W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 10:51 pm BST

PDB ID	:	5ECE
Title	:	Tankyrase 1 with Phthalazinone 1
Authors	:	Kazmirski, S.L.; Johannes, J.; Read, J.A.; Howard, T.; Larsen, N.A.; Ferguson, A.D.
Deposited on	:	2015-10-20
Resolution	:	2.20 Å(reported)

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

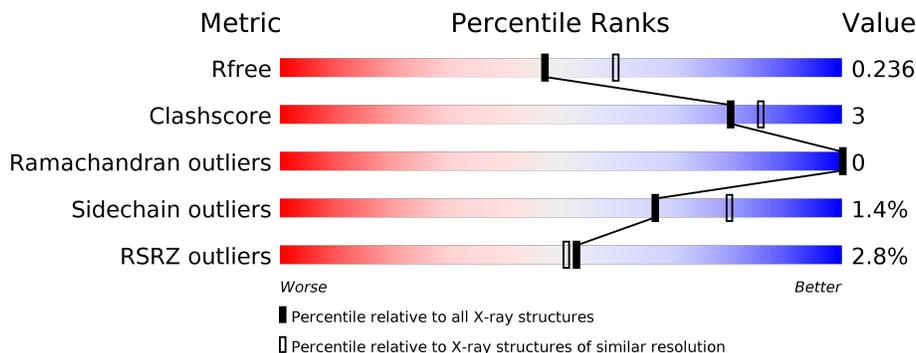|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.4%
RSRZ outliers		2.8%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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 <=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	213	3% — 90% — 7% ··
1	B	213	3% — 87% — 6% — 7%
1	C	213	2% — 90% — 6% — 5%
1	D	213	3% — 89% — 6% — 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7057 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.
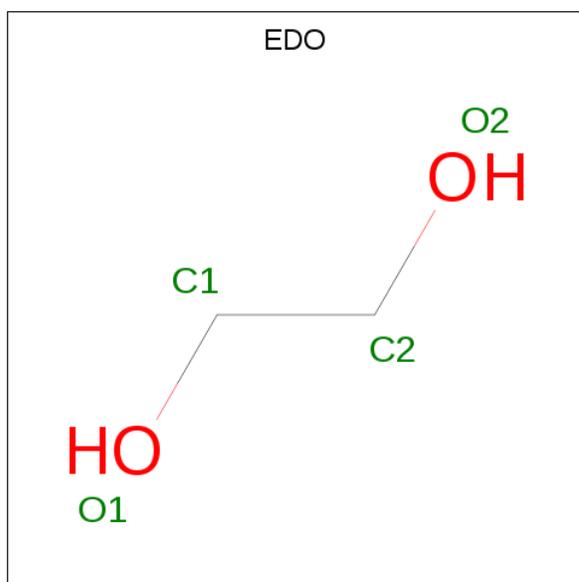
- Molecule 1 is a protein called Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1681	1057	310	304	10			
1	B	199	Total	C	N	O	S	0	0	0
			1612	1013	297	292	10			
1	C	203	Total	C	N	O	S	0	0	0
			1638	1030	301	297	10			
1	D	202	Total	C	N	O	S	0	1	0
			1640	1032	303	295	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1104	ALA	-	expression tag	UNP O95271
A	1266	ILE	MET	conflict	UNP O95271
B	1104	ALA	-	expression tag	UNP O95271
B	1266	ILE	MET	conflict	UNP O95271
C	1104	ALA	-	expression tag	UNP O95271
C	1266	ILE	MET	conflict	UNP O95271
D	1104	ALA	-	expression tag	UNP O95271
D	1266	ILE	MET	conflict	UNP O95271

