



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:59 PM EDT

PDB ID : 4EOR / pdb_00004eor
Title : Thr 160 phosphorylated CDK2 WT - human cyclin A3 complex with the inhibitor NU6102
Authors : Echalier, A.; Cot, E.; Camasses, A.; Hodimont, E.; Hoh, F.; Sheinerman, F.; Krasinska, L.; Fisher, D.
Deposited on : 2012-04-14
Resolution : 2.20 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

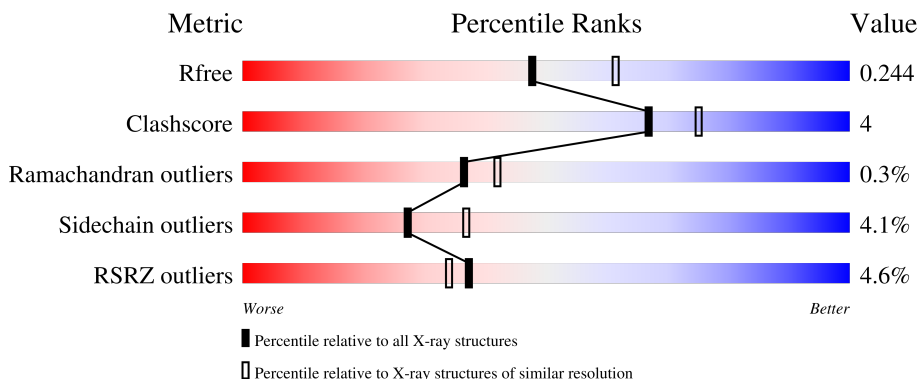
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

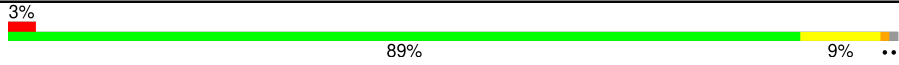



The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	298	 3% 89% 9% ..
1	C	298	 6% 74% 13% 9%
2	B	258	 3% 88% 10% .
2	D	258	 5% 88% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8899 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	
			Total	C	N	O	P				S
1	A	294	2401	1560	412	420	1	8	0	3	0
1	C	271	2171	1406	370	387	1	7	0	1	0

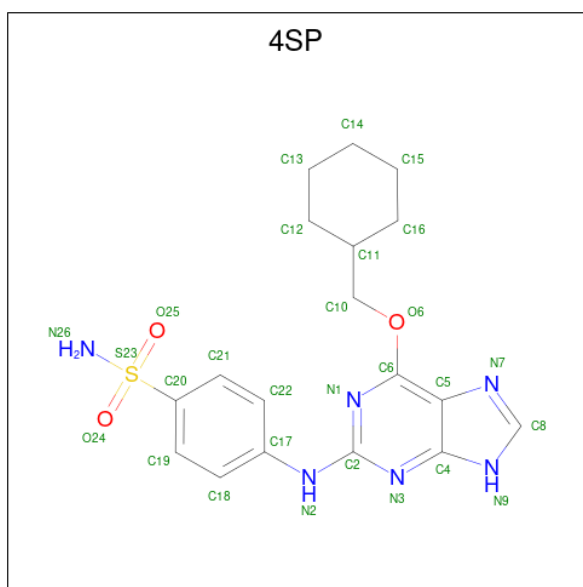
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	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
			Total	C	N	O	S			
2	B	257	2083	1349	339	384	11	0	1	0
2	D	255	2059	1334	335	379	11	0	0	0

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (CCD ID: 4SP) (formula: C₁₈H₂₂N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	28	18	6	3	1	0	0
3	C	1	28	18	6	3	1	0	0

