



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:08 AM UTC

PDB ID : 9ICN / pdb_00009icn
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX + 2',3'-DIDEOXYCYTIDINE-5'-TRIPHOSPHATE, SOAKED IN THE PRESENCE OF DDCTP AND MGCL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-16
Resolution : 3.00 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 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

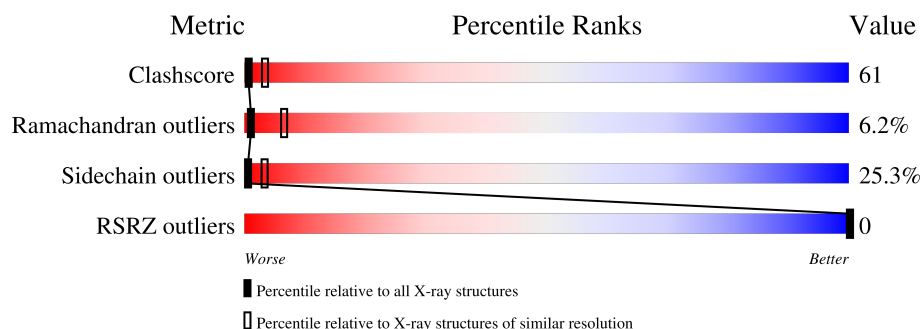
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

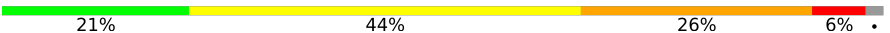
The reported resolution of this entry is 3.00 Å.

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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 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	T	7	
2	P	6	
3	A	335	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3032 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 DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	P	0	0	0
			126	59	25	36	6			

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	26	0	0
			2623	1657	458	499	9			

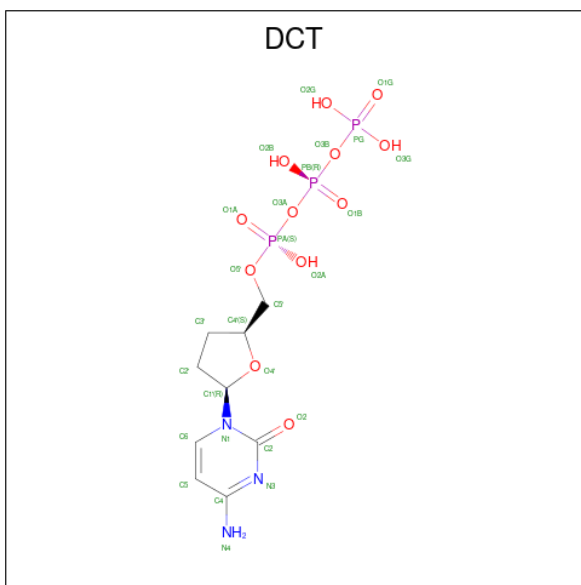
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			13	10	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	10	Total O 10 10	0	0
7	P	21	Total O 21 21	0	0
7	A	114	Total O 114 114	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.90Å 57.69Å 48.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.00-3.00) 86.3 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.150 , (Not available) 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 190.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3032	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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, NA, DCT

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	T	0.95	0/135	1.93	5/207 (2.4%)
2	P	1.18	1/141 (0.7%)	2.39	8/214 (3.7%)
3	A	1.60	16/2672 (0.6%)	2.10	98/3590 (2.7%)
All	All	1.56	17/2948 (0.6%)	2.10	111/4011 (2.8%)

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
3	A	4	0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	234	LYS	CA-C	-7.77	1.43	1.52
3	A	138	ILE	CA-CB	-7.21	1.45	1.54
2	P	1	DC	OP3-P	6.74	1.61	1.48
3	A	65	VAL	CA-C	-6.73	1.45	1.52
3	A	242	PRO	N-CA	-6.25	1.39	1.47
3	A	233	THR	CA-C	-6.06	1.44	1.52
3	A	24	ASN	CA-C	-5.96	1.45	1.52
3	A	119	ILE	CA-C	-5.76	1.46	1.52
3	A	241	LEU	C-N	-5.70	1.26	1.33
3	A	91	ASP	CA-C	-5.50	1.45	1.52
3	A	196	THR	CA-C	-5.45	1.45	1.52
3	A	24	ASN	C-N	-5.41	1.26	1.33
3	A	115	VAL	CA-CB	-5.18	1.47	1.54
3	A	160	ASP	CG-OD2	5.13	1.35	1.25
3	A	35	LYS	CA-C	-5.10	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	326	LYS	CE-NZ	-5.04	1.34	1.49
3	A	119	ILE	CA-CB	-5.01	1.48	1.53

