



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:21 AM UTC

PDB ID : 3V6J / pdb_00003v6j
Title : Replication of N2,3-Ethenoguanine by DNA Polymerases
Authors : Zhao, L.
Deposited on : 2011-12-19
Resolution : 2.30 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 types of validation reports are described at

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

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

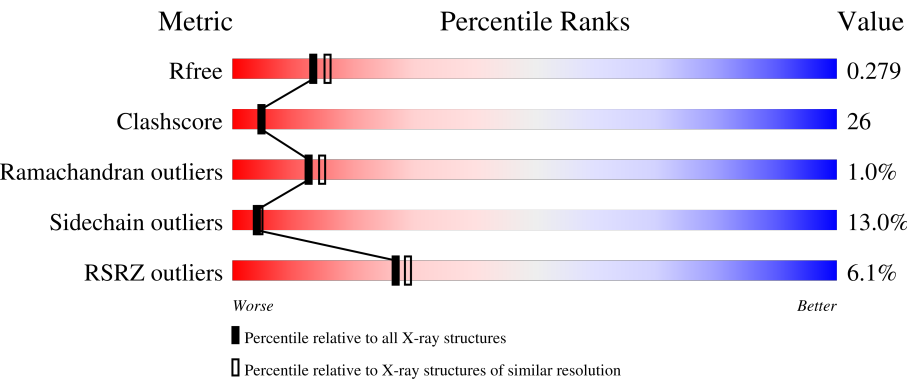
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	348	4% 63% 30% 5%
1	J	348	7% 63% 25% 10%
2	K	12	25% 17% 58% 17% 8%
2	P	12	8% 33% 25% 42%
3	B	17	12% 35% 18% 47%

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Mol	Chain	Length	Quality of chain
3	M	17	

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
2	DOC	K	13	-	-	X	-
3	EFG	M	5	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6824 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	2	0	0
			2762	1771	476	508	7			
1	J	343	Total	C	N	O	S	1	0	0
			2754	1765	474	508	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q97W02
A	-4	HIS	-	expression tag	UNP Q97W02
A	-3	HIS	-	expression tag	UNP Q97W02
A	-2	HIS	-	expression tag	UNP Q97W02
A	-1	HIS	-	expression tag	UNP Q97W02
A	0	HIS	-	expression tag	UNP Q97W02
J	-5	HIS	-	expression tag	UNP Q97W02
J	-4	HIS	-	expression tag	UNP Q97W02
J	-3	HIS	-	expression tag	UNP Q97W02
J	-2	HIS	-	expression tag	UNP Q97W02
J	-1	HIS	-	expression tag	UNP Q97W02
J	0	HIS	-	expression tag	UNP Q97W02

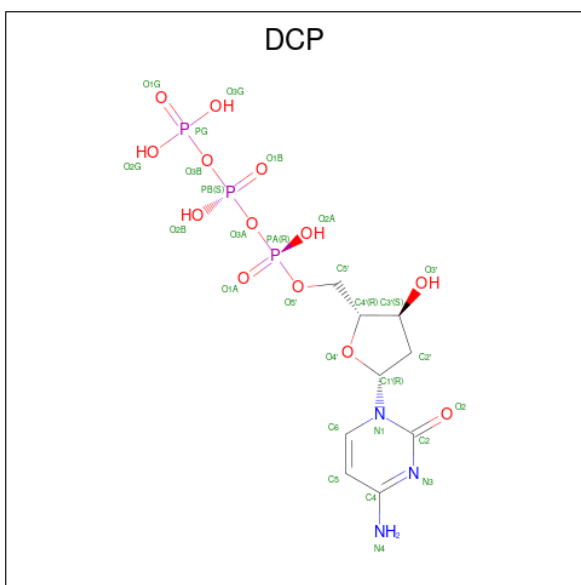
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	P	0	0	0
			250	119	52	68	11			
2	K	11	Total	C	N	O	P	0	0	0
			231	109	47	64	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	17	Total 340	C 165	F 1	N 56	O 102	P 16	0	0	0
3	M	13	Total 264	C 127	F 1	N 43	O 80	P 13	0	0	0

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
4	J	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	J	2	Total Mg 2 2	0	0
5	K	1	Total Mg 1 1	0	0

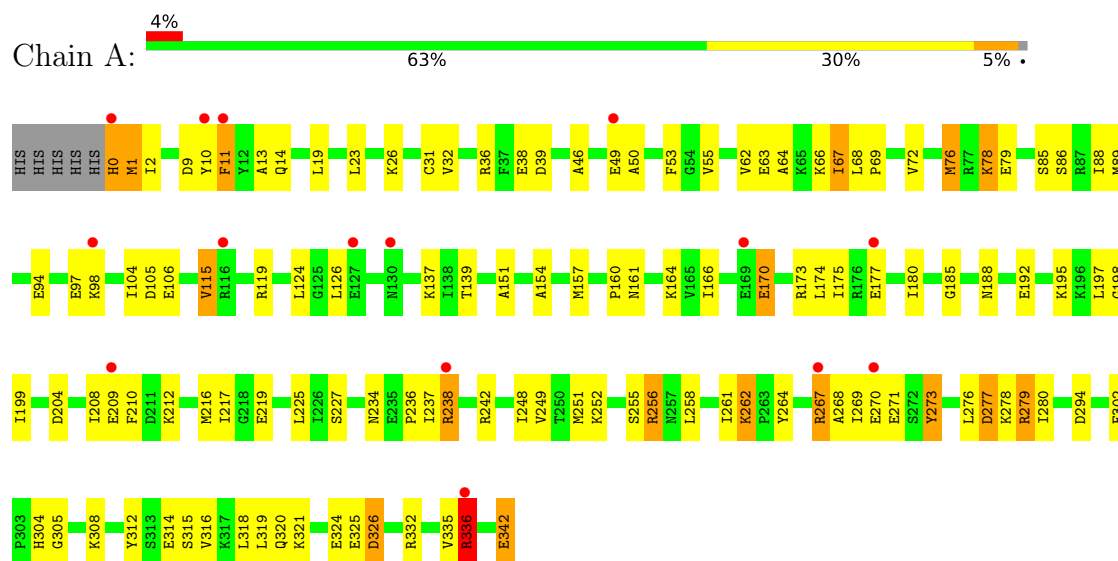
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total 99	O 99	0	0
6	J	43	Total 43	O 43	0	0
6	P	7	Total 7	O 7	0	0
6	B	8	Total 8	O 8	0	0
6	K	3	Total 3	O 3	0	0
6	M	2	Total 2	O 2	0	0

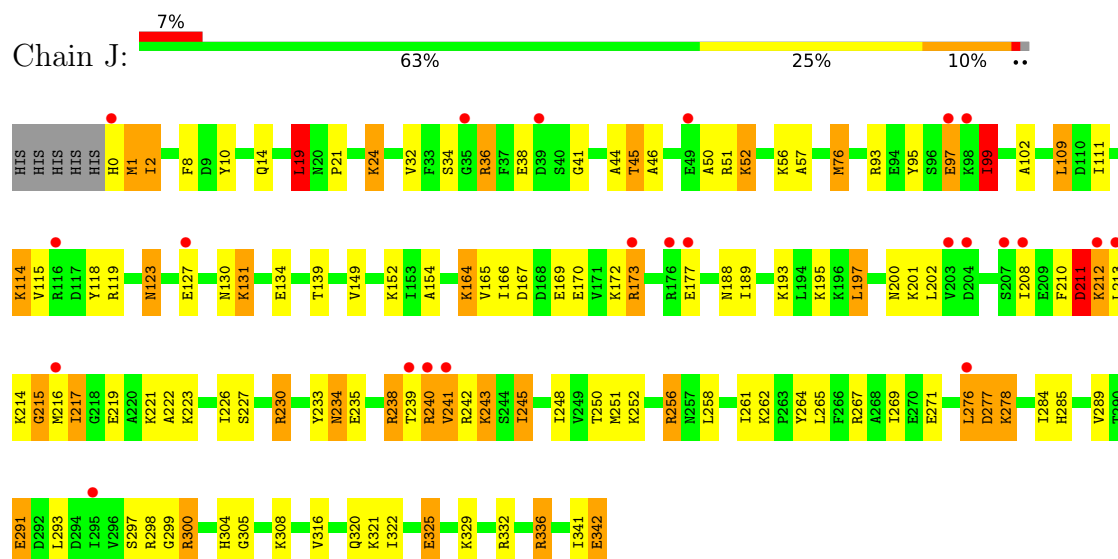
3 Residue-property plots [i](#)

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.

