



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2021 – 10:08 AM EDT

PDB ID : 7L28  
Title : Crystal structure of the catalytic domain of human PDE3A bound to Trequinsin  
Authors : Horner, S.W.; Garvie, C.  
Deposited on : 2020-12-16  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.20  
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) : 2.20

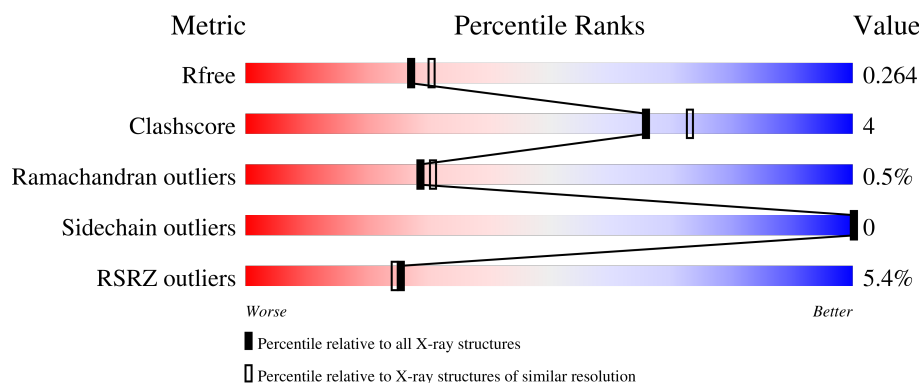
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	380	<div> <div>8%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	B	380	<div> <div>3%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	C	380	<div> <div>5%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	D	380	<div> <div>5%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12165 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2937	1894	492	533	18			
1	B	369	Total	C	N	O	S	0	0	0
			2977	1917	499	543	18			
1	C	375	Total	C	N	O	S	0	0	0
			3018	1938	511	551	18			
1	D	370	Total	C	N	O	S	0	1	0
			2982	1919	501	543	19			

There are 52 discrepancies between the modelled and reference sequences:

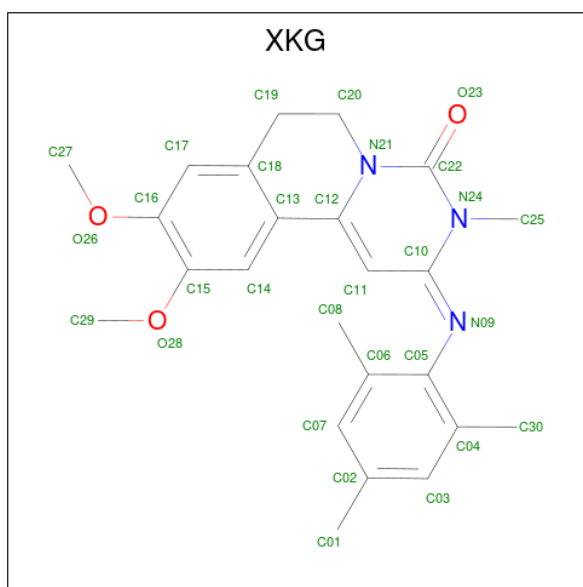
Chain	Residue	Modelled	Actual	Comment	Reference
A	668	GLY	-	expression tag	UNP Q14432
A	795	GLY	-	linker	UNP Q14432
A	796	GLY	-	linker	UNP Q14432
A	797	SER	-	linker	UNP Q14432
A	798	GLY	-	linker	UNP Q14432
A	799	GLY	-	linker	UNP Q14432
A	800	SER	-	linker	UNP Q14432
A	1062	GLY	-	linker	UNP Q14432
A	1063	GLY	-	linker	UNP Q14432
A	1064	SER	-	linker	UNP Q14432
A	1065	GLY	-	linker	UNP Q14432
A	1066	GLY	-	linker	UNP Q14432
A	1067	SER	-	linker	UNP Q14432
B	668	GLY	-	expression tag	UNP Q14432
B	780	GLY	-	linker	UNP Q14432
B	781	GLY	-	linker	UNP Q14432
B	782	SER	-	linker	UNP Q14432
B	798	GLY	-	linker	UNP Q14432
B	799	GLY	-	linker	UNP Q14432
B	800	SER	-	linker	UNP Q14432
B	1062	GLY	-	linker	UNP Q14432

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1063	GLY	-	linker	UNP Q14432
B	1064	SER	-	linker	UNP Q14432
B	1065	GLY	-	linker	UNP Q14432
B	1066	GLY	-	linker	UNP Q14432
B	1067	SER	-	linker	UNP Q14432
C	668	GLY	-	expression tag	UNP Q14432
C	780	GLY	-	linker	UNP Q14432
C	781	GLY	-	linker	UNP Q14432
C	782	SER	-	linker	UNP Q14432
C	783	GLY	-	linker	UNP Q14432
C	784	GLY	-	linker	UNP Q14432
C	785	SER	-	linker	UNP Q14432
C	1029	GLY	-	linker	UNP Q14432
C	1063	GLY	-	linker	UNP Q14432
C	1064	SER	-	linker	UNP Q14432
C	1065	GLY	-	linker	UNP Q14432
C	1066	GLY	-	linker	UNP Q14432
C	1067	SER	-	linker	UNP Q14432
D	668	GLY	-	expression tag	UNP Q14432
D	780	GLY	-	linker	UNP Q14432
D	781	GLY	-	linker	UNP Q14432
D	782	SER	-	linker	UNP Q14432
D	783	GLY	-	linker	UNP Q14432
D	784	GLY	-	linker	UNP Q14432
D	785	SER	-	linker	UNP Q14432
D	1062	GLY	-	linker	UNP Q14432
D	1063	GLY	-	linker	UNP Q14432
D	1064	SER	-	linker	UNP Q14432
D	1065	GLY	-	linker	UNP Q14432
D	1066	GLY	-	linker	UNP Q14432
D	1067	SER	-	linker	UNP Q14432

- Molecule 2 is (2E)-9,10-dimethoxy-3-methyl-2-[(2,4,6-trimethylphenyl)imino]-2,3,6,7-tetrahydro-4H-pyrimido[6,1-a]isoquinolin-4-one (three-letter code: XKG) (formula: C<sub>24</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	24	3	3		
2	B	1	Total	C	N	O	0	0
			30	24	3	3		
2	C	1	Total	C	N	O	0	0
			30	24	3	3		
2	D	1	Total	C	N	O	0	0
			30	24	3	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

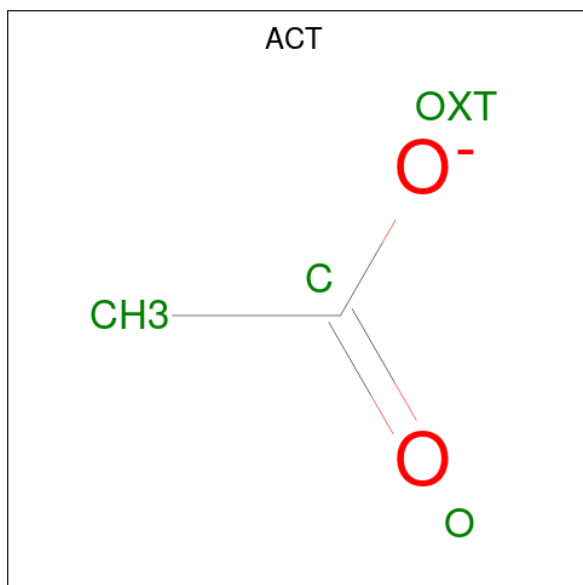
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	28	Total	O	0	0
			28	28		

