WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 10, 2020 – 09:03 PM GMT

PDB ID	:	6TU6
Title	:	Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole
Authors	:	Bloch, J.S.; Hilvert, D.
Deposited on	:	2020-01-02
Resolution	:	1.05 Å(reported)

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

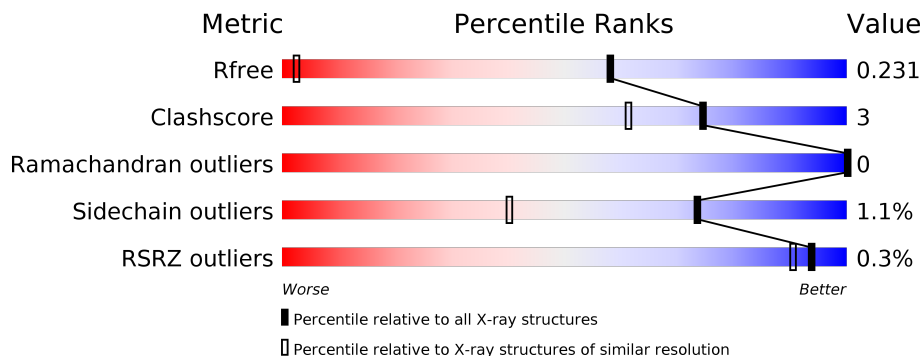|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.05 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		0.231
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		0.3%

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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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	317	89% 6% 5%
1	B	317	87% 7% 5%
1	C	317	88% 6% 5%
1	D	317	90% • 5%
1	E	317	89% 5% 5%
1	F	317	89% 5% 5%

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| Mol	Chain	Length	Quality of chain
1	G	317	87% · · · 7% · 5%
1	H	317	88% · · · 6% · 5%
1	I	317	87% · · · 8% · 5%
1	J	317	90% · · · 5% · 5%
1	K	317	89% · · · 5% · 5%
1	L	317	91% · · · · · 5%
1	M	317	90% · · · 5% · 5%
1	N	317	84% · · · 10% · 5%
1	O	317	88% · · · 7% · 5%
1	P	317	89% · · · 6% · 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 84548 atoms, of which 38676 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 Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total 4859	C 1547	H 2413	N 420	O 465	S 14	0	40	0
1	B	300	Total 4861	C 1544	H 2416	N 426	O 461	S 14	0	40	1
1	C	300	Total 4847	C 1541	H 2410	N 423	O 460	S 13	0	38	1
1	D	300	Total 4806	C 1527	H 2390	N 418	O 458	S 13	0	35	1
1	E	300	Total 4833	C 1539	H 2403	N 417	O 461	S 13	0	40	1
1	F	300	Total 4827	C 1539	H 2395	N 416	O 462	S 15	0	39	0
1	G	300	Total 4772	C 1521	H 2371	N 411	O 456	S 13	0	32	1
1	H	301	Total 4877	C 1550	H 2426	N 420	O 466	S 15	0	42	0
1	I	300	Total 4856	C 1543	H 2418	N 418	O 464	S 13	0	40	0
1	J	300	Total 4832	C 1537	H 2405	N 415	O 460	S 15	0	38	0
1	K	300	Total 4884	C 1551	H 2427	N 423	O 469	S 14	0	45	0
1	L	300	Total 4806	C 1529	H 2388	N 416	O 459	S 14	0	36	0
1	M	300	Total 4864	C 1543	H 2420	N 423	O 465	S 13	0	43	1
1	N	300	Total 4871	C 1546	H 2423	N 422	O 466	S 14	0	43	0
1	O	301	Total 4908	C 1558	H 2445	N 422	O 468	S 15	0	46	0
1	P	300	Total 4948	C 1568	H 2462	N 433	O 472	S 13	0	50	1

• Molecule 2 is 6-NITROBENZOTRIAZOLE (three-letter code: 6NT) (formula: $C_6H_4N_4O_2$) (labeled as "Ligand of Interest" by author).
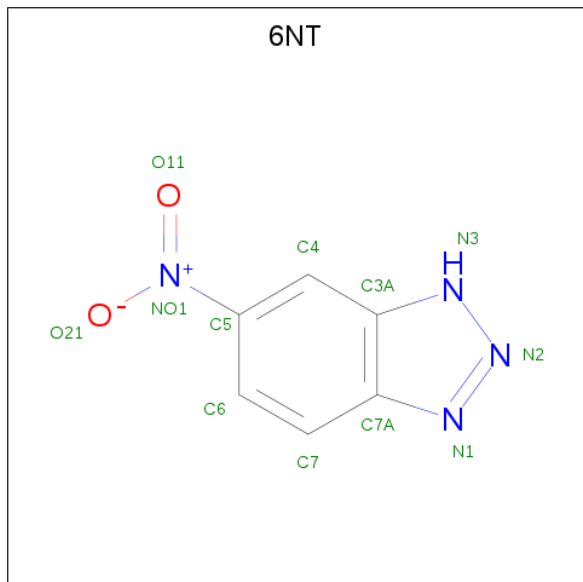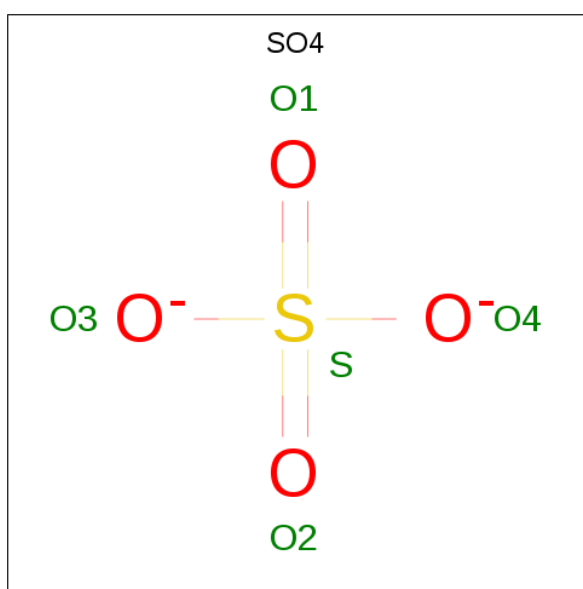

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	B	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	C	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	D	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	E	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	F	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	G	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	H	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	I	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	J	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	K	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	L	1	Total 16	C 6	H 4	N 4	O 2	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	N	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	O	1	Total 16	C 6	H 4	N 4	O 2	0	1
2	P	1	Total 16	C 6	H 4	N 4	O 2	0	1

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	H	1	Total 5	O 4	S 1	0	0
3	H	1	Total 5	O 4	S 1	0	0
3	I	1	Total 5	O 4	S 1	0	0
3	I	1	Total 5	O 4	S 1	0	0
3	J	1	Total 5	O 4	S 1	0	0
3	L	1	Total 5	O 4	S 1	0	0
3	M	1	Total 5	O 4	S 1	0	0
3	M	1	Total 5	O 4	S 1	0	0
3	N	1	Total 5	O 4	S 1	0	0
3	N	1	Total 5	O 4	S 1	0	0
3	O	1	Total 5	O 4	S 1	0	0
3	P	1	Total 5	O 4	S 1	0	0
3	P	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	458	Total 459	O 459	0	2
4	B	439	Total 439	O 439	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	432	Total 434	O 434	0	2
4	D	406	Total 407	O 407	0	2
4	E	443	Total 445	O 445	0	2
4	F	394	Total 394	O 394	0	0
4	G	390	Total 390	O 390	0	0
4	H	390	Total 390	O 390	0	0
4	I	378	Total 378	O 378	0	0
4	J	376	Total 376	O 376	0	0
4	K	374	Total 374	O 374	0	0
4	L	409	Total 409	O 409	0	0
4	M	463	Total 464	O 464	0	2
4	N	371	Total 372	O 372	0	1
4	O	372	Total 372	O 372	0	0
4	P	416	Total 418	O 418	0	2

