



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:21 AM UTC

PDB ID : 9HZH / pdb\_00009hzh  
Title : Protein kinase CK2 catalytic subunit alpha (CSNK2A1 gene product) in complex with F2X-Entry screen fragment F02 and CX-4945 (Silmitasertib)  
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Deposited on : 2025-01-13  
Resolution : 2.07 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

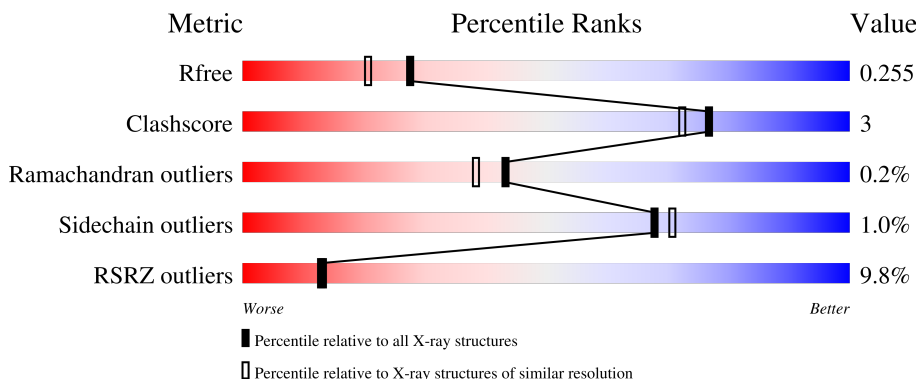
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	355	 8% 85% 8% 7%
1	B	355	 10% 85% 8% 7%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6081 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2799	1792	492	504	11			
1	B	331	Total	C	N	O	S	0	0	0
			2793	1789	491	502	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P68400
A	-18	GLY	-	expression tag	UNP P68400
A	-17	SER	-	expression tag	UNP P68400
A	-16	SER	-	expression tag	UNP P68400
A	-15	HIS	-	expression tag	UNP P68400
A	-14	HIS	-	expression tag	UNP P68400
A	-13	HIS	-	expression tag	UNP P68400
A	-12	HIS	-	expression tag	UNP P68400
A	-11	HIS	-	expression tag	UNP P68400
A	-10	HIS	-	expression tag	UNP P68400
A	-9	SER	-	expression tag	UNP P68400
A	-8	SER	-	expression tag	UNP P68400
A	-7	GLY	-	expression tag	UNP P68400
A	-6	LEU	-	expression tag	UNP P68400
A	-5	VAL	-	expression tag	UNP P68400
A	-4	PRO	-	expression tag	UNP P68400
A	-3	ARG	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	HIS	-	expression tag	UNP P68400
B	-19	MET	-	initiating methionine	UNP P68400
B	-18	GLY	-	expression tag	UNP P68400
B	-17	SER	-	expression tag	UNP P68400
B	-16	SER	-	expression tag	UNP P68400
B	-15	HIS	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P68400
B	-13	HIS	-	expression tag	UNP P68400
B	-12	HIS	-	expression tag	UNP P68400
B	-11	HIS	-	expression tag	UNP P68400
B	-10	HIS	-	expression tag	UNP P68400
B	-9	SER	-	expression tag	UNP P68400
B	-8	SER	-	expression tag	UNP P68400
B	-7	GLY	-	expression tag	UNP P68400
B	-6	LEU	-	expression tag	UNP P68400
B	-5	VAL	-	expression tag	UNP P68400
B	-4	PRO	-	expression tag	UNP P68400
B	-3	ARG	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	HIS	-	expression tag	UNP P68400

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



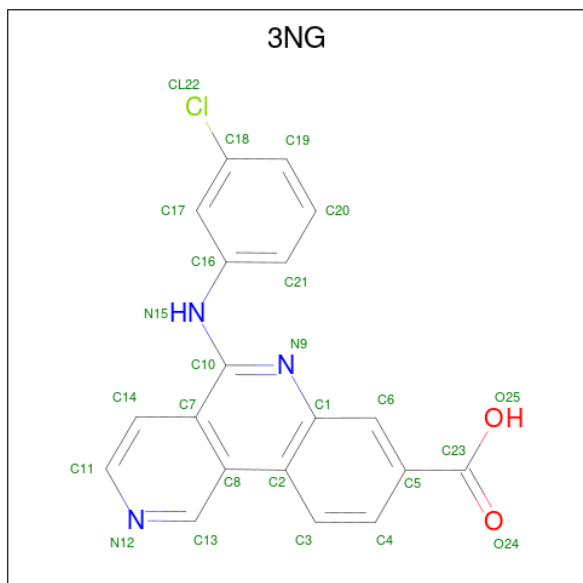
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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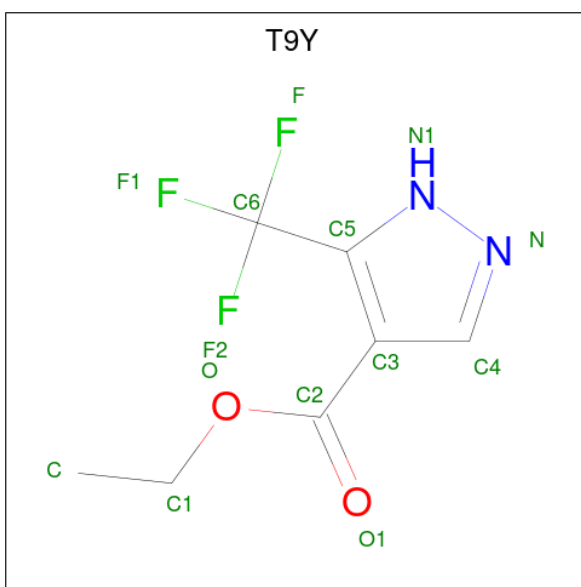
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5-[(3-chlorophenyl)amino]benzo[c][2,6]naphthyridine-8-carboxylic acid (CCD ID: 3NG) (formula:  $C_{19}H_{12}ClN_3O_2$ ).