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	C6-N1-C1'	-14.87	97.04	119.35
2	P	5	DT	C2-N1-C1'	14.76	141.49	119.35
3	A	49	TYR	CA-C-N	12.56	133.10	119.28
3	A	49	TYR	C-N-CA	12.56	133.10	119.28
3	A	20	THR	N-CA-CB	10.87	125.78	109.91
3	A	40	ARG	N-CA-C	9.72	121.57	110.97
1	T	4	DT	C6-N1-C1'	-9.57	104.99	119.35
3	A	30	SER	CA-C-N	-9.43	107.90	122.60
3	A	30	SER	C-N-CA	-9.43	107.90	122.60
3	A	34	HIS	CA-CB-CG	-9.33	104.47	113.80
3	A	152	ARG	N-CA-CB	8.77	124.00	110.14
3	A	204	SER	CA-C-N	-8.64	109.19	121.72
3	A	204	SER	C-N-CA	-8.64	109.19	121.72
1	T	2	DC	C2-N1-C1'	8.55	132.53	119.70
3	A	292	THR	CB-CA-C	8.53	124.57	109.65
3	A	20	THR	CB-CA-C	8.41	123.91	110.96
3	A	269	VAL	CB-CA-C	-8.33	100.90	112.14
3	A	161	ILE	N-CA-C	8.26	118.18	110.42
1	T	4	DT	C2-N1-C1'	8.20	131.64	119.35
1	T	2	DC	C6-N1-C1'	-8.19	107.42	119.70
3	A	65	VAL	N-CA-C	8.18	119.32	106.88
3	A	303	VAL	CB-CA-C	8.06	118.15	111.06
2	P	2	DA	C8-N9-C1'	7.87	138.85	127.05
2	P	2	DA	C4-N9-C1'	-7.86	115.26	127.05
3	A	291	PHE	N-CA-C	7.77	119.81	108.86
2	P	1	DC	C2-N1-C1'	7.74	131.30	119.70
3	A	117	GLU	N-CA-C	-7.65	103.29	114.39
3	A	279	ASN	N-CA-C	7.62	119.28	110.97
3	A	197	HIS	CA-C-N	7.56	127.20	119.19
3	A	197	HIS	C-N-CA	7.56	127.20	119.19
3	A	65	VAL	N-CA-CB	7.45	120.55	111.60
3	A	49	TYR	O-C-N	7.40	127.75	121.31
3	A	138	ILE	CB-CA-C	-7.34	102.08	112.22
3	A	201	THR	N-CA-C	7.22	119.14	108.60
2	P	1	DC	C6-N1-C1'	-7.21	108.88	119.70
3	A	24	ASN	CA-CB-CG	-7.21	105.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	30	SER	N-CA-C	-6.98	101.53	110.19
3	A	304	THR	N-CA-CB	-6.93	98.77	110.49
3	A	32	ALA	N-CA-C	6.92	125.53	110.80
3	A	49	TYR	CA-C-O	6.90	126.27	119.51
3	A	28	ASN	N-CA-C	6.59	118.25	111.14
3	A	138	ILE	O-C-N	6.27	128.29	121.83
3	A	296	TYR	CB-CA-C	-6.24	98.58	109.07
3	A	40	ARG	N-CA-CB	6.21	118.97	109.91
3	A	168	LYS	N-CA-CB	6.20	119.36	110.06
3	A	146	PHE	CA-CB-CG	-6.18	107.62	113.80
3	A	266	TYR	CA-CB-CG	-6.17	102.79	113.90
3	A	205	THR	N-CA-CB	6.15	119.89	109.87
3	A	243	SER	N-CA-C	-6.12	99.89	109.25
3	A	153	GLU	N-CA-CB	6.04	119.52	110.22
3	A	160	ASP	N-CA-C	-6.01	104.73	111.28
3	A	309	GLU	CA-C-N	5.95	127.28	119.84
3	A	309	GLU	C-N-CA	5.95	127.28	119.84
3	A	197	HIS	O-C-N	5.89	126.43	121.83
3	A	313	VAL	N-CA-C	5.87	116.31	107.80
3	A	246	ASP	N-CA-C	5.86	123.27	110.80
3	A	311	LEU	CA-C-N	5.85	128.40	120.79
3	A	311	LEU	C-N-CA	5.85	128.40	120.79
3	A	258	ARG	N-CA-C	5.84	117.92	108.34
3	A	207	GLN	CA-C-N	5.83	125.20	118.85
3	A	207	GLN	C-N-CA	5.83	125.20	118.85
3	A	250	TYR	N-CA-C	5.78	118.10	110.36
1	T	7	DG	P-O3'-C3'	-5.72	111.61	120.20
3	A	279	ASN	CA-CB-CG	-5.71	106.89	112.60
3	A	193	VAL	N-CA-C	5.68	116.48	108.36
3	A	109	SER	O-C-N	5.67	128.15	122.08
2	P	4	DA	O4'-C1'-N9	-5.66	99.91	108.40
3	A	228	LEU	N-CA-C	-5.65	106.06	113.12
3	A	193	VAL	N-CA-CB	-5.64	104.22	110.99
3	A	303	VAL	N-CA-C	5.64	118.60	112.96
3	A	64	GLY	N-CA-C	-5.54	108.49	115.08
3	A	202	SER	O-C-N	5.54	129.96	122.59
3	A	279	ASN	O-C-N	5.50	127.75	122.03
3	A	92	ASP	N-CA-CB	5.48	118.18	110.12
3	A	250	TYR	CA-C-O	5.43	126.88	120.96
3	A	238	VAL	CA-C-N	-5.42	113.80	122.53
3	A	238	VAL	C-N-CA	-5.42	113.80	122.53
3	A	74	ASP	N-CA-CB	5.41	117.81	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	296	TYR	N-CA-C	5.40	120.88	113.97
3	A	297	THR	N-CA-C	5.37	116.15	108.74
3	A	272	PHE	CA-CB-CG	-5.36	108.44	113.80
3	A	87	LYS	CB-CA-C	5.34	119.66	110.79
3	A	194	LEU	CA-C-N	-5.33	113.20	122.37
3	A	194	LEU	C-N-CA	-5.33	113.20	122.37
3	A	15	ILE	N-CA-CB	5.33	116.78	110.55
3	A	40	ARG	CB-CA-C	5.32	119.14	110.96
2	P	2	DA	C5'-C4'-O4'	-5.29	101.47	109.40
3	A	320	PHE	O-C-N	5.28	128.19	122.11
3	A	39	TYR	CA-CB-CG	-5.27	104.41	113.90
3	A	68	LYS	N-CA-C	5.26	117.10	111.36
3	A	222	HIS	CB-CA-C	-5.26	99.95	110.42
3	A	263	ASP	N-CA-C	5.25	119.44	113.19
3	A	313	VAL	N-CA-CB	-5.22	104.88	111.46
3	A	181	PHE	CA-C-N	5.21	127.69	120.29
3	A	181	PHE	C-N-CA	5.21	127.69	120.29
3	A	37	ASN	N-CA-C	-5.17	105.76	111.71
3	A	286	ALA	CA-C-N	5.14	127.59	120.29
3	A	286	ALA	C-N-CA	5.14	127.59	120.29
3	A	329	GLU	N-CA-C	-5.14	102.70	109.84
3	A	282	MET	N-CA-C	-5.13	105.60	111.14
3	A	159	GLN	CB-CA-C	-5.12	102.28	110.79
3	A	27	LYS	CB-CA-C	5.11	118.91	110.88
3	A	214	VAL	N-CA-CB	5.11	119.09	110.56
3	A	92	ASP	CB-CA-C	5.10	119.26	110.79
3	A	115	VAL	CB-CA-C	-5.08	105.21	112.22
3	A	26	GLU	N-CA-CB	5.05	117.34	110.01
3	A	93	THR	N-CA-CB	5.04	117.32	110.01
3	A	224	ILE	CA-CB-CG1	-5.02	101.87	110.40
3	A	292	THR	N-CA-C	5.01	117.56	108.69
3	A	86	GLU	N-CA-CB	5.01	117.58	110.16
3	A	146	PHE	N-CA-C	5.00	117.62	111.82

