Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2026 – 06:08 pm GMT

PDB ID	:	32SH / pdb_000032sh
Title	:	Crystal structure of YTHDF2 in complex with compound 4 (FE-462)
Authors	:	Nai, F.; Errani, F.; Caflisch, A.
Deposited on	:	2026-07-22
Resolution	:	1.61 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 (i) 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 (i)) were used in the production of this report:

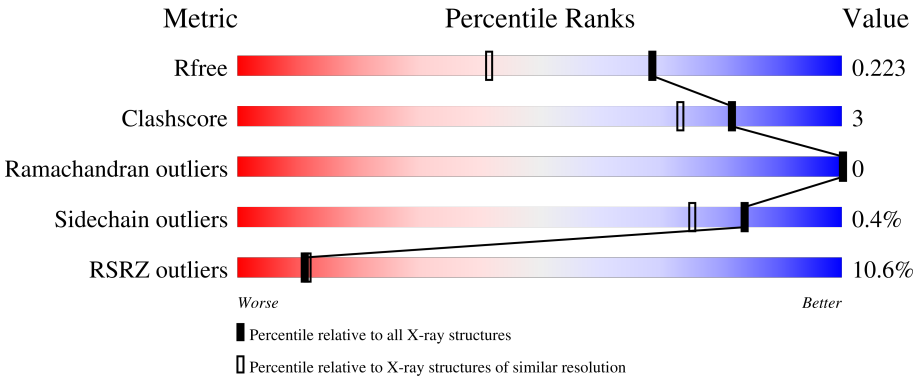
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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 <=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	167	9% 84% 6% 10%
1	B	167	10% 87% · 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	603	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2692 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 YTH domain-containing family protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	5	0
			1233	779	222	227	5			
1	B	150	Total	C	N	O	S	0	1	0
			1179	753	205	215	6			

There are 44 discrepancies between the modelled and reference sequences:

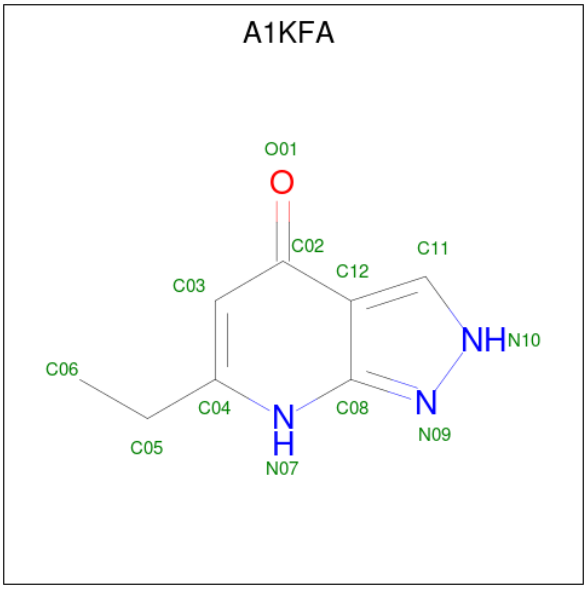
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	initiating methionine	UNP Q9Y5A9
A	387	GLY	-	expression tag	UNP Q9Y5A9
A	388	SER	-	expression tag	UNP Q9Y5A9
A	389	SER	-	expression tag	UNP Q9Y5A9
A	390	TYR	-	expression tag	UNP Q9Y5A9
A	391	HIS	-	expression tag	UNP Q9Y5A9
A	392	HIS	-	expression tag	UNP Q9Y5A9
A	393	HIS	-	expression tag	UNP Q9Y5A9
A	394	HIS	-	expression tag	UNP Q9Y5A9
A	395	HIS	-	expression tag	UNP Q9Y5A9
A	396	HIS	-	expression tag	UNP Q9Y5A9
A	397	SER	-	expression tag	UNP Q9Y5A9
A	398	SER	-	expression tag	UNP Q9Y5A9
A	399	GLY	-	expression tag	UNP Q9Y5A9
A	400	GLU	-	expression tag	UNP Q9Y5A9
A	401	ASN	-	expression tag	UNP Q9Y5A9
A	402	LEU	-	expression tag	UNP Q9Y5A9
A	403	TYR	-	expression tag	UNP Q9Y5A9
A	404	PHE	-	expression tag	UNP Q9Y5A9
A	405	GLN	-	expression tag	UNP Q9Y5A9
A	406	HIS	-	expression tag	UNP Q9Y5A9
A	407	MET	-	expression tag	UNP Q9Y5A9
B	386	MET	-	initiating methionine	UNP Q9Y5A9
B	387	GLY	-	expression tag	UNP Q9Y5A9
B	388	SER	-	expression tag	UNP Q9Y5A9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	389	SER	-	expression tag	UNP Q9Y5A9
B	390	TYR	-	expression tag	UNP Q9Y5A9
B	391	HIS	-	expression tag	UNP Q9Y5A9
B	392	HIS	-	expression tag	UNP Q9Y5A9
B	393	HIS	-	expression tag	UNP Q9Y5A9
B	394	HIS	-	expression tag	UNP Q9Y5A9
B	395	HIS	-	expression tag	UNP Q9Y5A9
B	396	HIS	-	expression tag	UNP Q9Y5A9
B	397	SER	-	expression tag	UNP Q9Y5A9
B	398	SER	-	expression tag	UNP Q9Y5A9
B	399	GLY	-	expression tag	UNP Q9Y5A9
B	400	GLU	-	expression tag	UNP Q9Y5A9
B	401	ASN	-	expression tag	UNP Q9Y5A9
B	402	LEU	-	expression tag	UNP Q9Y5A9
B	403	TYR	-	expression tag	UNP Q9Y5A9
B	404	PHE	-	expression tag	UNP Q9Y5A9
B	405	GLN	-	expression tag	UNP Q9Y5A9
B	406	HIS	-	expression tag	UNP Q9Y5A9
B	407	MET	-	expression tag	UNP Q9Y5A9

