



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 07:29 pm GMT

PDB ID : 5OKT
Title : Crystal structure of human Casein Kinase I delta in complex with IWP-2
Authors : Pichlo, C.; Brunstein, E.; Baumann, U.
Deposited on : 2017-07-25
Resolution : 2.13 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

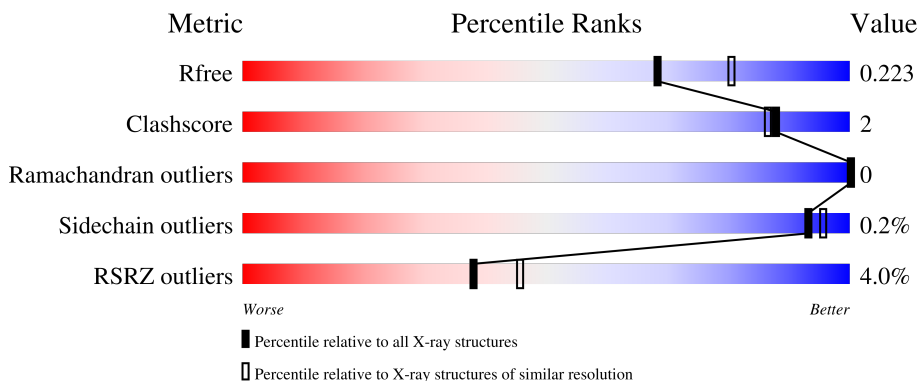
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


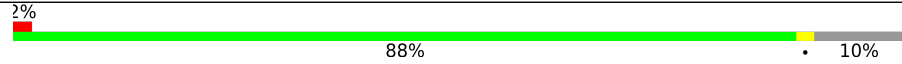
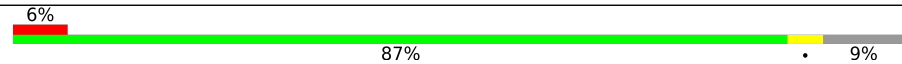

The reported resolution of this entry is 2.13 Å.

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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	314	 87% 9%
1	B	314	 88% 10%
2	C	314	 87% 9%
2	D	314	 85% 5% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	9XK	D	301	-	-	-	X
5	ACT	A	307	-	-	X	-
6	GOL	C	309	-	-	-	X
6	GOL	D	307	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18845 atoms, of which 9090 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 Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S			
1	A	286	4603	1489	2284	396	417	1	16	1	2	0
1	B	282	4491	1454	2226	386	410	1	14	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P48730
A	-18	GLY	-	expression tag	UNP P48730
A	-17	SER	-	expression tag	UNP P48730
A	-16	SER	-	expression tag	UNP P48730
A	-15	HIS	-	expression tag	UNP P48730
A	-14	HIS	-	expression tag	UNP P48730
A	-13	HIS	-	expression tag	UNP P48730
A	-12	HIS	-	expression tag	UNP P48730
A	-11	HIS	-	expression tag	UNP P48730
A	-10	HIS	-	expression tag	UNP P48730
A	-9	SER	-	expression tag	UNP P48730
A	-8	SER	-	expression tag	UNP P48730
A	-7	GLY	-	expression tag	UNP P48730
A	-6	LEU	-	expression tag	UNP P48730
A	-5	VAL	-	expression tag	UNP P48730
A	-4	PRO	-	expression tag	UNP P48730
A	-3	ARG	-	expression tag	UNP P48730
A	-2	GLY	-	expression tag	UNP P48730
A	-1	SER	-	expression tag	UNP P48730
A	0	HIS	-	expression tag	UNP P48730
B	-19	MET	-	initiating methionine	UNP P48730
B	-18	GLY	-	expression tag	UNP P48730
B	-17	SER	-	expression tag	UNP P48730
B	-16	SER	-	expression tag	UNP P48730
B	-15	HIS	-	expression tag	UNP P48730

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P48730
B	-13	HIS	-	expression tag	UNP P48730
B	-12	HIS	-	expression tag	UNP P48730
B	-11	HIS	-	expression tag	UNP P48730
B	-10	HIS	-	expression tag	UNP P48730
B	-9	SER	-	expression tag	UNP P48730
B	-8	SER	-	expression tag	UNP P48730
B	-7	GLY	-	expression tag	UNP P48730
B	-6	LEU	-	expression tag	UNP P48730
B	-5	VAL	-	expression tag	UNP P48730
B	-4	PRO	-	expression tag	UNP P48730
B	-3	ARG	-	expression tag	UNP P48730
B	-2	GLY	-	expression tag	UNP P48730
B	-1	SER	-	expression tag	UNP P48730
B	0	HIS	-	expression tag	UNP P48730

- Molecule 2 is a protein called Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	285	4547	1474	2253	395	411	14	4	0	0
2	D	282	4480	1450	2217	391	408	14	4	0	0

There are 40 discrepancies between the modelled and reference sequences:

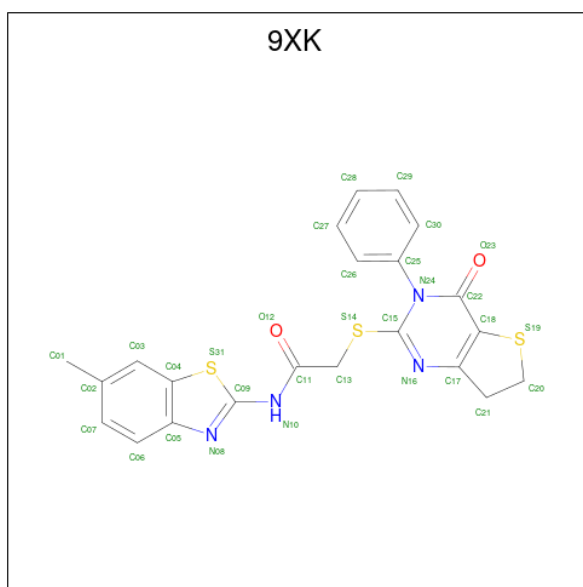
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP P48730
C	-18	GLY	-	expression tag	UNP P48730
C	-17	SER	-	expression tag	UNP P48730
C	-16	SER	-	expression tag	UNP P48730
C	-15	HIS	-	expression tag	UNP P48730
C	-14	HIS	-	expression tag	UNP P48730
C	-13	HIS	-	expression tag	UNP P48730
C	-12	HIS	-	expression tag	UNP P48730
C	-11	HIS	-	expression tag	UNP P48730
C	-10	HIS	-	expression tag	UNP P48730
C	-9	SER	-	expression tag	UNP P48730
C	-8	SER	-	expression tag	UNP P48730
C	-7	GLY	-	expression tag	UNP P48730
C	-6	LEU	-	expression tag	UNP P48730
C	-5	VAL	-	expression tag	UNP P48730