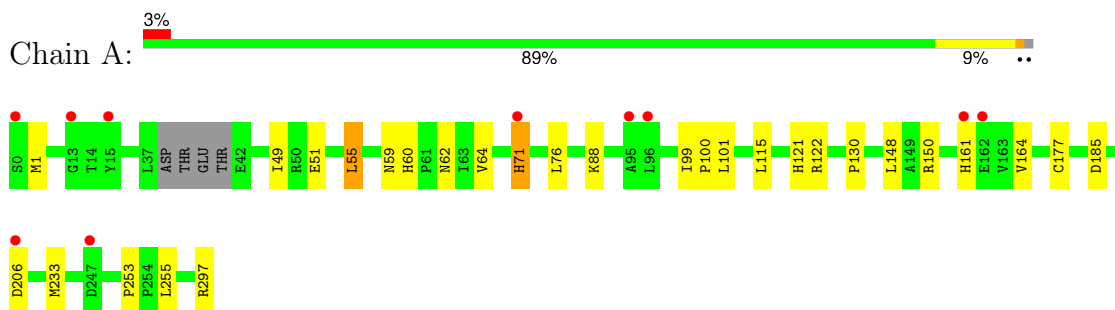
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	52	52	52	0	0
4	B	46	46	46	0	0
4	C	19	19	19	0	0
4	D	12	12	12	0	0

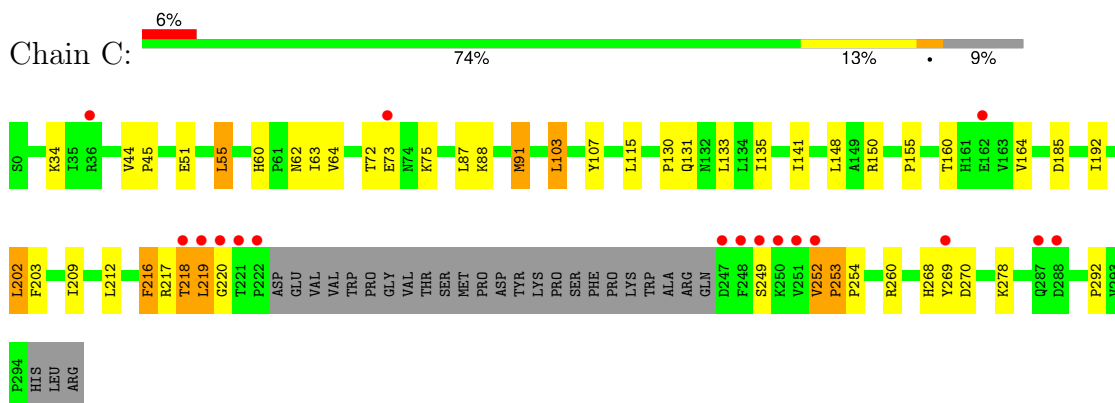
3 Residue-property plots [i](#)

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.

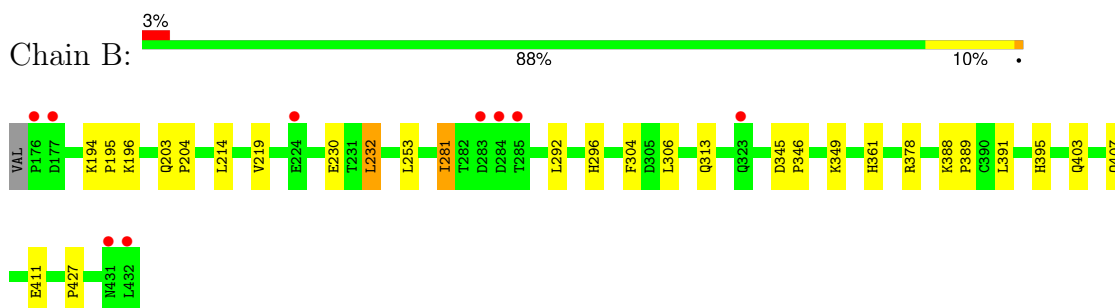
- Molecule 1: Cyclin-dependent kinase 2



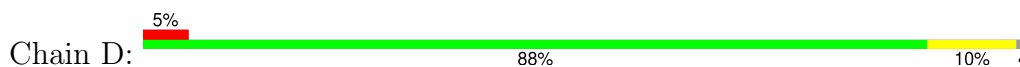
- Molecule 1: Cyclin-dependent kinase 2

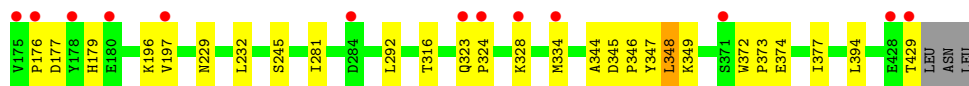


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.97Å 135.44Å 149.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.00-2.20) 89.0 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.245 0.218 , 0.244	Depositor DCC
R_{free} test set	3851 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8899	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4SP, TPO

