



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 8DC6 / pdb\_00008dc6  
Title : Crystal structure of p53 Y220C covalently bound to indole KG6  
Authors : Guiley, K.Z.; Shokat, K.M.  
Deposited on : 2022-06-15  
Resolution : 1.60 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

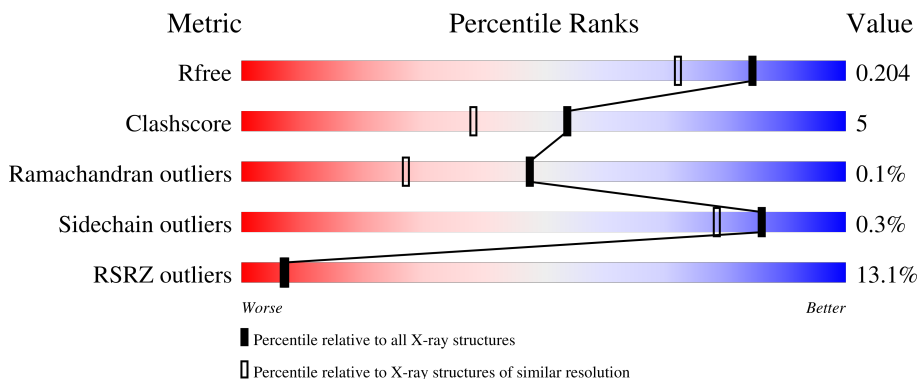
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	223	 13% 76% 10% 13%
1	B	223	 12% 75% 10% 13%
1	C	223	 11% 75% 10% 14%
1	D	223	 9% 79% 7% 14%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6875 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	1527	945	277	293	12	0	4	0
1	B	193	1532	947	279	294	12	0	4	0
1	C	192	1525	943	278	292	12	0	4	0
1	D	192	1534	949	278	295	12	0	6	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLY	-	expression tag	UNP P04637
A	91	ALA	-	expression tag	UNP P04637
A	92	HIS	-	expression tag	UNP P04637
A	93	MET	-	expression tag	UNP P04637
A	124	SER	CYS	conflict	UNP P04637
A	133	LEU	MET	conflict	UNP P04637
A	182	SER	CYS	conflict	UNP P04637
A	220	CYS	TYR	engineered mutation	UNP P04637
A	229	SER	CYS	conflict	UNP P04637
A	239	TYR	ASN	conflict	UNP P04637
A	268	ASP	ASN	conflict	UNP P04637
A	275	SER	CYS	conflict	UNP P04637
A	277	SER	CYS	conflict	UNP P04637
B	90	GLY	-	expression tag	UNP P04637
B	91	ALA	-	expression tag	UNP P04637
B	92	HIS	-	expression tag	UNP P04637
B	93	MET	-	expression tag	UNP P04637
B	124	SER	CYS	conflict	UNP P04637
B	133	LEU	MET	conflict	UNP P04637
B	182	SER	CYS	conflict	UNP P04637
B	220	CYS	TYR	engineered mutation	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
B	229	SER	CYS	conflict	UNP P04637
B	239	TYR	ASN	conflict	UNP P04637
B	268	ASP	ASN	conflict	UNP P04637
B	275	SER	CYS	conflict	UNP P04637
B	277	SER	CYS	conflict	UNP P04637
C	90	GLY	-	expression tag	UNP P04637
C	91	ALA	-	expression tag	UNP P04637
C	92	HIS	-	expression tag	UNP P04637
C	93	MET	-	expression tag	UNP P04637
C	124	SER	CYS	conflict	UNP P04637
C	133	LEU	MET	conflict	UNP P04637
C	182	SER	CYS	conflict	UNP P04637
C	220	CYS	TYR	engineered mutation	UNP P04637
C	229	SER	CYS	conflict	UNP P04637
C	239	TYR	ASN	conflict	UNP P04637
C	268	ASP	ASN	conflict	UNP P04637
C	275	SER	CYS	conflict	UNP P04637
C	277	SER	CYS	conflict	UNP P04637
D	90	GLY	-	expression tag	UNP P04637
D	91	ALA	-	expression tag	UNP P04637
D	92	HIS	-	expression tag	UNP P04637
D	93	MET	-	expression tag	UNP P04637
D	124	SER	CYS	conflict	UNP P04637
D	133	LEU	MET	conflict	UNP P04637
D	182	SER	CYS	conflict	UNP P04637
D	220	CYS	TYR	engineered mutation	UNP P04637
D	229	SER	CYS	conflict	UNP P04637
D	239	TYR	ASN	conflict	UNP P04637
D	268	ASP	ASN	conflict	UNP P04637
D	275	SER	CYS	conflict	UNP P04637
D	277	SER	CYS	conflict	UNP P04637

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



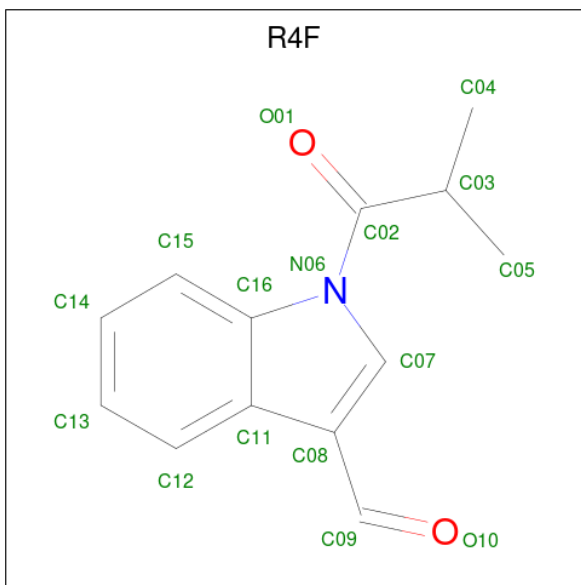
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1-(2-methylprop-2-enoyl)-1H-indole-3-carbaldehyde, bound form (CCD ID: R4F) (formula: C<sub>13</sub>H<sub>13</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	13	1	2		
4	B	1	Total	C	N	O	0	0
			16	13	1	2		
4	C	1	Total	C	N	O	0	0
			16	13	1	2		
4	D	1	Total	C	N	O	0	0
			16	13	1	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

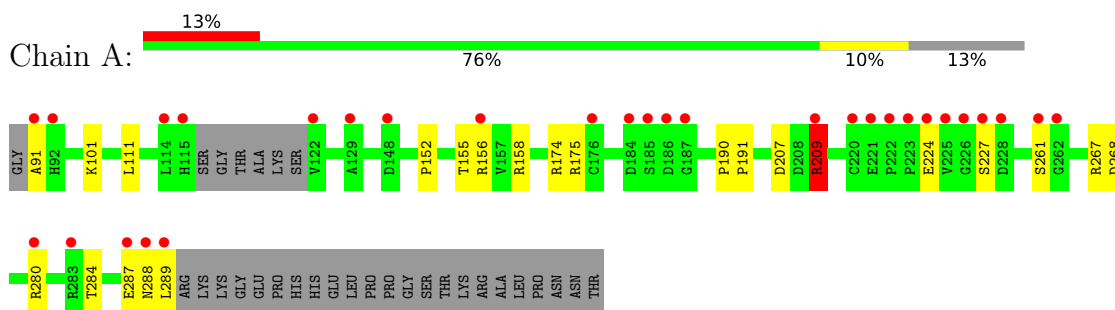
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total 157	O 157	0	0
6	B	155	Total 155	O 155	0	0
6	C	154	Total 154	O 154	0	0
6	D	156	Total 156	O 156	0	0