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

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

- Molecule 3 is 2-[4-[3-[(4-oxidanylidene-3 {H}-phthalazin-1-yl)methyl]phenyl]carbonylpiperazin-1-yl]pyridine-3-carbonitrile (three-letter code: 5N2) (formula: $C_{26}H_{22}N_6O_2$).
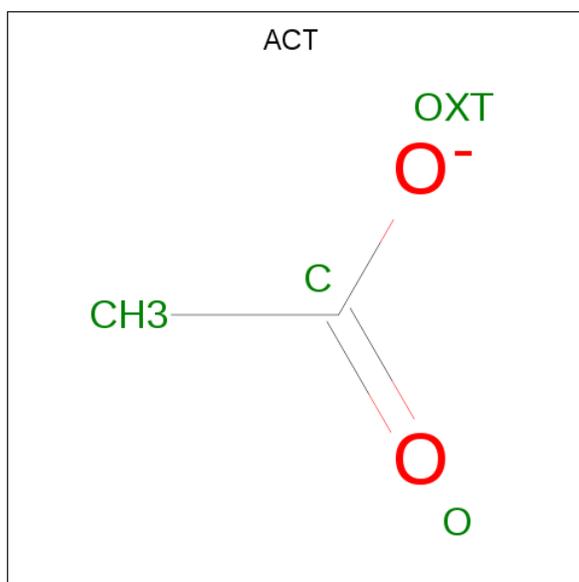
5N2
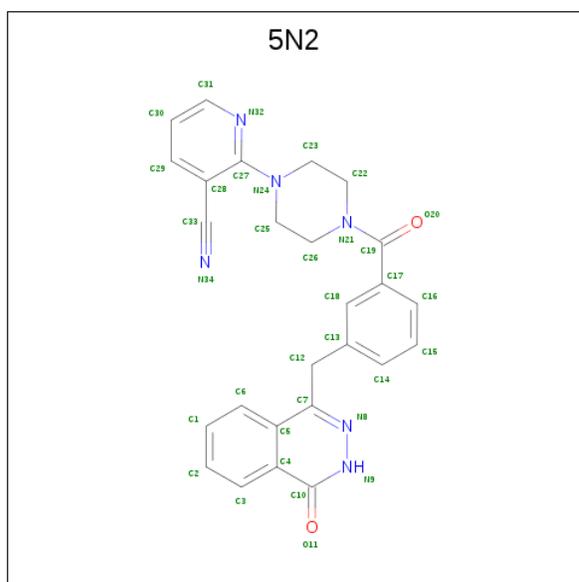
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	26	6	2		
3	B	1	Total	C	N	O	0	0
			34	26	6	2		
3	C	1	Total	C	N	O	0	0
			34	26	6	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total O		0	0
			85	85		
6	B	99	Total O		0	0
			99	99		
6	C	85	Total O		0	0
			85	85		
6	D	79	Total O		0	0
			79	79		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
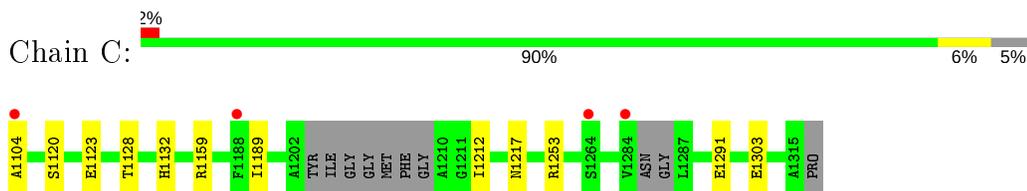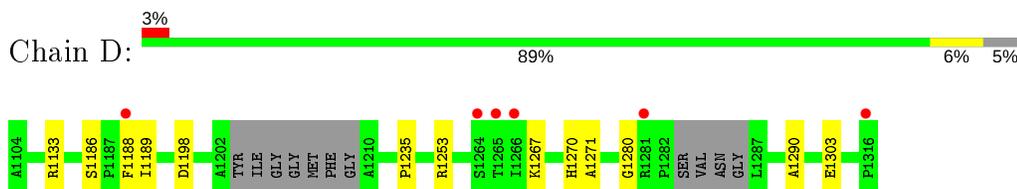
- Molecule 1: Tankyrase-1

Chain A:

- Molecule 1: Tankyrase-1

Chain B:

- Molecule 1: Tankyrase-1

Chain C:

- Molecule 1: Tankyrase-1

Chain D:
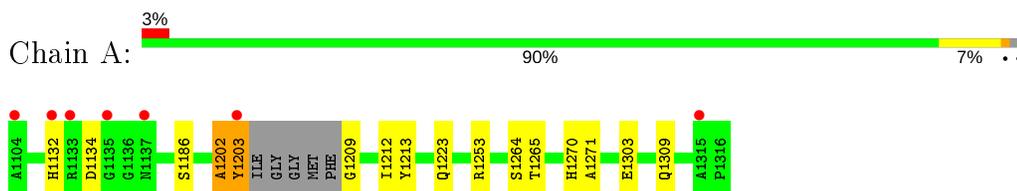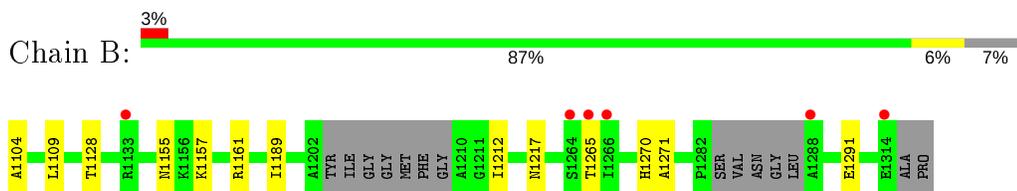
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.97Å 59.98Å 77.19Å 86.21° 78.89° 89.06°	Depositor
Resolution (Å)	44.00 – 2.20 40.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (44.00-2.20) 96.6 (40.39-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$<I/\sigma(I)>$ [1]	2.12 (at 2.20Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.181 , 0.224 0.191 , 0.236	Depositor DCC
R_{free} test set	2366 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.3	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7057	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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, 5N2, EDO, ACT