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
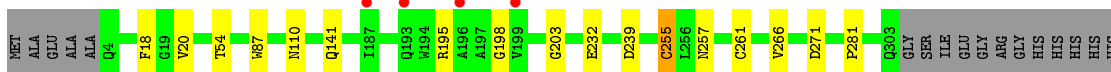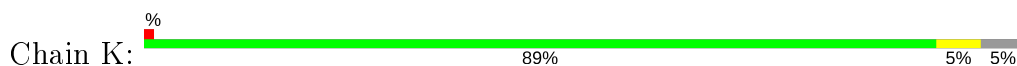
• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain A:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain B:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole
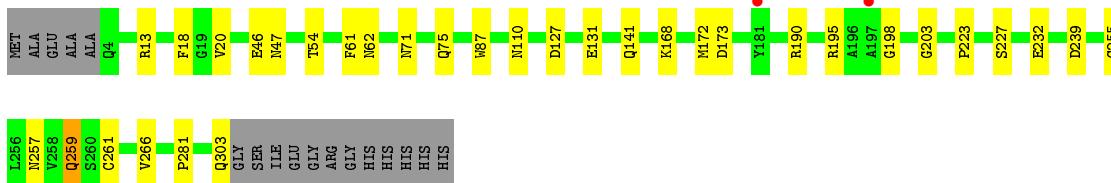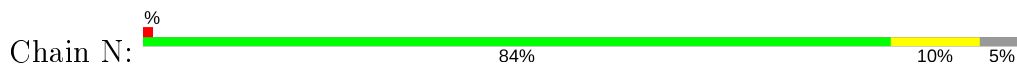
Chain C:
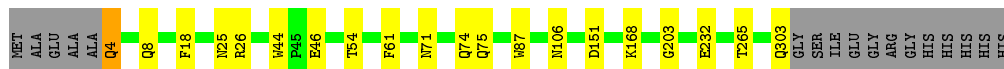
• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole
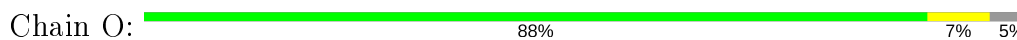
Chain D:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain E:

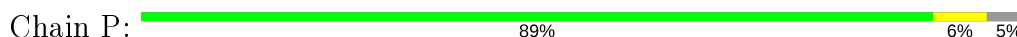• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain F:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain G:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain H:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain I:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain J:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain K:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain L:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain M:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain N:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain O:

• Molecule 1: Kemp Eliminase HG3.17 mutant Q50M, E47N, N300D Complexed with Transition State Analog 6-Nitrobenzotriazole

Chain P:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	98.37Å 108.69Å 108.72Å 88.53° 90.16° 89.82°	Depositor
Resolution (Å)	49.18 – 1.05 49.18 – 1.05	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.18-1.05) 94.1 (49.18-1.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.196 , 0.231 0.196 , 0.231	Depositor DCC
R_{free} test set	1975 reflections (0.10%)	wwPDB-VP
Wilson B-factor (Å^2)	8.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 45.9	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.022 for h,-l,k 0.022 for h,l,-k 0.477 for h,-k,-l 0.022 for -h,k,-l 0.023 for -h,-k,l 0.477 for -h,-l,-k 0.479 for -h,l,k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	84548	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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 94.85 % 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 2.1339e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6NT, 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	0.38	0/2637	0.64	0/3596
1	B	0.39	0/2625	0.65	0/3578
1	C	0.38	0/2606	0.63	0/3553
1	D	0.38	0/2565	0.64	0/3495
1	E	0.39	0/2606	0.64	0/3553
1	F	0.40	0/2602	0.64	0/3547
1	G	0.42	2/2547 (0.1%)	0.63	0/3473
1	H	0.42	2/2627 (0.1%)	0.64	0/3583
1	I	0.39	0/2621	0.62	0/3574
1	J	0.42	2/2599 (0.1%)	0.63	0/3543
1	K	0.42	2/2666 (0.1%)	0.63	0/3635
1	L	0.39	0/2578	0.63	0/3514
1	M	0.41	1/2626 (0.0%)	0.64	0/3579
1	N	0.40	0/2639	0.62	0/3597
1	O	0.42	2/2658 (0.1%)	0.63	0/3624
1	P	0.38	0/2701	0.62	0/3681
All	All	0.40	11/41903 (0.0%)	0.63	0/57125

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	50[A]	MET	CG-SD	6.72	1.98	1.81
1	K	255[A]	CYS	CB-SG	6.44	1.93	1.82
1	K	255[B]	CYS	CB-SG	6.44	1.93	1.82
1	H	261[A]	CYS	CB-SG	6.43	1.93	1.82
1	H	261[B]	CYS	CB-SG	6.43	1.93	1.82

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	2446	2413	2252	20	0
1	B	2445	2416	2254	18	0
1	C	2437	2410	2267	15	0
1	D	2416	2390	2260	12	0
1	E	2430	2403	2250	12	0
1	F	2432	2395	2240	14	0
1	G	2401	2371	2241	17	0
1	H	2451	2426	2266	15	0
1	I	2438	2418	2260	20	0
1	J	2427	2405	2250	13	0
1	K	2457	2427	2252	14	0
1	L	2418	2388	2251	9	0
1	M	2444	2420	2260	11	0
1	N	2448	2423	2262	23	0
1	O	2463	2445	2262	19	0
1	P	2486	2462	2271	14	0
2	A	12	4	4	0	0
2	B	12	4	4	0	0
2	C	12	4	4	0	0
2	D	12	4	4	0	0
2	E	12	4	4	0	0
2	F	12	4	4	0	0
2	G	12	4	4	0	0
2	H	12	4	4	0	0
2	I	12	4	4	0	0
2	J	12	4	4	0	0
2	K	12	4	4	0	0
2	L	12	4	4	0	0
2	M	12	4	4	0	0
2	N	12	4	4	0	0
2	O	12	4	4	0	0
2	P	12	4	4	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	15	0	0	1	0
3	D	15	0	0	1	0
3	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	5	0	0	0	0
3	H	10	0	0	0	0
3	I	10	0	0	1	0
3	J	5	0	0	0	0
3	L	5	0	0	0	0
3	M	10	0	0	1	0
3	N	10	0	0	1	0
3	O	5	0	0	0	0
3	P	10	0	0	1	0
4	A	459	0	0	13	4
4	B	439	0	0	10	3
4	C	434	0	0	10	2
4	D	407	0	0	10	5
4	E	445	0	0	8	3
4	F	394	0	0	3	5
4	G	390	0	0	12	3
4	H	390	0	0	10	1
4	I	378	0	0	15	3
4	J	376	0	0	4	3
4	K	374	0	0	9	4
4	L	409	0	0	6	6
4	M	464	0	0	9	2
4	N	372	0	0	16	1
4	O	372	0	0	5	1
4	P	418	0	0	8	2
All	All	45872	38676	36162	249	24

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.

