



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 11, 2024 – 09:36 PM EST

PDB ID : 3G4G  
Title : Crystal structure of human phosphodiesterase 4d with regulatory domain and d155871  
Authors : Staker, B.L.  
Deposited on : 2009-02-03  
Resolution : 2.30 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467  
Mogul : 1.8.5 (274361), 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

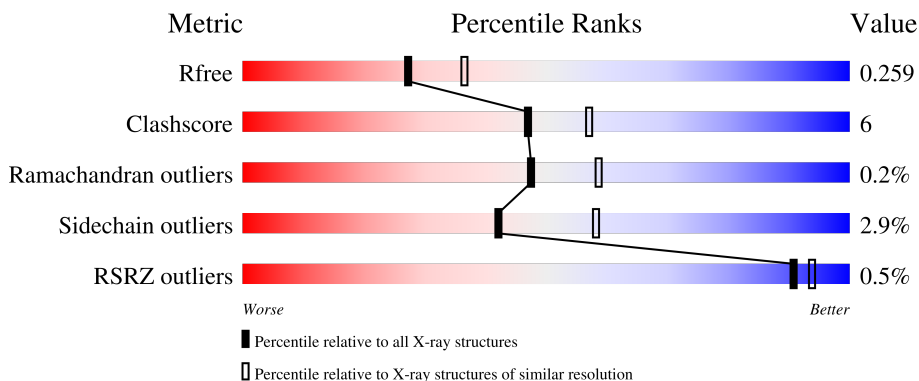
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	421	 71% 8% • 20%
1	B	421	 64% 16% 20%
1	C	421	 71% 9% • 19%
1	D	421	 70% 9% • 20%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11183 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	Total 2725	C 1724	N 464	O 523	S 14	0	0	0
1	B	336	Total 2712	C 1718	N 462	O 518	S 14	0	0	0
1	C	339	Total 2739	C 1733	N 468	O 524	S 14	0	0	0
1	D	337	Total 2716	C 1720	N 464	O 518	S 14	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MET	-	expression tag	UNP Q08499
A	215	LYS	-	linker	UNP Q08499
A	216	VAL	-	linker	UNP Q08499
A	217	THR	-	linker	UNP Q08499
A	218	ALA	-	linker	UNP Q08499
A	219	GLU	-	linker	UNP Q08499
A	220	GLU	-	linker	UNP Q08499
A	221	ALA	-	linker	UNP Q08499
A	222	PRO	-	linker	UNP Q08499
A	223	GLN	-	linker	UNP Q08499
A	579	ALA	-	expression tag	UNP Q08499
A	580	HIS	-	expression tag	UNP Q08499
A	581	HIS	-	expression tag	UNP Q08499
A	582	HIS	-	expression tag	UNP Q08499
A	583	HIS	-	expression tag	UNP Q08499
A	584	HIS	-	expression tag	UNP Q08499
A	585	HIS	-	expression tag	UNP Q08499
B	162	MET	-	expression tag	UNP Q08499
B	215	LYS	-	linker	UNP Q08499
B	216	VAL	-	linker	UNP Q08499
B	217	THR	-	linker	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
B	218	ALA	-	linker	UNP Q08499
B	219	GLU	-	linker	UNP Q08499
B	220	GLU	-	linker	UNP Q08499
B	221	ALA	-	linker	UNP Q08499
B	222	PRO	-	linker	UNP Q08499
B	223	GLN	-	linker	UNP Q08499
B	579	ALA	-	expression tag	UNP Q08499
B	580	HIS	-	expression tag	UNP Q08499
B	581	HIS	-	expression tag	UNP Q08499
B	582	HIS	-	expression tag	UNP Q08499
B	583	HIS	-	expression tag	UNP Q08499
B	584	HIS	-	expression tag	UNP Q08499
B	585	HIS	-	expression tag	UNP Q08499
C	162	MET	-	expression tag	UNP Q08499
C	215	LYS	-	linker	UNP Q08499
C	216	VAL	-	linker	UNP Q08499
C	217	THR	-	linker	UNP Q08499
C	218	ALA	-	linker	UNP Q08499
C	219	GLU	-	linker	UNP Q08499
C	220	GLU	-	linker	UNP Q08499
C	221	ALA	-	linker	UNP Q08499
C	222	PRO	-	linker	UNP Q08499
C	223	GLN	-	linker	UNP Q08499
C	579	ALA	-	expression tag	UNP Q08499
C	580	HIS	-	expression tag	UNP Q08499
C	581	HIS	-	expression tag	UNP Q08499
C	582	HIS	-	expression tag	UNP Q08499
C	583	HIS	-	expression tag	UNP Q08499
C	584	HIS	-	expression tag	UNP Q08499
C	585	HIS	-	expression tag	UNP Q08499
D	162	MET	-	expression tag	UNP Q08499
D	215	LYS	-	linker	UNP Q08499
D	216	VAL	-	linker	UNP Q08499
D	217	THR	-	linker	UNP Q08499
D	218	ALA	-	linker	UNP Q08499
D	219	GLU	-	linker	UNP Q08499
D	220	GLU	-	linker	UNP Q08499
D	221	ALA	-	linker	UNP Q08499
D	222	PRO	-	linker	UNP Q08499
D	223	GLN	-	linker	UNP Q08499
D	579	ALA	-	expression tag	UNP Q08499
D	580	HIS	-	expression tag	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
D	581	HIS	-	expression tag	UNP Q08499
D	582	HIS	-	expression tag	UNP Q08499
D	583	HIS	-	expression tag	UNP Q08499
D	584	HIS	-	expression tag	UNP Q08499
D	585	HIS	-	expression tag	UNP Q08499