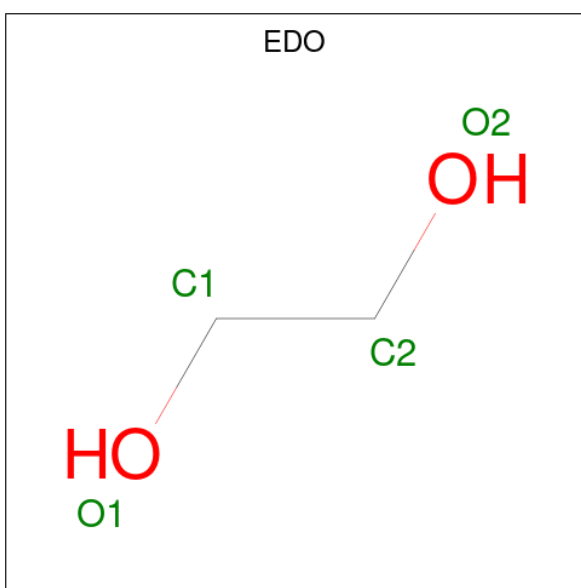
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			25	19	1	3	2	
3	B	1	Total	C	Cl	N	O	0
			25	19	1	3	2	

- Molecule 4 is ethyl 5-(trifluoromethyl)-1H-pyrazole-4-carboxylate (CCD ID: T9Y) (formula:  $C_7H_7F_3N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0
			14	7	3	2	2	
4	B	1	Total	C	F	N	O	0
			14	7	3	2	2	

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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		

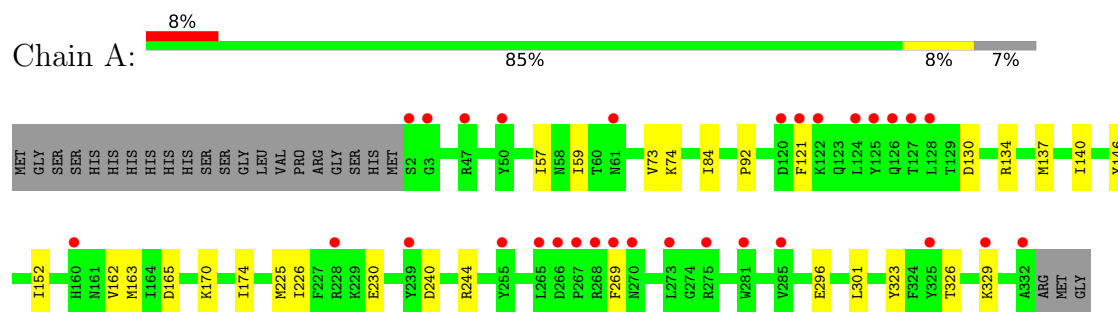
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	172	Total 172	O 172	0	0
6	B	201	Total 201	O 201	0	0

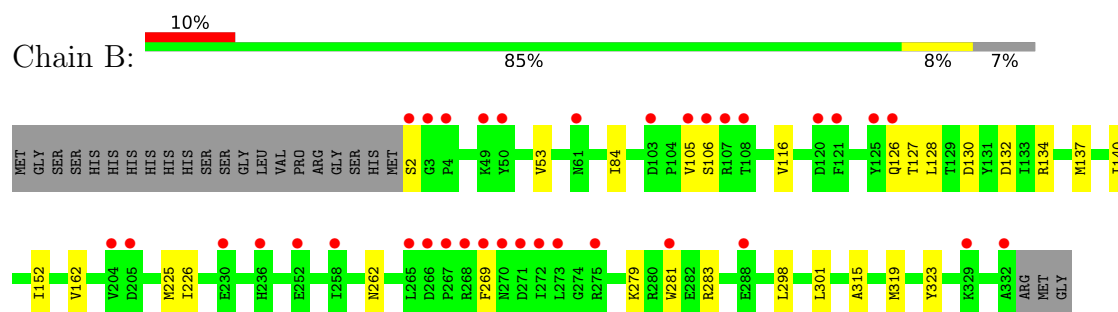
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Casein kinase II subunit alpha



#### • Molecule 1: Casein kinase II subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.49Å 129.49Å 123.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.56 – 2.07 91.56 – 2.07	Depositor EDS
% Data completeness (in resolution range)	71.6 (91.56-2.07) 68.5 (91.56-2.07)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.04 (at 2.07Å)	Xtriage
Refinement program	PHENIX 2.0_5885	Depositor
R, $R_{free}$	0.215 , 0.256 0.214 , 0.255	Depositor DCC
$R_{free}$ test set	1163 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6081	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6432e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: SO4, T9Y, 3NG, EDO

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	0.09	0/2874	0.25	0/3887
1	B	0.09	0/2868	0.26	0/3879
All	All	0.09	0/5742	0.26	0/7766

