Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 08:08 PM EDT

PDB ID	:	5NEV
Title	:	CDK2/Cyclin A in complex with compound 73
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Deposited on	:	2017-03-12
Resolution	:	2.97 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 (1)) were used in the production of this report:

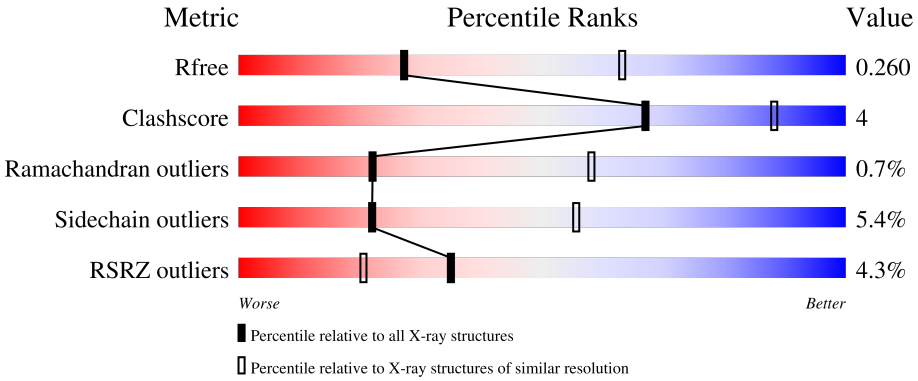
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	303	2% 76% 19%
1	C	303	4% 82% 14%
2	B	260	2% 89% 8%
2	D	260	9% 87% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8966 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2380	1544	403	424	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

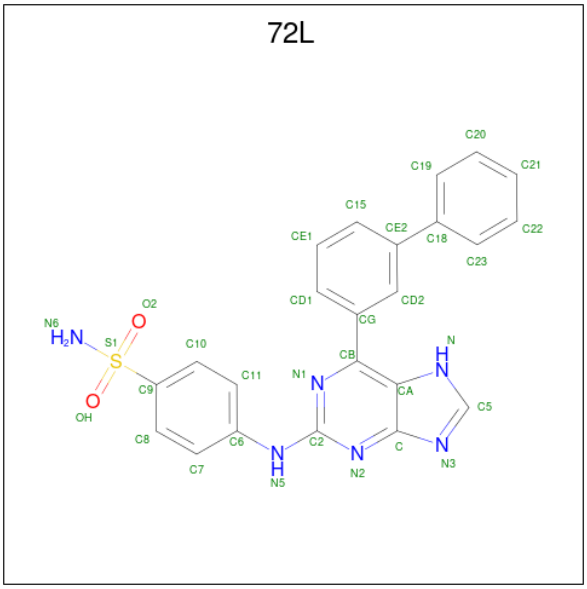
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	0	0
			2059	1334	335	379	11			
2	D	255	Total	C	N	O	S	0	0	0
			2059	1334	335	379	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	initiating methionine	UNP P20248
D	173	MET	-	initiating methionine	UNP P20248

- Molecule 3 is 4-[[6-(3-phenylphenyl)-7 {H}-purin-2-yl]amino]benzenesulfonamide (three-letter code: 72L) (formula: $C_{23}H_{18}N_6O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	23	6	2	1		
3	C	1	Total	C	N	O	S	0	0
			32	23	6	2	1		

- Molecule 4 is water.

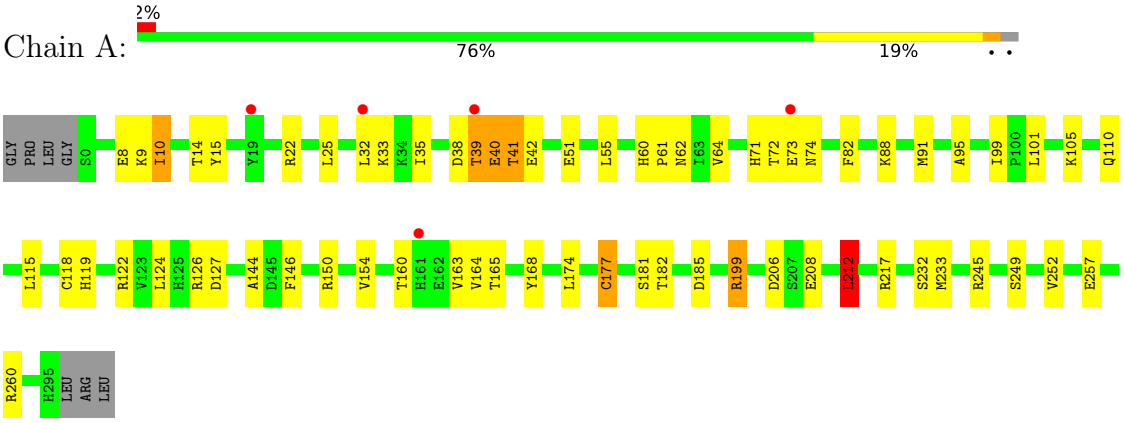
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	2	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

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.