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	0.49	0/2452	0.80	1/3323 (0.0%)
1	C	0.51	0/2210	0.84	5/2994 (0.2%)
2	B	0.47	0/2133	0.82	0/2896
2	D	0.44	0/2109	0.83	0/2864
All	All	0.48	0/8904	0.82	6/12077 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	GLY	N-CA-C	9.76	128.48	111.50
1	C	253	PRO	N-CA-C	6.41	118.52	110.70
1	C	252	VAL	CA-C-N	5.95	126.51	120.38
1	C	252	VAL	C-N-CA	5.95	126.51	120.38
1	A	253	PRO	N-CA-C	5.93	117.94	110.70
1	C	219	LEU	N-CA-CB	-5.14	101.76	110.50

There are no chirality outliers.

There are no planarity outliers.

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	2401	0	2444	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2171	0	2207	29	0
2	B	2083	0	2105	14	0
2	D	2059	0	2079	10	0
3	A	28	0	22	2	0
3	C	28	0	22	2	0
4	A	52	0	0	0	0
4	B	46	0	0	0	0
4	C	19	0	0	1	0
4	D	12	0	0	0	0
All	All	8899	0	8879	65	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 (65) 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:C:218:THR:HB	1:C:219:LEU:CB	2.14	0.77
1:C:218:THR:CA	1:C:219:LEU:CB	2.70	0.68
1:C:219:LEU:H	1:C:269:TYR:HE2	1.42	0.68
1:C:60:HIS:HD2	1:C:62:ASN:H	1.40	0.67
1:A:60:HIS:HD2	1:A:62:ASN:H	1.40	0.67
1:A:60:HIS:CD2	1:A:62:ASN:H	2.15	0.65
1:C:60:HIS:CD2	1:C:62:ASN:H	2.15	0.64
1:C:218:THR:CB	1:C:219:LEU:CB	2.79	0.60
1:C:218:THR:HG21	1:C:249:SER:O	2.01	0.59
1:C:218:THR:HA	1:C:219:LEU:CB	2.34	0.57
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.87	0.57
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.89	0.54
1:A:64:VAL:HG21	3:A:301:ASP:C8	2.38	0.53
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.43	0.53
1:A:177:CYS:HB2	1:A:233:MET:CE	2.40	0.52
1:C:64:VAL:HG21	3:C:301:ASP:C8	2.40	0.52
2:D:176:PRO:HA	2:D:179:HIS:CE1	2.46	0.51
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.93	0.51
1:C:64:VAL:HG21	3:C:301:ASP:H8	1.93	0.50
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.94	0.49
2:D:346:PRO:O	2:D:349:LYS:HG2	2.11	0.49
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.93	0.49
1:C:155:PRO:HD2	2:D:316:THR:HB	1.96	0.48
1:C:216:PHE:O	1:C:219:LEU:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:HIS:HE1	2:B:427:PRO:O	1.97	0.47
1:A:71:HIS:CE1	2:B:304:PHE:HZ	2.33	0.47
1:C:107:TYR:CZ	1:C:135:ILE:HD12	2.50	0.47
1:A:64:VAL:HG21	3:A:301:ASP:H8	1.95	0.47
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.97	0.47
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.97	0.47
1:C:268:HIS:HD2	1:C:270:ASP:H	1.62	0.46
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.97	0.46
1:C:252:VAL:H	1:C:260:ARG:HD3	1.81	0.46
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.52	0.45
2:B:345:ASP:HA	2:B:346:PRO:HA	1.71	0.45
1:C:87:LEU:O	1:C:91:MET:HG2	2.16	0.45
1:C:103:LEU:HD23	1:C:292:PRO:HG2	1.99	0.44
1:C:72:THR:HG22	1:C:73:GLU:H	1.82	0.44
2:D:372:TRP:HA	2:D:373:PRO:HD3	1.81	0.44
1:C:51:GLU:O	1:C:55:LEU:HB2	2.18	0.43
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.93	0.42
2:D:345:ASP:HA	2:D:346:PRO:HA	1.82	0.42
2:B:281:ILE:H	2:B:281:ILE:HG13	1.75	0.42
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
2:D:347:TYR:OH	2:D:394:LEU:HA	2.20	0.42
2:B:346:PRO:O	2:B:349:LYS:HG2	2.19	0.42
1:C:34:LYS:HD3	1:C:75:LYS:HE3	2.01	0.42
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.02	0.42
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.02	0.42
2:D:229:ASN:HD22	2:D:334:MET:HE2	1.83	0.42
1:A:99:ILE:HA	1:A:100:PRO:HD2	1.92	0.42
1:A:115:LEU:HD21	1:A:185:ASP:HB3	2.00	0.42
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.02	0.41
1:C:115:LEU:HD21	1:C:185:ASP:HB3	2.01	0.41
1:C:135:ILE:HD11	1:C:141:ILE:HD12	2.02	0.41
1:C:60:HIS:HB3	1:C:63:ILE:HD12	2.02	0.41
1:A:161[A]:HIS:CD2	1:A:161[A]:HIS:C	2.98	0.41
1:C:135:ILE:HG23	4:C:402:HOH:O	2.19	0.41
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.92	0.41
2:B:203:GLN:HA	2:B:204:PRO:HD3	1.95	0.41
2:B:407:GLN:O	2:B:411:GLU:HG2	2.21	0.41
2:D:323:GLN:HA	2:D:324:PRO:HA	1.85	0.41
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.54	0.40
1:A:121:HIS:C	1:A:122:ARG:HG3	2.46	0.40
1:C:202:LEU:HD12	1:C:203:PHE:CZ	2.57	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	292/298 (98%)	284 (97%)	7 (2%)	1 (0%)	36	42
1	C	267/298 (90%)	253 (95%)	12 (4%)	2 (1%)	18	19
2	B	256/258 (99%)	255 (100%)	1 (0%)	0	100	100
2	D	253/258 (98%)	249 (98%)	4 (2%)	0	100	100
All	All	1068/1112 (96%)	1041 (98%)	24 (2%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL
1	C	216	PHE

