



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:14 am BST

PDB ID : 1S9F
Title : DPO with AT matched
Authors : Trincao, J.; Johnson, R.E.; Wolffe, W.T.; Escalante, C.R.; Prakash, S.;
Prakash, L.; Aggarwal, A.K.
Deposited on : 2004-02-04
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

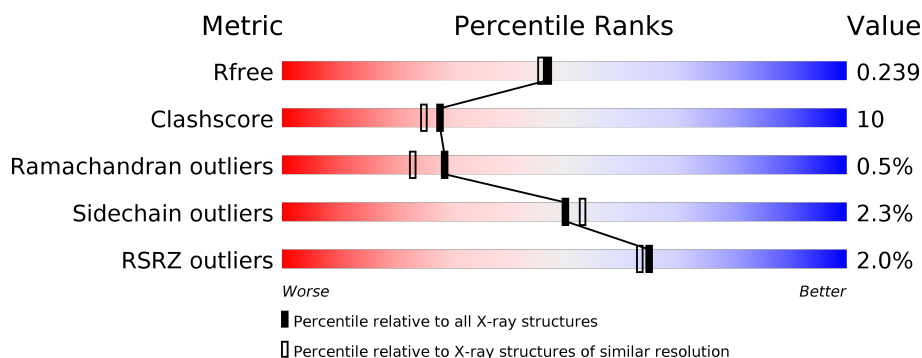
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	E	13	<div> <div></div> <div>54%46%</div> </div>
1	F	13	<div> <div></div> <div>54%46%</div> </div>
1	G	13	<div> <div></div> <div>77%23%</div> </div>
1	H	13	<div> <div></div> <div>77%23%</div> </div>
2	I	18	<div> <div>11%</div> <div>78%17%6%</div> </div>
2	J	18	<div> <div>11%</div> <div>72%22%6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	18	<div><div></div><div>6%</div><div>67%</div><div>22%</div><div>6%</div><div>6%</div></div>
2	L	18	<div><div></div><div>67%</div><div>28%</div><div>6%</div></div>
3	A	352	<div><div></div><div>%</div><div>80%</div><div>16%</div><div>• •</div></div>
3	B	352	<div><div></div><div>2%</div><div>77%</div><div>18%</div><div>• •</div></div>
3	C	352	<div><div></div><div>3%</div><div>74%</div><div>21%</div><div>• •</div></div>
3	D	352	<div><div></div><div>%</div><div>74%</div><div>23%</div><div>• •</div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14599 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 DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			
1	F	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			
1	G	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			
1	H	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			

- Molecule 2 is a DNA chain called 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			
2	J	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			
2	K	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			
2	L	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2733	1754	468	504	7			
3	B	341	Total	C	N	O	S	0	0	0
			2739	1757	471	504	7			
3	C	341	Total	C	N	O	S	0	0	0
			2733	1755	469	502	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	341	Total	C	N	O	S	0	0	0
			2729	1752	468	502	7			

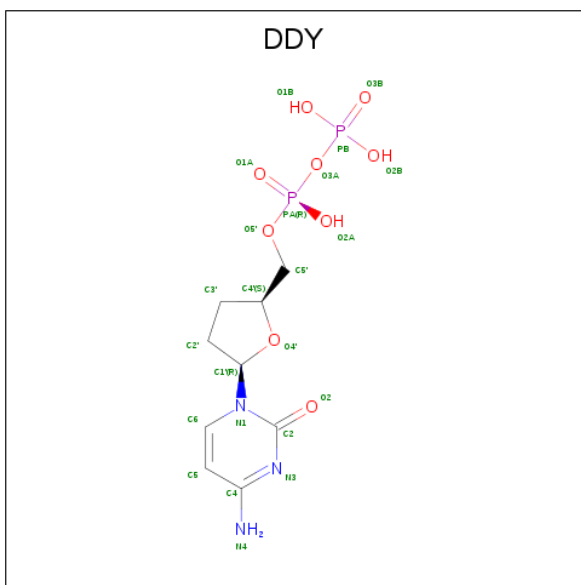
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2',3'-DIDEOXYCYTOSINE-5'-DIPHOSPHATE (three-letter code: DDY) (formula: C₉H₁₅N₃O₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 23	C 9	N 3	O 9	P 2	0	0
6	B	1	Total 23	C 9	N 3	O 9	P 2	0	0
6	C	1	Total 23	C 9	N 3	O 9	P 2	0	0
6	D	1	Total 23	C 9	N 3	O 9	P 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	36	Total O 36 36	0	0
7	I	36	Total O 36 36	0	0
7	F	49	Total O 49 49	0	0
7	J	32	Total O 32 32	0	0
7	G	35	Total O 35 35	0	0
7	K	51	Total O 51 51	0	0
7	H	33	Total O 33 33	0	0
7	L	50	Total O 50 50	0	0

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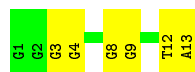
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	240	Total 240	O 240	0	0
7	B	180	Total 180	O 180	0	0
7	C	181	Total 181	O 181	0	0
7	D	206	Total 206	O 206	0	0

3 Residue-property plots

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

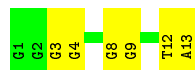
- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain E: 




- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain F: 




- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain G: 




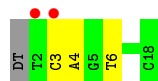
- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain H: 

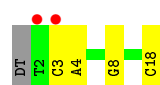


- Molecule 2: 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'

Chain I: 



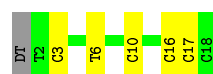
- Molecule 2: 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'



- Molecule 2: 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'



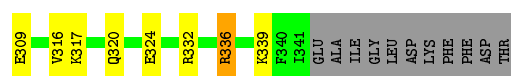
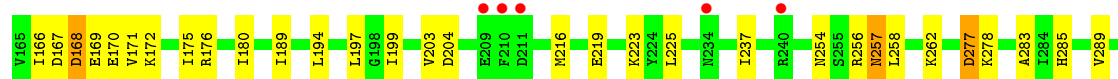
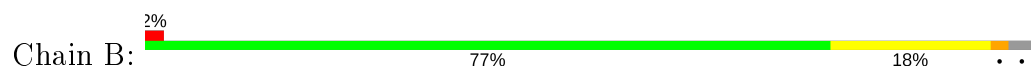
- Molecule 2: 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'