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

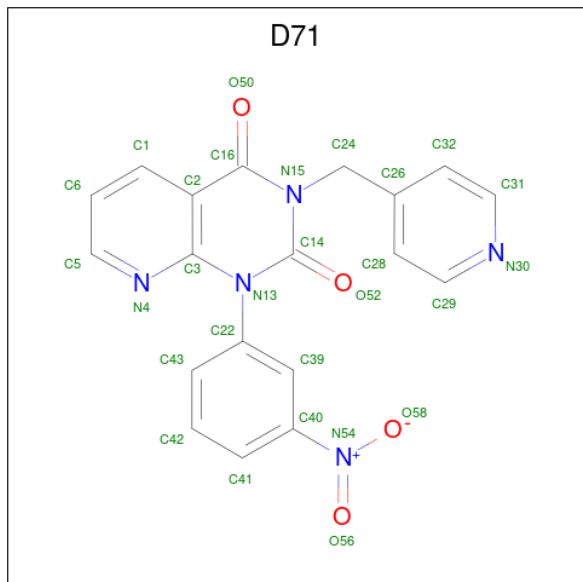
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 1-(3-nitrophenyl)-3-(pyridin-4-ylmethyl)pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione (three-letter code: D71) (formula: C<sub>19</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			28	19	5	4		
5	B	1	Total	C	N	O	0	0
			28	19	5	4		
5	C	1	Total	C	N	O	0	0
			28	19	5	4		
5	D	1	Total	C	N	O	0	0
			28	19	5	4		

- Molecule 6 is water.

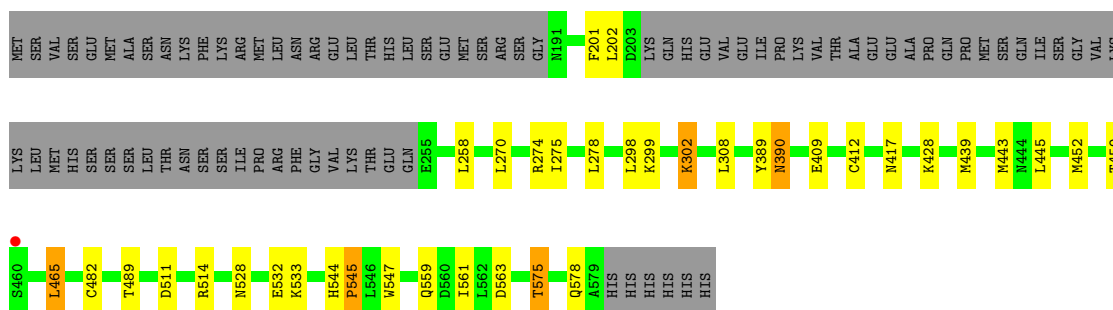
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	39	Total	O	0	0
			39	39		
6	B	35	Total	O	0	0
			35	35		
6	C	48	Total	O	0	0
			48	48		
6	D	45	Total	O	0	0
			45	45		

### 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.

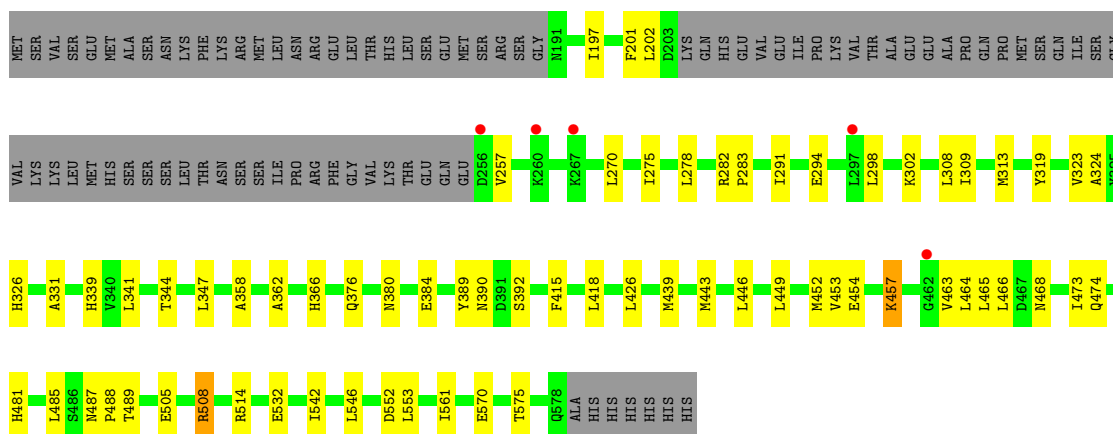
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A: 



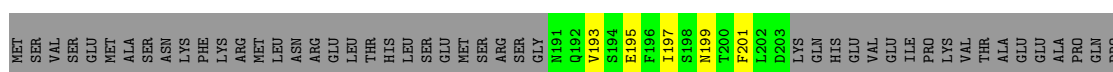
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

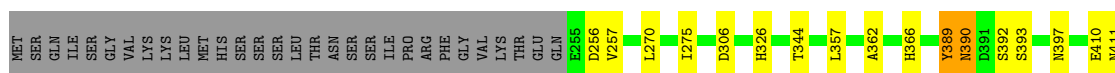
Chain B: 