- Molecule 2 is 6-ethyl-2,7-dihydropyrazolo[3,4-b]pyridin-4-one (CCD ID: A1KFA) (formula: $C_8H_9N_3O$) (labeled as "Ligand of Interest" by depositor).



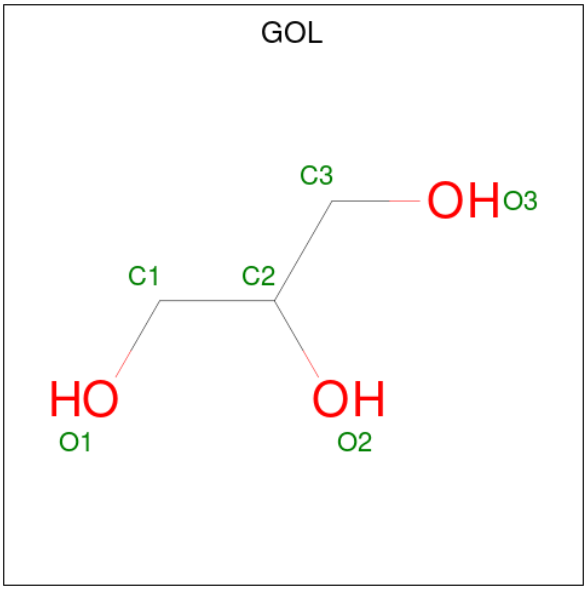
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	8	3	1		

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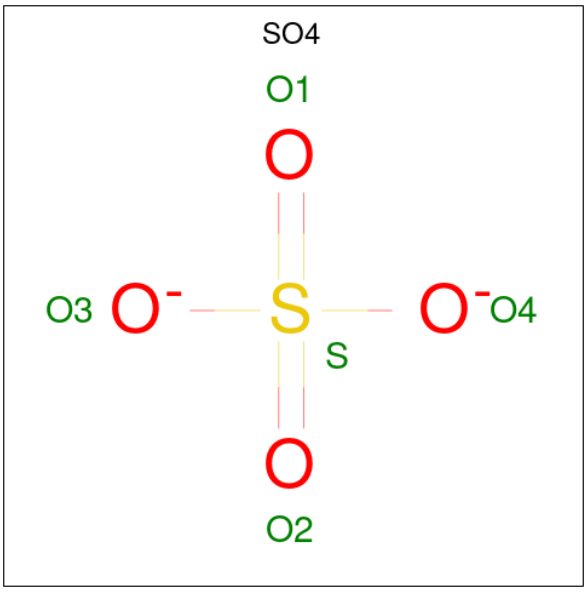
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			24	16	6	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

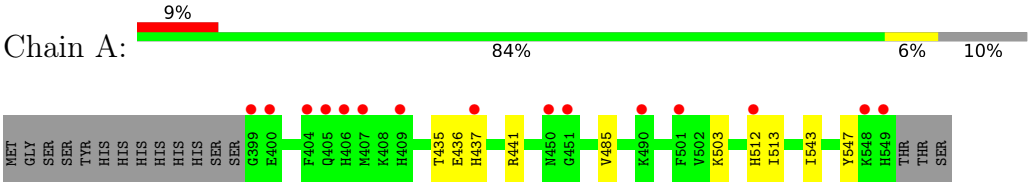
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	105	Total O 105 105	0	0
6	B	96	Total O 96 96	0	0