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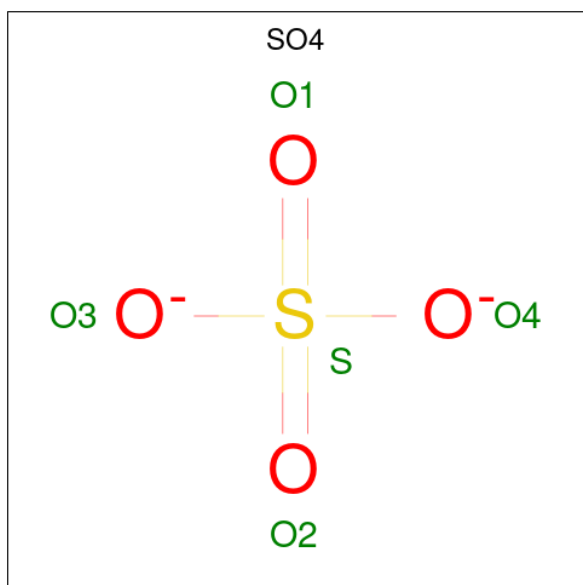
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP P48730
C	-3	ARG	-	expression tag	UNP P48730
C	-2	GLY	-	expression tag	UNP P48730
C	-1	SER	-	expression tag	UNP P48730
C	0	HIS	-	expression tag	UNP P48730
D	-19	MET	-	initiating methionine	UNP P48730
D	-18	GLY	-	expression tag	UNP P48730
D	-17	SER	-	expression tag	UNP P48730
D	-16	SER	-	expression tag	UNP P48730
D	-15	HIS	-	expression tag	UNP P48730
D	-14	HIS	-	expression tag	UNP P48730
D	-13	HIS	-	expression tag	UNP P48730
D	-12	HIS	-	expression tag	UNP P48730
D	-11	HIS	-	expression tag	UNP P48730
D	-10	HIS	-	expression tag	UNP P48730
D	-9	SER	-	expression tag	UNP P48730
D	-8	SER	-	expression tag	UNP P48730
D	-7	GLY	-	expression tag	UNP P48730
D	-6	LEU	-	expression tag	UNP P48730
D	-5	VAL	-	expression tag	UNP P48730
D	-4	PRO	-	expression tag	UNP P48730
D	-3	ARG	-	expression tag	UNP P48730
D	-2	GLY	-	expression tag	UNP P48730
D	-1	SER	-	expression tag	UNP P48730
D	0	HIS	-	expression tag	UNP P48730

- Molecule 3 is {N}-(6-methyl-1,3-benzothiazol-2-yl)-2-[(4-oxidanylidene-3-phenyl-6,7-dihydrothieno[3,2-d]pyrimidin-2-yl)sulfanyl]ethanamide (three-letter code: 9XK) (formula: C₂₂H₁₈N₄O₂S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	A	1	Total	C	H	N	O	S	0	0
			49	22	18	4	2	3		
3	B	1	Total	C	H	N	O	S	0	0
			49	22	18	4	2	3		
3	C	1	Total	C	H	N	O	S	0	0
			49	22	18	4	2	3		
3	D	1	Total	C	H	N	O	S	0	0
			49	22	18	4	2	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



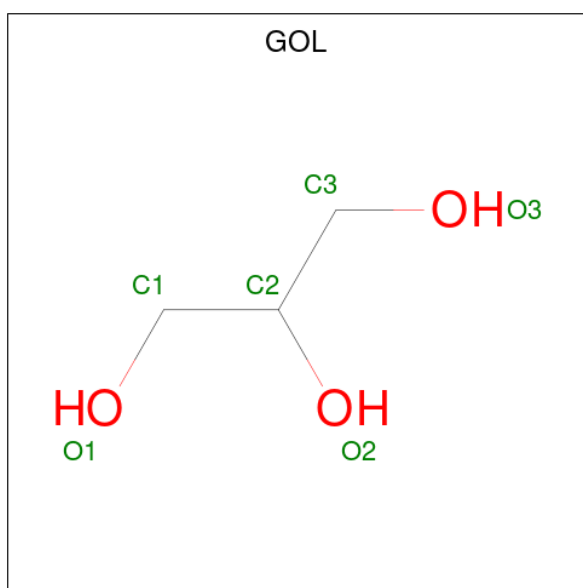
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total 5 4 1	0	0
4	A	1	Total 5 4 1	0	0
4	A	1	Total 5 4 1	0	0
4	A	1	Total 5 4 1	0	0
4	A	1	Total 5 4 1	0	0
4	B	1	Total 5 4 1	0	0
4	B	1	Total 5 4 1	0	0
4	B	1	Total 5 4 1	0	0
4	C	1	Total 5 4 1	0	0
4	C	1	Total 5 4 1	0	0
4	C	1	Total 5 4 1	0	0
4	C	1	Total 5 4 1	0	0
4	C	1	Total 5 4 1	0	0
4	C	1	Total 5 4 1	0	0
4	D	1	Total 5 4 1	0	0
4	D	1	Total 5 4 1	0	0
4	D	1	Total 5 4 1	0	0
4	D	1	Total 5 4 1	0	0
4	D	1	Total 5 4 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	7	2	3	2	0	0
5	A	1	7	2	3	2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	14	3	8	3	0	0
6	C	1	14	3	8	3	0	0

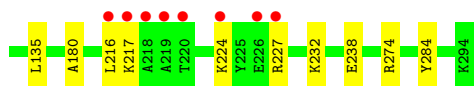
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	101	Total	O	0	0
			101	101		
7	B	90	Total	O	0	0
			90	90		
7	C	91	Total	O	0	0
			91	91		
7	D	81	Total	O	0	0
			81	81		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.11Å 82.73Å 89.64Å 89.73° 74.14° 86.57°	Depositor
Resolution (Å)	47.16 – 2.13 47.15 – 2.13	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.16-2.13) 94.8 (47.15-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.14Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.193 , 0.221 0.195 , 0.223	Depositor DCC
R_{free} test set	2012 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtrriage
Anisotropy	0.907	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,-h+l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18845	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: TPO, SO4, GOL, 9XK, ACT

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	0.27	0/2360	0.47	0/3173
1	B	0.27	0/2304	0.47	0/3098
2	C	0.27	0/2346	0.47	0/3156
2	D	0.27	0/2313	0.45	0/3115
All	All	0.27	0/9323	0.46	0/12542

There are no bond length outliers.

There are no bond angle outliers.

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	2319	2284	2282	10	0
1	B	2265	2226	2222	3	0
2	C	2294	2253	2255	8	0
2	D	2263	2217	2211	11	0
3	A	31	18	0	0	0
3	B	31	18	0	0	0
3	C	31	18	0	2	0
3	D	31	18	0	5	0
4	A	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	0	0	0
4	C	30	0	0	1	0
4	D	25	0	0	0	0
5	A	8	6	6	2	0
6	B	6	8	8	0	0
6	C	12	16	16	0	0
6	D	6	8	8	0	0
7	A	101	0	0	1	0
7	B	90	0	0	0	0
7	C	91	0	0	2	0
7	D	81	0	0	2	0
All	All	9755	9090	9008	37	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 2.