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	0.53	0/1726	0.69	1/2323 (0.0%)
1	B	0.52	0/1651	0.65	0/2218
1	C	0.56	1/1677 (0.1%)	0.66	0/2254
1	D	0.51	0/1683	0.70	1/2262 (0.0%)
All	All	0.53	1/6737 (0.0%)	0.67	2/9057 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1123	GLU	CD-OE2	6.59	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1202	ALA	C-N-CA	5.55	135.58	121.70
1	D	1133	ARG	C-N-CA	5.07	134.38	121.70

There are no chirality outliers.

There are no planarity outliers.

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	1681	0	1622	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1612	0	1550	9	0
1	C	1638	0	1580	8	0
1	D	1640	0	1586	6	0
2	A	4	0	6	1	0
2	B	8	0	12	0	0
2	C	4	0	6	1	0
2	D	12	0	18	1	0
3	A	34	0	22	3	0
3	B	34	0	22	3	0
3	C	34	0	22	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	4	0	3	1	0
6	A	85	0	0	0	0
6	B	99	0	0	2	0
6	C	85	0	0	1	0
6	D	79	0	0	2	0
All	All	7057	0	6449	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (36) 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)
3:A:1402:5N2:C33	3:A:1402:5N2:H18	2.16	0.76
1:D:1198:ASP:H	2:D:1401:EDO:H11	1.56	0.70
3:C:1403:5N2:C33	3:C:1403:5N2:H18	2.22	0.69
1:A:1132:HIS:CD2	1:A:1223:GLN:HE22	2.16	0.64
3:B:1403:5N2:C33	3:B:1403:5N2:H17	2.29	0.62
1:A:1202:ALA:HA	1:A:1203:TYR:C	2.20	0.62
1:C:1212:ILE:HG23	3:C:1403:5N2:H20	1.87	0.56
1:A:1309:GLN:HE22	2:A:1401:EDO:H12	1.71	0.55
1:D:1235:PRO:HD2	6:D:1542:HOH:O	2.07	0.54
1:A:1132:HIS:CD2	1:A:1134:ASP:HB2	2.44	0.53
1:C:1104:ALA:HB1	6:C:1529:HOH:O	2.09	0.52
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.91	0.52
1:C:1291:GLU:OE1	3:C:1403:5N2:H1	2.10	0.51
1:D:1270:HIS:HD2	1:D:1271:ALA:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1270:HIS:HD2	1:B:1271:ALA:O	1.96	0.49
1:C:1132:HIS:HD1	2:C:1402:EDO:H11	1.79	0.48
3:A:1402:5N2:C33	3:A:1402:5N2:C25	2.91	0.48
1:D:1253:ARG:HG3	1:D:1303:GLU:HG3	1.96	0.48
1:C:1128:THR:HB	1:C:1217:ASN:HA	1.95	0.48
1:B:1212:ILE:HG23	3:B:1403:5N2:H9	1.96	0.47
1:A:1270:HIS:HD2	1:A:1271:ALA:O	1.97	0.47
1:D:1267:LYS:HG2	6:D:1558:HOH:O	2.15	0.47
1:C:1253:ARG:HG3	1:C:1303:GLU:HG3	1.97	0.46
1:A:1253:ARG:HG3	1:A:1303:GLU:HG3	1.97	0.45
1:A:1132:HIS:HD2	1:A:1134:ASP:HB2	1.81	0.45
1:B:1291:GLU:OE1	3:B:1403:5N2:H1	2.16	0.45
1:B:1104:ALA:HB3	1:B:1155:ASN:HD21	1.81	0.45
1:B:1104:ALA:HB1	6:B:1581:HOH:O	2.18	0.44
1:A:1212:ILE:HG23	3:A:1402:5N2:H20	2.00	0.43
1:B:1157:LYS:HD3	1:B:1161:ARG:HH11	1.84	0.42
1:A:1132:HIS:HD2	1:A:1223:GLN:HE22	1.67	0.42
1:C:1120:SER:OG	5:C:1401:ACT:H2	2.19	0.42
1:B:1270:HIS:HB3	6:B:1586:HOH:O	2.20	0.42
1:A:1209:GLY:N	1:A:1213:TYR:HH	2.17	0.41
1:D:1280:GLY:O	1:D:1290:ALA:HA	2.21	0.41
1:B:1109:LEU:HD22	1:C:1159:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/213 (96%)	204 (100%)	1 (0%)	0	100	100
1	B	193/213 (91%)	190 (98%)	3 (2%)	0	100	100
1	C	197/213 (92%)	195 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	197/213 (92%)	193 (98%)	4 (2%)	0	100	100
All	All	792/852 (93%)	782 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	177/179 (99%)	173 (98%)	4 (2%)	50	63
1	B	170/179 (95%)	168 (99%)	2 (1%)	71	83
1	C	173/179 (97%)	172 (99%)	1 (1%)	86	93
1	D	173/179 (97%)	170 (98%)	3 (2%)	60	74
All	All	693/716 (97%)	683 (99%)	10 (1%)	67	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1186	SER
1	A	1203	TYR
1	A	1264	SER
1	A	1265	THR
1	B	1189	ILE
1	B	1265	THR
1	C	1189	ILE
1	D	1186	SER
1	D	1188	PHE
1	D	1189	ILE

