%)
1	B	0.62	0/2878	1.09	2/3912 (0.1%)
1	C	0.51	0/2781	1.02	3/3791 (0.1%)
1	D	0.53	0/2850	1.06	5/3875 (0.1%)
All	All	0.56	0/11329	1.06	15/15418 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	THR	CB-CA-C	7.19	119.70	108.84
1	D	45	LEU	CA-C-N	6.64	129.72	120.29
1	D	45	LEU	C-N-CA	6.64	129.72	120.29
1	B	218	ASP	CA-CB-CG	6.38	118.98	112.60
1	D	319	PHE	CA-CB-CG	6.17	119.97	113.80
1	C	355	ASN	CB-CA-C	6.11	121.24	110.85
1	A	285	ASP	CB-CA-C	-5.63	101.44	110.79
1	D	95	GLU	N-CA-C	-5.44	106.36	114.64
1	A	79	ASN	CB-CA-C	5.33	121.12	109.99
1	C	45	LEU	CA-C-N	5.27	127.78	120.29
1	C	45	LEU	C-N-CA	5.27	127.78	120.29
1	A	272	GLU	CB-CA-C	5.26	118.21	109.53
1	A	33	ILE	CB-CA-C	5.16	118.30	110.62
1	A	238	ASN	CA-CB-CG	-5.15	107.45	112.60
1	B	192	PRO	CB-CA-C	-5.08	104.30	110.95

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	29	0
1	B	2810	0	2784	23	0
1	C	2714	0	2614	26	0
1	D	2784	0	2728	39	0
2	A	46	0	0	1	0
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	117	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 (117) 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:N6	2:A:401[B]:P1K:F16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:357:ILE:O	1:B:358:LYS:HB2	1.95	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
1:A:23:TYR:OH	1:A:345:GLU:OE2	2.20	0.57
1:D:12:VAL:HG21	1:D:41:MET:HE3	1.86	0.57
1:A:185:LYS:HB3	3:A:699:HOH:O	2.03	0.57
1:A:242:GLN:HA	1:A:249:GLN:CD	2.28	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:D:101:ILE:C	1:D:103:GLN:H	2.14	0.54
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	1.93	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:34:GLN:HB2	1:C:331:ILE:HG13	1.93	0.51
1:C:237:ALA:HA	1:C:244:TYR:CE1	2.46	0.51
1:C:12:VAL:HG11	1:C:41:MET:HG3	1.92	0.50
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:B:79:ASN:C	1:B:250:ARG:HH22	2.19	0.49
1:A:287:ASN:ND2	1:A:313:THR:HG21	2.27	0.49
1:A:12:VAL:HG21	1:A:41:MET:HE3	1.95	0.48
1:D:109:LEU:HD13	1:D:157:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:THR:O	1:A:260:TYR:OH	2.29	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:A:127:THR:HG22	1:A:130:GLN:CD	2.41	0.46
1:B:279:THR:H	1:D:208:GLN:NE2	2.14	0.46
1:D:115:GLY:HA2	3:D:624:HOH:O	2.16	0.46
1:C:284:LEU:HD23	1:C:347:ILE:HG21	1.98	0.46
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.97	0.46
1:B:219:ALA:HA	1:B:223:GLY:HA3	1.98	0.46
1:C:176:LYS:HD3	1:C:176:LYS:HA	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:A:287:ASN:CG	3:A:506:HOH:O	2.60	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:A:116:ASN:CG	1:A:141:LYS:HG3	2.41	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: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:B:311:HIS:CD2	1:B:311:HIS:C	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:242:GLN:H	1:A:242:GLN:CD	2.28	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:99:THR:CG2	1:D:101:ILE:HG22	2.49	0.41
1:D:131:VAL:O	1:D:134:PHE:HB3	2.19	0.41
1:D:101:ILE:HB	1:D:138:TRP:CE3	2.55	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:101:ILE:C	1:D:103:GLN:N	2.78	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
3:A:651:HOH:O	1:C:49:GLN:CG	2.67	0.40
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%)	16	4
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%)	36	23
All	All	1415/1444 (98%)	1351 (96%)	60 (4%)	4 (0%)	36	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 ⓘ

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%)	284 (97%)	10 (3%)	32	10
1	B	307/319 (96%)	303 (99%)	4 (1%)	61	43
1	C	284/319 (89%)	276 (97%)	8 (3%)	38	15
1	D	298/319 (93%)	289 (97%)	9 (3%)	36	12
All	All	1183/1276 (93%)	1152 (97%)	31 (3%)	40	17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	127	THR
1	A	141	LYS
1	A	165	SER
1	A	197	GLN
1	A	210	ILE
1	A	240	ASN
1	A	243	LYS
1	A	311	HIS
1	A	330	ASN
1	B	94	LYS
1	B	218	ASP
1	B	298	VAL
1	B	311	HIS
1	C	41	MET
1	C	82	LYS

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Mol	Chain	Res	Type
1	C	94	LYS
1	C	240	ASN
1	C	265	MET
1	C	282	THR
1	C	347	ILE
1	C	354	LEU
1	D	84	SER
1	D	144	ILE
1	D	165	SER
1	D	210	ILE
1	D	306	SER
1	D	308	LYS
1	D	311	HIS
1	D	328	LYS
1	D	358	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	34	GLN
1	A	195	GLN
1	A	197	GLN
1	A	198	ASN
1	A	249	GLN
1	A	281	GLN
1	A	287	ASN
1	A	330	ASN
1	B	198	ASN
1	C	15	ASN
1	C	103	GLN
1	C	213	ASN
1	C	249	GLN
1	C	253	ASN
1	C	290	GLN
1	C	296	ASN
1	C	330	ASN
1	C	355	ASN
1	D	142	ASN
1	D	197	GLN
1	D	205	GLN
1	D	208	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 ⓘ