All (37) 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)
2:D:135:LEU:HD21	3:D:301:9XK:O12	1.45	1.14
2:D:135:LEU:CD2	3:D:301:9XK:O12	2.17	0.93
5:A:307:ACT:OXT	7:A:401:HOH:O	2.03	0.76
1:A:220:TPO:O3P	1:A:222:ARG:N	2.26	0.69
2:D:14:LYS:O	7:D:402:HOH:O	2.11	0.69
2:D:238:GLU:OE2	7:D:401:HOH:O	2.10	0.68
2:C:40:GLU:OE1	7:C:401:HOH:O	2.14	0.64
1:A:68:ILE:HD11	1:A:71[B]:CYS:SG	2.43	0.59
2:D:68:ILE:HD11	2:D:71:CYS:SG	2.44	0.58
3:D:301:9XK:S14	3:D:301:9XK:C30	2.93	0.57
2:C:68:ILE:HD11	2:C:71:CYS:SG	2.45	0.57
3:C:301:9XK:C13	3:C:301:9XK:C25	2.85	0.54
2:D:180:ALA:O	2:D:232:LYS:NZ	2.40	0.51
1:A:223:GLN:O	1:A:227:ARG:HG2	2.10	0.51
2:D:217:LYS:O	2:D:227:ARG:NH1	2.44	0.50
1:B:12:GLY:N	1:B:25:LEU:O	2.45	0.49
2:C:57:LYS:HA	2:C:60:GLN:HG2	1.95	0.48
1:A:220:TPO:O3P	1:A:220:TPO:O	2.31	0.48
1:A:220:TPO:O3P	1:A:222:ARG:CB	2.62	0.47
2:D:84:LEU:HD21	3:D:301:9XK:C27	2.45	0.47
2:C:270:ARG:NE	4:C:306:SO4:O1	2.44	0.47
2:C:220:THR:HG23	2:C:223:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:HD3	1:A:146:TYR:OH	2.17	0.45
2:C:5:VAL:HG21	2:C:11:LEU:HD23	1.98	0.45
2:D:216:LEU:O	2:D:224:LYS:NZ	2.40	0.44
1:B:14:LYS:NZ	1:B:22:ASP:OD2	2.46	0.43
2:C:238:GLU:OE1	7:C:402:HOH:O	2.21	0.43
1:B:19:SER:OG	1:B:149:ASP:OD1	2.24	0.43
1:A:204:MET:CE	1:A:248:PHE:CB	2.97	0.42
1:A:220:TPO:O3P	1:A:220:TPO:C	2.67	0.42
2:C:5:VAL:CG1	2:C:79:VAL:HG11	2.49	0.42
1:A:237:ILE:N	5:A:307:ACT:OXT	2.49	0.42
2:D:55:ILE:O	2:D:59:MET:HG2	2.20	0.42
2:D:274:ARG:HG2	2:D:284:TYR:OH	2.20	0.42
3:D:301:9XK:O12	3:D:301:9XK:S31	2.78	0.40
3:C:301:9XK:O12	3:C:301:9XK:S31	2.79	0.40
1:A:53:SER:O	1:A:57:LYS:HG3	2.22	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	283/314 (90%)	274 (97%)	9 (3%)	0	100	100
1	B	275/314 (88%)	268 (98%)	7 (2%)	0	100	100
2	C	279/314 (89%)	268 (96%)	11 (4%)	0	100	100
2	D	276/314 (88%)	269 (98%)	7 (2%)	0	100	100
All	All	1113/1256 (89%)	1079 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/274 (89%)	243 (100%)	1 (0%)	91	93
1	B	238/274 (87%)	238 (100%)	0	100	100
2	C	241/275 (88%)	240 (100%)	1 (0%)	91	93
2	D	237/275 (86%)	237 (100%)	0	100	100
All	All	960/1098 (87%)	958 (100%)	2 (0%)	93	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
2	C	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	278	HIS

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	B	220	1	8,10,11	1.58	1 (12%)	10,14,16	1.49	2 (20%)
1	TPO	A	220	1	8,10,11	1.54	1 (12%)	10,14,16	1.80	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	B	220	1	-	5/9/11/13	-
1	TPO	A	220	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	TPO	P-O1P	3.38	1.61	1.50
1	B	220	TPO	P-O1P	3.37	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	TPO	P-OG1-CB	-4.90	108.40	123.21
1	B	220	TPO	P-OG1-CB	-3.52	112.57	123.21
1	B	220	TPO	CG2-CB-CA	-2.22	108.78	113.16