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	2799	0	2739	17	0
1	B	2793	0	2735	15	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	25	0	11	1	0
3	B	25	0	11	1	0
4	A	14	0	0	0	0
4	B	14	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	172	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	201	0	0	0	0
All	All	6081	0	5508	32	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 3.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.36	0.61
1:A:163:MET:HE2	1:A:174:ILE:HG21	1.84	0.59
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.39	0.58
1:A:140:ILE:HD11	1:A:162:VAL:HG11	1.89	0.55
1:B:137:MET:HE3	1:B:225:MET:HE1	1.90	0.53
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.92	0.52
1:A:121:PHE:HZ	1:A:230:GLU:HG3	1.76	0.50
1:B:2:SER:HB3	1:B:262:ASN:HD21	1.76	0.50
1:A:226:ILE:HD11	1:A:301:LEU:HD22	1.94	0.50
1:B:137:MET:HA	1:B:137:MET:HE2	1.95	0.49
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.95	0.48
1:A:240:ASP:O	1:A:244:ARG:HG2	2.14	0.48
1:A:137:MET:HE3	1:A:225:MET:HE1	1.96	0.47
1:A:326:THR:HA	1:A:329:LYS:HE2	1.96	0.47
1:A:130:ASP:O	1:A:134:ARG:HG3	2.15	0.47
1:B:140:ILE:HD11	1:B:162:VAL:HG11	1.96	0.46
1:A:137:MET:HE2	1:A:140:ILE:HD12	1.96	0.46
1:B:130:ASP:O	1:B:134:ARG:HG3	2.16	0.45
1:B:128:LEU:HD22	1:B:132:ASP:HB3	1.99	0.44
1:B:126:GLN:HG3	1:B:127:THR:HG23	1.98	0.44
1:A:134:ARG:HD3	1:A:323:TYR:O	2.18	0.44
1:A:73:VAL:HG22	1:A:74:LYS:H	1.83	0.43
1:A:163:MET:HE1	3:A:403:3NG:C13	2.49	0.42
1:A:165:ASP:HB3	1:A:170:LYS:HB3	2.02	0.42
1:A:59:ILE:H	1:A:59:ILE:HG13	1.66	0.42
1:B:53:VAL:HG21	3:B:403:3NG:H21	2.02	0.42
1:A:92:PRO:HD2	1:A:146:TYR:CG	2.55	0.42
1:B:279:LYS:HE2	1:B:283:ARG:HH22	1.86	0.41
1:B:226:ILE:HD11	1:B:301:LEU:HD22	2.03	0.41
1:B:281:TRP:HB2	1:B:298:LEU:HD13	2.03	0.40
1:B:134:ARG:HD3	1:B:323:TYR:O	2.21	0.40
1:B:315:ALA:O	1:B:319:MET:HG3	2.20	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	330/355 (93%)	322 (98%)	8 (2%)	0	100	100
1	B	329/355 (93%)	318 (97%)	10 (3%)	1 (0%)	36	30
All	All	659/710 (93%)	640 (97%)	18 (3%)	1 (0%)	43	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	SER

### 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	305/324 (94%)	302 (99%)	3 (1%)	68	71
1	B	304/324 (94%)	301 (99%)	3 (1%)	68	71
All	All	609/648 (94%)	603 (99%)	6 (1%)	68	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	269	PHE

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Mol	Chain	Res	Type
1	A	296	GLU
1	B	105	VAL
1	B	116	VAL
1	B	269	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	262	ASN
1	B	186	GLN
1	B	236	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	406	-	4,4,4	0.67	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	3NG	B	403	-	28,28,28	0.89	1 (3%)	39,40,40	1.02	2 (5%)
2	SO4	B	402	-	4,4,4	0.67	0	6,6,6	0.08	0
3	3NG	A	403	-	28,28,28	0.88	1 (3%)	39,40,40	1.29	5 (12%)
2	SO4	B	401	-	4,4,4	0.66	0	6,6,6	0.09	0
5	EDO	B	405	-	3,3,3	0.25	0	2,2,2	0.29	0
2	SO4	B	406	-	4,4,4	0.67	0	6,6,6	0.10	0
5	EDO	A	405	-	3,3,3	0.26	0	2,2,2	0.27	0
2	SO4	A	402	-	4,4,4	0.67	0	6,6,6	0.08	0
2	SO4	A	401	-	4,4,4	0.67	0	6,6,6	0.09	0
4	T9Y	B	404	-	13,14,14	2.34	5 (38%)	16,20,20	2.20	5 (31%)
4	T9Y	A	404	-	13,14,14	2.34	5 (38%)	16,20,20	2.09	4 (25%)

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	3NG	B	403	-	-	0/8/8/8	0/4/4/4
3	3NG	A	403	-	-	0/8/8/8	0/4/4/4
5	EDO	B	405	-	-	0/1/1/1	-
4	T9Y	A	404	-	-	6/13/13/13	0/1/1/1
4	T9Y	B	404	-	-	6/13/13/13	0/1/1/1
5	EDO	A	405	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	T9Y	C5-N1	-5.15	1.29	1.34
4	A	404	T9Y	C5-N1	-5.15	1.29	1.34
4	A	404	T9Y	O-C2	3.52	1.40	1.33
4	B	404	T9Y	O-C2	3.47	1.40	1.33
4	A	404	T9Y	C4-N	2.79	1.38	1.33
4	B	404	T9Y	C4-N	2.76	1.38	1.33
3	B	403	3NG	C10-N9	-2.41	1.29	1.32
3	A	403	3NG	C10-N9	-2.37	1.29	1.32
4	A	404	T9Y	C3-C2	2.33	1.53	1.48
4	B	404	T9Y	C3-C2	2.29	1.53	1.48
4	A	404	T9Y	O-C1	-2.06	1.40	1.46
4	B	404	T9Y	O-C1	-2.06	1.40	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	T9Y	O-C2-C3	4.62	120.64	112.40
4	A	404	T9Y	O-C2-C3	4.16	119.83	112.40
3	A	403	3NG	N15-C10-N9	4.10	122.19	118.55
4	B	404	T9Y	C4-C3-C5	3.99	108.40	104.77
4	A	404	T9Y	C4-C3-C5	3.86	108.28	104.77
4	B	404	T9Y	C3-C4-N	-3.62	106.06	111.12
3	A	403	3NG	C7-C10-N15	-3.57	116.15	119.77
4	A	404	T9Y	C3-C4-N	-3.57	106.14	111.12
3	A	403	3NG	C16-N15-C10	2.59	134.85	128.22
4	B	404	T9Y	O1-C2-C3	-2.48	119.71	124.78
3	B	403	3NG	C10-N9-C1	2.28	121.40	116.81
4	A	404	T9Y	O1-C2-C3	-2.26	120.16	124.78
3	B	403	3NG	N15-C10-N9	2.15	120.46	118.55
3	A	403	3NG	C10-N9-C1	2.14	121.12	116.81
3	A	403	3NG	C16-C17-C18	2.07	120.41	118.72
4	B	404	T9Y	O-C2-O1	-2.07	119.65	123.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