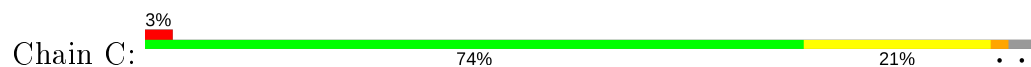
- Molecule 3: DNA polymerase IV

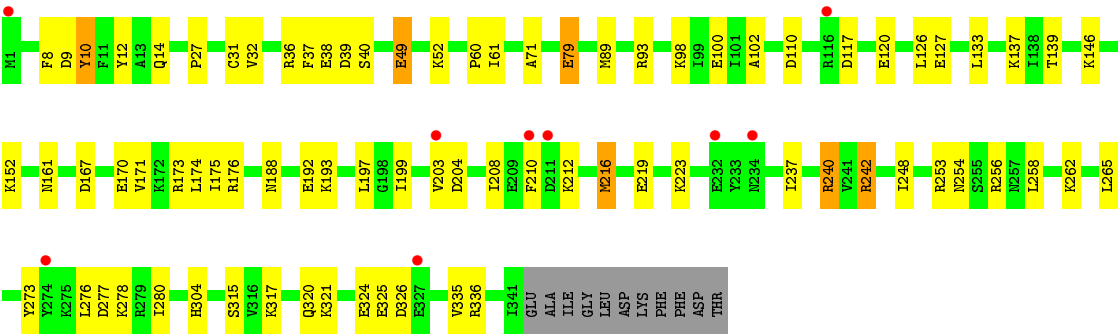


- Molecule 3: DNA polymerase IV

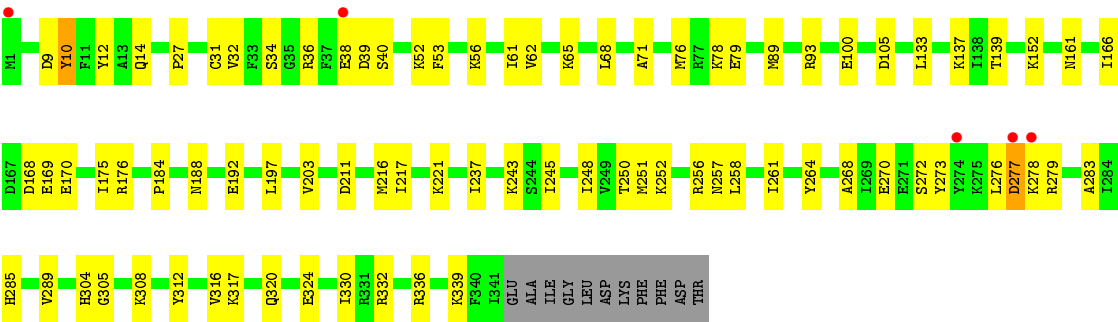


- Molecule 3: DNA polymerase IV





● Molecule 3: DNA polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.80 Å 100.30 Å 110.80 Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	44.6 (30.00-2.00) 92.9 (30.00-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.00 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.239 0.204 , 0.239	Depositor DCC
R_{free} test set	3529 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14599	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, DDY

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	E	0.32	0/310	0.71	0/479
1	F	0.34	0/310	0.74	0/479
1	G	0.34	0/310	0.74	0/479
1	H	0.35	0/310	0.77	0/479
2	I	0.31	0/372	0.70	0/570
2	J	0.32	0/372	0.75	0/570
2	K	0.33	0/372	0.75	0/570
2	L	0.33	0/372	0.69	0/570
3	A	0.32	0/2772	0.56	0/3725
3	B	0.32	0/2778	0.55	0/3732
3	C	0.33	0/2772	0.56	0/3724
3	D	0.33	0/2768	0.57	0/3720
All	All	0.33	0/13818	0.60	0/19097

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
2	K	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	12	DT	Sidechain
1	F	12	DT	Sidechain
2	K	8	DG	Sidechain