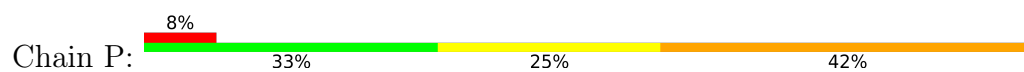
• Molecule 1: DNA polymerase IV



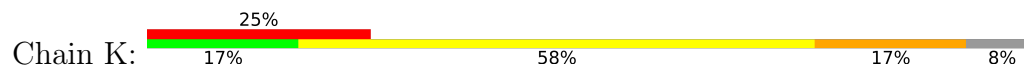
• Molecule 1: DNA polymerase IV



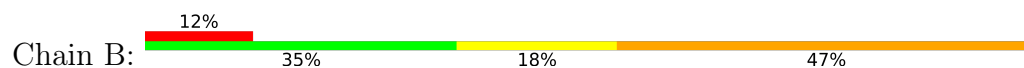
• Molecule 2: DNA (5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC))-3')



● Molecule 2: DNA (5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC))-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.70Å 111.42Å 98.81Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	29.84 – 2.30 29.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.84-2.30) 97.8 (29.84-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.273 0.220 , 0.279	Depositor DCC
R_{free} test set	2456 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DCP, MG, EFG, DOC

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	1.24	5/2802 (0.2%)	1.38	18/3763 (0.5%)
1	J	0.97	3/2794 (0.1%)	1.19	9/3755 (0.2%)
2	K	0.38	0/240	1.04	2/370 (0.5%)
2	P	0.77	1/262 (0.4%)	1.25	5/405 (1.2%)
3	B	0.60	0/349	1.59	13/532 (2.4%)
3	M	0.76	2/264 (0.8%)	1.19	2/401 (0.5%)
All	All	1.05	11/6711 (0.2%)	1.29	49/9226 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	4	DG	O3'-P	-8.49	1.48	1.61
3	M	7	DA	O3'-P	-8.01	1.49	1.61
1	A	76	MET	N-CA	-6.81	1.37	1.46
1	J	278	LYS	N-CA	6.76	1.54	1.46
3	M	6	DG	O3'-P	6.71	1.71	1.61
1	A	86	SER	C-O	-5.85	1.17	1.24
1	A	124	LEU	CA-C	5.72	1.60	1.52
1	A	335	VAL	C-O	-5.54	1.18	1.24
1	A	62	VAL	CA-CB	5.51	1.60	1.54
1	J	56	LYS	CA-C	5.43	1.59	1.52
1	J	19	LEU	C-O	-5.26	1.17	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	240	ARG	N-CA-C	11.89	128.50	112.68
3	M	6	DG	P-O3'-C3'	10.42	135.83	120.20
2	P	3	DG	P-O3'-C3'	8.87	133.50	120.20
3	B	2	DC	O3'-P-O5'	8.50	116.75	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	277	ASP	CA-C-N	-8.05	112.21	126.45
1	J	277	ASP	C-N-CA	-8.05	112.21	126.45
1	A	271	GLU	N-CA-C	-8.02	102.40	112.90
3	B	1	DT	P-O3'-C3'	7.89	132.04	120.20
1	A	2	ILE	N-CA-C	7.70	120.01	108.23
3	B	8	DA	O3'-P-O5'	-7.45	92.83	104.00
3	B	10	DC	C4'-C3'-O3'	7.28	120.92	110.00
1	J	322	ILE	N-CA-C	-7.12	106.13	111.90
1	A	262	LYS	CA-C-N	-7.05	111.52	119.28
1	A	262	LYS	C-N-CA	-7.05	111.52	119.28
2	P	2	DG	O3'-P-O5'	6.94	114.41	104.00
1	A	67	ILE	CB-CA-C	-6.92	100.88	112.16
1	A	217	ILE	N-CA-C	6.83	119.72	113.10
3	B	11	DC	O3'-P-O5'	-6.78	93.83	104.00
3	B	10	DC	C2'-C3'-O3'	-6.73	101.41	111.50
3	B	6	DG	C4'-C3'-O3'	-6.57	100.15	110.00
2	P	2	DG	P-O3'-C3'	6.54	130.00	120.20
1	A	13	ALA	N-CA-C	-6.32	104.47	111.36
1	A	185	GLY	N-CA-C	-6.21	106.75	115.32
1	J	316	VAL	N-CA-C	-6.13	104.77	110.53
2	K	11	DT	P-O3'-C3'	6.09	129.33	120.20
1	J	57	ALA	CA-C-N	-6.06	116.23	123.44
1	J	57	ALA	C-N-CA	-6.06	116.23	123.44
1	J	256	ARG	N-CA-C	-6.00	105.69	114.39
3	B	9	DT	O3'-P-O5'	5.93	112.89	104.00
2	P	11	DT	P-O3'-C3'	5.90	129.06	120.20
3	B	8	DA	C2'-C3'-O3'	-5.89	102.67	111.50
3	B	10	DC	P-O3'-C3'	-5.88	111.38	120.20
1	A	31	CYS	N-CA-C	5.86	119.02	109.59
1	A	126	LEU	CA-C-O	-5.72	114.36	120.42
3	B	1	DT	C4'-C3'-O3'	-5.68	101.47	110.00
3	M	14	DC	P-O3'-C3'	5.63	128.64	120.20
1	A	161	ASN	CA-C-N	-5.58	116.53	122.67
1	A	161	ASN	C-N-CA	-5.58	116.53	122.67
1	A	11	PHE	N-CA-C	5.58	122.68	110.80
1	J	217	ILE	N-CA-C	5.53	117.53	111.77
1	A	106	GLU	N-CA-C	5.52	117.65	108.99
1	A	336	ARG	CG-CD-NE	-5.46	99.99	112.00
2	K	11	DT	C2'-C3'-O3'	5.44	119.66	111.50
1	A	88	ILE	N-CA-C	-5.32	105.20	111.00
1	A	115	VAL	N-CA-C	-5.30	101.35	108.35
3	B	9	DT	C5'-C4'-C3'	-5.26	107.00	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	10	DA	P-O3'-C3'	5.22	128.03	120.20
1	A	151	ALA	N-CA-C	-5.11	105.80	111.36
3	B	6	DG	N9-C1'-C2'	5.00	121.01	113.50

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	2762	0	2902	102	0
1	J	2754	0	2880	128	0
2	K	231	0	124	35	0
2	P	250	0	136	20	0
3	B	340	0	193	44	0
3	M	264	0	147	35	0
4	A	28	0	12	2	0
4	J	28	0	12	6	0
5	A	2	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
6	A	99	0	0	12	0
6	B	8	0	0	2	0
6	J	43	0	0	6	0
6	K	3	0	0	1	0
6	M	2	0	0	0	0
6	P	7	0	0	0	0
All	All	6824	0	6406	325	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 26.