The worst 5 of 249 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:I:193:GLN:O	4:I:501:HOH:O	1.52	1.20
1:K:195:ARG:O	4:K:501:HOH:O	1.72	1.03
1:H:110[A]:ASN:ND2	4:H:503:HOH:O	1.88	1.03
1:I:110[A]:ASN:ND2	4:I:503:HOH:O	1.92	1.02
1:G:195:ARG:O	4:G:501:HOH:O	1.75	1.01

The worst 5 of 24 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)
4:K:502:HOH:O	4:P:662:HOH:O[1_665]	1.97	0.23
4:F:658:HOH:O	4:L:690:HOH:O[1_556]	2.01	0.19
4:F:558:HOH:O	4:L:806:HOH:O[1_556]	2.01	0.19
4:B:771:HOH:O	4:M:813:HOH:O[1_655]	2.02	0.18
4:C:792:HOH:O	4:G:702:HOH:O[1_545]	2.02	0.18

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/317 (105%)	326 (98%)	8 (2%)	0	100	100
1	B	334/317 (105%)	329 (98%)	5 (2%)	0	100	100
1	C	332/317 (105%)	327 (98%)	5 (2%)	0	100	100
1	D	329/317 (104%)	324 (98%)	5 (2%)	0	100	100
1	E	334/317 (105%)	329 (98%)	5 (2%)	0	100	100
1	F	333/317 (105%)	329 (99%)	4 (1%)	0	100	100
1	G	326/317 (103%)	321 (98%)	5 (2%)	0	100	100
1	H	337/317 (106%)	332 (98%)	5 (2%)	0	100	100
1	I	334/317 (105%)	330 (99%)	4 (1%)	0	100	100
1	J	332/317 (105%)	327 (98%)	5 (2%)	0	100	100
1	K	339/317 (107%)	334 (98%)	5 (2%)	0	100	100
1	L	330/317 (104%)	327 (99%)	3 (1%)	0	100	100
1	M	335/317 (106%)	330 (98%)	5 (2%)	0	100	100
1	N	337/317 (106%)	332 (98%)	5 (2%)	0	100	100
1	O	339/317 (107%)	334 (98%)	5 (2%)	0	100	100
1	P	344/317 (108%)	339 (98%)	5 (2%)	0	100	100
All	All	5349/5072 (106%)	5270 (98%)	79 (2%)	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	275/254 (108%)	273 (99%)	2 (1%)	84	57
1	B	274/254 (108%)	271 (99%)	3 (1%)	73	40
1	C	271/254 (107%)	268 (99%)	3 (1%)	73	40
1	D	269/254 (106%)	267 (99%)	2 (1%)	84	57
1	E	273/254 (108%)	271 (99%)	2 (1%)	84	57
1	F	273/254 (108%)	271 (99%)	2 (1%)	84	57
1	G	266/254 (105%)	260 (98%)	6 (2%)	50	13
1	H	276/254 (109%)	271 (98%)	5 (2%)	59	21
1	I	275/254 (108%)	271 (98%)	4 (2%)	65	26
1	J	273/254 (108%)	271 (99%)	2 (1%)	84	57
1	K	280/254 (110%)	278 (99%)	2 (1%)	84	57
1	L	270/254 (106%)	268 (99%)	2 (1%)	84	57
1	M	275/254 (108%)	273 (99%)	2 (1%)	84	57
1	N	276/254 (109%)	270 (98%)	6 (2%)	52	14
1	O	279/254 (110%)	277 (99%)	2 (1%)	84	57
1	P	283/254 (111%)	281 (99%)	2 (1%)	84	57
All	All	4388/4064 (108%)	4341 (99%)	47 (1%)	73	40

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	62	ASN
1	I	62	ASN
1	O	18	PHE
1	H	185[A]	GLN
1	I	87	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

40 ligands are modelled in this entry.

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	$\#|Z| > 2$
2	6NT	F	401[B]	-	8,13,13	1.17	0	10,18,18	1.76	2 (20%)
3	SO4	E	403	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	O	402	-	4,4,4	0.14	0	6,6,6	0.08	0
2	6NT	K	401[B]	-	8,13,13	1.24	1 (12%)	10,18,18	2.17	1 (10%)
2	6NT	N	401[B]	-	8,13,13	1.24	1 (12%)	10,18,18	1.96	1 (10%)
3	SO4	C	404	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	I	403	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	N	403	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	C	403	-	4,4,4	0.13	0	6,6,6	0.08	0
2	6NT	P	401[B]	-	8,13,13	1.26	0	10,18,18	1.41	1 (10%)
3	SO4	H	402	-	4,4,4	0.15	0	6,6,6	0.34	0
3	SO4	D	404	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	E	402	-	4,4,4	0.16	0	6,6,6	0.20	0
2	6NT	A	401[B]	-	8,13,13	1.35	0	10,18,18	1.49	1 (10%)
3	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	J	402	-	4,4,4	0.14	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|>2$	Counts	RMSZ	#$|Z|>2$
3	SO4	N	402	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	A	402	-	4,4,4	0.15	0	6,6,6	0.16	0
2	6NT	M	401[B]	-	8,13,13	1.11	0	10,18,18	1.63	1 (10%)
2	6NT	H	401[B]	-	8,13,13	1.20	0	10,18,18	1.97	2 (20%)
3	SO4	F	402	-	4,4,4	0.14	0	6,6,6	0.32	0
3	SO4	M	402	-	4,4,4	0.17	0	6,6,6	0.32	0
3	SO4	M	403	-	4,4,4	0.16	0	6,6,6	0.24	0
2	6NT	G	401[B]	-	8,13,13	1.28	1 (12%)	10,18,18	1.84	1 (10%)
3	SO4	H	403	-	4,4,4	0.16	0	6,6,6	0.17	0
2	6NT	J	401[B]	-	8,13,13	1.22	0	10,18,18	1.63	1 (10%)
3	SO4	P	402	-	4,4,4	0.15	0	6,6,6	0.15	0
2	6NT	O	401[B]	-	8,13,13	1.27	0	10,18,18	1.81	1 (10%)
3	SO4	I	402	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	L	402	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	B	402	-	4,4,4	0.13	0	6,6,6	0.12	0
2	6NT	B	401[B]	-	8,13,13	1.12	0	10,18,18	1.44	1 (10%)
3	SO4	D	403	-	4,4,4	0.16	0	6,6,6	0.19	0
3	SO4	P	403	-	4,4,4	0.15	0	6,6,6	0.12	0
2	6NT	E	401[B]	-	8,13,13	1.47	1 (12%)	10,18,18	1.50	1 (10%)
2	6NT	I	401[B]	-	8,13,13	1.26	0	10,18,18	1.97	2 (20%)
2	6NT	D	401[B]	-	8,13,13	1.23	0	10,18,18	1.56	1 (10%)
2	6NT	L	401[B]	-	8,13,13	1.22	0	10,18,18	1.67	1 (10%)
3	SO4	D	402	-	4,4,4	0.17	0	6,6,6	0.36	0
2	6NT	C	401[B]	-	8,13,13	1.24	0	10,18,18	1.52	1 (10%)

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
2	6NT	F	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	G	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	J	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	K	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	A	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	N	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	O	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	E	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	I	401[B]	-	-	0/2/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6NT	D	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	M	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	H	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	L	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	B	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	C	401[B]	-	-	0/2/4/4	0/2/2/2
2	6NT	P	401[B]	-	-	0/2/4/4	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401[B]	6NT	C7-C7A	-2.36	1.37	1.41
2	K	401[B]	6NT	C5-NO1	-2.12	1.40	1.45
2	G	401[B]	6NT	C5-NO1	-2.01	1.40	1.45
2	N	401[B]	6NT	C5-NO1	-2.01	1.40	1.45

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401[B]	6NT	N3-N2-N1	-6.22	103.18	111.25
2	N	401[B]	6NT	N3-N2-N1	-5.64	103.93	111.25
2	G	401[B]	6NT	N3-N2-N1	-5.44	104.19	111.25
2	I	401[B]	6NT	N3-N2-N1	-5.20	104.50	111.25
2	L	401[B]	6NT	N3-N2-N1	-4.65	105.22	111.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	SO4	1	0
3	N	402	SO4	1	0
3	A	402	SO4	1	0
3	M	403	SO4	1	0
3	I	402	SO4	1	0
3	P	403	SO4	1	0
3	D	402	SO4	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 6NT F 401 (B)