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	261/262 (100%)	251 (96%)	10 (4%)	29	40
1	C	235/262 (90%)	223 (95%)	12 (5%)	21	27
2	B	232/232 (100%)	225 (97%)	7 (3%)	36	49
2	D	229/232 (99%)	219 (96%)	10 (4%)	25	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	957/988 (97%)	918 (96%)	39 (4%)	27 37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	55	LEU
1	A	59	ASN
1	A	71	HIS
1	A	101	LEU
1	A	148	LEU
1	A	150	ARG
1	A	206	ASP
1	A	255	LEU
1	A	297	ARG
2	B	196	LYS
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	296	HIS
2	B	378	ARG
2	B	403	GLN
1	C	55	LEU
1	C	91	MET
1	C	103	LEU
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
1	C	202	LEU
1	C	209	ILE
1	C	212	LEU
1	C	217	ARG
1	C	218	THR
1	C	278	LYS
2	D	177	ASP
2	D	196	LYS
2	D	197	VAL
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	292	LEU
2	D	328	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	348	LEU
2	D	429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	84	HIS
1	A	246	GLN
1	A	265	GLN
1	A	268	HIS
2	B	228	GLN
2	B	254	GLN
2	B	290	GLN
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	60	HIS
1	C	71	HIS
1	C	74	ASN
1	C	265	GLN
1	C	268	HIS
2	D	254	GLN
2	D	317	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](#)

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	C	160	1	8,10,11	0.88	0	10,14,16	1.02	1 (10%)
1	TPO	A	160	1	8,10,11	0.83	0	10,14,16	1.15	0