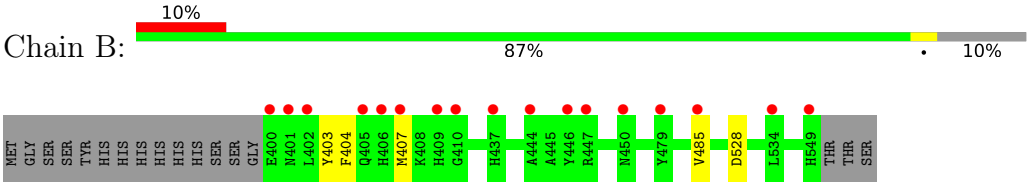
3 Residue-property plots (i)

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: YTH domain-containing family protein 2



• Molecule 1: YTH domain-containing family protein 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	80.85Å 80.85Å 113.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.10 – 1.61 44.10 – 1.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.10-1.61) 100.0 (44.10-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.61Å)	Xtriage
Refinement program	PHENIX 2.1_6048	Depositor
R, R_{free}	0.203 , 0.220 0.205 , 0.223	Depositor DCC
R_{free} test set	2690 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2692	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4, GOL, A1KFA, CL

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	0.27	0/1263	0.45	0/1709
1	B	0.27	0/1208	0.46	0/1635
All	All	0.27	0/2471	0.46	0/3344

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1233	0	1146	9	0
1	B	1179	0	1097	3	0
2	A	12	0	0	0	0
2	B	24	0	0	1	0
3	A	12	0	16	4	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
5	A	1	0	0	0	0
6	A	105	0	0	2	0
6	B	96	0	0	1	0
All	All	2692	0	2259	12	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 (12) 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:436:GLU:H	3:A:603:GOL:H12	1.62	0.65
1:A:512[A]:HIS:ND1	4:A:606:SO4:O1	2.33	0.61
1:A:503:LYS:NZ	1:A:547:TYR:O	2.42	0.52
1:A:441:ARG:NH1	6:A:701:HOH:O	2.43	0.51
1:A:436:GLU:HB3	3:A:603:GOL:H32	1.93	0.51
1:A:435:THR:HB	3:A:603:GOL:H12	1.96	0.48
1:A:513:ILE:HD11	1:A:543:ILE:HD12	1.98	0.45
1:B:404:PHE:HB3	1:B:407:MET:HE2	2.02	0.42
1:B:528:ASP:OD2	2:B:601[A]:A1KFA:N10	2.54	0.41
1:A:485:VAL:HG22	6:A:758:HOH:O	2.21	0.41
1:B:403:TYR:OH	6:B:701:HOH:O	2.22	0.40
1:A:437:HIS:HD2	3:A:603:GOL:O3	2.03	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	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	B	149/167 (89%)	147 (99%)	2 (1%)	0	100	100
All	All	303/334 (91%)	299 (99%)	4 (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	125/149 (84%)	125 (100%)	0	100	100
1	B	118/149 (79%)	117 (99%)	1 (1%)	73	59
All	All	243/298 (82%)	242 (100%)	1 (0%)	84	75

