



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 08:13 AM EDT

PDB ID : 4F5R / pdb\_00004f5r  
Title : Open and closed ternary complex of R283K DNA polymerase beta with a dCTP analog in the same asymmetric unit  
Authors : Freudenthal, B.D.; Beard, W.A.; Wilson, S.H.  
Deposited on : 2012-05-13  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

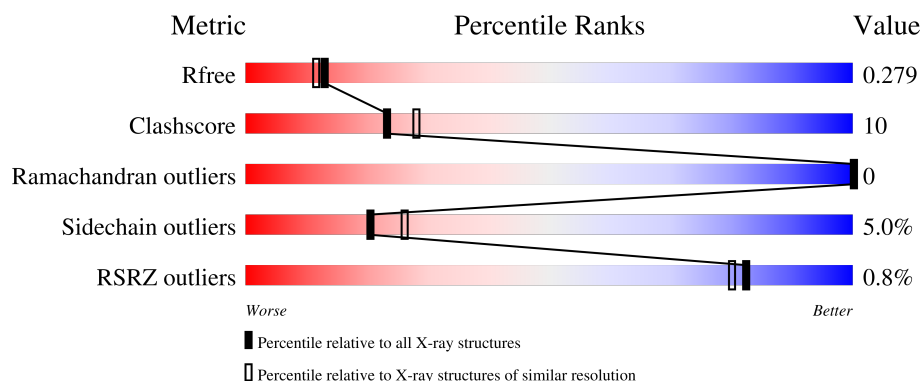
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	335	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>..</div> </div> </div>
2	C	5	<div> <div></div> <div>40%</div> <div>60%</div> </div>
2	D	5	<div> <div></div> <div>100%</div> </div>
3	G	10	<div> <div></div> <div>80%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	10	 70% 30%
4	F	16	 69% 31%
4	T	16	 81% 19%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6910 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 DNA polymerase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2581	1635	450	487	9			
1	B	321	Total	C	N	O	S	0	1	0
			2583	1636	449	489	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LYS	ARG	engineered mutation	UNP P06746
B	283	LYS	ARG	engineered mutation	UNP P06746

- Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*TP\*CP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			
2	C	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			
3	G	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

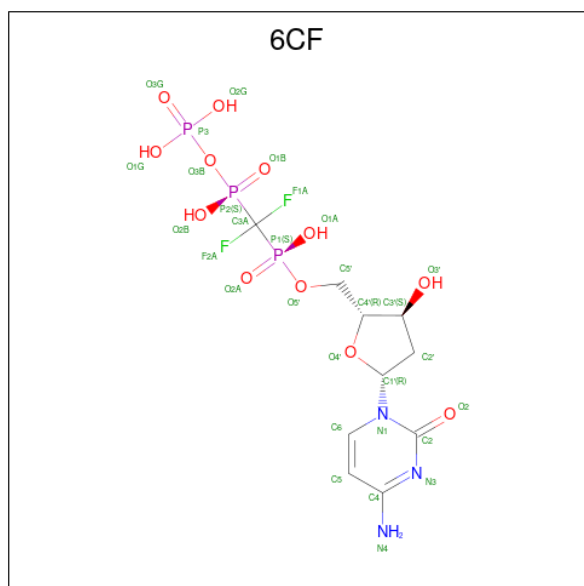
- Molecule 4 is a DNA chain called DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	16	Total	C	N	O	P	0	0	0
			323	153	63	92	15			
4	F	16	Total	C	N	O	P	0	0	0
			323	153	63	92	15			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	T	1	Total	Na	0	0
			1	1		
5	G	1	Total	Na	0	0
			1	1		

- Molecule 6 is 2'-deoxy-5'-O-[(S)-{difluoro[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}(hydroxy)phosphoryl]cytidine (CCD ID: 6CF) (formula: C<sub>10</sub>H<sub>16</sub>F<sub>2</sub>N<sub>3</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Mn 2	0	0
7	D	1	Total 1	Mn 1	0	0
7	T	1	Total 1	Mn 1	0	0