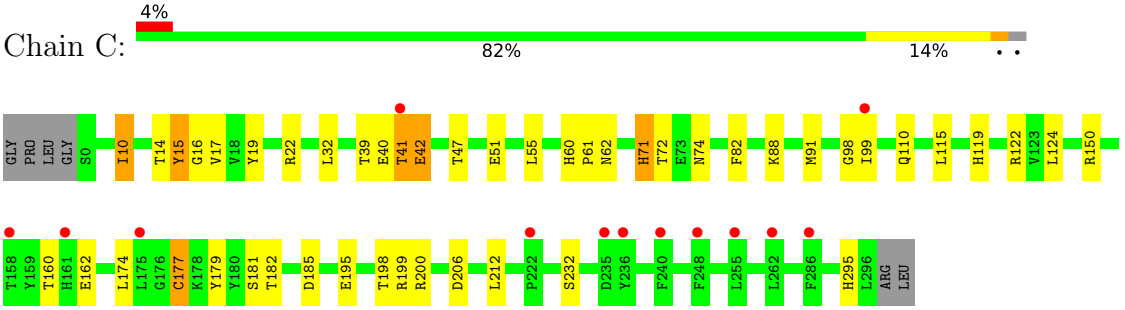
• Molecule 1: Cyclin-dependent kinase 2

Chain A:



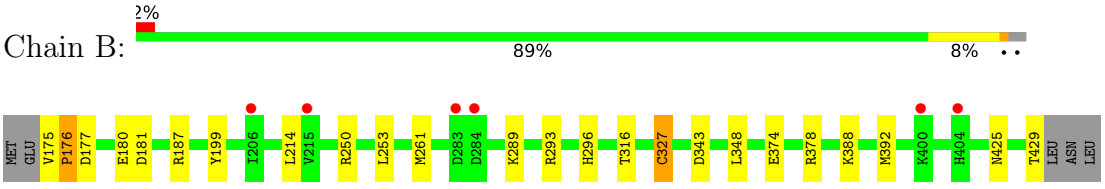
• Molecule 1: Cyclin-dependent kinase 2

Chain C:



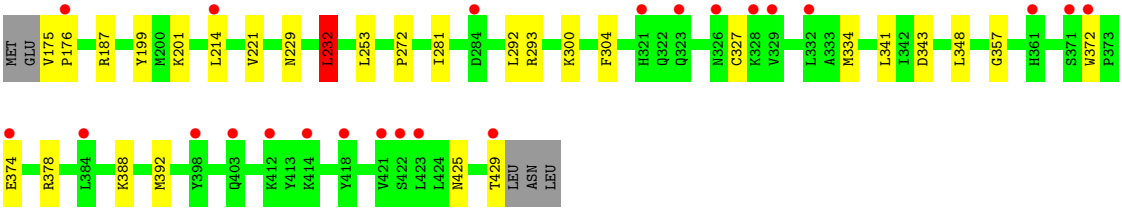
• Molecule 2: Cyclin-A2

Chain B:



• Molecule 2: Cyclin-A2

Chain D:


MET GLU V175 P176 R187 Y199 M200 K201 L214 V221 N229 L232 L253 P272 I281 D284 L292 R293 K300 F304 H321 Q322 Q323 N326 C327 K328 V329 L332 A333 M334 L341 I342 D343 L348 G357 H361 S371 W372 P373
E374 R378 L384 K388 M392 Y398 Q403 K412 Y413 K414 Y418 V421 S422 L423 L424 M425 T429 LEU ASN LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.53Å 132.05Å 149.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.03 – 2.97 66.03 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.03-2.97) 100.0 (66.03-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.218 , 0.261 0.216 , 0.260	Depositor DCC
R_{free} test set	1544 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	65.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8966	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: TPO, 72L

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.06	3/2430 (0.1%)	1.07	8/3297 (0.2%)
1	C	0.81	0/2438	0.97	2/3308 (0.1%)
2	B	0.92	4/2109 (0.2%)	0.93	6/2864 (0.2%)
2	D	0.73	0/2109	0.88	5/2864 (0.2%)
All	All	0.89	7/9086 (0.1%)	0.97	21/12333 (0.2%)