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	485	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	HIS
1	A	488	GLN
1	B	530	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is 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			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	603	-	4,4,4	0.67	0	6,6,6	0.15	0
4	SO4	A	606	-	4,4,4	0.65	0	6,6,6	0.09	0
2	A1KFA	A	601	-	13,13,13	3.34	6 (46%)	12,18,18	3.16	5 (41%)
3	GOL	A	603	-	5,5,5	0.34	0	5,5,5	0.48	0
4	SO4	A	605	-	4,4,4	0.64	0	6,6,6	0.08	0
4	SO4	B	604	-	4,4,4	0.63	0	6,6,6	0.06	0
2	A1KFA	B	601[B]	-	13,13,13	3.47	6 (46%)	12,18,18	3.34	5 (41%)
4	SO4	A	604	-	4,4,4	0.61	0	6,6,6	0.20	0
3	GOL	A	602	-	5,5,5	0.40	0	5,5,5	0.53	0
2	A1KFA	B	601[A]	-	13,13,13	3.35	6 (46%)	12,18,18	3.11	5 (41%)
4	SO4	B	602	-	4,4,4	0.70	0	6,6,6	0.27	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
2	A1KFA	A	601	-	-	1/2/2/2	0/2/2/2
3	GOL	A	603	-	-	0/4/4/4	-
2	A1KFA	B	601[B]	-	-	1/2/2/2	0/2/2/2
3	GOL	A	602	-	-	2/4/4/4	-
2	A1KFA	B	601[A]	-	-	1/2/2/2	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1KFA	C03-C04	7.31	1.48	1.36
2	B	601[A]	A1KFA	C03-C04	6.95	1.47	1.36
2	B	601[B]	A1KFA	C03-C04	6.88	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601[B]	A1KFA	C08-N07	6.78	1.53	1.38
2	B	601[A]	A1KFA	C08-N07	6.46	1.52	1.38
2	A	601	A1KFA	C08-N07	6.28	1.52	1.38
2	B	601[B]	A1KFA	C04-N07	5.30	1.45	1.37
2	B	601[A]	A1KFA	C04-N07	5.05	1.45	1.37
2	A	601	A1KFA	C04-N07	4.93	1.45	1.37
2	B	601[A]	A1KFA	C12-C08	-3.25	1.39	1.46
2	B	601[B]	A1KFA	C12-C08	-3.17	1.40	1.46
2	B	601[B]	A1KFA	N10-N09	2.94	1.40	1.36
2	B	601[A]	A1KFA	N10-N09	2.89	1.40	1.36
2	A	601	A1KFA	C12-C08	-2.61	1.41	1.46
2	B	601[B]	A1KFA	C12-C02	2.61	1.55	1.47
2	A	601	A1KFA	N10-N09	2.59	1.40	1.36
2	A	601	A1KFA	C12-C02	2.53	1.55	1.47
2	B	601[A]	A1KFA	C12-C02	2.24	1.54	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601[B]	A1KFA	N07-C08-N09	8.14	130.19	123.31
2	A	601	A1KFA	N07-C08-N09	7.79	129.89	123.31
2	B	601[A]	A1KFA	N07-C08-N09	7.46	129.61	123.31
2	B	601[A]	A1KFA	C08-N09-N10	5.64	107.30	103.28
2	B	601[B]	A1KFA	C08-N09-N10	5.61	107.28	103.28
2	A	601	A1KFA	C08-N09-N10	4.47	106.47	103.28
2	A	601	A1KFA	C03-C04-N07	3.37	122.29	119.62
2	B	601[A]	A1KFA	C12-C08-N09	-3.34	109.20	113.58
2	B	601[B]	A1KFA	C12-C08-N09	-3.22	109.35	113.58
2	A	601	A1KFA	C12-C08-N09	-3.13	109.46	113.58
2	A	601	A1KFA	C05-C04-C03	-3.03	120.45	125.14
2	B	601[B]	A1KFA	C05-C04-C03	-2.52	121.23	125.14
2	B	601[B]	A1KFA	C11-N10-N09	-2.48	108.47	112.43
2	B	601[A]	A1KFA	C11-N10-N09	-2.34	108.70	112.43
2	B	601[A]	A1KFA	C05-C04-C03	-2.18	121.77	125.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-C3
2	A	601	A1KFA	N07-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
2	B	601[A]	A1KFA	N07-C04-C05-C06
2	B	601[B]	A1KFA	N07-C04-C05-C06

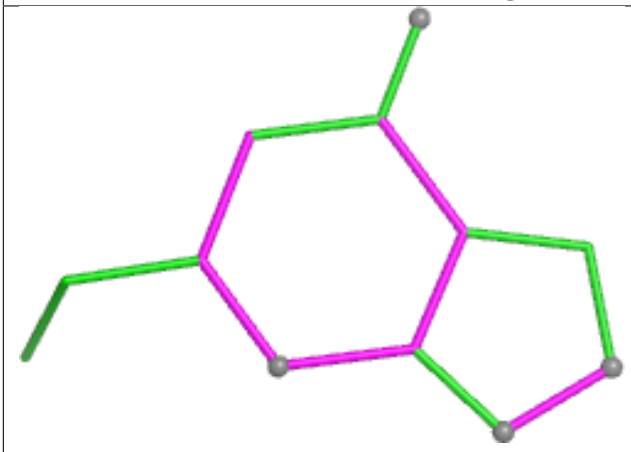
There are no ring outliers.

3 monomers are involved in 6 short contacts:

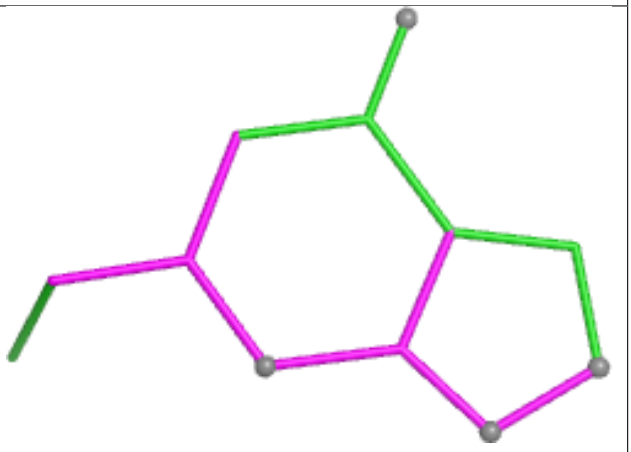
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	SO4	1	0
3	A	603	GOL	4	0
2	B	601[A]	A1KFA	1	0

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.