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	20	THR	CA
3	A	40	ARG	CA
3	A	65	VAL	CA
3	A	292	THR	CA

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	T	122	0	69	3	0
2	P	126	0	68	11	0
3	A	2623	0	2641	330	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	13	0	0	0	0
7	A	114	0	0	18	0
7	P	21	0	0	1	0
7	T	10	0	0	1	0
All	All	3032	0	2778	343	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 61.

All (343) 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:A:191:MET:HG2	3:A:255:ILE:HG13	1.35	1.04
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.56	1.04
2:P:5:DT:H2''	2:P:6:DG:H5'	1.39	0.99
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.11	0.96
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.47	0.93
3:A:282:MET:HE3	3:A:323:ILE:HD11	1.52	0.91
3:A:259:LEU:HD12	3:A:260:ILE:N	1.85	0.91
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.52	0.90
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.54	0.90
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.54	0.89
3:A:259:LEU:HD12	3:A:260:ILE:H	1.38	0.88
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.09	0.88
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.89	0.86
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.72	0.86
3:A:41:LYS:HD3	3:A:42:ALA:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.07	0.83
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.76	0.83
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.59	0.81
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.10	0.81
3:A:271:TYR:HB2	7:A:592:HOH:O	1.80	0.80
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.47	0.80
3:A:278:PHE:HB2	3:A:333:ARG:O	1.82	0.79
3:A:41:LYS:HD3	3:A:42:ALA:N	1.98	0.79
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.64	0.79
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.13	0.78
3:A:18:MET:HE1	3:A:76:PHE:CB	2.13	0.77
3:A:33:ILE:O	3:A:37:ASN:HB2	1.86	0.76
3:A:68:LYS:O	3:A:72:LYS:HE3	1.86	0.76
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.14	0.75
3:A:245:ASN:N	3:A:245:ASN:HD22	1.84	0.75
2:P:5:DT:H2''	2:P:6:DG:C5'	2.16	0.75
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.69	0.75
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.17	0.75
3:A:260:ILE:HG22	3:A:261:PRO:HD2	1.69	0.75
3:A:227:THR:HG23	3:A:235:PHE:CE2	2.22	0.74
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.69	0.74
3:A:279:ASN:O	3:A:283:ARG:HG3	1.87	0.74
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.22	0.74
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.52	0.74
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.32	0.74
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.23	0.73
3:A:75:GLU:O	3:A:79:THR:HG23	1.89	0.73
3:A:242:PRO:HG2	7:A:589:HOH:O	1.88	0.73
2:P:1:DC:C2'	2:P:2:DA:H5''	2.19	0.73
3:A:179:GLY:O	3:A:182:ARG:HB3	1.89	0.73
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.71	0.72
2:P:2:DA:C8	2:P:2:DA:H5'	2.24	0.72
3:A:172:GLU:HG2	3:A:198:PRO:HG3	1.70	0.72
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.20	0.72
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.54	0.72
3:A:111:ALA:O	3:A:115:VAL:HG23	1.90	0.71
3:A:217:GLN:O	3:A:221:VAL:HG22	1.90	0.71
2:P:1:DC:H2''	2:P:2:DA:H5''	1.71	0.70
3:A:155:MET:HE3	3:A:188:SER:OG	1.90	0.70
3:A:292:THR:C	3:A:293:ILE:HD13	2.15	0.70
3:A:27:LYS:HB3	3:A:36:TYR:CG	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.72	0.69
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.74	0.69
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.27	0.69
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.75	0.69
3:A:292:THR:O	3:A:298:ILE:HA	1.92	0.69
3:A:227:THR:HG23	3:A:235:PHE:HE2	1.55	0.68
3:A:80:GLY:O	3:A:81:LYS:HG2	1.92	0.68
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.75	0.68
3:A:164:ASN:O	3:A:168:LYS:HG2	1.94	0.67
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.24	0.67
3:A:31:GLN:HG3	3:A:112:ARG:HH22	1.59	0.67
3:A:201:THR:HA	3:A:261:PRO:CB	2.25	0.67
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.41	0.67
3:A:172:GLU:CG	3:A:198:PRO:HG3	2.25	0.67
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.25	0.67
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.95	0.67
2:P:5:DT:C2'	2:P:6:DG:H5'	2.21	0.66
3:A:11:LEU:HD23	3:A:11:LEU:H	1.58	0.66
3:A:319:ILE:O	3:A:322:TYR:HB2	1.95	0.66