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	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O3P-P-O2P	2.12	115.76	107.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	4SP	C	301	-	31,31,31	2.51	8 (25%)	43,44,44	2.07	10 (23%)
3	4SP	A	301	-	31,31,31	3.48	9 (29%)	43,44,44	2.41	15 (34%)

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	4SP	C	301	-	-	3/15/23/23	0/4/4/4
3	4SP	A	301	-	-	4/15/23/23	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	4SP	C20-S23	-12.90	1.57	1.77
3	C	301	4SP	C20-S23	-10.26	1.61	1.77
3	A	301	4SP	S23-N26	-9.02	1.42	1.60
3	C	301	4SP	C5-C4	5.02	1.47	1.39
3	A	301	4SP	C5-N7	-4.97	1.30	1.39
3	A	301	4SP	C4-N9	-4.33	1.30	1.36
3	C	301	4SP	S23-N26	-4.13	1.52	1.60
3	A	301	4SP	C5-C6	-3.70	1.34	1.41
3	A	301	4SP	C17-N2	-3.70	1.32	1.40
3	A	301	4SP	O24-S23	-3.45	1.37	1.43
3	A	301	4SP	O25-S23	-3.31	1.37	1.43
3	C	301	4SP	C6-N1	2.84	1.36	1.32
3	C	301	4SP	O25-S23	2.44	1.48	1.43
3	C	301	4SP	O24-S23	2.39	1.47	1.43
3	A	301	4SP	C5-C4	2.34	1.42	1.39
3	C	301	4SP	C5-N7	-2.34	1.34	1.39
3	C	301	4SP	C8-N7	2.06	1.36	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	4SP	O25-S23-O24	-6.48	108.84	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	4SP	O25-S23-C20	6.18	114.34	107.35
3	A	301	4SP	O24-S23-C20	5.55	113.62	107.35
3	A	301	4SP	O25-S23-O24	-5.37	110.53	118.80
3	C	301	4SP	C2-N1-C6	4.76	123.58	115.38
3	C	301	4SP	C5-C4-N3	-4.64	122.00	126.55
3	A	301	4SP	C5-C4-N3	-4.30	122.34	126.55
3	A	301	4SP	C2-N1-C6	4.29	122.77	115.38
3	A	301	4SP	C5-N7-C8	3.87	107.84	103.48
3	A	301	4SP	C5-C6-N1	-3.61	118.66	123.49
3	C	301	4SP	C5-N7-C8	3.58	107.52	103.48
3	C	301	4SP	C5-C6-N1	-3.56	118.72	123.49
3	C	301	4SP	N3-C2-N1	-3.44	120.62	126.26
3	A	301	4SP	C4-C5-N7	-3.24	106.17	110.67
3	C	301	4SP	C4-C5-N7	-3.23	106.18	110.67
3	A	301	4SP	C13-C12-C11	-3.21	105.33	112.08
3	A	301	4SP	O6-C6-C5	3.14	120.88	116.73
3	A	301	4SP	C6-C5-N7	2.93	137.27	133.82
3	C	301	4SP	C6-C5-N7	2.68	136.97	133.82
3	C	301	4SP	O25-S23-C20	2.65	110.35	107.35
3	A	301	4SP	C18-C19-C20	2.58	121.94	119.44
3	C	301	4SP	O6-C6-C5	2.40	119.90	116.73
3	A	301	4SP	N3-C2-N1	-2.35	122.41	126.26
3	A	301	4SP	O24-S23-N26	-2.27	104.08	107.35
3	A	301	4SP	C21-C20-C19	-2.20	117.60	120.47

There are no chirality outliers.