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	C	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	GLU	CG-CD	7.67	1.63	1.51
1	A	168	TYR	CE1-CZ	-6.70	1.29	1.38
2	B	374	GLU	CD-OE2	6.04	1.32	1.25
1	A	208	GLU	CD-OE2	5.34	1.31	1.25
2	B	176	PRO	N-CA	5.26	1.56	1.47
2	B	378	ARG	CD-NE	5.08	1.55	1.46
2	B	374	GLU	CD-OE1	5.05	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	378	ARG	CG-CD-NE	7.48	127.52	111.80
2	D	187	ARG	NE-CZ-NH2	-7.20	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	ARG	NE-CZ-NH2	6.52	123.56	120.30
2	D	187	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	22	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	D	232	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	22	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	22	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	212	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	A	245	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	199	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	B	250	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	B	187	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	245	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	126	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	261	MET	CG-SD-CE	5.23	108.57	100.20
2	D	378	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	B	327	CYS	CA-CB-SG	5.16	123.28	114.00
2	D	334	MET	CA-CB-CG	5.10	121.97	113.30
2	B	293	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	144	ALA	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	16	GLY	Peptide
1	C	71	HIS	Peptide

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	2380	0	2419	36	0
1	C	2388	0	2430	23	0
2	B	2059	0	2079	8	0
2	D	2059	0	2079	9	0
3	A	32	0	0	1	0
3	C	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8966	0	9007	70	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 4.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:CYS:SG	1:A:233:MET:CE	2.21	1.27
1:A:177:CYS:SG	1:A:233:MET:HE3	1.77	1.25
1:A:15:TYR:OH	1:A:51:GLU:OE1	1.83	0.95
1:C:40:GLU:O	1:C:42:GLU:N	1.99	0.95
1:A:177:CYS:SG	1:A:233:MET:HE1	2.15	0.84
1:A:39:THR:HG21	2:B:289:LYS:HD3	1.66	0.78
1:C:15:TYR:OH	1:C:51:GLU:OE1	2.05	0.71
1:A:174:LEU:HB3	1:A:212:LEU:HD12	1.74	0.69
1:A:40:GLU:O	1:A:42:GLU:N	2.21	0.69
1:A:25:LEU:HD11	2:D:293:ARG:HB3	1.76	0.68
1:A:154:VAL:O	2:B:316:THR:HG22	1.96	0.65
1:C:10:ILE:HD11	1:C:82:PHE:HE1	1.63	0.61
2:D:214:LEU:HD22	2:D:253:LEU:HG	1.83	0.60
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.84	0.59
1:C:15:TYR:HD2	1:C:47:THR:HG1	1.50	0.58
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.04	0.57
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.69	0.57
1:A:177:CYS:HG	1:A:233:MET:CE	2.17	0.56
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.88	0.56
1:C:195:GLU:O	1:C:198:THR:O	2.24	0.56
1:C:15:TYR:OH	1:C:51:GLU:CD	2.45	0.55
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.88	0.55
1:C:181:SER:OG	1:C:182:THR:N	2.39	0.54
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.43	0.54
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.90	0.53
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.77	0.52
1:C:51:GLU:O	1:C:55:LEU:HB2	2.10	0.52
1:A:15:TYR:OH	1:A:51:GLU:CD	2.49	0.51
1:A:181:SER:OG	1:A:182:THR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.25	0.51
1:A:177:CYS:HG	1:A:233:MET:HE1	1.72	0.51
1:A:15:TYR:CD1	1:A:35:ILE:CD1	2.95	0.50
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.28	0.49
1:C:177:CYS:SG	1:C:179:TYR:O	2.71	0.49
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.48	0.48
1:C:17:VAL:HG13	1:C:19:TYR:CE1	2.48	0.48
1:A:51:GLU:O	1:A:55:LEU:HB2	2.14	0.48
1:A:64:VAL:HG11	3:A:301:72L:C5	2.44	0.47
1:A:15:TYR:CE1	1:A:33:LYS:HD3	2.49	0.47
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.96	0.47
1:C:119:HIS:CD2	1:C:182:THR:HB	2.50	0.47
1:A:177:CYS:SG	1:A:233:MET:HE2	2.41	0.47
1:A:119:HIS:CD2	1:A:182:THR:HB	2.51	0.46
1:C:60:HIS:CD2	1:C:62:ASN:H	2.34	0.46
1:A:95:ALA:O	1:A:199:ARG:NH1	2.49	0.45
1:C:60:HIS:HD2	1:C:62:ASN:H	1.64	0.44
1:A:60:HIS:CD2	1:A:62:ASN:H	2.35	0.44
1:C:91:MET:HG2	1:C:99:ILE:HD11	1.99	0.44
2:D:221:VAL:HG21	2:D:281:ILE:HD13	2.00	0.44
1:C:174:LEU:HB3	1:C:212:LEU:HD13	1.99	0.44
1:C:198:THR:O	1:C:198:THR:OG1	2.36	0.43
1:A:101:LEU:CD1	1:A:105:LYS:HE3	2.48	0.43
2:D:232:LEU:HD13	2:D:341:LEU:HD12	2.00	0.43
2:D:388:LYS:O	2:D:392:MET:HG2	2.19	0.43
1:C:17:VAL:HG13	1:C:19:TYR:HE1	1.84	0.43
1:A:60:HIS:HD2	1:A:62:ASN:H	1.65	0.43
1:A:38:ASP:HB2	1:A:41:THR:HG22	2.00	0.42
1:A:39:THR:CG2	2:B:289:LYS:HD3	2.44	0.42
2:B:388:LYS:O	2:B:392:MET:HG2	2.19	0.42
1:C:15:TYR:HD2	1:C:47:THR:OG1	2.03	0.42
1:A:40:GLU:C	1:A:42:GLU:N	2.73	0.42
1:A:118:CYS:HG	1:A:146:PHE:HE1	1.67	0.42
1:C:71:HIS:NE2	2:D:304:PHE:CE2	2.87	0.42
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.55	0.42
1:A:164:VAL:HG12	1:A:165:THR:N	2.35	0.41
1:A:249:SER:HA	1:A:260:ARG:HD3	2.03	0.41
2:B:175:VAL:HG13	2:B:175:VAL:O	2.21	0.41
2:D:175:VAL:HG13	2:D:175:VAL:O	2.21	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.40
2:D:357:GLY:HA2	2:D:372:TRP:CZ3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/303 (97%)	276 (94%)	13 (4%)	4 (1%)	11	41
1	C	294/303 (97%)	280 (95%)	12 (4%)	2 (1%)	22	58
2	B	253/260 (97%)	246 (97%)	6 (2%)	1 (0%)	34	70
2	D	253/260 (97%)	247 (98%)	5 (2%)	1 (0%)	34	70
All	All	1093/1126 (97%)	1049 (96%)	36 (3%)	8 (1%)	22	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	C	39	THR
1	C	41	THR
1	A	39	THR
2	D	176	PRO
1	A	177	CYS
1	A	40	GLU
2	B	176	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	260/265 (98%)	243 (94%)	17 (6%)	17 48
1	C	261/265 (98%)	243 (93%)	18 (7%)	15 46
2	B	229/234 (98%)	222 (97%)	7 (3%)	40 73
2	D	229/234 (98%)	218 (95%)	11 (5%)	25 60
All	All	979/998 (98%)	926 (95%)	53 (5%)	22 55