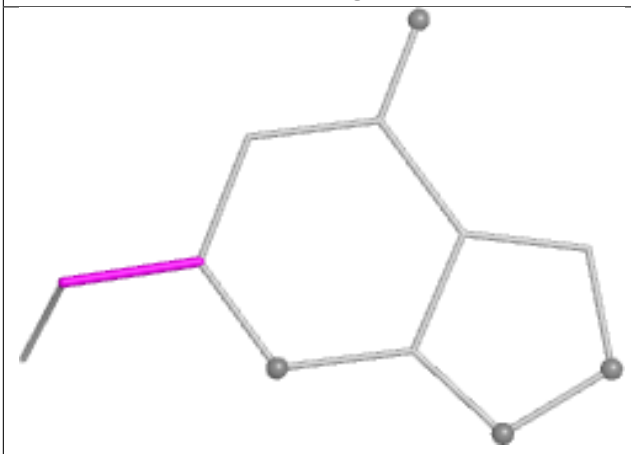
Ligand A1KFA A 601



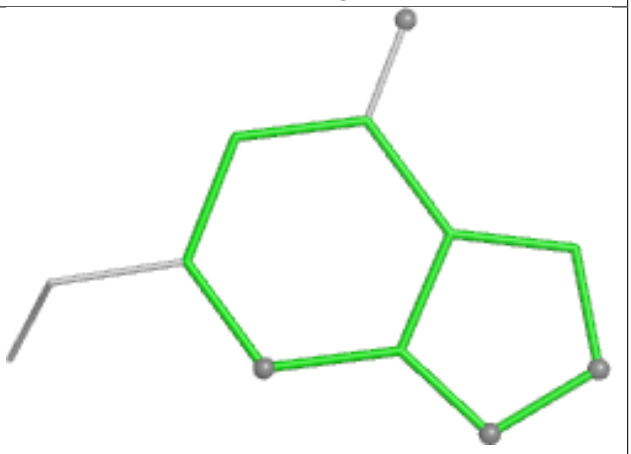
Bond lengths



Bond angles

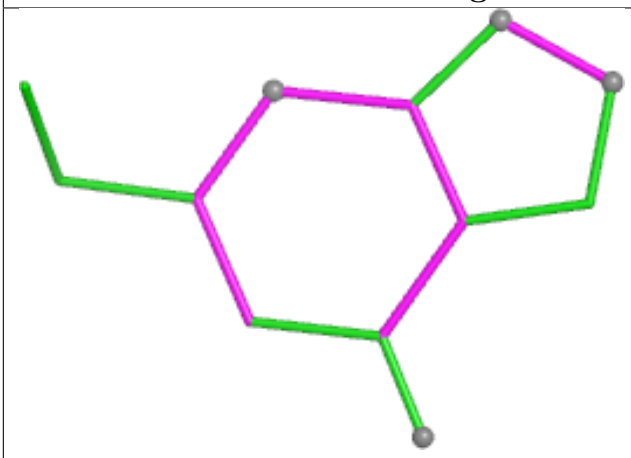


Torsions

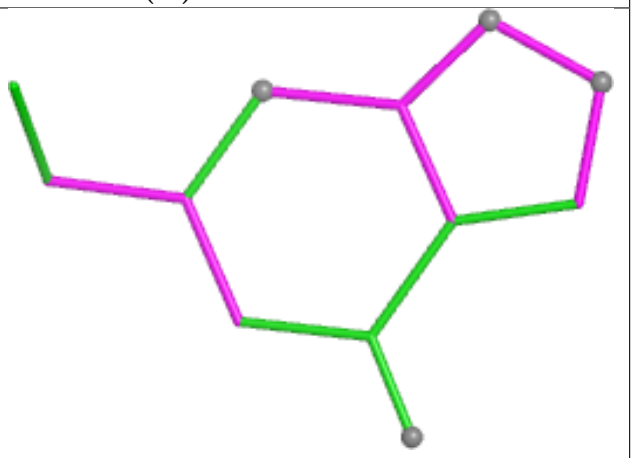


Rings

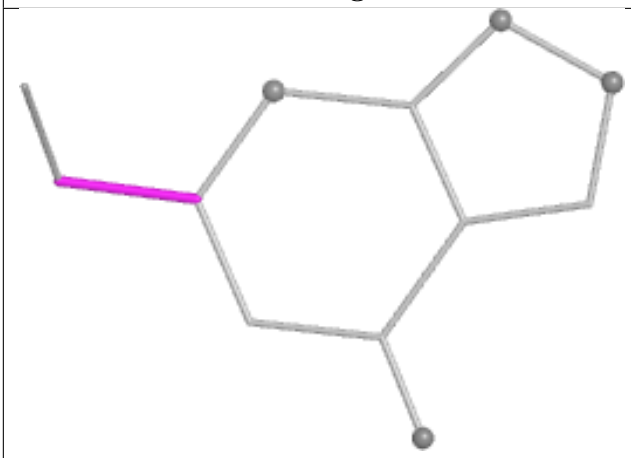
Ligand A1KFA B 601 (B)