All (325) 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:B:10:DC:C6	3:B:10:DC:H5''	1.67	1.27
1:A:66:LYS:HA	6:A:573:HOH:O	1.36	1.25
2:K:9:DG:H2'	6:K:202:HOH:O	1.36	1.21
1:A:195:LYS:HE2	6:A:585:HOH:O	1.36	1.20
1:J:341:ILE:CG2	1:J:342:GLU:H	1.55	1.19
2:K:12:DT:H2''	2:K:13:DOC:H6	1.26	1.16
1:A:248:ILE:HD11	6:A:512:HOH:O	1.47	1.15
1:J:342:GLU:HG3	1:J:342:GLU:O	1.48	1.11
3:B:10:DC:H3'	6:B:101:HOH:O	1.48	1.10
1:J:164:LYS:HD2	1:J:165:VAL:O	1.53	1.07
3:B:10:DC:H4'	3:B:10:DC:OP1	1.30	1.07
1:J:211:ASP:OD1	1:J:211:ASP:C	2.00	1.02
1:J:341:ILE:HG22	1:J:342:GLU:N	1.54	1.02
2:P:12:DT:N3	3:B:7:DA:H2	1.56	1.01
3:B:10:DC:H6	3:B:10:DC:C5'	1.73	1.00
2:K:12:DT:H2''	2:K:13:DOC:C6	1.91	1.00
1:J:170:GLU:HG2	1:J:173:ARG:HD2	1.44	1.00
1:J:14:GLN:HE22	1:J:139:THR:H	1.01	0.99
3:B:10:DC:OP1	3:B:10:DC:C4'	2.10	0.99
1:A:264:TYR:O	1:A:267:ARG:HG3	1.61	0.98
2:P:12:DT:N3	3:B:7:DA:C2	2.28	0.98
2:K:11:DT:H3	3:M:8:DA:H2	0.96	0.95
1:J:238:ARG:HG3	1:J:238:ARG:O	1.65	0.95
3:B:10:DC:H5''	3:B:10:DC:H6	0.78	0.94
1:A:157:MET:CE	1:A:164:LYS:HE3	1.99	0.93
2:K:12:DT:H2'	2:K:13:DOC:H5	1.52	0.92
3:B:9:DT:H5''	3:B:9:DT:H6	1.32	0.92
1:J:341:ILE:HG22	1:J:342:GLU:H	0.76	0.91
2:P:2:DG:H2'	2:P:3:DG:O4'	1.71	0.91
1:J:173:ARG:HH11	1:J:173:ARG:CG	1.81	0.90
1:J:164:LYS:CD	1:J:165:VAL:O	2.20	0.90
1:J:189:ILE:O	1:J:193:LYS:HG3	1.71	0.89
1:J:173:ARG:HH11	1:J:173:ARG:HG2	1.35	0.89
3:M:5:EFG:H10	3:M:5:EFG:H1'	1.55	0.89
2:K:12:DT:O2	3:M:7:DA:H2	1.56	0.88
1:J:164:LYS:HE3	1:J:165:VAL:O	1.74	0.87
1:A:270:GLU:CD	1:A:312:TYR:HH	1.83	0.87
4:J:401:DCP:H5'2	6:J:503:HOH:O	1.75	0.86
2:P:12:DT:H3	3:B:7:DA:H2	0.90	0.84
1:J:99:ILE:HG13	1:J:109:LEU:CD2	2.08	0.83
1:J:211:ASP:OD1	1:J:211:ASP:O	1.97	0.82
1:J:336:ARG:HH22	3:M:8:DA:P	2.03	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PRO:HA	6:A:564:HOH:O	1.79	0.81
1:J:164:LYS:CE	1:J:165:VAL:O	2.29	0.81
1:A:1:MET:HE2	1:A:234:ASN:OD1	1.81	0.80
1:A:264:TYR:O	1:A:267:ARG:CG	2.30	0.80
1:A:10:TYR:CZ	1:A:14:GLN:HG3	2.17	0.80
3:M:12:DT:H1'	3:M:13:DT:H5'	1.64	0.80
2:K:11:DT:H2'	2:K:12:DT:H71	1.64	0.80
2:K:12:DT:N3	3:M:7:DA:C2	2.50	0.80
1:A:10:TYR:OH	1:A:14:GLN:HG3	1.82	0.79
1:J:238:ARG:HD2	1:J:239:THR:O	1.83	0.79
1:J:99:ILE:HG13	1:J:109:LEU:HD22	1.62	0.79
1:J:300:ARG:HG3	6:J:530:HOH:O	1.83	0.79
2:K:12:DT:C2'	2:K:13:DOC:C6	2.61	0.79
2:K:12:DT:C2	3:M:7:DA:H2	2.00	0.79
1:A:0:HIS:O	1:A:1:MET:HB3	1.82	0.78
1:A:0:HIS:O	1:A:1:MET:CB	2.32	0.78
1:A:157:MET:HE3	1:A:164:LYS:HE3	1.63	0.77
1:J:24:LYS:HA	6:J:521:HOH:O	1.84	0.77
1:J:14:GLN:NE2	1:J:139:THR:H	1.82	0.77
2:P:2:DG:H2'	2:P:3:DG:C4'	2.14	0.77
1:A:249:VAL:HG11	1:A:267:ARG:NE	2.00	0.77
1:A:63:GLU:OE2	1:A:66:LYS:HE2	1.85	0.76
4:J:401:DCP:H1'	2:K:13:DOC:H2'	1.67	0.76
1:J:251:MET:HG2	1:J:264:TYR:CD2	2.20	0.76
2:K:12:DT:C2'	2:K:13:DOC:C5	2.64	0.75
1:J:114:LYS:HA	1:J:114:LYS:HE2	1.67	0.75
1:J:173:ARG:CG	1:J:173:ARG:NH1	2.46	0.74
1:A:248:ILE:HD11	6:A:565:HOH:O	1.86	0.74
1:J:164:LYS:HD2	1:J:165:VAL:N	2.02	0.74
1:J:52:LYS:HD2	6:J:537:HOH:O	1.86	0.74
1:A:277:ASP:O	1:A:278:LYS:HB2	1.88	0.74
1:J:210:PHE:CE1	1:J:214:LYS:HB2	2.22	0.74
4:J:401:DCP:C1'	2:K:13:DOC:H2'	2.18	0.74
1:J:291:GLU:HG2	1:J:329:LYS:HB2	1.69	0.73
2:K:12:DT:H2'	2:K:13:DOC:C5	2.18	0.73
3:M:12:DT:H2''	3:M:13:DT:OP2	1.89	0.73
3:M:5:EFG:H1'	3:M:5:EFG:C9	2.19	0.72
1:J:277:ASP:O	1:J:278:LYS:CB	2.34	0.72
3:B:10:DC:C6	3:B:10:DC:C5'	2.59	0.72
1:A:154:ALA:HB2	1:A:166:ILE:HD12	1.70	0.72
1:A:67:ILE:O	1:A:67:ILE:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:NH1	3:B:6:DG:H21	1.87	0.71
1:A:270:GLU:CD	1:A:312:TYR:OH	2.32	0.71
3:B:1:DT:C6	3:B:1:DT:C5'	2.74	0.71
2:P:12:DT:C2	3:B:7:DA:H2	2.08	0.71
1:A:14:GLN:HE22	1:A:139:THR:H	1.39	0.70
1:A:157:MET:HE1	1:A:164:LYS:HE3	1.74	0.70
1:J:267:ARG:NH1	1:J:271:GLU:OE2	2.24	0.70
1:J:211:ASP:CG	1:J:212:LYS:HD3	2.16	0.69
1:J:336:ARG:NH2	3:M:8:DA:OP2	2.26	0.69
2:P:3:DG:C2'	2:P:4:DG:C8	2.76	0.69
1:J:21:PRO:O	1:J:24:LYS:HB2	1.92	0.69
1:J:219:GLU:OE2	1:J:223:LYS:HE2	1.91	0.69
1:A:302:PHE:HZ	1:A:314:GLU:HG3	1.58	0.69
1:A:38:GLU:O	1:A:39:ASP:HB2	1.93	0.68
1:J:298:ARG:HD2	1:J:321:LYS:HE3	1.76	0.67
1:J:243:LYS:N	3:M:9:DT:OP1	2.21	0.67
3:B:1:DT:H2''	3:B:2:DC:H5'	1.76	0.67
1:J:332:ARG:HH21	3:M:5:EFG:H2'	1.60	0.66
1:J:154:ALA:HB2	1:J:166:ILE:HD12	1.77	0.66
1:J:332:ARG:NH2	3:M:6:DG:OP2	2.28	0.66
1:J:300:ARG:CG	6:J:530:HOH:O	2.42	0.66
2:P:3:DG:H2'	2:P:4:DG:C8	2.30	0.66
1:A:302:PHE:CZ	1:A:314:GLU:HG3	2.31	0.66
3:B:1:DT:H5''	3:B:1:DT:H6	1.61	0.65
3:B:5:EFG:O5'	3:B:5:EFG:H8	1.95	0.65
1:J:238:ARG:O	1:J:238:ARG:CG	2.40	0.65
2:P:11:DT:H3	3:B:8:DA:H2	1.41	0.65
1:A:248:ILE:CD1	6:A:512:HOH:O	2.21	0.65