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	E	274	0	146	8	0
1	F	274	0	146	7	0
1	G	274	0	146	3	0
1	H	274	0	146	4	0
2	I	335	0	194	5	0
2	J	335	0	194	7	0
2	K	335	0	194	10	0
2	L	335	0	194	7	0
3	A	2733	0	2867	45	0
3	B	2739	0	2878	61	0
3	C	2733	0	2874	70	0
3	D	2729	0	2863	61	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	23	0	12	2	0
6	B	23	0	12	4	0
6	C	23	0	12	1	0
6	D	23	0	12	1	0
7	A	240	0	0	4	0
7	B	180	0	0	6	0
7	C	181	0	0	2	0
7	D	206	0	0	6	0
7	E	36	0	0	0	0
7	F	49	0	0	1	0
7	G	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	33	0	0	0	0
7	I	36	0	0	0	0
7	J	32	0	0	0	0
7	K	51	0	0	1	0
7	L	50	0	0	0	0
All	All	14599	0	12890	260	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 (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:14:GLN:HE22	3:D:139:THR:H	1.06	1.03
3:C:14:GLN:HE22	3:C:139:THR:H	0.97	0.95
2:L:16:DC:H2''	2:L:17:DC:H5'	1.46	0.95
3:B:176:ARG:HG2	3:B:203:VAL:HG21	1.50	0.93
3:C:176:ARG:HG2	3:C:203:VAL:HG11	1.49	0.93
3:A:14:GLN:HE22	3:A:139:THR:H	0.99	0.92
3:D:176:ARG:HG2	3:D:203:VAL:HG11	1.55	0.89
2:K:8:DG:H2'	3:C:336:ARG:HH21	1.41	0.85
3:B:197:LEU:HD11	3:B:216:MET:HG3	1.58	0.84
2:J:18:DC:H6	2:J:18:DC:H5'	1.46	0.81
2:L:16:DC:H2''	2:L:17:DC:C5'	2.10	0.80
1:H:3:DG:H2''	1:H:4:DG:H5'	1.63	0.80
3:A:88:ILE:HD11	3:A:138:ILE:HD12	1.64	0.80
3:A:79:GLU:H	3:A:79:GLU:CD	1.86	0.79
3:C:79:GLU:CD	3:C:79:GLU:H	1.82	0.79
1:F:13:DA:H2''	6:B:4011:DDY:H4'	1.64	0.79
3:C:36:ARG:HH22	3:C:254:ASN:ND2	1.81	0.78
3:D:316:VAL:O	3:D:320:GLN:HG3	1.85	0.76
1:E:3:DG:H2''	1:E:4:DG:H5'	1.68	0.76
2:K:8:DG:H2'	3:C:336:ARG:NH2	2.00	0.76
3:B:79:GLU:H	3:B:79:GLU:CD	1.90	0.76
3:D:14:GLN:NE2	3:D:139:THR:H	1.83	0.75
3:C:175:ILE:HG22	3:C:203:VAL:HG13	1.69	0.74
3:B:175:ILE:O	3:B:203:VAL:HG23	1.88	0.73
3:C:14:GLN:HE22	3:C:139:THR:N	1.81	0.72
3:D:79:GLU:H	3:D:79:GLU:CD	1.92	0.71
3:A:14:GLN:HE22	3:A:139:THR:N	1.83	0.71
3:A:320:GLN:O	3:A:324:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:TYR:CE2	6:C:4012:DDY:H2'1	2.26	0.70
3:D:34:SER:HB2	3:D:40:SER:OG	1.93	0.68
1:E:8:DG:H2''	1:E:9:DG:C5'	2.24	0.68
3:A:304:HIS:HD2	3:A:305:GLY:O	1.77	0.67
2:I:3:DC:H4'	3:A:62:VAL:HG21	1.78	0.65
1:E:8:DG:H2''	1:E:9:DG:H5'	1.79	0.65
3:A:317:LYS:HA	3:A:320:GLN:HE21	1.61	0.64
3:B:175:ILE:HG22	3:B:203:VAL:HG22	1.80	0.64
3:D:270:GLU:OE2	3:D:308:LYS:HE2	1.97	0.64
3:C:36:ARG:NH2	3:C:254:ASN:ND2	2.46	0.64
3:C:117:ASP:OD2	3:C:120:GLU:HG3	1.98	0.64
3:B:316:VAL:O	3:B:320:GLN:HG3	1.99	0.63
3:A:12:TYR:CE2	6:A:4010:DDY:H2'1	2.34	0.63
3:A:214:LYS:HD2	3:A:219:GLU:HB2	1.79	0.63
2:J:18:DC:C6	2:J:18:DC:H5'	2.33	0.63
3:D:12:TYR:CE2	6:D:4013:DDY:H2'1	2.34	0.63
3:D:320:GLN:O	3:D:324:GLU:HG3	1.98	0.62
3:D:304:HIS:HD2	3:D:305:GLY:O	1.81	0.62
2:J:8:DG:P	3:B:336:ARG:HH22	2.23	0.62
3:A:257:ASN:C	3:A:257:ASN:HD22	2.02	0.61
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.82	0.61
3:C:133:LEU:O	3:C:137:LYS:HD2	2.00	0.61
3:D:188:ASN:O	3:D:192:GLU:HG2	2.01	0.61
3:A:164:LYS:HD3	3:A:165:VAL:N	2.16	0.61
3:B:14:GLN:HE22	3:B:139:THR:H	1.48	0.61
3:B:285:HIS:HD2	7:B:4095:HOH:O	1.84	0.60
3:C:49:GLU:OE1	3:C:52:LYS:HE2	2.02	0.60
3:B:133:LEU:O	3:B:137:LYS:HD2	2.01	0.60
3:C:242:ARG:HG2	3:C:242:ARG:HH11	1.67	0.60
3:B:122:TYR:O	3:B:126:LEU:HD13	2.02	0.59
3:B:257:ASN:HD22	3:B:257:ASN:C	2.06	0.59
3:C:102:ALA:HA	3:C:240:ARG:NH1	2.18	0.59
3:A:69:PRO:CG	3:B:309:GLU:HG2	2.32	0.59
3:C:175:ILE:HG22	3:C:203:VAL:CG1	2.32	0.59
3:B:88:ILE:HD11	3:B:138:ILE:HD12	1.85	0.59
3:B:126:LEU:HD12	3:B:163:ILE:HD13	1.84	0.59
3:C:304:HIS:HB3	7:C:4021:HOH:O	2.04	0.58
3:C:265:LEU:HD21	3:C:315:SER:HB3	1.86	0.58
3:C:321:LYS:O	3:C:325:GLU:HG3	2.03	0.58
3:D:261:ILE:HD13	3:D:330:ILE:HD12	1.86	0.57
3:D:268:ALA:O	3:D:272:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:DG:H2''	1:F:9:DG:H5'	1.85	0.57
3:C:256:ARG:NH2	3:C:326:ASP:O	2.38	0.57
3:D:175:ILE:O	3:D:203:VAL:HG13	2.05	0.57
3:D:175:ILE:HG22	3:D:203:VAL:HG13	1.87	0.57
3:D:336:ARG:HD2	7:D:4191:HOH:O	2.05	0.56
2:L:10:DC:OP2	3:D:243:LYS:HD2	2.05	0.56
3:B:277:ASP:O	3:B:278:LYS:HB2	2.06	0.56
3:C:240:ARG:HG2	3:C:240:ARG:HH11	1.71	0.56
3:B:82:GLN:HB2	7:B:4138:HOH:O	2.06	0.55
3:B:289:VAL:HB	3:B:332:ARG:HB2	1.89	0.54
3:C:188:ASN:O	3:C:192:GLU:HG2	2.08	0.54
1:F:8:DG:H2''	1:F:9:DG:C5'	2.36	0.54
3:B:175:ILE:HG22	3:B:203:VAL:CG2	2.36	0.54
3:B:21:PRO:O	3:B:24:LYS:HG2	2.07	0.54
3:A:2:ILE:H	3:A:112:SER:HB3	1.73	0.54
3:C:100:GLU:HB2	3:C:237:ILE:HG23	1.89	0.54
3:B:219:GLU:O	3:B:223:LYS:HG3	2.08	0.54
3:A:327:GLU:HG3	7:A:4157:HOH:O	2.08	0.54
2:I:3:DC:H4'	3:A:62:VAL:CG2	2.38	0.53
3:A:69:PRO:HG3	3:B:309:GLU:HG2	1.90	0.53
3:D:252:LYS:HE3	7:D:4193:HOH:O	2.08	0.53
3:B:142:VAL:HG22	3:B:163:ILE:HG13	1.90	0.53
3:B:169:GLU:HG2	7:B:4145:HOH:O	2.08	0.53
3:D:317:LYS:HA	3:D:320:GLN:HE21	1.74	0.53
3:C:199:ILE:HD11	3:C:208:ILE:HG13	1.90	0.53
3:A:158:ALA:HB2	3:A:164:LYS:HB2	1.91	0.52
3:B:180:ILE:HD13	3:B:194:LEU:HD13	1.91	0.52
3:D:89:MET:O	3:D:93:ARG:HG3	2.09	0.52
3:B:14:GLN:NE2	3:B:139:THR:H	2.05	0.52
3:C:280:ILE:HD12	3:D:52:LYS:HD3	1.91	0.52
3:C:175:ILE:O	3:C:203:VAL:HG13	2.10	0.52
3:A:257:ASN:HD22	3:A:258:LEU:N	2.07	0.51
3:C:277:ASP:O	3:C:278:LYS:HB2	2.10	0.51
3:B:153:ILE:O	3:B:157:MET:HG3	2.10	0.51
3:D:248:ILE:HG23	3:D:332:ARG:NH2	2.26	0.51
3:B:9:ASP:O	3:B:10:TYR:C	2.49	0.51
3:B:116:ARG:NH2	7:B:4126:HOH:O	2.44	0.51
3:B:320:GLN:O	3:B:324:GLU:HG3	2.11	0.51
3:B:317:LYS:HA	3:B:320:GLN:HE21	1.75	0.51
3:C:193:LYS:HB3	3:C:216:MET:SD	2.50	0.51
3:D:27:PRO:HG2	3:D:71:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:GLU:O	3:C:223:LYS:HG3	2.10	0.51
3:D:175:ILE:HG22	3:D:203:VAL:CG1	2.40	0.51
3:A:76:MET:HE3	3:A:78:LYS:HB2	1.93	0.51
3:C:317:LYS:HA	3:C:320:GLN:HE21	1.75	0.51
3:D:38:GLU:O	3:D:39:ASP:HB2	2.11	0.51
3:B:27:PRO:HG2	3:B:71:ALA:HA	1.92	0.50
3:C:210:PHE:HZ	3:C:219:GLU:HG3	1.76	0.50
1:F:13:DA:H5''	3:B:106:GLU:CD	2.31	0.50
3:B:171:VAL:O	3:B:175:ILE:HG13	2.10	0.50
2:I:6:DT:H5'	3:A:32:VAL:HG11	1.94	0.50
3:C:38:GLU:O	3:C:39:ASP:HB2	2.11	0.50
3:D:197:LEU:HD21	3:D:216:MET:HG3	1.94	0.50
1:H:13:DA:OP1	3:D:152:LYS:HE2	2.11	0.50
3:B:219:GLU:HG2	3:B:223:LYS:HD2	1.94	0.50
1:F:13:DA:H2''	6:B:4011:DDY:C4'	2.40	0.50