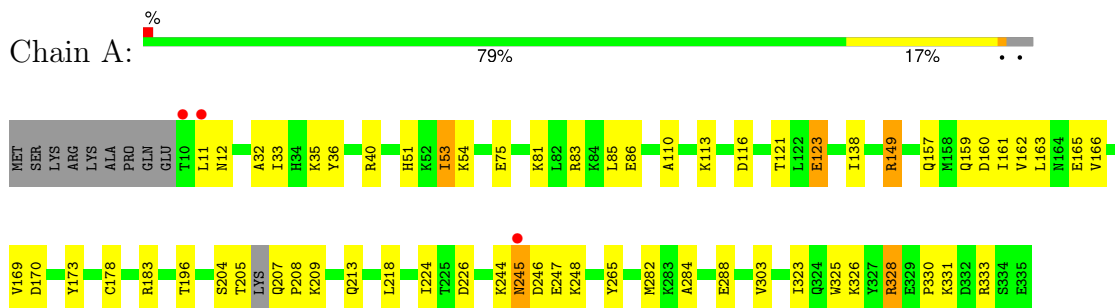
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	184	Total 184	O 184	0	0
8	B	120	Total 120	O 120	0	0
8	D	17	Total 17	O 17	0	0
8	P	19	Total 19	O 19	0	0
8	T	41	Total 41	O 41	0	0
8	C	4	Total 4	O 4	0	0
8	G	12	Total 12	O 12	0	0
8	F	17	Total 17	O 17	0	0

### 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: DNA polymerase beta



- Molecule 1: DNA polymerase beta



- Molecule 2: DNA (5'-D(P\*GP\*TP\*CP\*GP\*G)-3')



There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(P\*GP\*TP\*CP\*GP\*G)-3')




- Molecule 3: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*C)-3')

Chain P:  70% 30%




- Molecule 3: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*C)-3')

Chain G:  80% 20%



- Molecule 4: DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3')

Chain T:  81% 19%



- Molecule 4: DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3')

Chain F:  69% 31%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.03Å 79.45Å 102.09Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	21.36 – 2.20 21.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.8 (21.36-2.20) 85.0 (21.36-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650), CNS	Depositor
R, $R_{free}$	0.210 , 0.278 0.215 , 0.279	Depositor DCC
$R_{free}$ test set	1604 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MN, 6CF

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	0.46	1/2629 (0.0%)	0.79	2/3534 (0.1%)
1	B	0.50	3/2632 (0.1%)	0.79	7/3538 (0.2%)
2	C	0.25	0/118	0.80	0/179
2	D	0.30	0/118	0.94	0/179
3	G	0.40	0/227	0.75	0/349
3	P	0.31	0/227	0.96	1/349 (0.3%)
4	F	0.26	0/362	0.81	0/556
4	T	0.27	0/362	0.89	1/556 (0.2%)
All	All	0.45	4/6675 (0.1%)	0.80	11/9240 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	ASP	C-N	10.43	1.47	1.33
1	B	255	ILE	C-N	6.72	1.42	1.33
1	B	189	GLY	C-N	-5.92	1.26	1.33
1	A	149	ARG	C-N	-5.52	1.27	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	ASN	N-CA-C	9.06	121.23	111.36
1	B	245	ASN	CB-CA-C	-6.32	109.30	116.63
1	A	204	SER	N-CA-C	6.26	119.54	110.28
1	B	79	THR	N-CA-C	-6.23	101.76	110.35
1	B	255	ILE	O-C-N	5.73	129.39	123.20
1	B	189	GLY	O-C-N	5.72	128.92	122.34
3	P	6	DT	N1-C1'-C2'	5.31	121.46	113.50
1	B	255	ILE	CA-C-N	-5.30	115.25	122.93
1	B	255	ILE	C-N-CA	-5.30	115.25	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	12	DT	P-O5'-C5'	-5.13	112.31	120.00
1	A	245	ASN	CB-CA-C	-5.11	100.68	110.65

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	2581	0	2590	43	0
1	B	2583	0	2587	69	0
2	C	106	0	57	4	0
2	D	106	0	57	0	0
3	G	203	0	113	1	0
3	P	203	0	114	1	0
4	F	323	0	179	7	0
4	T	323	0	179	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	T	1	0	0	0	0
6	A	30	0	12	3	0
6	B	30	0	12	0	0
7	B	2	0	0	0	0
7	D	1	0	0	0	0
7	T	1	0	0	0	0
8	A	184	0	0	8	0
8	B	120	0	0	3	0
8	C	4	0	0	1	0
8	D	17	0	0	0	0
8	F	17	0	0	0	0
8	G	12	0	0	0	0
8	P	19	0	0	1	0
8	T	41	0	0	1	0
All	All	6910	0	5900	125	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 10.