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.77	0.65
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.11	0.65
3:A:282:MET:CE	3:A:323:ILE:HD11	2.25	0.65
3:A:11:LEU:H	3:A:11:LEU:CD2	2.10	0.65
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.10	0.65
3:A:295:GLU:CD	3:A:295:GLU:H	2.04	0.65
1:T:3:DA:H1'	7:T:617:HOH:O	1.97	0.64
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.77	0.64
3:A:31:GLN:N	7:A:641:HOH:O	2.30	0.64
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.79	0.64
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.35	0.64
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.63	0.64
3:A:326:LYS:HG3	3:A:326:LYS:O	1.97	0.64
3:A:243:SER:HB3	3:A:249:GLU:HA	1.79	0.64
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.28	0.63
3:A:330:PRO:O	3:A:333:ARG:HG3	1.99	0.63
3:A:44:SER:O	3:A:47:ALA:HB3	1.98	0.63
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.81	0.63
3:A:306:VAL:HG23	3:A:307:ALA:N	2.13	0.63
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.28	0.62
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.39	0.62
3:A:212:HIS:HB3	7:A:541:HOH:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.30	0.62
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.30	0.62
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.13	0.62
3:A:152:ARG:NH2	3:A:181:PHE:O	2.32	0.61
3:A:286:ALA:HB2	3:A:323:ILE:HD13	1.82	0.61
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.82	0.61
3:A:259:LEU:O	3:A:260:ILE:HD13	2.00	0.61
3:A:165:GLU:O	3:A:169:VAL:HG12	2.01	0.61
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.35	0.61
3:A:215:VAL:O	3:A:219:GLN:HG3	2.00	0.61
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.36	0.61
3:A:207:GLN:O	3:A:210:LEU:HB2	2.01	0.61
3:A:18:MET:CE	3:A:76:PHE:HB2	2.31	0.60
3:A:58:GLU:O	3:A:61:LYS:HB2	2.00	0.60
3:A:157:GLN:O	3:A:161:ILE:HG13	2.01	0.60
3:A:12:ASN:HD21	3:A:53:ILE:H	1.49	0.60
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.16	0.60
3:A:79:THR:O	3:A:81:LYS:N	2.34	0.60
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.82	0.60
3:A:286:ALA:HB1	3:A:323:ILE:HG21	1.84	0.59
3:A:262:LYS:O	3:A:262:LYS:HG3	2.02	0.59
3:A:176:THR:HG22	3:A:178:CYS:SG	2.42	0.59
3:A:23:ALA:O	3:A:36:TYR:HD1	1.86	0.59
3:A:331:LYS:HD2	3:A:332:ASP:N	2.18	0.59
3:A:150:ILE:HG21	3:A:158:MET:CE	2.33	0.58
3:A:248:LYS:O	3:A:248:LYS:HG2	2.03	0.58
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.85	0.58
3:A:245:ASN:N	3:A:245:ASN:ND2	2.50	0.58
3:A:282:MET:HE1	3:A:320:PHE:CD1	2.38	0.58
3:A:276:ASP:O	3:A:279:ASN:HB2	2.03	0.58
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.38	0.58
3:A:201:THR:HA	3:A:261:PRO:HB3	1.85	0.58
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.39	0.57
3:A:303:VAL:C	3:A:305:GLY:H	2.12	0.57
3:A:157:GLN:O	3:A:160:ASP:HB3	2.05	0.57
3:A:253:ARG:HH11	3:A:253:ARG:HG2	1.69	0.57
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.40	0.56
3:A:133:ASN:H	3:A:136:GLN:NE2	2.03	0.56
3:A:286:ALA:O	3:A:291:PHE:HB2	2.06	0.56
3:A:18:MET:HE3	3:A:76:PHE:CD1	2.40	0.56
3:A:254:ARG:NH2	7:A:549:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:133:ASN:H	3:A:136:GLN:HE21	1.53	0.56
3:A:155:MET:SD	3:A:158:MET:HE3	2.45	0.56
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.36	0.56
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.30	0.56
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.87	0.56
2:P:4:DA:H2''	2:P:5:DT:O5'	2.05	0.56
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.21	0.56
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.88	0.56
3:A:165:GLU:OE1	3:A:168:LYS:NZ	2.39	0.56
3:A:211:LEU:HD12	3:A:211:LEU:O	2.06	0.56
3:A:158:MET:HG2	3:A:241:LEU:HD21	1.89	0.55
3:A:115:VAL:C	3:A:117:GLU:H	2.14	0.55
3:A:288:GLU:C	3:A:290:GLY:H	2.15	0.55
3:A:79:THR:C	3:A:81:LYS:H	2.14	0.55
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.71	0.55
3:A:154:GLU:O	3:A:158:MET:HG3	2.07	0.55
3:A:241:LEU:HB3	3:A:242:PRO:HD2	1.89	0.55
3:A:207:GLN:OE1	3:A:210:LEU:HG	2.06	0.54
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.89	0.54
3:A:85:LEU:HD23	3:A:89:ARG:HH21	1.73	0.54
3:A:282:MET:HG2	7:A:555:HOH:O	2.08	0.54
3:A:325:TRP:HD1	7:A:583:HOH:O	1.90	0.54
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.43	0.53
3:A:194:LEU:N	3:A:194:LEU:HD13	2.23	0.53
3:A:265:TYR:O	3:A:269:VAL:HG23	2.08	0.53
3:A:280:LYS:O	3:A:283:ARG:N	2.42	0.53