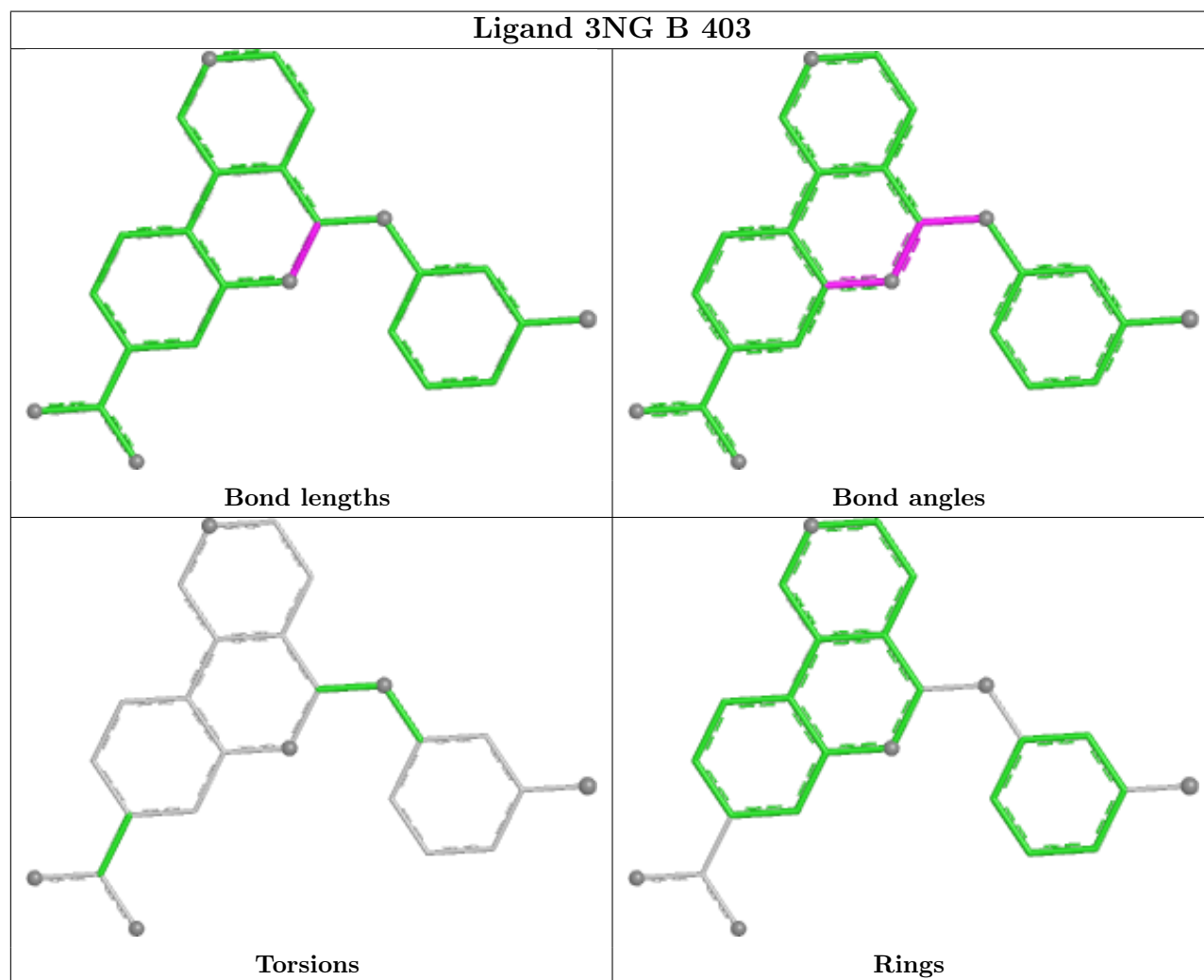
Mol	Chain	Res	Type	Atoms
4	A	404	T9Y	O1-C2-C3-C4
4	A	404	T9Y	O-C2-C3-C4
4	A	404	T9Y	O1-C2-C3-C5
4	A	404	T9Y	O-C2-C3-C5
4	B	404	T9Y	O1-C2-C3-C4
4	B	404	T9Y	O-C2-C3-C4
4	A	404	T9Y	C3-C2-O-C1
4	A	404	T9Y	O1-C2-O-C1
4	B	404	T9Y	O1-C2-C3-C5
4	B	404	T9Y	O-C2-C3-C5
4	B	404	T9Y	C3-C2-O-C1
4	B	404	T9Y	O1-C2-O-C1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