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	C	401	1	21,23,23	2.52	5 (23%)	22,35,35	2.45	6 (27%)
2	P1K	D	401	1	21,23,23	2.62	5 (23%)	22,35,35	3.04	7 (31%)
2	P1K	A	401[A]	1	21,23,23	2.63	6 (28%)	22,35,35	2.83	7 (31%)
2	P1K	B	401	1	21,23,23	2.49	7 (33%)	22,35,35	3.76	10 (45%)
2	P1K	A	401[B]	1	21,23,23	3.00	7 (33%)	22,35,35	1.99	3 (13%)

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	C	401	1	-	6/12/21/21	0/1/1/1
2	P1K	D	401	1	-	7/12/21/21	0/1/1/1
2	P1K	A	401[A]	1	-	8/12/21/21	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P1K	B	401	1	-	6/12/21/21	0/1/1/1
2	P1K	A	401[B]	1	-	9/12/21/21	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	P1K	P1-O2	8.67	1.64	1.56
2	A	401[A]	P1K	P1-O2	6.57	1.62	1.56
2	B	401	P1K	N6-N5	6.26	1.42	1.32
2	C	401	P1K	P1-O2	6.08	1.62	1.56
2	D	401	P1K	N6-N5	6.04	1.41	1.32
2	D	401	P1K	C12-S11	-5.79	1.69	1.78
2	A	401[A]	P1K	N6-N5	5.77	1.41	1.32
2	A	401[B]	P1K	N6-N5	5.72	1.41	1.32
2	C	401	P1K	C12-S11	-5.49	1.69	1.78
2	A	401[B]	P1K	C12-S11	-5.45	1.69	1.78
2	D	401	P1K	P1-O2	5.43	1.61	1.56
2	C	401	P1K	N6-N5	4.94	1.40	1.32
2	B	401	P1K	C12-C13	4.86	1.58	1.48
2	A	401[A]	P1K	C12-S11	-4.75	1.71	1.78
2	B	401	P1K	C12-S11	-4.58	1.71	1.78
2	A	401[A]	P1K	C12-C13	4.21	1.57	1.48
2	D	401	P1K	C12-C13	3.97	1.56	1.48
2	A	401[A]	P1K	N4-N5	3.87	1.41	1.34
2	C	401	P1K	C12-C13	3.70	1.56	1.48
2	B	401	P1K	P1-O2	3.62	1.59	1.56
2	C	401	P1K	N4-N5	3.57	1.40	1.34
2	A	401[B]	P1K	C12-C13	3.56	1.55	1.48
2	A	401[B]	P1K	N4-N5	3.31	1.40	1.34
2	B	401	P1K	N4-N5	3.29	1.40	1.34
2	D	401	P1K	N4-N5	3.09	1.39	1.34
2	A	401[B]	P1K	B1-C1	3.01	1.62	1.57
2	B	401	P1K	C1-N4	-2.89	1.42	1.46
2	A	401[A]	P1K	C8-C7	2.36	1.40	1.36
2	B	401	P1K	C8-C7	2.25	1.40	1.36
2	A	401[B]	P1K	C1-N4	2.04	1.48	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	P1K	O15-S11-O14	-13.51	100.44	119.34
2	D	401	P1K	O15-S11-O14	-10.46	104.71	119.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	P1K	O15-S11-O14	-9.77	105.67	119.34
2	C	401	P1K	O15-S11-O14	-8.49	107.47	119.34
2	A	401[B]	P1K	O15-S11-O14	-7.35	109.06	119.34
2	B	401	P1K	C1-N4-N5	-5.42	113.08	119.86
2	D	401	P1K	C1-N4-N5	-5.08	113.50	119.86
2	B	401	P1K	O14-S11-C12	4.63	116.53	108.06
2	A	401[A]	P1K	C1-N4-N5	-4.48	114.25	119.86
2	D	401	P1K	N4-N5-N6	-4.47	103.00	107.02
2	B	401	P1K	O15-S11-N10	4.29	116.73	107.02
2	B	401	P1K	C7-C9-N10	-4.16	102.71	112.27
2	A	401[A]	P1K	N4-N5-N6	-3.92	103.50	107.02
2	C	401	P1K	C1-N4-N5	-3.81	115.09	119.86
2	C	401	P1K	N4-N5-N6	-3.46	103.91	107.02
2	A	401[A]	P1K	C7-C9-N10	-3.44	104.36	112.27
2	A	401[B]	P1K	C1-N4-N5	-3.42	115.58	119.86
2	D	401	P1K	C9-C7-C8	-3.32	123.89	130.03
2	D	401	P1K	C9-C7-N6	3.24	127.99	121.61
2	A	401[A]	P1K	O15-S11-C12	3.21	113.94	108.06
2	B	401	P1K	N4-N5-N6	-3.13	104.21	107.02
2	C	401	P1K	O14-S11-N10	3.09	114.02	107.02
2	B	401	P1K	C9-C7-C8	-2.97	124.53	130.03
2	C	401	P1K	C9-C7-C8	-2.74	124.97	130.03
2	B	401	P1K	O15-S11-C12	2.57	112.77	108.06
2	A	401[A]	P1K	C9-C7-C8	-2.54	125.32	130.03
2	D	401	P1K	C8-N4-N5	2.44	113.13	110.75
2	D	401	P1K	O14-S11-C12	2.21	112.12	108.06
2	A	401[B]	P1K	C7-C8-N4	2.21	108.43	105.33
2	C	401	P1K	C9-C7-N6	2.09	125.72	121.61
2	A	401[A]	P1K	C8-N4-N5	2.07	112.78	110.75
2	B	401	P1K	C9-C7-N6	2.06	125.66	121.61
2	B	401	P1K	C8-N4-N5	2.03	112.74	110.75