3:A:221:LYS:NZ	3:A:221:LYS:HB2	2.26	0.50
3:A:257:ASN:ND2	3:A:257:ASN:C	2.65	0.50
3:B:158:ALA:HB2	3:B:164:LYS:HB2	1.94	0.50
3:A:69:PRO:HG2	3:B:309:GLU:HG2	1.92	0.50
3:A:252:LYS:HE3	7:A:4199:HOH:O	2.12	0.49
3:A:12:TYR:OH	3:A:78:LYS:HE2	2.11	0.49
2:L:6:DT:H5'	3:D:32:VAL:HG11	1.94	0.49
2:I:3:DC:H2''	2:I:4:DA:O5'	2.12	0.49
3:A:277:ASP:O	3:A:278:LYS:HB2	2.12	0.49
3:A:27:PRO:HG2	3:A:71:ALA:HA	1.93	0.49
3:D:9:ASP:O	3:D:10:TYR:C	2.51	0.49
3:C:197:LEU:HD11	3:C:216:MET:HG3	1.95	0.49
3:D:258:LEU:HD13	3:D:258:LEU:C	2.32	0.48
3:D:251:MET:HG2	3:D:264:TYR:CD2	2.48	0.48
3:C:9:ASP:O	3:C:10:TYR:C	2.51	0.48
3:C:100:GLU:HG3	3:C:240:ARG:HD3	1.93	0.48
3:A:253:ARG:HD2	7:A:4095:HOH:O	2.12	0.48
3:D:39:ASP:CG	3:D:65:LYS:HE3	2.34	0.48
3:A:9:ASP:O	3:A:10:TYR:C	2.52	0.47
3:B:100:GLU:HB2	3:B:237:ILE:HG23	1.95	0.47
3:C:170:GLU:O	3:C:174:LEU:HG	2.14	0.47
3:C:258:LEU:HD11	3:C:262:LYS:HD2	1.95	0.47
3:A:180:ILE:HD13	3:A:194:LEU:HD13	1.95	0.47
2:L:16:DC:C2'	2:L:17:DC:C5'	2.87	0.47
3:C:14:GLN:NE2	3:C:139:THR:H	1.83	0.47
1:H:13:DA:OP1	3:D:152:LYS:CE	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:304:HIS:CD2	3:D:53:PHE:O	2.68	0.47
3:B:8:PHE:N	3:B:8:PHE:CD1	2.81	0.47
3:B:126:LEU:CD1	3:B:163:ILE:HD13	2.45	0.47
3:B:199:ILE:HG23	3:B:204:ASP:HB2	1.96	0.47
3:C:197:LEU:HD22	3:C:212:LYS:HE2	1.96	0.47
3:C:27:PRO:HG2	3:C:71:ALA:HA	1.97	0.47
1:G:3:DG:H2''	1:G:4:DG:H5'	1.96	0.47
3:A:190:THR:HG21	3:A:221:LYS:HD3	1.96	0.46
3:B:283:ALA:HB2	3:B:339:LYS:HD2	1.97	0.46
3:A:191:ALA:O	3:A:195:LYS:HD3	2.15	0.46
3:B:36:ARG:HH22	3:B:254:ASN:ND2	2.14	0.46
6:B:4011:DDY:H2'1	7:B:4094:HOH:O	2.16	0.46
3:C:199:ILE:HG23	3:C:204:ASP:HB2	1.97	0.46
2:K:8:DG:H5''	3:C:242:ARG:NH2	2.31	0.46
3:B:257:ASN:C	3:B:257:ASN:ND2	2.68	0.46
3:C:171:VAL:O	3:C:175:ILE:HG13	2.16	0.46
3:D:285:HIS:HD2	7:D:4119:HOH:O	1.97	0.46
3:D:283:ALA:HB2	3:D:339:LYS:HD2	1.98	0.46
2:J:3:DC:H5'	2:J:3:DC:H6	1.81	0.46
3:C:320:GLN:O	3:C:324:GLU:HG3	2.16	0.46
3:B:168:ASP:O	3:B:172:LYS:HG3	2.15	0.45
1:E:3:DG:H2''	1:E:4:DG:C5'	2.43	0.45
2:I:6:DT:H5'	3:A:32:VAL:CG1	2.46	0.45
3:D:100:GLU:HB2	3:D:237:ILE:HG23	1.97	0.45
3:D:276:LEU:O	3:D:277:ASP:O	2.35	0.45
3:D:248:ILE:HG21	7:D:4043:HOH:O	2.17	0.45
3:B:13:ALA:O	3:B:17:GLU:HG3	2.16	0.45
2:K:3:DC:O2	3:C:60:PRO:HG2	2.17	0.45
3:A:257:ASN:ND2	3:A:259:GLU:H	2.14	0.45
3:C:240:ARG:HG2	3:C:240:ARG:NH1	2.31	0.45
3:D:217:ILE:HD12	3:D:221:LYS:HB3	1.98	0.45
1:G:13:DA:OP1	3:C:152:LYS:HE2	2.17	0.45
3:C:31:CYS:HB3	3:C:61:ILE:HD11	1.98	0.45
3:C:324:GLU:HG3	7:C:4140:HOH:O	2.17	0.45
3:C:8:PHE:CD1	3:C:8:PHE:N	2.84	0.45
3:D:245:ILE:CD1	3:D:279:ARG:HH21	2.30	0.45
2:K:3:DC:H2''	2:K:4:DA:O5'	2.17	0.45
3:B:176:ARG:CG	3:B:203:VAL:HG21	2.35	0.44
7:K:455:HOH:O	3:C:248:ILE:HG22	2.16	0.44
2:K:2:DT:H72	3:C:253:ARG:HB3	1.99	0.44
3:C:242:ARG:NH1	3:C:242:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:8:DG:OP2	3:B:336:ARG:NH2	2.44	0.44
3:A:97:GLU:HA	3:A:97:GLU:OE1	2.18	0.44
1:E:8:DG:C2'	1:E:9:DG:H5''	2.47	0.44
3:D:133:LEU:O	3:D:137:LYS:HD2	2.18	0.44
3:D:36:ARG:HD2	3:D:250:THR:CG2	2.48	0.44
2:L:3:DC:H4'	3:D:62:VAL:HG21	2.00	0.43
3:D:277:ASP:O	3:D:278:LYS:HB2	2.17	0.43
1:E:8:DG:H2''	1:E:9:DG:H5''	1.99	0.43
3:D:68:LEU:HD13	3:D:71:ALA:HB2	2.00	0.43
3:B:180:ILE:HD11	3:B:225:LEU:HD13	2.01	0.43
2:J:8:DG:O5'	3:B:336:ARG:NH2	2.51	0.43
2:K:2:DT:H72	3:C:253:ARG:CB	2.49	0.43
7:F:489:HOH:O	3:B:189:ILE:HD13	2.18	0.43
3:D:76:MET:HE3	3:D:78:LYS:HB2	2.01	0.43
1:E:13:DA:H2''	6:A:4010:DDY:O4'	2.19	0.43
3:A:8:PHE:CD1	3:A:8:PHE:N	2.83	0.43
3:B:167:ASP:O	3:B:171:VAL:HG23	2.17	0.43
3:C:173:ARG:HH11	3:C:173:ARG:HG2	1.84	0.43
2:L:16:DC:H1'	2:L:17:DC:H5''	2.00	0.43
3:D:166:ILE:HG23	3:D:170:GLU:HB3	2.00	0.43
3:A:167:ASP:HB2	7:A:4195:HOH:O	2.19	0.42
3:C:273:TYR:HA	3:C:276:LEU:HD12	2.01	0.42
3:C:89:MET:O	3:C:93:ARG:HG3	2.19	0.42
3:A:245:ILE:HD12	3:A:276:LEU:HD23	2.00	0.42
3:A:256:ARG:NH2	3:A:326:ASP:O	2.44	0.42
3:D:251:MET:HE2	3:D:330:ILE:HG22	2.00	0.42
3:D:289:VAL:HB	3:D:332:ARG:HB2	2.00	0.42
3:A:208:ILE:HD11	3:A:212:LYS:HG2	2.02	0.42
3:C:167:ASP:O	3:C:171:VAL:HG23	2.20	0.42
3:C:335:VAL:HG22	3:C:336:ARG:N	2.34	0.42
3:D:39:ASP:OD1	3:D:65:LYS:HE3	2.19	0.42
2:K:8:DG:H5''	3:C:242:ARG:CZ	2.49	0.42
3:D:245:ILE:HD11	3:D:279:ARG:HH21	1.84	0.42
3:C:98:LYS:CB	3:C:110:ASP:HB3	2.50	0.42
3:B:258:LEU:CD1	3:B:262:LYS:HD2	2.50	0.41
1:E:8:DG:H1'	1:E:9:DG:H5''	2.02	0.41
3:B:176:ARG:HB2	3:B:176:ARG:NH1	2.35	0.41
3:C:197:LEU:CD2	3:C:212:LYS:HE2	2.49	0.41
3:D:31:CYS:HB3	3:D:61:ILE:CD1	2.51	0.41
1:G:3:DG:H2''	1:G:4:DG:C5'	2.50	0.41
1:F:13:DA:H5''	3:B:106:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:79:GLU:N	3:B:79:GLU:CD	2.68	0.41
6:B:4011:DDY:H5'2	7:B:4168:HOH:O	2.20	0.41
2:K:2:DT:O2	3:C:37:PHE:HB3	2.21	0.41
1:H:3:DG:C2'	1:H:4:DG:H5'	2.44	0.41
3:D:31:CYS:HB3	3:D:61:ILE:HD11	2.03	0.41
3:C:37:PHE:CD2	3:C:40:SER:HB3	2.56	0.41
3:D:184:PRO:HG3	7:D:4209:HOH:O	2.21	0.41
3:C:280:ILE:HD12	3:D:52:LYS:CD	2.50	0.41
3:D:221:LYS:HE2	7:D:4200:HOH:O	2.20	0.41
1:F:3:DG:H2''	1:F:4:DG:H5'	2.02	0.41
3:A:88:ILE:HD11	3:A:138:ILE:CD1	2.43	0.41
3:B:189:ILE:N	3:B:189:ILE:HD12	2.36	0.41
3:D:169:GLU:CD	3:D:169:GLU:H	2.23	0.41
3:D:261:ILE:CD1	3:D:330:ILE:HD12	2.51	0.41
2:J:3:DC:H2''	2:J:4:DA:O5'	2.21	0.41
3:B:122:TYR:CZ	3:B:126:LEU:HD11	2.56	0.41
3:B:126:LEU:HD12	3:B:163:ILE:CD1	2.51	0.41
2:K:6:DT:H5'	3:C:32:VAL:HG11	2.03	0.41
3:D:270:GLU:OE2	3:D:312:TYR:OH	2.33	0.40
3:B:83:GLN:O	3:B:87:ARG:HG3	2.22	0.40
3:C:258:LEU:CD1	3:C:262:LYS:HD2	2.52	0.40
3:D:176:ARG:CG	3:D:203:VAL:HG11	2.40	0.40
3:C:173:ARG:NH1	3:C:173:ARG:HG2	2.36	0.40
3:C:31:CYS:HB3	3:C:61:ILE:CD1	2.51	0.40
3:A:13:ALA:O	3:A:17:GLU:HG3	2.20	0.40
3:A:321:LYS:O	3:A:325:GLU:HG3	2.22	0.40
3:B:166:ILE:HG23	3:B:170:GLU:HB3	2.02	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	
3	A	339/352 (96%)	329 (97%)	8 (2%)	2 (1%)	25	19
3	B	339/352 (96%)	331 (98%)	6 (2%)	2 (1%)	25	19
3	C	339/352 (96%)	322 (95%)	16 (5%)	1 (0%)	41	37
3	D	339/352 (96%)	328 (97%)	9 (3%)	2 (1%)	25	19
All	All	1356/1408 (96%)	1310 (97%)	39 (3%)	7 (0%)	29	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	277	ASP
3	D	277	ASP
3	B	277	ASP
3	C	10	TYR
3	D	10	TYR
3	A	10	TYR
3	B	10	TYR