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	LYS
1	A	10	ILE
1	A	14	THR
1	A	32	LEU
1	A	72	THR
1	A	73	GLU
1	A	74	ASN
1	A	88	LYS
1	A	122	ARG
1	A	124	LEU
1	A	150	ARG
1	A	163	VAL
1	A	206	ASP
1	A	212	LEU
1	A	232	SER
1	A	252	VAL
2	B	177	ASP
2	B	180	GLU
2	B	181	ASP
2	B	327	CYS
2	B	343	ASP
2	B	425	ASN
2	B	429	THR
1	C	10	ILE
1	C	14	THR
1	C	15	TYR
1	C	32	LEU
1	C	41	THR
1	C	42	GLU
1	C	72	THR
1	C	74	ASN
1	C	88	LYS

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Mol	Chain	Res	Type
1	C	122	ARG
1	C	124	LEU
1	C	150	ARG
1	C	162	GLU
1	C	177	CYS
1	C	200	ARG
1	C	206	ASP
1	C	232	SER
1	C	295	HIS
2	D	201	LYS
2	D	229	ASN
2	D	232	LEU
2	D	272	PRO
2	D	292	LEU
2	D	300	LYS
2	D	327	CYS
2	D	343	ASP
2	D	374	GLU
2	D	425	ASN
2	D	429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	119	HIS
2	B	179	HIS
2	B	317	GLN
2	B	322	GLN
2	B	370	GLN
2	B	396	GLN
2	B	419	HIS
1	C	5	GLN
1	C	60	HIS
1	C	119	HIS
1	C	125	HIS
2	D	233	HIS
2	D	317	GLN
2	D	322	GLN
2	D	370	GLN
2	D	396	GLN

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Mol	Chain	Res	Type
2	D	419	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	A	160	1	8,10,11	1.15	0	10,14,16	1.81	3 (30%)
1	TPO	C	160	1	8,10,11	0.80	0	10,14,16	1.55	1 (10%)

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
1	TPO	A	160	1	-	1/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	P-OG1-CB	-3.42	112.87	123.21
1	A	160	TPO	P-OG1-CB	-3.28	113.29	123.21
1	A	160	TPO	O2P-P-O1P	2.23	119.43	110.68
1	A	160	TPO	O-C-CA	-2.08	119.33	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	72L	C	301	-	33,36,36	1.50	4 (12%)	41,52,52	1.79	10 (24%)
3	72L	A	301	-	33,36,36	1.60	6 (18%)	41,52,52	2.61	18 (43%)