Ligand 6NT K 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT N 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT P 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT A 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT M 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT H 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT G 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT J 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT O 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT B 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT E 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT I 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT D 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT L 401 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NT C 401 (B)

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(Å²)	Q<0.9
1	A	300/317 (94%)	-0.29	0	100	100	5, 10, 18, 36	0
1	B	300/317 (94%)	-0.27	0	100	100	5, 10, 18, 34	0
1	C	300/317 (94%)	-0.27	0	100	100	5, 10, 18, 34	0
1	D	300/317 (94%)	-0.29	0	100	100	5, 10, 19, 35	0
1	E	300/317 (94%)	-0.31	0	100	100	5, 10, 18, 31	0
1	F	300/317 (94%)	-0.08	1 (0%)	94	90	7, 10, 18, 37	0
1	G	300/317 (94%)	0.01	3 (1%)	82	77	7, 11, 20, 32	0
1	H	301/317 (94%)	-0.07	2 (0%)	87	84	7, 10, 18, 38	0
1	I	300/317 (94%)	-0.04	2 (0%)	87	84	6, 11, 20, 38	0
1	J	300/317 (94%)	-0.09	0	100	100	6, 10, 18, 36	0
1	K	300/317 (94%)	0.01	4 (1%)	77	71	7, 11, 20, 40	0
1	L	300/317 (94%)	-0.28	0	100	100	5, 10, 19, 34	0
1	M	300/317 (94%)	-0.30	0	100	100	5, 10, 18, 33	0
1	N	300/317 (94%)	-0.00	2 (0%)	87	84	7, 11, 19, 46	0
1	O	301/317 (94%)	-0.05	1 (0%)	94	90	7, 10, 18, 37	1 (0%)
1	P	300/317 (94%)	-0.28	0	100	100	5, 10, 17, 31	0
All	All	4802/5072 (94%)	-0.16	15 (0%)	94	90	5, 10, 19, 46	1 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	199	VAL	3.4
1	H	3	ALA	3.1
1	I	197	ALA	3.0
1	K	193[A]	GLN	2.9
1	N	197	ALA	2.8

