



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 12:24 PM EDT

PDB ID : 8DC6
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

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>.

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 : 2.31.2
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) : 2.31.2

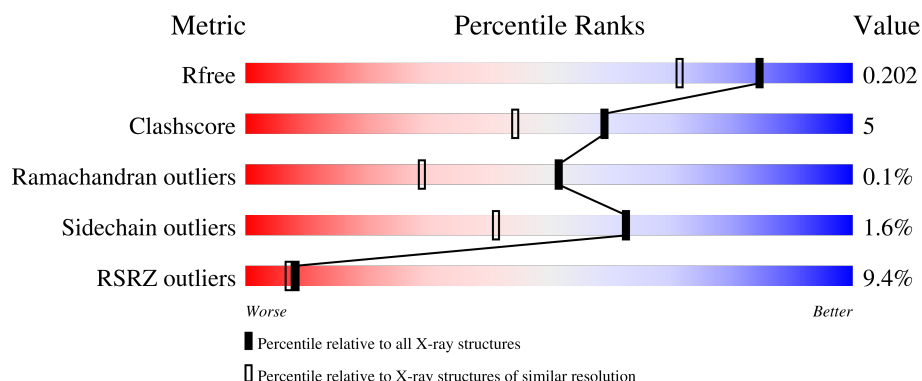
1 Overall quality at a glance

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 ≥ 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	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>13%</div> </div> </div>
1	B	223	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>13%</div> </div> </div>
1	C	223	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>14%</div> </div> </div>
1	D	223	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> </div>

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

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 (three-letter code: 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 (three-letter code: SO4) (formula: O₄S).



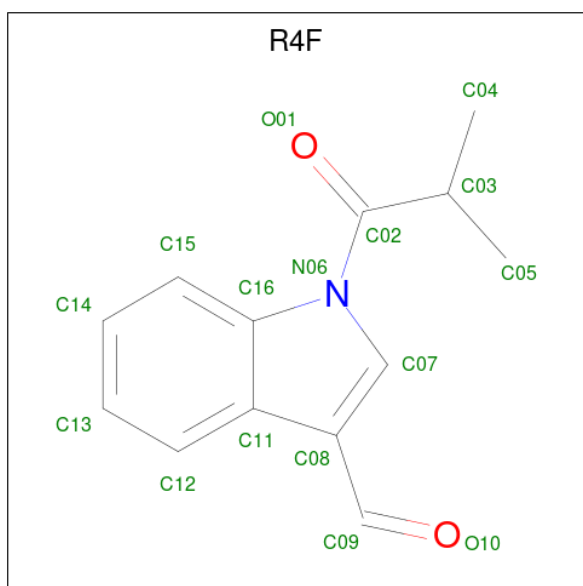
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	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 (three-letter code: R4F) (formula: C₁₃H₁₃NO₂) (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 (three-letter code: 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		

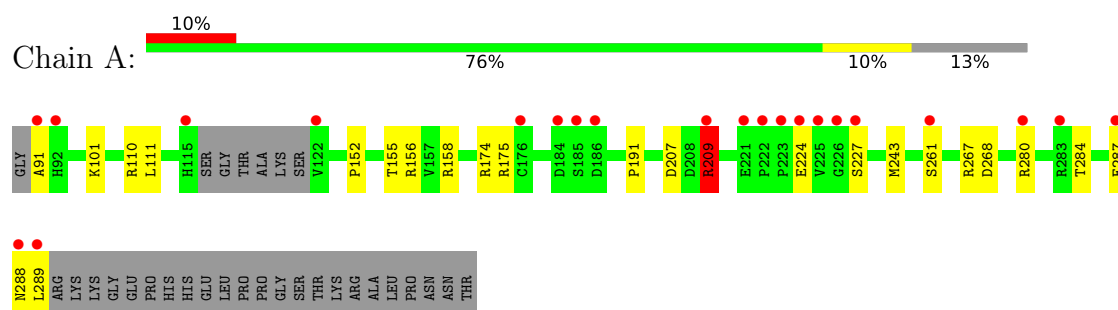
- Molecule 6 is water.

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

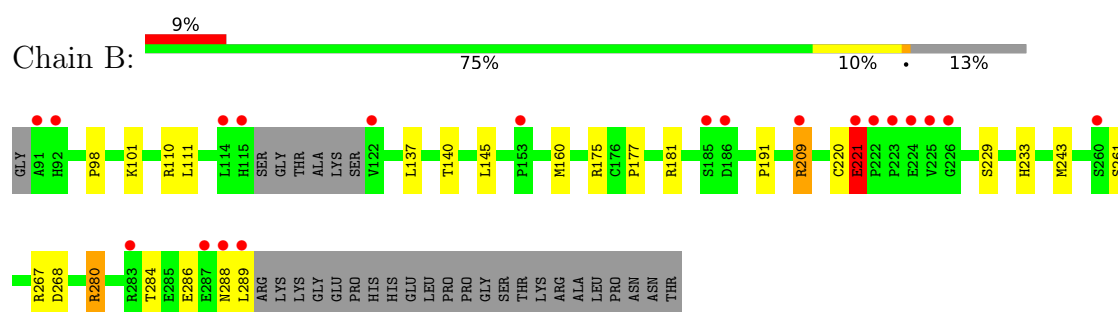
3 Residue-property plots [i](#)

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.

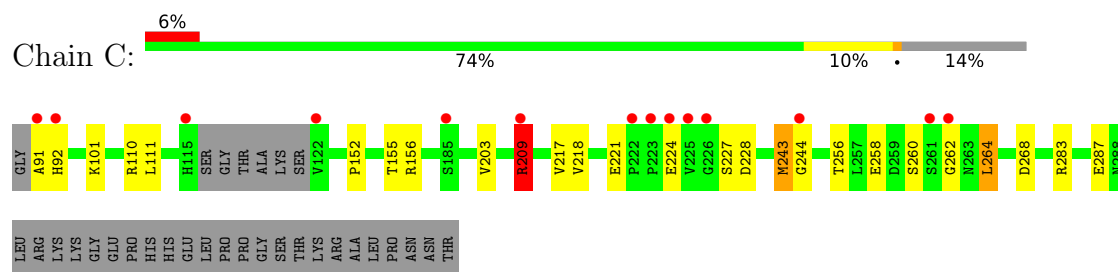
• Molecule 1: Cellular tumor antigen p53



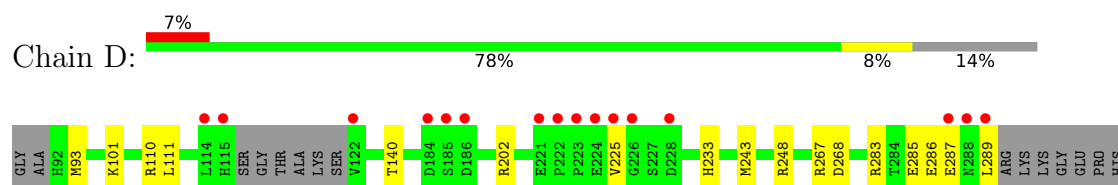
• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53