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

Mol	Chain	Res	Type
1	A	1132	HIS

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Mol	Chain	Res	Type
1	A	1270	HIS
1	B	1178	ASN
1	B	1262	GLN
1	B	1270	HIS
1	D	1270	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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 Counts	Bond lengths RMSZ	Bond lengths #$|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles #$|Z| > 2$
3	5N2	A	1402	-	36,38,38	1.16	3 (8%)	43,53,53	1.65	2 (4%)
2	EDO	D	1403	-	3,3,3	0.60	0	2,2,2	0.23	0
5	ACT	C	1401	-	1,3,3	5.06	1 (100%)	0,3,3	0.00	-
2	EDO	D	1401	-	3,3,3	0.59	0	2,2,2	0.39	0
2	EDO	D	1402	-	3,3,3	0.50	0	2,2,2	0.70	0
2	EDO	B	1402	-	3,3,3	0.78	0	2,2,2	0.12	0
2	EDO	B	1401	-	3,3,3	0.65	0	2,2,2	0.22	0
2	EDO	A	1401	-	3,3,3	0.71	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	5N2	C	1403	-	36,38,38	1.12	3 (8%)	43,53,53	1.53	3 (6%)
3	5N2	B	1403	-	36,38,38	1.19	4 (11%)	43,53,53	1.57	3 (6%)
2	EDO	C	1402	-	3,3,3	0.62	0	2,2,2	0.07	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
3	5N2	A	1402	-	-	0/17/28/28	0/5/5/5
2	EDO	D	1403	-	-	0/1/1/1	-
2	EDO	D	1401	-	-	0/1/1/1	-
2	EDO	D	1402	-	-	0/1/1/1	-
2	EDO	B	1402	-	-	0/1/1/1	-
2	EDO	B	1401	-	-	1/1/1/1	-
2	EDO	A	1401	-	-	0/1/1/1	-
3	5N2	C	1403	-	-	0/17/28/28	0/5/5/5
3	5N2	B	1403	-	-	0/17/28/28	0/5/5/5
2	EDO	C	1402	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	ACT	CH3-C	5.06	1.55	1.48
3	B	1403	5N2	C7-C5	4.75	1.48	1.43
3	A	1402	5N2	C7-C5	4.74	1.48	1.43
3	C	1403	5N2	C7-C5	4.53	1.48	1.43
3	B	1403	5N2	N9-N8	3.33	1.42	1.34
3	C	1403	5N2	N9-N8	3.02	1.42	1.34
3	A	1402	5N2	N9-N8	2.94	1.41	1.34
3	A	1402	5N2	C7-N8	-2.26	1.29	1.32
3	C	1403	5N2	C7-N8	-2.26	1.29	1.32
3	B	1403	5N2	C7-N8	-2.22	1.29	1.32
3	B	1403	5N2	C27-N24	2.13	1.43	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	5N2	C10-N9-N8	8.62	127.24	119.32
3	C	1403	5N2	C10-N9-N8	8.42	127.05	119.32
3	B	1403	5N2	C10-N9-N8	8.18	126.83	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	5N2	C28-C27-N24	-3.38	119.41	124.11
3	B	1403	5N2	C28-C27-N24	-2.82	120.19	124.11
3	C	1403	5N2	C25-N24-C27	2.31	127.10	119.05
3	B	1403	5N2	C18-C17-C19	-2.23	115.17	120.14
3	C	1403	5N2	C28-C27-N24	-2.11	121.17	124.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1402	EDO	O1-C1-C2-O2
2	B	1401	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	5N2	3	0
5	C	1401	ACT	1	0
2	D	1401	EDO	1	0
2	A	1401	EDO	1	0
3	C	1403	5N2	3	0
3	B	1403	5N2	3	0
2	C	1402	EDO	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 5N2 A 1402