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	220	TPO	N-CA-CB-CG2
1	B	220	TPO	N-CA-CB-OG1
1	B	220	TPO	C-CA-CB-CG2
1	B	220	TPO	CB-OG1-P-O1P
1	B	220	TPO	CB-OG1-P-O2P
1	A	220	TPO	CB-OG1-P-O3P
1	A	220	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	220	TPO	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
5	ACT	A	308	-	3,3,3	0.74	0	3,3,3	1.37	0
4	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	306	-	4,4,4	0.14	0	6,6,6	0.05	0
3	9XK	C	301	-	31,35,35	3.63	11 (35%)	35,50,50	2.95	10 (28%)
4	SO4	C	306	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	D	306	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.06	0
6	GOL	C	309	-	5,5,5	0.36	0	5,5,5	0.20	0
6	GOL	D	307	-	5,5,5	0.37	0	5,5,5	0.20	0
4	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	D	305	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	D	302	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.06	0
3	9XK	B	301	-	31,35,35	3.42	12 (38%)	35,50,50	3.42	14 (40%)
3	9XK	D	301	-	31,35,35	3.46	10 (32%)	35,50,50	3.88	15 (42%)
4	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.07	0
6	GOL	C	308	-	5,5,5	0.39	0	5,5,5	0.29	0
4	SO4	C	305	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	C	307	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.04	0
5	ACT	A	307	-	3,3,3	0.76	0	3,3,3	1.39	0
6	GOL	B	305	-	5,5,5	0.37	0	5,5,5	0.21	0
3	9XK	A	301	-	31,35,35	3.63	11 (35%)	35,50,50	3.26	13 (37%)
4	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	D	303	-	4,4,4	0.14	0	6,6,6	0.06	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
3	9XK	A	301	-	-	0/11/19/19	0/5/5/5
6	GOL	C	308	-	-	0/4/4/4	-
6	GOL	C	309	-	-	0/4/4/4	-
6	GOL	D	307	-	-	4/4/4/4	-
3	9XK	B	301	-	-	1/11/19/19	0/5/5/5
3	9XK	D	301	-	-	3/11/19/19	0/5/5/5
3	9XK	C	301	-	-	4/11/19/19	0/5/5/5
6	GOL	B	305	-	-	0/4/4/4	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	9XK	C21-C17	10.54	1.67	1.50
3	D	301	9XK	C21-C17	10.47	1.67	1.50
3	C	301	9XK	C21-C17	10.13	1.66	1.50
3	B	301	9XK	C21-C17	9.81	1.66	1.50
3	C	301	9XK	C15-N24	8.78	1.51	1.39
3	C	301	9XK	C18-C17	8.46	1.55	1.38
3	A	301	9XK	C15-N24	8.45	1.51	1.39
3	A	301	9XK	C18-C17	8.15	1.54	1.38
3	D	301	9XK	C18-C17	8.11	1.54	1.38
3	B	301	9XK	C18-C17	7.38	1.53	1.38
3	C	301	9XK	C15-N16	6.42	1.50	1.32
3	B	301	9XK	C15-N24	6.41	1.48	1.39
3	B	301	9XK	C09-N10	6.27	1.47	1.36
3	D	301	9XK	C15-N24	6.25	1.48	1.39
3	D	301	9XK	C15-N16	6.10	1.49	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	9XK	C15-N16	6.02	1.49	1.32
3	C	301	9XK	C15-S14	5.93	1.83	1.74
3	D	301	9XK	C11-N10	5.82	1.48	1.35
3	A	301	9XK	C09-N10	5.37	1.46	1.36
3	B	301	9XK	C15-N16	5.32	1.47	1.32
3	B	301	9XK	C20-S19	-4.93	1.65	1.80
3	A	301	9XK	C15-S14	4.64	1.81	1.74
3	A	301	9XK	C11-N10	4.62	1.45	1.35
3	C	301	9XK	C11-N10	4.40	1.45	1.35
3	D	301	9XK	C15-S14	4.33	1.81	1.74
3	B	301	9XK	C13-C11	4.24	1.56	1.51
3	D	301	9XK	C20-S19	-4.24	1.67	1.80
3	B	301	9XK	C11-N10	3.97	1.44	1.35
3	D	301	9XK	C09-N10	3.97	1.43	1.36
3	A	301	9XK	C20-S19	-3.92	1.68	1.80
3	C	301	9XK	C20-S19	-3.92	1.68	1.80
3	D	301	9XK	O23-C22	-3.23	1.16	1.23
3	C	301	9XK	C09-N10	3.17	1.42	1.36
3	B	301	9XK	O12-C11	-2.97	1.17	1.23
3	B	301	9XK	O23-C22	-2.96	1.16	1.23
3	C	301	9XK	O23-C22	-2.86	1.17	1.23
3	C	301	9XK	O12-C11	-2.83	1.17	1.23
3	B	301	9XK	C15-S14	2.79	1.78	1.74
3	A	301	9XK	C22-N24	2.55	1.46	1.42
3	D	301	9XK	C17-N16	2.44	1.45	1.38
3	B	301	9XK	C05-C04	-2.24	1.35	1.42
3	C	301	9XK	C17-N16	2.23	1.44	1.38
3	A	301	9XK	C17-N16	2.11	1.44	1.38
3	A	301	9XK	O12-C11	-2.08	1.19	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	9XK	C18-C22-N24	12.73	119.88	112.20
3	D	301	9XK	C18-C22-N24	12.57	119.79	112.20
3	B	301	9XK	C18-C22-N24	12.18	119.55	112.20
3	C	301	9XK	C18-C22-N24	10.97	118.82	112.20
3	D	301	9XK	C13-S14-C15	10.56	121.16	99.09
3	C	301	9XK	C18-C17-N16	-7.20	119.09	123.93
3	D	301	9XK	C18-C17-N16	-7.08	119.17	123.93
3	A	301	9XK	C18-C17-N16	-7.04	119.19	123.93
3	B	301	9XK	C18-C17-N16	-6.74	119.40	123.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	9XK	C17-C18-S19	-6.06	106.56	109.64
3	D	301	9XK	C25-N24-C22	5.89	125.23	116.55
3	B	301	9XK	O12-C11-N10	-5.67	113.28	123.63
3	D	301	9XK	C09-N10-C11	-5.63	114.33	129.54
3	B	301	9XK	C03-C04-S31	5.36	135.83	125.10
3	B	301	9XK	C13-C11-N10	5.10	121.40	114.41
3	A	301	9XK	C03-C04-S31	5.09	135.28	125.10
3	D	301	9XK	C05-C04-S31	-5.01	105.20	111.85
3	A	301	9XK	C05-C04-S31	-4.67	105.66	111.85
3	A	301	9XK	C17-C18-S19	-4.58	107.31	109.64
3	B	301	9XK	C25-N24-C22	4.48	123.16	116.55
3	C	301	9XK	C05-C04-S31	-4.32	106.12	111.85
3	D	301	9XK	C13-C11-N10	4.32	120.33	114.41
3	C	301	9XK	C03-C04-S31	4.30	133.70	125.10
3	C	301	9XK	C13-C11-N10	4.09	120.01	114.41
3	D	301	9XK	C04-C05-N08	4.06	117.50	108.04
3	C	301	9XK	N24-C15-N16	-4.02	120.30	124.58
3	B	301	9XK	C05-C04-S31	-3.95	106.61	111.85
3	D	301	9XK	C25-N24-C15	-3.76	113.71	119.80
3	A	301	9XK	C13-C11-N10	3.75	119.56	114.41
3	A	301	9XK	N24-C15-N16	-3.73	120.60	124.58
3	C	301	9XK	C09-N10-C11	-3.57	119.89	129.54
3	A	301	9XK	C04-C05-N08	3.51	116.22	108.04
3	C	301	9XK	C04-C05-N08	3.43	116.03	108.04
3	D	301	9XK	C03-C04-S31	3.22	131.55	125.10
3	C	301	9XK	C13-S14-C15	3.12	105.61	99.09
3	D	301	9XK	N24-C15-N16	-2.96	121.42	124.58
3	A	301	9XK	C13-S14-C15	2.82	104.99	99.09
3	A	301	9XK	C06-C05-N08	-2.76	122.78	130.78
3	B	301	9XK	O23-C22-C18	-2.73	118.99	125.44
3	D	301	9XK	C17-C18-S19	-2.71	108.26	109.64
3	C	301	9XK	C06-C05-N08	-2.65	123.09	130.78
3	B	301	9XK	C09-N10-C11	-2.64	122.42	129.54
3	B	301	9XK	C06-C05-N08	-2.56	123.35	130.78
3	A	301	9XK	C25-N24-C22	2.56	120.33	116.55
3	B	301	9XK	C04-C05-N08	2.56	113.99	108.04
3	D	301	9XK	C11-C13-S14	-2.47	101.59	111.42
3	A	301	9XK	C09-N10-C11	-2.45	122.91	129.54
3	D	301	9XK	C02-C03-C04	-2.42	118.67	121.18
3	B	301	9XK	N24-C15-N16	-2.25	122.18	124.58
3	A	301	9XK	O23-C22-C18	-2.24	120.15	125.44
3	D	301	9XK	C06-C05-N08	-2.22	124.33	130.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	9XK	O12-C11-C13	2.14	125.27	121.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