HIS
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, α , β , γ	91.04Å 105.75Å 105.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.60 52.88 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.29-1.60) 99.4 (52.88-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.181 , 0.202 0.182 , 0.202	Depositor DCC
R_{free} test set	6610 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6875	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, R4F, SO4, MG

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	0.42	0/1574	1.05	6/2134 (0.3%)
1	B	0.50	2/1579 (0.1%)	0.93	8/2141 (0.4%)
1	C	0.42	2/1573 (0.1%)	0.68	4/2133 (0.2%)
1	D	0.37	0/1584	0.62	1/2148 (0.0%)
All	All	0.43	4/6310 (0.1%)	0.84	19/8556 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ARG	CZ-NH1	-6.16	1.25	1.33
1	B	209	ARG	CB-CG	-5.66	1.37	1.52
1	C	209	ARG	CG-CD	-5.58	1.38	1.51
1	C	209	ARG	CZ-NH2	5.18	1.39	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ARG	NE-CZ-NH1	-23.58	108.51	120.30
1	B	209	ARG	NE-CZ-NH1	-23.03	108.78	120.30
1	A	209	ARG	NE-CZ-NH2	20.07	130.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ARG	CA-CB-CG	-14.91	80.59	113.40
1	B	209	ARG	CG-CD-NE	13.83	140.84	111.80
1	A	209	ARG	CG-CD-NE	13.04	139.18	111.80
1	A	209	ARG	CD-NE-CZ	-9.25	110.65	123.60
1	C	209	ARG	CG-CD-NE	9.20	131.12	111.80
1	A	209	ARG	CB-CG-CD	9.06	135.16	111.60
1	B	209	ARG	CA-CB-CG	-7.26	97.42	113.40
1	C	209	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	B	220	CYS	C-N-CA	6.75	138.57	121.70
1	D	93	MET	CG-SD-CE	5.92	109.67	100.20
1	B	261	SER	CB-CA-C	-5.40	99.84	110.10
1	C	264	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	221	GLU	N-CA-CB	-5.32	101.03	110.60
1	B	221	GLU	CG-CD-OE2	-5.32	107.67	118.30
1	B	209	ARG	CB-CG-CD	5.30	125.39	111.60
1	C	243	MET	C-N-CA	-5.17	111.44	122.30

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 [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	1527	0	1487	20	0
1	B	1532	0	1491	10	1
1	C	1525	0	1483	23	0
1	D	1534	0	1494	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
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	6	1
6	D	156	0	0	2	1
All	All	6875	0	5955	57	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 (57) 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:C:101:LYS:NZ	6:C:503:HOH:O	2.27	0.67
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:156:ARG:HH11	1:A:158:ARG:NH2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:140:THR:HG23	1:B:233:HIS:HB3	1.86	0.57
1:A:280:ARG:HH21	1:C:260:SER:C	2.08	0.56
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: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:B:98:PRO:HG2	1:B:160:MET:HE3	1.96	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: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:A:191:PRO:HD3	1:D:243:MET:HE1	2.00	0.43
1:D:283:ARG:O	1:D:287:GLU:HG2	2.18	0.43
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%)	29	11
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%)	51	29

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%)	175 (99%)	2 (1%)	73	57
1	B	178/198 (90%)	175 (98%)	3 (2%)	60	38
1	C	177/198 (89%)	173 (98%)	4 (2%)	50	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	179/198 (90%)	177 (99%)	2 (1%)	73	57
All	All	711/792 (90%)	700 (98%)	11 (2%)	62	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	243	MET
1	B	110	ARG
1	B	243	MET
1	B	280	ARG
1	C	92	HIS
1	C	110	ARG
1	C	209	ARG
1	C	243	MET
1	D	110	ARG
1	D	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	92	HIS
1	C	178	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	A	402	-	4,4,4	0.14	0	6,6,6	0.24	0
3	SO4	C	403	-	4,4,4	0.19	0	6,6,6	0.51	0
3	SO4	D	404	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.41	0
3	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	D	403	-	4,4,4	0.13	0	6,6,6	0.20	0
3	SO4	A	406	-	4,4,4	0.12	0	6,6,6	0.22	0
4	R4F	A	407	1	14,17,17	1.28	2 (14%)	13,24,24	0.64	0
4	R4F	D	405	1	14,17,17	1.44	2 (14%)	13,24,24	0.72	0
3	SO4	C	402	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.20	0
3	SO4	B	402	-	4,4,4	0.12	0	6,6,6	0.37	0
3	SO4	A	405	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	402	-	4,4,4	0.16	0	6,6,6	0.36	0
4	R4F	C	404	1	14,17,17	1.17	2 (14%)	13,24,24	0.66	0
4	R4F	B	405	1	14,17,17	1.36	2 (14%)	13,24,24	0.65	0
3	SO4	A	403	-	4,4,4	0.15	0	6,6,6	0.22	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	D	405	1	-	1/5/10/10	0/2/2/2
4	R4F	A	407	1	-	0/5/10/10	0/2/2/2
4	R4F	C	404	1	-	1/5/10/10	0/2/2/2
4	R4F	B	405	1	-	1/5/10/10	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	C07-N06	3.90	1.44	1.39
4	B	405	R4F	C07-N06	3.78	1.44	1.39
4	A	407	R4F	C07-N06	2.90	1.43	1.39
4	A	407	R4F	C08-C11	2.71	1.47	1.41
4	C	404	R4F	C08-C11	2.55	1.47	1.41
4	C	404	R4F	C07-N06	2.54	1.42	1.39
4	B	405	R4F	C08-C11	2.50	1.47	1.41
4	D	405	R4F	C08-C11	2.15	1.46	1.41

There are no bond angle outliers.

There are no chirality outliers.