1:J:211:ASP:OD1	1:J:212:LYS:HD3	1.98	0.64
1:J:304:HIS:HD2	1:J:305:GLY:O	1.79	0.64
3:B:15:DC:H2''	3:B:16:DC:C5	2.31	0.64
1:J:341:ILE:CG2	1:J:342:GLU:N	2.27	0.64
2:K:10:DA:H2'	2:K:11:DT:H71	1.78	0.64
4:A:401:DCP:HN41	3:B:5:EFG:H1	1.46	0.63
3:B:5:EFG:H1'	3:B:5:EFG:H10	1.81	0.63
1:A:10:TYR:CE2	1:A:14:GLN:HB2	2.33	0.63
1:A:316:VAL:O	1:A:320:GLN:HG3	1.97	0.63
2:K:11:DT:N3	3:M:8:DA:H2	1.81	0.63
2:P:2:DG:N2	2:P:3:DG:C6	2.67	0.63
1:A:32:VAL:HG21	3:B:5:EFG:C9	2.29	0.62
1:A:267:ARG:HG3	1:A:268:ALA:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:TYR:HA	1:A:267:ARG:HG2	1.80	0.62
1:J:46:ALA:HB1	1:J:50:ALA:HB3	1.80	0.62
3:B:15:DC:H2''	3:B:16:DC:C6	2.35	0.62
2:K:11:DT:N3	3:M:8:DA:C2	2.58	0.62
1:A:248:ILE:CD1	6:A:565:HOH:O	2.46	0.62
2:K:13:DOC:O2	3:M:6:DG:N7	2.33	0.62
1:J:188:ASN:HB3	6:J:518:HOH:O	1.98	0.61
1:J:342:GLU:O	1:J:342:GLU:CG	2.36	0.61
1:J:341:ILE:O	1:J:342:GLU:C	2.43	0.61
3:B:9:DT:H5''	3:B:9:DT:C6	2.24	0.61
3:B:1:DT:C6	3:B:1:DT:H5''	2.35	0.61
3:B:10:DC:H2''	3:B:11:DC:O5'	2.00	0.61
2:K:12:DT:C2	3:M:7:DA:C2	2.83	0.60
2:K:12:DT:O2	3:M:7:DA:C2	2.47	0.60
3:B:9:DT:H6	3:B:9:DT:C5'	2.10	0.60
1:A:11:PHE:HE2	1:A:104:ILE:HG12	1.66	0.60
1:J:164:LYS:HD2	1:J:165:VAL:C	2.25	0.60
1:J:2:ILE:HG22	1:J:111:ILE:HG13	1.85	0.59
1:J:32:VAL:HG21	3:M:5:EFG:H9	1.84	0.59
1:J:245:ILE:HB	1:J:276:LEU:HD21	1.84	0.59
1:J:285:HIS:CD2	1:J:299:GLY:HA3	2.37	0.59
1:A:10:TYR:CZ	1:A:14:GLN:CG	2.86	0.58
2:P:2:DG:H2'	2:P:3:DG:H5''	1.84	0.58
1:A:10:TYR:CE2	1:A:14:GLN:CB	2.87	0.57
1:J:44:ALA:C	1:J:45:THR:HG22	2.29	0.57
4:J:401:DCP:O4'	2:K:13:DOC:H2'	2.05	0.57
3:M:14:DC:H1'	3:M:15:DC:O5'	2.04	0.57
1:A:67:ILE:O	1:A:67:ILE:CG2	2.52	0.57
1:J:245:ILE:HB	1:J:276:LEU:CD2	2.35	0.57
1:A:0:HIS:N	1:A:0:HIS:CD2	2.72	0.57
1:J:214:LYS:HG3	1:J:219:GLU:HA	1.86	0.57
2:P:3:DG:H2''	2:P:4:DG:C8	2.40	0.57
2:K:5:DG:H1	3:M:14:DC:N4	2.02	0.57
1:A:332:ARG:NH1	3:B:6:DG:N2	2.53	0.56
1:J:34:SER:HB3	3:M:5:EFG:H4'	1.87	0.56
1:J:289:VAL:HB	1:J:332:ARG:HB2	1.86	0.56
2:K:11:DT:O4	3:M:8:DA:N1	2.38	0.56
3:M:8:DA:H2''	3:M:9:DT:C6	2.40	0.56
1:J:130:ASN:O	1:J:130:ASN:ND2	2.36	0.56
1:J:173:ARG:NH1	1:J:173:ARG:HG3	2.20	0.56
2:P:2:DG:H2'	2:P:3:DG:C5'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:164:LYS:HD2	1:J:164:LYS:C	2.31	0.55
1:J:241:VAL:CG1	1:J:242:ARG:N	2.69	0.55
1:J:170:GLU:HA	1:J:173:ARG:HB3	1.89	0.55
1:J:210:PHE:CD1	1:J:210:PHE:C	2.84	0.55
3:B:1:DT:C5'	3:B:1:DT:H6	2.16	0.55
1:A:197:LEU:CD1	1:A:216:MET:HG2	2.38	0.54
1:J:210:PHE:O	1:J:213:LEU:N	2.40	0.54
1:A:9:ASP:O	1:A:10:TYR:C	2.51	0.54
2:K:11:DT:H2''	2:K:12:DT:H6	1.73	0.54
1:A:166:ILE:HG23	1:A:170:GLU:HB3	1.90	0.53
1:A:342:GLU:HA	6:A:558:HOH:O	2.08	0.53
2:K:7:DA:N1	3:M:13:DT:O2	2.41	0.53
3:B:1:DT:H2''	3:B:2:DC:C5'	2.38	0.53
1:A:320:GLN:O	1:A:324:GLU:HG2	2.09	0.53
1:A:195:LYS:O	1:A:198:GLY:N	2.35	0.53
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.92	0.52
3:M:11:DC:H2''	3:M:12:DT:C5	2.45	0.52
1:J:321:LYS:O	1:J:321:LYS:HG2	2.10	0.52
1:A:269:ILE:HD11	1:A:315:SER:OG	2.10	0.52
1:J:210:PHE:HD1	1:J:211:ASP:N	2.08	0.52
2:P:11:DT:O4	3:B:8:DA:N1	2.43	0.52
6:A:589:HOH:O	1:J:19:LEU:HG	2.09	0.51
1:A:173:ARG:HG2	1:A:177:GLU:OE1	2.10	0.51
1:J:211:ASP:OD1	1:J:212:LYS:CD	2.58	0.51
1:J:230:ARG:CB	1:J:230:ARG:HH11	2.23	0.51
2:P:2:DG:C2'	2:P:3:DG:C4'	2.87	0.51
1:J:210:PHE:CD1	1:J:211:ASP:N	2.79	0.51
1:A:68:LEU:O	1:A:69:PRO:C	2.52	0.50
1:A:10:TYR:CE2	1:A:14:GLN:HG3	2.46	0.50
1:A:276:LEU:O	1:A:279:ARG:CD	2.59	0.50
1:J:169:GLU:O	1:J:172:LYS:HB2	2.11	0.50
1:J:213:LEU:HD23	1:J:222:ALA:HB1	1.93	0.50
2:K:10:DA:C2'	2:K:11:DT:H71	2.41	0.50
1:A:302:PHE:HZ	1:A:314:GLU:CG	2.22	0.50
2:P:12:DT:H2''	2:P:13:DOC:OP1	2.10	0.49
2:K:11:DT:C6	2:K:12:DT:C7	2.96	0.49
3:M:5:EFG:H10	3:M:5:EFG:C1'	2.35	0.49
1:A:238:ARG:CG	6:A:566:HOH:O	2.60	0.49
1:J:41:GLY:HA2	3:M:5:EFG:H4'	1.95	0.49
1:J:214:LYS:HE3	1:J:219:GLU:HG3	1.93	0.49
3:M:9:DT:H2''	3:M:10:DC:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:O	1:A:66:LYS:HG2	2.13	0.49
1:J:14:GLN:HE22	1:J:139:THR:N	1.86	0.49
1:J:118:TYR:CE2	1:J:167:ASP:HA	2.47	0.49
2:P:11:DT:N3	3:B:8:DA:C2	2.70	0.49
1:A:249:VAL:HG11	1:A:267:ARG:HE	1.78	0.49
1:A:157:MET:HE3	1:A:164:LYS:CE	2.38	0.48
1:J:127:GLU:O	1:J:131:LYS:HB2	2.12	0.48
1:A:258:LEU:O	1:A:262:LYS:HG3	2.12	0.48
1:A:55:VAL:HG21	1:A:68:LEU:HD12	1.96	0.48
3:B:10:DC:H2''	3:B:11:DC:C5'	2.44	0.48
1:J:230:ARG:HH11	1:J:230:ARG:HB2	1.79	0.48
1:A:1:MET:O	1:A:1:MET:HG3	2.14	0.48
1:J:114:LYS:HA	1:J:114:LYS:CE	2.41	0.48
1:J:265:LEU:O	1:J:269:ILE:HG13	2.14	0.48
1:A:32:VAL:HG21	3:B:5:EFG:C10	2.44	0.47
1:A:236:PRO:HB2	1:A:238:ARG:HE	1.79	0.47