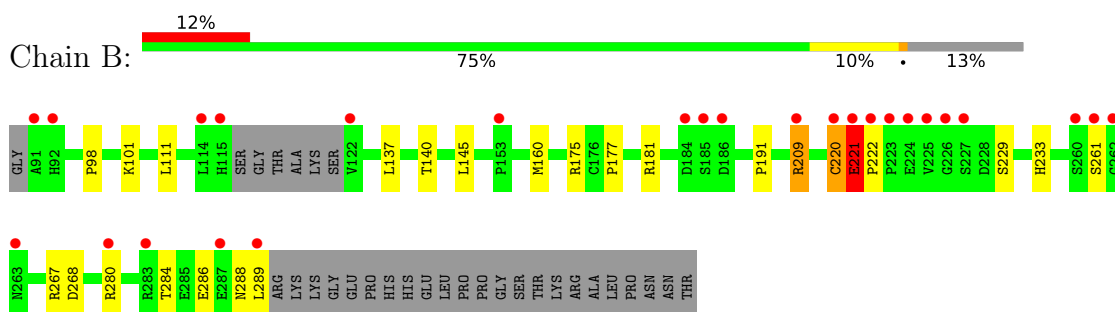
### 3 Residue-property plots [i](#)

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

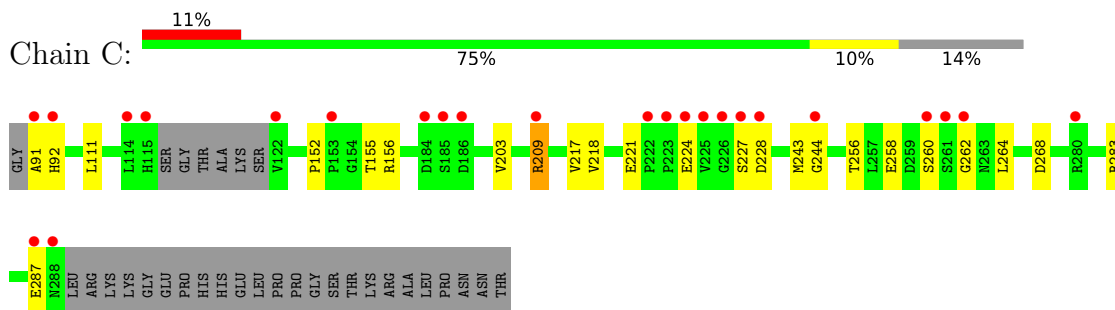
- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53

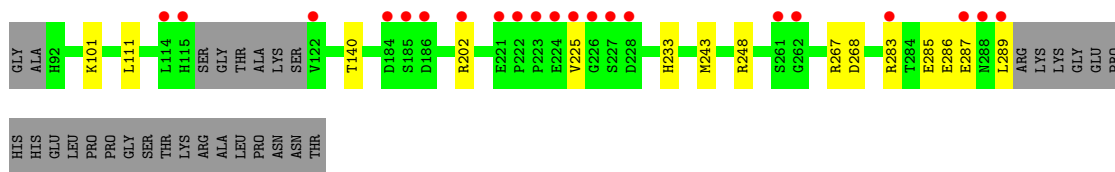


- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53





HIS  
HIS  
GLU  
LEU  
PRO  
PRO  
GLY  
SER  
THR  
LYS  
ARG  
ALA  
LEU  
PRO  
ASN  
THR

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.04Å 105.75Å 105.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.60 47.29 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.29-1.60) 99.4 (47.29-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.20.1	Depositor
R, $R_{free}$	0.181 , 0.202 0.184 , 0.204	Depositor DCC
$R_{free}$ test set	6610 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.032 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.21 % 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 1.5769e-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: MG, ZN, R4F, SO4

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	0.37	1/1574 (0.1%)	0.90	6/2134 (0.3%)
1	B	0.45	2/1579 (0.1%)	0.83	8/2141 (0.4%)
1	C	0.38	0/1573	0.62	3/2133 (0.1%)
1	D	0.30	0/1584	0.57	0/2148
All	All	0.38	3/6310 (0.0%)	0.74	17/8556 (0.2%)

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	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ARG	NE-CZ	-5.77	1.26	1.33
1	B	209	ARG	CZ-NH1	-5.50	1.25	1.32
1	B	209	ARG	CB-CG	-5.06	1.37	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ARG	CA-CB-CG	-16.75	80.59	114.10
1	B	209	ARG	CG-CD-NE	13.11	140.84	112.00
1	A	209	ARG	NE-CZ-NH1	-12.99	108.51	121.50
1	B	209	ARG	NE-CZ-NH1	-12.71	108.78	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ARG	NE-CZ-NH2	12.37	130.34	119.20
1	A	209	ARG	CG-CD-NE	12.36	139.18	112.00
1	A	209	ARG	CB-CG-CD	10.37	135.16	111.30
1	A	209	ARG	CD-NE-CZ	-9.82	110.65	124.40
1	C	209	ARG	CG-CD-NE	8.70	131.13	112.00
1	B	209	ARG	CA-CB-CG	-8.34	97.42	114.10
1	B	220	CYS	CA-C-N	6.87	138.57	121.80
1	B	220	CYS	C-N-CA	6.87	138.57	121.80
1	B	209	ARG	CB-CG-CD	6.12	125.39	111.30
1	B	261	SER	CB-CA-C	-5.41	99.84	110.11
1	B	221	GLU	N-CA-CB	-5.25	101.03	110.37
1	C	243	MET	CA-C-N	-5.22	111.44	121.78
1	C	243	MET	C-N-CA	-5.22	111.44	121.78

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	221	GLU	Sidechain

## 5.2 Too-close contacts

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	1527	0	1487	21	0
1	B	1532	0	1492	12	1
1	C	1525	0	1483	23	0
1	D	1534	0	1494	11	1
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	25	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	15	0	0	0	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	0	0
4	D	16	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	157	0	0	5	0
6	B	155	0	0	1	0
6	C	154	0	0	5	1
6	D	156	0	0	2	1
All	All	6875	0	5956	60	2

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 5.