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.88	0.53
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.36	0.53
3:A:308:GLY:O	3:A:309:GLU:HB2	2.09	0.52
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.91	0.52
3:A:194:LEU:HD11	3:A:258:ARG:CD	2.31	0.52
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.92	0.52
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.92	0.52
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.45	0.51
3:A:155:MET:HE3	3:A:188:SER:CB	2.40	0.51
3:A:36:TYR:CD2	3:A:37:ASN:N	2.79	0.51
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.93	0.51
3:A:243:SER:CB	3:A:249:GLU:HA	2.41	0.51
3:A:119:ILE:HA	3:A:124:ASP:HB3	1.92	0.51
3:A:205:THR:O	3:A:206:LYS:O	2.29	0.51
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:296:TYR:CD1	3:A:296:TYR:N	2.78	0.50
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.53	0.50
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.11	0.50
3:A:156:LEU:HD23	3:A:181:PHE:HE1	1.76	0.50
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.94	0.50
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.43	0.50
3:A:255:ILE:HG12	3:A:256:ASP:N	2.26	0.50
3:A:11:LEU:HD23	3:A:11:LEU:N	2.27	0.49
3:A:174:ILE:O	3:A:195:LEU:HD12	2.13	0.49
3:A:204:SER:O	3:A:204:SER:OG	2.28	0.49
3:A:133:ASN:O	3:A:137:ARG:HG3	2.12	0.49
3:A:194:LEU:HD12	3:A:258:ARG:CG	2.42	0.49
3:A:243:SER:OG	3:A:249:GLU:HG3	2.12	0.49
3:A:275:SER:HB2	3:A:277:ILE:HD13	1.94	0.49
3:A:76:PHE:O	3:A:79:THR:O	2.29	0.49
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.48	0.49
3:A:152:ARG:HA	3:A:155:MET:HB2	1.94	0.49
3:A:283:ARG:HB2	7:A:630:HOH:O	2.13	0.48
3:A:157:GLN:HE22	3:A:244:LYS:HZ3	1.57	0.48
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.48	0.48
3:A:85:LEU:HD23	3:A:89:ARG:NH2	2.28	0.48
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.96	0.48
3:A:18:MET:CG	3:A:22:LEU:HD23	2.42	0.48
3:A:200:PHE:HB2	7:A:625:HOH:O	2.13	0.48
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.47	0.48
3:A:26:GLU:HA	3:A:30:SER:OG	2.14	0.48
3:A:292:THR:O	3:A:293:ILE:HD13	2.13	0.48
3:A:201:THR:HA	3:A:261:PRO:HB2	1.96	0.47
3:A:280:LYS:O	3:A:283:ARG:HB2	2.13	0.47
3:A:298:ILE:HG21	3:A:322:TYR:CD2	2.47	0.47
3:A:321:ASP:O	3:A:324:GLN:N	2.45	0.47
3:A:41:LYS:O	3:A:45:VAL:HG13	2.14	0.47
3:A:201:THR:OG1	3:A:202:SER:N	2.47	0.47
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.29	0.47
3:A:31:GLN:HG3	3:A:112:ARG:NH2	2.27	0.47
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.35	0.47
3:A:322:TYR:C	3:A:324:GLN:H	2.21	0.47
3:A:95:SER:HA	7:A:639:HOH:O	2.15	0.47
3:A:195:LEU:O	3:A:260:ILE:N	2.41	0.47
3:A:264:GLN:HB3	3:A:296:TYR:O	2.15	0.47
3:A:12:ASN:CB	3:A:46:ILE:HD12	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:85:LEU:CD2	3:A:89:ARG:HH21	2.28	0.47
3:A:216:GLU:O	3:A:220:LYS:N	2.48	0.47
3:A:269:VAL:HG12	3:A:269:VAL:O	2.14	0.47
3:A:272:PHE:HA	7:A:532:HOH:O	2.14	0.47
3:A:46:ILE:HD13	3:A:53:ILE:HD12	1.97	0.47
3:A:155:MET:CE	3:A:188:SER:HB2	2.45	0.47
3:A:254:ARG:NH1	3:A:255:ILE:H	2.12	0.47
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.50	0.47
3:A:35:LYS:O	3:A:38:ALA:HB3	2.15	0.46
3:A:59:ALA:O	3:A:62:LEU:HB2	2.14	0.46
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.13	0.46
3:A:311:LEU:HA	3:A:312:PRO:HD2	1.70	0.46
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.51	0.46
3:A:121:THR:H	3:A:124:ASP:HB2	1.80	0.46
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.27	0.46
3:A:180:SER:HB2	3:A:185:ALA:HB3	1.98	0.46
3:A:56:GLY:O	3:A:59:ALA:N	2.48	0.46
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.94	0.46
3:A:60:LYS:CA	3:A:65:VAL:HG22	2.39	0.46
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.50	0.46
3:A:191:MET:HB2	3:A:191:MET:HE3	1.66	0.46
3:A:259:LEU:HD12	3:A:259:LEU:C	2.28	0.46
3:A:18:MET:CE	3:A:76:PHE:CD1	2.99	0.46
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.46	0.46
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.80	0.45
3:A:85:LEU:O	3:A:89:ARG:HG3	2.17	0.45
3:A:58:GLU:O	3:A:58:GLU:HG2	2.17	0.45
3:A:100:LEU:HA	3:A:100:LEU:HD12	1.51	0.45
3:A:86:GLU:O	3:A:90:GLN:HG3	2.17	0.45
3:A:18:MET:HE1	3:A:76:PHE:CG	2.52	0.45
3:A:18:MET:HG2	3:A:22:LEU:CD2	2.43	0.45
3:A:270:LEU:HD22	3:A:319:ILE:CD1	2.47	0.45
3:A:206:LYS:O	3:A:207:GLN:HB2	2.15	0.45
3:A:244:LYS:C	3:A:245:ASN:HD22	2.25	0.45
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.84	0.45