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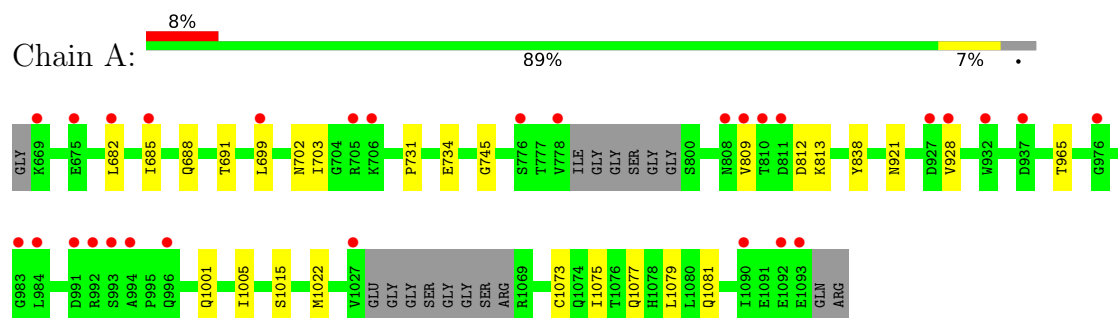
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	25	Total	O	0	0
			25	25		
6	D	24	Total	O	0	0
			24	24		

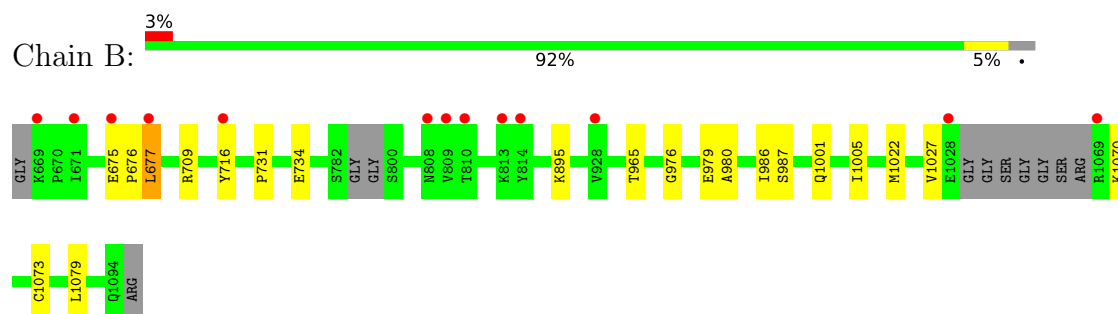
### 3 Residue-property plots [i](#)

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.

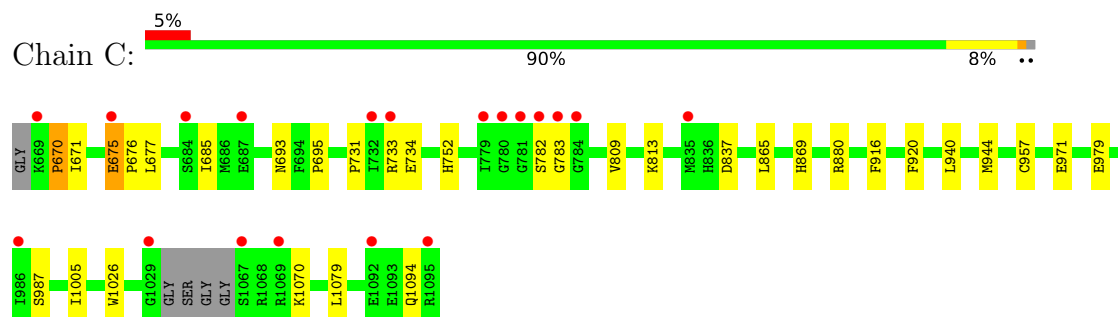
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



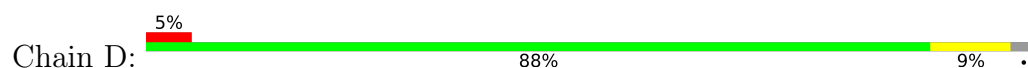
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



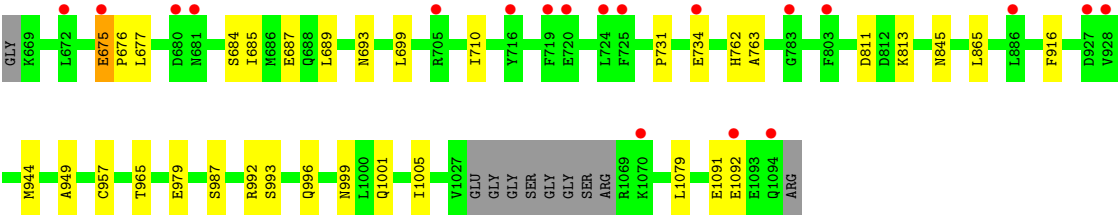
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.24Å 59.65Å 158.12Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	46.29 – 2.20 46.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.29-2.20) 98.7 (46.29-2.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.233 , 0.263 0.237 , 0.264	Depositor DCC
$R_{free}$ test set	3894 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN, ACT, MG, XKG

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	0/3016	0.63	0/4096
1	B	0.51	0/3056	0.66	0/4149
1	C	0.52	0/3098	0.65	0/4203
1	D	0.49	0/3062	0.63	0/4158
All	All	0.50	0/12232	0.64	0/16606