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	SO4	H	403	5/5	0.69	0.15	41,42,61,89	0
3	SO4	N	403	5/5	0.77	0.15	42,60,69,94	0
3	SO4	C	404	5/5	0.82	0.19	37,39,65,76	0
3	SO4	O	402	5/5	0.85	0.21	49,59,71,96	0
3	SO4	D	403	5/5	0.85	0.19	66,69,76,78	0
3	SO4	E	402	5/5	0.87	0.14	28,38,57,61	0
3	SO4	E	403	5/5	0.88	0.23	30,42,68,69	0
3	SO4	B	402	5/5	0.89	0.14	36,46,63,84	0
3	SO4	D	404	5/5	0.90	0.12	56,57,69,76	0
3	SO4	J	402	5/5	0.91	0.19	39,49,72,84	0
3	SO4	P	402	5/5	0.91	0.12	25,30,70,87	0
3	SO4	P	403	5/5	0.91	0.10	33,52,73,80	0
3	SO4	L	402	5/5	0.92	0.20	30,41,78,79	0
3	SO4	C	402	5/5	0.92	0.14	51,51,51,51	0
3	SO4	I	403	5/5	0.93	0.18	34,44,82,85	0
3	SO4	C	403	5/5	0.93	0.10	27,35,64,79	0
3	SO4	M	403	5/5	0.93	0.10	25,43,74,76	0
3	SO4	A	402	5/5	0.94	0.10	42,42,42,42	0
3	SO4	I	402	5/5	0.94	0.10	47,47,47,47	0
3	SO4	N	402	5/5	0.95	0.09	44,44,45,45	0
3	SO4	F	402	5/5	0.95	0.12	34,34,35,35	0
3	SO4	D	402	5/5	0.95	0.11	30,30,31,31	0
3	SO4	M	402	5/5	0.96	0.09	29,30,31,31	0
3	SO4	H	402	5/5	0.96	0.11	30,31,31,31	0
2	6NT	H	401[B]	12/12	0.97	0.06	10,11,12,12	0
2	6NT	J	401[B]	12/12	0.97	0.08	10,11,12,12	0
2	6NT	N	401[B]	12/12	0.97	0.08	10,11,12,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6NT	O	401[B]	12/12	0.97	0.07	9,10,11,12	0
2	6NT	I	401[B]	12/12	0.97	0.08	11,12,13,13	0
2	6NT	G	401[B]	12/12	0.97	0.07	10,11,12,13	0
2	6NT	A	401[B]	12/12	0.98	0.07	6,7,8,8	0
2	6NT	F	401[B]	12/12	0.98	0.06	10,11,12,12	0
2	6NT	K	401[B]	12/12	0.98	0.06	10,12,12,14	0
2	6NT	C	401[B]	12/12	0.98	0.05	7,8,8,9	0
2	6NT	E	401[B]	12/12	0.99	0.05	6,7,8,8	0
2	6NT	B	401[B]	12/12	0.99	0.05	7,7,8,9	0
2	6NT	D	401[B]	12/12	0.99	0.05	7,8,8,9	0
2	6NT	L	401[B]	12/12	0.99	0.05	7,8,9,9	0