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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Mol	Chain	Res	Type	Atoms
2	A	401[B]	P1K	C13-C12-S11-N10
2	A	401[B]	P1K	C9-N10-S11-O14
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-O14
2	A	401[B]	P1K	C13-C12-S11-O15
2	D	401	P1K	C8-C7-C9-N10
2	A	401[A]	P1K	N6-C7-C9-N10
2	D	401	P1K	N6-C7-C9-N10
2	A	401[B]	P1K	C9-N10-S11-C12
2	A	401[A]	P1K	C8-C7-C9-N10
2	A	401[B]	P1K	C7-C9-N10-S11
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
2	B	401	P1K	N6-C7-C9-N10
2	A	401[B]	P1K	S11-C12-C13-F18
2	A	401[B]	P1K	S11-C12-C13-F17

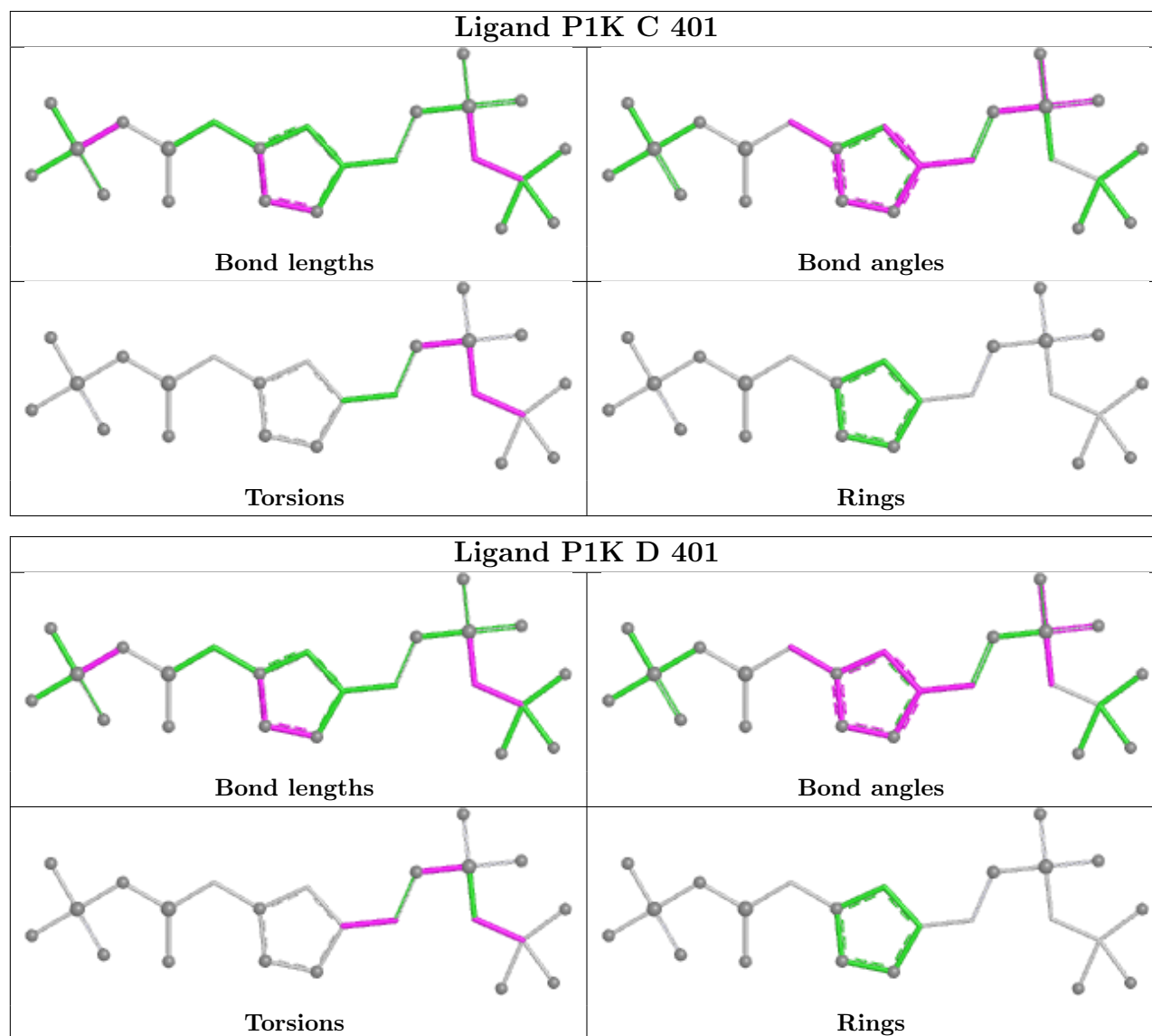
There are no ring outliers.