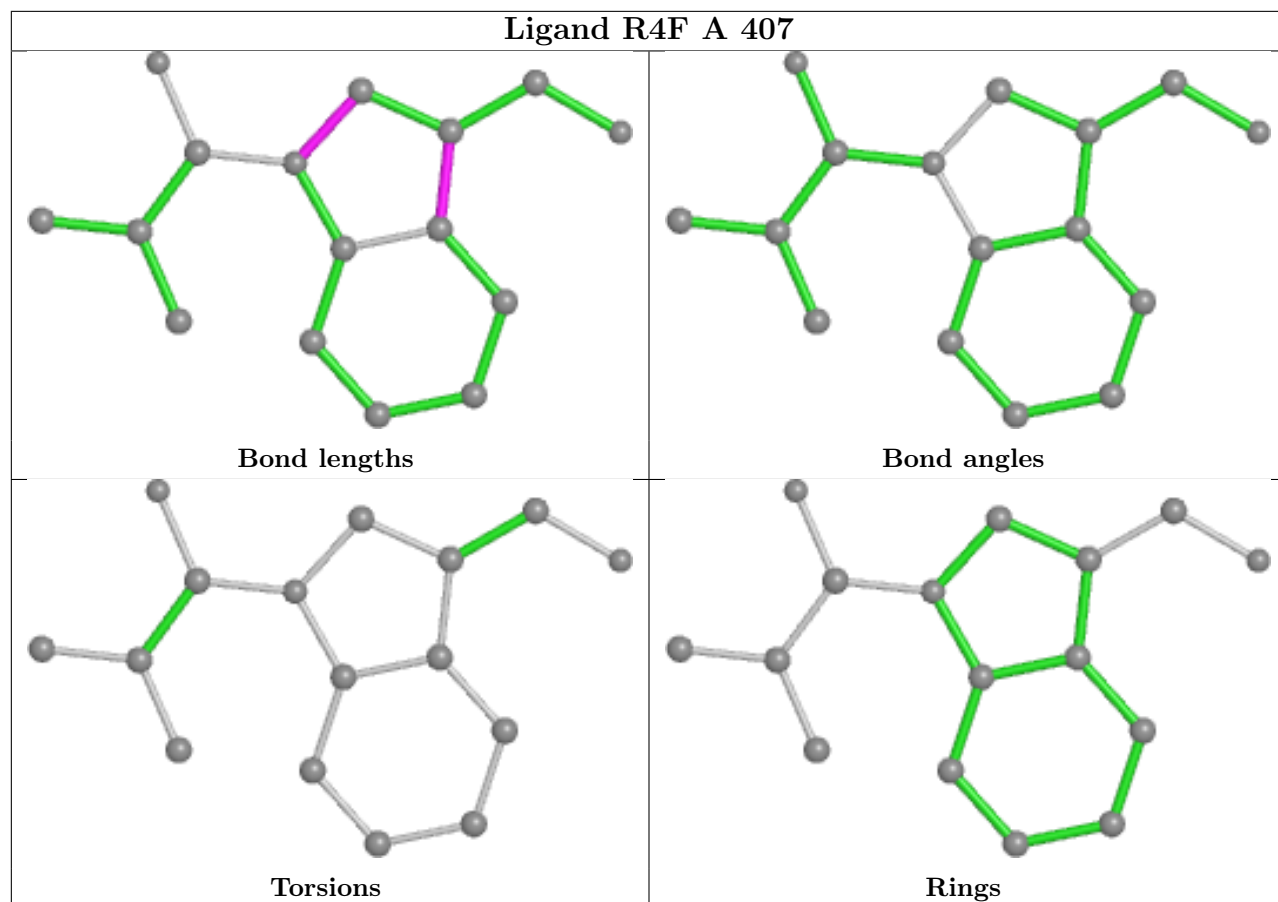
All (3) torsion outliers are listed below:

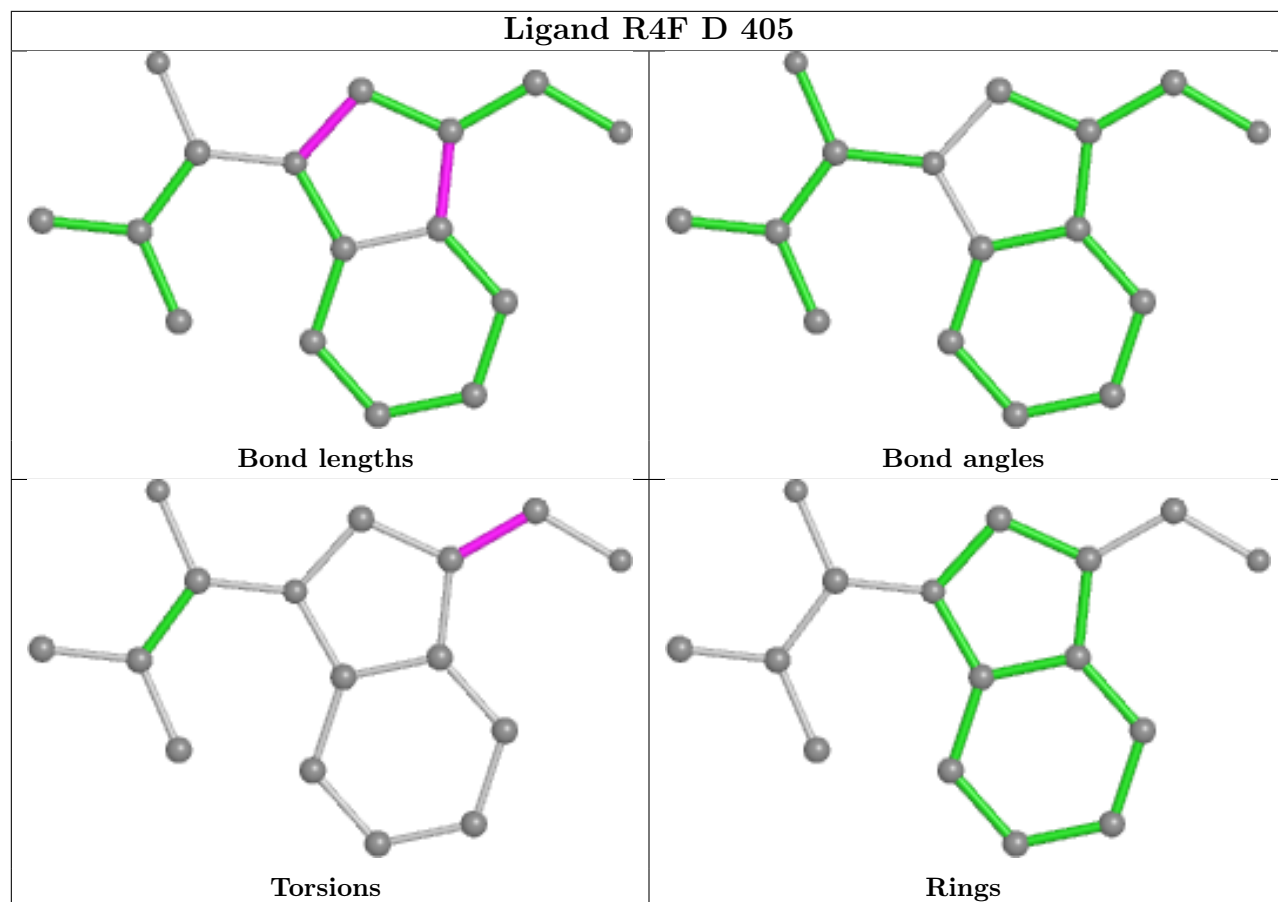
Mol	Chain	Res	Type	Atoms
4	B	405	R4F	C07-C08-C09-O10
4	C	404	R4F	C07-C08-C09-O10
4	D	405	R4F	C07-C08-C09-O10