5.3.2 Protein sidechains ⓘ

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	
3	A	298/309 (96%)	295 (99%)	3 (1%)	76	81
3	B	299/309 (97%)	292 (98%)	7 (2%)	50	53
3	C	298/309 (96%)	289 (97%)	9 (3%)	41	41
3	D	297/309 (96%)	289 (97%)	8 (3%)	44	46
All	All	1192/1236 (96%)	1165 (98%)	27 (2%)	50	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	161	ASN
3	A	168	ASP
3	A	257	ASN
3	B	142	VAL

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Mol	Chain	Res	Type
3	B	161	ASN
3	B	164	LYS
3	B	168	ASP
3	B	256	ARG
3	B	257	ASN
3	B	336	ARG
3	C	49	GLU
3	C	79	GLU
3	C	126	LEU
3	C	127	GLU
3	C	146	LYS
3	C	161	ASN
3	C	216	MET
3	C	240	ARG
3	C	242	ARG
3	D	56	LYS
3	D	105	ASP
3	D	161	ASN
3	D	168	ASP
3	D	211	ASP
3	D	256	ARG
3	D	257	ASN
3	D	273	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	83	GLN
3	A	161	ASN
3	A	254	ASN
3	A	257	ASN
3	A	304	HIS
3	A	320	GLN
3	B	14	GLN
3	B	70	ASN
3	B	82	GLN
3	B	83	GLN
3	B	161	ASN
3	B	188	ASN
3	B	254	ASN
3	B	257	ASN

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Mol	Chain	Res	Type
3	B	285	HIS
3	B	320	GLN
3	C	14	GLN
3	C	70	ASN
3	C	130	ASN
3	C	161	ASN
3	C	254	ASN
3	C	304	HIS
3	C	320	GLN
3	D	14	GLN
3	D	70	ASN
3	D	83	GLN
3	D	161	ASN
3	D	254	ASN
3	D	257	ASN
3	D	285	HIS
3	D	304	HIS
3	D	320	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	DDY	A	4010	4	20,24,24	3.20	6 (30%)	24,36,36	2.60	7 (29%)
6	DDY	C	4012	4	20,24,24	3.22	7 (35%)	24,36,36	2.60	8 (33%)
6	DDY	B	4011	4	20,24,24	3.21	6 (30%)	24,36,36	2.73	9 (37%)
6	DDY	D	4013	4	20,24,24	3.24	6 (30%)	24,36,36	2.59	8 (33%)