Bond lengths

Bond angles

Torsions

Rings

Ligand 5N2 C 1403

Bond lengths

Bond angles

Torsions

Rings

Ligand 5N2 B 1403

Bond lengths

Bond angles

Torsions

Rings
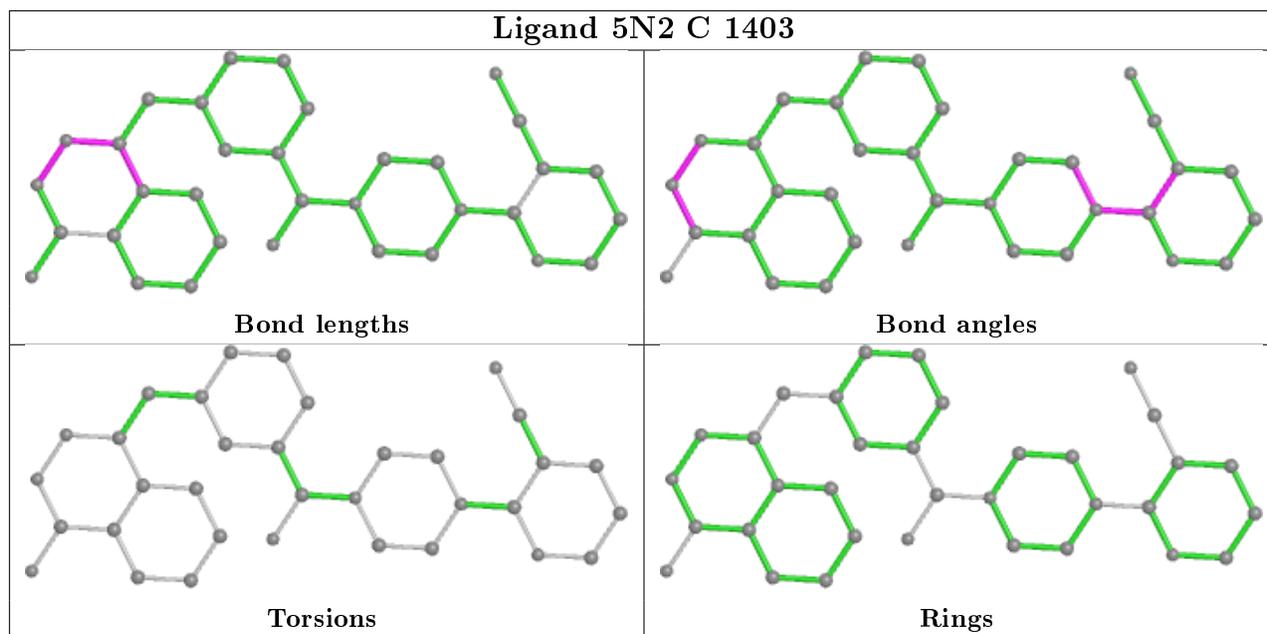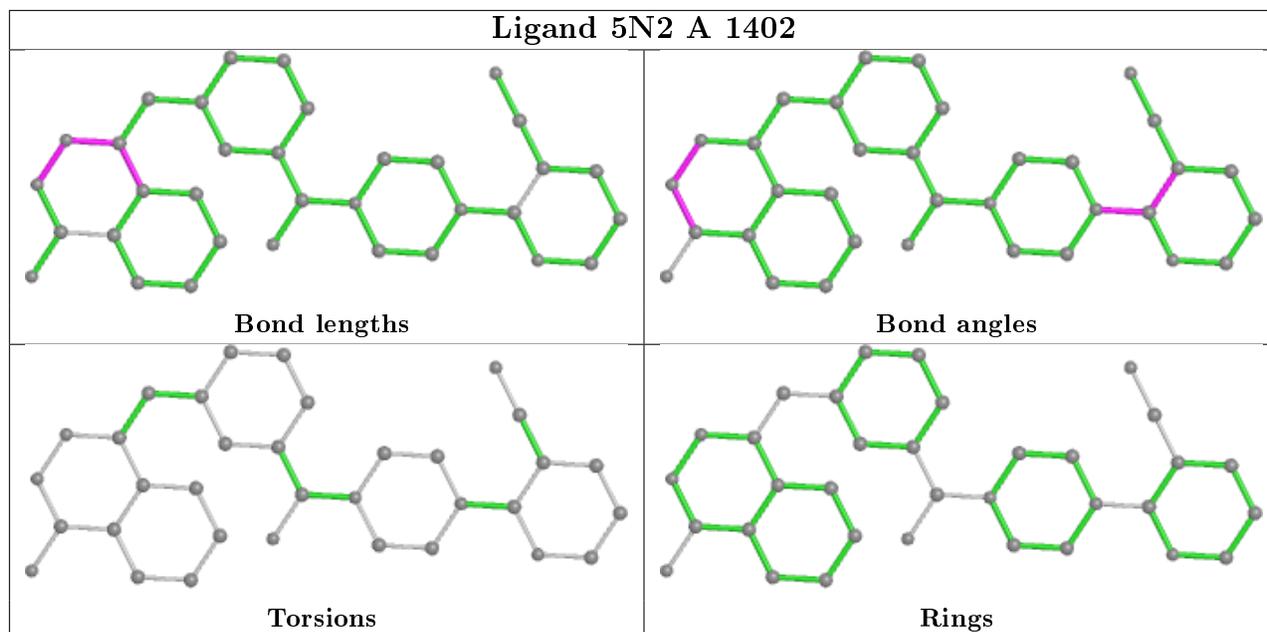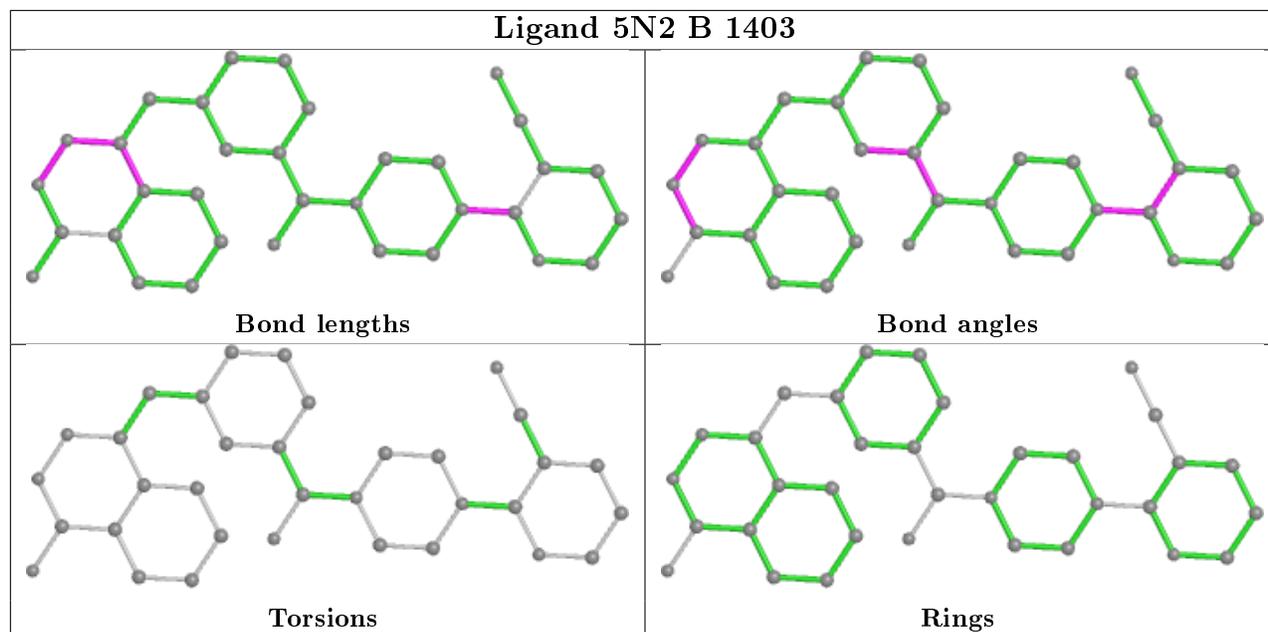
5.7 Other polymers (i)

