



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 04:39 PM EDT

PDB ID : 8DC4
Title : Crystal structure of p53 Y220C covalently bound to carbazole KG3
Authors : Guiley, K.Z.; Shokat, K.M.
Deposited on : 2022-06-15
Resolution : 2.40 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

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

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

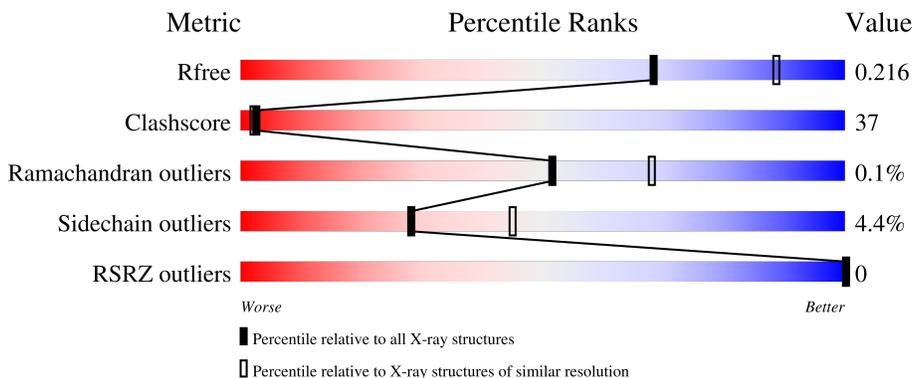
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	 37% 49% 12%
1	B	223	 45% 41% 12%
1	C	223	 45% 41% 12%
1	D	223	 44% 42% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6769 atoms, of which 52 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	B	197	1577	976	283	306	12	17	9	0
1	A	197	1588	981	287	308	12	24	10	0
1	C	197	1595	986	287	310	12	14	11	0
1	D	197	1603	992	287	311	13	34	13	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

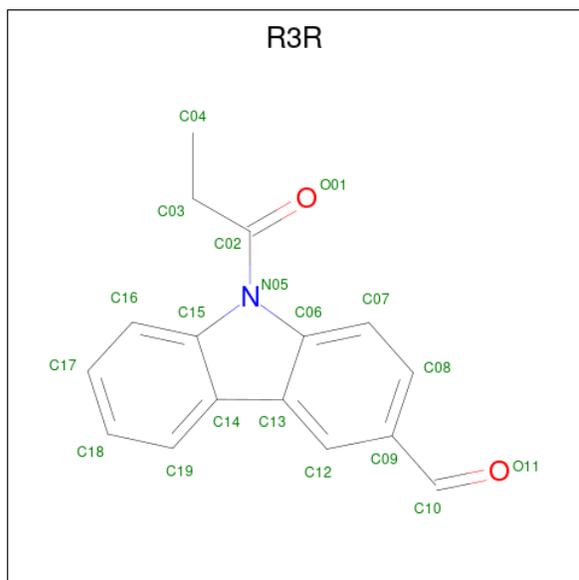
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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

- Molecule 3 is 9-propanoyl-9H-carbazole-3-carbaldehyde, bound form (three-letter code: R3R) (formula: C₁₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	B	1	Total	C	H	N	O	0	0
			32	16	13	1	2		
3	A	1	Total	C	H	N	O	0	0
			32	16	13	1	2		
3	C	1	Total	C	H	N	O	0	0
			32	16	13	1	2		
3	D	1	Total	C	H	N	O	0	0
			32	16	13	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	68	Total	O	0	0
			68	68		
4	A	72	Total	O	0	0
			72	72		
4	C	65	Total	O	0	0
			65	65		
4	D	69	Total	O	0	0
			69	69		

4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	68.56Å 68.56Å 220.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.37 – 2.40 59.37 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.37-2.40) 97.6 (59.37-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.40Å)	Xtrriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.161 , 0.231 0.155 , 0.216	Depositor DCC
R_{free} test set	2292 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	0.438 for -h,-k,l 0.447 for h,-h-k,-l 0.439 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6769	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, R3R

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	0.59	0/1645	0.69	0/2231
1	B	0.57	0/1637	0.71	0/2220
1	C	0.57	0/1655	0.69	0/2245
1	D	0.58	0/1669	0.72	0/2263
All	All	0.58	0/6606	0.70	0/8959

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	1588	0	1556	141	0
1	B	1577	0	1550	116	0
1	C	1595	0	1564	109	0
1	D	1603	0	1578	105	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	19	13	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	13	0	1	0
3	C	19	13	0	1	0
3	D	19	13	0	1	0
4	A	72	0	0	29	0
4	B	68	0	0	26	0
4	C	65	0	0	24	0
4	D	69	0	0	21	0
All	All	6717	52	6248	457	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 37.

The worst 5 of 457 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:242:CYS:SG	4:A:565:HOH:O	2.02	1.16
1:B:209:ARG:H	1:B:209:ARG:HD3	1.20	1.06
1:D:256[A]:THR:HG22	1:D:267:ARG:HG3	1.37	1.05
1:A:101:LYS:O	1:A:267:ARG:NH1	1.90	1.04
1:D:172:VAL:O	4:D:501:HOH:O	1.78	0.98

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	205/223 (92%)	197 (96%)	6 (3%)	2 (1%)	15	23
1	B	204/223 (92%)	198 (97%)	6 (3%)	0	100	100
1	C	206/223 (92%)	198 (96%)	8 (4%)	0	100	100
1	D	208/223 (93%)	200 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	823/892 (92%)	793 (96%)	28 (3%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182[A]	SER
1	A	182[B]	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	187/198 (94%)	179 (96%)	8 (4%)	29	46
1	B	186/198 (94%)	178 (96%)	8 (4%)	29	46
1	C	188/198 (95%)	179 (95%)	9 (5%)	25	41
1	D	190/198 (96%)	182 (96%)	8 (4%)	30	47
All	All	751/792 (95%)	718 (96%)	33 (4%)	28	45

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	209	ARG
1	D	238	CYS
1	D	289	LEU
1	A	209	ARG
1	A	198	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	C	192	GLN
1	D	115	HIS