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	2937	0	2861	26	0
1	B	2977	0	2897	17	0
1	C	3018	0	2938	28	0
1	D	2982	0	2902	24	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	1	0
6	A	30	0	0	0	0
6	B	28	0	0	0	0
6	C	25	0	0	1	0
6	D	24	0	0	1	0
All	All	12165	0	11610	95	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 (95) 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:677:LEU:HD11	1:C:733:ARG:CD	1.78	1.14
1:C:677:LEU:HD11	1:C:733:ARG:HD2	1.11	1.07
1:C:677:LEU:CD1	1:C:733:ARG:HD2	1.89	1.03
1:C:675:GLU:HB3	1:C:676:PRO:HD2	1.44	0.99
1:A:682:LEU:HD21	1:A:703:ILE:HG12	1.50	0.92
1:B:980:ALA:HB2	1:B:986:ILE:HD11	1.54	0.90
1:A:688:GLN:O	1:A:691:THR:HG22	1.73	0.89
1:C:675:GLU:HB3	1:C:676:PRO:CD	2.03	0.88
1:A:1022:MET:HE1	1:A:1075:ILE:HB	1.68	0.75
1:A:1022:MET:CE	1:A:1075:ILE:HB	2.17	0.75
1:C:685:ILE:HD11	1:C:695:PRO:HG2	1.68	0.75
1:D:845:ASN:HD21	1:D:865:LEU:H	1.37	0.73
1:B:1027:VAL:HG22	1:B:1070:LYS:HB2	1.71	0.70
1:B:676:PRO:HB2	1:B:709:ARG:HH22	1.60	0.67
1:B:1027:VAL:CG2	1:B:1070:LYS:HB2	2.25	0.66
1:A:809:VAL:HG12	1:A:809:VAL:O	1.96	0.66
1:A:1022:MET:HE2	1:A:1073:CYS:SG	2.43	0.58
1:D:689:LEU:O	1:D:762:HIS:HE1	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:LEU:HD22	1:A:699:LEU:CD1	2.35	0.57
1:D:992:ARG:HG3	1:D:993:SER:N	2.19	0.55
1:C:752:HIS:HD2	1:C:971:GLU:OE1	1.89	0.54
1:B:976:GLY:O	1:B:986:ILE:HD12	2.07	0.54
1:A:965:THR:HG23	1:A:1001:GLN:NE2	2.23	0.54
1:D:677:LEU:HA	6:D:1211:HOH:O	2.08	0.54
1:B:965:THR:HG23	1:B:1001:GLN:NE2	2.24	0.52
1:B:979:GLU:OE2	1:B:987:SER:OG	2.27	0.52
1:D:1091:GLU:O	1:D:1092:GLU:HB2	2.08	0.52
1:A:1022:MET:HE3	1:A:1075:ILE:HB	1.93	0.51
1:D:965:THR:HG23	1:D:1001:GLN:NE2	2.25	0.51
1:B:976:GLY:O	1:B:986:ILE:CD1	2.59	0.51
1:B:731:PRO:HB2	1:B:734:GLU:OE1	2.10	0.51
1:A:731:PRO:HB2	1:A:734:GLU:OE1	2.10	0.51
1:C:731:PRO:HB2	1:C:734:GLU:OE1	2.10	0.51
1:D:979:GLU:OE2	1:D:987:SER:OG	2.27	0.51
1:A:965:THR:HG23	1:A:1001:GLN:HE21	1.75	0.51
1:C:979:GLU:OE2	1:C:987:SER:OG	2.27	0.51
1:B:965:THR:HG23	1:B:1001:GLN:HE21	1.76	0.51
1:A:682:LEU:CD2	1:A:703:ILE:HG12	2.34	0.50
1:D:684:SER:O	1:D:687:GLU:HG2	2.12	0.50
1:A:813:LYS:HE2	1:A:813:LYS:HA	1.94	0.50
1:D:731:PRO:HB2	1:D:734:GLU:OE1	2.10	0.50
1:C:920:PHE:HB2	1:C:944:MET:SD	2.52	0.50
1:D:996:GLN:HB3	1:D:999:ASN:HB2	1.93	0.49
1:C:677:LEU:CD1	1:C:733:ARG:CD	2.66	0.49
1:C:693:ASN:ND2	1:C:957:CYS:H	2.10	0.49
1:A:682:LEU:HD22	1:A:699:LEU:HD11	1.96	0.48
1:A:1022:MET:HE1	1:A:1075:ILE:CB	2.40	0.48
1:B:675:GLU:O	1:B:677:LEU:HD13	2.13	0.48
1:C:1070:LYS:HA	1:C:1070:LYS:HD3	1.71	0.47
1:D:710:ILE:HB	5:D:1104:ACT:H3	1.97	0.47
1:C:813:LYS:HE2	1:C:1026:TRP:CD1	2.51	0.46
1:D:693:ASN:ND2	1:D:957:CYS:H	2.12	0.46
1:A:1077:GLN:HG3	1:A:1081:GLN:HE21	1.79	0.46
1:D:965:THR:HG23	1:D:1001:GLN:HE21	1.81	0.46
1:A:921:ASN:HD21	1:A:1015:SER:CB	2.29	0.46
1:D:675:GLU:HB3	1:D:676:PRO:HD3	1.97	0.45
1:A:685:ILE:HG21	1:A:699:LEU:HB2	1.99	0.45
1:A:809:VAL:O	1:A:809:VAL:CG1	2.62	0.45
1:C:916:PHE:HB3	1:C:944:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:ASN:HD21	1:C:957:CYS:H	1.64	0.45
1:A:685:ILE:HD12	1:A:702:ASN:HD22	1.81	0.45
1:A:812:ASP:OD1	1:A:813:LYS:N	2.49	0.45
1:C:670:PRO:HB2	1:C:671:ILE:H	1.63	0.44
1:D:845:ASN:HD22	1:D:845:ASN:HA	1.59	0.44
1:A:1022:MET:HE1	1:A:1075:ILE:CG2	2.48	0.44
1:C:1094:GLN:HE21	1:C:1094:GLN:HB2	1.60	0.44
1:C:677:LEU:HD11	1:C:733:ARG:NE	2.29	0.44
1:C:865:LEU:HD23	1:C:865:LEU:HA	1.78	0.44
1:A:682:LEU:HD22	1:A:699:LEU:HD12	2.00	0.44
1:B:716:TYR:C	1:B:716:TYR:CD1	2.91	0.43
1:D:916:PHE:HB3	1:D:944:MET:CE	2.48	0.43
1:D:693:ASN:HD21	1:D:957:CYS:H	1.66	0.43
1:C:675:GLU:CB	1:C:676:PRO:HD2	2.30	0.42
1:A:1005:ILE:HG23	1:A:1079:LEU:HD11	2.00	0.42
1:C:837:ASP:HA	1:C:869:HIS:CD2	2.54	0.42
1:D:811:ASP:OD2	1:D:813:LYS:NZ	2.45	0.42
1:C:809:VAL:HG12	1:C:809:VAL:O	2.19	0.42
1:C:670:PRO:HG3	1:C:880:ARG:HE	1.85	0.42
1:C:752:HIS:CE1	6:C:1225:HOH:O	2.72	0.42
1:B:1005:ILE:HG23	1:B:1079:LEU:HD11	2.01	0.41
1:D:1005:ILE:HG23	1:D:1079:LEU:HD11	2.01	0.41
1:C:1005:ILE:HG23	1:C:1079:LEU:HD11	2.02	0.41
1:D:992:ARG:CG	1:D:993:SER:N	2.82	0.41
1:B:1022:MET:HG3	1:B:1073:CYS:SG	2.60	0.41
1:C:920:PHE:CD1	1:C:944:MET:HG3	2.55	0.41
1:D:685:ILE:HD13	1:D:699:LEU:HA	2.03	0.41
1:A:1022:MET:CE	1:A:1073:CYS:SG	3.08	0.41
1:D:689:LEU:O	1:D:762:HIS:CE1	2.72	0.41
1:B:895:LYS:HB3	1:B:895:LYS:HE3	1.91	0.41
1:D:865:LEU:HA	1:D:865:LEU:HD23	1.87	0.41
1:A:745:GLY:HA3	1:A:838:TYR:CE1	2.56	0.40
1:C:940:LEU:O	1:C:944:MET:HG2	2.21	0.40
1:D:763:ALA:HB3	1:D:949:ALA:HB1	2.02	0.40
1:B:675:GLU:O	1:B:677:LEU:CD1	2.70	0.40
1:B:1027:VAL:HG21	1:B:1070:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	357/380 (94%)	346 (97%)	10 (3%)	1 (0%)	41	46
1	B	363/380 (96%)	353 (97%)	9 (2%)	1 (0%)	41	46
1	C	371/380 (98%)	355 (96%)	12 (3%)	4 (1%)	14	12
1	D	367/380 (97%)	353 (96%)	13 (4%)	1 (0%)	41	46
All	All	1458/1520 (96%)	1407 (96%)	44 (3%)	7 (0%)	29	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	928	VAL
1	C	670	PRO
1	C	675	GLU
1	C	782	SER
1	B	677	LEU
1	C	783	GLY
1	D	675	GLU