All (60) 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:207:ASP:O	6:A:501:HOH:O	1.91	0.86
1:C:209:ARG:HD3	1:C:209:ARG:H	1.41	0.84
1:A:280:ARG:NH2	1:C:260:SER:O	2.12	0.83
1:A:280:ARG:HH22	1:C:156:ARG:HH12	1.29	0.81
1:C:209:ARG:HD3	1:C:209:ARG:N	1.96	0.78
1:C:256[B]:THR:HG22	1:C:258:GLU:HG3	1.71	0.71
1:C:221:GLU:OE2	6:C:501:HOH:O	2.09	0.70
1:A:91:ALA:N	6:A:503:HOH:O	2.26	0.69
1:A:289:LEU:O	6:A:502:HOH:O	2.13	0.67
1:D:202:ARG:NH1	6:D:504:HOH:O	2.27	0.66
1:B:280:ARG:NH1	6:B:501:HOH:O	2.29	0.65
1:B:177:PRO:O	1:B:181:ARG:HG3	1.98	0.64
1:C:91:ALA:N	6:C:504:HOH:O	2.30	0.64
1:C:283:ARG:O	1:C:287:GLU:HG3	1.97	0.64
1:A:261:SER:HB3	1:D:283:ARG:NH2	2.13	0.64
1:C:111:LEU:HG	1:C:268:ASP:HB3	1.81	0.63
1:C:156:ARG:HD3	1:C:217:VAL:HG11	1.82	0.61
1:A:280:ARG:HH21	1:C:260:SER:C	2.08	0.61
1:A:190:PRO:HA	1:D:243:MET:HE3	1.83	0.61
1:A:156:ARG:HH11	1:A:158:ARG:NH2	2.01	0.59
1:C:209:ARG:H	1:C:209:ARG:CD	2.15	0.58
1:D:285:GLU:OE1	6:D:501:HOH:O	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PRO:HG3	1:B:160:MET:HE1	1.85	0.57
1:B:140:THR:HG23	1:B:233:HIS:HB3	1.86	0.57
1:A:111:LEU:HG	1:A:268:ASP:HB3	1.88	0.56
1:D:140:THR:HG23	1:D:233:HIS:HB3	1.88	0.55
1:A:224:GLU:O	1:A:227:SER:HB2	2.07	0.55
1:C:156:ARG:HD2	6:C:521:HOH:O	2.08	0.53
1:C:228:ASP:HB2	6:C:623:HOH:O	2.08	0.53
1:C:203:VAL:HG12	1:C:218:VAL:HG22	1.90	0.52
1:A:156:ARG:NH1	1:A:158:ARG:NH2	2.58	0.51
1:C:224:GLU:HB3	1:C:227:SER:HB2	1.92	0.51
1:B:284:THR:O	1:B:288:ASN:ND2	2.37	0.50
1:A:284:THR:O	1:A:287:GLU:HG2	2.10	0.50
1:C:156:ARG:HD3	1:C:217:VAL:CG1	2.42	0.50
1:D:286:GLU:O	1:D:289:LEU:HG	2.13	0.48
1:D:243:MET:HB2	1:D:243:MET:HE2	1.79	0.48
1:C:244:GLY:HA2	6:C:618:HOH:O	2.12	0.48
1:A:174:ARG:HD3	6:A:511:HOH:O	2.13	0.47
1:A:209:ARG:HH11	1:A:209:ARG:HD3	1.11	0.47
1:C:152:PRO:O	1:C:155:THR:HG23	2.14	0.47
1:A:280:ARG:NH2	1:C:262:GLY:N	2.64	0.46
1:C:256[B]:THR:HG23	1:C:264:LEU:CD2	2.46	0.46
1:A:152:PRO:O	1:A:155:THR:HG23	2.16	0.45
1:B:286:GLU:O	1:B:289:LEU:HG	2.16	0.45
1:B:98:PRO:CG	1:B:160:MET:HE1	2.46	0.44
1:D:111:LEU:HG	1:D:268:ASP:HB3	1.99	0.44
6:A:501:HOH:O	1:D:248:ARG:NH2	2.24	0.44
1:A:287:GLU:HG3	1:A:288:ASN:OD1	2.18	0.44
1:C:209:ARG:N	1:C:209:ARG:CD	2.76	0.44
1:D:283:ARG:O	1:D:287:GLU:HG2	2.18	0.43
1:A:280:ARG:NH2	1:C:260:SER:C	2.71	0.42
1:B:220:CYS:C	1:B:222:PRO:HD3	2.44	0.42
1:D:101:LYS:O	1:D:267:ARG:HD2	2.19	0.42
1:B:175:ARG:HD3	1:B:191:PRO:O	2.20	0.41
1:A:175:ARG:HD3	1:A:191:PRO:O	2.21	0.41
1:B:145:LEU:O	1:B:229:SER:HA	2.21	0.41
1:B:111:LEU:HG	1:B:268:ASP:HB3	2.02	0.41
1:B:101:LYS:O	1:B:267:ARG:HD2	2.21	0.41
1:A:101:LYS:O	1:A:267:ARG:HD2	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:633:HOH:O	6:D:647:HOH:O[2_554]	2.08	0.12
1:B:137:LEU:O	1:D:202:ARG:NH1[2_555]	2.19	0.01

### 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	193/223 (86%)	191 (99%)	2 (1%)	0	100	100
1	B	193/223 (86%)	188 (97%)	4 (2%)	1 (0%)	24	10
1	C	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
1	D	194/223 (87%)	191 (98%)	3 (2%)	0	100	100
All	All	772/892 (86%)	761 (99%)	10 (1%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	221	GLU

#### 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	177/198 (89%)	177 (100%)	0	100	100
1	B	178/198 (90%)	178 (100%)	0	100	100
1	C	177/198 (89%)	176 (99%)	1 (1%)	78	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	179/198 (90%)	178 (99%)	1 (1%)	78	66
All	All	711/792 (90%)	709 (100%)	2 (0%)	86	78

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

Mol	Chain	Res	Type
1	C	92	HIS
1	D	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	263	ASN
1	B	233	HIS
1	C	92	HIS
1	C	178	HIS
1	D	233	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](#)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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
3	SO4	C	402	-	4,4,4	0.27	0	6,6,6	0.16	0
4	R4F	C	404	1	17,17,17	1.01	2 (11%)	22,24,24	1.00	2 (9%)
3	SO4	A	406	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.39	0
3	SO4	A	404	-	4,4,4	0.30	0	6,6,6	0.39	0
3	SO4	A	405	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.51	0
4	R4F	B	405	1	17,17,17	1.26	2 (11%)	22,24,24	1.03	2 (9%)
3	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.37	0
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.25	0
4	R4F	A	407	1	17,17,17	1.08	2 (11%)	22,24,24	0.99	1 (4%)
3	SO4	D	404	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	A	403	-	4,4,4	0.26	0	6,6,6	0.26	0
4	R4F	D	405	1	17,17,17	1.49	2 (11%)	22,24,24	1.14	3 (13%)
3	SO4	B	404	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	403	-	4,4,4	0.24	0	6,6,6	0.18	0
3	SO4	B	403	-	4,4,4	0.24	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	R4F	C	404	1	-	2/10/10/10	0/2/2/2
4	R4F	B	405	1	-	2/10/10/10	0/2/2/2
4	R4F	A	407	1	-	0/10/10/10	0/2/2/2
4	R4F	D	405	1	-	2/10/10/10	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	405	R4F	C02-N06	4.63	1.47	1.38
4	B	405	R4F	C02-N06	3.57	1.45	1.38
4	D	405	R4F	C07-N06	2.87	1.44	1.38
4	B	405	R4F	C07-N06	2.79	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	407	R4F	C07-N06	2.26	1.43	1.38
4	C	404	R4F	C02-N06	2.17	1.42	1.38
4	A	407	R4F	C02-N06	2.14	1.42	1.38
4	C	404	R4F	C07-N06	2.03	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	405	R4F	C11-C16-N06	2.48	109.57	107.33
4	D	405	R4F	C16-N06-C07	-2.43	106.47	108.03
4	B	405	R4F	C11-C16-N06	2.21	109.33	107.33
4	C	404	R4F	C07-N06-C02	-2.12	123.99	126.31
4	A	407	R4F	C11-C16-N06	2.12	109.24	107.33
4	C	404	R4F	C11-C16-N06	2.10	109.23	107.33
4	D	405	R4F	O10-C09-C08	-2.09	122.61	125.41
4	B	405	R4F	O10-C09-C08	-2.07	122.63	125.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