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Mol	Chain	Res	Type
1	A	136	GLN
1	A	144	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 8 ligands modelled in this entry, 4 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
3	R3R	B	402	1	19,21,21	1.13	3 (15%)	22,30,30	1.54	3 (13%)
3	R3R	A	402	1	19,21,21	1.31	3 (15%)	22,30,30	1.32	2 (9%)
3	R3R	D	402	1	19,21,21	1.20	3 (15%)	22,30,30	1.24	2 (9%)
3	R3R	C	402	1	19,21,21	1.09	1 (5%)	22,30,30	1.47	2 (9%)

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	R3R	B	402	1	-	2/4/8/8	0/3/3/3
3	R3R	A	402	1	-	4/4/8/8	0/3/3/3
3	R3R	D	402	1	-	2/4/8/8	0/3/3/3
3	R3R	C	402	1	-	4/4/8/8	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	R3R	C14-C15	-2.54	1.36	1.41
3	D	402	R3R	C14-C15	-2.30	1.37	1.41
3	B	402	R3R	C06-N05	-2.28	1.36	1.39
3	D	402	R3R	C13-C06	-2.22	1.37	1.41
3	A	402	R3R	C06-N05	-2.19	1.36	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	R3R	C03-C02-N05	4.90	125.20	117.60
3	C	402	R3R	C03-C02-N05	4.84	125.11	117.60
3	A	402	R3R	C03-C02-N05	4.28	124.24	117.60
3	D	402	R3R	C03-C02-N05	3.80	123.50	117.60
3	B	402	R3R	C04-C03-C02	-3.22	106.77	112.72

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

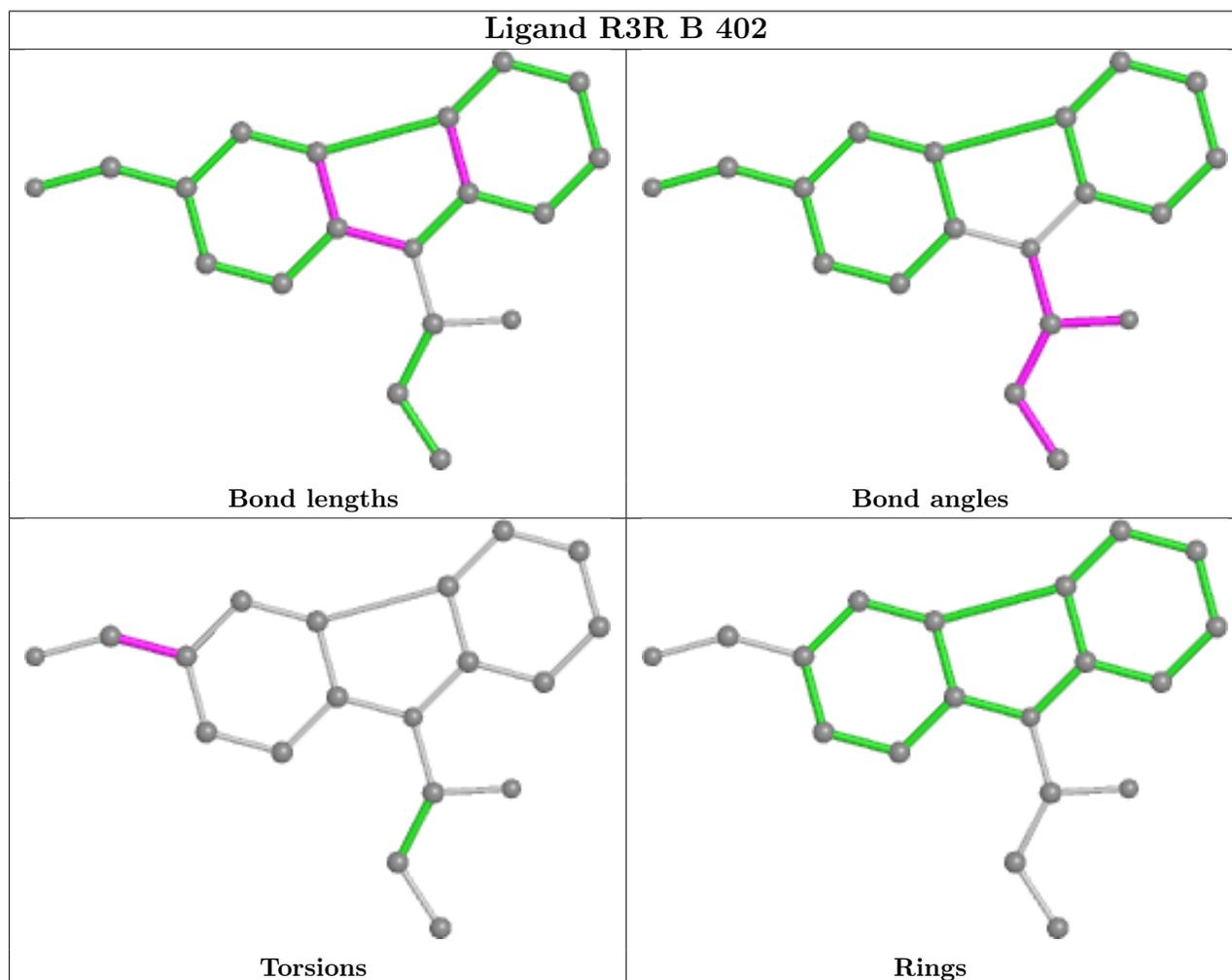
Mol	Chain	Res	Type	Atoms
3	D	402	R3R	C12-C09-C10-O11
3	B	402	R3R	C08-C09-C10-O11
3	B	402	R3R	C12-C09-C10-O11
3	D	402	R3R	C08-C09-C10-O11
3	A	402	R3R	N05-C02-C03-C04