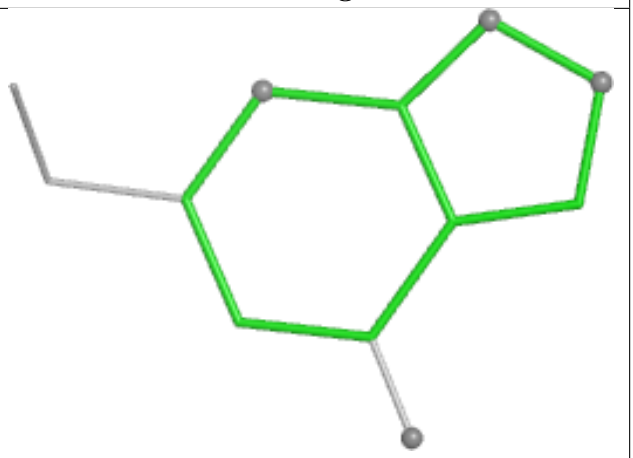
Bond lengths



Bond angles

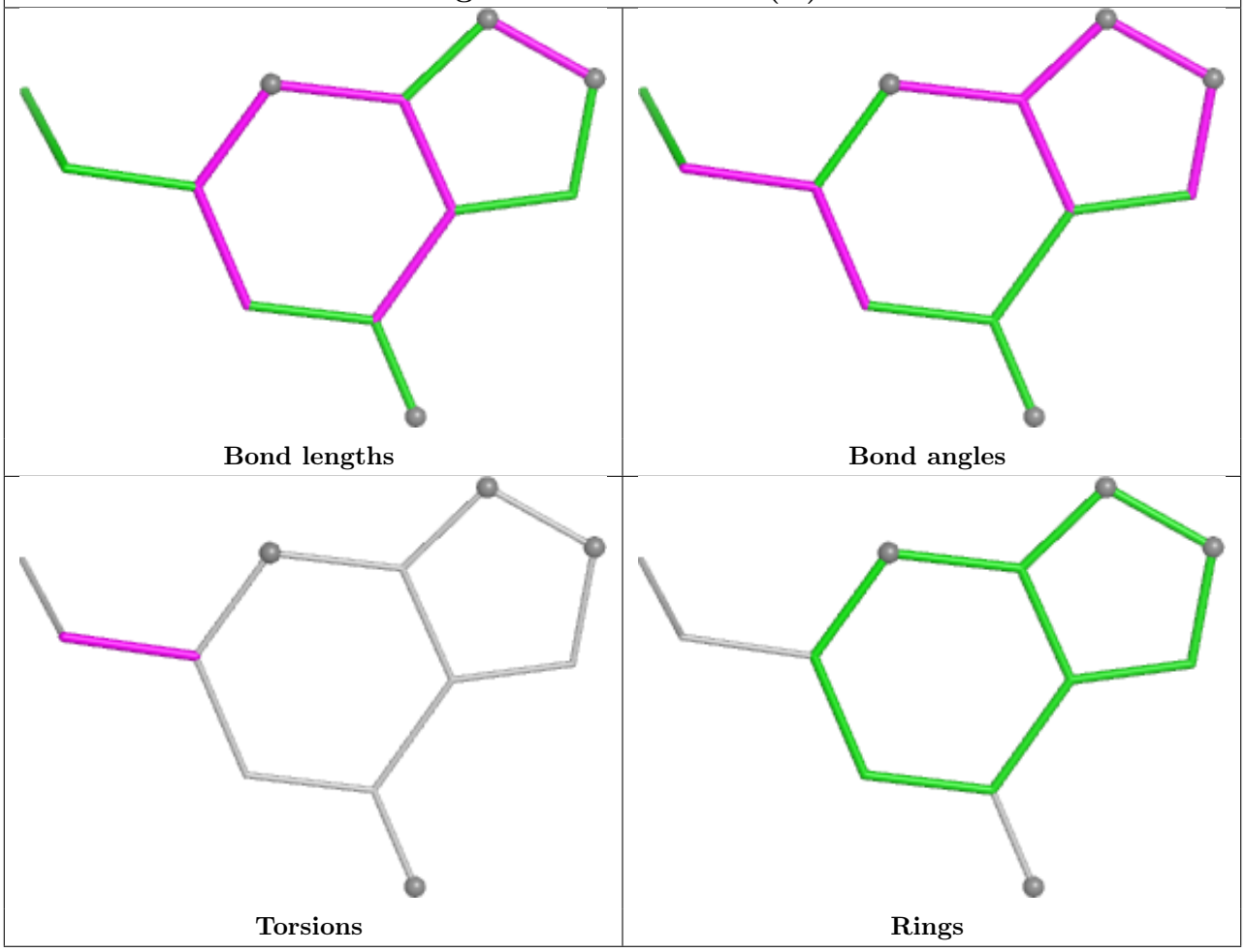


Torsions



Rings

Ligand A1KFA B 601 (A)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	151/167 (90%)	0.55	15 (9%)	13	13	12, 29, 46, 58	5 (3%)
1	B	150/167 (89%)	0.77	17 (11%)	10	10	12, 31, 47, 61	1 (0%)
All	All	301/334 (90%)	0.66	32 (10%)	11	11	12, 30, 47, 61	6 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	PHE	3.9
1	A	409	HIS	3.8
1	A	549	HIS	3.7
1	B	402	LEU	3.6
1	B	549	HIS	3.6
1	A	407	MET	3.5
1	A	512[A]	HIS	3.4
1	A	451	GLY	3.4
1	B	401	ASN	3.3
1	B	406	HIS	3.1
1	A	406	HIS	2.9
1	A	404	PHE	2.9
1	B	410	GLY	2.8
1	B	400	GLU	2.8
1	A	399	GLY	2.8
1	B	450	ASN	2.6
1	B	447	ARG	2.6
1	B	409	HIS	2.5
1	B	437	HIS	2.5
1	A	450	ASN	2.5
1	A	490	LYS	2.5
1	A	437	HIS	2.4
1	B	444	ALA	2.4