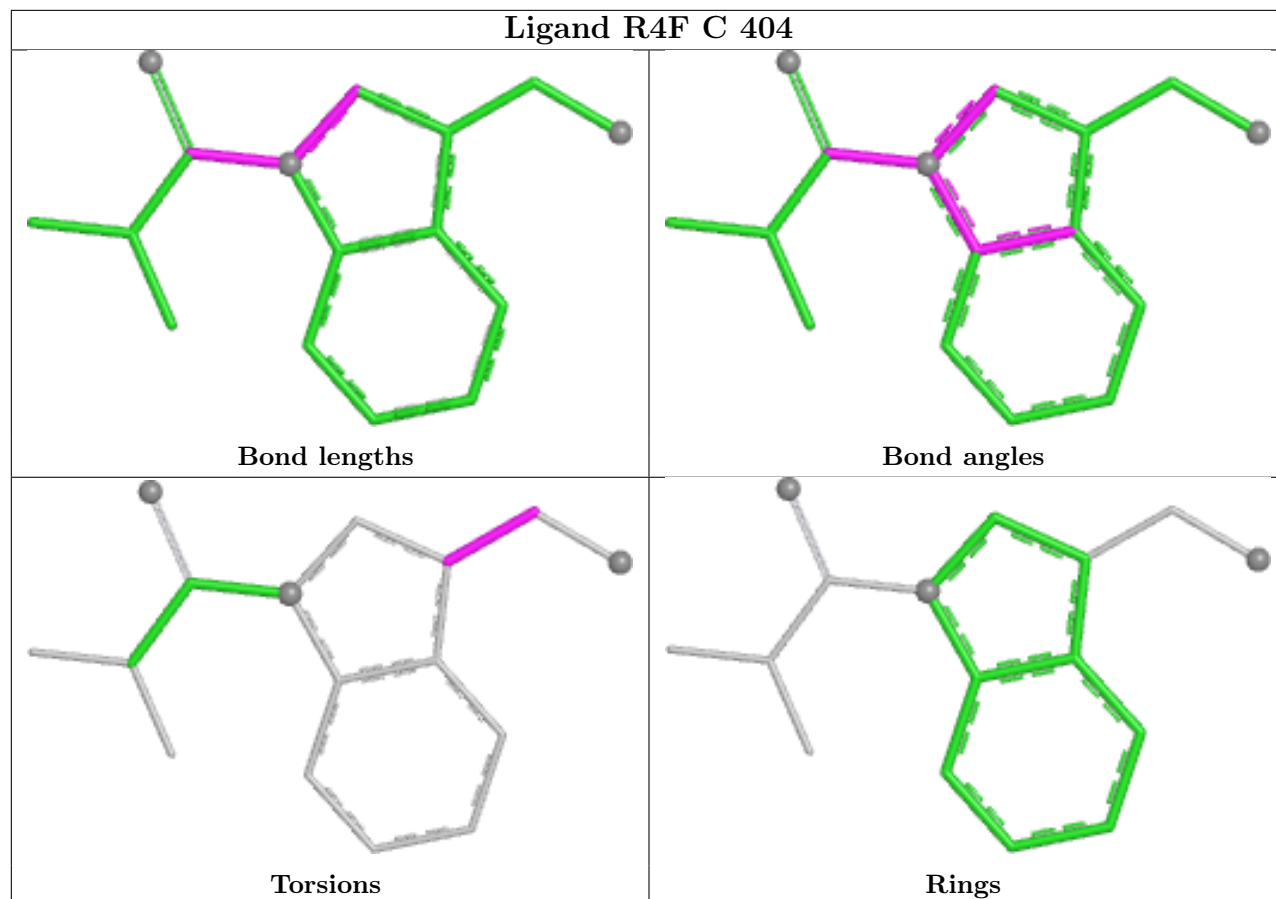
Mol	Chain	Res	Type	Atoms
4	C	404	R4F	C07-C08-C09-O10
4	C	404	R4F	C11-C08-C09-O10
4	D	405	R4F	C07-C08-C09-O10
4	D	405	R4F	C11-C08-C09-O10
4	B	405	R4F	C11-C08-C09-O10
4	B	405	R4F	C07-C08-C09-O10

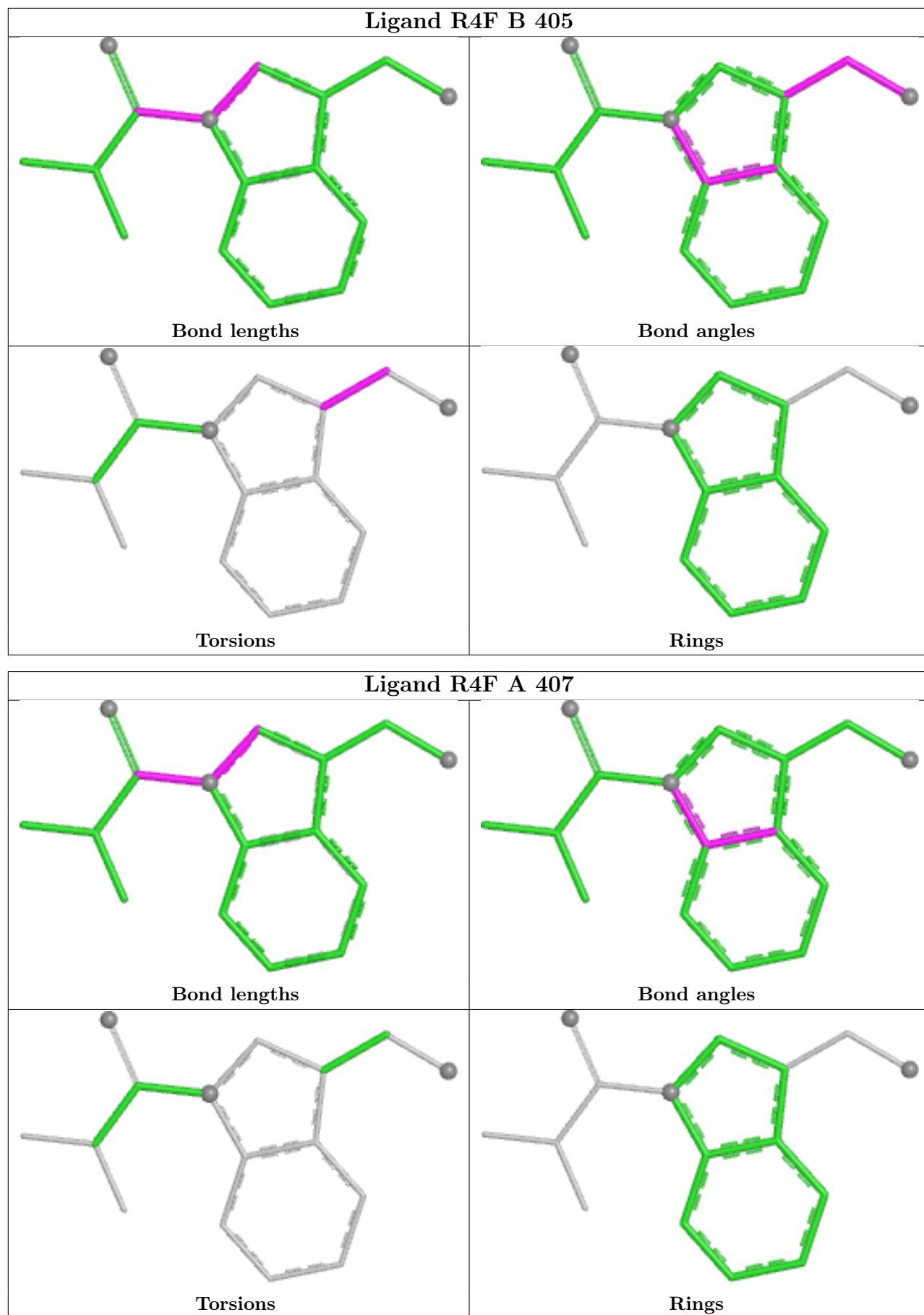
There are no ring outliers.