All (125) 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:B:292:THR:HB	1:B:301:LEU:HD21	1.49	0.95
1:B:287:LEU:HD23	1:B:301:LEU:CD1	1.98	0.93
1:B:10:THR:HG22	1:B:10:THR:O	1.68	0.91
1:B:174:ILE:HB	1:B:196:THR:HG22	1.54	0.89
1:B:292:THR:CB	1:B:301:LEU:HD21	2.10	0.81
1:A:328:ARG:HH11	1:A:328:ARG:HB2	1.46	0.79
1:B:287:LEU:CD2	1:B:301:LEU:CD1	2.60	0.79
1:B:292:THR:CG2	1:B:301:LEU:HD21	2.13	0.79
1:B:282:MET:HB2	1:B:325:TRP:CZ3	2.17	0.79
1:A:36:TYR:CE1	1:A:40:ARG:HD2	2.20	0.76
1:B:287:LEU:HD23	1:B:301:LEU:HD11	1.69	0.72
1:A:116:ASP:HB2	8:A:667:HOH:O	1.90	0.71
1:A:33:ILE:HG22	8:A:664:HOH:O	1.91	0.71
4:F:2:DC:H4'	4:F:3:DG:OP1	1.92	0.69
4:T:6:DG:N7	8:T:201:HOH:O	2.26	0.68
1:B:244:LYS:O	1:B:247:GLU:HB2	1.94	0.66
4:F:2:DC:H2''	4:F:3:DG:C8	2.30	0.66
1:A:207:GLN:N	1:A:208:PRO:HD3	2.10	0.66
1:B:83:ARG:NH1	1:B:83:ARG:HB3	2.11	0.65
1:B:10:THR:O	1:B:10:THR:CG2	2.42	0.64
1:A:75:GLU:OE2	1:A:83:ARG:HG2	1.96	0.64
1:A:81:LYS:NZ	1:A:86:GLU:HG3	2.12	0.64
1:B:174:ILE:HB	1:B:196:THR:CG2	2.28	0.64
1:B:206:LYS:HB3	1:B:206:LYS:NZ	2.13	0.64
1:B:206:LYS:HB3	1:B:206:LYS:HZ3	1.63	0.62
1:B:194:LEU:HD11	1:B:260:ILE:HG12	1.81	0.62
1:B:12:ASN:HD21	1:B:53:ILE:H	1.48	0.61
1:A:36:TYR:CZ	1:A:40:ARG:CD	2.85	0.60
1:A:196:THR:HB	1:A:265:TYR:CD1	2.36	0.60
1:A:245:ASN:O	8:A:614:HOH:O	2.17	0.59
1:B:236:MET:HE3	1:B:254:ARG:NH2	2.18	0.59
1:B:194:LEU:HD11	1:B:260:ILE:CG1	2.33	0.58
1:B:287:LEU:CD2	1:B:301:LEU:HD13	2.32	0.58
3:P:2:DC:H2'	3:P:3:DT:H71	1.84	0.58
1:B:36:TYR:CZ	1:B:40:ARG:HD2	2.39	0.58
1:B:36:TYR:CE1	1:B:40:ARG:HD2	2.39	0.57
1:B:194:LEU:CD1	1:B:260:ILE:HG12	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:402:6CF:H6	6:A:402:6CF:O5'	2.04	0.57
1:A:244:LYS:CB	1:A:247:GLU:H	2.18	0.57
1:B:195:LEU:O	1:B:259:LEU:HD12	2.04	0.57
1:B:12:ASN:ND2	1:B:53:ILE:H	2.02	0.56
1:A:36:TYR:CZ	1:A:40:ARG:HD2	2.40	0.56
1:A:328:ARG:HB2	1:A:328:ARG:NH1	2.18	0.56
1:B:287:LEU:CD2	1:B:301:LEU:HD11	2.31	0.55
1:B:195:LEU:HD21	1:B:214:VAL:HG21	1.87	0.55
2:C:5:DG:H1	4:F:1:DC:H42	1.53	0.55
1:B:18:MET:SD	1:B:82:LEU:HG	2.47	0.55
1:A:244:LYS:O	1:A:245:ASN:CB	2.55	0.54
1:B:142:TYR:OH	1:B:226:ASP:OD2	2.27	0.53
1:A:36:TYR:CE1	1:A:40:ARG:CD	2.92	0.53
1:B:292:THR:HB	1:B:301:LEU:HD11	1.90	0.53
1:A:282:MET:HE3	1:A:323:ILE:HD11	1.89	0.52
1:B:199:SER:OG	1:B:210:LEU:HD11	2.09	0.52
3:G:3:DT:H2''	3:G:4:DG:C8	2.45	0.52
1:B:292:THR:HB	1:B:301:LEU:CD2	2.31	0.52
1:A:159:GLN:O	1:A:163:LEU:HG	2.10	0.52
1:A:32:ALA:HB1	1:A:35:LYS:HG3	1.91	0.52
1:B:163:LEU:HD22	1:B:175:ALA:HB3	1.93	0.51
1:A:51:HIS:NE2	8:A:647:HOH:O	2.34	0.50
1:B:161:ILE:O	1:B:165:GLU:HG2	2.11	0.50
1:B:291:PHE:C	1:B:301:LEU:CD1	2.84	0.50
1:B:260:ILE:HG23	1:B:261:PRO:HD2	1.93	0.50
1:B:135:HIS:HD2	8:B:556:HOH:O	1.93	0.50
1:A:165:GLU:O	1:A:169:VAL:HG23	2.12	0.49
1:A:121:THR:HB	8:A:668:HOH:O	2.12	0.49
1:B:284:ALA:O	1:B:288:GLU:HG3	2.13	0.48
1:A:288:GLU:HG3	8:A:644:HOH:O	2.13	0.48