3:A:331:LYS:HD2	3:A:332:ASP:H	1.81	0.45
3:A:133:ASN:ND2	7:A:512:HOH:O	2.48	0.45
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.99	0.44
3:A:123:GLU:HG3	7:A:623:HOH:O	2.16	0.44
3:A:218:LEU:N	3:A:218:LEU:CD1	2.80	0.44
2:P:5:DT:P	3:A:107:GLY:HA3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:282:MET:HB3	7:A:555:HOH:O	2.17	0.44
3:A:265:TYR:C	3:A:269:VAL:HG23	2.42	0.44
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.98	0.44
3:A:150:ILE:O	3:A:187:SER:HA	2.17	0.44
3:A:45:VAL:CG2	3:A:46:ILE:N	2.80	0.44
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.24	0.44
3:A:156:LEU:HD23	3:A:181:PHE:CE1	2.52	0.44
3:A:285:HIS:NE2	3:A:323:ILE:O	2.47	0.44
2:P:2:DA:H5'	2:P:2:DA:H8	1.78	0.43
3:A:237:GLY:O	3:A:254:ARG:NH1	2.50	0.43
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.98	0.43
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.69	0.43
3:A:127:LYS:HD2	3:A:127:LYS:HA	1.73	0.43
3:A:80:GLY:C	3:A:81:LYS:HG2	2.43	0.43
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.48	0.43
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.34	0.43
1:T:6:DT:H2''	1:T:7:DG:C8	2.53	0.43
2:P:2:DA:C8	2:P:2:DA:C5'	2.99	0.43
3:A:113:LYS:O	3:A:117:GLU:HG3	2.18	0.43
3:A:235:PHE:CD1	3:A:235:PHE:C	2.94	0.43
3:A:316:GLU:O	3:A:320:PHE:HD2	2.02	0.43
3:A:33:ILE:H	3:A:33:ILE:HG22	1.54	0.43
3:A:79:THR:C	3:A:81:LYS:N	2.77	0.43
3:A:286:ALA:O	3:A:291:PHE:N	2.52	0.43
3:A:303:VAL:O	3:A:305:GLY:N	2.52	0.42
3:A:306:VAL:O	3:A:307:ALA:HB2	2.18	0.42
3:A:145:ASP:HB3	3:A:252:HIS:O	2.18	0.42
3:A:253:ARG:NH1	7:A:503:HOH:O	2.51	0.42
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.35	0.42
3:A:239:CYS:O	3:A:240:GLN:HB2	2.20	0.42
3:A:255:ILE:HG23	3:A:255:ILE:HD13	1.85	0.42
3:A:331:LYS:CD	3:A:332:ASP:N	2.83	0.42
3:A:30:SER:HA	7:A:641:HOH:O	2.18	0.42
3:A:152:ARG:O	3:A:155:MET:HB2	2.20	0.42
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.49	0.42
3:A:218:LEU:HB2	3:A:224:ILE:HD12	2.01	0.42
3:A:201:THR:HG23	3:A:204:SER:HB3	2.02	0.42
3:A:150:ILE:HB	3:A:155:MET:HE2	2.02	0.41
1:T:4:DT:H2''	1:T:5:DC:O5'	2.21	0.41
3:A:115:VAL:C	3:A:117:GLU:N	2.75	0.41
3:A:196:THR:OG1	3:A:262:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:221:VAL:O	3:A:222:HIS:HB2	2.20	0.41
3:A:327:TYR:HD1	3:A:328:ARG:N	2.18	0.41
3:A:99:PHE:CD1	3:A:99:PHE:C	2.98	0.41
3:A:177:VAL:HG11	3:A:191:MET:HE2	2.02	0.41
3:A:280:LYS:H	3:A:280:LYS:HG3	1.65	0.41
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.62	0.41
3:A:15:ILE:HG21	3:A:46:ILE:CD1	2.50	0.41
3:A:163:LEU:N	3:A:163:LEU:HD23	2.33	0.41
3:A:271:TYR:CD2	3:A:271:TYR:C	2.95	0.41
3:A:277:ILE:HG13	3:A:335:GLU:HB3	2.02	0.41
3:A:41:LYS:O	3:A:44:SER:HB3	2.19	0.41
3:A:135:HIS:C	3:A:135:HIS:CD2	2.98	0.41
3:A:154:GLU:HB3	3:A:241:LEU:HD11	2.03	0.41
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.50	0.41
3:A:330:PRO:C	3:A:333:ARG:HG3	2.44	0.41
3:A:181:PHE:HA	7:A:530:HOH:O	2.20	0.41
3:A:223:PHE:O	3:A:239:CYS:HA	2.20	0.41
3:A:293:ILE:CD1	3:A:298:ILE:CG1	2.99	0.41
2:P:3:DG:H1'	7:P:511:HOH:O	2.21	0.41
3:A:25:PHE:CD1	3:A:25:PHE:C	2.99	0.41
3:A:42:ALA:O	3:A:46:ILE:HG23	2.21	0.41
3:A:83:ARG:HA	3:A:86:GLU:HG2	2.02	0.41
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.09	0.41
3:A:228:LEU:HB2	3:A:236:MET:O	2.21	0.41
3:A:53:ILE:N	7:A:554:HOH:O	2.54	0.41
3:A:125:LEU:HA	3:A:125:LEU:HD23	1.81	0.41
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.56	0.41
3:A:194:LEU:CD1	3:A:258:ARG:CG	2.99	0.41
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.65	0.40
3:A:255:ILE:HG23	3:A:255:ILE:O	2.20	0.40
3:A:266:TYR:O	3:A:270:LEU:N	2.45	0.40
3:A:289:LYS:HG3	3:A:323:ILE:O	2.20	0.40
3:A:18:MET:CG	3:A:22:LEU:CD2	2.99	0.40
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.99	0.40
3:A:208:PRO:O	3:A:212:HIS:HD2	2.03	0.40
3:A:18:MET:CE	3:A:76:PHE:CG	3.05	0.40
3:A:194:LEU:CD1	3:A:258:ARG:CD	2.97	0.40
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.99	0.40
3:A:18:MET:O	3:A:21:GLU:HB2	2.22	0.40
3:A:83:ARG:O	3:A:86:GLU:N	2.54	0.40
3:A:294:ASN:C	3:A:294:ASN:HD22	2.29	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	325/335 (97%)	269 (83%)	36 (11%)	20 (6%)	1 6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU
3	A	309	GLU
3	A	10	THR
3	A	80	GLY
3	A	185	ALA
3	A	202	SER
3	A	246	ASP
3	A	289	LYS
3	A	304	THR
3	A	91	ASP
3	A	310	PRO
3	A	265	TYR
3	A	307	ALA
3	A	334	SER
3	A	204	SER
3	A	207	GLN
3	A	295	GLU