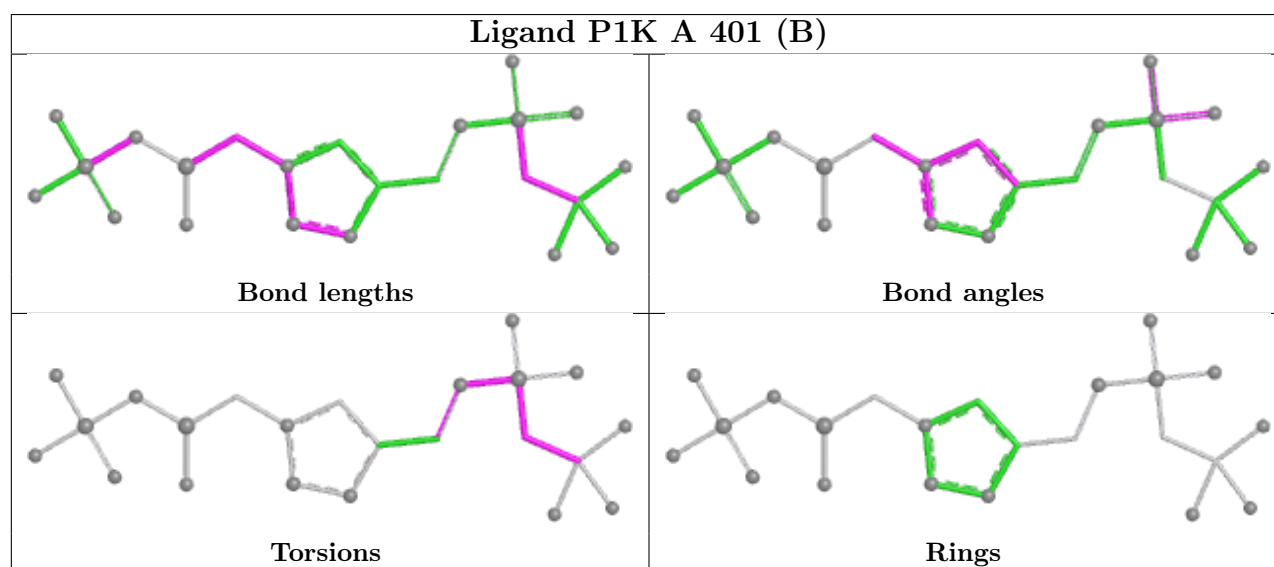
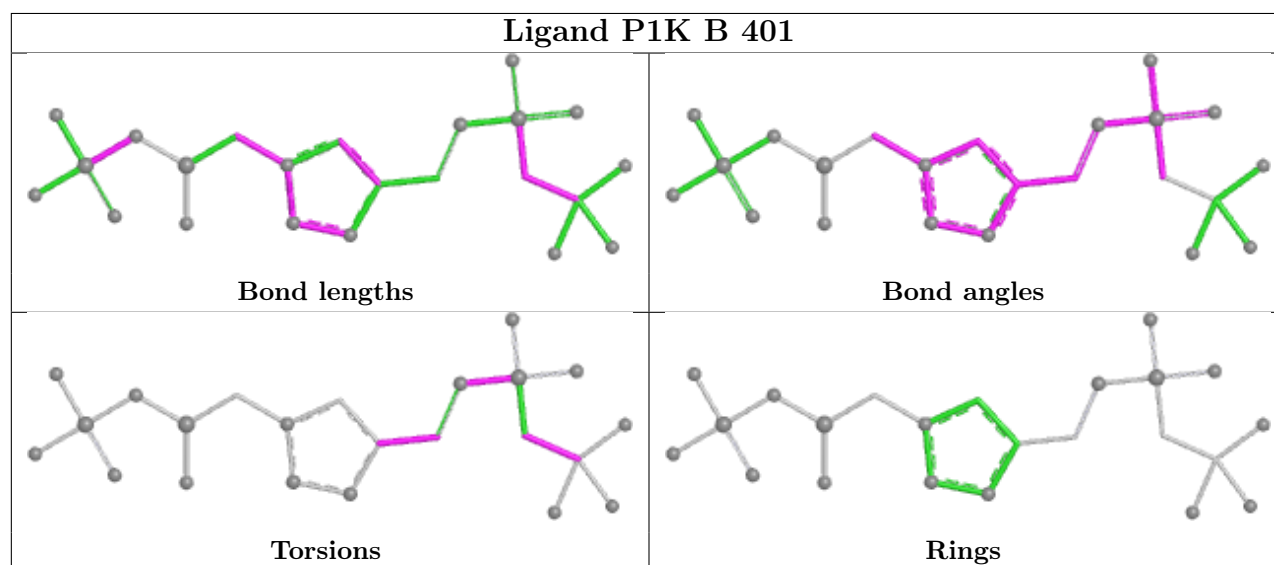
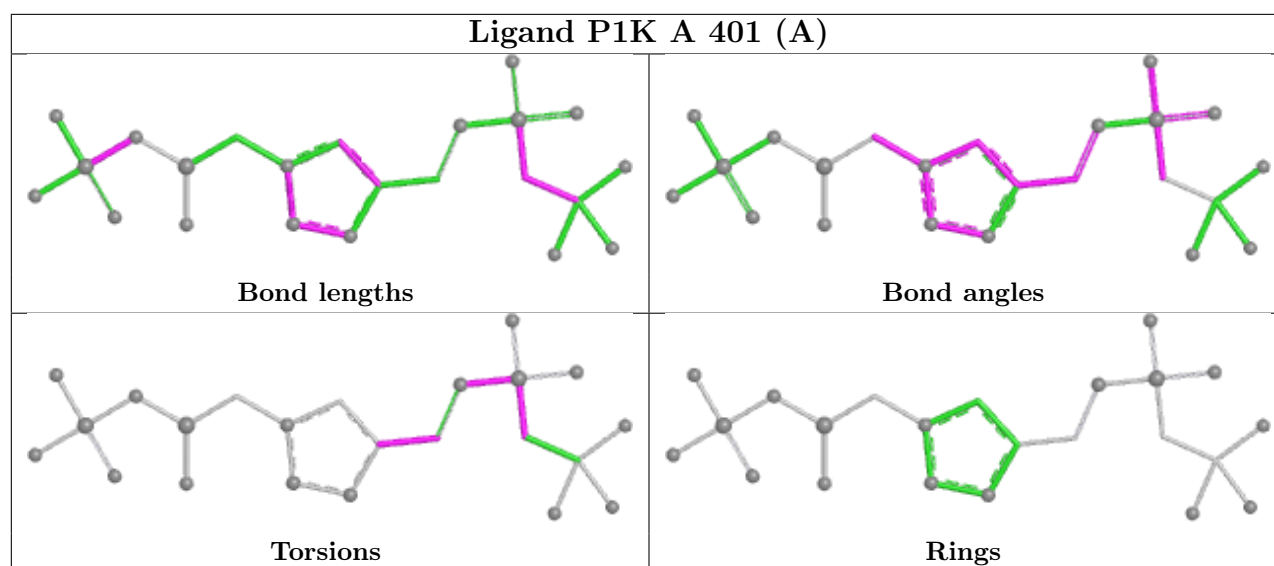
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	P1K	1	0
2	B	401	P1K	1	0
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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	355/361 (98%)	1.29	77 (21%) 2 3	23, 37, 57, 71	0
1	B	357/361 (98%)	0.38	2 (0%) 85 90	21, 29, 42, 58	0
1	C	354/361 (98%)	1.72	133 (37%) 1 1	26, 48, 65, 89	0
1	D	357/361 (98%)	1.50	105 (29%) 1 1	25, 45, 66, 79	0
All	All	1423/1444 (98%)	1.22	317 (22%) 2 3	21, 38, 62, 89	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	VAL	5.3
1	D	2	THR	5.1
1	C	39	TYR	5.1
1	A	135	PHE	4.8
1	C	306	SER	4.7
1	C	307	VAL	4.6
1	D	135	PHE	4.6
1	D	138	TRP	4.5
1	C	356	ALA	4.5
1	D	140	PRO	4.5
1	A	143	PRO	4.4
1	D	132	LEU	4.4
1	C	77	ALA	4.4
1	A	138	TRP	4.4
1	A	93	TRP	4.3
1	D	101	ILE	4.3
1	C	73	ALA	4.2
1	D	298	VAL	4.2
1	D	96	LEU	4.1
1	A	132	LEU	4.0
1	D	85	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	144	ILE	3.9
1	D	164	LEU	3.9
1	C	325	PHE	3.9
1	D	291	ILE	3.9
1	A	96	LEU	3.9
1	A	263	ASN	3.9
1	C	354	LEU	3.8
1	C	305	PRO	3.8
1	C	8	ILE	3.8
1	C	33	ILE	3.7
1	A	295	PRO	3.7
1	A	101	ILE	3.7
1	C	11	LEU	3.7
1	D	143	PRO	3.7
1	C	301	ILE	3.6
1	A	357	ILE	3.6
1	C	351	TYR	3.6
1	C	246	THR	3.6
1	A	140	PRO	3.5
1	C	248	ILE	3.5
1	A	262	VAL	3.5
1	C	326	ILE	3.5
1	C	234	PHE	3.5
1	A	95	GLU	3.5
1	D	81	GLY	3.5
1	C	104	VAL	3.5
1	C	300	ALA	3.4
1	A	131	VAL	3.4
1	D	147	TYR	3.4
1	D	83	ILE	3.4
1	A	133	THR	3.4
1	C	182	LEU	3.4
1	C	279	THR	3.4
1	C	32	VAL	3.4
1	C	302	SER	3.4
1	C	282	THR	3.3
1	D	117	LEU	3.3
1	C	251	ALA	3.3
1	D	99	THR	3.3
1	A	109	LEU	3.3
1	C	333	LEU	3.3
1	D	157	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	147	TYR	3.3
1	D	92	TYR	3.3
1	C	298	VAL	3.3
1	D	93	TRP	3.2
1	C	3	PRO	3.2
1	A	134	PHE	3.2
1	C	237	ALA	3.2
1	C	304	GLU	3.2
1	C	352	VAL	3.2
1	D	115	GLY	3.2
1	C	328	LYS	3.2
1	C	76	TYR	3.2
1	C	255	THR	3.2
1	A	100	PRO	3.2
1	C	135	PHE	3.2
1	A	99	THR	3.2
1	C	232	LEU	3.2
1	C	274	PHE	3.2
1	D	295	PRO	3.1
1	C	83	ILE	3.1
1	A	117	LEU	3.1
1	D	110	ALA	3.1
1	A	121	PHE	3.1
1	D	279	THR	3.1
1	D	131	VAL	3.1
1	D	161	VAL	3.1
1	C	180	PRO	3.1
1	A	248	ILE	3.1
1	A	110	ALA	3.1
1	C	327	PRO	3.0
1	C	353	VAL	3.0
1	A	94	LYS	3.0
1	D	88	THR	3.0
1	C	332	GLY	3.0
1	C	266	TYR	3.0
1	C	331	ILE	3.0
1	D	357	ILE	3.0
1	A	158	PHE	3.0
1	D	145	GLY	3.0
1	C	93	TRP	3.0
1	D	133	THR	3.0
1	D	20	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	103	GLN	3.0
1	C	252	ILE	3.0
1	D	3	PRO	3.0
1	D	98	ASN	3.0
1	D	134	PHE	3.0
1	A	118	ALA	2.9
1	C	81	GLY	2.9
1	C	85	PHE	2.9
1	A	246	THR	2.9
1	C	347	ILE	2.9
1	D	154	SER	2.9
1	C	35	ASN	2.9
1	C	324	VAL	2.9
1	D	292	VAL	2.9
1	C	258	GLY	2.8
1	C	43	TYR	2.8
1	C	244	TYR	2.8
1	D	112	TYR	2.8
1	C	239	LEU	2.8
1	C	269	LEU	2.8
1	C	243	LYS	2.8
1	D	356	ALA	2.8
1	A	161	VAL	2.8
1	A	292	VAL	2.8
1	A	298	VAL	2.8
1	D	109	LEU	2.8
1	C	25	VAL	2.8
1	C	115	GLY	2.8
1	C	183	GLY	2.8
1	A	287	ASN	2.7
1	A	104	VAL	2.7
1	A	92	TYR	2.7
1	D	106	LEU	2.7
1	D	269	LEU	2.7
1	A	210	ILE	2.7
1	A	5	ASP	2.7
1	C	276	TYR	2.7
1	D	217	LEU	2.7