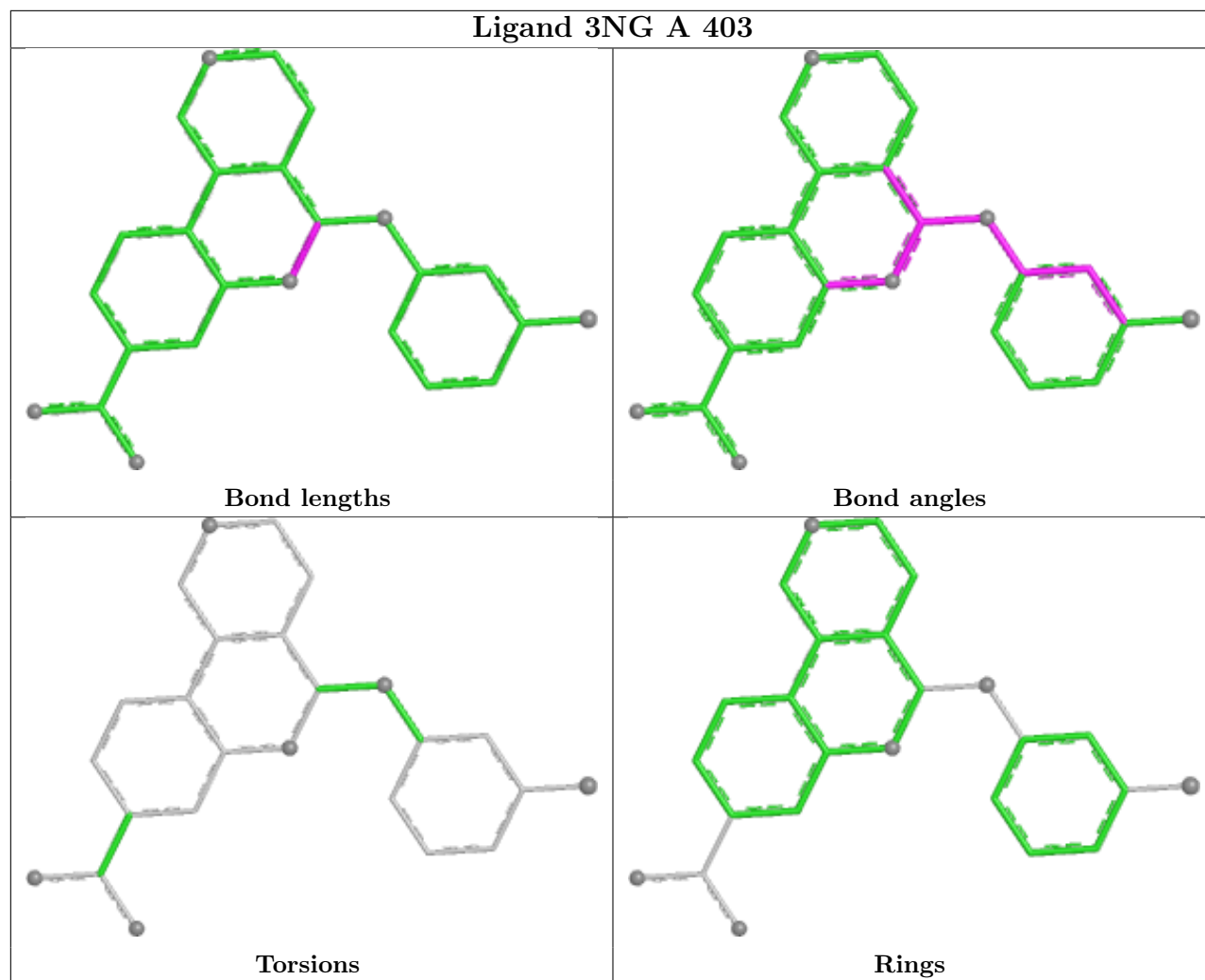
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	3NG	1	0
3	A	403	3NG	1	0

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.