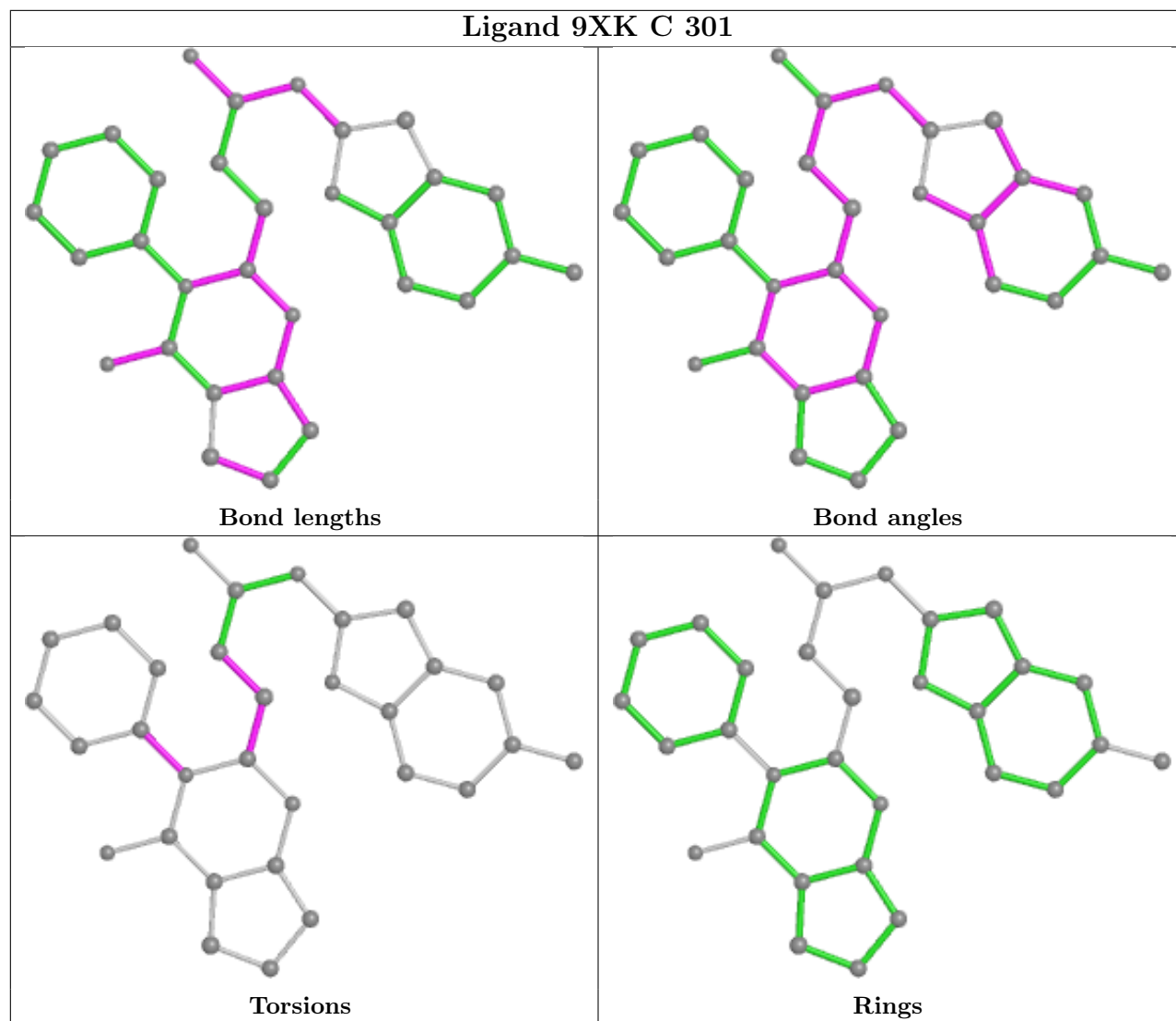
Mol	Chain	Res	Type	Atoms
3	C	301	9XK	C11-C13-S14-C15
3	C	301	9XK	N16-C15-S14-C13
3	C	301	9XK	N24-C15-S14-C13
3	D	301	9XK	C11-C13-S14-C15
6	D	307	GOL	O1-C1-C2-C3
6	D	307	GOL	C1-C2-C3-O3
6	D	307	GOL	O2-C2-C3-O3
3	D	301	9XK	O12-C11-C13-S14
6	D	307	GOL	O1-C1-C2-O2
3	D	301	9XK	N10-C11-C13-S14
3	B	301	9XK	O12-C11-C13-S14
3	C	301	9XK	C30-C25-N24-C15

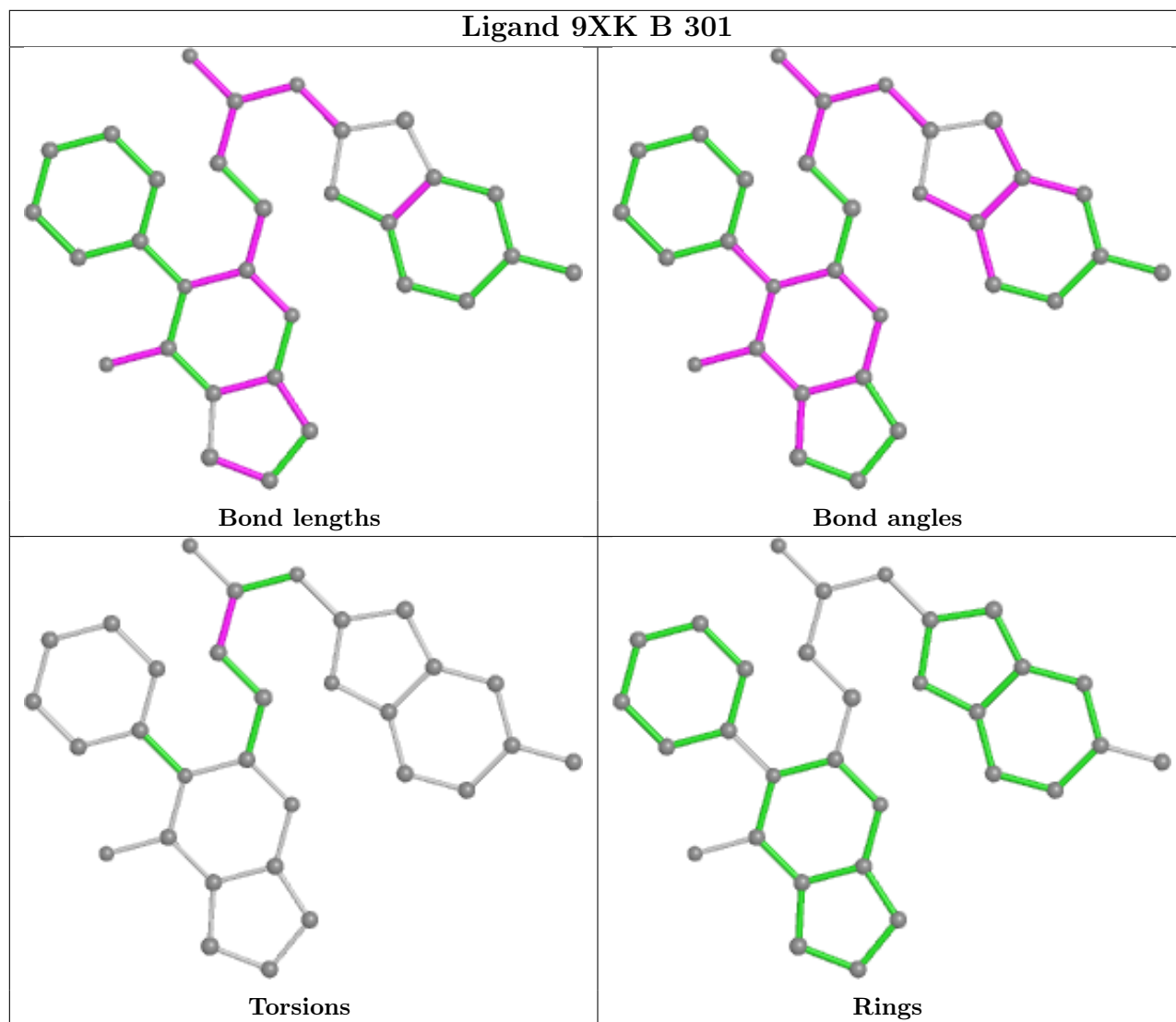
There are no ring outliers.