2	6NT	P	401[B]	12/12	0.99	0.04	7,8,8,9	0
2	6NT	M	401[B]	12/12	0.99	0.05	6,7,8,9	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.
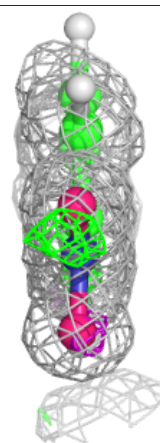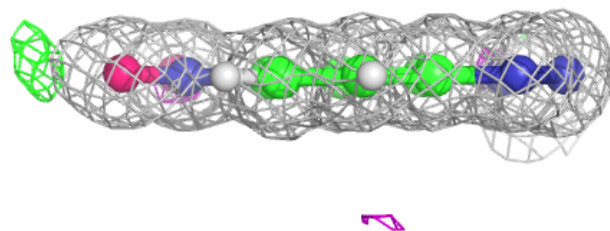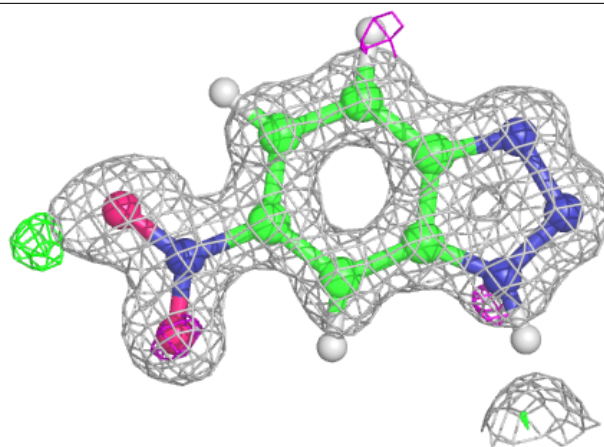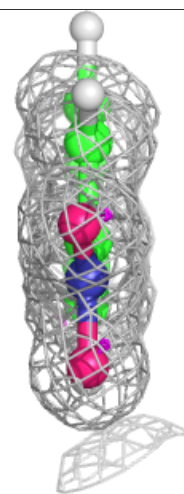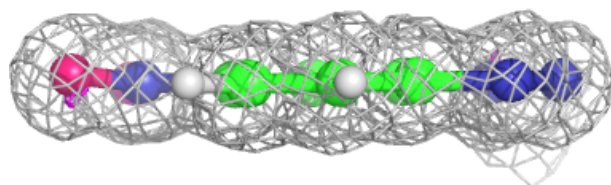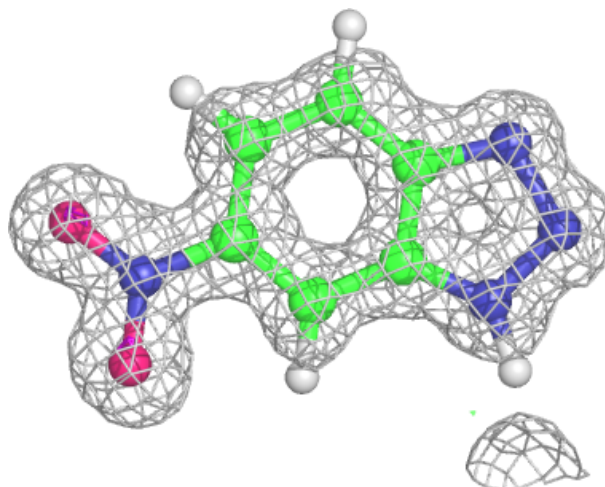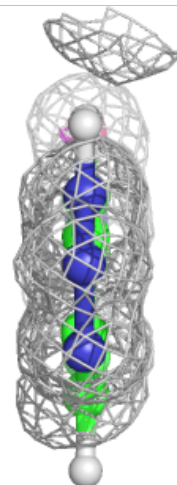
Electron density around 6NT H 401 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
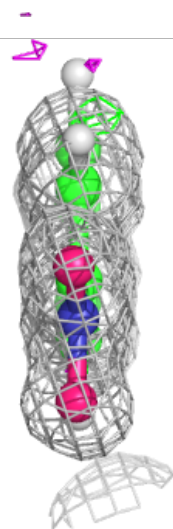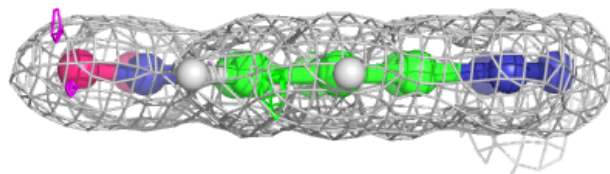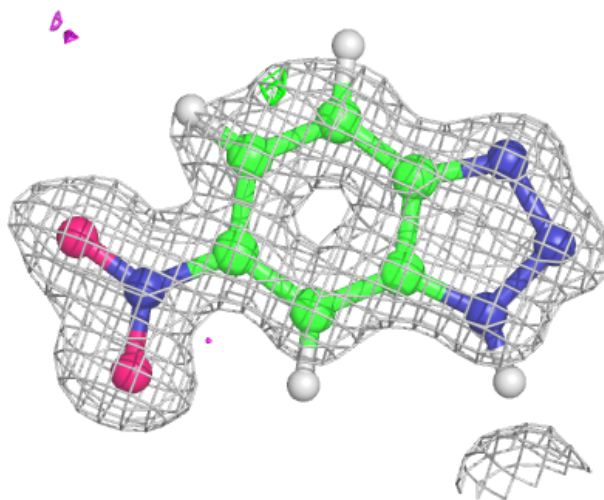
Electron density around 6NT J 401 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
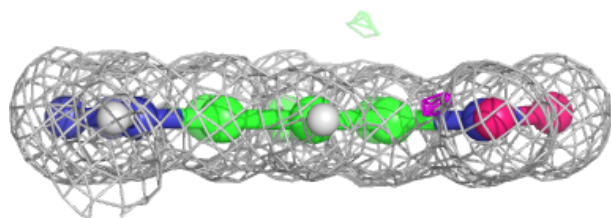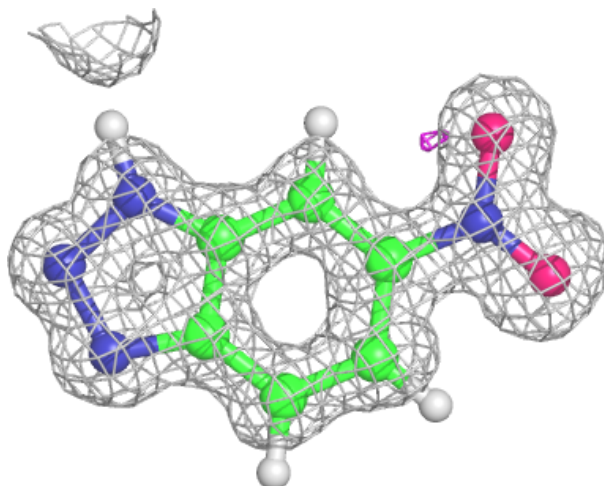and green (positive)
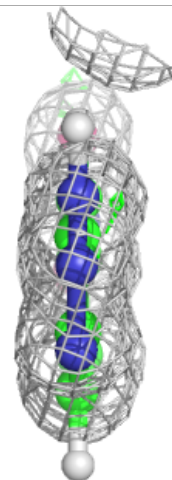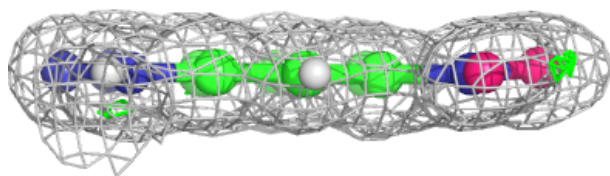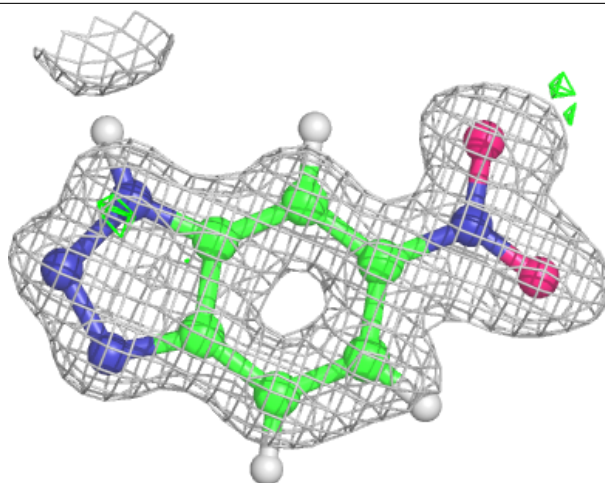
Electron density around 6NT N 401 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
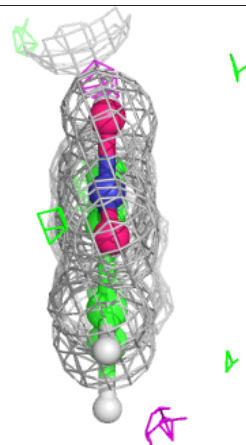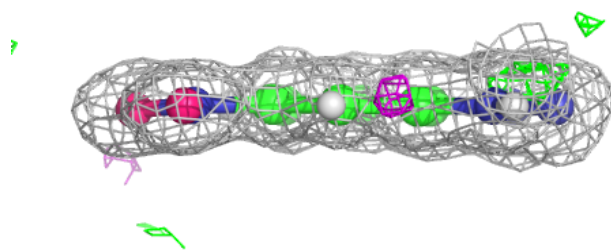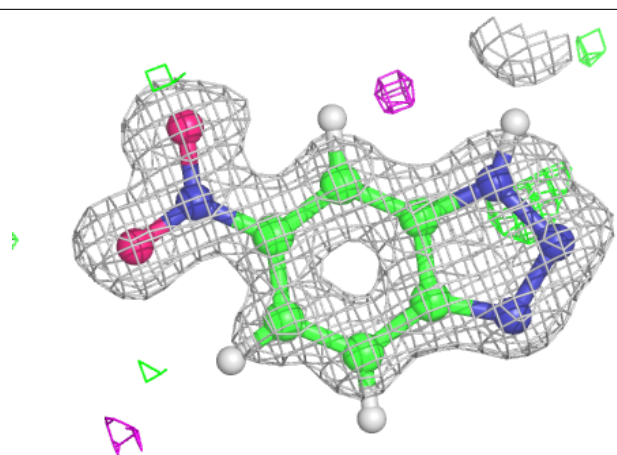
Electron density around 6NT O 401 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
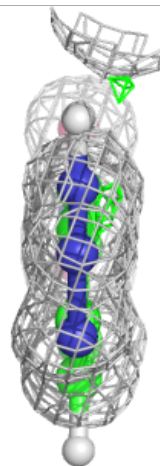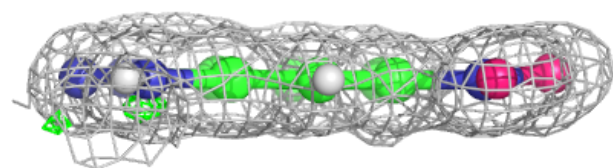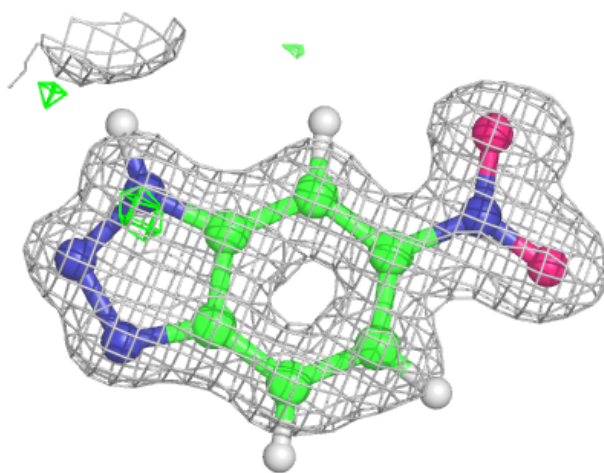
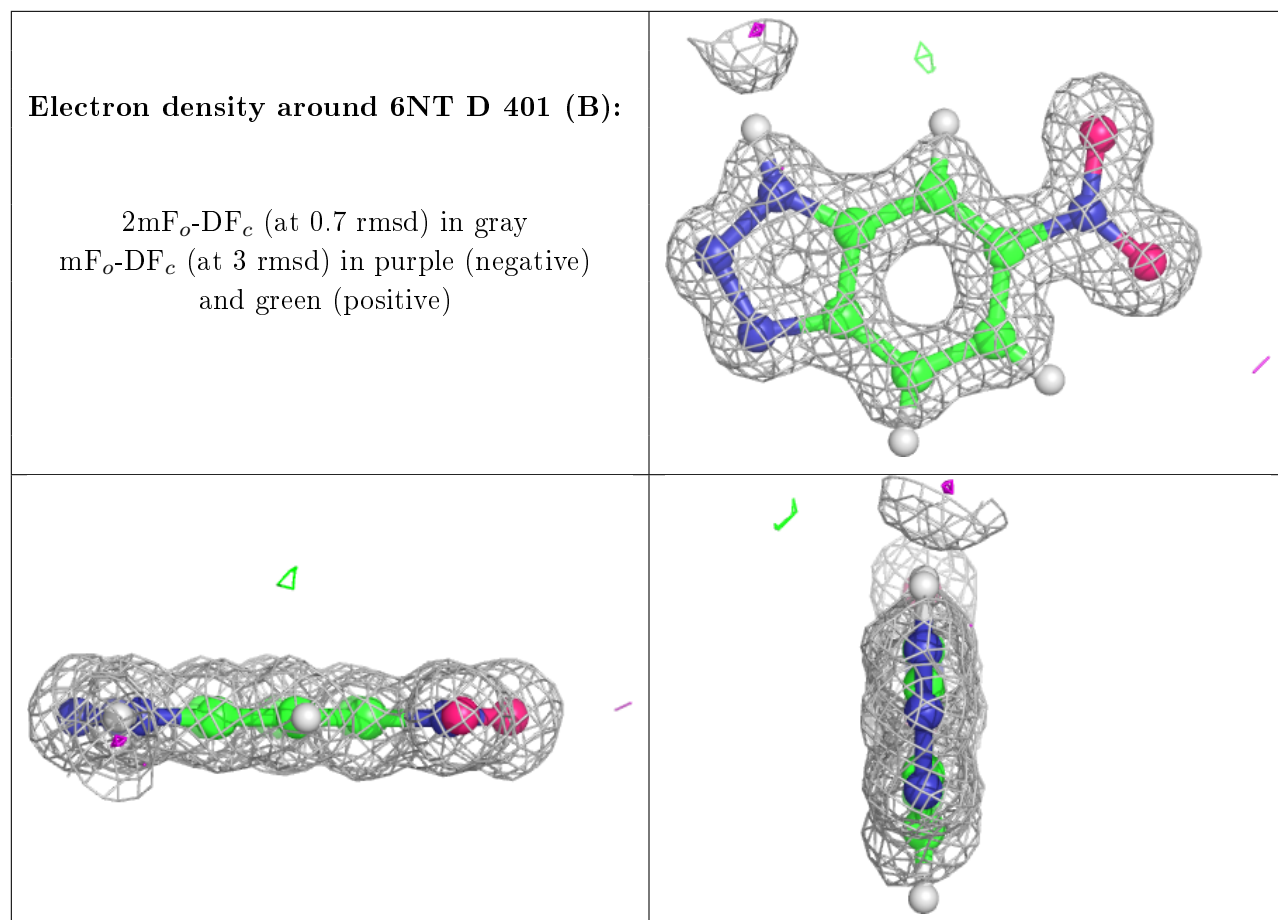**Electron density around 6NT I 401 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
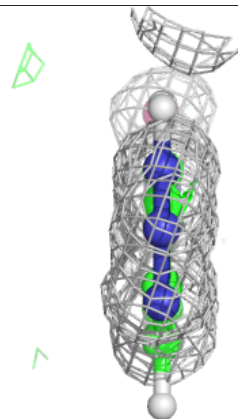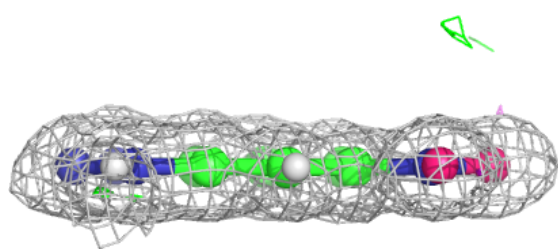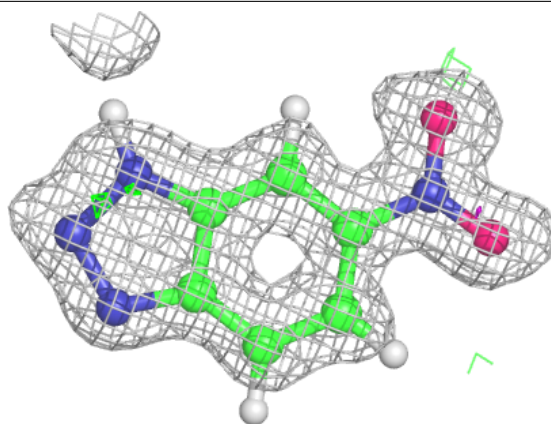
Electron density around 6NT G 401 (B):