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	DDY	A	4010	4	-	3/13/25/25	0/2/2/2
6	DDY	C	4012	4	-	3/13/25/25	0/2/2/2
6	DDY	B	4011	4	-	2/13/25/25	0/2/2/2
6	DDY	D	4013	4	-	3/13/25/25	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	4013	DDY	C2'-C1'	-8.17	1.33	1.51
6	A	4010	DDY	C2'-C1'	-8.16	1.33	1.51
6	C	4012	DDY	C2'-C1'	-8.15	1.33	1.51
6	D	4013	DDY	C2'-C3'	-7.95	1.32	1.54
6	B	4011	DDY	C2'-C3'	-7.91	1.32	1.54
6	A	4010	DDY	C2'-C3'	-7.89	1.32	1.54
6	B	4011	DDY	C2'-C1'	-7.85	1.33	1.51
6	C	4012	DDY	C2'-C3'	-7.85	1.32	1.54
6	B	4011	DDY	C6-N1	5.38	1.42	1.35
6	D	4013	DDY	C6-N1	5.31	1.42	1.35
6	C	4012	DDY	C6-N1	5.16	1.42	1.35
6	A	4010	DDY	C6-N1	5.04	1.42	1.35
6	B	4011	DDY	C4-N3	3.73	1.41	1.35
6	C	4012	DDY	C4-N3	3.72	1.41	1.35
6	D	4013	DDY	C4-N3	3.70	1.41	1.35
6	B	4011	DDY	C3'-C4'	-3.65	1.33	1.52
6	C	4012	DDY	C3'-C4'	-3.54	1.33	1.52
6	D	4013	DDY	C3'-C4'	-3.52	1.33	1.52
6	A	4010	DDY	C3'-C4'	-3.47	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4010	DDY	C4-N3	3.39	1.41	1.35
6	B	4011	DDY	PB-O3B	3.20	1.60	1.50
6	D	4013	DDY	PB-O3B	3.04	1.60	1.50
6	C	4012	DDY	PB-O3B	2.98	1.60	1.50
6	A	4010	DDY	PB-O3B	2.96	1.60	1.50
6	C	4012	DDY	PB-O1B	-2.12	1.46	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4011	DDY	C3'-C2'-C1'	7.74	111.73	102.78
6	C	4012	DDY	C3'-C2'-C1'	7.73	111.71	102.78
6	A	4010	DDY	C3'-C2'-C1'	7.53	111.48	102.78
6	D	4013	DDY	C3'-C2'-C1'	7.45	111.40	102.78
6	B	4011	DDY	C4'-O4'-C1'	-5.75	104.38	109.81
6	D	4013	DDY	C4'-O4'-C1'	-5.72	104.41	109.81
6	A	4010	DDY	C4'-O4'-C1'	-5.47	104.65	109.81
6	C	4012	DDY	C4'-O4'-C1'	-5.03	105.06	109.81
6	A	4010	DDY	C2'-C3'-C4'	4.91	111.92	102.72
6	C	4012	DDY	C2'-C3'-C4'	4.89	111.89	102.72
6	D	4013	DDY	C2'-C3'-C4'	4.72	111.56	102.72
6	B	4011	DDY	C2'-C3'-C4'	4.41	111.00	102.72
6	B	4011	DDY	C2-N3-C4	4.12	120.51	116.34
6	A	4010	DDY	C2-N3-C4	4.00	120.39	116.34
6	C	4012	DDY	C2-N3-C4	3.92	120.31	116.34
6	D	4013	DDY	C2-N3-C4	3.86	120.25	116.34
6	B	4011	DDY	O4'-C1'-C2'	-3.44	102.95	106.67
6	B	4011	DDY	O2B-PB-O1B	2.90	118.71	107.64
6	C	4012	DDY	O4'-C1'-C2'	-2.77	103.67	106.67
6	D	4013	DDY	O4'-C1'-C2'	-2.70	103.75	106.67
6	A	4010	DDY	O2B-PB-O1B	2.67	117.83	107.64
6	D	4013	DDY	O2B-PB-O1B	2.63	117.69	107.64
6	A	4010	DDY	O4'-C1'-C2'	-2.63	103.83	106.67
6	C	4012	DDY	O2B-PB-O1B	2.58	117.51	107.64
6	B	4011	DDY	PA-O3A-PB	-2.55	124.08	132.83
6	C	4012	DDY	PA-O3A-PB	-2.39	124.64	132.83
6	C	4012	DDY	N4-C4-N3	2.12	119.84	116.49
6	A	4010	DDY	PA-O3A-PB	-2.12	125.56	132.83
6	D	4013	DDY	N4-C4-N3	2.08	119.78	116.49
6	B	4011	DDY	N4-C4-N3	2.06	119.75	116.49
6	D	4013	DDY	PA-O3A-PB	-2.05	125.80	132.83
6	B	4011	DDY	O4'-C4'-C5'	2.03	112.85	109.52

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4010	DDY	C5'-O5'-PA-O1A
6	A	4010	DDY	C5'-O5'-PA-O2A
6	C	4012	DDY	C5'-O5'-PA-O1A
6	C	4012	DDY	C5'-O5'-PA-O2A
6	D	4013	DDY	C5'-O5'-PA-O1A
6	D	4013	DDY	C5'-O5'-PA-O2A
6	B	4011	DDY	PA-O3A-PB-O1B
6	A	4010	DDY	C5'-O5'-PA-O3A
6	C	4012	DDY	C5'-O5'-PA-O3A
6	D	4013	DDY	C5'-O5'-PA-O3A
6	B	4011	DDY	PA-O3A-PB-O3B

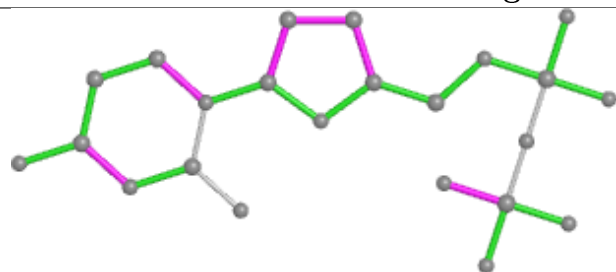
There are no ring outliers.

4 monomers are involved in 8 short contacts:

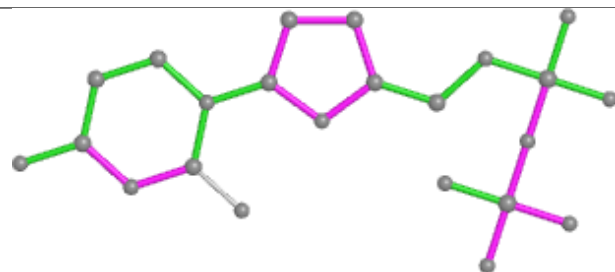
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4010	DDY	2	0
6	C	4012	DDY	1	0
6	B	4011	DDY	4	0
6	D	4013	DDY	1	0

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 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.