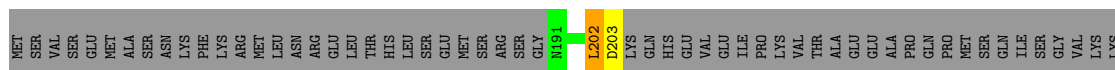
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain C: 





- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.13Å 75.31Å 162.56Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	48.80 – 2.30 46.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.80-2.30) 95.0 (46.76-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.188 , 0.257 0.193 , 0.259	Depositor DCC
$R_{free}$ test set	3262 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.094 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: ZN, CA, MG, D71

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	0.76	1/2780 (0.0%)	0.74	1/3778 (0.0%)
1	B	0.69	0/2767	0.72	4/3759 (0.1%)
1	C	0.75	0/2795	0.76	1/3797 (0.0%)
1	D	0.73	0/2771	0.73	2/3765 (0.1%)
All	All	0.73	1/11113 (0.0%)	0.74	8/15099 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	CYS	CB-SG	-5.32	1.73	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ASN	N-CA-C	-8.64	87.66	111.00
1	D	390	ASN	N-CA-C	-6.88	92.43	111.00
1	B	508	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	390	ASN	N-CA-C	-5.99	94.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ARG	NE-CZ-NH1	5.82	123.21	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	TYR	Peptide
1	B	389	TYR	Peptide
1	C	389	TYR	Peptide
1	D	389	TYR	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2725	0	2663	26	0
1	B	2712	0	2659	47	0
1	C	2739	0	2681	33	0
1	D	2716	0	2661	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
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	28	0	13	0	0
5	B	28	0	13	1	0
5	C	28	0	13	0	0
5	D	28	0	13	0	0
6	A	39	0	0	0	0
6	B	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	48	0	0	0	0
6	D	45	0	0	0	0
All	All	11183	0	10716	135	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 6.

The worst 5 of 135 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:GLU:HG2	1:A:575:THR:HG22	1.51	0.92
1:D:532:GLU:HG2	1:D:575:THR:CG2	2.02	0.90
1:C:201:PHE:CE1	1:C:542:ILE:HD13	2.13	0.82
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.63	0.81
1:B:532:GLU:HG2	1:B:575:THR:HG22	1.65	0.79

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	334/421 (79%)	329 (98%)	4 (1%)	1 (0%)	41 50
1	B	332/421 (79%)	326 (98%)	6 (2%)	0	100 100
1	C	335/421 (80%)	329 (98%)	5 (2%)	1 (0%)	41 50
1	D	333/421 (79%)	323 (97%)	9 (3%)	1 (0%)	41 50
All	All	1334/1684 (79%)	1307 (98%)	24 (2%)	3 (0%)	47 58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	D	390	ASN
1	C	390	ASN

### 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	307/386 (80%)	295 (96%)	12 (4%)	32	46
1	B	306/386 (79%)	298 (97%)	8 (3%)	46	63
1	C	309/386 (80%)	302 (98%)	7 (2%)	50	67
1	D	306/386 (79%)	298 (97%)	8 (3%)	46	63
All	All	1228/1544 (80%)	1193 (97%)	35 (3%)	42	58

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	203	ASP
1	D	344	THR
1	D	470	SER
1	B	294	GLU
1	A	578	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	271	HIS
1	D	509	GLN
1	D	411	ASN
1	C	271	HIS
1	C	559	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 [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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
5	D71	B	902	-	29,31,31	2.90	14 (48%)	35,44,44	1.57	7 (20%)
5	D71	D	904	-	29,31,31	2.87	15 (51%)	35,44,44	2.05	15 (42%)
5	D71	A	901	-	29,31,31	3.18	14 (48%)	35,44,44	1.53	8 (22%)
5	D71	C	903	-	29,31,31	3.07	15 (51%)	35,44,44	1.79	9 (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
5	D71	B	902	-	-	0/10/12/12	0/4/4/4
5	D71	D	904	-	-	0/10/12/12	0/4/4/4
5	D71	A	901	-	-	0/10/12/12	0/4/4/4
5	D71	C	903	-	-	0/10/12/12	0/4/4/4

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	D71	C2-C3	6.82	1.49	1.40
5	A	901	D71	C2-C3	6.62	1.49	1.40
5	A	901	D71	C32-C31	5.98	1.50	1.38
5	B	902	D71	C2-C3	5.74	1.48	1.40
5	A	901	D71	C41-C40	5.25	1.48	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903	D71	O52-C14-N15	-3.53	117.08	121.99
5	D	904	D71	C39-C40-N54	3.53	121.85	118.75
5	D	904	D71	C39-C22-N13	3.50	123.44	119.49
5	D	904	D71	C5-N4-C3	3.46	123.15	115.14
5	D	904	D71	C24-C26-C28	-3.39	114.40	120.77

There are no chirality outliers.