1	B	407	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	446	TYR	2.3
1	B	485	VAL	2.3
1	B	479	TYR	2.3
1	A	548	LYS	2.3
1	B	534	LEU	2.2
1	B	405	GLN	2.1
1	A	400	GLU	2.0
1	A	405	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

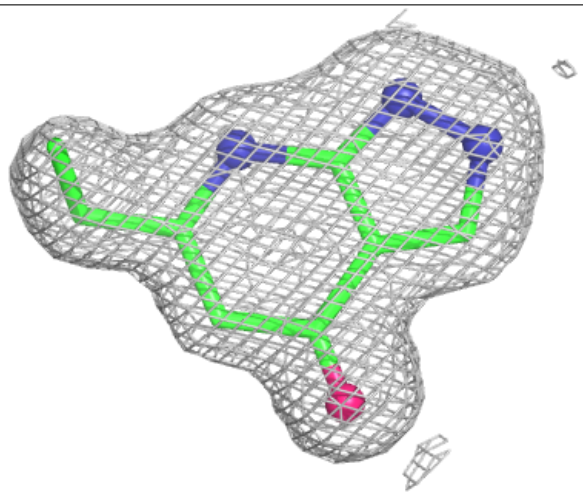
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	606	5/5	0.60	0.15	59,59,68,75	0
4	SO4	A	605	5/5	0.75	0.12	57,58,65,71	0
4	SO4	B	603	5/5	0.76	0.14	49,50,62,70	0
3	GOL	A	602	6/6	0.79	0.20	30,42,48,52	0
3	GOL	A	603	6/6	0.80	0.16	34,47,52,55	0
4	SO4	B	604	5/5	0.80	0.12	43,60,65,66	0
4	SO4	B	602	5/5	0.90	0.11	35,38,39,40	0
4	SO4	A	604	5/5	0.95	0.08	29,32,35,37	0
2	A1KFA	B	601[B]	12/12	0.96	0.07	20,22,23,24	12
2	A1KFA	A	601	12/12	0.96	0.07	21,23,25,26	0
2	A1KFA	B	601[A]	12/12	0.96	0.07	21,22,23,23	12
5	CL	A	607	1/1	0.97	0.07	37,37,37,37	0