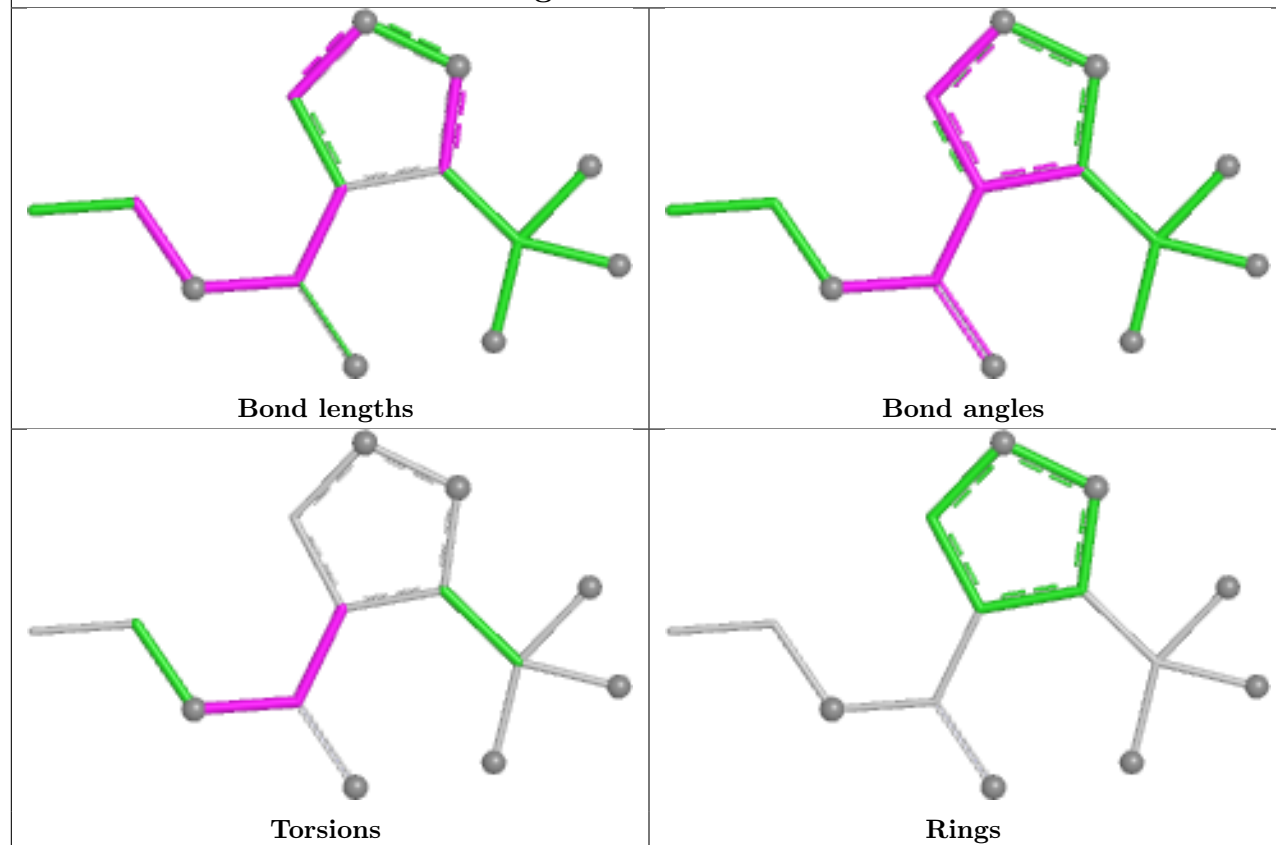




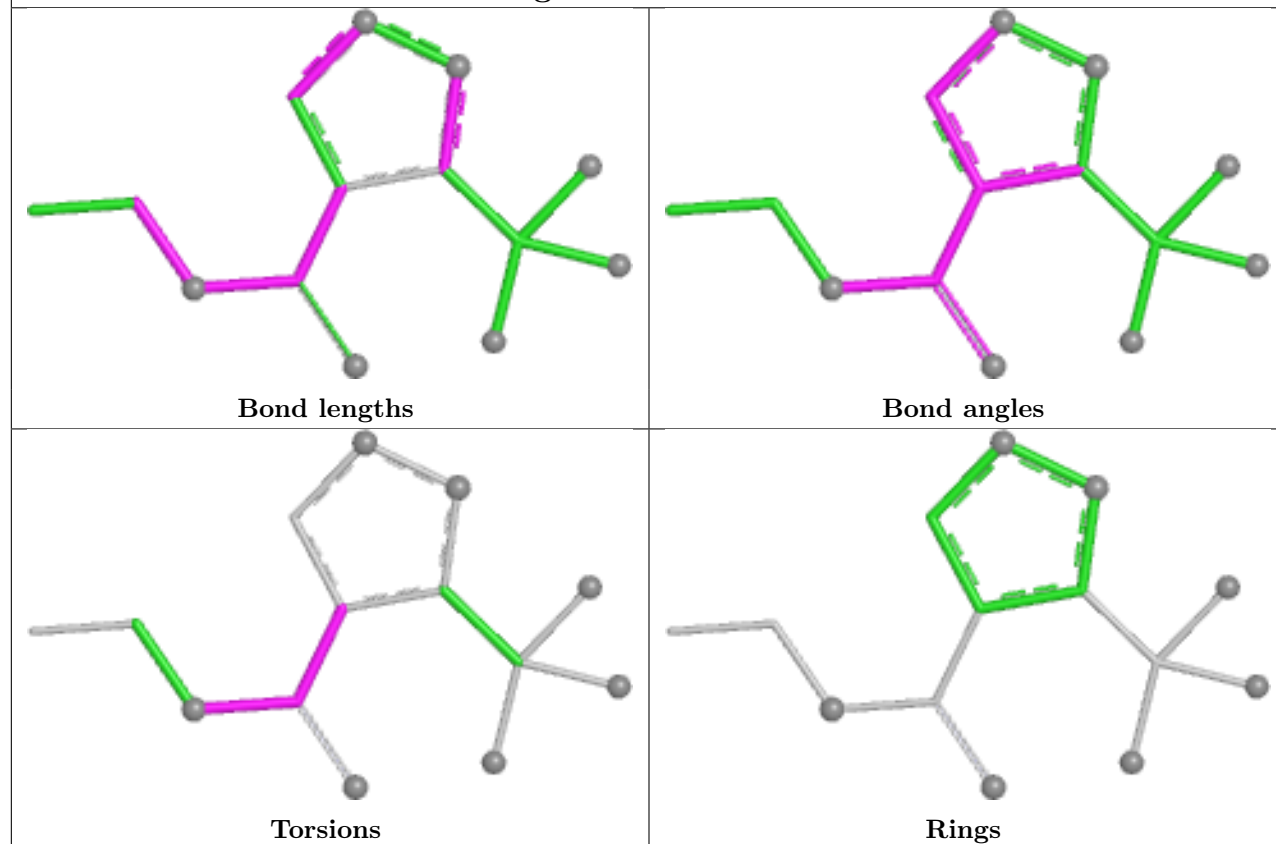
## Ligand 3NG A 403



## Ligand T9Y B 404



## Ligand T9Y A 404



## 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	331/355 (93%)	0.51	30 (9%) 15 15	16, 35, 76, 107	1 (0%)
1	B	331/355 (93%)	0.56	35 (10%) 11 11	17, 36, 71, 133	0
All	All	662/710 (93%)	0.53	65 (9%) 13 13	16, 35, 72, 133	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	VAL	5.8
1	B	3	GLY	5.0
1	A	332	ALA	4.8
1	A	255	TYR	4.7
1	A	2	SER	4.7
1	A	125	TYR	4.3
1	B	332	ALA	4.2
1	A	275	ARG	4.2
1	A	269	PHE	4.1
1	B	121	PHE	4.0
1	B	2	SER	4.0
1	A	121	PHE	3.9
1	B	50	TYR	3.7
1	B	126	GLN	3.7
1	B	125	TYR	3.6
1	A	128	LEU	3.4
1	A	266	ASP	3.3
1	A	3	GLY	3.3
1	B	267	PRO	3.3
1	A	127	THR	3.2
1	B	273	LEU	3.2
1	A	267	PRO	3.2
1	A	126	GLN	3.2
1	A	270	ASN	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	3.0
1	B	107	ARG	2.9
1	B	230	GLU	2.9
1	B	269	PHE	2.8
1	A	122	LYS	2.8
1	A	268	ARG	2.7
1	A	124	LEU	2.7
1	B	236	HIS	2.7
1	B	108	THR	2.7
1	B	265	LEU	2.7
1	A	281	TRP	2.7
1	B	120	ASP	2.6
1	B	288	GLU	2.6
1	B	49	LYS	2.6
1	B	271	ASP	2.6
1	A	273	LEU	2.5
1	A	120	ASP	2.5
1	B	106	SER	2.5
1	A	265	LEU	2.5
1	B	281	TRP	2.5
1	B	103	ASP	2.4
1	B	252	GLU	2.3
1	B	258	ILE	2.3
1	B	4	PRO	2.3
1	B	268	ARG	2.3
1	A	61	ASN	2.3
1	B	272	ILE	2.2
1	A	47	ARG	2.2
1	A	228	ARG	2.2
1	A	160	HIS	2.2
1	B	270	ASN	2.2
1	A	239	TYR	2.1
1	A	285	VAL	2.1
1	B	205	ASP	2.1
1	B	275	ARG	2.1
1	B	204	VAL	2.1
1	A	325	TYR	2.0
1	A	329	LYS	2.0
1	B	61	ASN	2.0
1	B	266	ASP	2.0
1	B	329	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