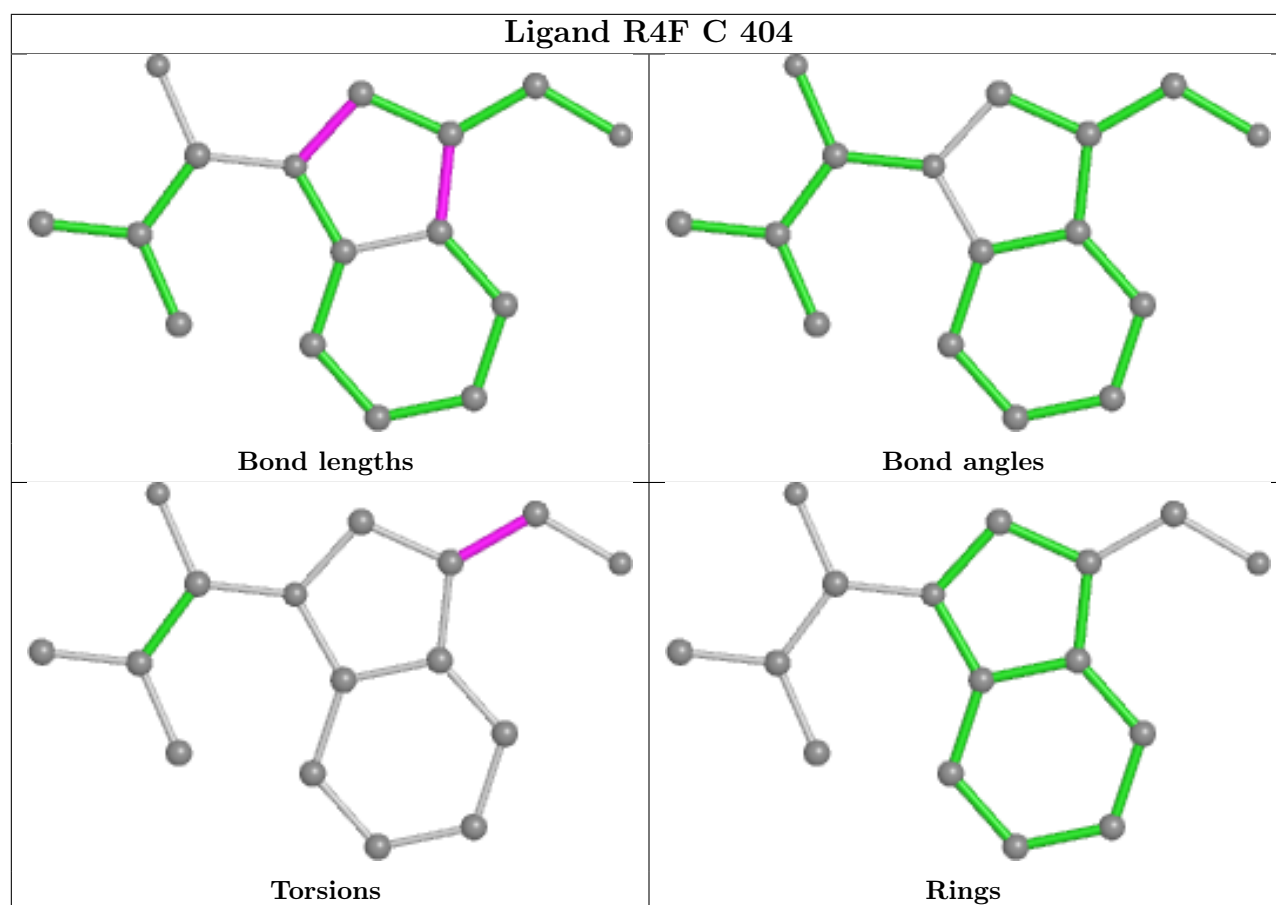
There are no ring outliers.

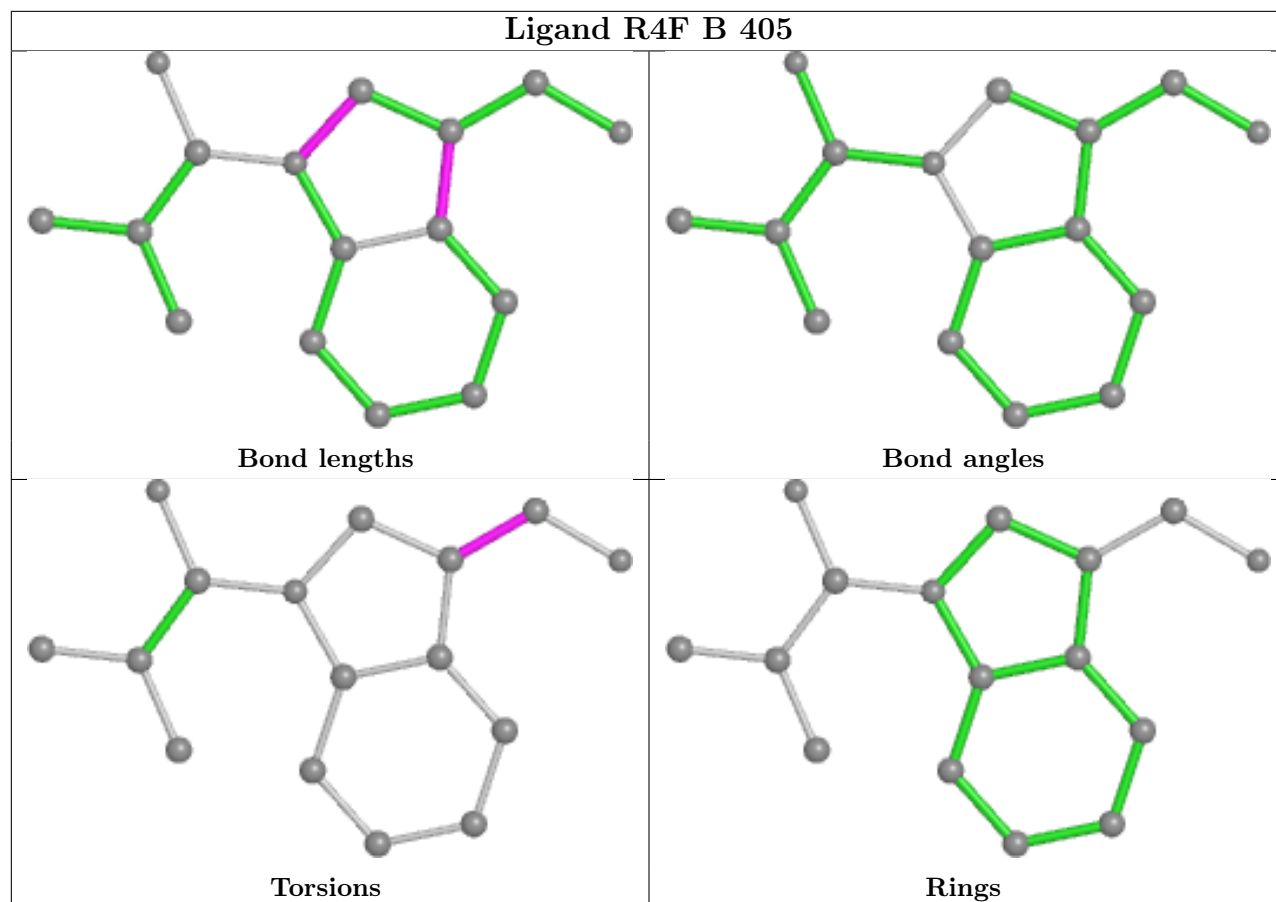
No monomer is involved in short contacts.