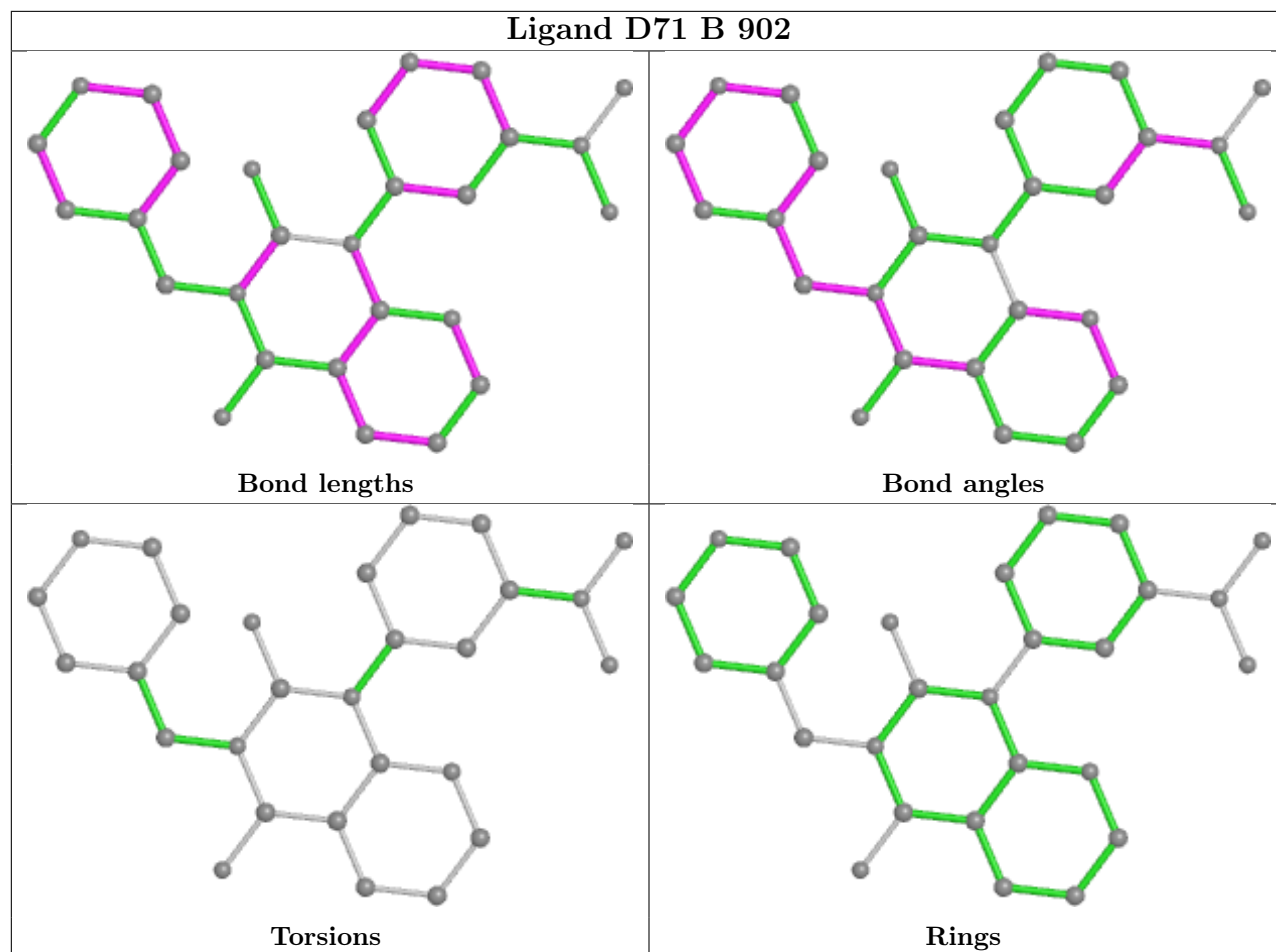
There are no torsion outliers.

There are no ring outliers.

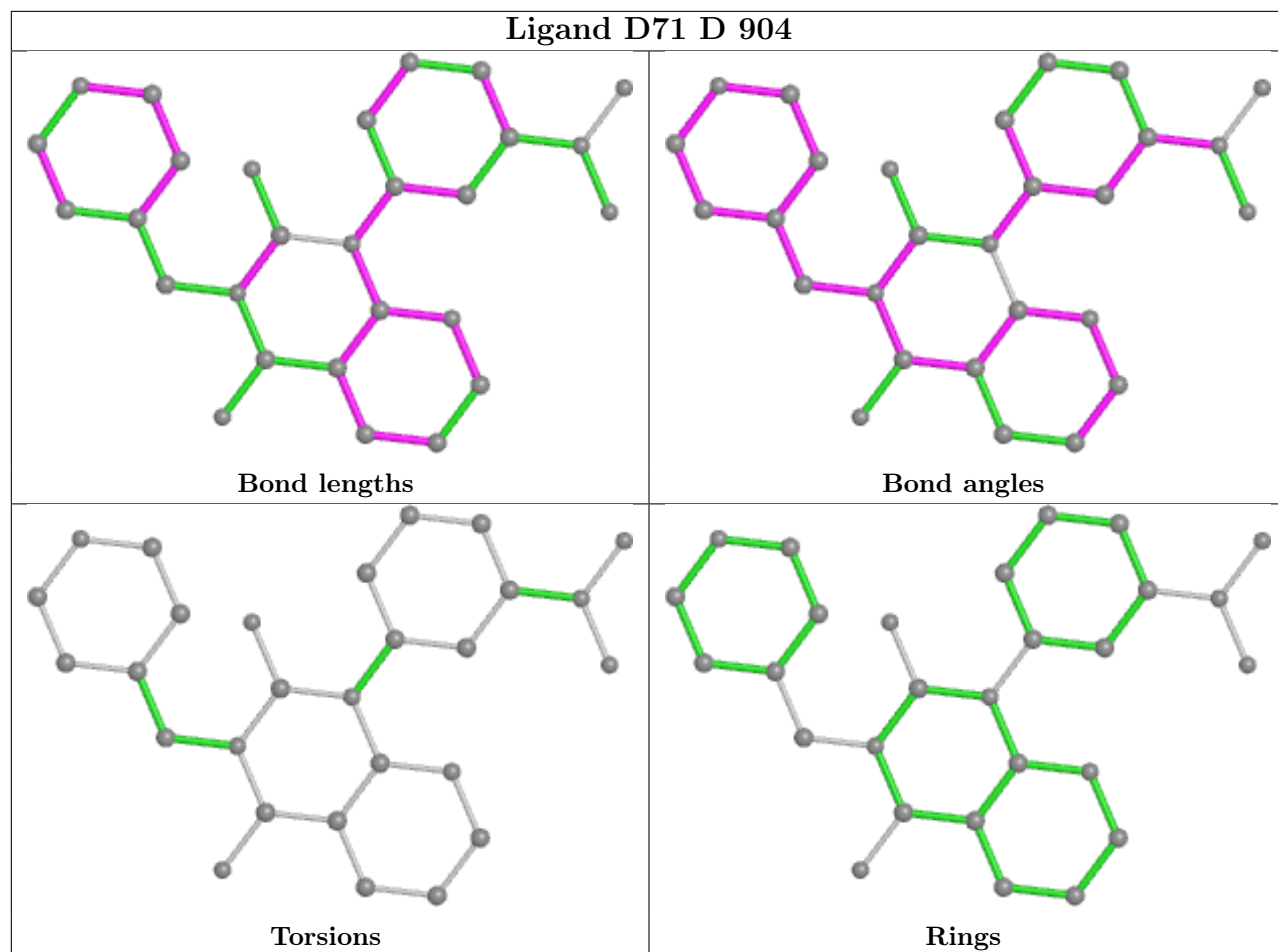
1 monomer is involved in 1 short contact:

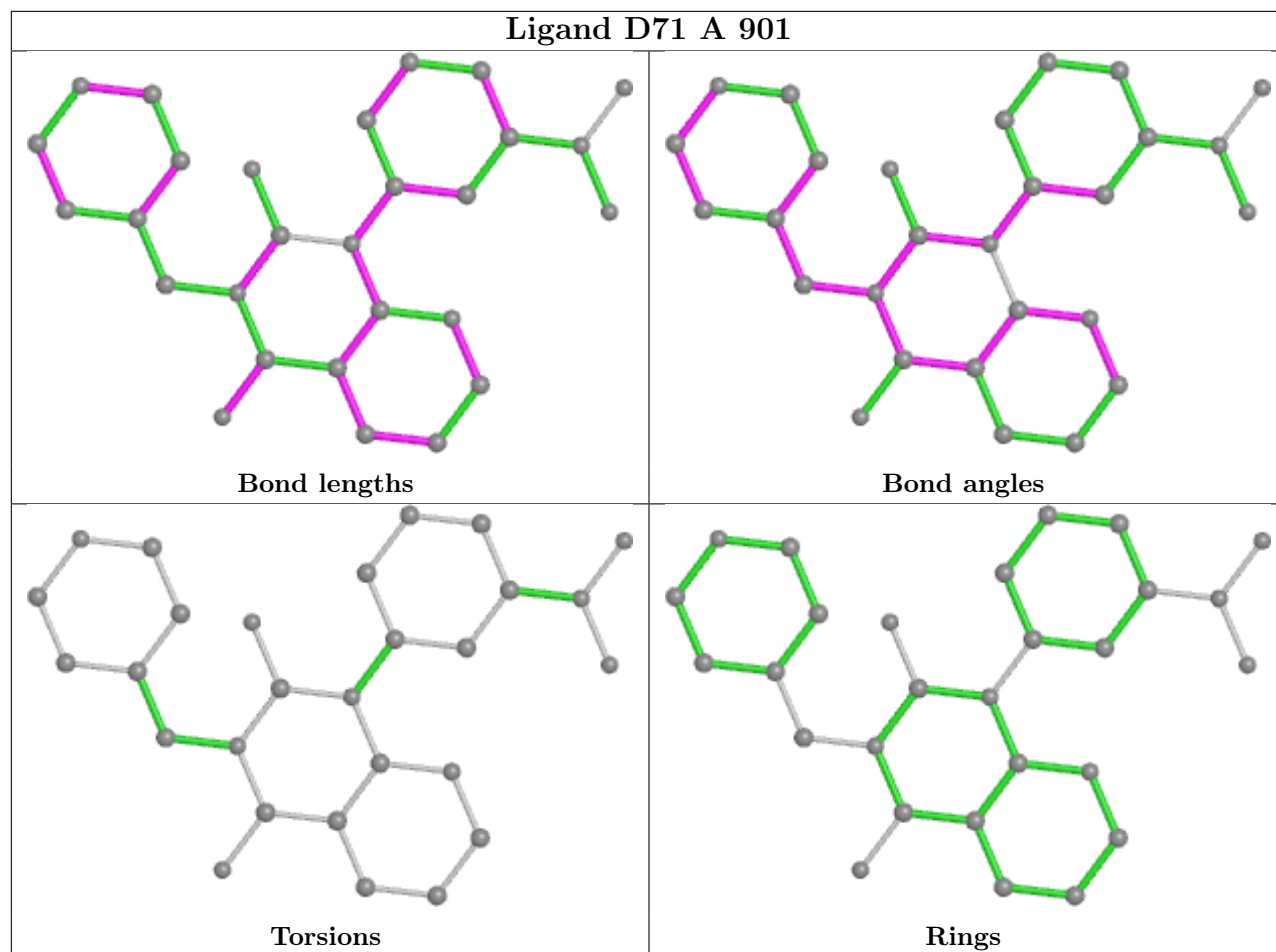
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	D71	1	0