1:B:209:LYS:HB3	1:B:212:HIS:HB3	1.93	0.48
1:A:218:LEU:HB2	1:A:224:ILE:HD12	1.95	0.48
1:B:48:LYS:O	1:B:50:PRO:HD3	2.14	0.48
2:C:4:DG:N7	8:C:102:HOH:O	2.34	0.48
1:B:278:PHE:HB2	1:B:335:GLU:HG3	1.96	0.48
1:A:209:LYS:O	1:A:213:GLN:HG3	2.14	0.48
1:B:287:LEU:HD22	1:B:301:LEU:HD13	1.96	0.47
1:A:33:ILE:O	1:A:36:TYR:HB3	2.15	0.47
1:A:81:LYS:HZ3	1:A:86:GLU:HG3	1.79	0.47
1:B:206:LYS:NZ	1:B:206:LYS:CB	2.77	0.47
1:A:162:VAL:O	1:A:166:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:NH2	8:B:577:HOH:O	2.48	0.47
6:A:402:6CF:O2	4:T:6:DG:N2	2.45	0.46
1:A:157:GLN:O	1:A:161:ILE:HG13	2.14	0.46
1:B:158:MET:O	1:B:162:VAL:HG23	2.16	0.45
1:B:314:ASP:HB2	8:B:616:HOH:O	2.17	0.45
1:A:110:ALA:HB2	8:P:103:HOH:O	2.16	0.45
2:C:5:DG:H1	4:F:1:DC:N4	2.15	0.45
1:A:244:LYS:C	1:A:246:ASP:H	2.23	0.45
1:B:283:LYS:HE3	4:F:6:DG:H21	1.82	0.45
1:B:197:HIS:CG	1:B:198:PRO:HD2	2.51	0.45
1:B:248:LYS:HE3	1:B:248:LYS:HB2	1.68	0.45
2:C:3:DC:H2'	2:C:4:DG:C8	2.51	0.44
1:B:292:THR:HG22	1:B:301:LEU:HD21	1.96	0.44
1:B:79:THR:OG1	1:B:81:LYS:HG2	2.18	0.44
1:B:104:SER:OG	1:B:135:HIS:HE1	1.99	0.44
1:B:83:ARG:HB3	1:B:83:ARG:CZ	2.47	0.43
1:B:12:ASN:HD21	1:B:53:ILE:N	2.15	0.43
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.80	0.43
1:B:83:ARG:NH1	1:B:83:ARG:CB	2.80	0.43
1:A:81:LYS:HE3	1:A:83:ARG:HD2	2.00	0.43
1:A:178:CYS:O	8:A:502:HOH:O	2.22	0.43
1:B:83:ARG:CB	1:B:83:ARG:HH11	2.31	0.43
1:B:165:GLU:OE1	1:B:221:VAL:HG11	2.19	0.43
1:B:154:GLU:O	1:B:158:MET:HG3	2.19	0.42
4:F:1:DC:H2''	4:F:2:DC:O5'	2.19	0.42
1:B:166:VAL:CG1	1:B:173:TYR:CB	2.97	0.42
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.84	0.42
1:A:284:ALA:HA	8:A:589:HOH:O	2.19	0.42
1:A:138:ILE:HD13	1:A:226:ASP:HB3	2.01	0.42
1:A:149:ARG:NH2	6:A:402:6CF:O2G	2.50	0.42
1:B:166:VAL:CG1	1:B:173:TYR:HB3	2.49	0.42
1:A:170:ASP:HB3	1:A:173:TYR:CD2	2.55	0.42
1:A:183:ARG:O	1:A:331:LYS:HA	2.20	0.42
1:A:123:GLU:H	1:A:123:GLU:HG3	1.64	0.41
1:B:155:MET:HE2	1:B:181:PHE:HB2	2.02	0.41
1:B:295:GLU:OE1	4:F:8:DC:H4'	2.20	0.41
1:A:81:LYS:HZ2	1:A:86:GLU:HG3	1.82	0.41
1:B:221:VAL:O	1:B:221:VAL:HG23	2.21	0.41
1:B:291:PHE:C	1:B:301:LEU:HD11	2.45	0.41
1:B:183:ARG:O	1:B:331:LYS:HD3	2.21	0.41
1:A:330:PRO:HA	1:A:333:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:ND2	1:A:53:ILE:HD12	2.35	0.41
4:T:5:DC:H2"	4:T:6:DG:OP1	2.21	0.41
1:B:287:LEU:HD23	1:B:301:LEU:HD12	1.94	0.40
1:A:81:LYS:CE	1:A:83:ARG:HD2	2.52	0.40
1:B:236:MET:HE3	1:B:254:ARG:HH22	1.85	0.40
1:B:276:ASP:OD2	1:B:277:ILE:N	2.54	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	321/335 (96%)	310 (97%)	11 (3%)	0	100	100
1	B	318/335 (95%)	308 (97%)	10 (3%)	0	100	100
All	All	639/670 (95%)	618 (97%)	21 (3%)	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	280/295 (95%)	268 (96%)	12 (4%)	25	32
1	B	282/295 (96%)	266 (94%)	16 (6%)	17	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	562/590 (95%)	534 (95%)	28 (5%)	20	26