1:J:213:LEU:O	1:J:214:LYS:C	2.56	0.47
4:J:401:DCP:H1'	2:K:13:DOC:C2'	2.43	0.47
2:P:2:DG:C2'	2:P:3:DG:O4'	2.55	0.47
2:P:4:DG:H2''	2:P:5:DG:C8	2.49	0.47
1:J:111:ILE:O	1:J:115:VAL:HG22	2.15	0.47
1:J:291:GLU:OE2	1:J:329:LYS:HD2	2.14	0.47
2:K:9:DG:C2'	2:K:10:DA:C8	2.98	0.47
1:A:238:ARG:HG3	6:A:566:HOH:O	2.15	0.47
1:A:276:LEU:O	1:A:279:ARG:HD2	2.15	0.47
1:J:193:LYS:HB3	1:J:216:MET:SD	2.55	0.47
2:K:9:DG:C2'	2:K:10:DA:H8	2.27	0.47
1:A:38:GLU:O	1:A:39:ASP:CB	2.63	0.46
1:J:164:LYS:CD	1:J:164:LYS:C	2.86	0.46
1:J:213:LEU:O	1:J:215:GLY:N	2.48	0.46
1:A:332:ARG:CZ	3:B:6:DG:H21	2.28	0.46
1:A:10:TYR:CD2	1:A:10:TYR:O	2.69	0.46
1:J:240:ARG:O	1:J:241:VAL:HB	2.14	0.46
1:J:36:ARG:HG2	1:J:250:THR:HG21	1.97	0.46
3:B:1:DT:C6	3:B:1:DT:C4'	2.98	0.46
1:A:237:ILE:O	1:A:237:ILE:HG22	2.15	0.46
1:A:336:ARG:HH22	3:B:8:DA:P	2.38	0.46
1:A:11:PHE:HB3	4:A:401:DCP:O3'	2.15	0.46
1:J:241:VAL:HG13	1:J:242:ARG:N	2.30	0.46
1:J:291:GLU:H	1:J:291:GLU:HG3	1.45	0.45
1:J:97:GLU:CD	1:J:97:GLU:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:173:ARG:HH12	1:J:177:GLU:CD	2.24	0.45
1:J:251:MET:HG2	1:J:264:TYR:CG	2.51	0.45
1:A:32:VAL:HG21	3:B:5:EFG:H10	1.99	0.45
1:J:212:LYS:HD3	1:J:212:LYS:N	2.32	0.45
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.98	0.45
1:A:256:ARG:NH2	1:A:326:ASP:O	2.50	0.45
1:A:251:MET:HE1	1:A:261:ILE:HG12	1.97	0.45
1:A:308:LYS:HD3	1:A:312:TYR:HE2	1.82	0.45
1:J:197:LEU:HD21	1:J:216:MET:HE3	1.98	0.45
1:J:24:LYS:HA	1:J:24:LYS:HD2	1.85	0.45
1:J:32:VAL:HG21	3:M:5:EFG:C10	2.47	0.45
1:J:217:ILE:HD12	1:J:221:LYS:HB3	1.98	0.45
1:J:261:ILE:O	1:J:262:LYS:C	2.60	0.45
2:K:11:DT:H2''	2:K:12:DT:C6	2.52	0.45
1:J:114:LYS:NZ	1:J:114:LYS:HB3	2.31	0.44
1:J:243:LYS:HB3	3:M:9:DT:P	2.57	0.44
3:M:8:DA:H2''	3:M:9:DT:H6	1.81	0.44
3:B:1:DT:H2'	3:B:2:DC:C6	2.52	0.44
2:K:5:DG:H2''	2:K:6:DA:C8	2.52	0.44
1:A:304:HIS:HD2	1:A:305:GLY:O	1.99	0.44
1:J:51:ARG:O	1:J:52:LYS:C	2.61	0.44
1:A:23:LEU:HD22	1:A:72:VAL:HG21	2.00	0.44
1:A:208:ILE:HD11	1:A:212:LYS:HG3	2.00	0.44
1:J:130:ASN:ND2	1:J:130:ASN:C	2.76	0.43
1:A:197:LEU:HD11	1:A:216:MET:HG2	1.98	0.43
1:A:267:ARG:HG3	1:A:268:ALA:H	1.83	0.43
3:B:8:DA:N6	6:B:108:HOH:O	2.52	0.43
1:A:258:LEU:HD12	1:A:319:LEU:HD23	2.00	0.43
1:J:123:ASN:N	1:J:123:ASN:HD22	2.15	0.43
1:A:273:TYR:HA	1:A:276:LEU:HD12	1.99	0.43
1:J:99:ILE:HG13	1:J:109:LEU:HD23	1.94	0.43
1:J:298:ARG:HH21	1:J:325:GLU:HB2	1.84	0.43
2:K:4:DG:H22	3:M:16:DC:H42	1.65	0.43
3:B:1:DT:C6	3:B:1:DT:O5'	2.71	0.43
1:J:130:ASN:C	1:J:130:ASN:HD22	2.17	0.42
1:A:276:LEU:O	1:A:277:ASP:C	2.62	0.42
3:B:16:DC:OP2	3:B:16:DC:H6	2.02	0.42
1:A:10:TYR:CD2	1:A:14:GLN:HB2	2.54	0.42
1:A:276:LEU:O	1:A:279:ARG:HD3	2.19	0.42
1:A:26:LYS:HE3	1:A:26:LYS:HB2	1.94	0.42
1:A:85:SER:O	1:A:89:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:O	1:A:192:GLU:HG2	2.19	0.42
1:A:197:LEU:HD12	1:A:216:MET:HG2	2.02	0.42
1:J:93:ARG:C	1:J:95:TYR:H	2.28	0.42
1:J:212:LYS:HD2	1:J:212:LYS:HA	1.84	0.42
1:J:227:SER:O	1:J:233:TYR:N	2.49	0.42
1:A:209:GLU:O	1:A:210:PHE:C	2.62	0.42
1:J:1:MET:CE	1:J:234:ASN:HD21	2.33	0.41
1:J:44:ALA:O	4:J:401:DCP:H2'1	2.20	0.41
1:J:154:ALA:HB1	1:J:164:LYS:HG3	2.01	0.41
1:J:233:TYR:CZ	1:J:235:GLU:HG2	2.55	0.41
1:J:258:LEU:HD21	1:J:320:GLN:HE21	1.85	0.41
1:A:23:LEU:CD2	1:A:72:VAL:HG21	2.51	0.41
1:A:63:GLU:O	1:A:64:ALA:C	2.62	0.41
1:J:93:ARG:C	1:J:95:TYR:N	2.79	0.41
1:J:149:VAL:O	1:J:152:LYS:HB3	2.20	0.41
1:J:210:PHE:CZ	1:J:214:LYS:HB2	2.55	0.41
1:J:238:ARG:O	1:J:239:THR:C	2.62	0.41
2:K:4:DG:H22	3:M:16:DC:N4	2.19	0.41
2:K:6:DA:H2'	2:K:7:DA:C8	2.55	0.41
1:J:99:ILE:HG23	1:J:99:ILE:O	2.20	0.41
3:M:12:DT:H1'	3:M:13:DT:C5'	2.43	0.41
2:P:11:DT:C4	3:B:8:DA:N1	2.88	0.41
1:A:0:HIS:CD2	1:A:0:HIS:H1	2.38	0.41
1:A:9:ASP:C	1:A:10:TYR:CD1	2.98	0.41
1:A:10:TYR:O	1:A:10:TYR:CG	2.72	0.41
1:A:174:LEU:O	1:A:175:ILE:C	2.63	0.41
1:A:180:ILE:HD11	1:A:225:LEU:HD13	2.02	0.41
1:A:336:ARG:NH2	3:B:8:DA:OP2	2.45	0.41
1:J:321:LYS:O	1:J:325:GLU:HG2	2.21	0.41
1:A:53:PHE:O	1:A:67:ILE:HG21	2.20	0.40
1:J:304:HIS:CD2	1:J:305:GLY:O	2.67	0.40
1:J:76:MET:HE2	1:J:76:MET:HB3	1.80	0.40
1:A:318:LEU:HG	6:A:588:HOH:O	2.21	0.40
1:J:102:ALA:HA	1:J:240:ARG:HD2	2.04	0.40
1:A:76:MET:HE3	1:A:78:LYS:HD3	2.04	0.40
1:A:280:ILE:CG2	1:A:305:GLY:HA3	2.51	0.40
1:J:222:ALA:O	1:J:226:ILE:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	341/348 (98%)	323 (95%)	16 (5%)	2 (1%)	21	27
1	J	341/348 (98%)	300 (88%)	36 (11%)	5 (2%)	8	8
All	All	682/696 (98%)	623 (91%)	52 (8%)	7 (1%)	12	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	J	241	VAL
1	A	277	ASP
1	J	211	ASP
1	J	215	GLY
1	J	10	TYR
1	J	99	ILE