All (7) torsion outliers are listed below:

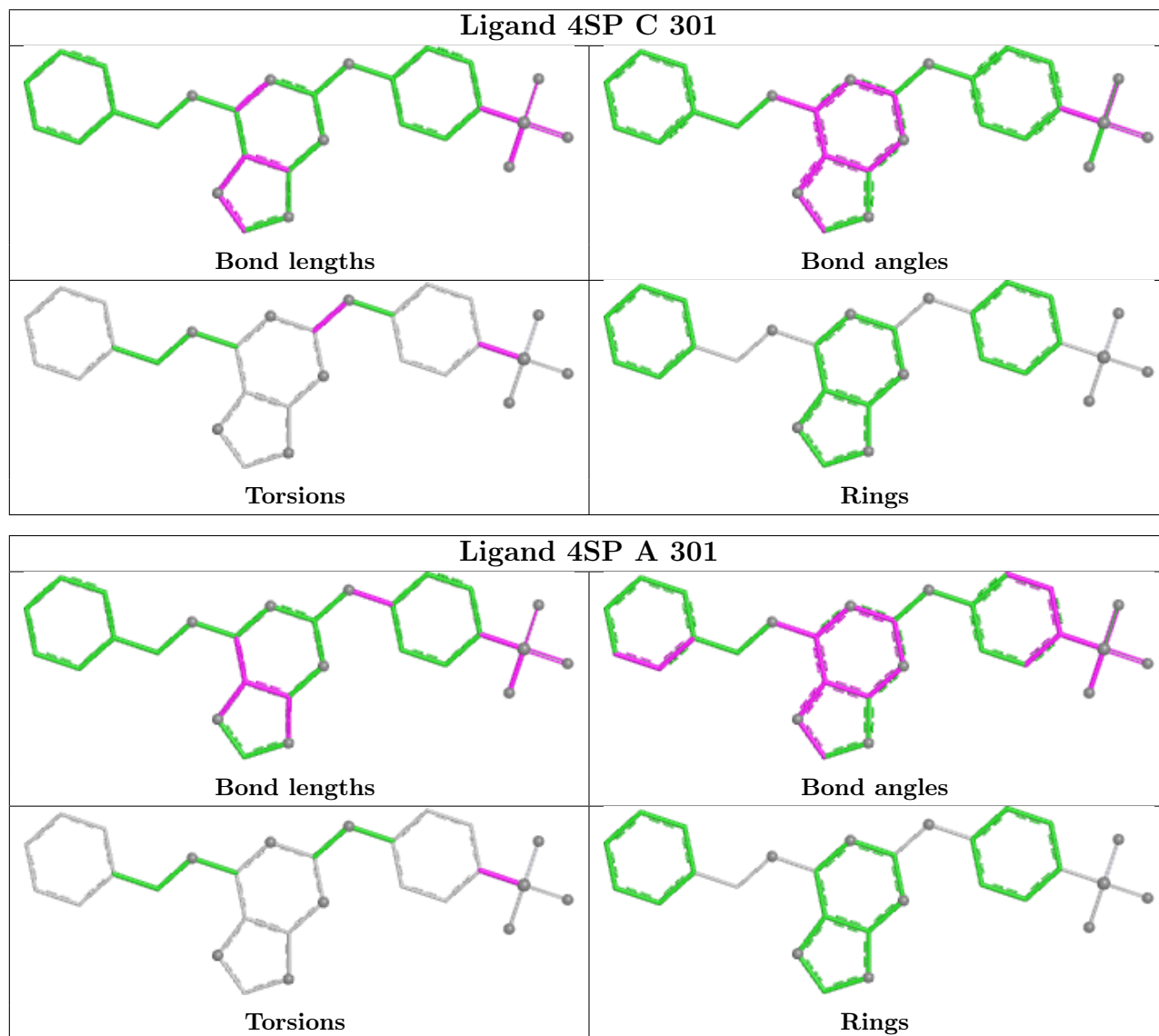
Mol	Chain	Res	Type	Atoms
3	A	301	4SP	C19-C20-S23-O24
3	A	301	4SP	C19-C20-S23-N26
3	A	301	4SP	C21-C20-S23-O24
3	A	301	4SP	C21-C20-S23-N26
3	C	301	4SP	N1-C2-N2-C17
3	C	301	4SP	N3-C2-N2-C17
3	C	301	4SP	C19-C20-S23-O24