1	A	264	THR	2.7
1	C	36	ASN	2.7
1	D	219	ALA	2.7
1	A	284	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	262	VAL	2.7
1	C	4	LYS	2.7
1	A	123	ASP	2.7
1	C	100	PRO	2.6
1	A	157	LEU	2.6
1	A	244	TYR	2.6
1	A	216	PRO	2.6
1	C	143	PRO	2.6
1	C	179	PHE	2.6
1	C	284	LEU	2.6
1	D	119	LEU	2.6
1	C	147	TYR	2.6
1	C	138	TRP	2.6
1	D	280	LEU	2.6
1	A	145	GLY	2.5
1	D	90	GLY	2.5
1	A	127	THR	2.5
1	D	94	LYS	2.5
1	D	266	TYR	2.5
1	C	262	VAL	2.5
1	C	241	PRO	2.5
1	A	116	ASN	2.5
1	A	112	TYR	2.5
1	A	222	TYR	2.5
1	A	83	ILE	2.5
1	A	163	ALA	2.5
1	C	245	PRO	2.5
1	D	301	ILE	2.5
1	C	303	LYS	2.5
1	D	354	LEU	2.5
1	C	229	PRO	2.5
1	D	89	PRO	2.5
1	C	144	ILE	2.5
1	D	113	THR	2.5
1	C	84	SER	2.5
1	D	151	SER	2.5
1	A	240	ASN	2.4
1	A	242	GLN	2.4
1	C	257	GLN	2.4
1	D	158	PHE	2.4
1	A	122	PRO	2.4
1	D	125	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	326	ILE	2.4
1	D	79	ASN	2.4
1	D	102	ASP	2.4
1	C	263	ASN	2.4
1	C	173	VAL	2.4
1	A	103	GLN	2.4
1	C	49	GLN	2.4
1	C	174	LEU	2.4
1	D	107	LEU	2.4
1	D	239	LEU	2.4
1	C	141	LYS	2.4
1	C	235	ILE	2.4
1	C	125	VAL	2.4
1	C	240	ASN	2.3
1	C	20	LEU	2.3
1	C	132	LEU	2.3
1	D	181	ALA	2.3
1	D	282	THR	2.3
1	C	37	LYS	2.3
1	C	322	TYR	2.3
1	D	260	TYR	2.3
1	A	291	ILE	2.3
1	A	125	VAL	2.3
1	C	48	VAL	2.3
1	C	205	GLN	2.3
1	D	165	SER	2.3
1	C	159	GLY	2.3
1	D	136	LYS	2.3
1	D	299	THR	2.3
1	C	278	ALA	2.3
1	D	129	GLN	2.3
1	A	144	ILE	2.3
1	C	101	ILE	2.3
1	D	84	SER	2.3
1	C	12	VAL	2.3
1	A	97	LYS	2.3
1	C	5	ASP	2.3
1	C	99	THR	2.3
1	C	236	HIS	2.3
1	C	34	GLN	2.3
1	A	170	PHE	2.3
1	A	139	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	92	TYR	2.3
1	A	293	MET	2.3
1	C	334	VAL	2.3
1	A	88	THR	2.2
1	A	77	ALA	2.2
1	A	106	LEU	2.2
1	C	19	LEU	2.2
1	C	157	LEU	2.2
1	D	294	LYS	2.2
1	D	39	TYR	2.2
1	C	178	ILE	2.2
1	C	131	VAL	2.2
1	D	307	VAL	2.2
1	D	305	PRO	2.2
1	C	238	ASN	2.2
1	D	105	ASN	2.2
1	D	142	ASN	2.2
1	D	300	ALA	2.2
1	C	280	LEU	2.2
1	D	258	GLY	2.2
1	C	155	ILE	2.2
1	D	100	PRO	2.2
1	C	292	VAL	2.2
1	D	302	SER	2.2
1	C	29	ALA	2.2
1	C	247	ASP	2.2
1	C	249	GLN	2.2
1	D	257	GLN	2.2
1	D	284	LEU	2.2
1	A	142	ASN	2.2
1	B	358	LYS	2.2
1	C	310	TYR	2.2
1	D	141	LYS	2.2
1	B	357	ILE	2.2
1	D	8	ILE	2.2
1	D	252	ILE	2.2
1	C	88	THR	2.2
1	A	114	SER	2.2
1	A	137	ASP	2.1
1	A	212	VAL	2.1
1	C	350	ALA	2.1
1	C	228	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	98	ASN	2.1
1	A	330	ASN	2.1
1	C	10	LYS	2.1
1	D	263	ASN	2.1
1	C	264	THR	2.1
1	C	260	TYR	2.1
1	D	248	ILE	2.1
1	D	347	ILE	2.1
1	C	53	ALA	2.1
1	C	181	ALA	2.1
1	D	71	ALA	2.1
1	C	78	LYS	2.1
1	C	308	LYS	2.1
1	C	330	ASN	2.1
1	D	86	ASP	2.1
1	C	250	ARG	2.1
1	D	122	PRO	2.1
1	D	73	ALA	2.1
1	D	114	SER	2.1
1	A	20	LEU	2.1
1	D	358	LYS	2.1
1	A	150	TYR	2.1
1	A	260	TYR	2.1
1	C	16	PHE	2.1
1	C	150	TYR	2.1
1	C	158	PHE	2.1
1	D	150	TYR	2.1
1	A	90	GLY	2.0
1	D	35	ASN	2.0
1	D	118	ALA	2.0
1	C	265	MET	2.0
1	C	103	GLN	2.0
1	A	317	SER	2.0
1	C	184	LEU	2.0
1	C	186	HIS	2.0
1	A	153	PRO	2.0
1	D	304	GLU	2.0
1	A	79	ASN	2.0
1	A	159	GLY	2.0
1	D	116	ASN	2.0
1	D	167	ASN	2.0
1	D	351	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	77	ALA	2.0
1	D	285	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