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	
1	A	302/307 (98%)	271 (90%)	31 (10%)	7	8
1	J	300/307 (98%)	253 (84%)	47 (16%)	2	2
All	All	602/614 (98%)	524 (87%)	78 (13%)	4	4

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	19	LEU
1	A	36	ARG
1	A	49	GLU
1	A	78	LYS
1	A	79	GLU
1	A	94	GLU
1	A	97	GLU
1	A	98	LYS
1	A	105	ASP
1	A	115	VAL
1	A	119	ARG
1	A	137	LYS
1	A	160	PRO
1	A	170	GLU
1	A	219	GLU
1	A	227	SER
1	A	238	ARG
1	A	242	ARG
1	A	252	LYS
1	A	255	SER
1	A	256	ARG
1	A	267	ARG
1	A	273	TYR
1	A	279	ARG
1	A	294	ASP
1	A	321	LYS
1	A	325	GLU
1	A	326	ASP
1	A	336	ARG
1	A	342	GLU
1	J	0	HIS
1	J	1	MET
1	J	2	ILE
1	J	8	PHE
1	J	19	LEU
1	J	24	LYS
1	J	36	ARG
1	J	38	GLU
1	J	45	THR
1	J	52	LYS
1	J	76	MET
1	J	97	GLU

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Mol	Chain	Res	Type
1	J	99	ILE
1	J	109	LEU
1	J	114	LYS
1	J	119	ARG
1	J	123	ASN
1	J	131	LYS
1	J	134	GLU
1	J	164	LYS
1	J	173	ARG
1	J	195	LYS
1	J	197	LEU
1	J	200	ASN
1	J	201	LYS
1	J	202	LEU
1	J	208	ILE
1	J	211	ASP
1	J	212	LYS
1	J	230	ARG
1	J	234	ASN
1	J	238	ARG
1	J	243	LYS
1	J	245	ILE
1	J	248	ILE
1	J	252	LYS
1	J	256	ARG
1	J	276	LEU
1	J	284	ILE
1	J	291	GLU
1	J	293	LEU
1	J	297	SER
1	J	300	ARG
1	J	308	LYS
1	J	325	GLU
1	J	336	ARG
1	J	342	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	14	GLN
1	A	82	GLN

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Mol	Chain	Res	Type
1	A	123	ASN
1	A	257	ASN
1	A	285	HIS
1	A	304	HIS
1	J	0	HIS
1	J	14	GLN
1	J	123	ASN
1	J	200	ASN
1	J	234	ASN
1	J	285	HIS
1	J	304	HIS
1	J	320	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EFG	B	5	3	24,28,29	3.15	14 (58%)	31,42,45	2.45	12 (38%)
3	EFG	M	5	3	24,28,29	2.20	7 (29%)	31,42,45	2.12	12 (38%)
2	DOC	P	13	3,2	16,19,20	0.90	0	20,26,29	1.33	2 (10%)
2	DOC	K	13	2	16,19,20	1.10	2 (12%)	20,26,29	2.61	9 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EFG	B	5	3	-	0/7/25/26	0/4/4/4
3	EFG	M	5	3	-	2/7/25/26	0/4/4/4
2	DOC	P	13	3,2	-	2/7/18/19	0/2/2/2
2	DOC	K	13	2	-	2/7/18/19	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	EFG	C9-N3	-6.65	1.28	1.39
3	B	5	EFG	C2'-C1'	-5.29	1.46	1.53
3	B	5	EFG	C2'-C3'	-5.01	1.46	1.52
3	B	5	EFG	C5-N7	-4.77	1.29	1.39
3	M	5	EFG	C2'-C1'	4.63	1.58	1.53
3	M	5	EFG	C1'-N9	4.36	1.59	1.47
3	B	5	EFG	C10-N2	-4.34	1.29	1.38
3	M	5	EFG	C9-N3	-4.28	1.32	1.39
3	B	5	EFG	C4-N3	-3.80	1.29	1.41
3	B	5	EFG	C8-N9	-3.57	1.29	1.37
3	B	5	EFG	C5-C4	-3.43	1.30	1.38
3	M	5	EFG	O4'-C1'	3.30	1.49	1.42
3	M	5	EFG	C10-N2	-3.29	1.31	1.38
3	B	5	EFG	C5-C6	-3.25	1.32	1.44
3	B	5	EFG	C6-N1	-3.21	1.32	1.38
3	M	5	EFG	C4-N3	-2.81	1.32	1.41
3	B	5	EFG	C2-N2	-2.64	1.29	1.33
3	B	5	EFG	O4'-C1'	-2.62	1.35	1.42
3	B	5	EFG	C4-N9	-2.54	1.31	1.38
2	K	13	DOC	C6-N1	-2.35	1.32	1.38
2	K	13	DOC	C5-C4	-2.33	1.37	1.42
3	M	5	EFG	O3'-C3'	2.10	1.48	1.43
3	B	5	EFG	O3'-C3'	-2.08	1.37	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	13	DOC	C4'-O4'-C1'	6.58	116.02	109.81
3	M	5	EFG	N3-C2-N2	-5.15	109.32	113.33
3	B	5	EFG	F-C2'-C3'	-5.03	99.22	109.14
3	B	5	EFG	O4'-C1'-N9	-5.00	97.03	108.36
3	B	5	EFG	N3-C2-N2	-4.91	109.51	113.33
3	B	5	EFG	C3'-C2'-C1'	4.87	108.75	103.10
3	M	5	EFG	O4'-C1'-N9	4.81	119.26	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	13	DOC	C3'-C2'-C1'	4.41	107.95	102.87
2	K	13	DOC	O2-C2-N3	-3.96	116.09	122.33
2	K	13	DOC	C1'-N1-C2	3.87	124.47	117.83
3	B	5	EFG	C5-C6-N1	3.76	122.82	113.25
3	B	5	EFG	N3-C4-N9	3.56	134.65	129.41
3	M	5	EFG	C10-N2-C2	3.07	107.09	103.26
2	P	13	DOC	C3'-C2'-C1'	2.88	106.19	102.87
2	K	13	DOC	O4'-C1'-C2'	-2.85	103.04	106.41
2	K	13	DOC	C2'-C1'-N1	2.75	117.62	112.40
3	M	5	EFG	C4'-O4'-C1'	-2.74	103.42	109.47
3	M	5	EFG	C5-C6-N1	2.74	120.22	113.25
3	M	5	EFG	O6-C6-N1	-2.72	115.00	120.11
3	B	5	EFG	C10-N2-C2	2.71	106.64	103.26
3	M	5	EFG	C9-N3-C2	-2.67	107.19	109.90
3	B	5	EFG	C10-C9-N3	2.50	107.72	105.02
3	B	5	EFG	O6-C6-N1	-2.42	115.56	120.11
3	M	5	EFG	C1'-N9-C8	2.40	133.56	126.73
3	B	5	EFG	C8-N7-C5	2.39	108.53	104.26
3	M	5	EFG	C10-C9-N3	2.34	107.55	105.02
3	B	5	EFG	N9-C8-N7	-2.33	109.08	113.40
2	K	13	DOC	O2-C2-N1	2.24	123.29	118.90
3	B	5	EFG	C9-N3-C2	-2.23	107.64	109.90
2	K	13	DOC	O4'-C4'-C5'	2.21	113.31	109.34
3	M	5	EFG	F-C2'-C1'	2.17	113.23	108.88
3	M	5	EFG	N1-C2-N2	2.08	131.83	128.74
2	P	13	DOC	C4'-O4'-C1'	2.08	111.77	109.81
2	K	13	DOC	C6-N1-C2	-2.06	116.99	120.46
3	M	5	EFG	C2'-C3'-C4'	-2.05	99.73	102.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	13	DOC	O4'-C4'-C5'-O5'
2	P	13	DOC	O4'-C4'-C5'-O5'
2	K	13	DOC	C3'-C4'-C5'-O5'
3	M	5	EFG	C4'-C5'-O5'-P
2	P	13	DOC	C3'-C4'-C5'-O5'
3	M	5	EFG	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5	EFG	6	0
3	M	5	EFG	8	0
2	P	13	DOC	1	0
2	K	13	DOC	11	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 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$
4	DCP	J	401	5	28,29,29	1.56	3 (10%)	41,45,45	1.53	7 (17%)
4	DCP	A	401	5	28,29,29	1.49	4 (14%)	41,45,45	1.46	6 (14%)