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, 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	193/223 (86%)	0.58	22 (11%) 5 4	9, 18, 44, 72	0
1	B	193/223 (86%)	0.51	20 (10%) 6 5	9, 17, 42, 65	0
1	C	192/223 (86%)	0.43	14 (7%) 15 13	9, 17, 41, 57	0
1	D	192/223 (86%)	0.43	16 (8%) 11 10	8, 18, 44, 63	0
All	All	770/892 (86%)	0.49	72 (9%) 8 7	8, 18, 42, 72	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PRO	8.2
1	A	224	GLU	7.7
1	B	289	LEU	7.5
1	A	289	LEU	6.3
1	D	225	VAL	6.2
1	A	226	GLY	6.1
1	C	115	HIS	6.0
1	B	225	VAL	6.0
1	B	115	HIS	5.9
1	B	224	GLU	5.6
1	A	225	VAL	5.5
1	B	223	PRO	5.4
1	D	223	PRO	5.4
1	D	224	GLU	5.3
1	D	115	HIS	5.2
1	D	122	VAL	5.2
1	C	225	VAL	4.8
1	C	224	GLU	4.7
1	B	221	GLU	4.6
1	D	114	LEU	4.2
1	A	176	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	4.0
1	A	261	SER	3.9
1	D	222	PRO	3.9
1	B	209	ARG	3.8
1	B	222	PRO	3.7
1	A	227	SER	3.6
1	A	221	GLU	3.6
1	C	91	ALA	3.5
1	B	122	VAL	3.5
1	C	185	SER	3.4
1	A	288	ASN	3.4
1	D	289	LEU	3.4
1	A	280	ARG	3.4
1	D	287	GLU	3.3
1	B	185	SER	3.3
1	C	222	PRO	3.3
1	D	226	GLY	3.2
1	B	153	PRO	3.2
1	C	244	GLY	3.1
1	C	209	ARG	3.1
1	C	223	PRO	3.0
1	A	122	VAL	3.0
1	C	92	HIS	3.0
1	A	185	SER	2.9
1	C	226	GLY	2.9
1	A	115	HIS	2.8
1	A	209	ARG	2.8
1	A	186	ASP	2.8
1	D	186	ASP	2.8
1	B	186	ASP	2.7
1	C	122	VAL	2.7
1	C	261	SER	2.7
1	B	92	HIS	2.7
1	B	226	GLY	2.6
1	D	184	ASP	2.6
1	A	91	ALA	2.6
1	A	287	GLU	2.5
1	D	221	GLU	2.5
1	A	184	ASP	2.5
1	B	283	ARG	2.4
1	C	262	GLY	2.4
1	B	288	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	185	SER	2.4
1	B	114	LEU	2.3
1	A	92	HIS	2.2
1	A	283	ARG	2.2
1	D	288	ASN	2.1
1	D	228	ASP	2.1
1	B	287	GLU	2.1
1	B	91	ALA	2.1
1	B	260	SER	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, 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
4	R4F	B	405	16/16	0.75	0.27	23,32,44,49	0
4	R4F	A	407	16/16	0.79	0.26	24,30,39,48	0
4	R4F	C	404	16/16	0.83	0.26	26,31,43,46	0
4	R4F	D	405	16/16	0.87	0.23	23,31,44,46	0
3	SO4	D	404	5/5	0.89	0.32	46,49,57,58	0
3	SO4	A	403	5/5	0.90	0.22	33,33,47,51	0
3	SO4	C	402	5/5	0.91	0.16	28,35,44,48	0
3	SO4	A	406	5/5	0.91	0.26	38,39,48,51	0
5	MG	C	405	1/1	0.91	0.06	36,36,36,36	0
3	SO4	A	402	5/5	0.92	0.22	37,39,43,46	0
3	SO4	A	404	5/5	0.92	0.14	24,30,38,38	0
3	SO4	D	403	5/5	0.93	0.14	28,29,41,49	0
3	SO4	A	405	5/5	0.94	0.22	47,48,54,55	0
3	SO4	B	403	5/5	0.94	0.17	26,28,39,46	0

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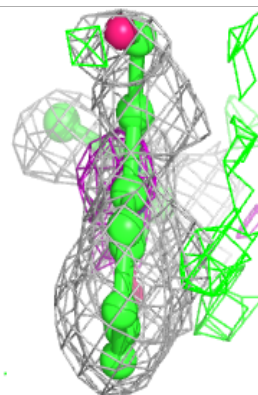
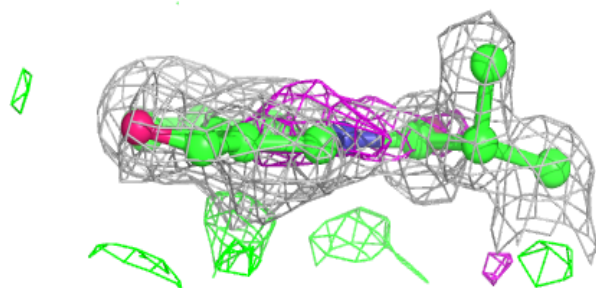
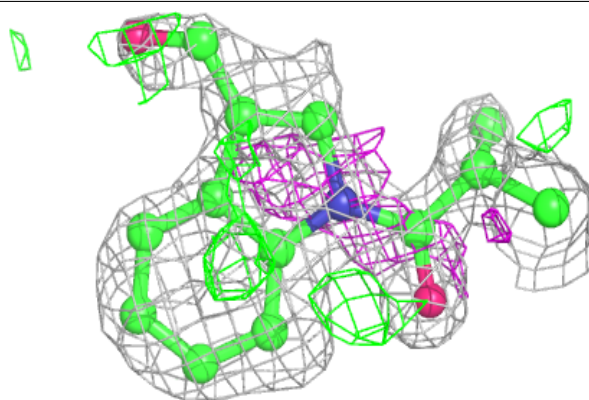
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	D	402	5/5	0.95	0.11	27,29,31,31	0
5	MG	B	406	1/1	0.95	0.23	25,25,25,25	0
3	SO4	B	402	5/5	0.95	0.10	23,25,28,32	0
3	SO4	B	404	5/5	0.96	0.15	37,46,48,51	0
3	SO4	C	403	5/5	0.97	0.08	19,20,24,29	0
2	ZN	D	401	1/1	1.00	0.12	12,12,12,12	0
2	ZN	A	401	1/1	1.00	0.11	11,11,11,11	0
2	ZN	B	401	1/1	1.00	0.12	12,12,12,12	0
2	ZN	C	401	1/1	1.00	0.11	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.