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
3	A	288/295 (98%)	215 (75%)	73 (25%)	0 3

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	15	ILE
3	A	18	MET
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	77	LEU
3	A	79	THR
3	A	93	THR
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	121	THR
3	A	122	LEU
3	A	130	ASP
3	A	131	LYS
3	A	138	ILE
3	A	150	ILE
3	A	153	GLU
3	A	168	LYS
3	A	169	VAL
3	A	171	SER

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Mol	Chain	Res	Type
3	A	172	GLU
3	A	174	ILE
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	201	THR
3	A	202	SER
3	A	207	GLN
3	A	209	LYS
3	A	214	VAL
3	A	218	LEU
3	A	219	GLN
3	A	228	LEU
3	A	230	LYS
3	A	233	THR
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	259	LEU
3	A	264	GLN
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	288	GLU
3	A	292	THR
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	296	TYR
3	A	298	ILE
3	A	301	LEU
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	98	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	252	HIS
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	DCT	A	338	4	10,12,28	1.19	0	17,20,43	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DCT	A	338	4	-	6/12/12/31	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

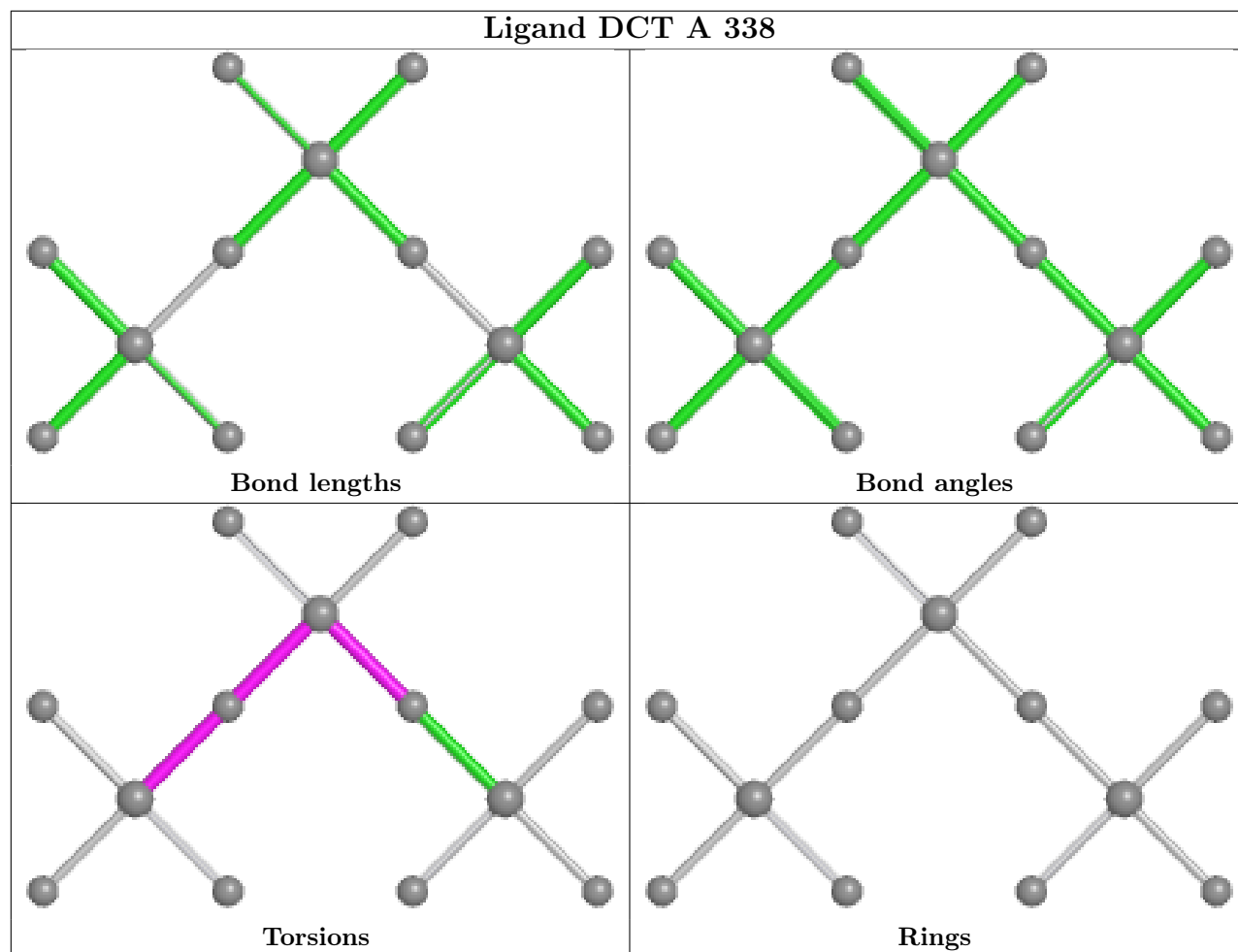
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	338	DCT	PB-O3B-PG-O2G
6	A	338	DCT	PG-O3B-PB-O2B
6	A	338	DCT	PA-O3A-PB-O2B
6	A	338	DCT	PB-O3B-PG-O1G
6	A	338	DCT	PG-O3B-PB-O1B
6	A	338	DCT	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	7/7 (100%)	-1.21	0 100 100	22, 36, 65, 98	0
2	P	6/6 (100%)	-1.36	0 100 100	20, 31, 34, 37	0
3	A	324/335 (96%)	-1.13	0 100 100	4, 35, 86, 100	0
All	All	337/348 (96%)	-1.14	0 100 100	4, 35, 87, 100	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