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
4	DCP	J	401	5	-	4/22/34/34	0/2/2/2
4	DCP	A	401	5	-	4/22/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	401	DCP	PA-O3A	4.97	1.64	1.59
4	J	401	DCP	PB-O3A	4.22	1.64	1.59
4	A	401	DCP	PA-O3A	-3.38	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	DCP	C6-C5	3.15	1.42	1.35
4	A	401	DCP	C2-N1	2.76	1.45	1.40
4	J	401	DCP	C6-C5	2.34	1.40	1.35
4	A	401	DCP	O3'-C3'	2.15	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	DCP	O2B-PB-O3A	4.32	118.95	107.27
4	J	401	DCP	O2-C2-N3	-3.84	116.27	122.33
4	J	401	DCP	O2G-PG-O3B	-3.18	93.97	104.64
4	A	401	DCP	O3'-C3'-C4'	2.76	120.53	110.07
4	J	401	DCP	C1'-N1-C2	2.70	122.46	117.83
4	J	401	DCP	O3G-PG-O2G	2.59	117.51	107.80
4	J	401	DCP	C2'-C3'-C4'	2.58	108.03	102.80
4	A	401	DCP	O3A-PA-O1A	-2.53	103.09	110.70
4	A	401	DCP	O2G-PG-O3B	-2.53	96.15	104.64
4	A	401	DCP	O4'-C1'-N1	2.39	112.10	107.86
4	J	401	DCP	O2B-PB-O3B	-2.36	100.89	107.27
4	J	401	DCP	N1-C2-N3	2.15	122.54	118.80
4	A	401	DCP	C6-C5-C4	2.14	121.04	117.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

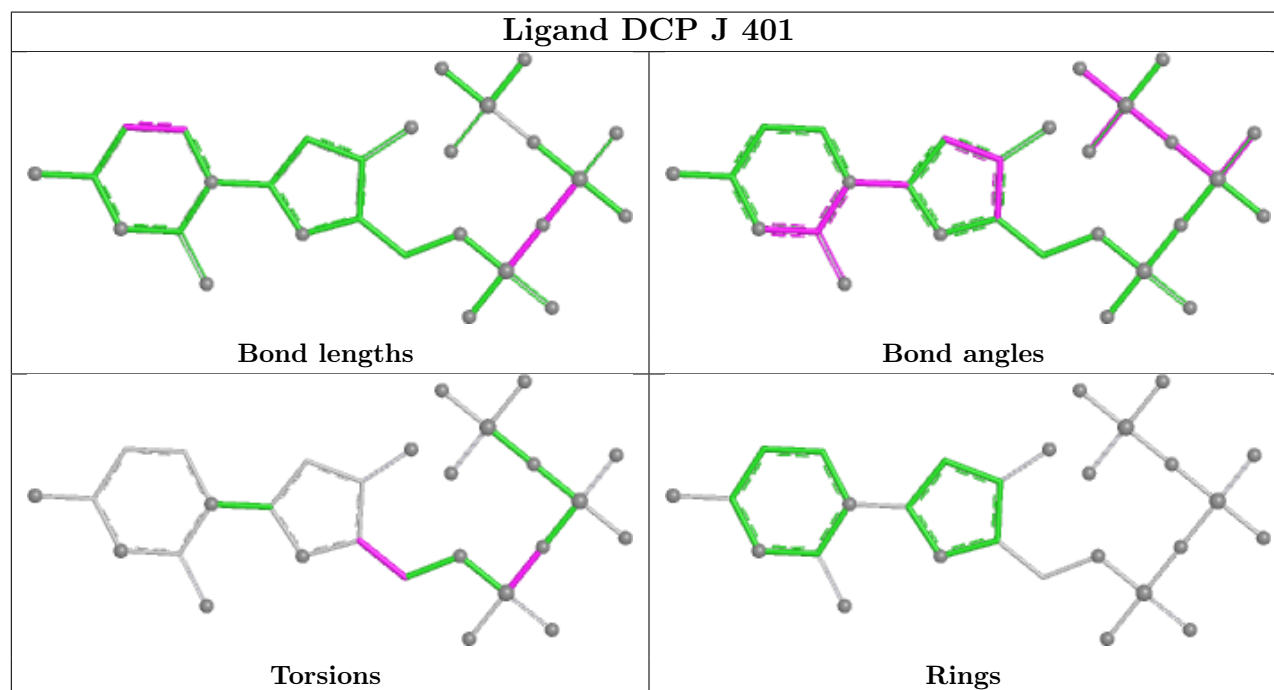
Mol	Chain	Res	Type	Atoms
4	J	401	DCP	C3'-C4'-C5'-O5'
4	J	401	DCP	O4'-C4'-C5'-O5'
4	J	401	DCP	PB-O3A-PA-O1A
4	A	401	DCP	PB-O3B-PG-O1G
4	J	401	DCP	PB-O3A-PA-O2A
4	A	401	DCP	PB-O3B-PG-O2G
4	A	401	DCP	PB-O3B-PG-O3G
4	A	401	DCP	PA-O3A-PB-O2B

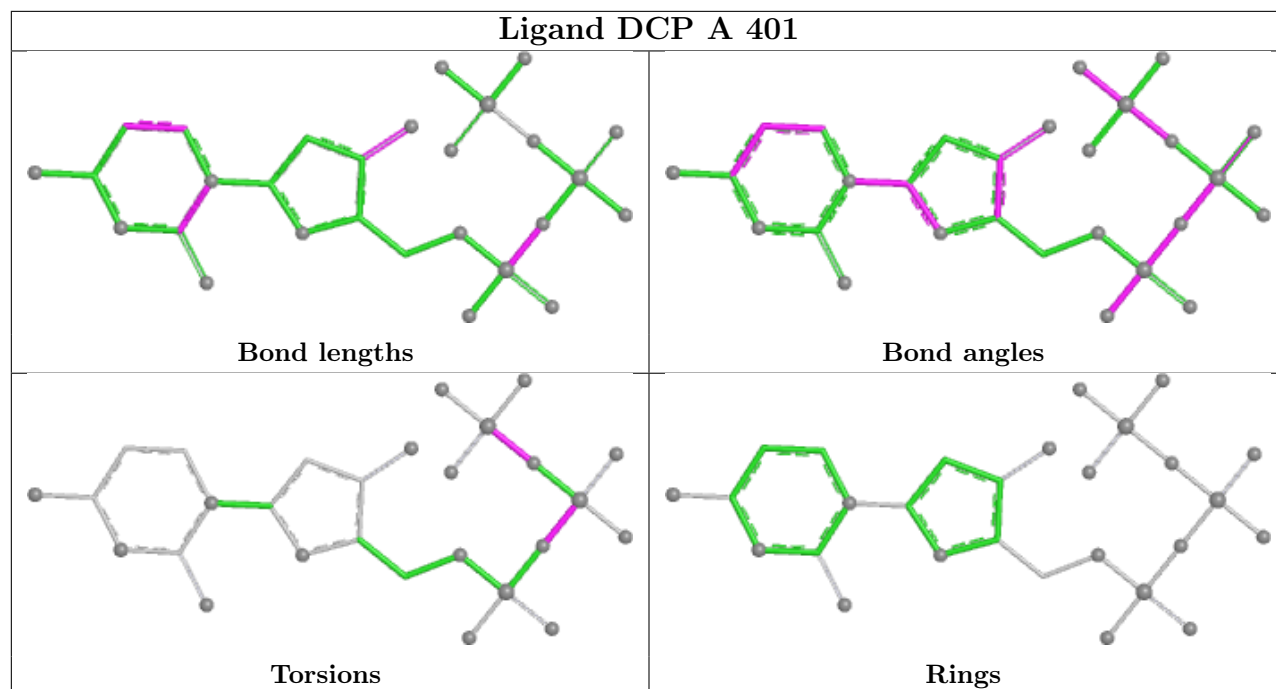
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	401	DCP	6	0
4	A	401	DCP	2	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.