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	54	LYS
1	A	85	LEU
1	A	113	LYS
1	A	123	GLU
1	A	160	ASP
1	A	205	THR
1	A	248	LYS
1	A	303	VAL
1	A	325	TRP
1	A	326	LYS
1	A	328	ARG
1	B	48	LYS
1	B	82	LEU
1	B	112	ARG
1	B	116	ASP
1	B	196	THR
1	B	203	GLU
1	B	205	THR
1	B	206	LYS
1	B	221	VAL
1	B	249	GLU
1	B	269	VAL
1	B	272	PHE
1	B	282	MET
1	B	295	GLU
1	B	325	TRP
1	B	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	264	GLN
1	A	285	HIS
1	B	12	ASN

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Mol	Chain	Res	Type
1	B	135	HIS
1	B	213	GLN
1	B	264	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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z  > 2$
6	6CF	B	404	7	26,31,31	2.32	8 (30%)	36,50,50	1.50	6 (16%)
6	6CF	A	402	-	26,31,31	2.32	8 (30%)	36,50,50	1.47	6 (16%)

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
6	6CF	B	404	7	-	6/23/46/46	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	6CF	A	402	-	-	1/23/46/46	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	6CF	O2-C2	7.60	1.37	1.23
6	B	404	6CF	O2-C2	7.33	1.37	1.23
6	A	402	6CF	C4-N4	4.67	1.45	1.33
6	B	404	6CF	C4-N4	4.34	1.44	1.33
6	B	404	6CF	P2-O1B	3.86	1.57	1.51
6	B	404	6CF	P1-O2A	3.34	1.56	1.51
6	A	402	6CF	P1-O2A	3.03	1.56	1.51
6	B	404	6CF	C2-N3	2.96	1.42	1.36
6	A	402	6CF	P2-O1B	2.88	1.55	1.51
6	A	402	6CF	C2-N3	2.87	1.42	1.36
6	A	402	6CF	O3'-C3'	-2.74	1.37	1.43
6	A	402	6CF	C6-C5	2.60	1.41	1.35
6	B	404	6CF	C6-C5	2.59	1.41	1.35
6	B	404	6CF	O3'-C3'	-2.56	1.38	1.43
6	A	402	6CF	O4'-C4'	-2.32	1.39	1.45
6	B	404	6CF	O4'-C4'	-2.31	1.39	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	404	6CF	O5'-P1-O2A	-4.87	106.52	115.44
6	A	402	6CF	O5'-P1-O2A	-4.68	106.86	115.44
6	A	402	6CF	P2-O3B-P3	-3.30	120.63	132.45
6	B	404	6CF	O1G-P3-O3B	3.21	115.41	104.64
6	A	402	6CF	O1G-P3-O3B	2.91	114.39	104.64
6	B	404	6CF	P2-O3B-P3	-2.81	122.37	132.45
6	B	404	6CF	O2G-P3-O3B	2.67	113.60	104.64
6	A	402	6CF	O5'-P1-C3A	2.34	109.20	102.57
6	B	404	6CF	O4'-C1'-N1	2.29	111.93	107.86
6	A	402	6CF	P1-C3A-P2	-2.21	107.47	112.87
6	A	402	6CF	O2G-P3-O3B	2.17	111.92	104.64
6	B	404	6CF	O2G-P3-O3G	-2.14	102.52	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	402	6CF	C5'-O5'-P1-C3A
6	B	404	6CF	F1A-C3A-P2-O1B
6	B	404	6CF	F2A-C3A-P2-O1B
6	B	404	6CF	F1A-C3A-P2-O3B
6	B	404	6CF	F2A-C3A-P2-O3B
6	B	404	6CF	P2-O3B-P3-O2G
6	B	404	6CF	C5'-O5'-P1-O2A