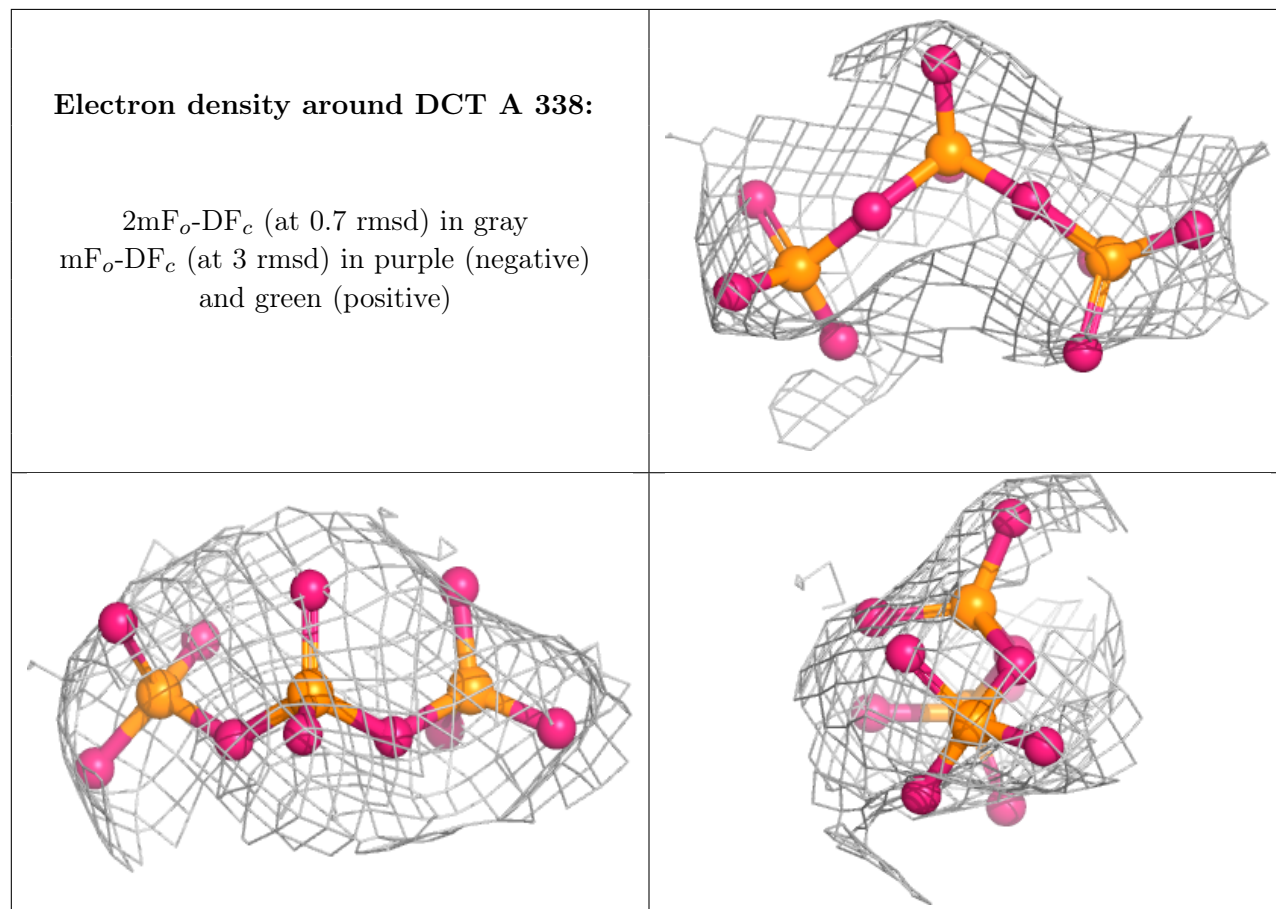
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	DCT	A	338	13/27	0.91	0.10	83,86,95,97	13
4	MG	A	339	1/1	0.96	0.06	30,30,30,30	1
5	NA	A	342	1/1	0.99	0.05	37,37,37,37	0
5	NA	A	341	1/1	0.99	0.03	21,21,21,21	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.