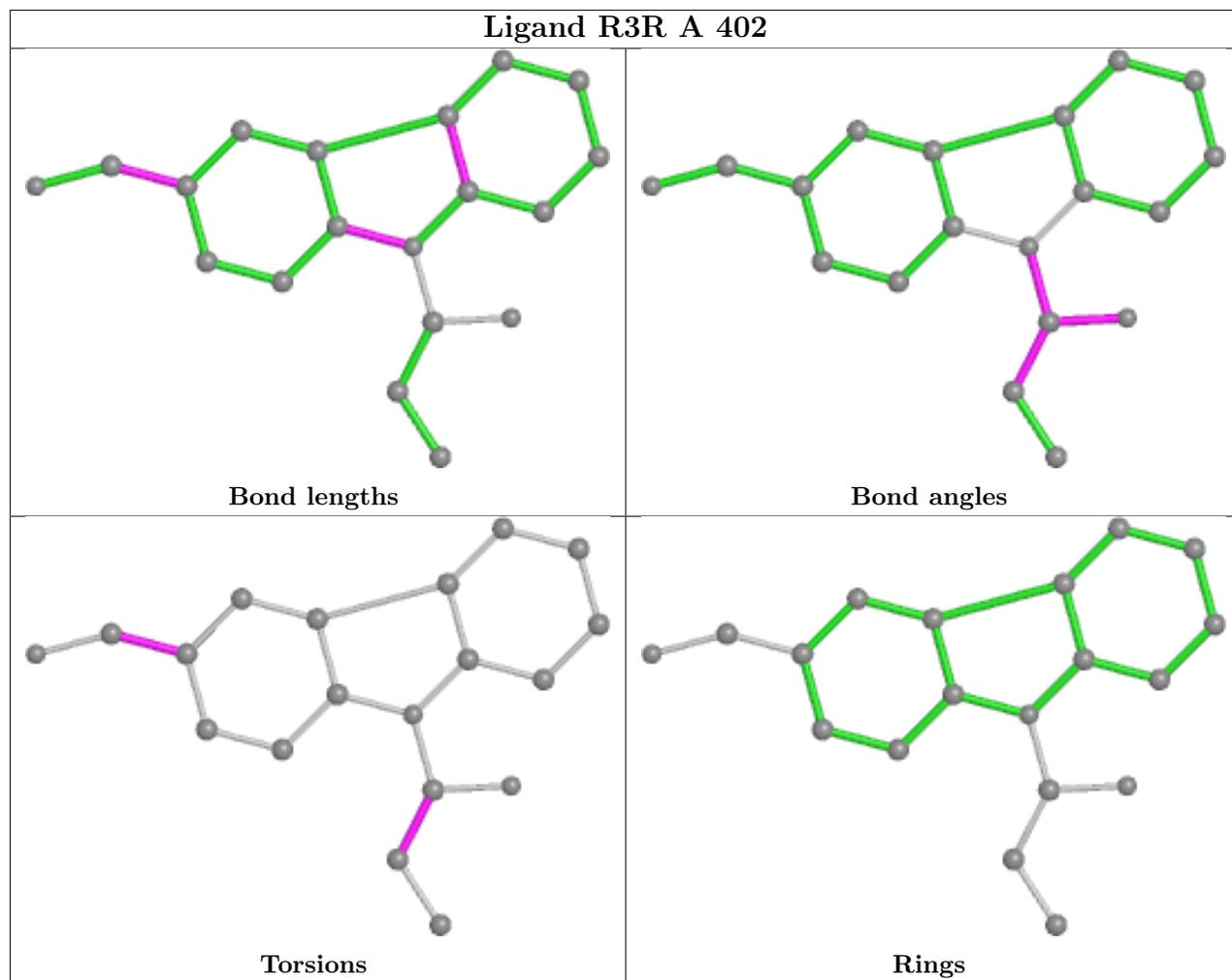
There are no ring outliers.

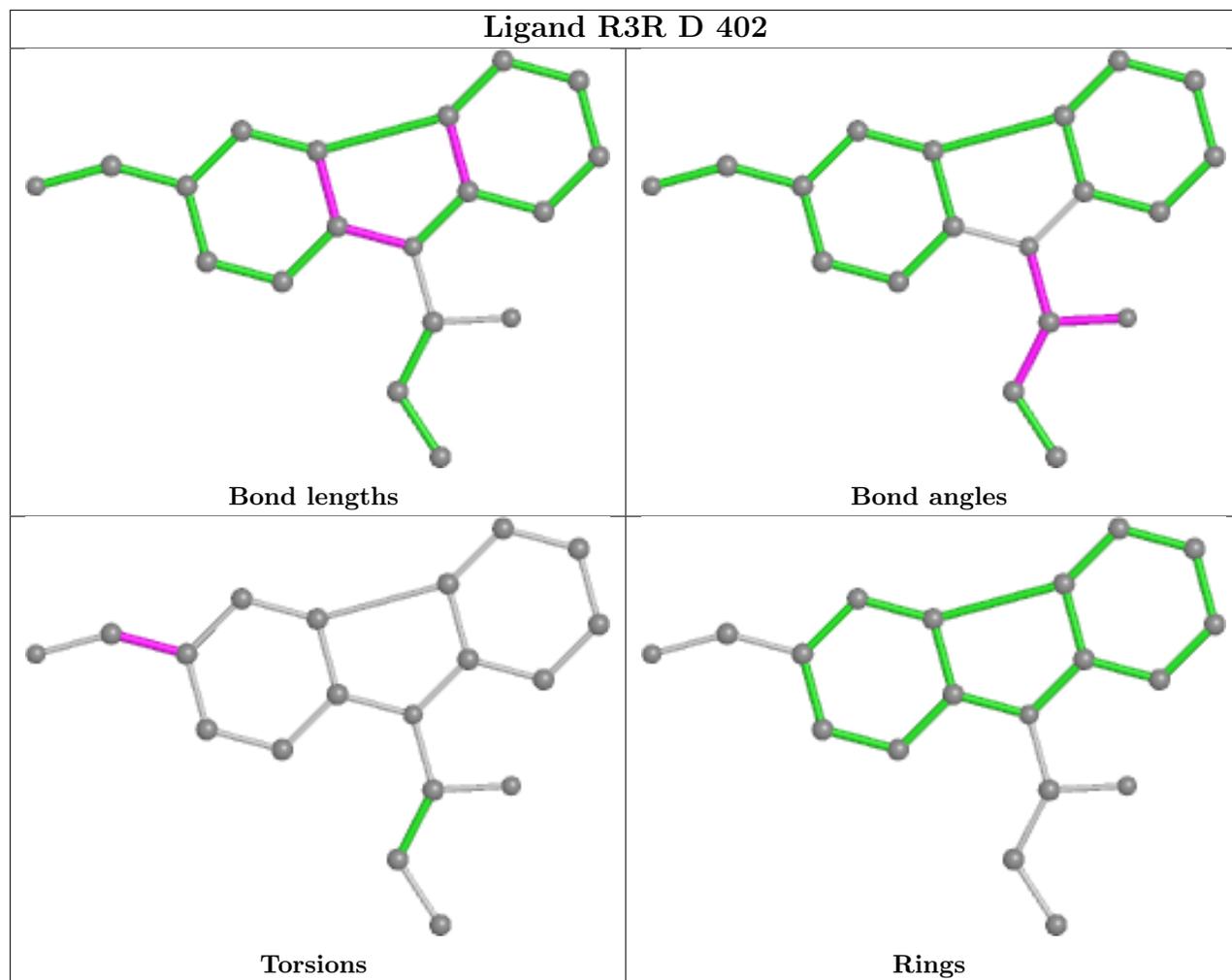
4 monomers are involved in 4 short contacts:

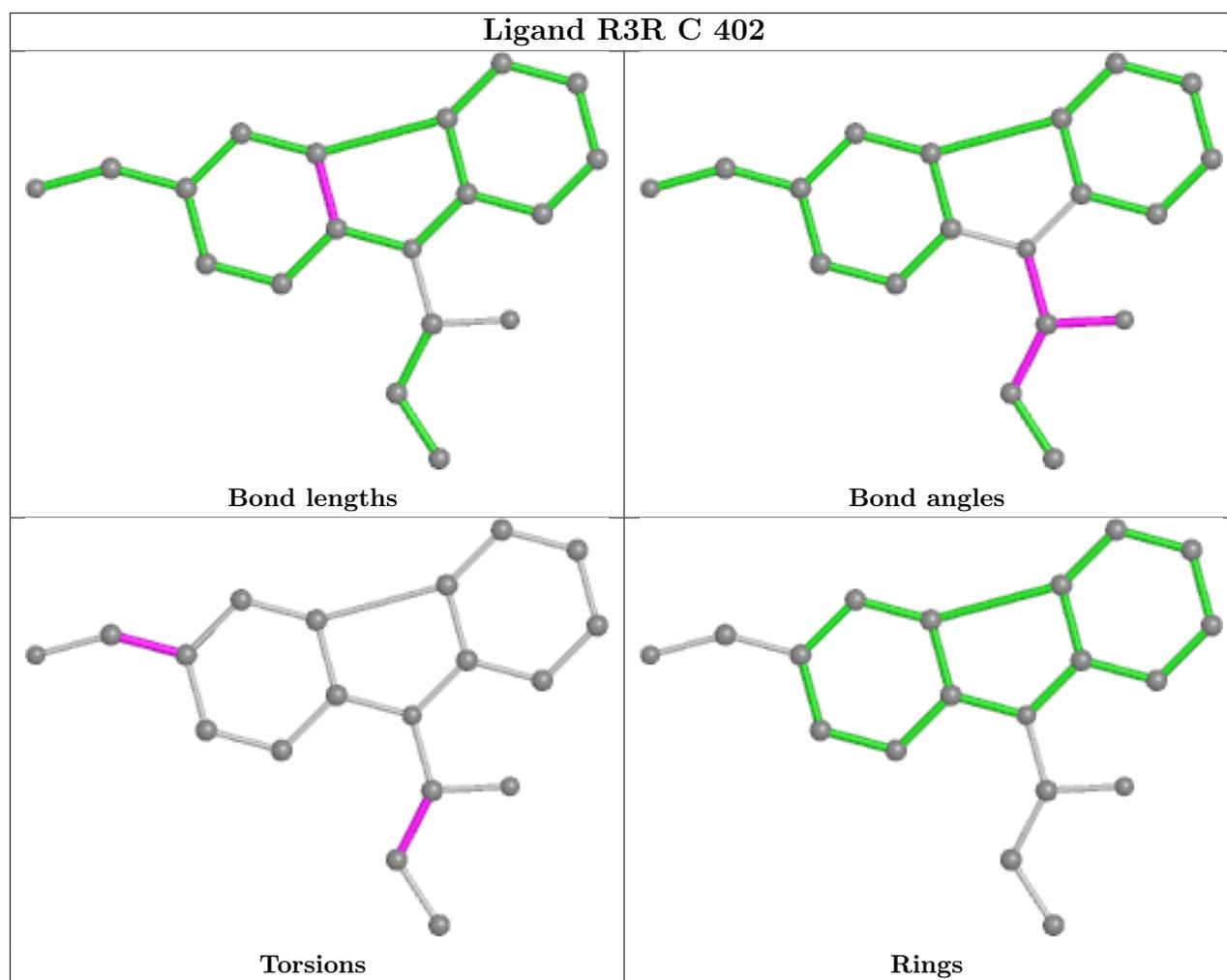
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	R3R	1	0
3	A	402	R3R	1	0
3	D	402	R3R	1	0
3	C	402	R3R	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	197/223 (88%)	-0.83	0 100 100	19, 30, 45, 58	0
1	B	197/223 (88%)	-0.83	0 100 100	21, 31, 50, 63	0
1	C	197/223 (88%)	-0.81	0 100 100	19, 30, 50, 70	0
1	D	197/223 (88%)	-0.84	0 100 100	20, 31, 46, 60	0
All	All	788/892 (88%)	-0.83	0 100 100	19, 30, 48, 70	0

There are no RSRZ outliers to report.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