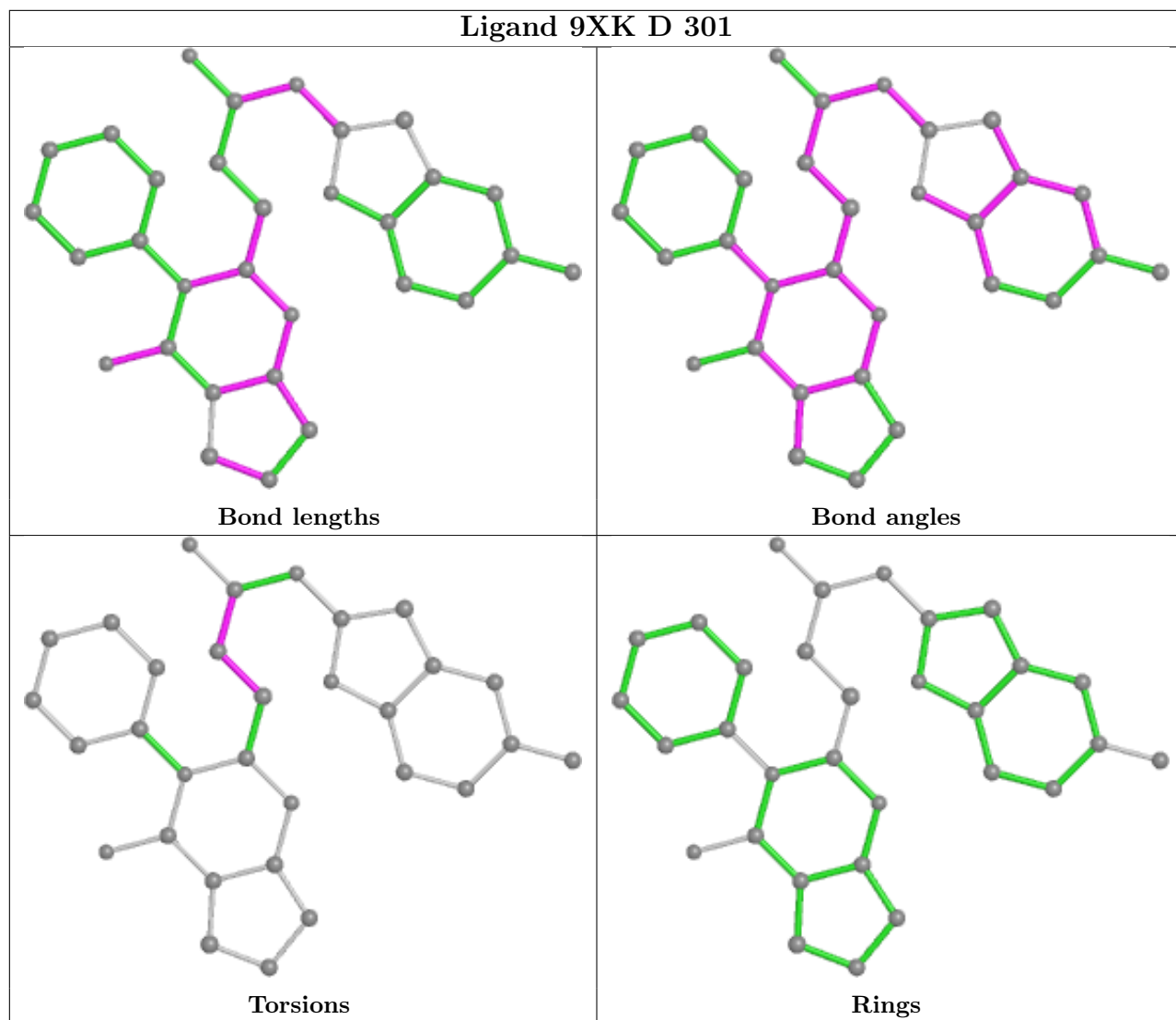
4 monomers are involved in 10 short contacts:

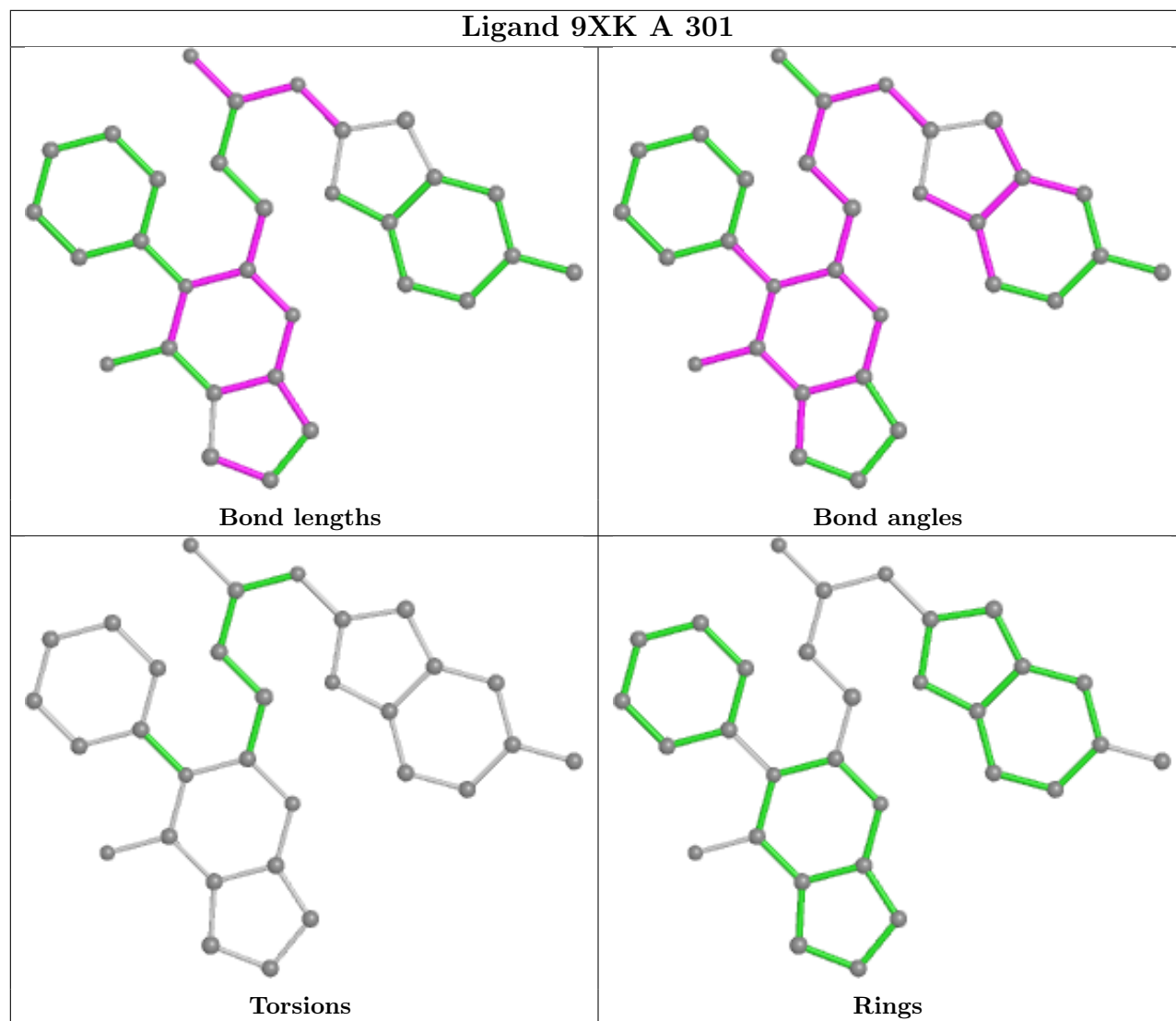
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	9XK	2	0
4	C	306	SO4	1	0
3	D	301	9XK	5	0
5	A	307	ACT	2	0