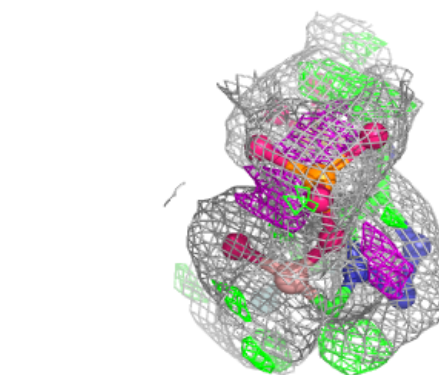
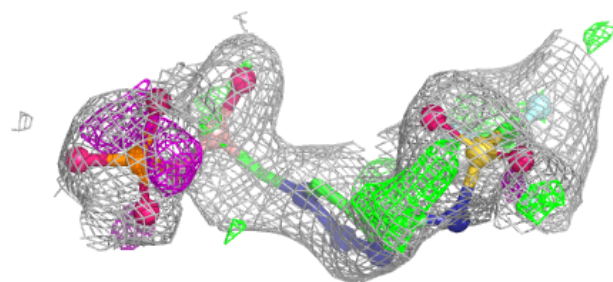
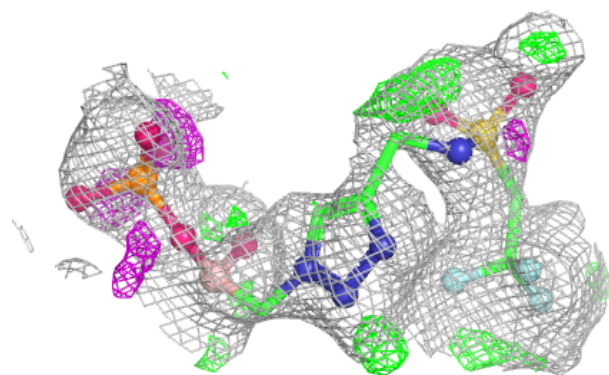
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	P1K	A	401[A]	23/23	0.78	0.19	35,45,61,62	23
2	P1K	A	401[B]	23/23	0.78	0.19	35,53,75,80	23
2	P1K	D	401	23/23	0.82	0.17	46,57,75,80	0
2	P1K	C	401	23/23	0.88	0.15	43,59,81,82	0
2	P1K	B	401	23/23	0.89	0.14	35,42,57,64	0