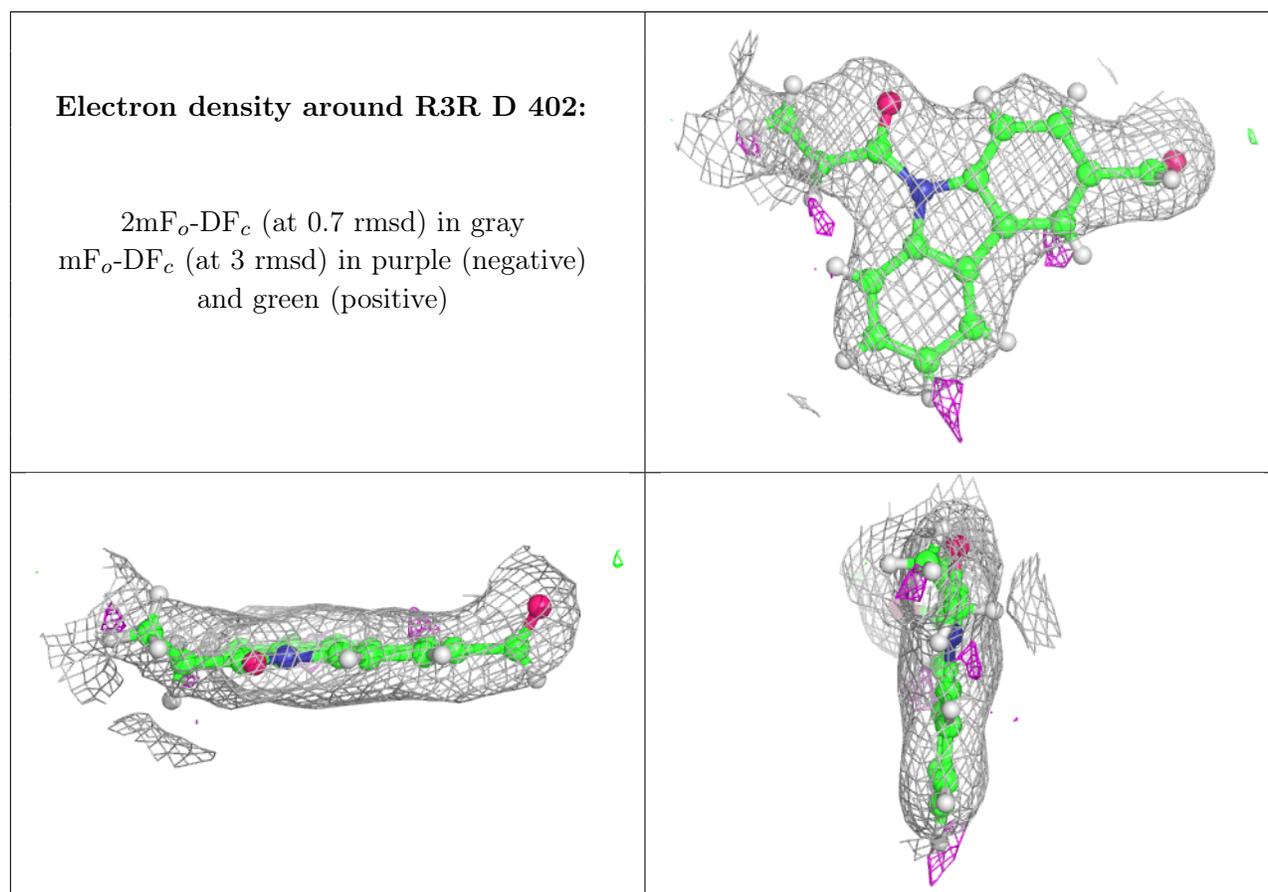
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	R3R	D	402	19/19	0.96	0.12	26,39,62,62	0
3	R3R	A	402	19/19	0.97	0.14	22,38,57,73	0
3	R3R	C	402	19/19	0.97	0.11	23,36,44,50	0
3	R3R	B	402	19/19	0.97	0.11	25,36,43,45	0

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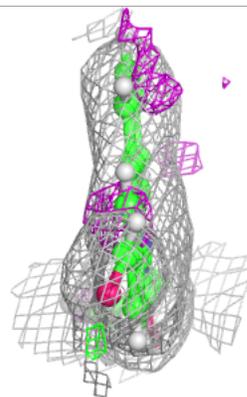
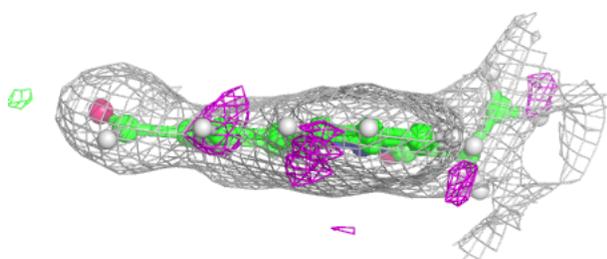
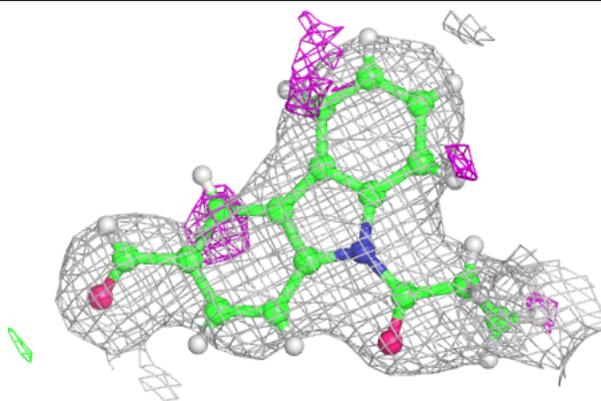
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	401	1/1	1.00	0.13	39,39,39,39	0
2	ZN	A	401	1/1	1.00	0.13	38,38,38,38	0
2	ZN	C	401	1/1	1.00	0.11	45,45,45,45	0
2	ZN	D	401	1/1	1.00	0.15	33,33,33,33	0

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.