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	208/213 (97%)	-0.01	7 (3%)	45	43	21, 33, 64, 94	0
1	B	199/213 (93%)	0.02	6 (3%)	50	48	20, 32, 68, 95	0
1	C	203/213 (95%)	-0.03	4 (1%)	65	63	19, 31, 60, 77	0
1	D	202/213 (94%)	0.08	6 (2%)	50	48	21, 35, 70, 93	0
All	All	812/852 (95%)	0.01	23 (2%)	53	51	19, 33, 67, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1266	ILE	7.0
1	B	1266	ILE	6.6
1	B	1265	THR	6.0
1	B	1264	SER	4.8
1	A	1203	TYR	4.5
1	D	1265	THR	4.5
1	B	1133	ARG	3.7
1	D	1316	PRO	3.3
1	C	1264	SER	3.3
1	D	1188	PHE	3.2
1	A	1315	ALA	3.1
1	B	1314	GLU	2.9
1	A	1104	ALA	2.7
1	A	1135	GLY	2.7
1	A	1137	ASN	2.6
1	A	1133	ARG	2.4
1	B	1288	ALA	2.4
1	C	1284	VAL	2.3
1	D	1264	SER	2.3
1	A	1132	HIS	2.2
1	C	1188	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1104	ALA	2.1
1	D	1281	ARG	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 carbohydrates 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.