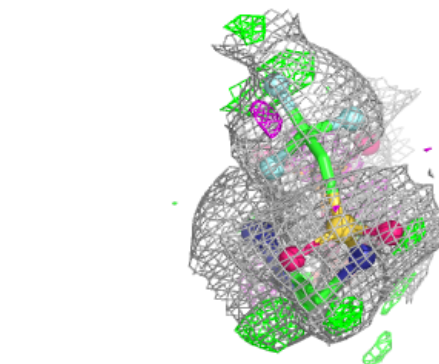
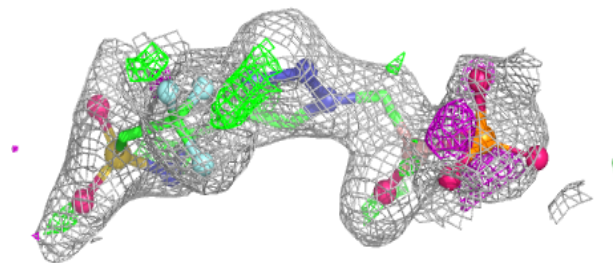
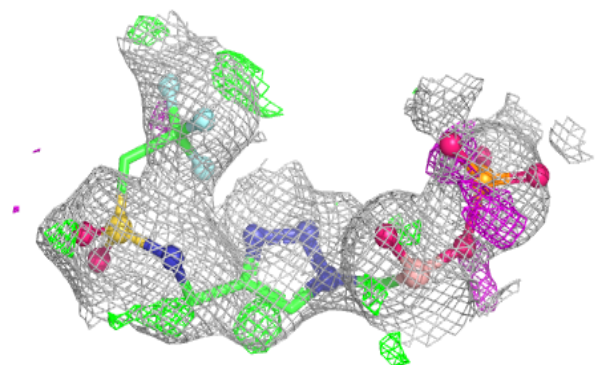
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P1K A 401 (A):