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/327 (98%)	319 (100%)	0	100	100
1	B	323/327 (99%)	323 (100%)	0	100	100
1	C	326/327 (100%)	326 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	323/327 (99%)	323 (100%)	0	100	100
All	All	1291/1308 (99%)	1291 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	702	ASN
1	A	921	ASN
1	A	970	ASN
1	A	1001	GLN
1	A	1081	GLN
1	B	860	ASN
1	B	1001	GLN
1	B	1083	HIS
1	C	693	ASN
1	C	752	HIS
1	C	867	ASN
1	C	1001	GLN
1	C	1094	GLN
1	D	693	ASN
1	D	762	HIS
1	D	845	ASN
1	D	860	ASN
1	D	970	ASN
1	D	1001	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	XKG	A	1101	-	29,33,33	2.90	7 (24%)	38,49,49	1.82	10 (26%)
2	XKG	C	1101	-	29,33,33	2.84	7 (24%)	38,49,49	1.59	9 (23%)
5	ACT	D	1104	-	1,3,3	3.29	1 (100%)	0,3,3	0.00	-
5	ACT	C	1104	-	1,3,3	4.02	1 (100%)	0,3,3	0.00	-
2	XKG	D	1101	-	29,33,33	2.62	8 (27%)	38,49,49	1.82	8 (21%)
2	XKG	B	1101	-	29,33,33	2.76	7 (24%)	38,49,49	1.44	7 (18%)
5	ACT	A	1104	-	1,3,3	4.09	1 (100%)	0,3,3	0.00	-
5	ACT	B	1104	-	1,3,3	3.52	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XKG	B	1101	-	-	2/6/17/17	0/4/4/4
2	XKG	A	1101	-	-	4/6/17/17	0/4/4/4
2	XKG	C	1101	-	-	0/6/17/17	0/4/4/4
2	XKG	D	1101	-	-	1/6/17/17	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	XKG	C11-C12	10.23	1.50	1.38
2	B	1101	XKG	C11-C12	9.75	1.49	1.38
2	C	1101	XKG	C11-C12	9.69	1.49	1.38
2	D	1101	XKG	C11-C12	8.10	1.47	1.38
2	C	1101	XKG	C11-C10	7.14	1.51	1.40
2	D	1101	XKG	C11-C10	7.05	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	XKG	C11-C10	6.95	1.50	1.40
2	B	1101	XKG	C11-C10	6.51	1.50	1.40
2	A	1101	XKG	C12-N21	5.68	1.46	1.37
2	C	1101	XKG	C12-N21	5.12	1.45	1.37
2	B	1101	XKG	C12-N21	5.03	1.45	1.37
2	D	1101	XKG	C13-C18	-4.47	1.34	1.40
5	A	1104	ACT	CH3-C	4.09	1.54	1.48
2	C	1101	XKG	C13-C18	-4.03	1.34	1.40
5	C	1104	ACT	CH3-C	4.02	1.53	1.48
2	D	1101	XKG	C12-N21	3.95	1.43	1.37
2	A	1101	XKG	C13-C18	-3.81	1.35	1.40
2	D	1101	XKG	C13-C12	3.73	1.54	1.47
2	B	1101	XKG	C13-C18	-3.63	1.35	1.40
2	C	1101	XKG	C13-C12	3.61	1.54	1.47
5	B	1104	ACT	CH3-C	3.52	1.53	1.48
2	B	1101	XKG	C13-C12	3.39	1.53	1.47
5	D	1104	ACT	CH3-C	3.29	1.52	1.48
2	A	1101	XKG	C13-C12	3.04	1.53	1.47
2	D	1101	XKG	C20-C19	2.84	1.54	1.51
2	C	1101	XKG	O26-C16	2.74	1.41	1.37
2	C	1101	XKG	C20-C19	2.64	1.54	1.51
2	B	1101	XKG	O28-C15	2.51	1.41	1.37
2	B	1101	XKG	C10-N09	-2.49	1.25	1.31
2	A	1101	XKG	O26-C16	2.49	1.41	1.37
2	A	1101	XKG	O28-C15	2.45	1.41	1.37
2	D	1101	XKG	O26-C16	2.33	1.40	1.37
2	D	1101	XKG	C10-N09	-2.20	1.25	1.31

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	XKG	C06-C07-C02	-5.31	116.73	122.17
2	A	1101	XKG	O26-C16-C15	4.99	122.36	115.41
2	D	1101	XKG	C20-N21-C12	-4.23	113.73	118.70
2	C	1101	XKG	O26-C16-C15	3.88	120.81	115.41
2	A	1101	XKG	O26-C16-C17	-3.80	117.59	124.12
2	A	1101	XKG	C12-C13-C18	-3.68	117.34	120.15
2	D	1101	XKG	C07-C02-C03	3.61	122.39	118.09
2	A	1101	XKG	O28-C15-C16	3.40	120.15	115.41
2	C	1101	XKG	C12-C13-C18	-3.39	117.57	120.15
2	B	1101	XKG	C12-C13-C18	-3.30	117.64	120.15
2	A	1101	XKG	C07-C02-C03	3.21	121.92	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	XKG	C20-N21-C12	-3.09	115.07	118.70
2	C	1101	XKG	C20-C19-C18	-3.02	106.34	109.79
2	B	1101	XKG	C04-C03-C02	-3.00	119.09	122.17
2	D	1101	XKG	C14-C13-C12	2.90	122.50	118.58
2	D	1101	XKG	C12-C13-C18	-2.84	117.98	120.15
2	A	1101	XKG	C06-C07-C02	-2.76	119.33	122.17
2	A	1101	XKG	C04-C03-C02	-2.73	119.37	122.17
2	D	1101	XKG	C07-C06-C05	2.60	121.22	118.42
2	C	1101	XKG	C07-C02-C03	2.60	121.19	118.09
2	C	1101	XKG	C06-C07-C02	-2.59	119.51	122.17
2	C	1101	XKG	C14-C13-C12	2.55	122.03	118.58
2	C	1101	XKG	O26-C16-C17	-2.55	119.74	124.12
2	B	1101	XKG	O26-C16-C15	2.51	118.90	115.41
2	C	1101	XKG	C04-C03-C02	-2.50	119.61	122.17
2	B	1101	XKG	C07-C02-C03	2.45	121.02	118.09
2	D	1101	XKG	O26-C16-C15	2.34	118.67	115.41
2	A	1101	XKG	C20-C19-C18	-2.33	107.13	109.79
2	A	1101	XKG	O28-C15-C14	-2.33	120.12	124.12
2	A	1101	XKG	C20-N21-C12	-2.32	115.97	118.70
2	B	1101	XKG	C14-C13-C12	2.31	121.70	118.58
2	B	1101	XKG	O26-C16-C17	-2.19	120.36	124.12
2	D	1101	XKG	C20-C19-C18	-2.15	107.33	109.79
2	B	1101	XKG	C20-C19-C18	-2.10	107.39	109.79

There are no chirality outliers.