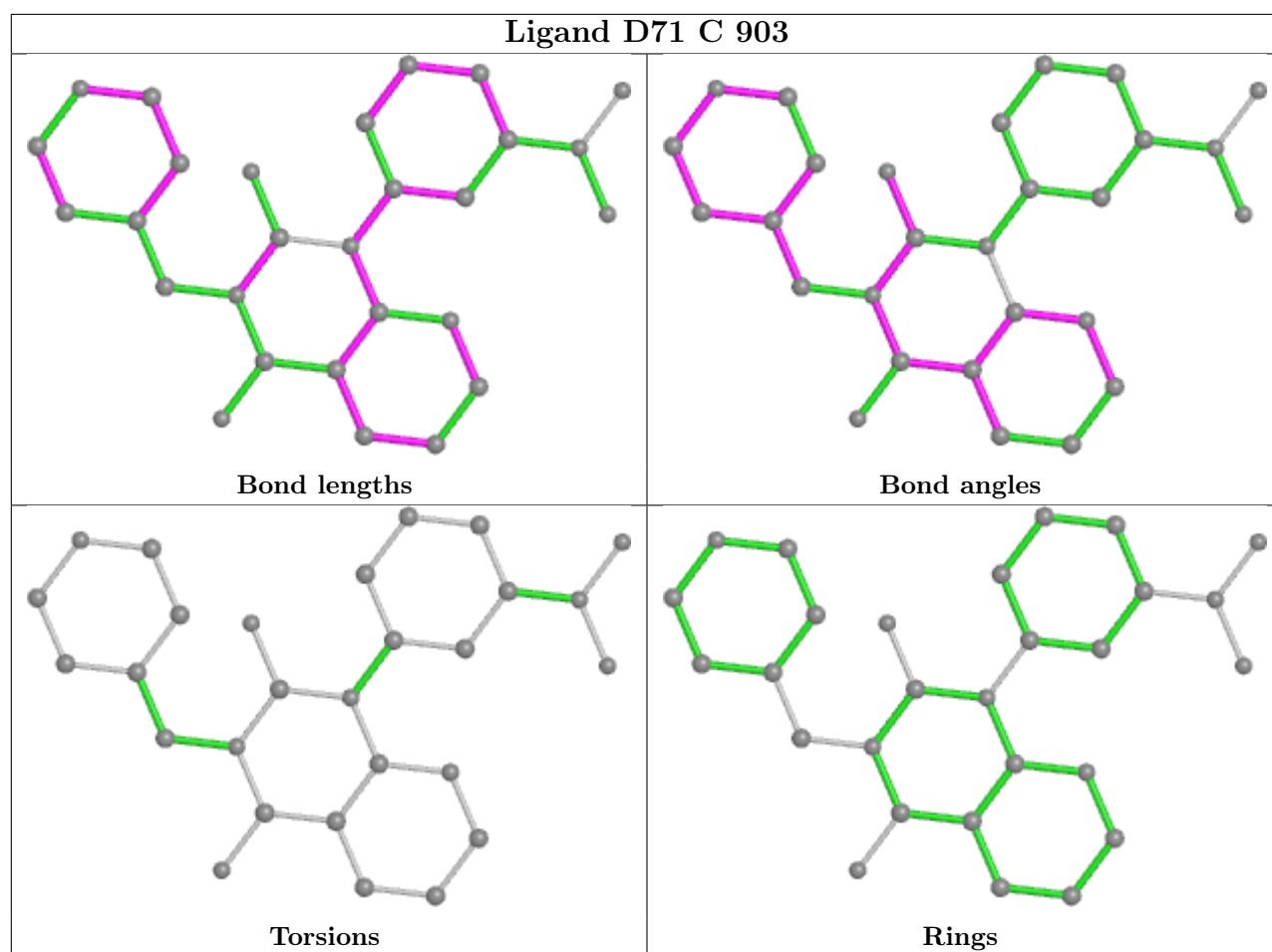
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	338/421 (80%)	-0.18	1 (0%) 94 96	11, 23, 38, 47	0
1	B	336/421 (79%)	-0.04	5 (1%) 73 79	14, 30, 46, 54	0
1	C	339/421 (80%)	-0.14	0 100 100	11, 25, 41, 49	0
1	D	337/421 (80%)	-0.22	1 (0%) 94 96	14, 26, 38, 45	0
All	All	1350/1684 (80%)	-0.14	7 (0%) 91 94	11, 26, 42, 54	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	LYS	2.5
1	B	267	LYS	2.4
1	B	462	GLY	2.1
1	D	256	ASP	2.1
1	B	297	LEU	2.1