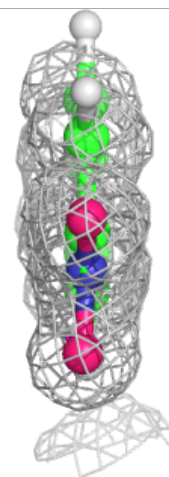$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
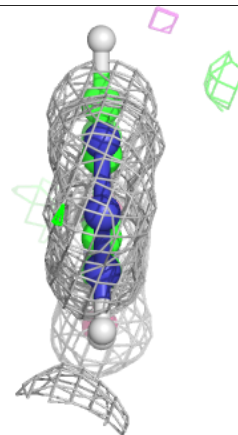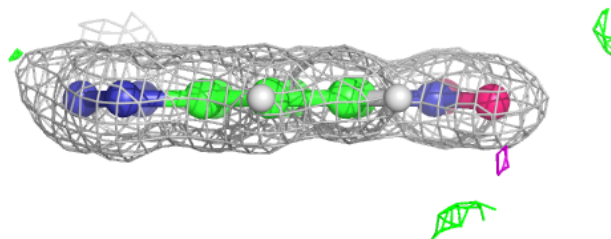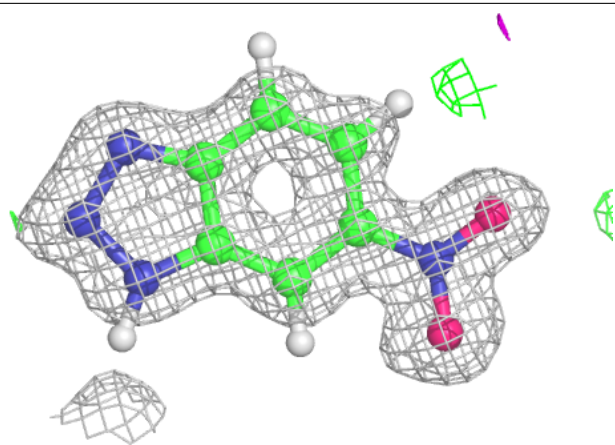
Electron density around 6NT A 401 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
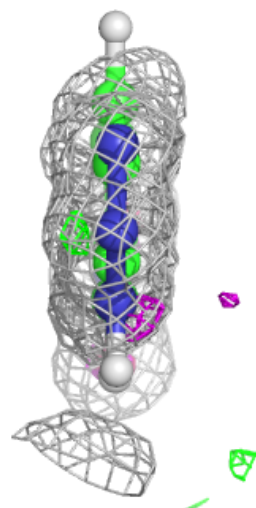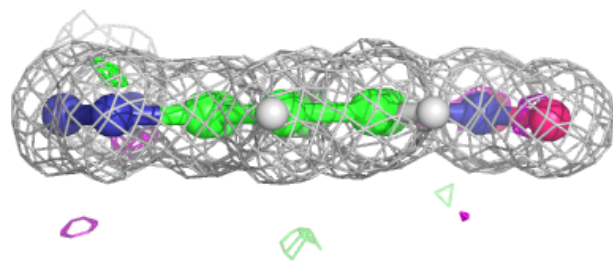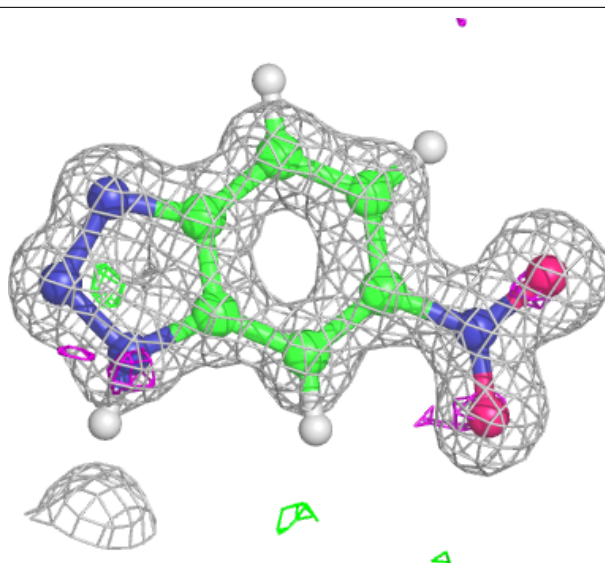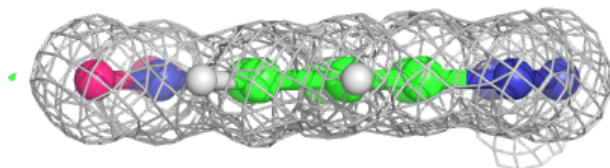
Electron density around 6NT F 401 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
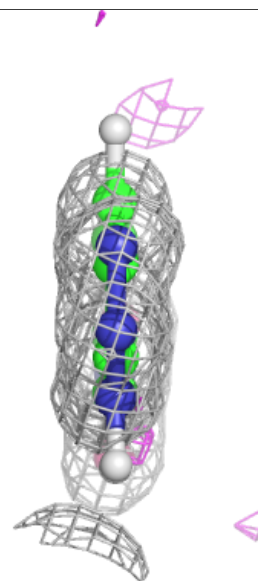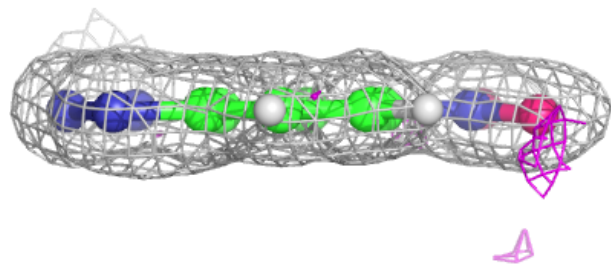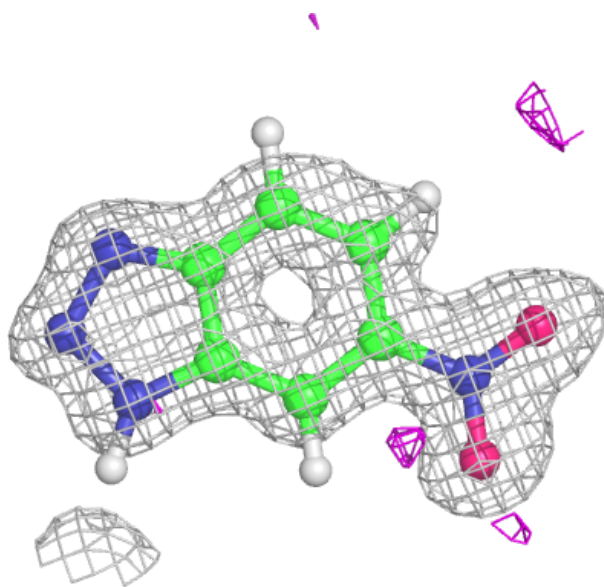
Electron density around 6NT K 401 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
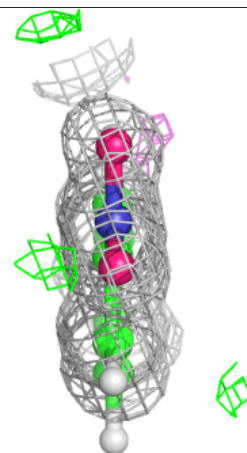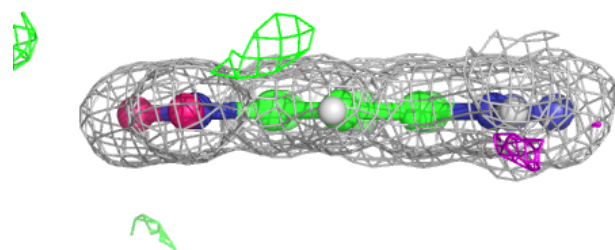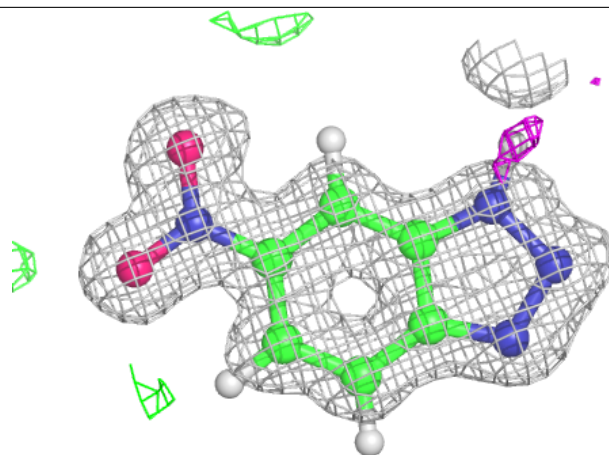
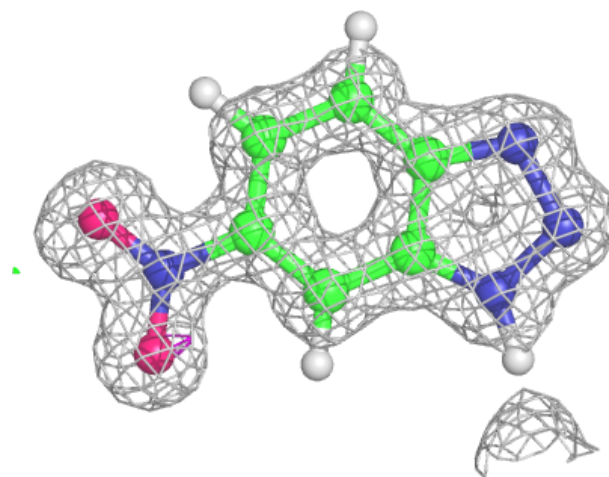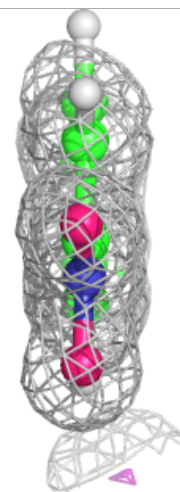**Electron density around 6NT C 401 (B):**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
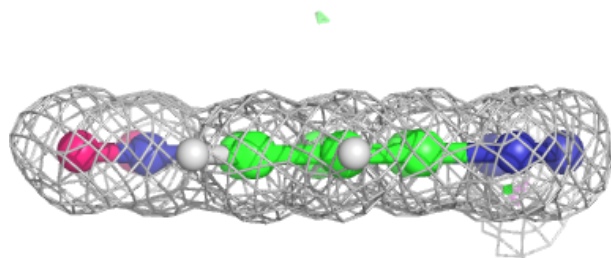
Electron density around 6NT E 401 (B):