All (7) torsion outliers are listed below:

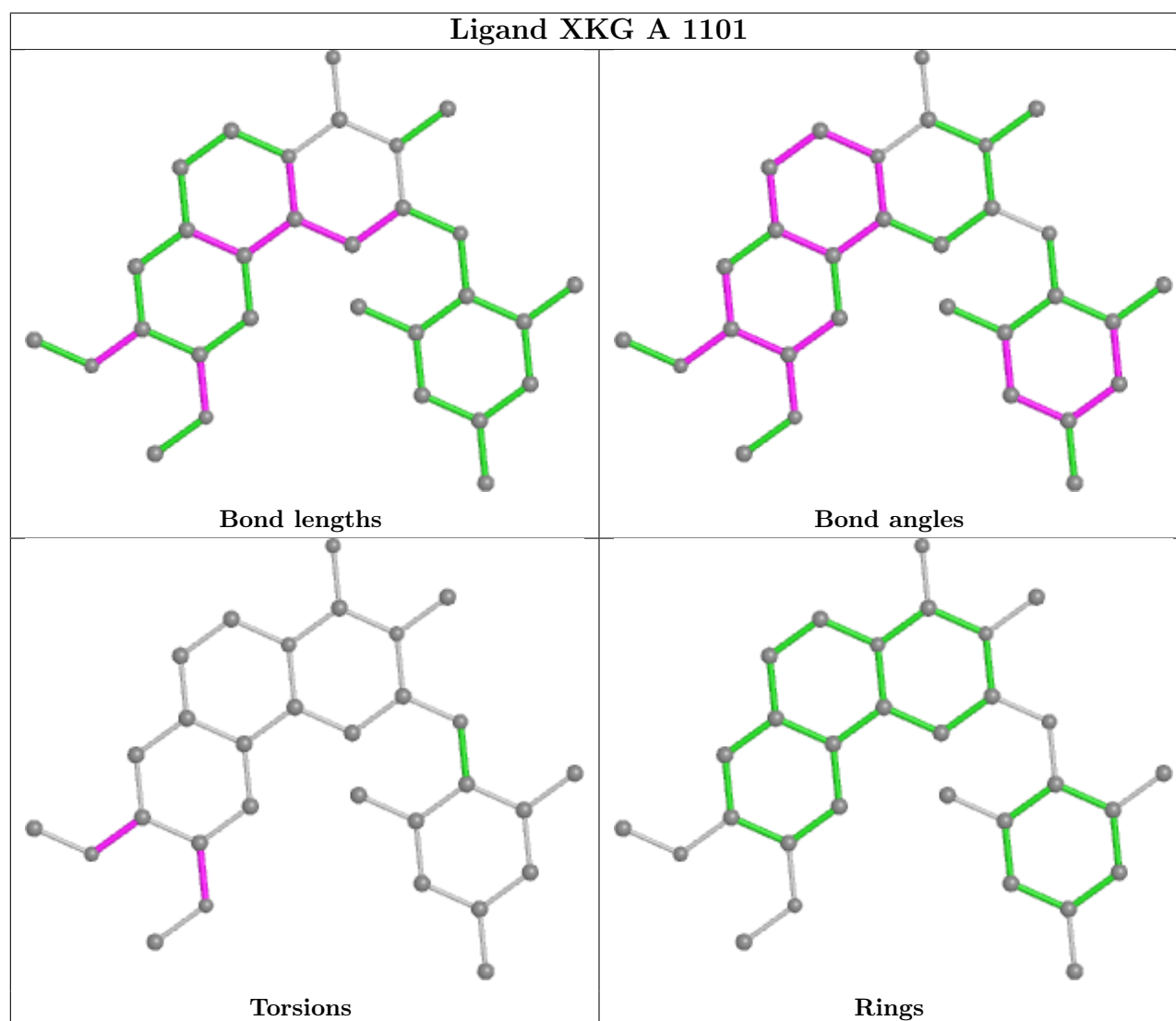
Mol	Chain	Res	Type	Atoms
2	A	1101	XKG	C15-C16-O26-C27
2	A	1101	XKG	C17-C16-O26-C27
2	A	1101	XKG	C16-C15-O28-C29
2	A	1101	XKG	C14-C15-O28-C29
2	B	1101	XKG	C15-C16-O26-C27
2	B	1101	XKG	C17-C16-O26-C27
2	D	1101	XKG	C16-C15-O28-C29

There are no ring outliers.

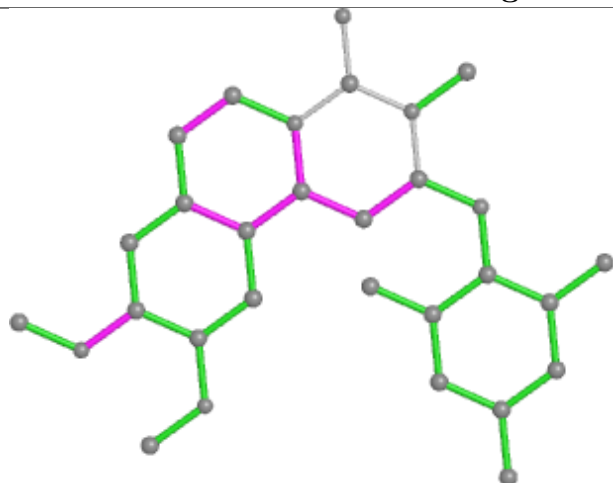
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1104	ACT	1	0

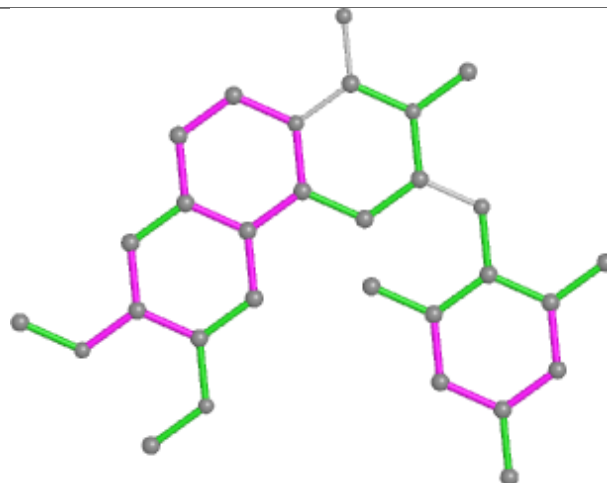
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