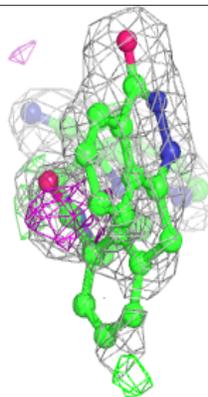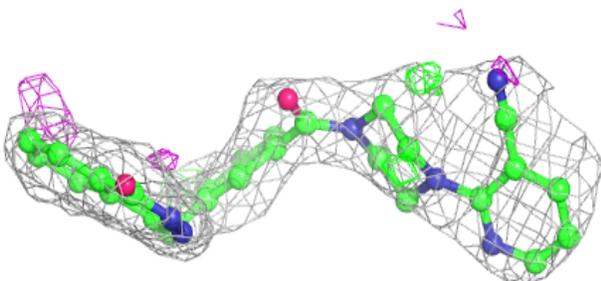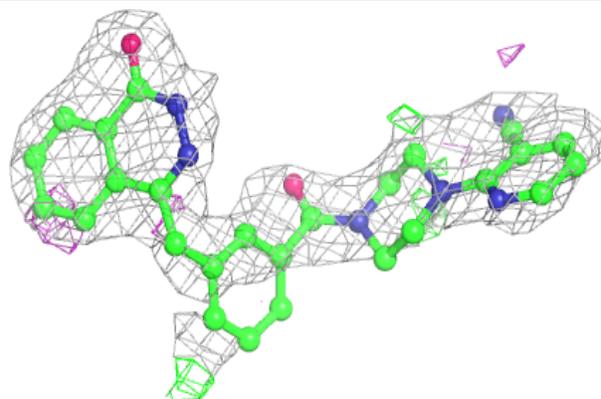| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	5N2	C	1403	34/34	0.69	0.35	46,81,89,90	0
2	EDO	A	1401	4/4	0.81	0.15	51,51,51,52	0
3	5N2	B	1403	34/34	0.81	0.29	35,59,69,73	0
2	EDO	D	1401	4/4	0.85	0.15	41,42,44,48	0
2	EDO	D	1403	4/4	0.85	0.22	57,57,58,60	0
2	EDO	B	1401	4/4	0.87	0.12	53,54,55,55	0
3	5N2	A	1402	34/34	0.89	0.20	32,43,53,54	0
2	EDO	B	1402	4/4	0.90	0.12	46,48,49,50	0
2	EDO	D	1402	4/4	0.92	0.14	34,38,41,44	0
5	ACT	C	1401	4/4	0.93	0.23	52,53,55,56	0
2	EDO	C	1402	4/4	0.97	0.16	23,25,29,32	0
4	ZN	C	1404	1/1	0.99	0.06	29,29,29,29	0
4	ZN	D	1404	1/1	0.99	0.07	33,33,33,33	0
4	ZN	A	1403	1/1	0.99	0.08	32,32,32,32	0
4	ZN	B	1404	1/1	1.00	0.09	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
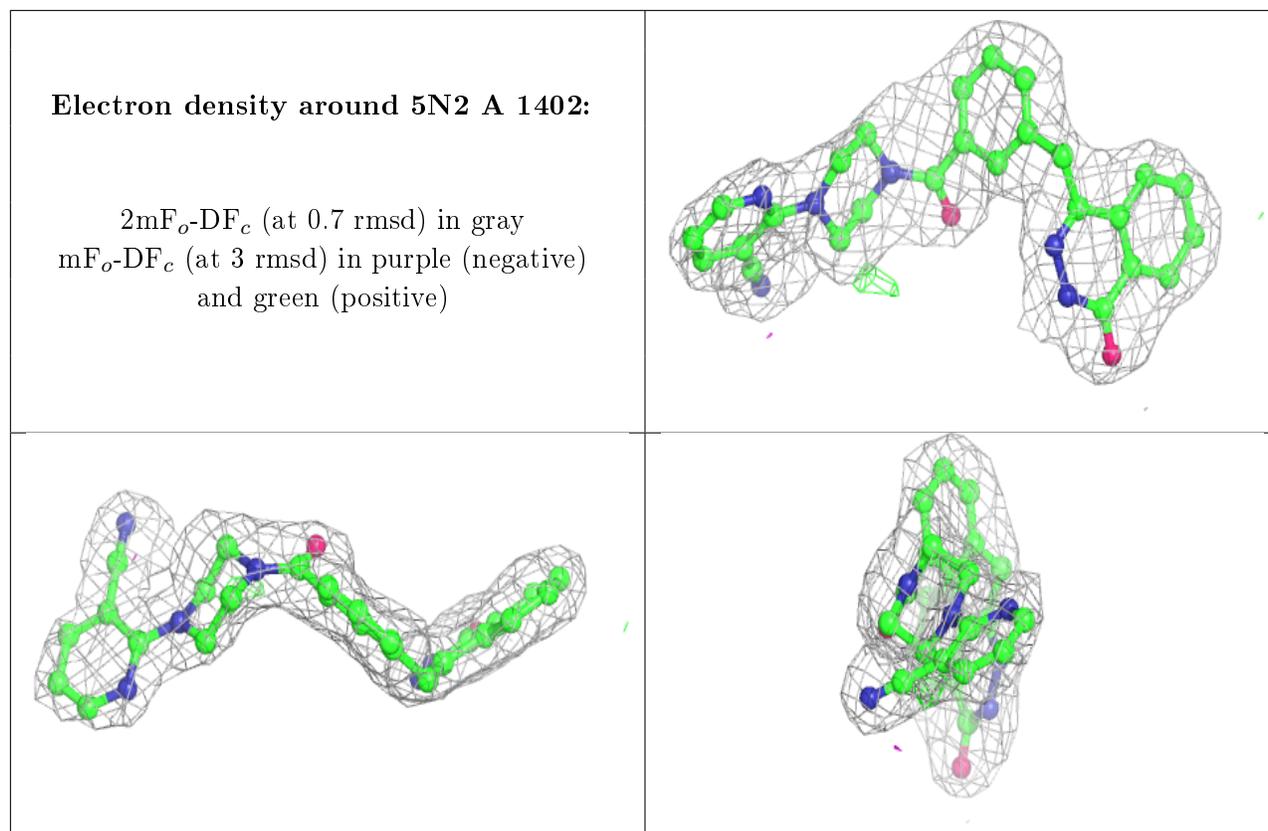
Electron density around 5N2 C 1403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
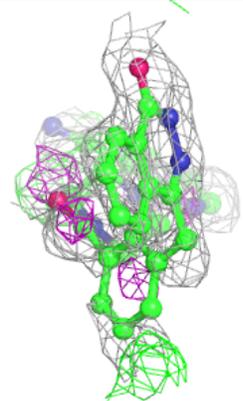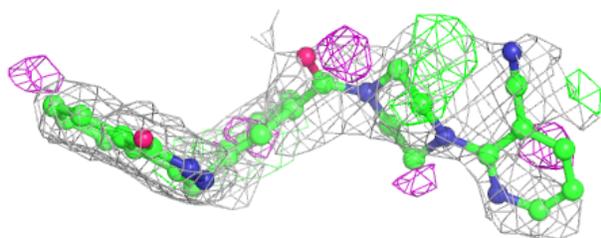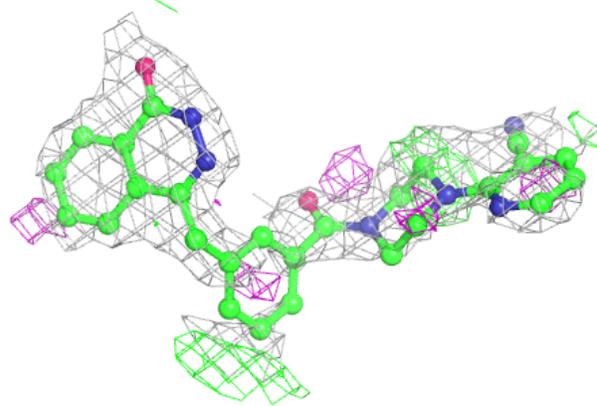
Electron density around 5N2 B 1403:

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 5N2 A 1402:

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.