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

Electron density around 6NT B 401 (B):

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

Electron density around 6NT D 401 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
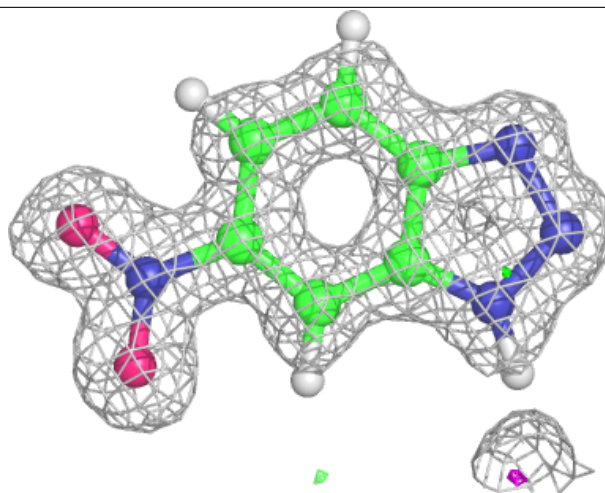$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
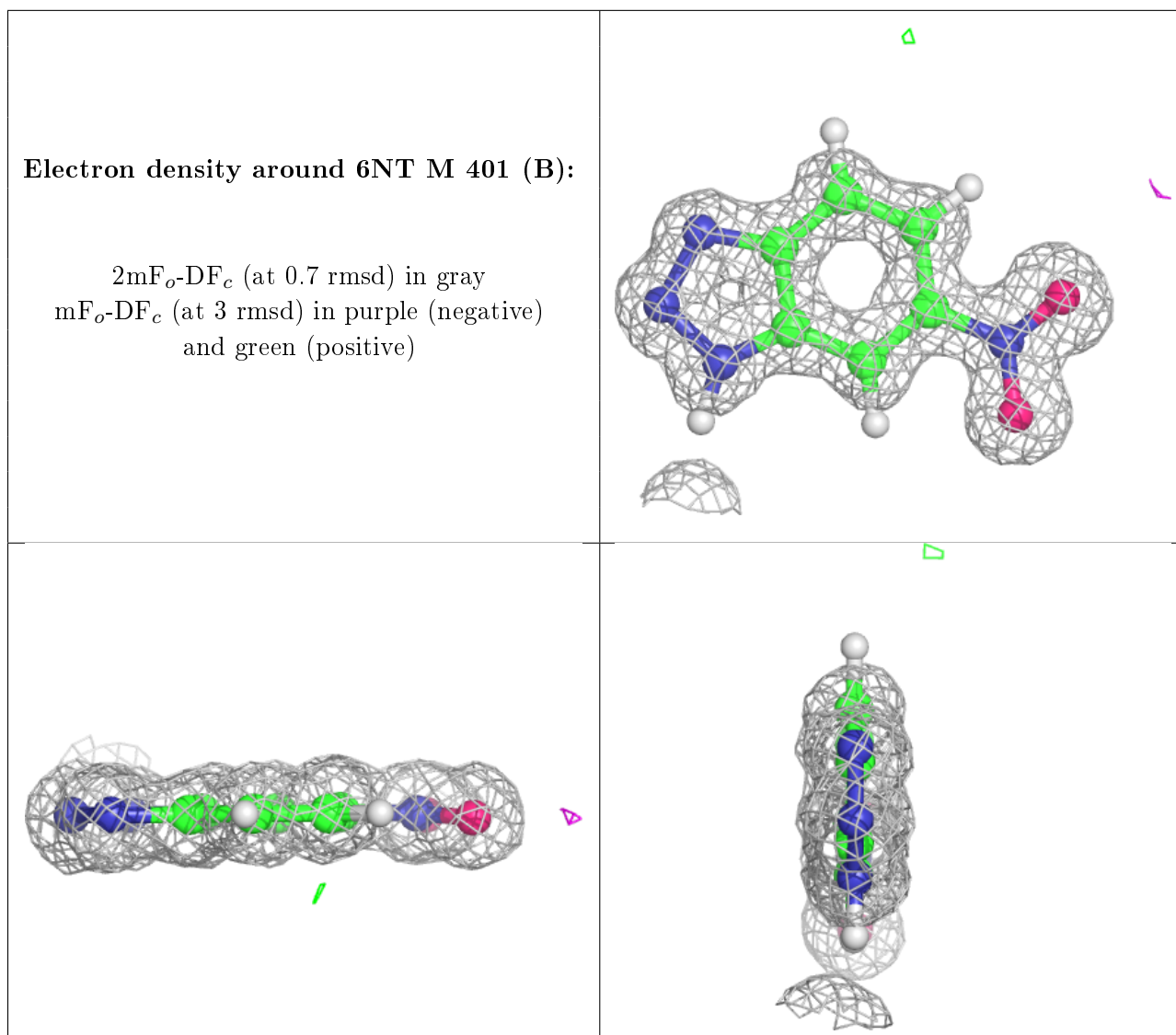
Electron density around 6NT L 401 (B):

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

Electron density around 6NT P 401 (B):

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

Electron density around 6NT M 401 (B):

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

6.5 Other polymers ⓘ

There are no such residues in this entry.