### 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](#)

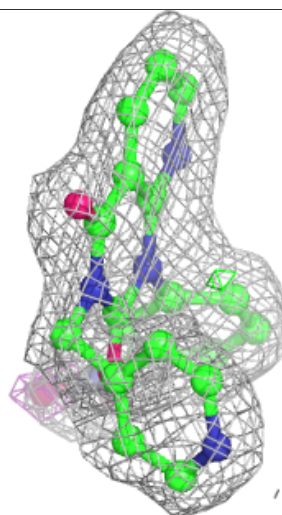
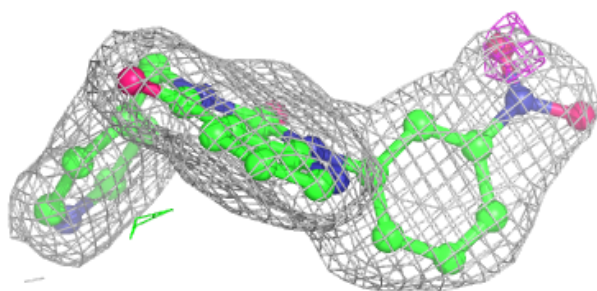
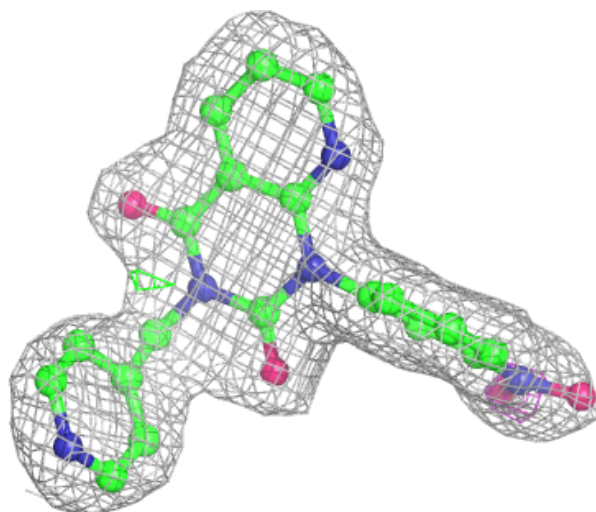
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
3	MG	A	802	1/1	0.92	0.29	12,12,12,12	0
4	CA	A	4	1/1	0.93	0.10	53,53,53,53	0
3	MG	B	804	1/1	0.94	0.24	17,17,17,17	0
4	CA	B	1	1/1	0.94	0.18	41,41,41,41	0
5	D71	C	903	28/28	0.94	0.13	14,20,31,36	0
5	D71	A	901	28/28	0.95	0.13	14,19,31,36	0
5	D71	B	902	28/28	0.95	0.12	16,19,24,27	0
3	MG	C	806	1/1	0.95	0.20	14,14,14,14	0
5	D71	D	904	28/28	0.95	0.13	14,16,21,24	0
4	CA	C	2	1/1	0.97	0.08	52,52,52,52	0
4	CA	D	3	1/1	0.98	0.20	35,35,35,35	0
3	MG	D	808	1/1	0.99	0.15	10,10,10,10	0
2	ZN	D	807	1/1	0.99	0.09	22,22,22,22	0
2	ZN	A	801	1/1	0.99	0.14	21,21,21,21	0
2	ZN	C	805	1/1	1.00	0.12	20,20,20,20	0
2	ZN	B	803	1/1	1.00	0.12	25,25,25,25	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.

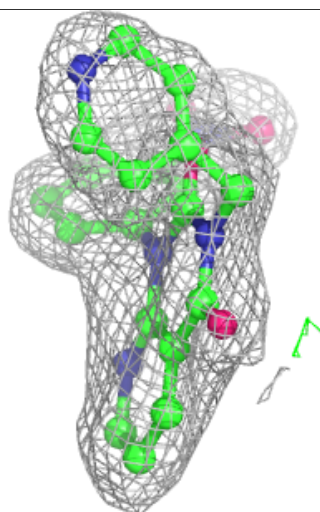
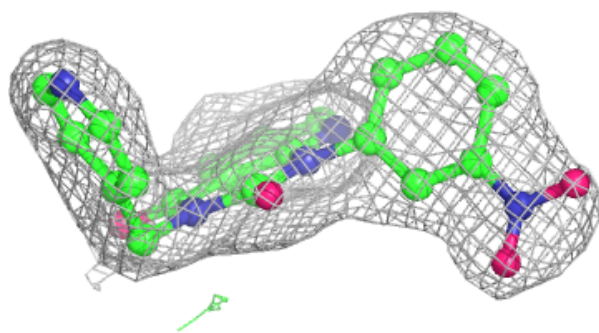
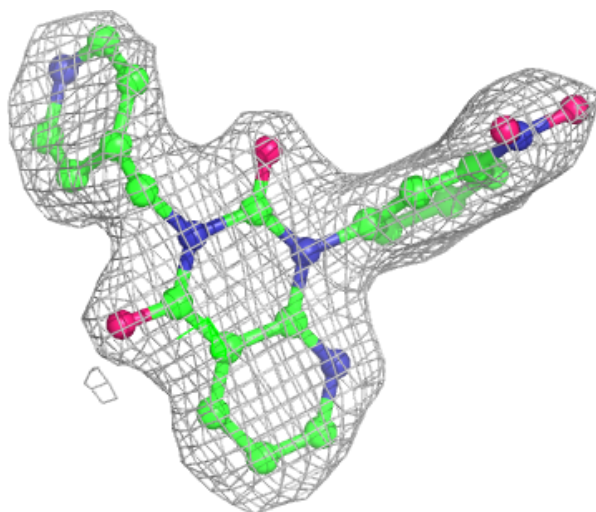
**Electron density around D71 C 903:**