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	4SP	2	0
3	A	301	4SP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/298 (98%)	-0.10	10 (3%) 48 45	10, 21, 39, 51	5 (1%)
1	C	270/298 (90%)	0.51	17 (6%) 26 23	17, 34, 59, 81	6 (2%)
2	B	257/258 (99%)	-0.05	9 (3%) 47 44	10, 25, 38, 49	4 (1%)
2	D	255/258 (98%)	0.45	13 (5%) 33 30	20, 37, 56, 67	0
All	All	1075/1112 (96%)	0.20	49 (4%) 37 34	10, 29, 51, 81	15 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	VAL	6.6
1	C	248	PHE	6.0
1	C	247	ASP	5.8
2	B	283	ASP	5.4
1	A	15[A]	TYR	5.4
1	A	0	SER	5.1
2	D	429	THR	4.5
1	C	252	VAL	4.4
1	C	220	GLY	4.3
1	C	249	SER	4.2
2	D	175	VAL	4.1
1	C	219	LEU	4.0
2	B	284	ASP	3.8
1	C	250	LYS	3.6
2	D	428	GLU	3.6
2	B	323	GLN	3.5
1	C	218	THR	3.5
1	C	222	PRO	3.5
1	A	71	HIS	3.4
1	A	96	LEU	3.4
1	C	287	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	431	ASN	3.3
1	A	162	GLU	3.0
1	C	269	TYR	3.0
1	C	288	ASP	3.0
1	A	206	ASP	2.9
2	B	432	LEU	2.9
2	B	177	ASP	2.8
2	D	284	ASP	2.7
2	D	323	GLN	2.7
2	B	176	PRO	2.6
1	A	95	ALA	2.6
2	D	371	SER	2.5
2	D	324	PRO	2.5
2	D	178	TYR	2.5
2	D	197	VAL	2.4
1	A	13	GLY	2.4
1	C	221	THR	2.4
1	A	247	ASP	2.4
1	C	73	GLU	2.4
2	D	334	MET	2.3
2	B	224	GLU	2.2
2	B	285	THR	2.1
1	A	161[A]	HIS	2.1
2	D	180	GLU	2.1
2	D	176	PRO	2.1
1	C	162	GLU	2.0
2	D	328	LYS	2.0
1	C	36	ARG	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, 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
1	TPO	C	160	11/12	0.96	0.07	27,30,32,33	0
1	TPO	A	160	11/12	0.98	0.06	15,18,19,20	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

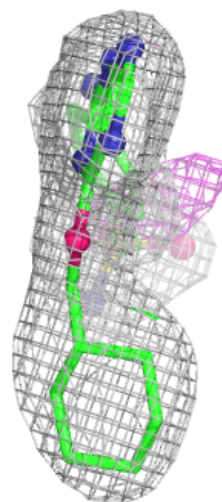
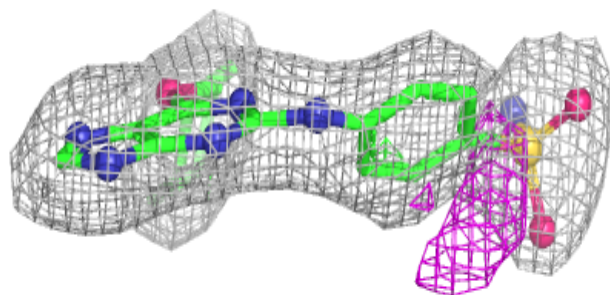
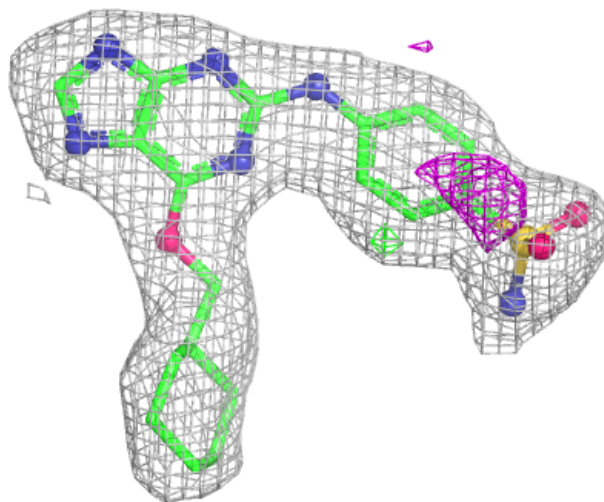
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