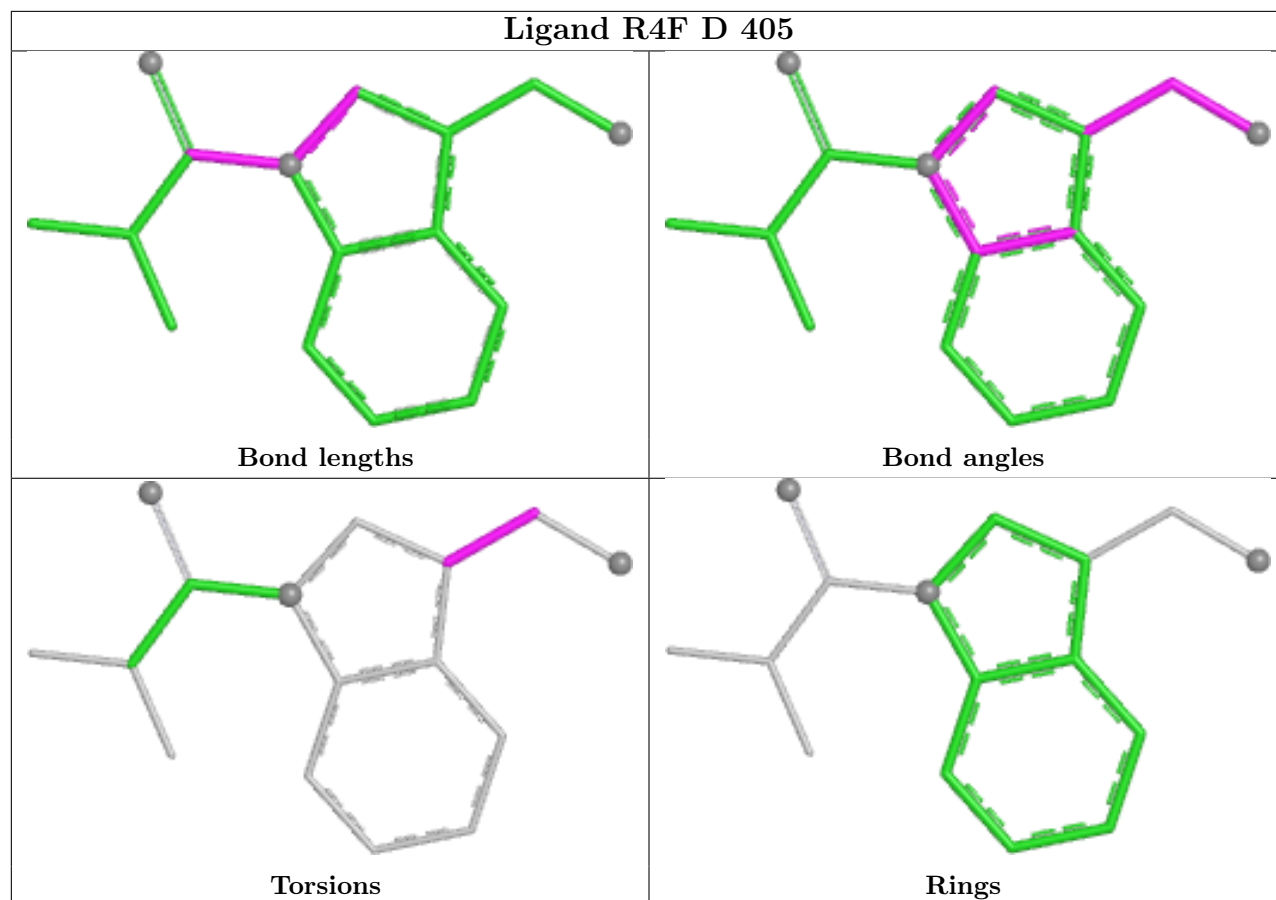
No monomer is involved in short contacts.

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

equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	193/223 (86%)	0.60	30 (15%) <b>5</b> <b>4</b>	9, 18, 44, 72	4 (2%)
1	B	193/223 (86%)	0.51	26 (13%) <b>7</b> <b>6</b>	7, 17, 42, 65	4 (2%)
1	C	192/223 (86%)	0.47	24 (12%) <b>8</b> <b>8</b>	7, 17, 41, 57	4 (2%)
1	D	192/223 (86%)	0.44	21 (10%) <b>10</b> <b>10</b>	7, 17, 44, 63	6 (3%)
All	All	770/892 (86%)	0.51	101 (13%) <b>7</b> <b>7</b>	7, 17, 42, 72	18 (2%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PRO	6.9
1	C	91	ALA	6.6
1	D	122	VAL	6.2
1	C	115	HIS	6.1
1	B	115	HIS	5.7
1	D	115	HIS	5.5
1	D	223	PRO	5.4
1	B	225	VAL	5.3
1	A	289	LEU	5.2
1	B	122	VAL	5.1
1	C	244	GLY	5.1
1	B	223	PRO	5.0
1	A	91	ALA	4.9
1	D	225	VAL	4.8
1	A	176	CYS	4.8
1	C	225	VAL	4.6
1	B	91	ALA	4.6
1	C	122	VAL	4.5
1	B	289	LEU	4.5
1	A	122	VAL	4.4
1	B	209	ARG	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	225	VAL	4.3
1	B	222	PRO	4.2
1	B	221	GLU	4.2
1	A	222	PRO	4.1
1	A	209	ARG	4.1
1	C	209	ARG	4.1
1	A	280	ARG	4.0
1	D	289	LEU	3.9
1	A	224	GLU	3.7
1	A	221	GLU	3.7
1	B	287	GLU	3.6
1	D	222	PRO	3.5
1	C	224	GLU	3.5
1	D	184	ASP	3.5
1	C	223	PRO	3.5
1	B	186	ASP	3.4
1	D	114	LEU	3.4
1	B	283	ARG	3.4
1	D	186	ASP	3.3
1	A	226	GLY	3.3
1	C	114	LEU	3.3
1	A	186	ASP	3.3
1	C	262	GLY	3.2
1	A	115	HIS	3.2
1	B	185	SER	3.2
1	A	187	GLY	3.2
1	C	226	GLY	3.2
1	D	287	GLU	3.2
1	B	224	GLU	3.1
1	A	261	SER	3.1
1	C	92	HIS	3.0
1	C	185	SER	3.0
1	D	185	SER	3.0
1	D	283	ARG	3.0
1	A	288	ASN	3.0
1	D	224	GLU	2.9
1	A	92	HIS	2.8
1	A	114	LEU	2.8
1	A	287	GLU	2.8
1	A	220	CYS	2.8
1	A	184	ASP	2.8
1	B	261	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	227	SER	2.8
1	D	221	GLU	2.7
1	D	226	GLY	2.7
1	C	184	ASP	2.7
1	A	185	SER	2.7
1	A	227	SER	2.7
1	B	220	CYS	2.7
1	B	92	HIS	2.6
1	B	260	SER	2.6
1	C	261	SER	2.6
1	B	262	GLY	2.6
1	A	228	ASP	2.6
1	C	287	GLU	2.6
1	C	280	ARG	2.6
1	C	288	ASN	2.6
1	A	156	ARG	2.6
1	B	184	ASP	2.5
1	C	228	ASP	2.5
1	A	262	GLY	2.5
1	B	114	LEU	2.4
1	B	263	ASN	2.4
1	D	261	SER	2.4
1	D	228	ASP	2.4
1	D	288	ASN	2.4
1	A	283	ARG	2.4
1	B	226	GLY	2.3
1	D	227	SER	2.2
1	C	222	PRO	2.2
1	B	227	SER	2.2
1	C	260	SER	2.2
1	D	202	ARG	2.2
1	B	153	PRO	2.1
1	D	262	GLY	2.1
1	C	186	ASP	2.1
1	B	280	ARG	2.1
1	C	153	PRO	2.1
1	A	129	ALA	2.0
1	A	148	ASP	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](#)