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
3	72L	C	301	-	-	4/18/18/18	0/5/5/5
3	72L	A	301	-	-	8/18/18/18	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	72L	S1-N6	4.96	1.70	1.60
3	C	301	72L	C2-N5	4.25	1.45	1.36
3	A	301	72L	CB-N1	4.03	1.36	1.32
3	A	301	72L	C2-N5	3.64	1.43	1.36
3	A	301	72L	S1-N6	3.46	1.67	1.60
3	C	301	72L	CB-N1	3.26	1.35	1.32
3	A	301	72L	C9-S1	-2.93	1.72	1.77
3	A	301	72L	C6-N5	2.77	1.46	1.40
3	A	301	72L	CA-N	2.28	1.48	1.39
3	C	301	72L	C6-N5	2.27	1.45	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	72L	C9-S1-N6	-7.20	98.20	108.38
3	A	301	72L	O2-S1-C9	6.12	114.18	107.35
3	A	301	72L	O2-S1-OH	-5.75	109.31	118.76
3	C	301	72L	O2-S1-OH	-4.99	110.56	118.76
3	C	301	72L	CG-CB-N1	4.49	119.88	115.50
3	A	301	72L	O2-S1-N6	4.41	113.90	107.36
3	A	301	72L	N2-C2-N1	-4.36	119.33	126.23
3	C	301	72L	N2-C2-N1	-4.13	119.70	126.23
3	A	301	72L	C2-N2-C	4.09	119.92	115.28
3	A	301	72L	CG-CB-N1	3.89	119.29	115.50
3	A	301	72L	C15-CE2-CD2	3.23	122.73	118.16
3	C	301	72L	O2-S1-C9	3.15	110.87	107.35
3	C	301	72L	C8-C9-S1	3.12	124.26	119.73
3	C	301	72L	C-CA-N	-2.96	106.32	109.40
3	C	301	72L	C2-N2-C	2.96	118.64	115.28
3	C	301	72L	OH-S1-C9	2.90	110.58	107.35
3	A	301	72L	C23-C18-C19	2.86	123.30	117.59
3	A	301	72L	OH-S1-C9	2.62	110.28	107.35
3	A	301	72L	C19-C18-CE2	-2.61	116.83	121.36
3	A	301	72L	CD1-CG-CB	2.55	124.81	120.65
3	C	301	72L	C10-C9-S1	-2.35	116.32	119.73
3	A	301	72L	C-CA-N	-2.32	106.98	109.40
3	A	301	72L	CD2-CE2-C18	-2.27	117.11	120.86
3	A	301	72L	C6-N5-C2	-2.26	122.67	129.23
3	A	301	72L	C8-C9-S1	-2.24	116.49	119.73
3	A	301	72L	C20-C19-C18	-2.17	117.83	120.56
3	A	301	72L	OH-S1-N6	2.16	110.57	107.36
3	C	301	72L	C6-N5-C2	-2.05	123.28	129.23

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	72L	N1-CB-CG-CD1
3	A	301	72L	N1-CB-CG-CD2
3	A	301	72L	CA-CB-CG-CD1
3	A	301	72L	CA-CB-CG-CD2
3	C	301	72L	N1-CB-CG-CD1
3	C	301	72L	CA-CB-CG-CD1
3	C	301	72L	CA-CB-CG-CD2
3	A	301	72L	C23-C18-CE2-C15
3	A	301	72L	C19-C18-CE2-C15
3	A	301	72L	C19-C18-CE2-CD2
3	A	301	72L	C23-C18-CE2-CD2
3	C	301	72L	N1-CB-CG-CD2