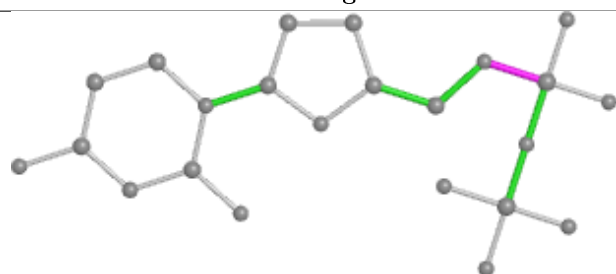
Ligand DDY A 4010



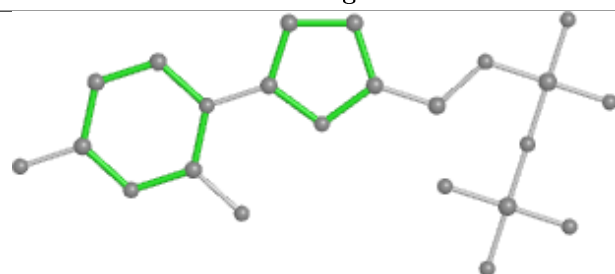
Bond lengths



Bond angles

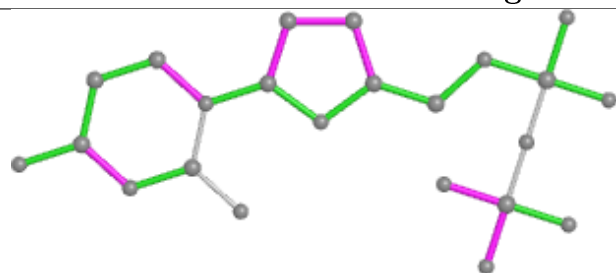


Torsions

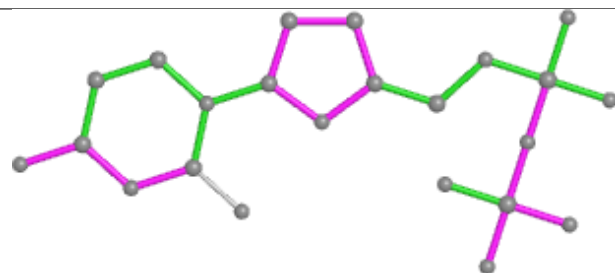


Rings

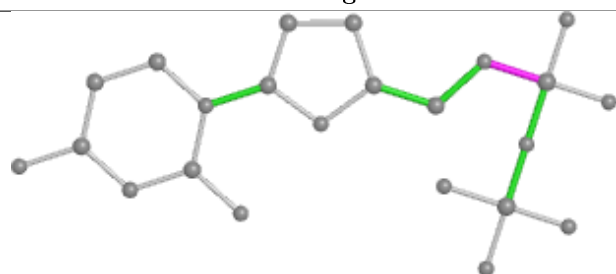
Ligand DDY C 4012



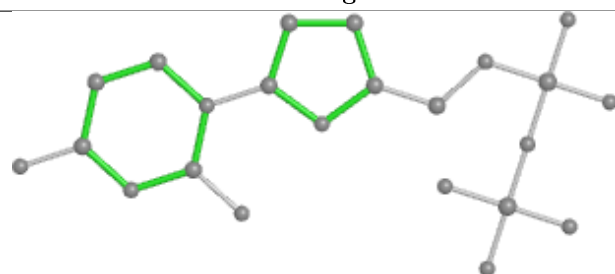
Bond lengths



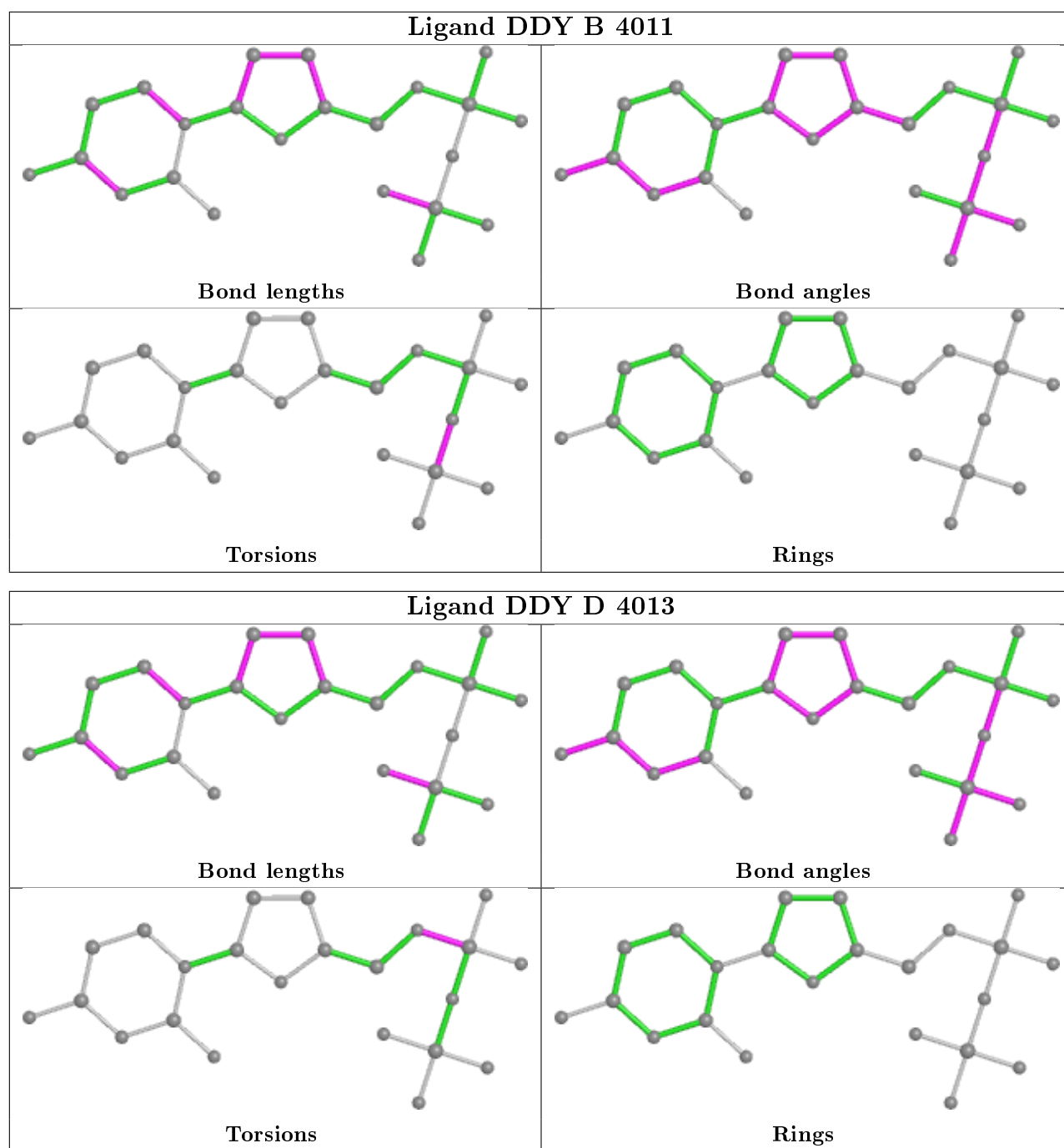
Bond angles



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	13/13 (100%)	-0.27	0 100 100	28, 33, 40, 40	0
1	F	13/13 (100%)	-0.36	0 100 100	27, 33, 39, 43	0
1	G	13/13 (100%)	-0.39	0 100 100	24, 31, 35, 37	0
1	H	13/13 (100%)	-0.19	0 100 100	28, 33, 43, 48	0
2	I	17/18 (94%)	0.30	2 (11%) 4 4	26, 34, 92, 103	0
2	J	17/18 (94%)	0.09	2 (11%) 4 4	24, 32, 70, 90	0
2	K	17/18 (94%)	-0.18	1 (5%) 22 21	22, 32, 64, 82	0
2	L	17/18 (94%)	-0.26	0 100 100	25, 33, 58, 69	0
3	A	341/352 (96%)	-0.11	3 (0%) 84 83	17, 29, 47, 54	1 (0%)
3	B	341/352 (96%)	-0.01	8 (2%) 60 59	18, 33, 50, 59	1 (0%)
3	C	341/352 (96%)	0.10	9 (2%) 56 54	17, 31, 52, 61	1 (0%)
3	D	341/352 (96%)	-0.06	5 (1%) 73 72	15, 29, 47, 62	1 (0%)
All	All	1484/1532 (96%)	-0.03	30 (2%) 65 63	15, 31, 49, 103	4 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	2	DT	4.7
2	I	3	DC	4.7
2	J	2	DT	4.6
3	D	277	ASP	3.9
3	B	240	ARG	3.7
3	D	38	GLU	3.6
3	D	1	MET	3.3
3	C	210	PHE	3.1
3	C	274	TYR	3.1
3	A	241	VAL	2.8
3	A	38	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	327	GLU	2.8
3	C	234	ASN	2.7
2	K	2	DT	2.6
3	B	211	ASP	2.6
3	B	1	MET	2.6
3	D	274	TYR	2.4
3	B	234	ASN	2.4
3	B	210	PHE	2.3
3	C	116	ARG	2.3
3	B	38	GLU	2.3
2	J	3	DC	2.2
3	B	97	GLU	2.2
3	D	278	LYS	2.2
3	C	1	MET	2.2
3	A	327	GLU	2.1
3	B	209	GLU	2.1
3	C	232	GLU	2.1
3	C	203	VAL	2.1
3	C	211	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	B	4008	1/1	0.88	0.11	39,39,39,39	0
6	DDY	B	4011	23/23	0.93	0.14	40,44,48,49	0
4	CA	B	4002	1/1	0.95	0.12	44,44,44,44	0
5	MG	A	4007	1/1	0.96	0.06	38,38,38,38	0