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

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	285/314 (90%)	0.23	4 (1%) 75 80	26, 40, 78, 119	0
1	B	281/314 (89%)	0.28	6 (2%) 63 69	29, 44, 82, 122	0
2	C	285/314 (90%)	0.45	18 (6%) 20 25	29, 47, 103, 120	1 (0%)
2	D	282/314 (89%)	0.43	17 (6%) 21 27	29, 48, 99, 140	1 (0%)
All	All	1133/1256 (90%)	0.35	45 (3%) 38 46	26, 44, 95, 140	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	218	ALA	7.2
2	D	41	CYS	6.3
1	B	5	VAL	4.8
2	C	41	CYS	4.2
2	D	21	GLY	4.1
2	C	21	GLY	3.8
2	C	16	GLY	3.4
2	D	216	LEU	3.3
2	C	218	ALA	3.3
2	C	20	PHE	3.2
1	B	15	ILE	3.2
2	D	220	THR	3.1
1	A	25	LEU	2.9
2	D	217	LYS	2.9
1	B	170	ASN	2.7
2	D	22	ASP	2.7
2	C	216	LEU	2.7
2	D	58	MET	2.7
2	D	219	ALA	2.6
2	C	24	TYR	2.6
2	D	224	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	225	TYR	2.6
2	C	173	LEU	2.6
2	C	224	LYS	2.5
1	B	227	ARG	2.5
2	C	217	LYS	2.5
2	C	23	ILE	2.5
2	D	226	GLU	2.4
1	A	15	ILE	2.4
2	C	77	TYR	2.4
1	A	225	TYR	2.4
2	D	25	LEU	2.3
2	D	119	ILE	2.3
1	A	171	LYS	2.3
2	D	76	ASP	2.3
2	D	50	HIS	2.2
2	D	227	ARG	2.1
2	C	25	LEU	2.1
1	B	53	SER	2.1
2	C	79	VAL	2.1
2	C	174	THR	2.1
2	D	24	TYR	2.1
2	C	19	SER	2.0
2	C	170	ASN	2.0
1	B	157	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	A	220	11/12	0.85	0.21	98,114,138,138	0
1	TPO	B	220	11/12	0.91	0.13	97,102,123,123	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands i

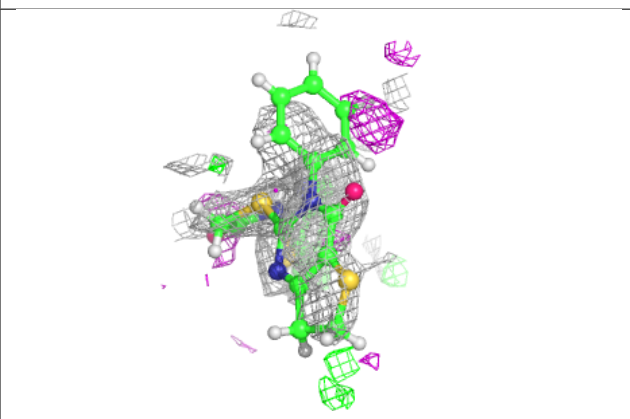
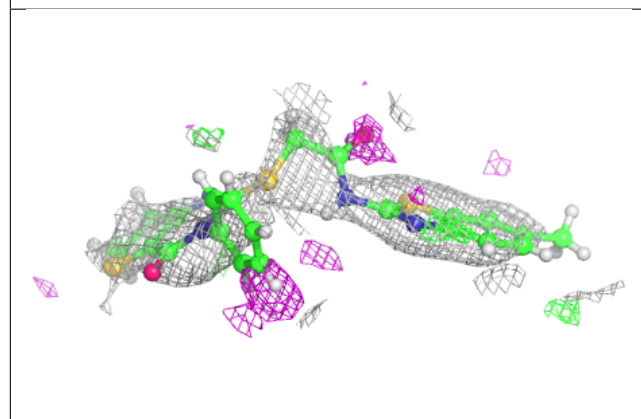
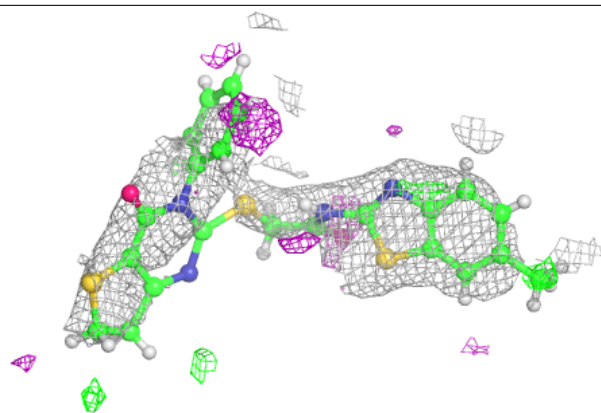
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	306	5/5	0.65	0.23	122,122,122,123	0
6	GOL	C	309	6/6	0.66	0.46	82,98,99,100	0
6	GOL	B	305	6/6	0.67	0.28	66,79,83,83	0
6	GOL	C	308	6/6	0.68	0.32	76,92,94,94	0
6	GOL	D	307	6/6	0.68	0.53	77,92,94,94	0
4	SO4	C	305	5/5	0.72	0.18	105,106,106,107	0
5	ACT	A	307	4/4	0.72	0.33	70,71,84,84	0
3	9XK	D	301	31/31	0.76	0.42	104,119,147,148	0
4	SO4	C	304	5/5	0.82	0.28	122,122,122,122	0
3	9XK	C	301	31/31	0.82	0.36	88,117,143,144	0
4	SO4	A	306	5/5	0.83	0.18	100,100,101,101	0
5	ACT	A	308	4/4	0.84	0.20	49,54,62,62	0
4	SO4	A	304	5/5	0.86	0.20	94,94,94,95	0
4	SO4	A	305	5/5	0.88	0.17	109,109,109,109	0
4	SO4	D	305	5/5	0.89	0.19	103,103,103,104	0
4	SO4	C	307	5/5	0.90	0.16	118,118,118,118	0
4	SO4	C	306	5/5	0.91	0.19	99,99,99,99	0
4	SO4	B	304	5/5	0.92	0.16	94,95,95,95	0
3	9XK	A	301	31/31	0.93	0.17	35,68,83,84	0
4	SO4	D	303	5/5	0.94	0.14	76,77,79,80	0
4	SO4	D	304	5/5	0.94	0.14	88,88,88,89	0
3	9XK	B	301	31/31	0.95	0.14	41,76,93,93	0
4	SO4	C	303	5/5	0.95	0.11	69,70,71,71	0
4	SO4	B	303	5/5	0.96	0.15	71,71,72,72	0
4	SO4	A	302	5/5	0.97	0.15	49,50,51,52	0
4	SO4	B	302	5/5	0.97	0.16	55,56,56,57	0
4	SO4	C	302	5/5	0.97	0.15	71,71,71,72	0
4	SO4	A	303	5/5	0.98	0.13	57,57,58,59	0
4	SO4	D	302	5/5	0.98	0.14	58,59,60,60	0