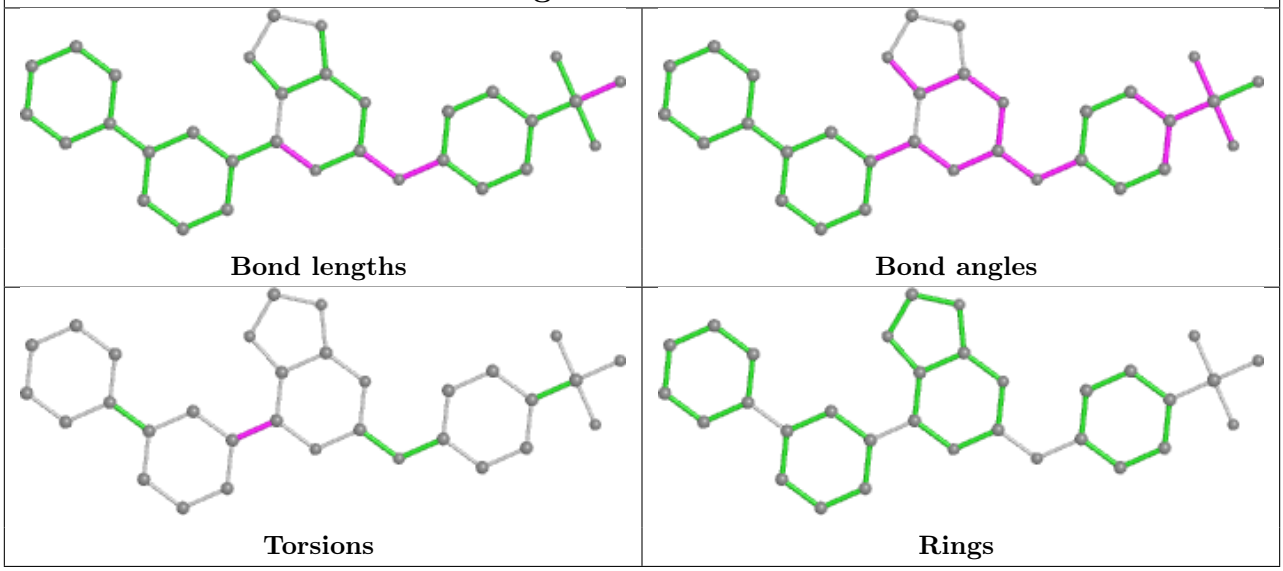
There are no ring outliers.

1 monomer is involved in 1 short contact:

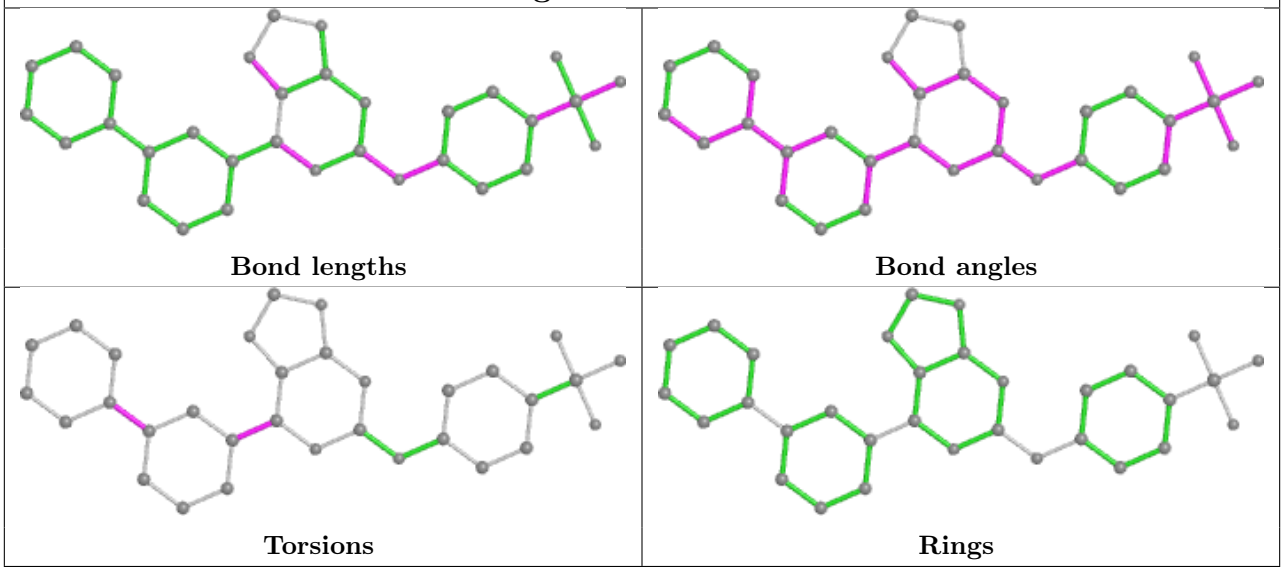
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	72L	1	0