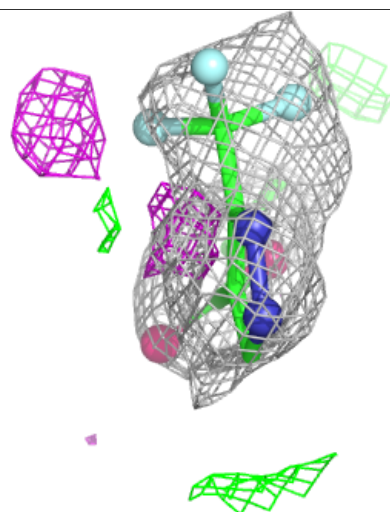
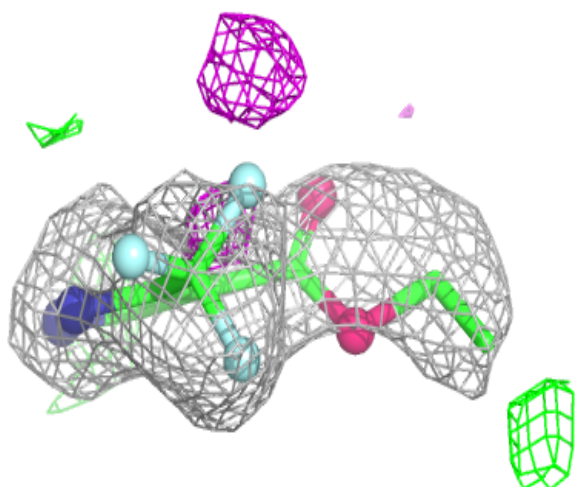
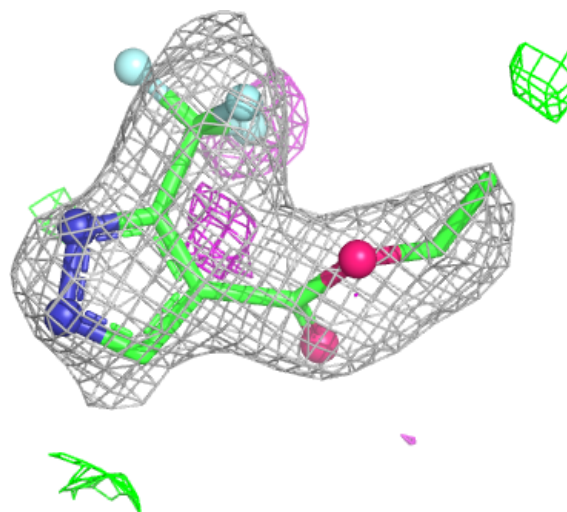
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	SO4	A	402	5/5	0.67	0.15	74,87,106,122	0
4	T9Y	B	404	14/14	0.76	0.20	40,75,84,89	0
2	SO4	B	402	5/5	0.77	0.14	63,86,93,108	0
2	SO4	B	406	5/5	0.78	0.14	60,70,76,80	0
5	EDO	A	405	4/4	0.79	0.19	45,46,47,52	0
2	SO4	A	406	5/5	0.85	0.12	40,52,87,103	0
4	T9Y	A	404	14/14	0.85	0.16	50,73,85,93	0
5	EDO	B	405	4/4	0.88	0.13	44,45,54,55	0
3	3NG	B	403	25/25	0.89	0.12	22,35,45,160	0
3	3NG	A	403	25/25	0.94	0.09	21,29,41,69	0
2	SO4	A	401	5/5	0.95	0.14	32,38,47,75	0
2	SO4	B	401	5/5	0.96	0.09	38,41,49,54	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.

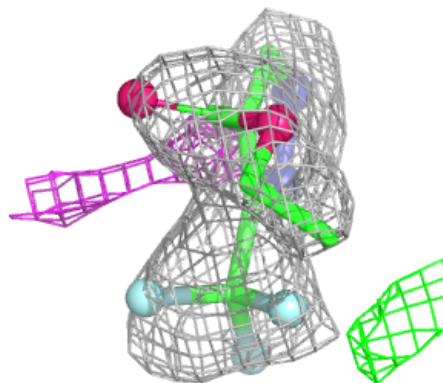
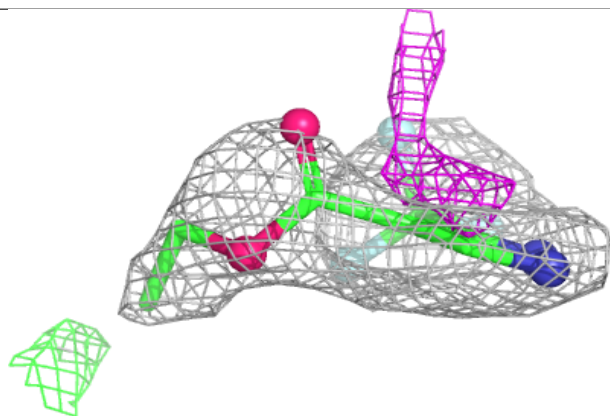
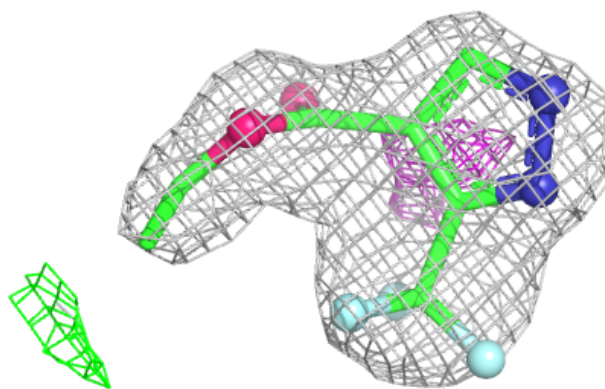
**Electron density around T9Y B 404:**