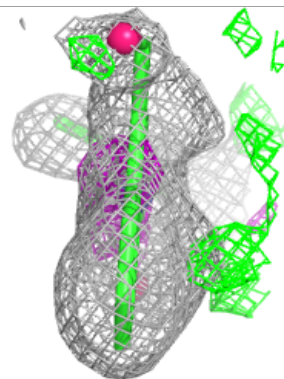
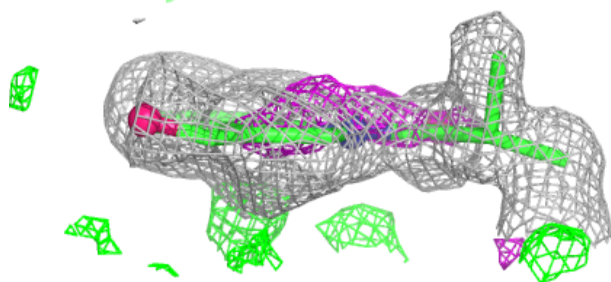
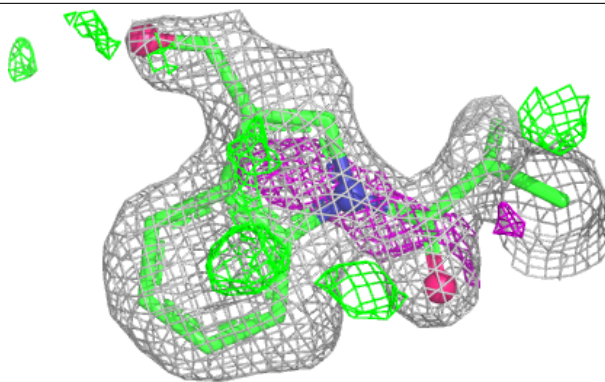
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	D	404	5/5	0.80	0.12	46,49,57,58	0
4	R4F	B	405	16/16	0.80	0.16	23,32,44,49	0
4	R4F	C	404	16/16	0.81	0.14	26,31,43,46	0
3	SO4	A	405	5/5	0.82	0.12	47,48,54,55	0
3	SO4	A	406	5/5	0.83	0.13	38,39,48,51	0
4	R4F	A	407	16/16	0.83	0.14	24,30,39,48	0
3	SO4	A	402	5/5	0.84	0.12	37,39,43,46	0
4	R4F	D	405	16/16	0.84	0.13	23,31,44,46	0
3	SO4	A	404	5/5	0.87	0.13	24,30,38,38	0
3	SO4	A	403	5/5	0.88	0.11	33,33,47,51	0
3	SO4	D	402	5/5	0.90	0.11	27,29,31,31	0
3	SO4	B	404	5/5	0.91	0.10	37,46,48,51	0
3	SO4	C	402	5/5	0.91	0.10	28,35,44,48	0
5	MG	C	405	1/1	0.92	0.08	36,36,36,36	0
3	SO4	D	403	5/5	0.93	0.09	28,29,41,49	0
3	SO4	B	402	5/5	0.94	0.12	23,25,28,32	0
3	SO4	B	403	5/5	0.94	0.09	26,28,39,46	0
5	MG	B	406	1/1	0.95	0.18	25,25,25,25	0
3	SO4	C	403	5/5	0.96	0.11	19,20,24,29	0
2	ZN	D	401	1/1	1.00	0.01	12,12,12,12	0
2	ZN	A	401	1/1	1.00	0.01	11,11,11,11	0
2	ZN	B	401	1/1	1.00	0.01	12,12,12,12	0
2	ZN	C	401	1/1	1.00	0.01	11,11,11,11	0

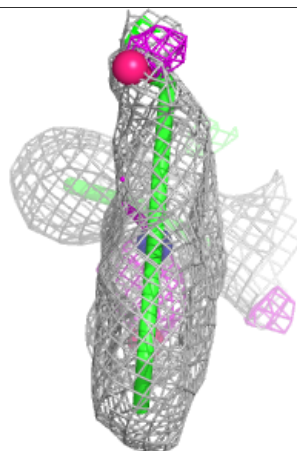
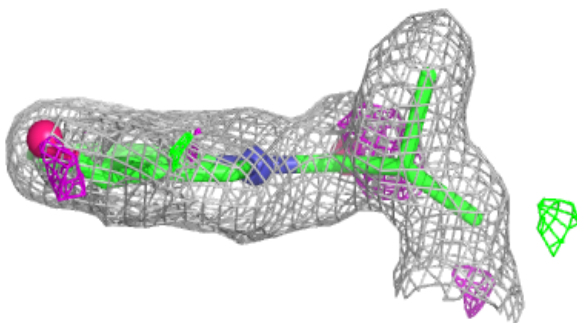
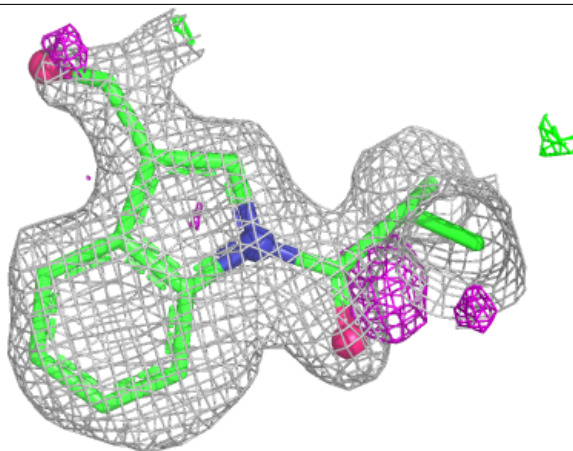
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around R4F B 405:**

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

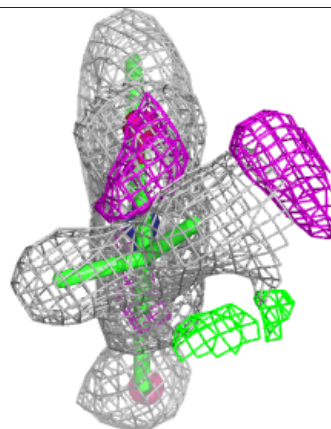
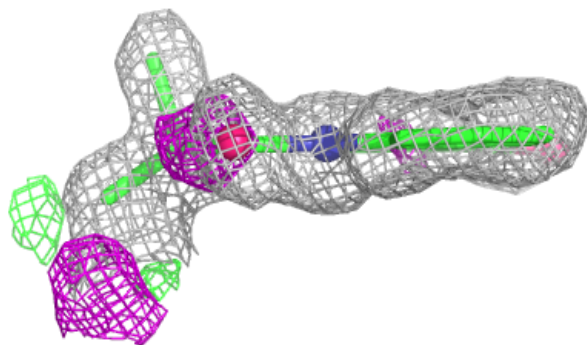
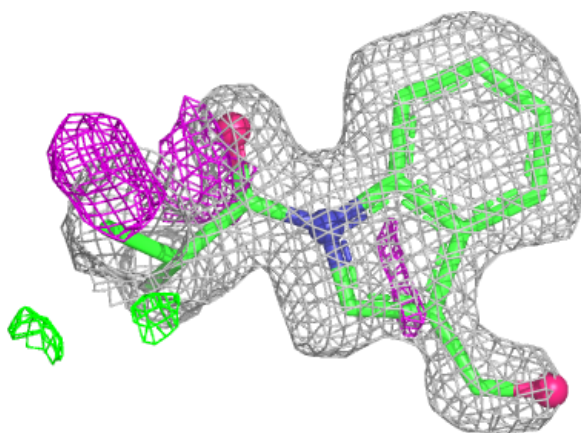
**Electron density around R4F C 404:**

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

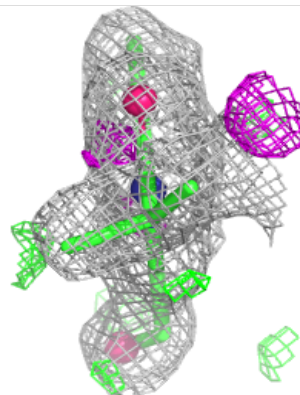
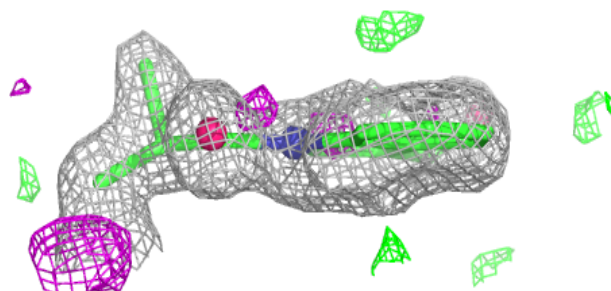
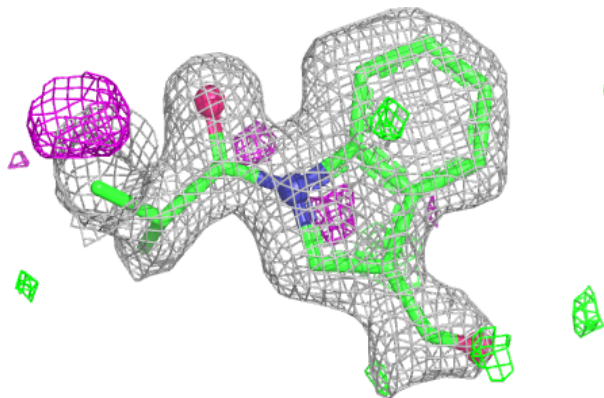