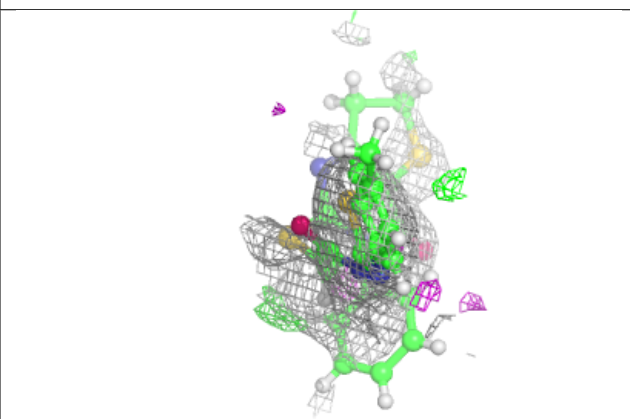
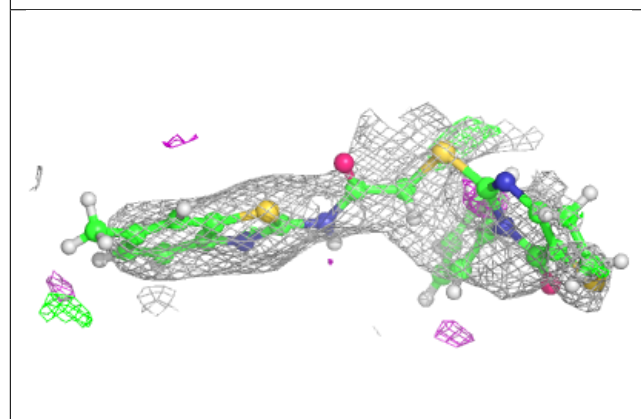
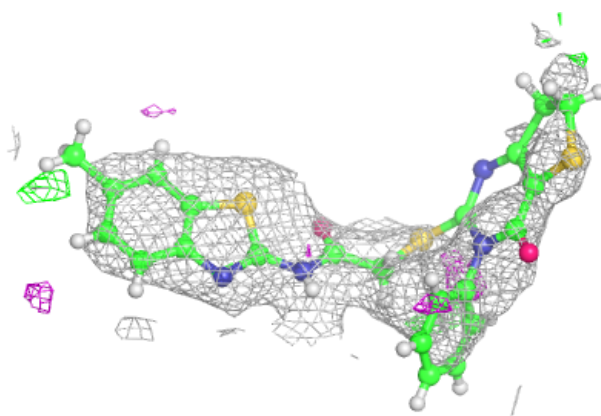
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9XK D 301:

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

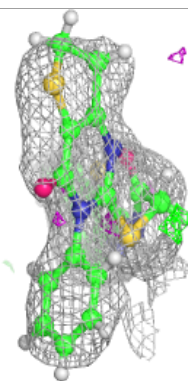
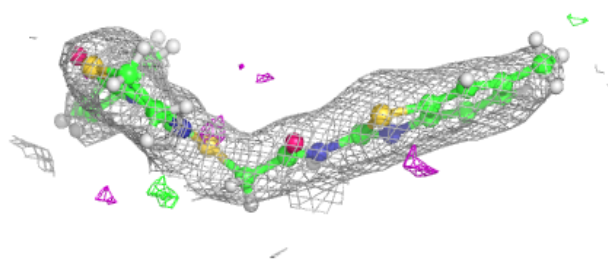
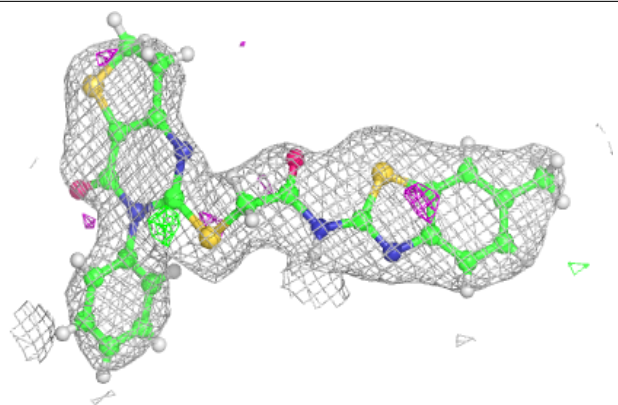
**Electron density around 9XK C 301:**

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

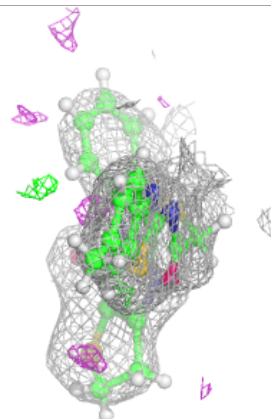
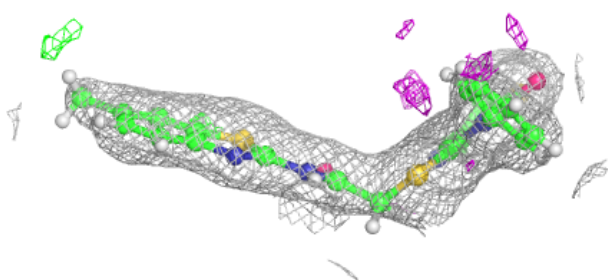
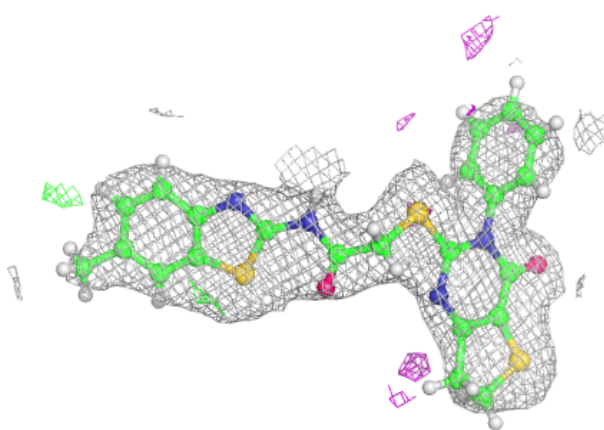


Electron density around 9XK A 301:

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

**Electron density around 9XK B 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.