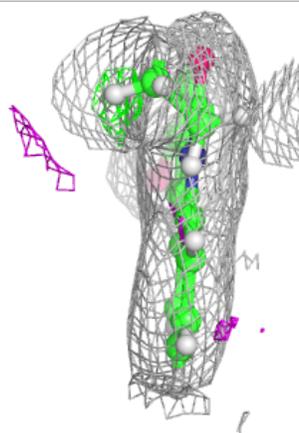
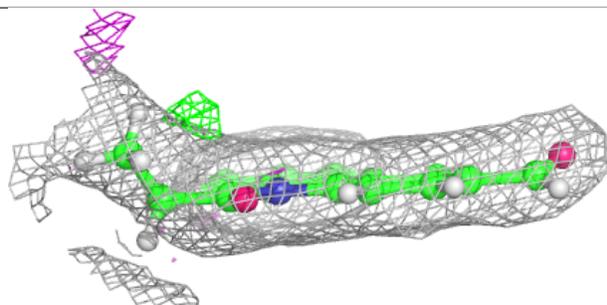
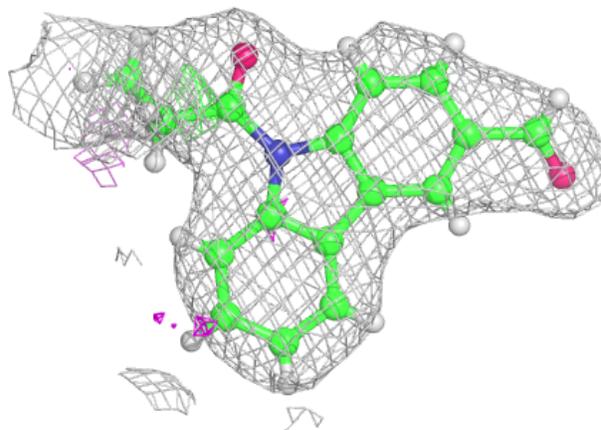


Electron density around R3R A 402:

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

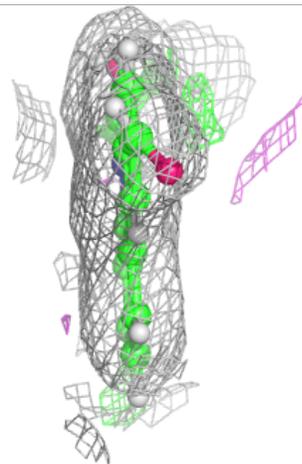
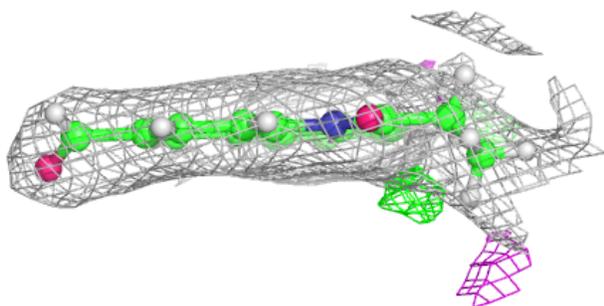
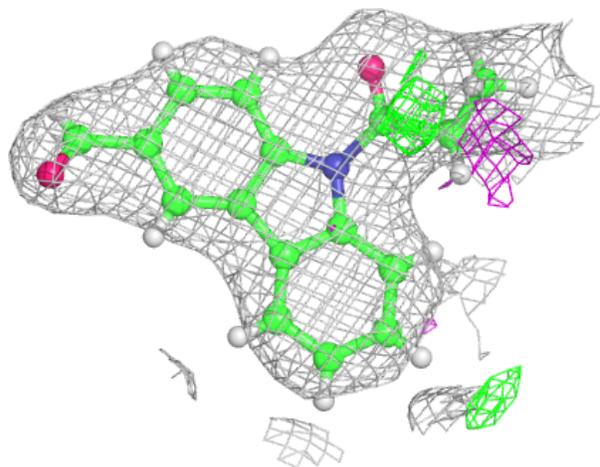
**Electron density around R3R C 402:**

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



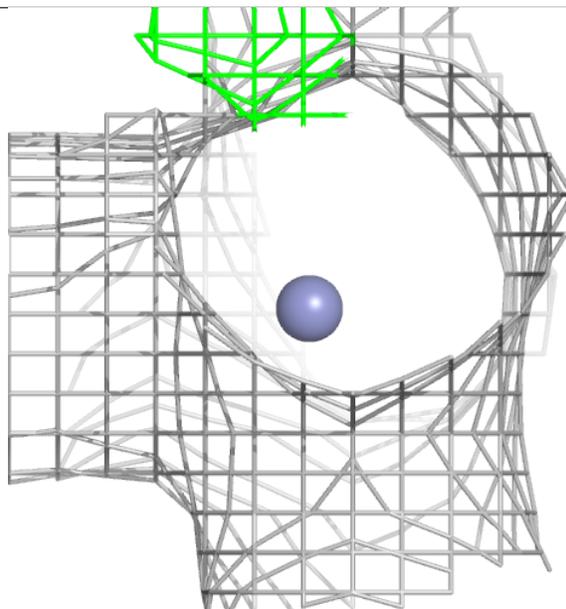
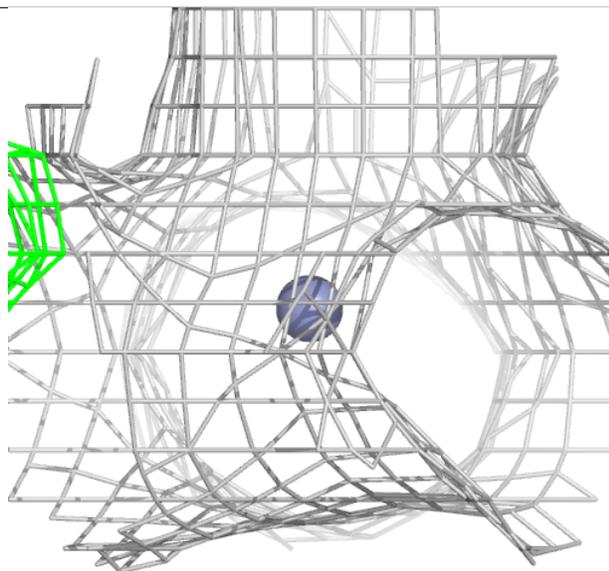
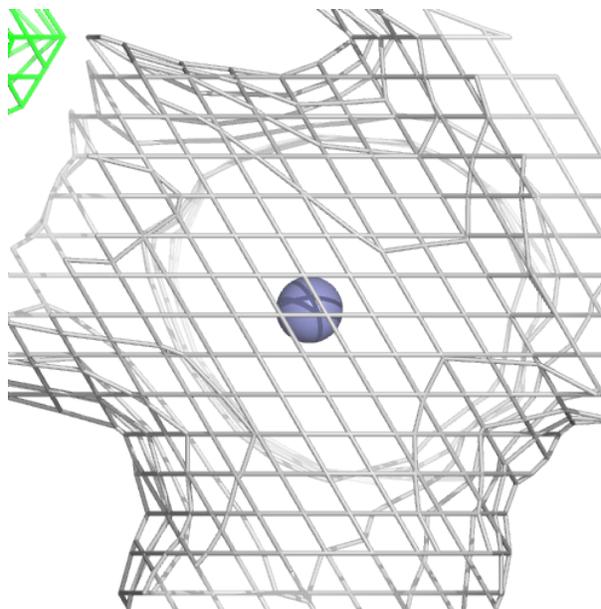
Electron density around R3R B 402:

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



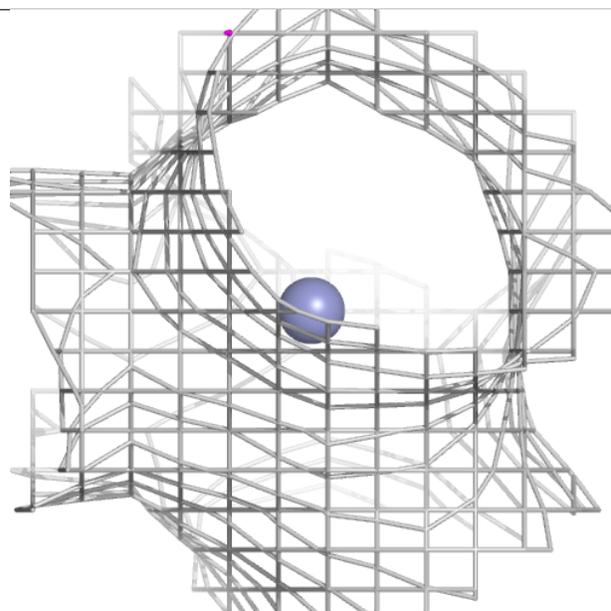
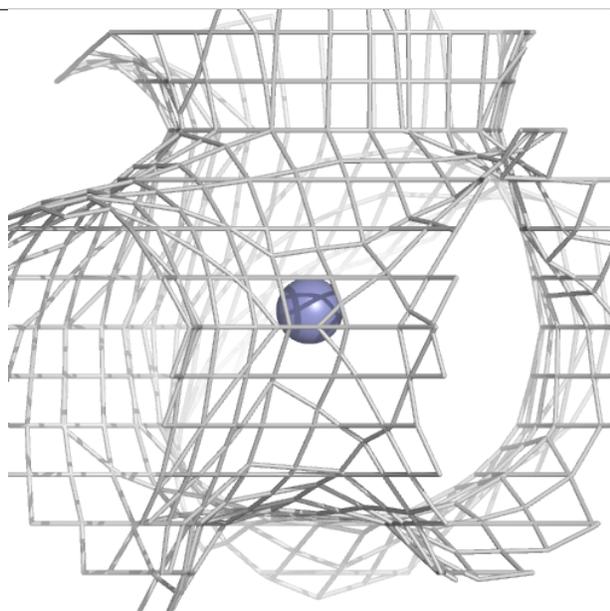
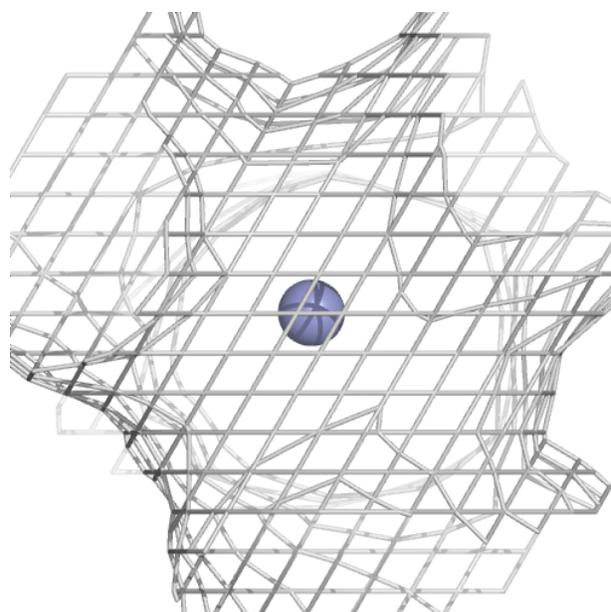
Electron density around ZN B 401:

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



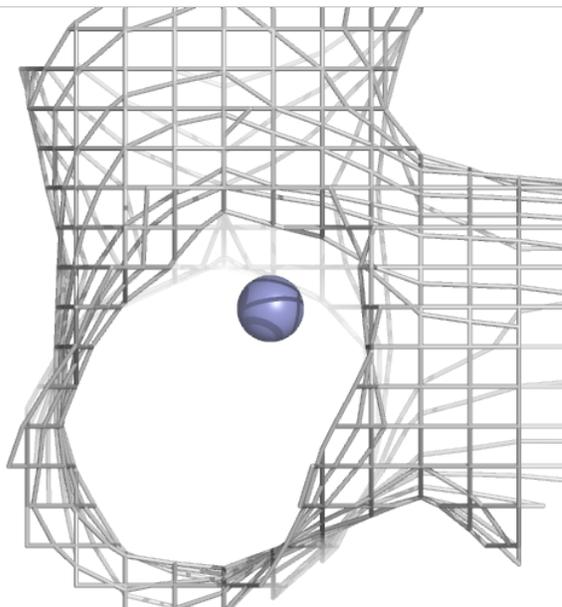
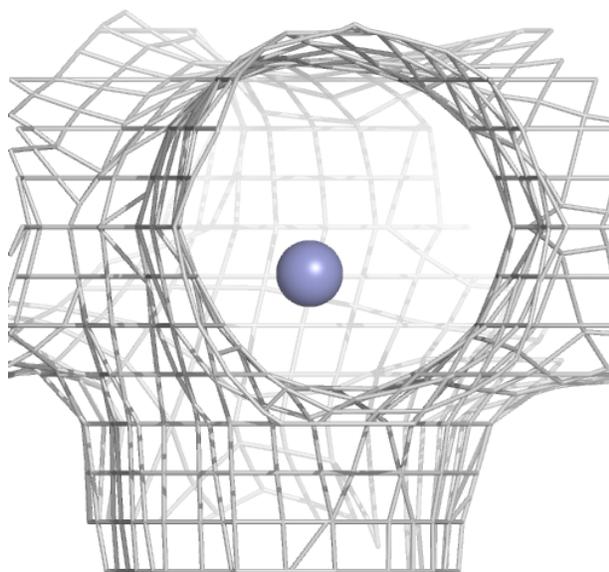
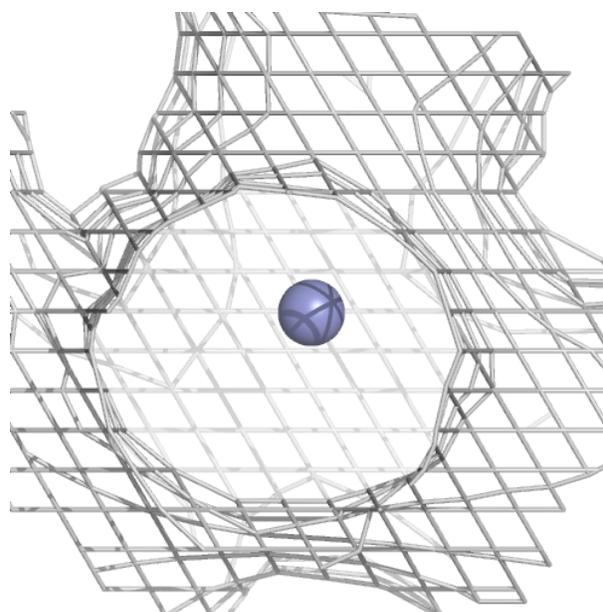
Electron density around ZN A 401:

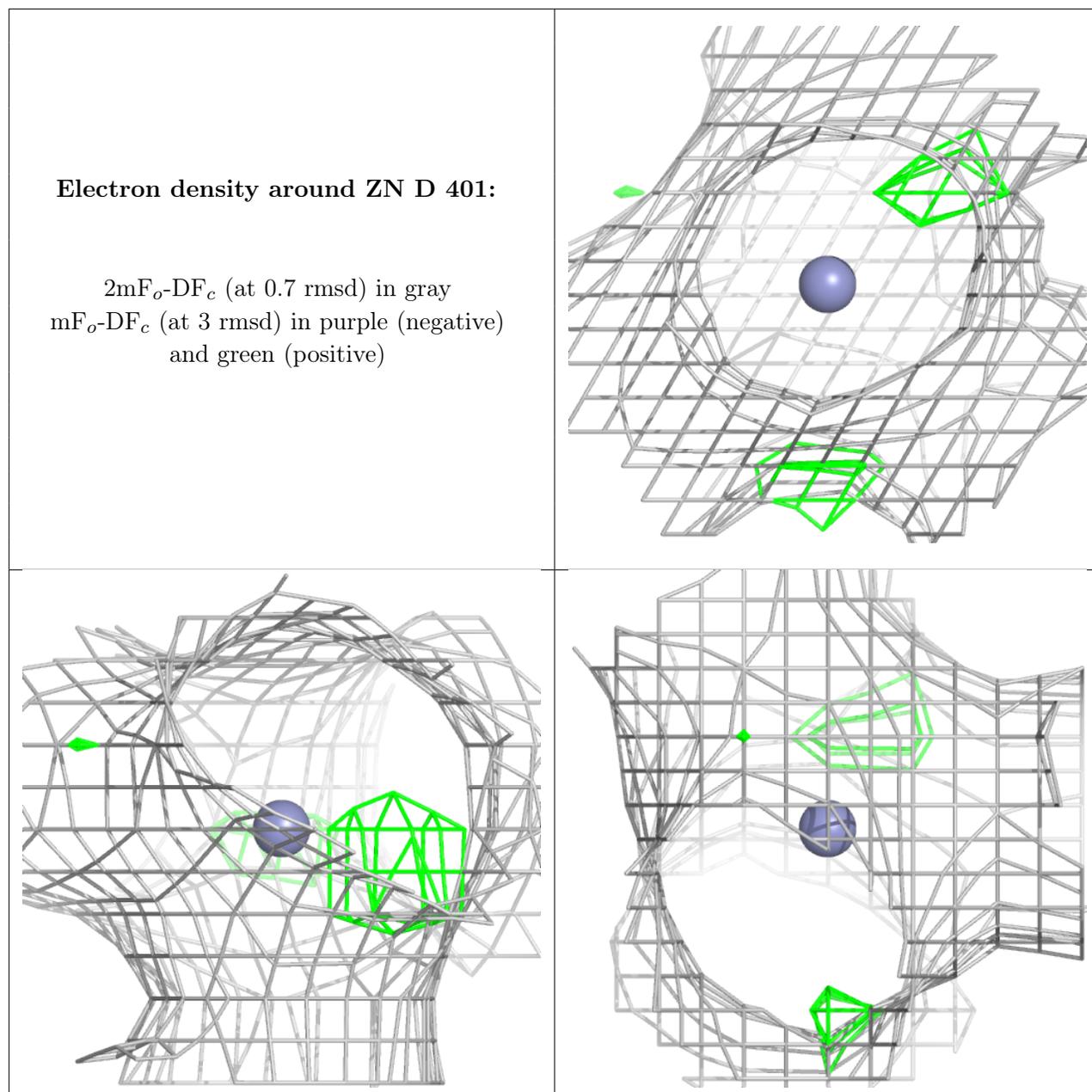
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 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.