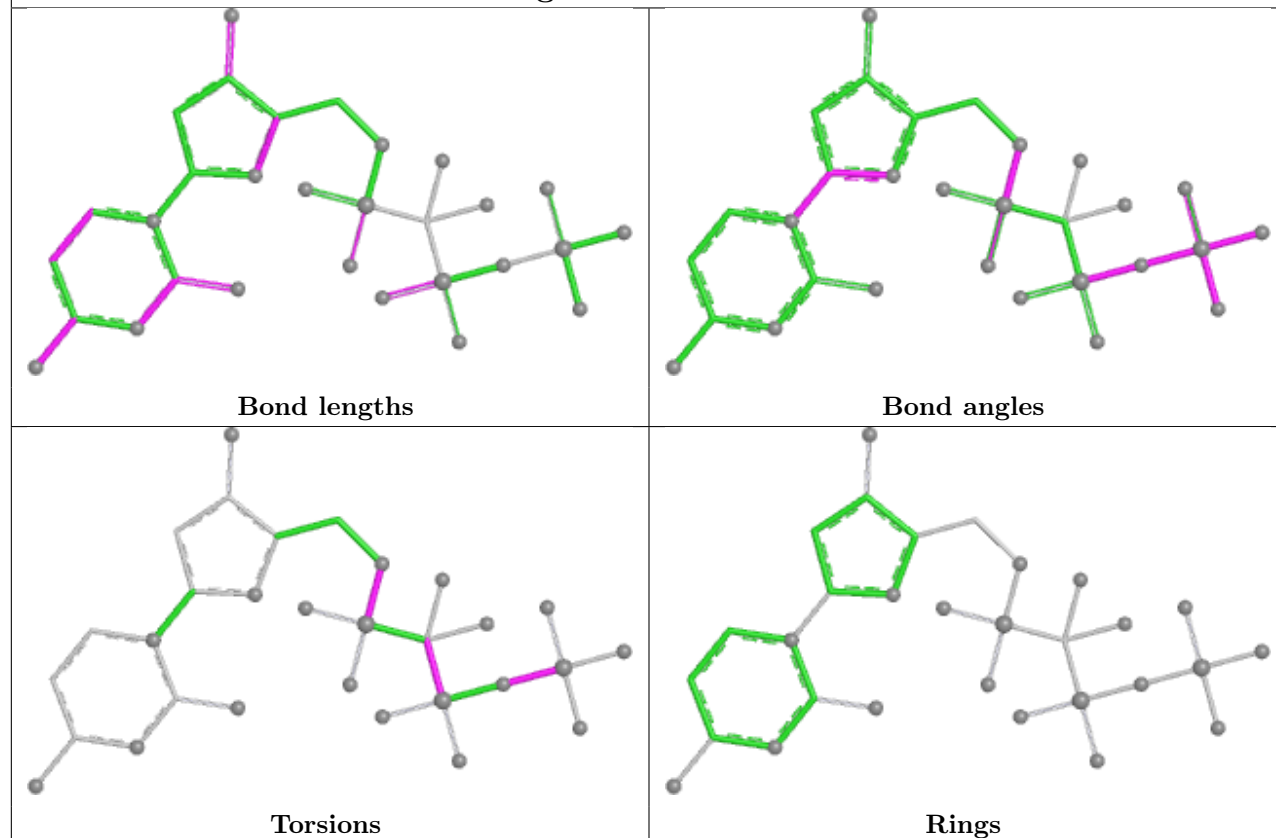
There are no ring outliers.