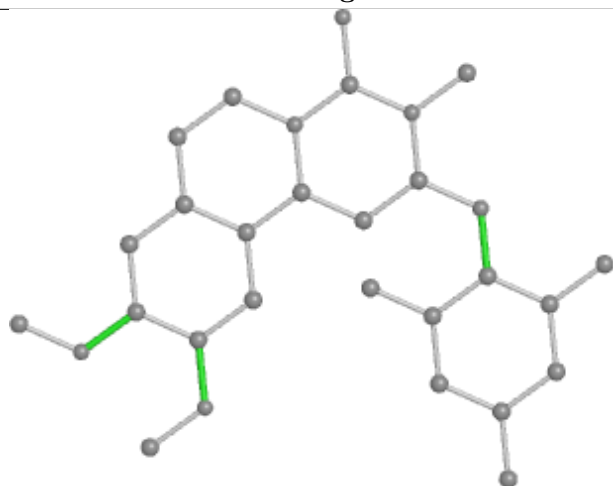
## Ligand XKG C 1101



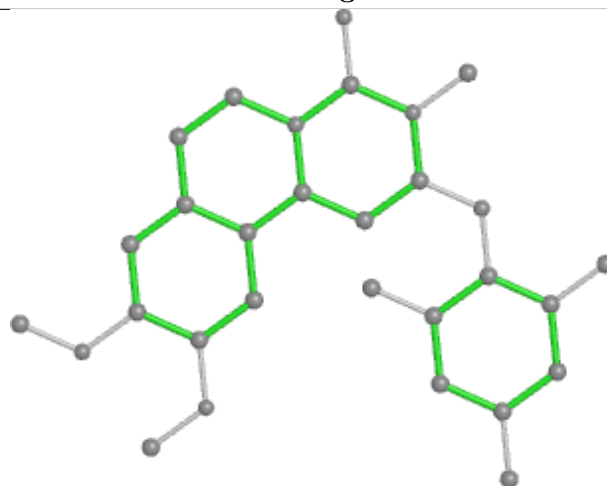
Bond lengths



Bond angles

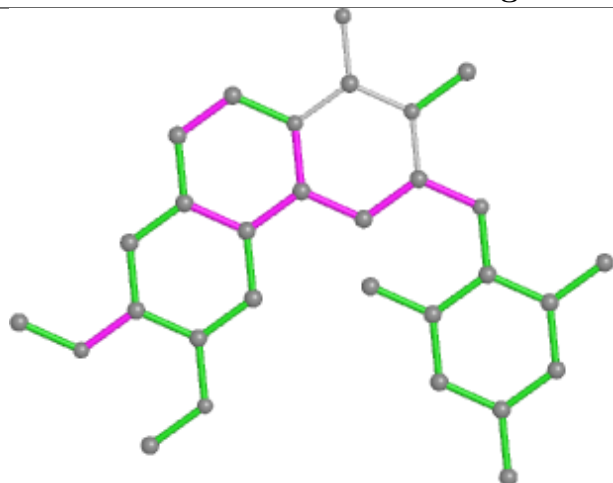


Torsions

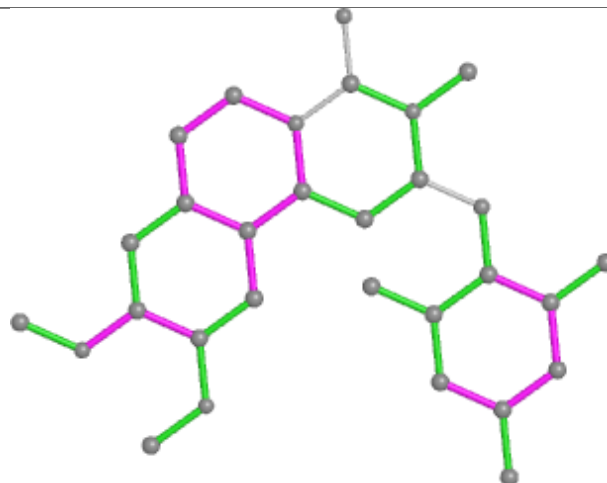


Rings

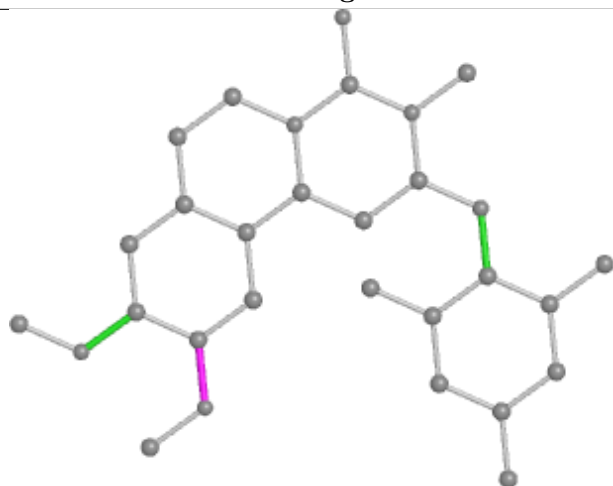
## Ligand XKG D 1101



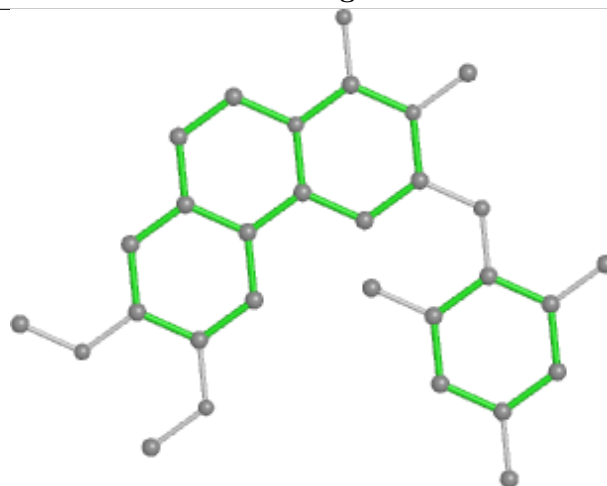
Bond lengths



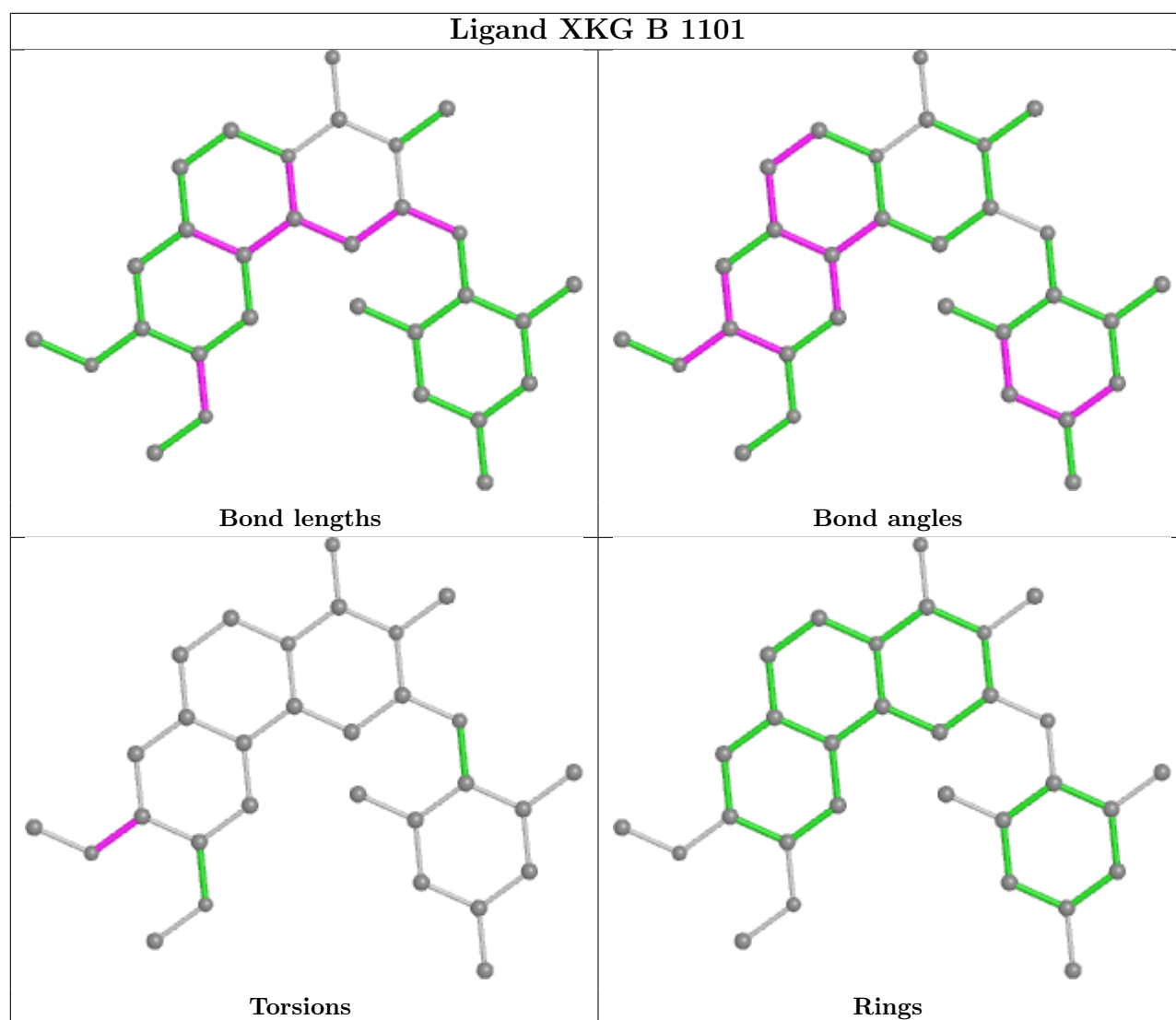
Bond angles



Torsions



Rings



## 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	363/380 (95%)	0.35	29 (7%)	12 11	39, 63, 98, 127	0
1	B	369/380 (97%)	0.23	13 (3%)	44 42	36, 58, 91, 135	0
1	C	375/380 (98%)	0.26	19 (5%)	28 26	30, 58, 97, 127	0
1	D	370/380 (97%)	0.32	19 (5%)	28 26	42, 62, 94, 115	0
All	All	1477/1520 (97%)	0.29	80 (5%)	25 24	30, 60, 97, 135	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	779	ILE	8.5
1	A	809	VAL	7.4
1	C	781	GLY	6.7
1	C	783	GLY	6.2
1	C	780	GLY	6.2
1	C	1029	GLY	6.0
1	C	669	LYS	5.8
1	C	1095	ARG	5.4
1	C	733	ARG	4.9
1	A	810	THR	4.8
1	D	675	GLU	4.7
1	C	1067	SER	4.6
1	C	782	SER	4.5
1	A	669	LYS	4.4
1	B	675	GLU	4.4
1	A	811	ASP	4.3
1	D	927	ASP	4.3
1	B	808	ASN	4.3
1	A	675	GLU	4.1
1	A	705	ARG	4.0
1	C	687	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	928	VAL	3.8
1	C	1069	ARG	3.8
1	C	1092	GLU	3.7
1	A	778	VAL	3.7
1	D	716	TYR	3.6
1	D	928	VAL	3.6
1	D	1092	GLU	3.5
1	C	835	MET	3.4
1	B	669	LYS	3.4
1	B	809	VAL	3.4
1	D	1094	GLN	3.3
1	A	776	SER	3.3
1	D	680	ASP	3.3
1	A	1093	GLU	3.3
1	A	808	ASN	3.2
1	A	983	GLY	3.0
1	B	810	THR	3.0
1	D	734	GLU	3.0
1	D	705	ARG	3.0
1	D	720	GLU	3.0
1	C	784	GLY	2.9
1	B	1028	GLU	2.8
1	C	684	SER	2.8
1	A	991	ASP	2.8