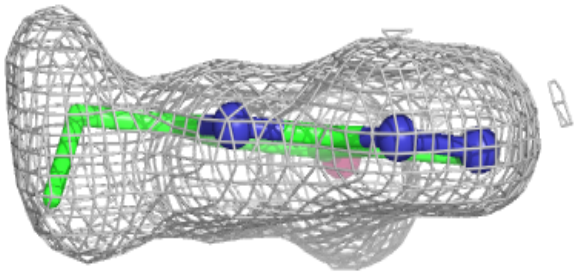
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

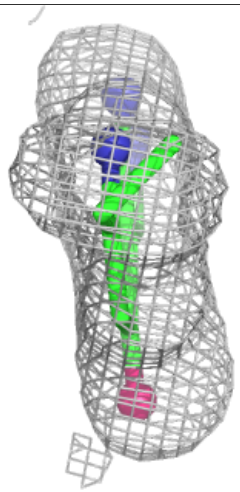
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1KFA B 601 (B):

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

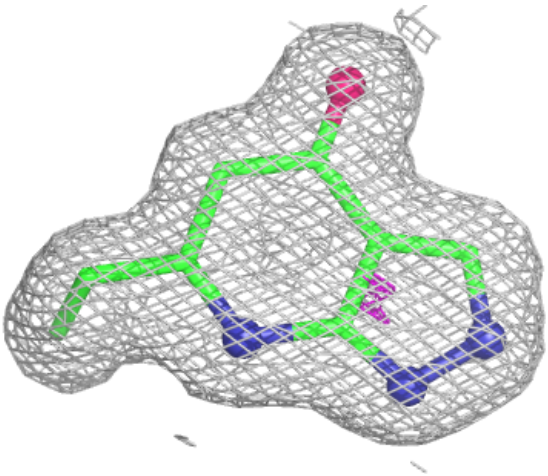


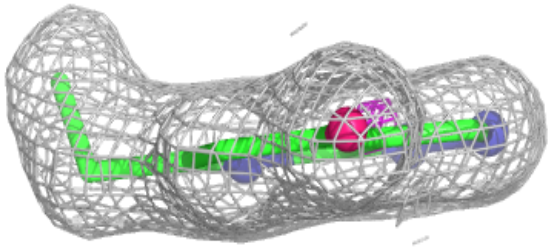


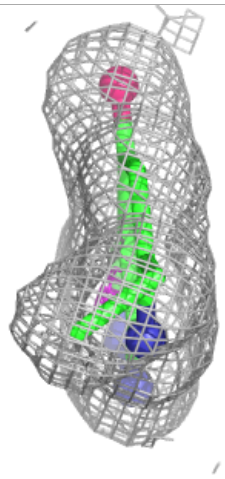


Electron density around A1KFA A 601:

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

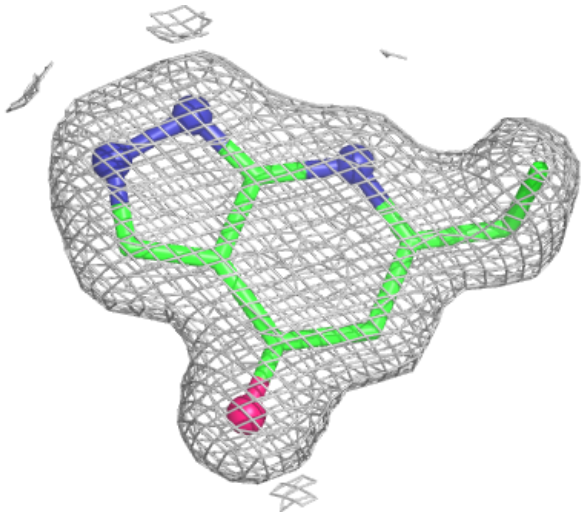


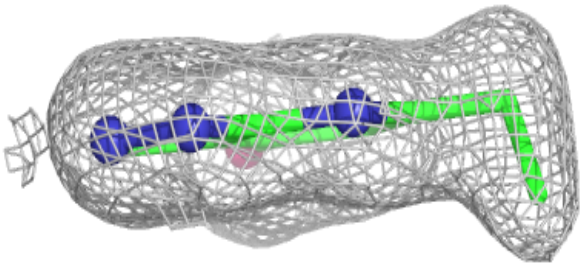


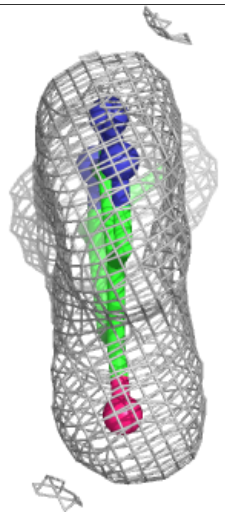


Electron density around A1KFA B 601 (A):

$2mF_o$-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.