1 monomer is involved in 3 short contacts:

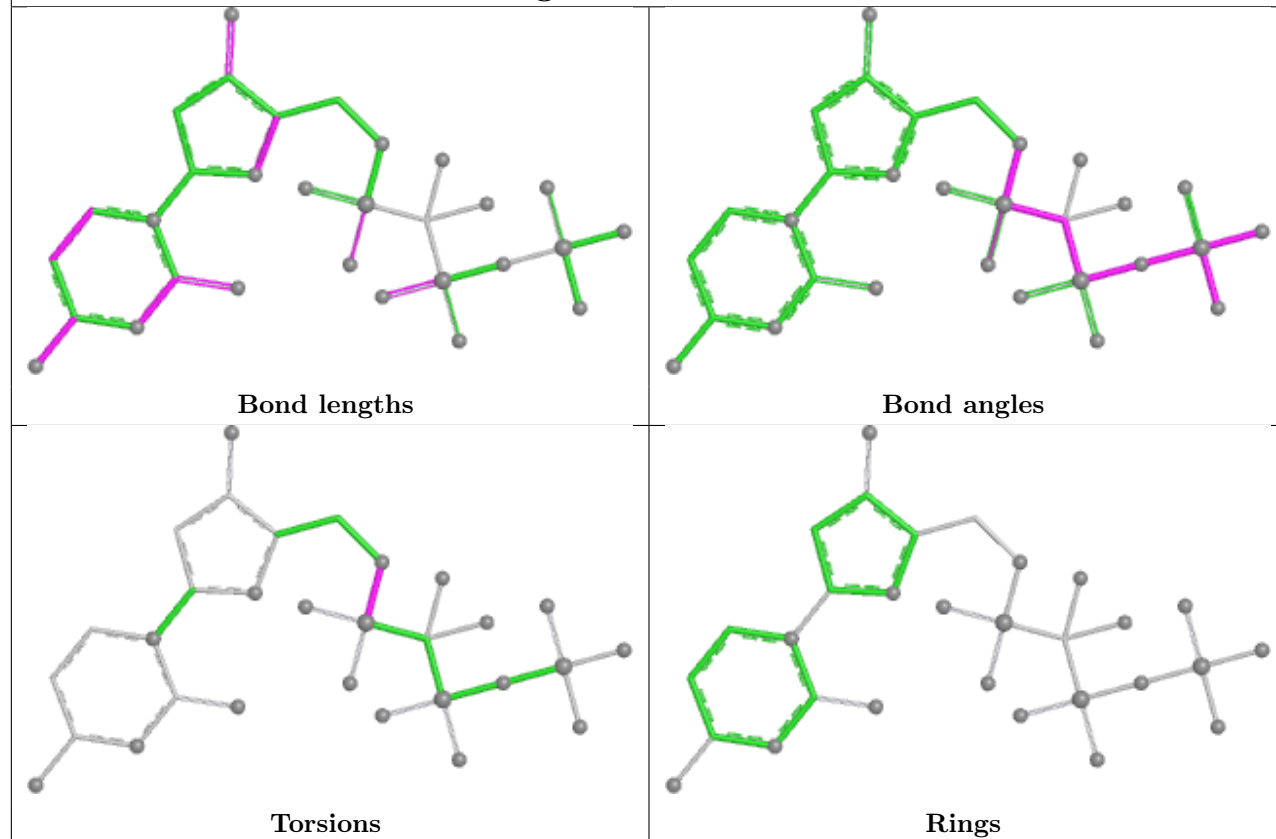
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	402	6CF	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand 6CF B 404



## Ligand 6CF A 402



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	325/335 (97%)	-0.25	3 (0%) 81 78	18, 31, 51, 80	0
1	B	321/335 (95%)	-0.06	3 (0%) 81 78	18, 37, 56, 68	1 (0%)
2	C	5/5 (100%)	-0.28	0 100 100	35, 36, 48, 51	0
2	D	5/5 (100%)	-0.97	0 100 100	22, 26, 31, 32	0
3	G	10/10 (100%)	-0.56	0 100 100	29, 39, 49, 49	0
3	P	10/10 (100%)	-0.84	0 100 100	24, 31, 36, 41	0
4	F	16/16 (100%)	-0.06	0 100 100	31, 46, 63, 65	0
4	T	16/16 (100%)	-0.75	0 100 100	24, 34, 41, 44	0
All	All	708/732 (96%)	-0.19	6 (0%) 82 80	18, 34, 55, 80	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	LEU	3.9
1	A	10	THR	3.9
1	A	245	ASN	3.6
1	B	10	THR	2.8
1	A	11	LEU	2.8
1	B	92	ASP	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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