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

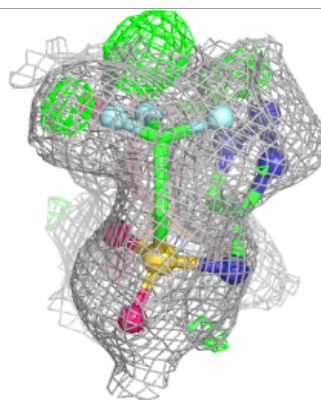
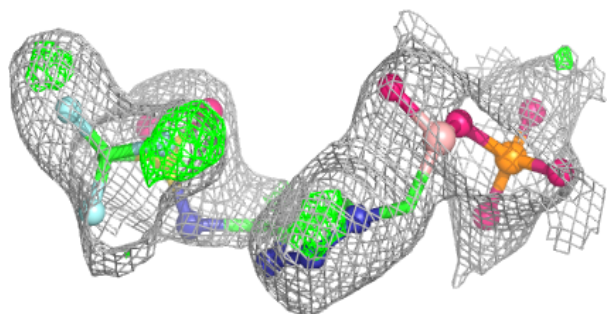
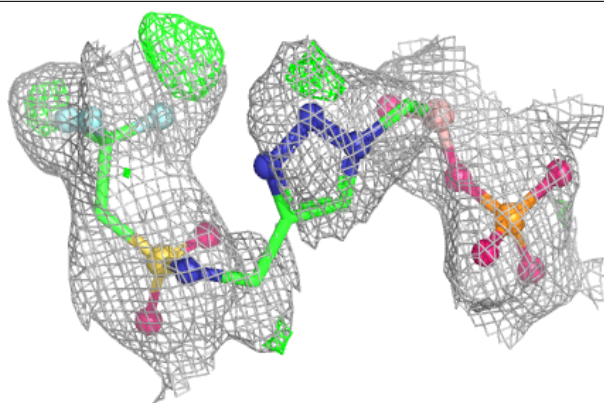
**Electron density around P1K A 401 (B):**

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

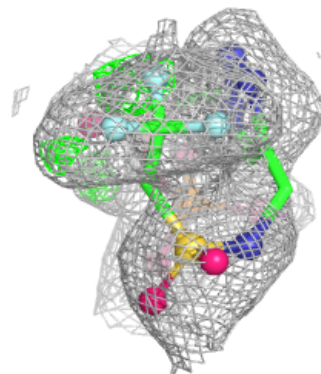
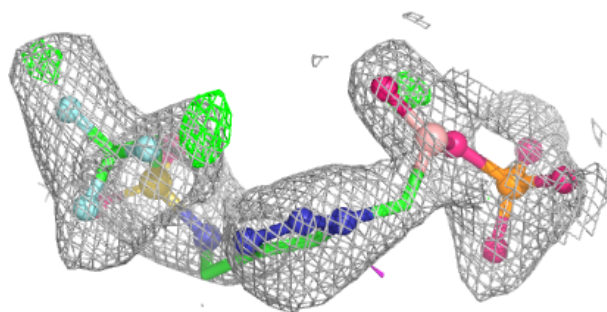
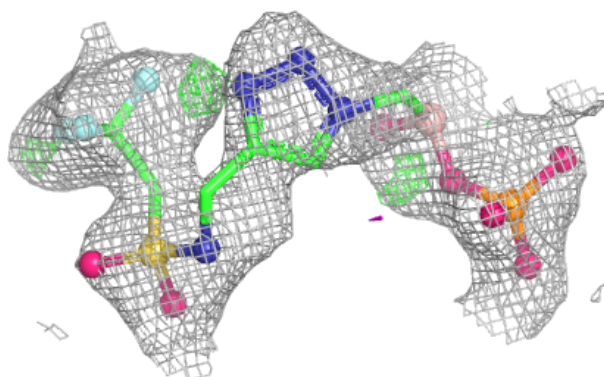


Electron density around P1K D 401:

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

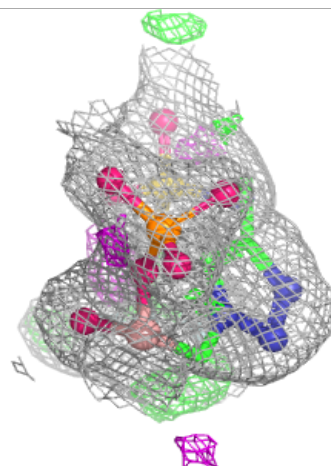
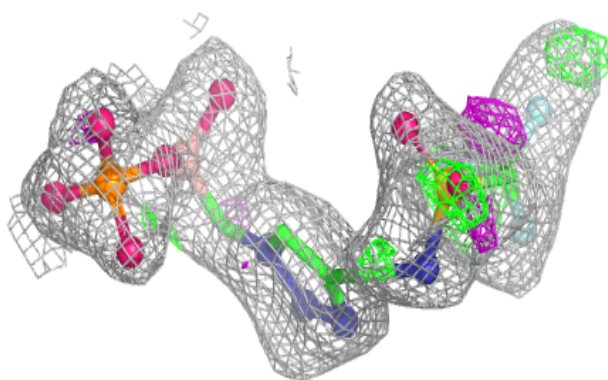
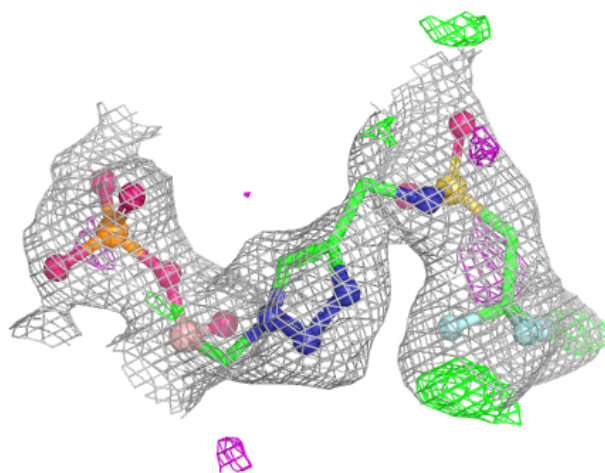
**Electron density around P1K C 401:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.