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



**Electron density around T9Y A 404:**

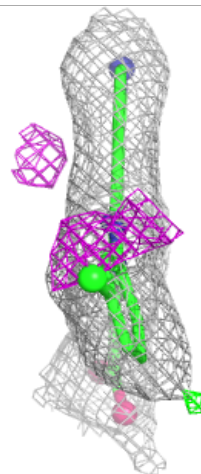
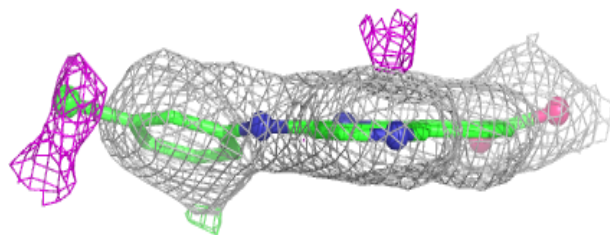
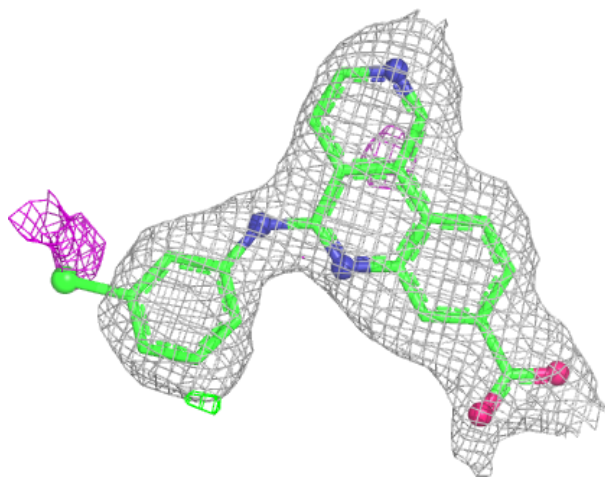
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

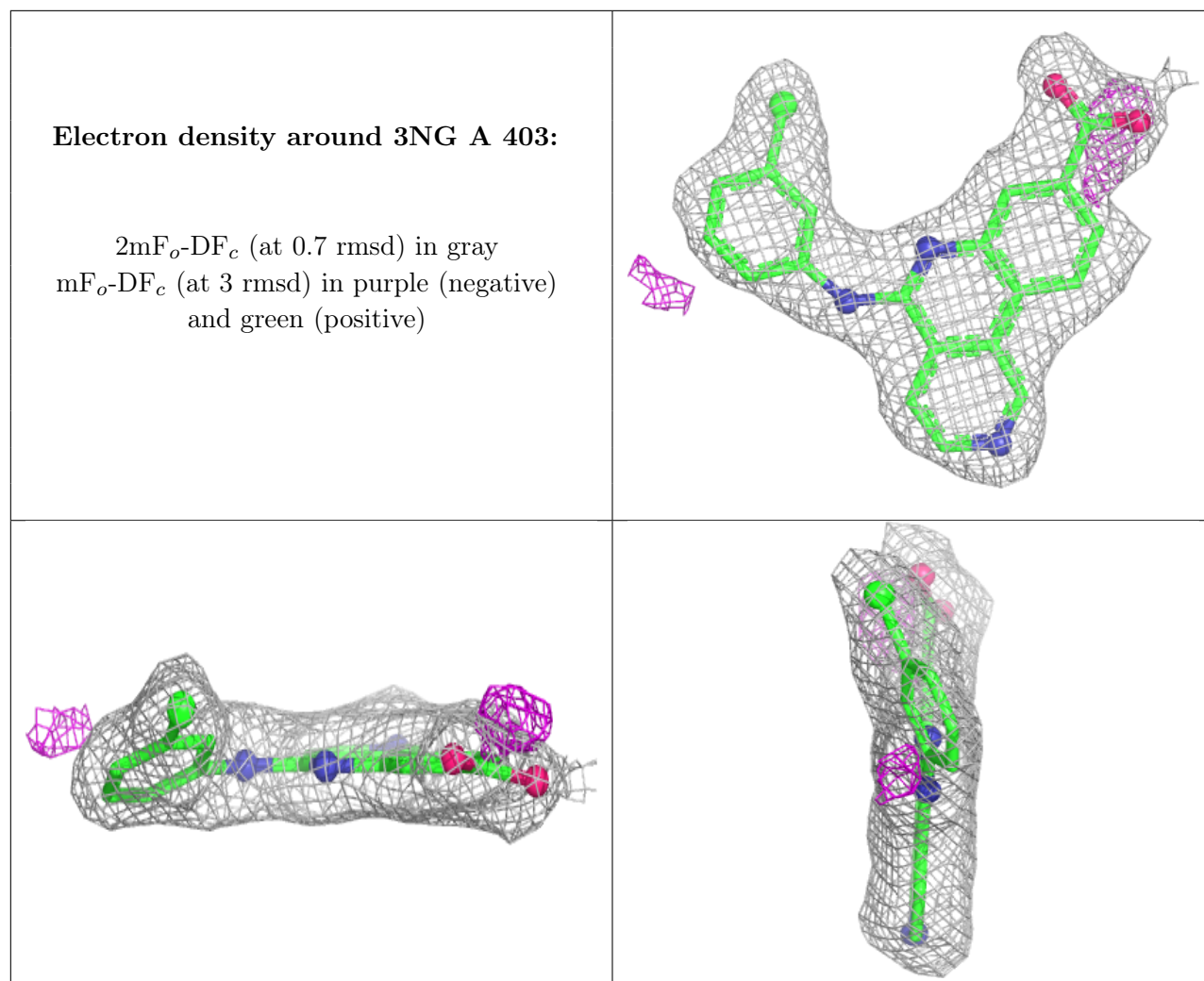




**Electron density around 3NG B 403:**

$2mF_o-DF_c$  (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.