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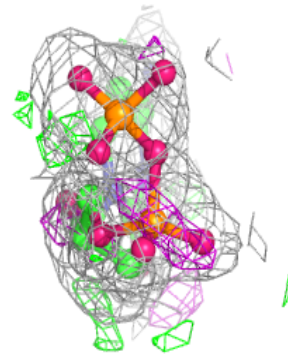
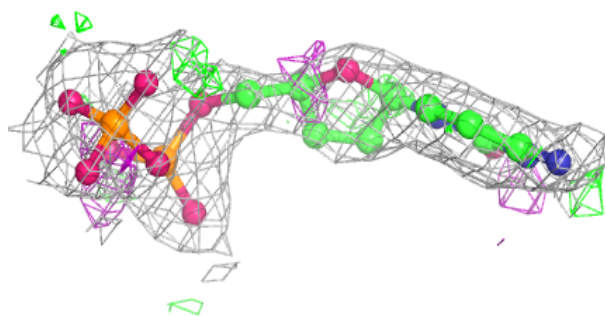
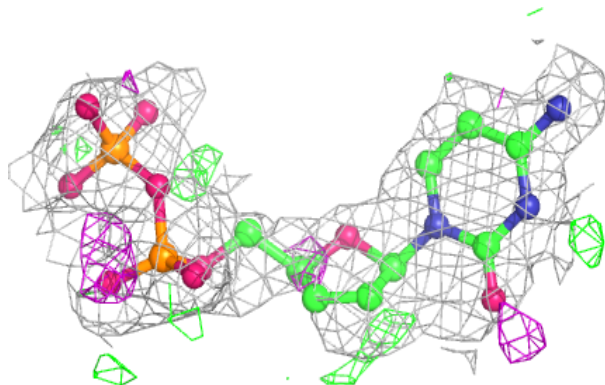
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	4005	1/1	0.96	0.12	28,28,28,28	0
6	DDY	D	4013	23/23	0.97	0.12	17,22,27,28	0
6	DDY	C	4012	23/23	0.97	0.10	20,26,29,31	0
6	DDY	A	4010	23/23	0.97	0.12	21,27,32,32	0
5	MG	D	4006	1/1	0.98	0.05	35,35,35,35	0
4	CA	A	4001	1/1	0.99	0.12	22,22,22,22	0
4	CA	C	4003	1/1	0.99	0.12	26,26,26,26	0
4	CA	D	4004	1/1	1.00	0.14	19,19,19,19	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.

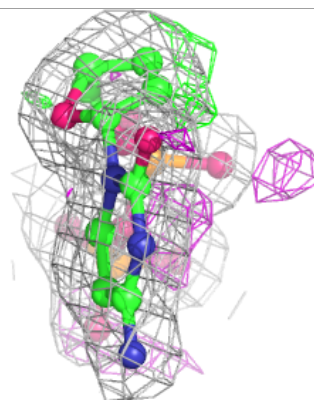
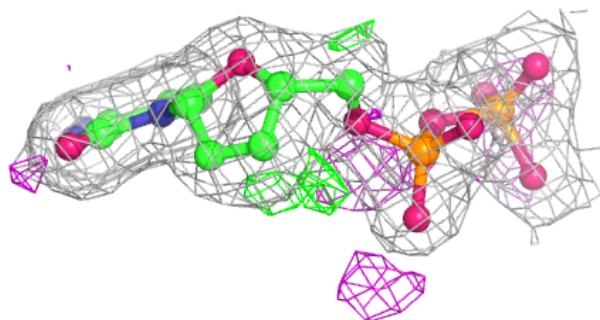
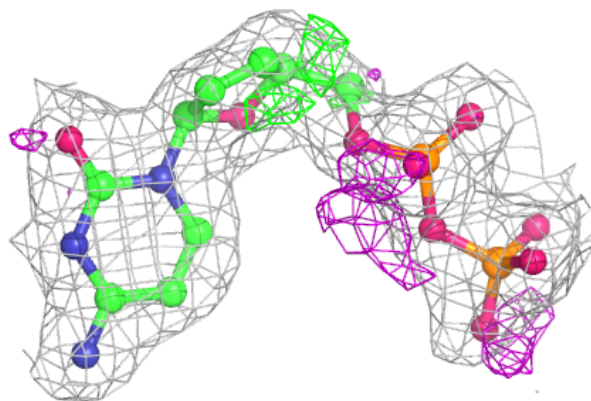
Electron density around DDY B 4011:

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

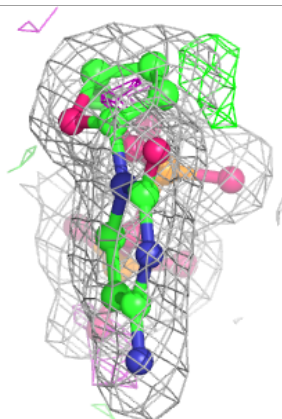
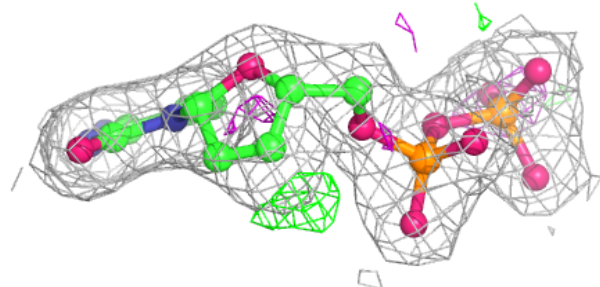
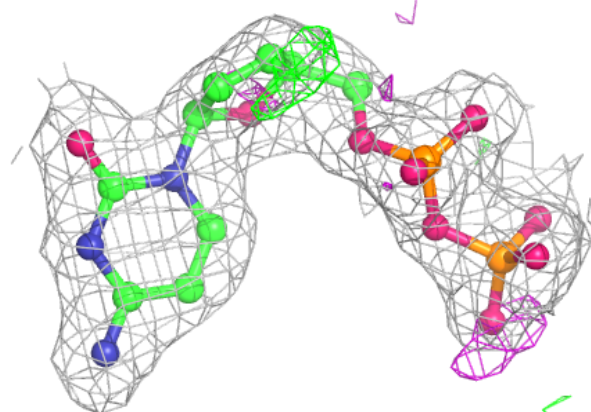


Electron density around DDY D 4013:

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

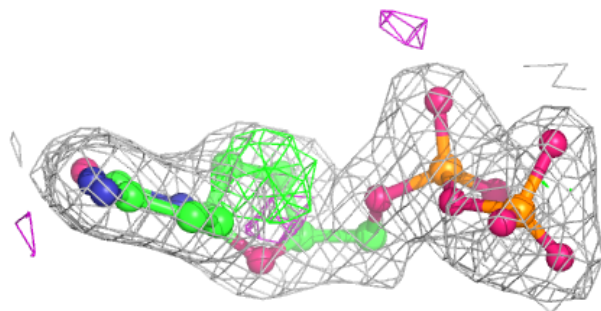
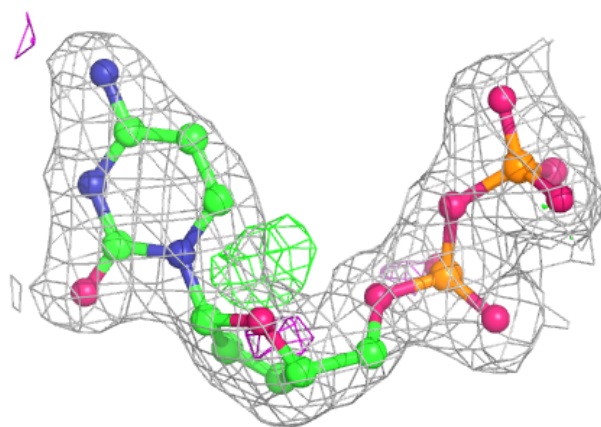
**Electron density around DDY C 4012:**

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



Electron density around DDY A 4010:

$2mF_o-DF_c$ (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.