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



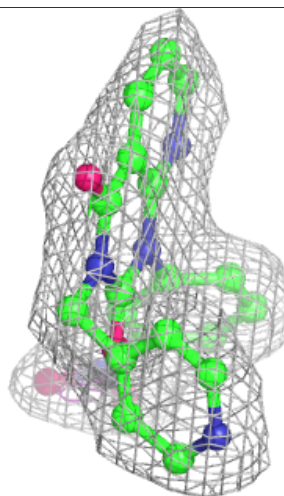
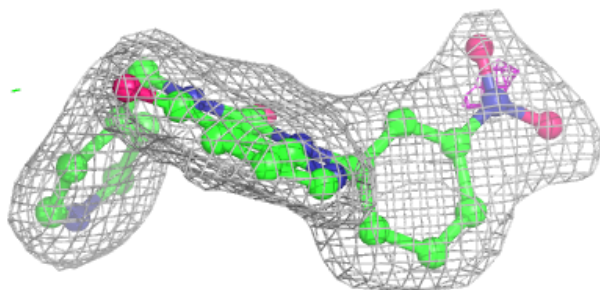
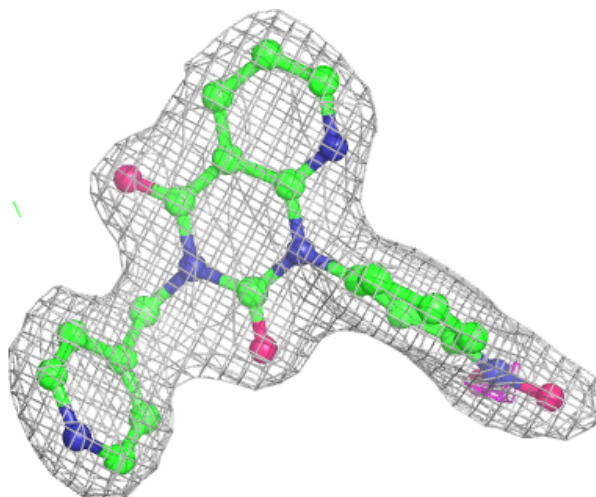
**Electron density around D71 A 901:**

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

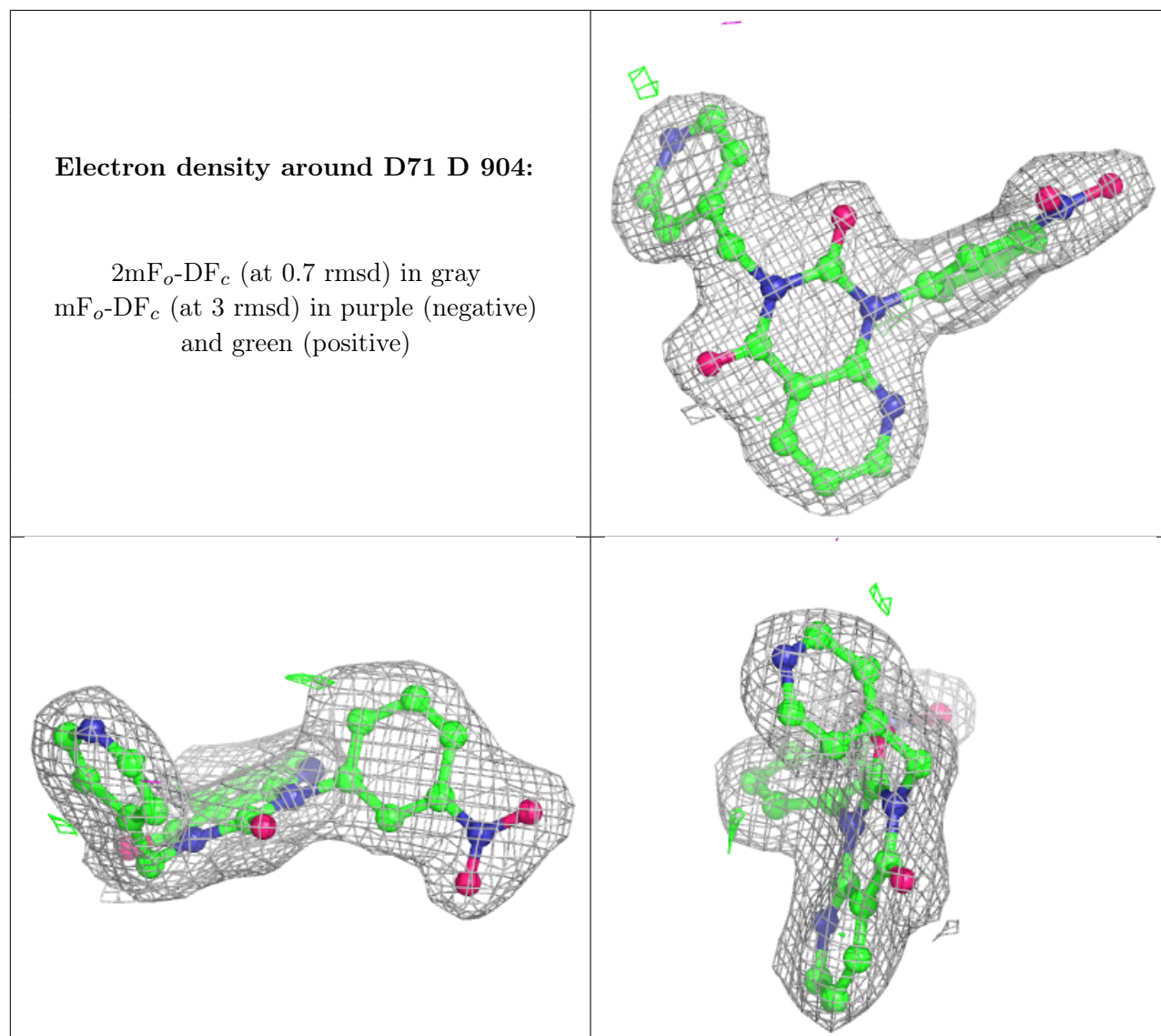


**Electron density around D71 B 902:**

$2mF_o-DF_c$  (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.