1	D	719	PHE	2.8
1	D	724	LEU	2.8
1	D	783	GLY	2.8
1	A	682	LEU	2.7
1	C	675	GLU	2.7
1	B	814	TYR	2.6
1	A	993	SER	2.6
1	B	813	LYS	2.6
1	D	1070	LYS	2.5
1	B	928	VAL	2.5
1	A	1090	ILE	2.5
1	C	986	ILE	2.5
1	A	937	ASP	2.5
1	A	699	LEU	2.4
1	A	992	ARG	2.4
1	A	1027	VAL	2.4
1	D	803	PHE	2.4
1	D	725	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	671	ILE	2.3
1	A	927	ASP	2.3
1	A	996	GLN	2.3
1	D	681	ASN	2.3
1	A	706	LYS	2.3
1	A	685	ILE	2.2
1	B	677	LEU	2.2
1	B	716	TYR	2.2
1	C	732	ILE	2.2
1	A	1092	GLU	2.2
1	A	994	ALA	2.2
1	D	672	LEU	2.1
1	A	976	GLY	2.1
1	B	1069	ARG	2.1
1	A	984	LEU	2.1
1	A	932	TRP	2.0
1	D	886	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	ACT	B	1104	4/4	0.83	0.27	59,61,63,64	0
5	ACT	D	1104	4/4	0.91	0.27	86,88,88,89	0
4	MG	D	1103	1/1	0.94	0.20	42,42,42,42	0
2	XKG	A	1101	30/30	0.94	0.14	56,60,63,65	0
4	MG	C	1103	1/1	0.94	0.23	39,39,39,39	0
5	ACT	A	1104	4/4	0.95	0.10	71,72,74,75	0

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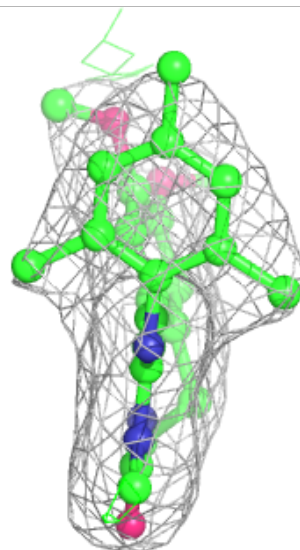
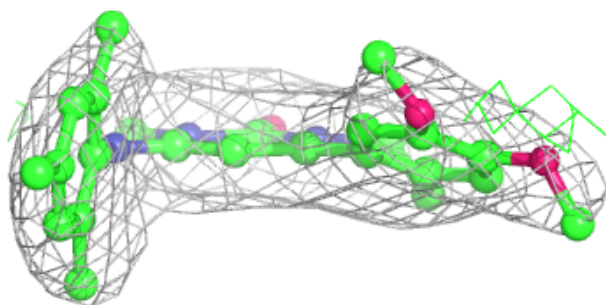
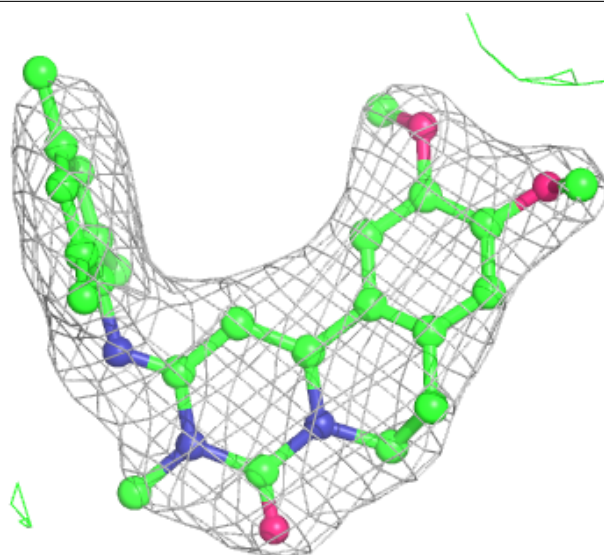
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XKG	C	1101	30/30	0.95	0.14	53,59,66,68	0
5	ACT	C	1104	4/4	0.95	0.14	65,66,69,73	0
2	XKG	D	1101	30/30	0.95	0.15	45,49,52,54	0
4	MG	B	1103	1/1	0.96	0.21	35,35,35,35	0
2	XKG	B	1101	30/30	0.97	0.13	42,47,56,59	0
4	MG	A	1103	1/1	0.99	0.12	36,36,36,36	0
3	MN	B	1102	1/1	0.99	0.14	40,40,40,40	0
3	MN	D	1102	1/1	1.00	0.18	46,46,46,46	0
3	MN	A	1102	1/1	1.00	0.14	47,47,47,47	0
3	MN	C	1102	1/1	1.00	0.14	46,46,46,46	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.