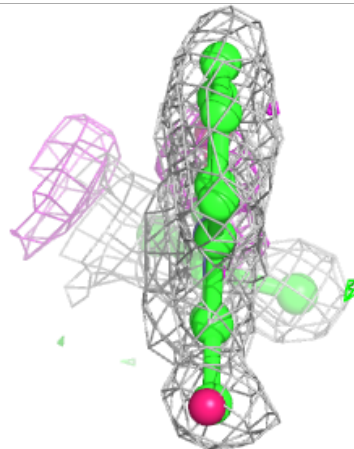
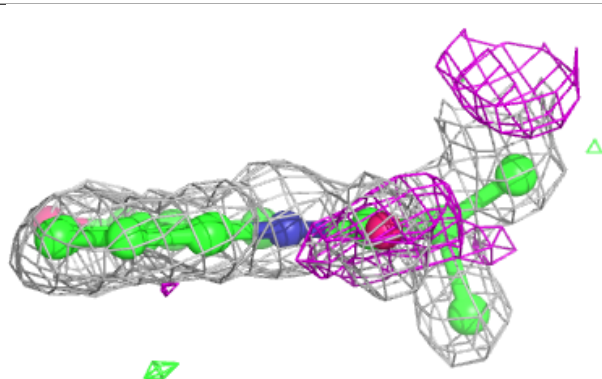
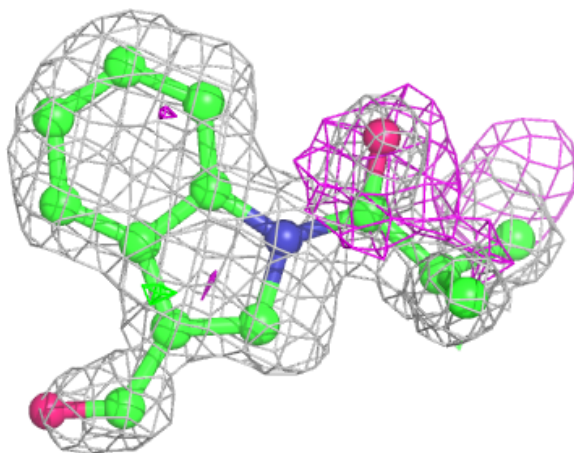
Electron density around R4F B 405:

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



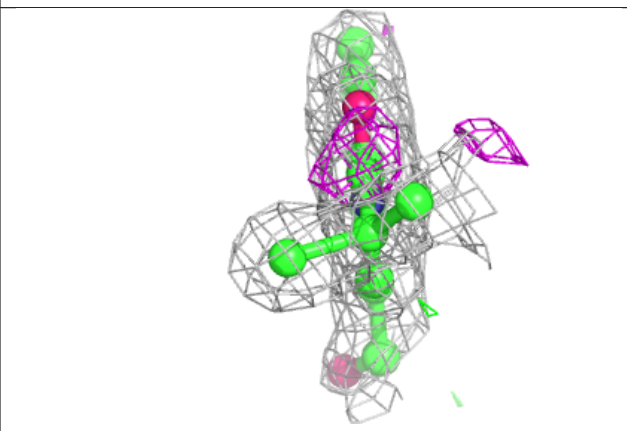
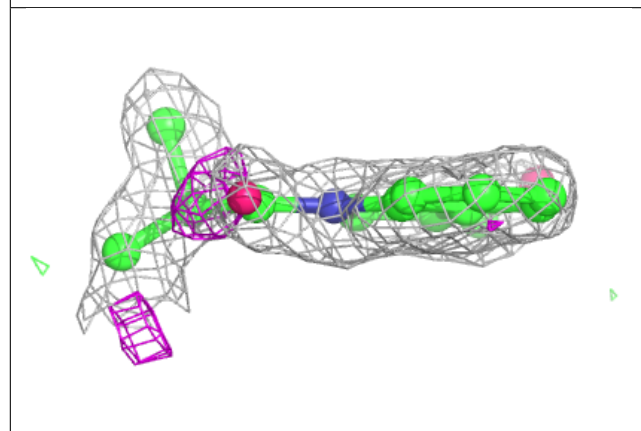
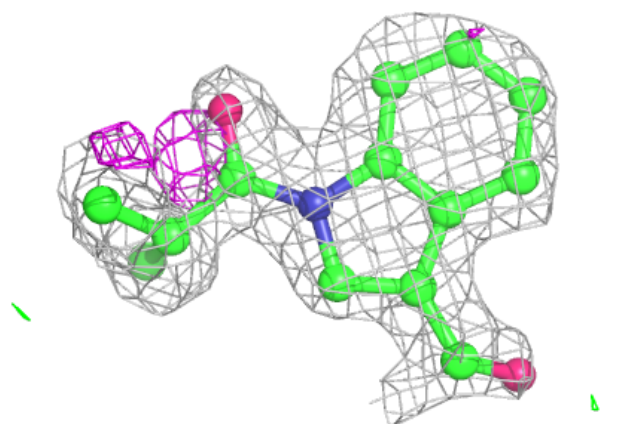
Electron density around R4F A 407:

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

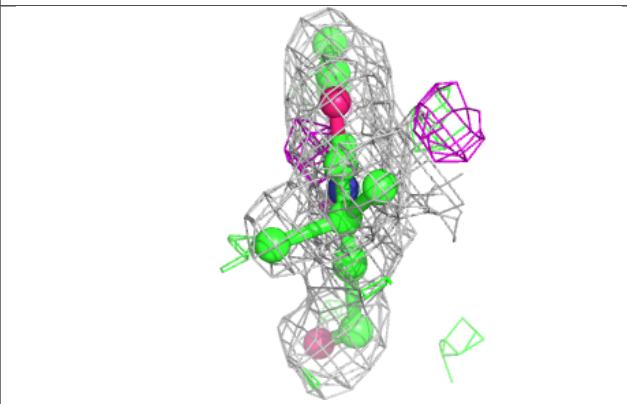
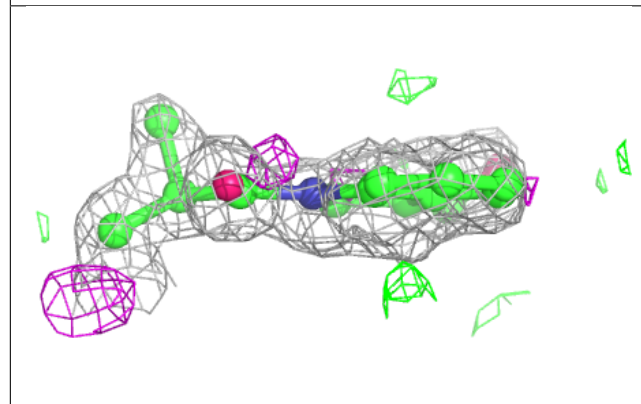
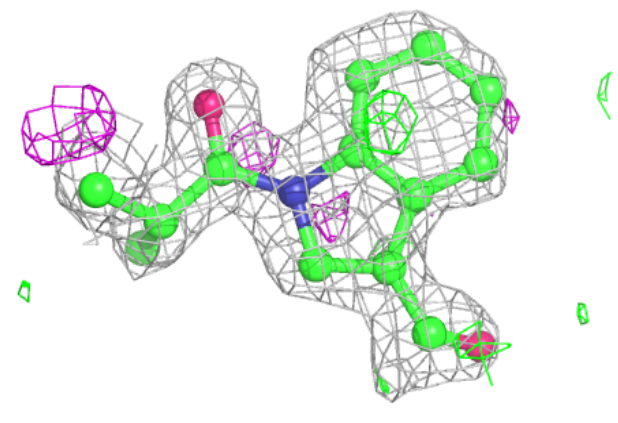


Electron density around R4F C 404:

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

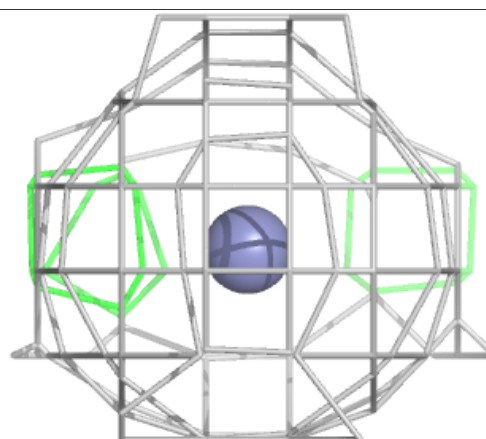
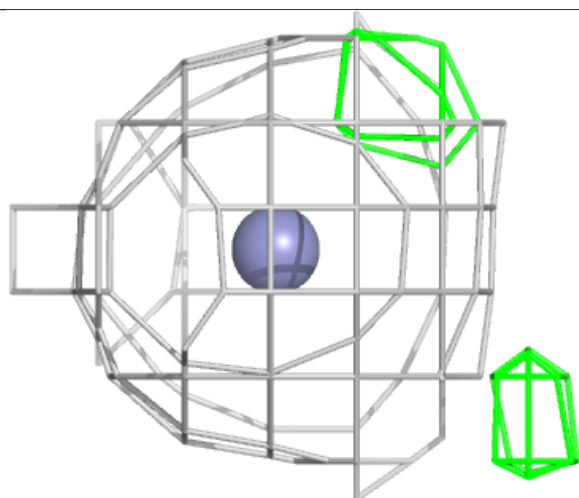
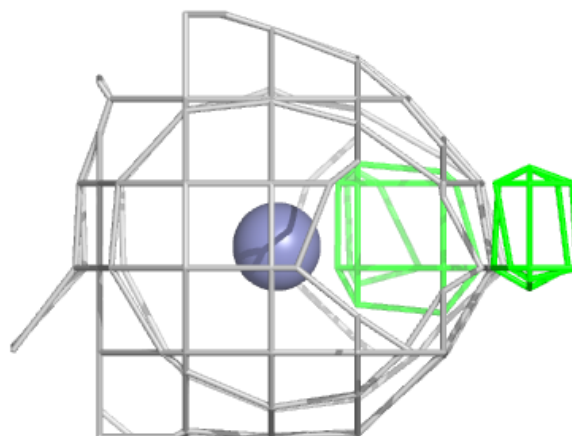
**Electron density around R4F D 405:**

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



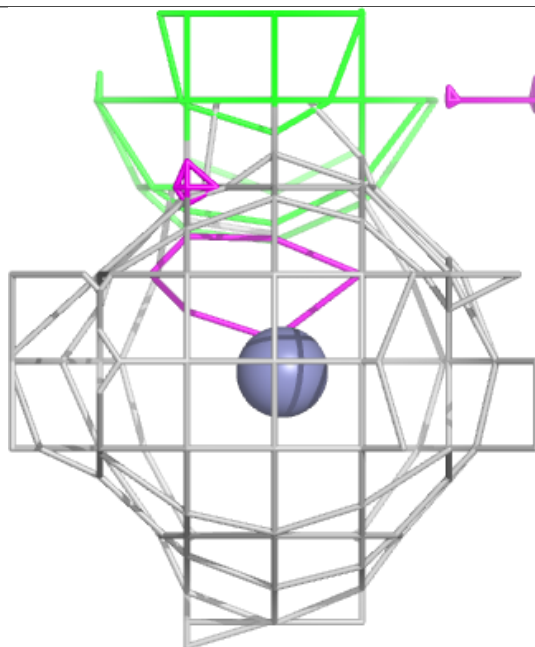
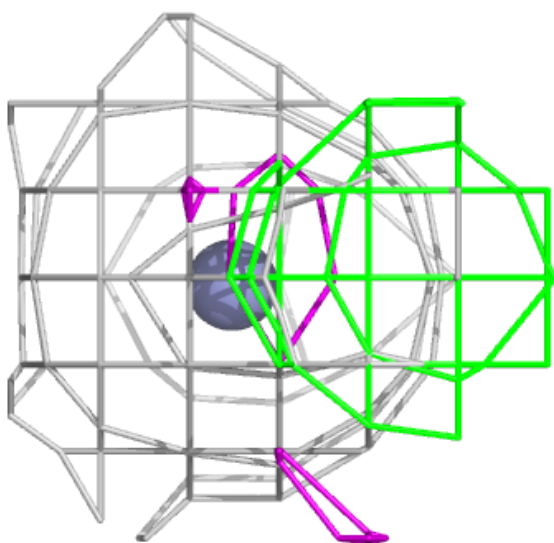
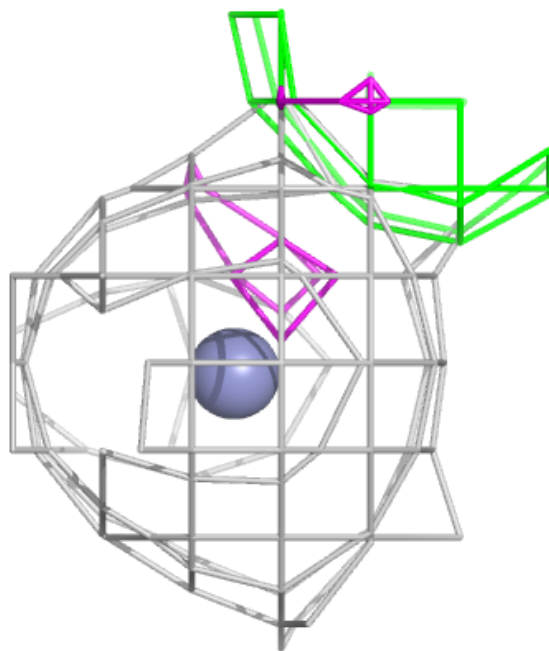
Electron density around ZN D 401:

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



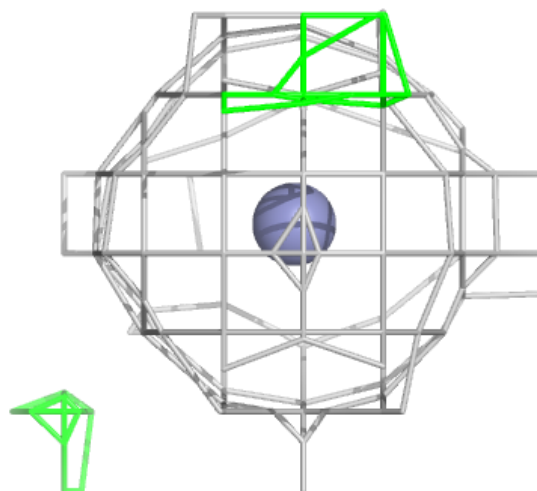
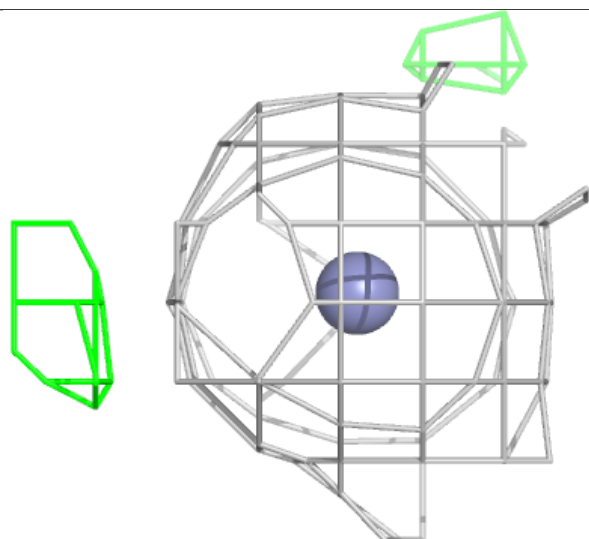
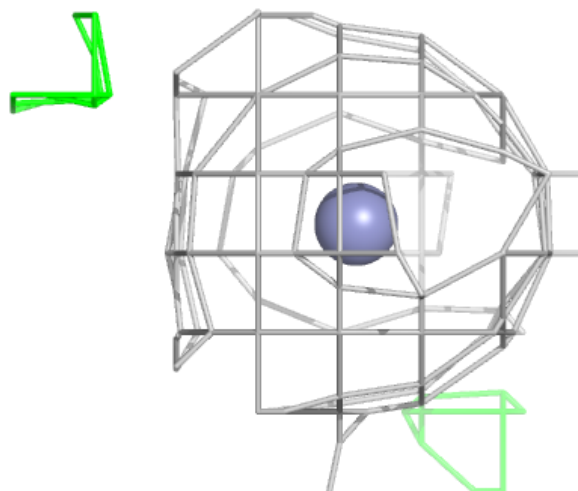
Electron density around ZN A 401:

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



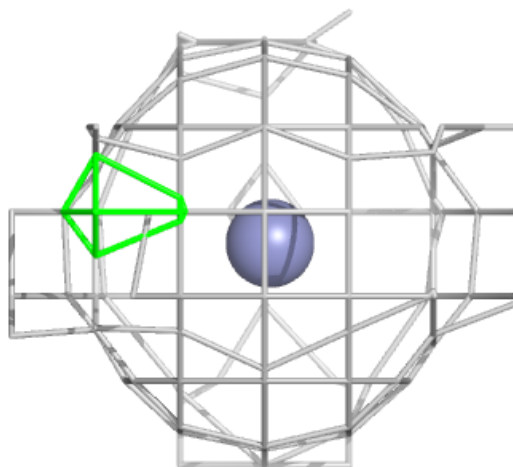
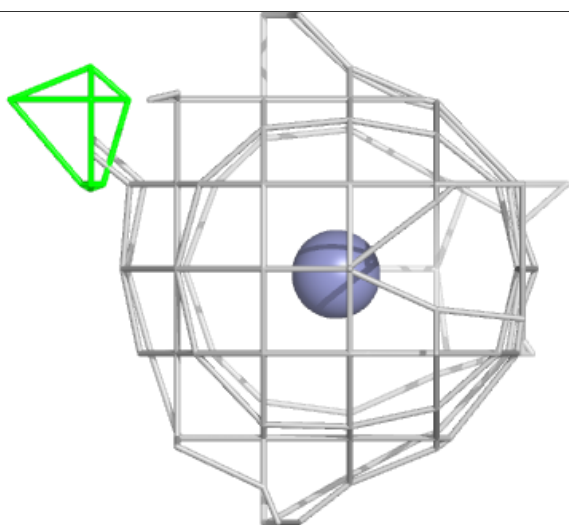
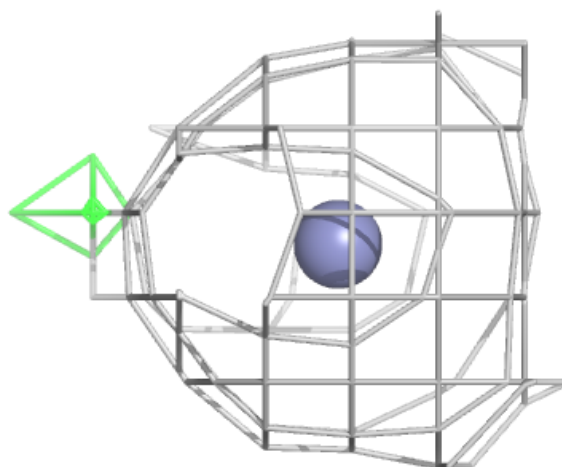
Electron density around ZN B 401:

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



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 [i](#)

There are no such residues in this entry.