**Electron density around R4F A 407:**

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

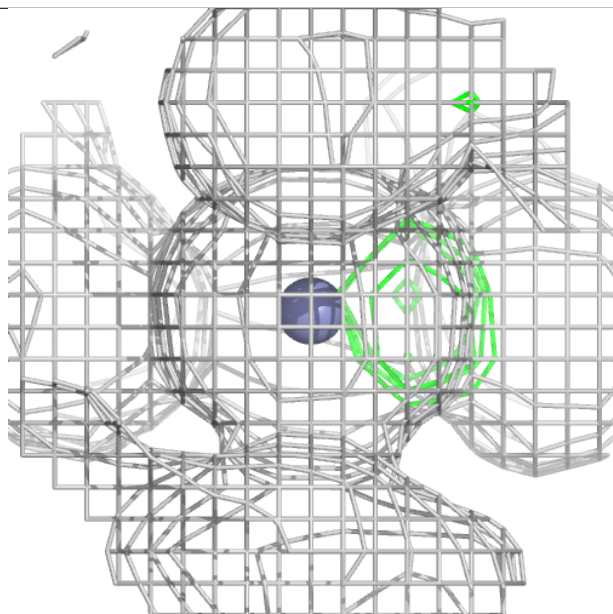
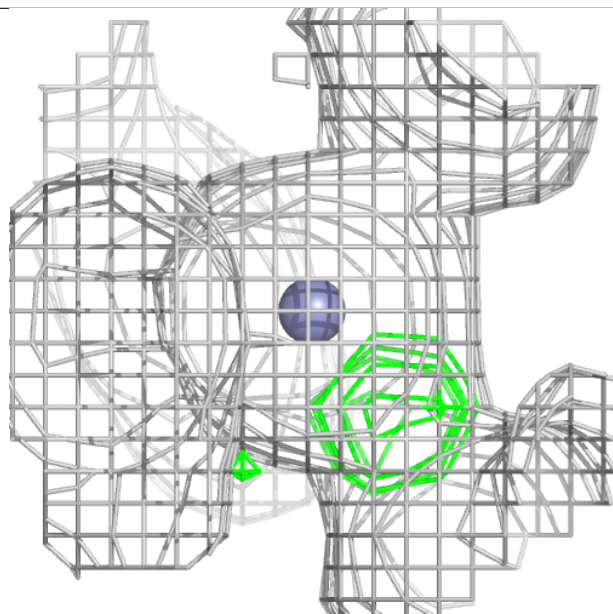
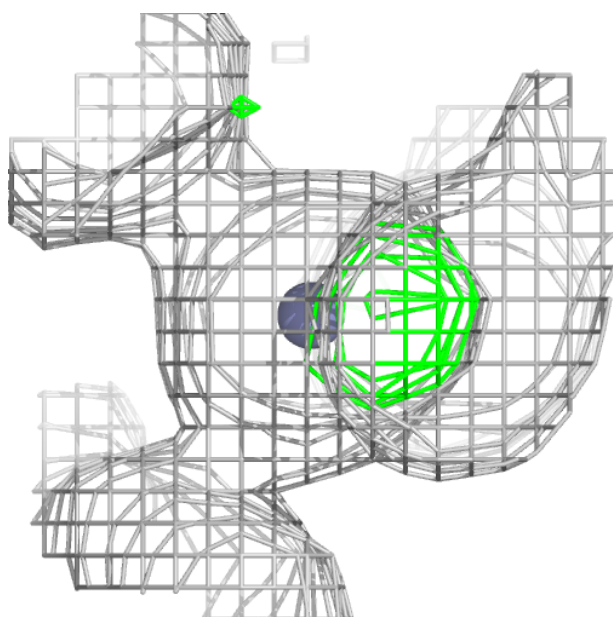
**Electron density around R4F D 405:**

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



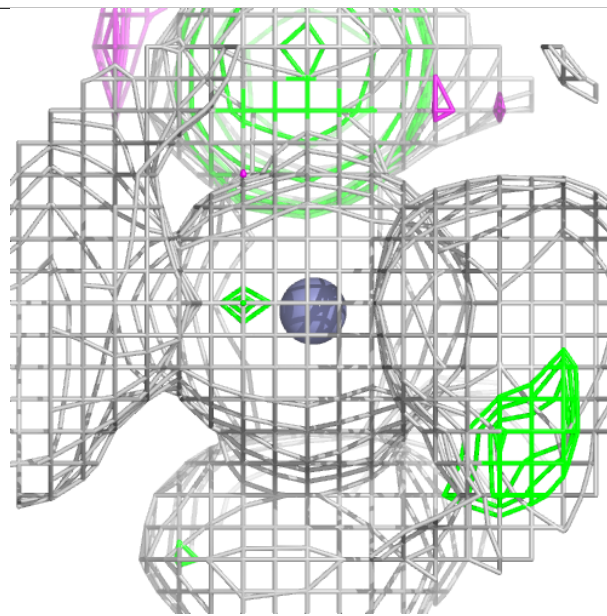
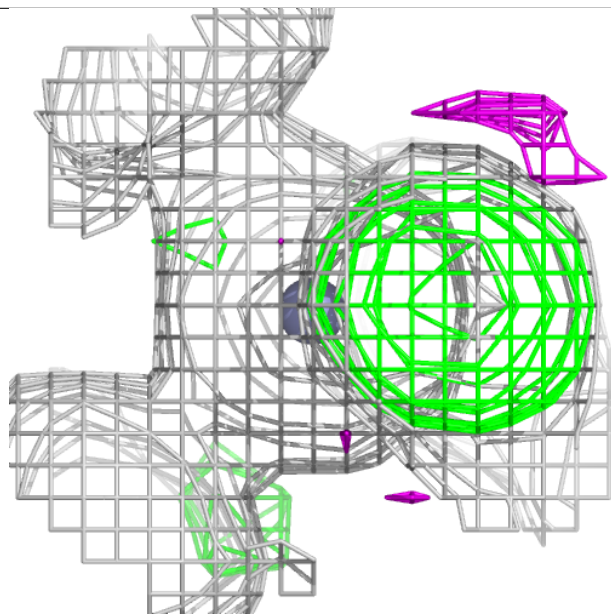
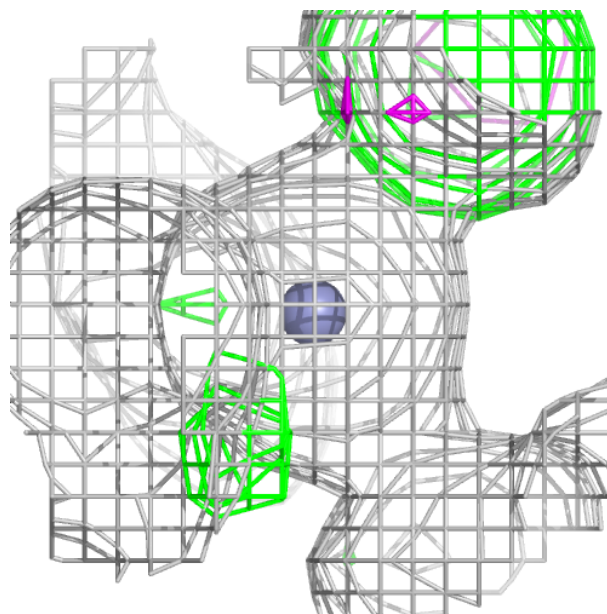
**Electron density around ZN D 401:**