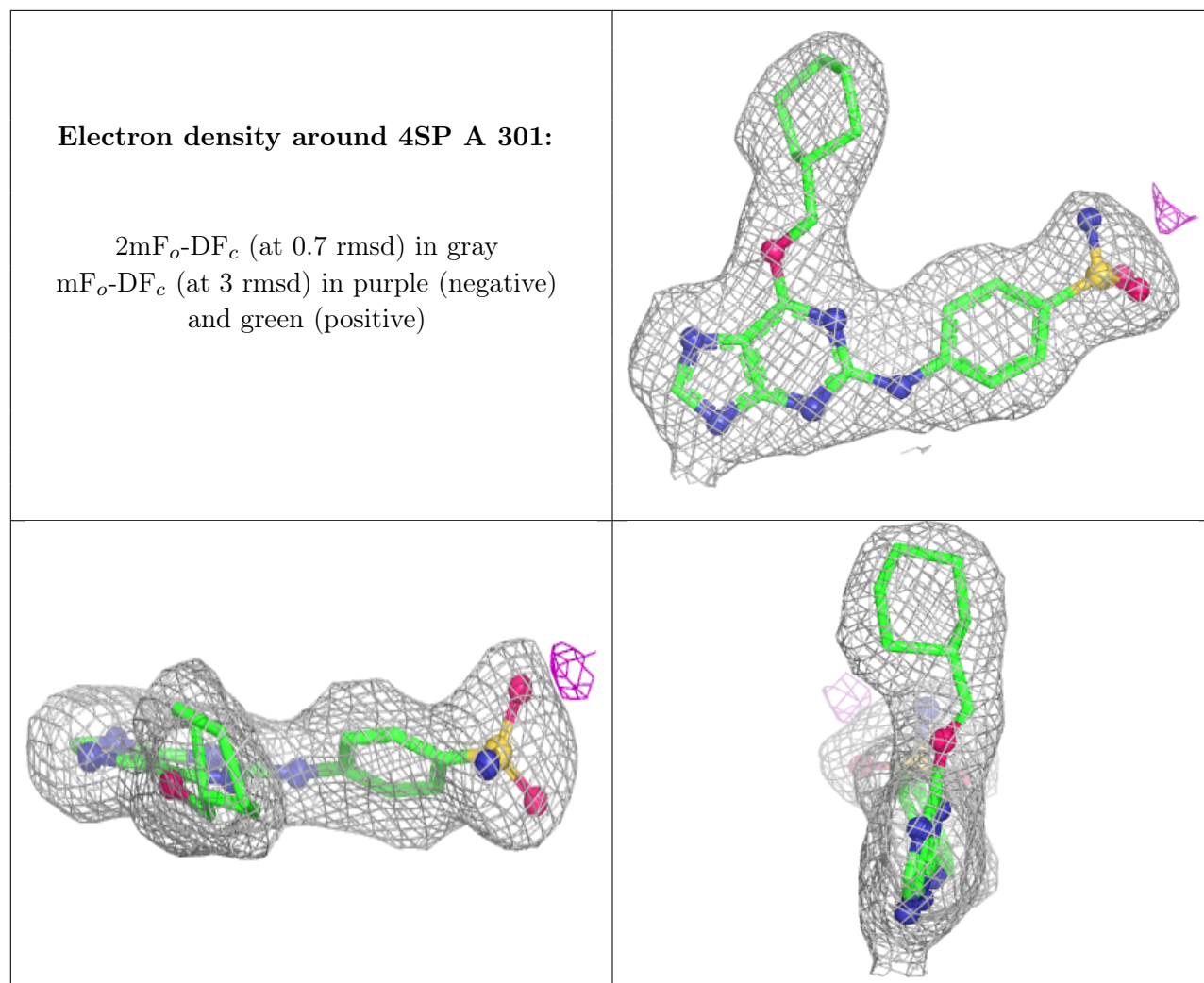
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	4SP	C	301	28/28	0.91	0.10	36,38,40,40	0
3	4SP	A	301	28/28	0.95	0.07	26,28,31,31	0

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

Electron density around 4SP 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.