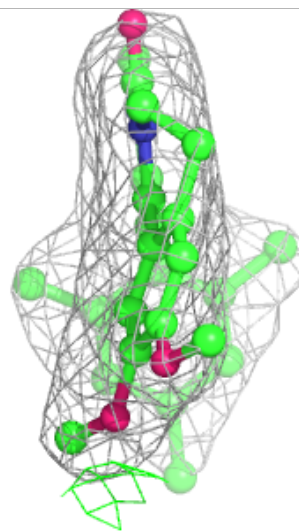
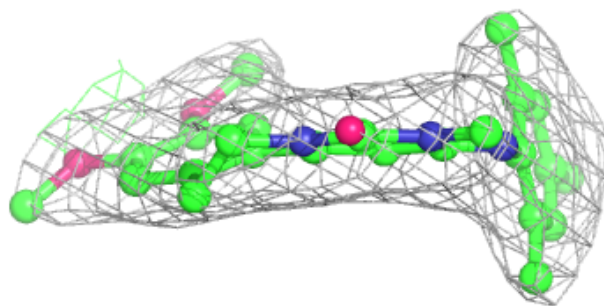
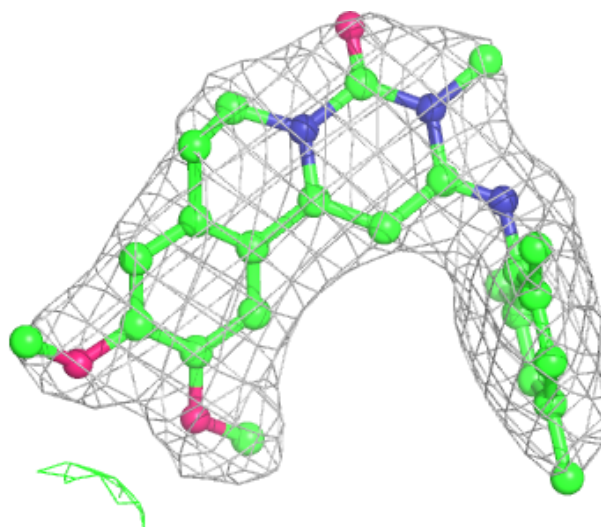
**Electron density around XKG A 1101:**

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



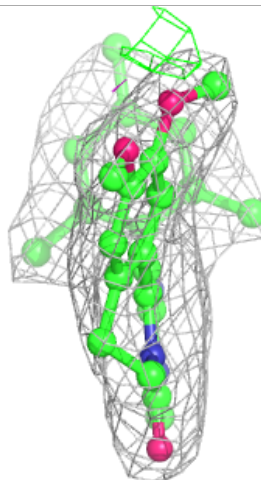
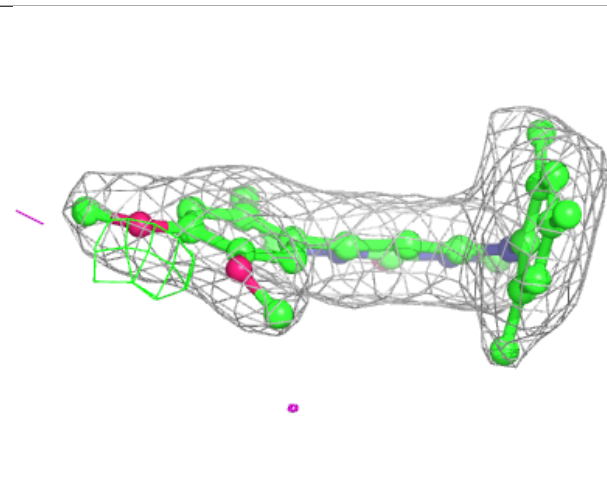
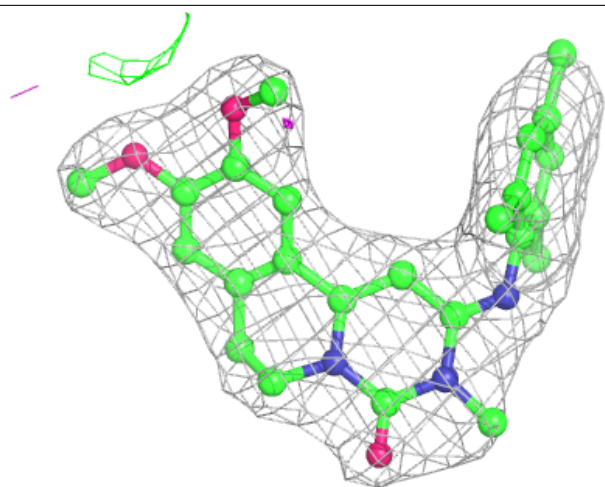
**Electron density around XKG C 1101:**

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



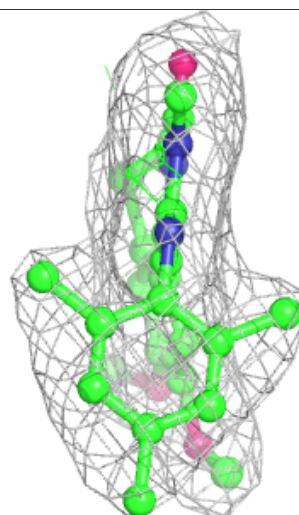
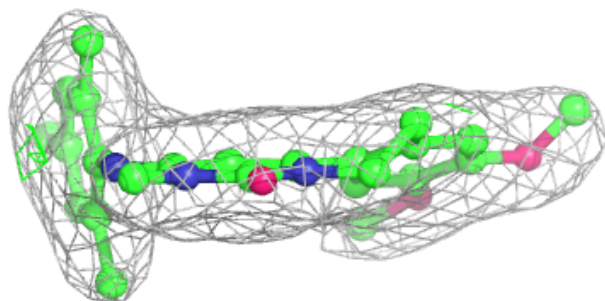
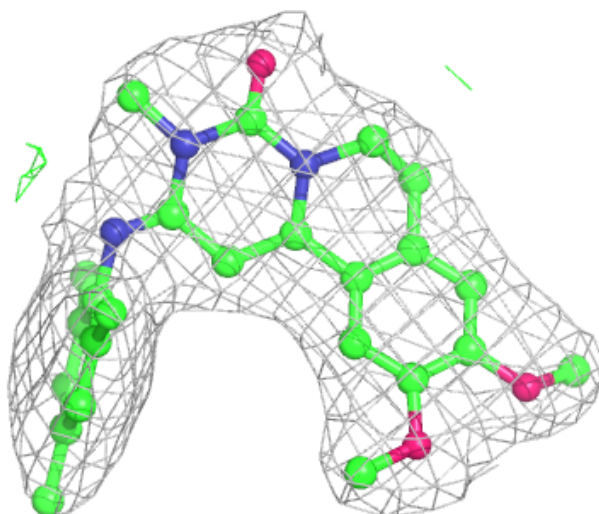
**Electron density around XKG D 1101:**

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



**Electron density around XKG B 1101:**

$2mF_o-DF_c$  (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.