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	A	343/348 (98%)	0.06	15 (4%) 39 41	11, 42, 68, 88	23 (6%)
1	J	343/348 (98%)	0.58	23 (6%) 24 26	20, 67, 100, 118	14 (4%)
2	K	10/12 (83%)	1.64	3 (30%) 1 1	63, 99, 123, 132	3 (30%)
2	P	11/12 (91%)	0.73	1 (9%) 15 16	49, 56, 107, 110	1 (9%)
3	B	16/17 (94%)	0.40	2 (12%) 8 9	37, 57, 105, 105	2 (12%)
3	M	12/17 (70%)	1.00	1 (8%) 17 19	51, 92, 171, 172	1 (8%)
All	All	735/754 (97%)	0.36	45 (6%) 27 29	11, 54, 100, 172	44 (5%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	ASN	6.7
2	P	2	DG	5.6
1	J	49	GLU	5.4
1	A	336	ARG	5.2
1	A	209	GLU	5.0
1	A	49	GLU	4.8
3	M	16	DC	4.6
1	A	169	GLU	4.6
1	A	177	GLU	4.4
2	K	3	DG	4.4
1	A	10	TYR	4.2
1	J	241	VAL	3.9
1	J	177	GLU	3.7
1	J	276	LEU	3.7
1	J	116	ARG	3.7
1	A	127	GLU	3.4
2	K	4	DG	3.2
1	J	295	ILE	3.1
1	J	208	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	98	LYS	3.0
1	J	239	THR	2.9
1	A	11	PHE	2.9
1	J	127	GLU	2.9
3	B	1	DT	2.9
1	A	267	ARG	2.8
1	J	176	ARG	2.8
1	J	216	MET	2.6
1	J	213	LEU	2.6
1	J	204	ASP	2.5
1	J	212	LYS	2.5
3	B	17	DC	2.5
1	A	0	HIS	2.5
1	J	203	VAL	2.4
1	J	97	GLU	2.4
1	A	116	ARG	2.3
1	A	238	ARG	2.3
2	K	5	DG	2.2
1	J	39	ASP	2.2
1	J	207	SER	2.2
1	J	173	ARG	2.1
1	A	270	GLU	2.1
1	J	240	ARG	2.1
1	J	35	GLY	2.1
1	A	98	LYS	2.0
1	J	0	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOC	K	13	18/19	0.73	0.20	61,76,86,87	0
2	DOC	P	13	18/19	0.75	0.18	35,43,87,90	0
3	EFG	M	5	25/26	0.87	0.13	48,70,96,98	0
3	EFG	B	5	25/26	0.90	0.11	35,40,51,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

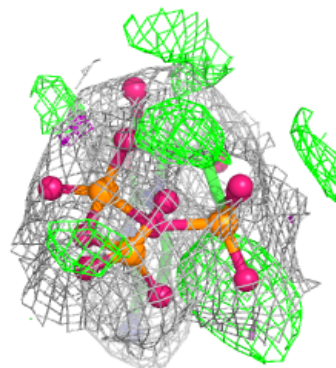
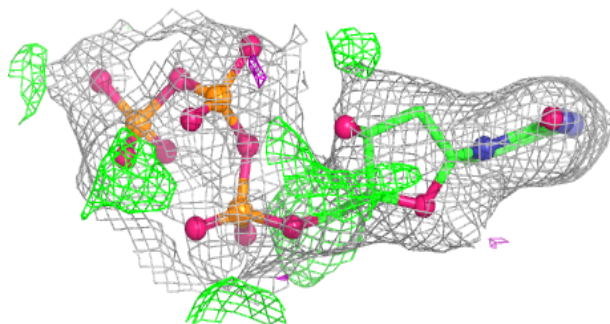
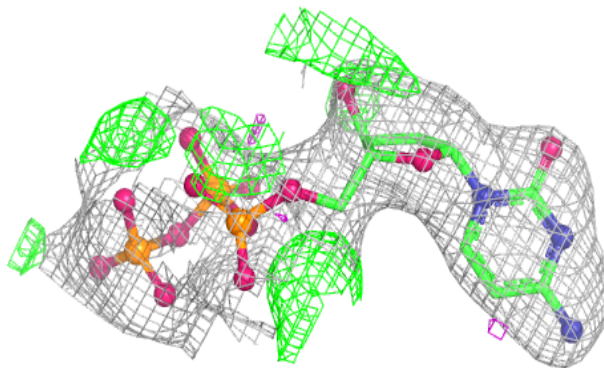
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	J	402	1/1	0.73	0.13	43,43,43,43	0
4	DCP	J	401	28/28	0.93	0.11	45,57,72,90	0
5	MG	K	101	1/1	0.93	0.23	49,49,49,49	0
5	MG	A	402	1/1	0.96	0.14	19,19,19,19	0
4	DCP	A	401	28/28	0.97	0.07	24,37,46,47	0
5	MG	J	403	1/1	0.98	0.10	28,28,28,28	0
5	MG	A	403	1/1	1.00	0.07	13,13,13,13	0

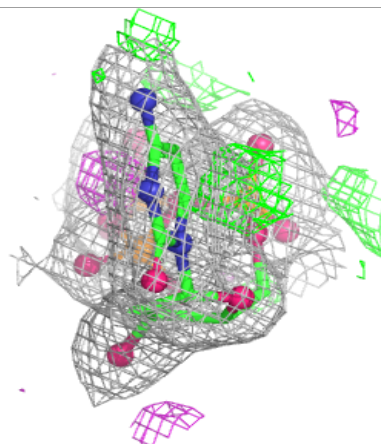
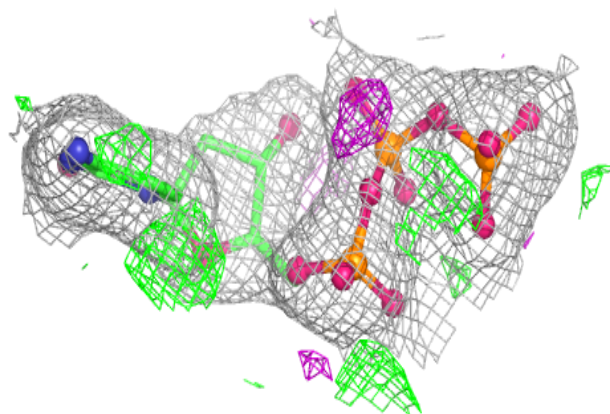
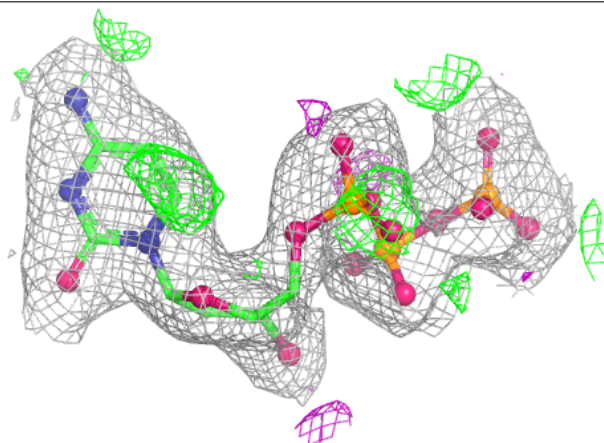
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCP J 401:

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

**Electron density around DCP A 401:**

$2mF_o-DF_c$ (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.