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 72L C 301



Ligand 72L A 301



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	295/303 (97%)	0.16	5 (1%) 70 50	36, 58, 105, 128	0
1	C	296/303 (97%)	0.53	13 (4%) 34 20	65, 92, 130, 152	0
2	B	255/260 (98%)	0.32	6 (2%) 59 39	40, 64, 88, 103	0
2	D	255/260 (98%)	0.56	23 (9%) 9 5	64, 101, 151, 171	0
All	All	1101/1126 (97%)	0.39	47 (4%) 35 20	36, 79, 133, 171	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	6.4
2	D	422	SER	4.7
2	D	326	ASN	4.1
1	C	161	HIS	4.1
2	D	403	GLN	3.7
1	C	235	ASP	3.4
2	D	214	LEU	3.3
2	D	412	LYS	3.3
2	D	372	TRP	3.3
1	C	41	THR	3.2
1	C	99	ILE	3.0
2	D	418	TYR	3.0
2	D	332	LEU	2.9
1	C	175	LEU	2.9
1	C	255	LEU	2.8
1	A	32	LEU	2.7
2	D	423	LEU	2.7
1	C	158	THR	2.7
2	D	321	HIS	2.7
1	C	286	PHE	2.6
1	A	161	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	236	TYR	2.5
1	A	19	TYR	2.5
1	C	222	PRO	2.5
2	D	284	ASP	2.5
2	D	176	PRO	2.4
2	D	384	LEU	2.5
2	D	323	GLN	2.4
2	D	328	LYS	2.4
2	D	329	VAL	2.3
2	D	421	VAL	2.3
1	C	262	LEU	2.3
1	C	240	PHE	2.3
2	B	283	ASP	2.3
2	D	429	THR	2.3
2	B	284	ASP	2.3
1	C	248	PHE	2.3
2	D	371	SER	2.2
2	B	400	LYS	2.2
1	A	73	GLU	2.2
2	B	206	ILE	2.2
2	D	374	GLU	2.1
2	D	361	HIS	2.1
2	D	398	TYR	2.1
2	D	414	LYS	2.1
2	B	404	HIS	2.0
2	B	215	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPO	C	160	11/12	0.96	0.17	86,92,97,99	0
1	TPO	A	160	11/12	0.98	0.17	51,54,56,58	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

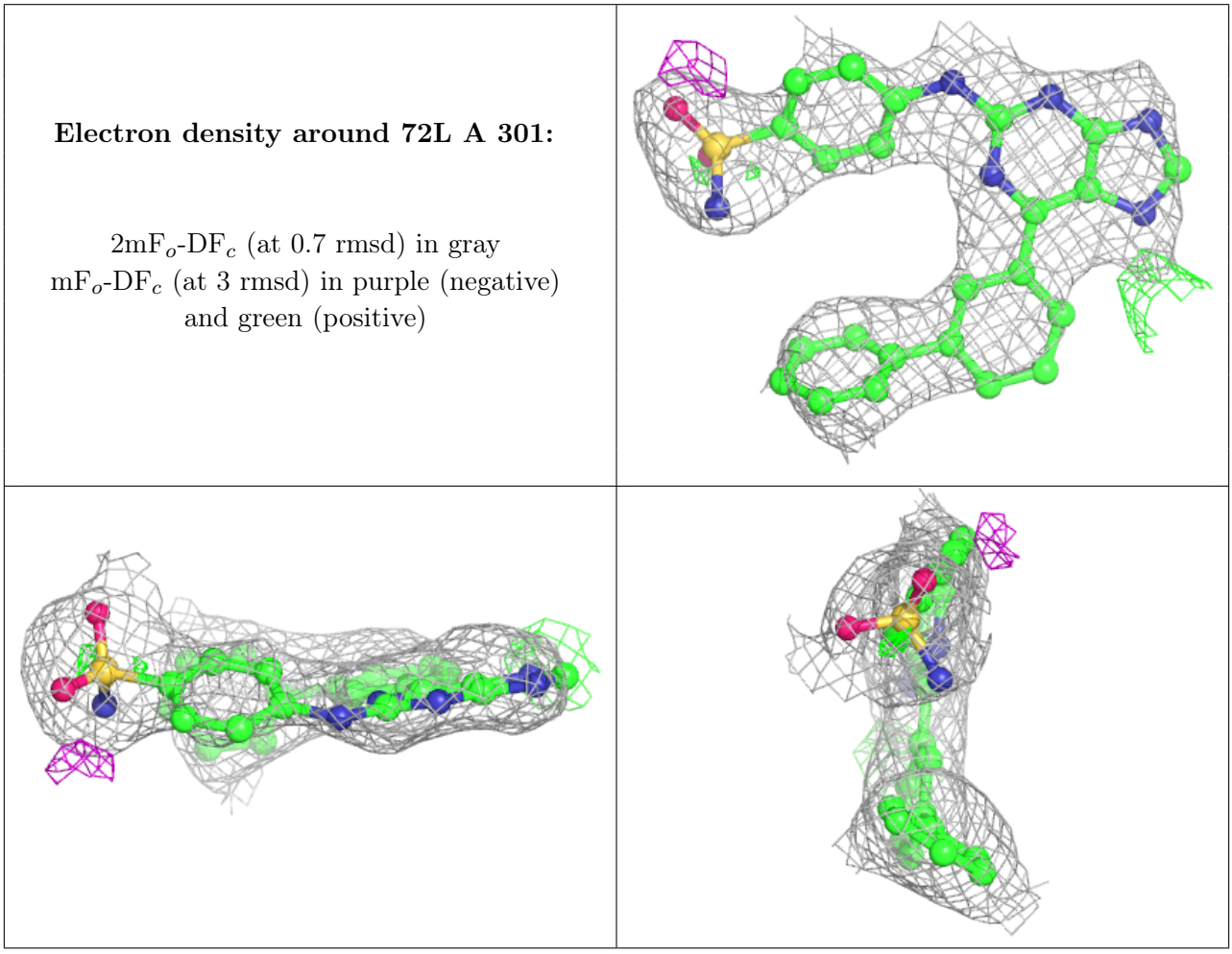
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	72L	A	301	32/32	0.89	0.28	99,115,129,130	0
3	72L	C	301	32/32	0.90	0.43	111,128,146,147	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.