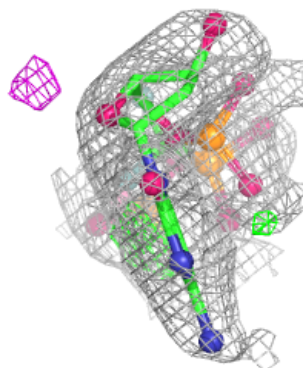
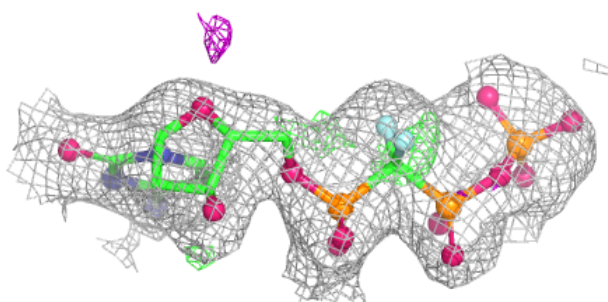
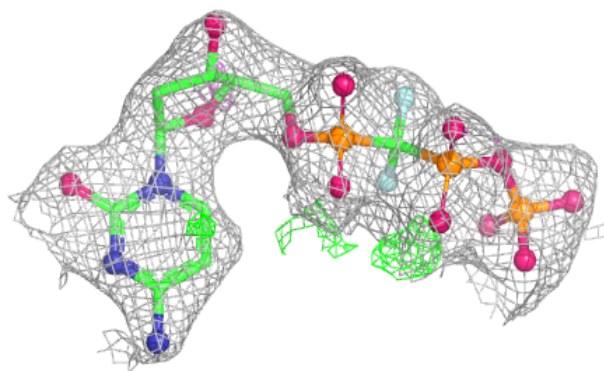
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	G	101	1/1	0.89	0.16	44,44,44,44	0
6	6CF	A	402	30/30	0.89	0.09	27,40,54,62	0
5	NA	B	403	1/1	0.91	0.10	33,33,33,33	0
5	NA	T	102	1/1	0.92	0.08	54,54,54,54	0
7	MN	B	402	1/1	0.93	0.06	29,29,29,29	0
6	6CF	B	404	30/30	0.94	0.08	26,32,37,41	0
7	MN	B	401	1/1	0.96	0.04	27,27,27,27	0
5	NA	A	401	1/1	0.98	0.09	22,22,22,22	0
7	MN	T	101	1/1	0.98	0.03	39,39,39,39	0
7	MN	D	101	1/1	0.99	0.02	36,36,36,36	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.

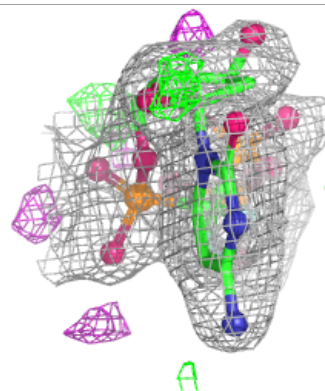
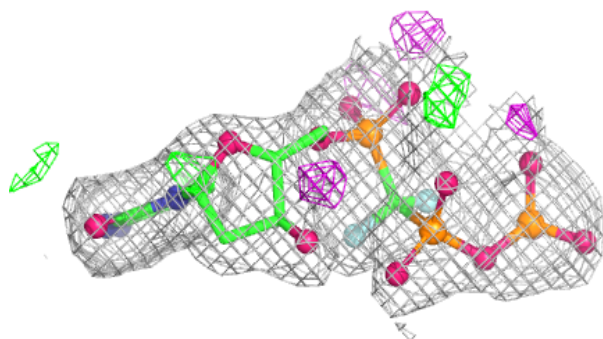
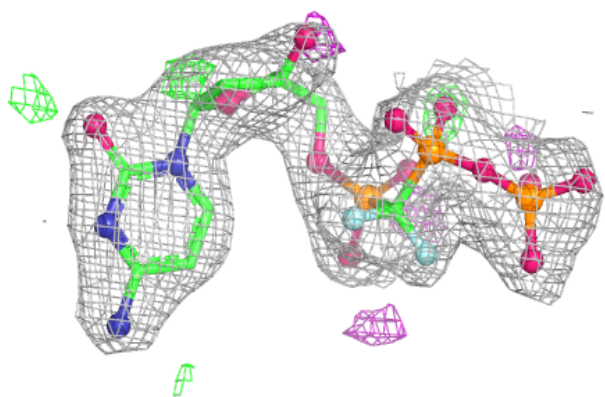
### Electron density around 6CF A 402:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 6CF B 404:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.