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



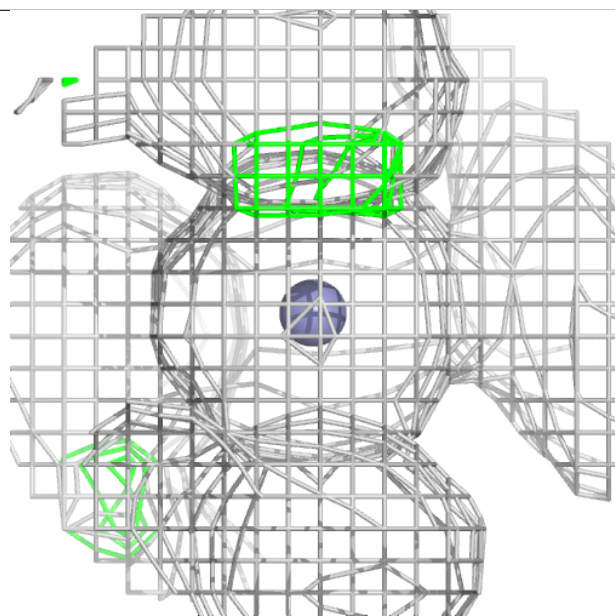
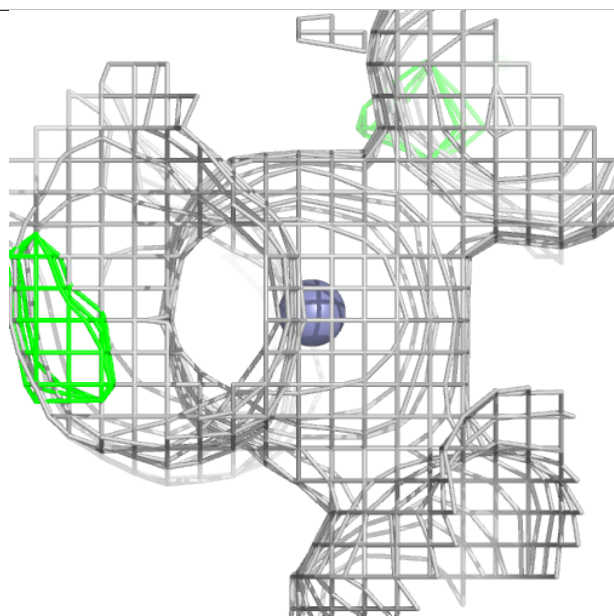
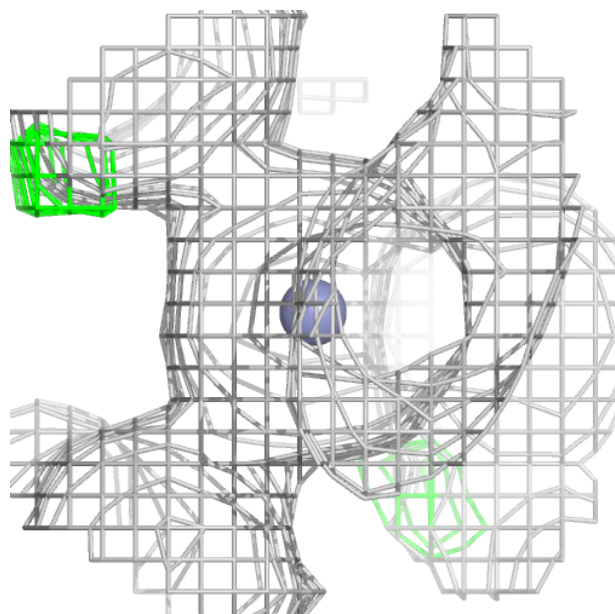
**Electron density around ZN A 401:**

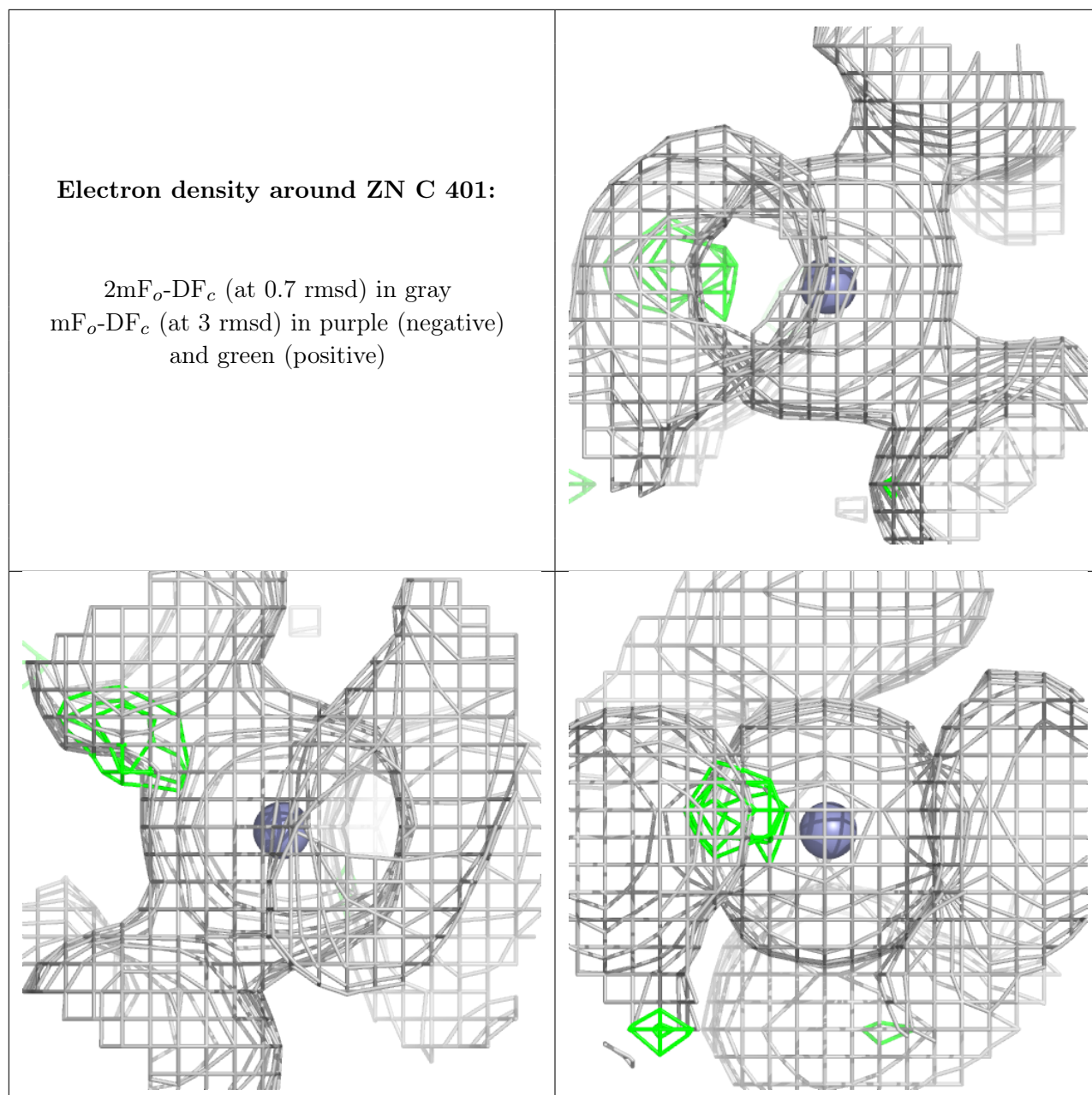
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN B 401:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.