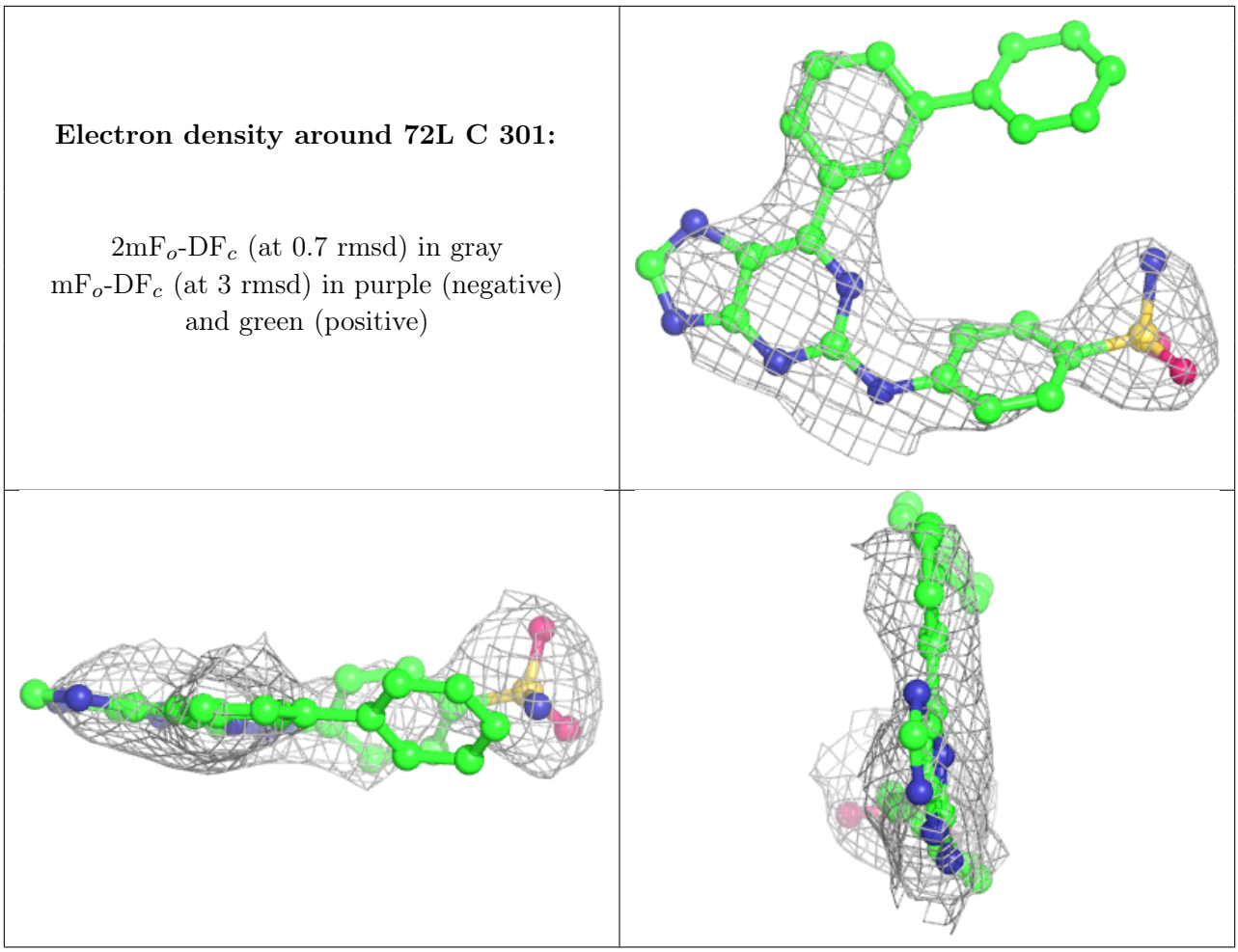
Electron density around 72L A 301:

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



Electron density around 72L C 301:

$2mF_o$-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.