



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:35 PM UTC

PDB ID : 2BPG / pdb_00002bpg
Title : STRUCTURES OF TERNARY COMPLEXES OF RAT DNA POLYMERASE BETA, A DNA TEMPLATE-PRIMER, AND DDCTP
Authors : Pelletier, H.; Sawaya, M.R.; Kumar, A.; Wilson, S.H.; Kraut, J.
Deposited on : 1994-05-19
Resolution : 3.60 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

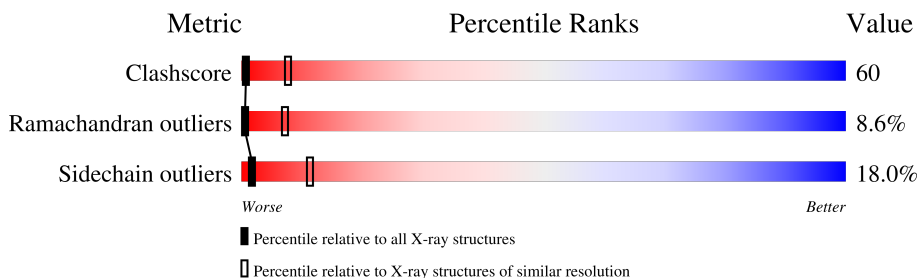
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	8	38% 38% 25%
1	T	8	12% 25% 38% 25%
2	D	7	14% 57% 29%
2	P	7	86% 14%
3	A	335	20% 42% 29% 6% .
3	B	335	26% 45% 21% 5% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5754 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(*GP*GP*GP*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	8	Total	C	N	O	P	0	0	0
			167	77	34	48	8			
1	C	8	Total	C	N	O	P	0	0	0
			167	77	34	48	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			
2	D	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			

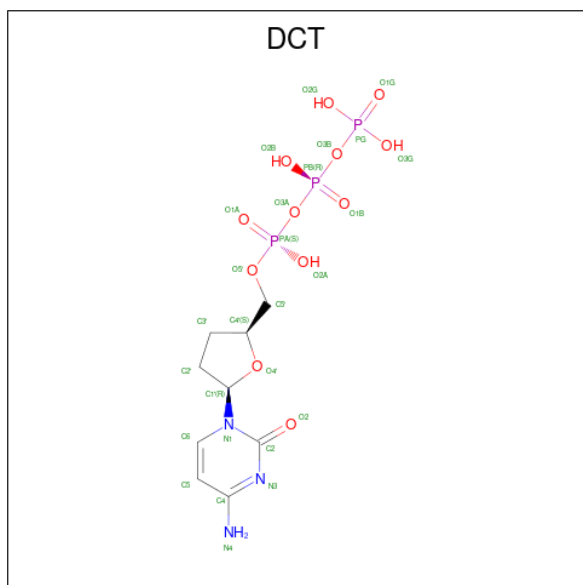
- Molecule 3 is a protein called DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	324	Total	C	N	O	S	0	0	0
			2542	1602	448	483	9			
3	B	324	Total	C	N	O	S	0	0	0
			2541	1601	448	483	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 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	27	9	3	12	3	0	0
5	B	1	27	9	3	12	3	0	0

- Molecule 6 is water.

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

Note EDS was not executed.

- Molecule 1: DNA (5'-D(*GP*GP*GP*CP*GP*CP*CP*G)-3')

Chain T: 




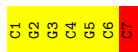
- Molecule 1: DNA (5'-D(*GP*GP*GP*CP*GP*CP*CP*G)-3')

Chain C: 



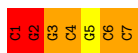
- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*GP*CP*C)-3')

Chain P: 




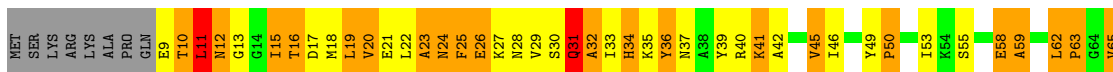
- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*GP*CP*C)-3')

Chain D: 



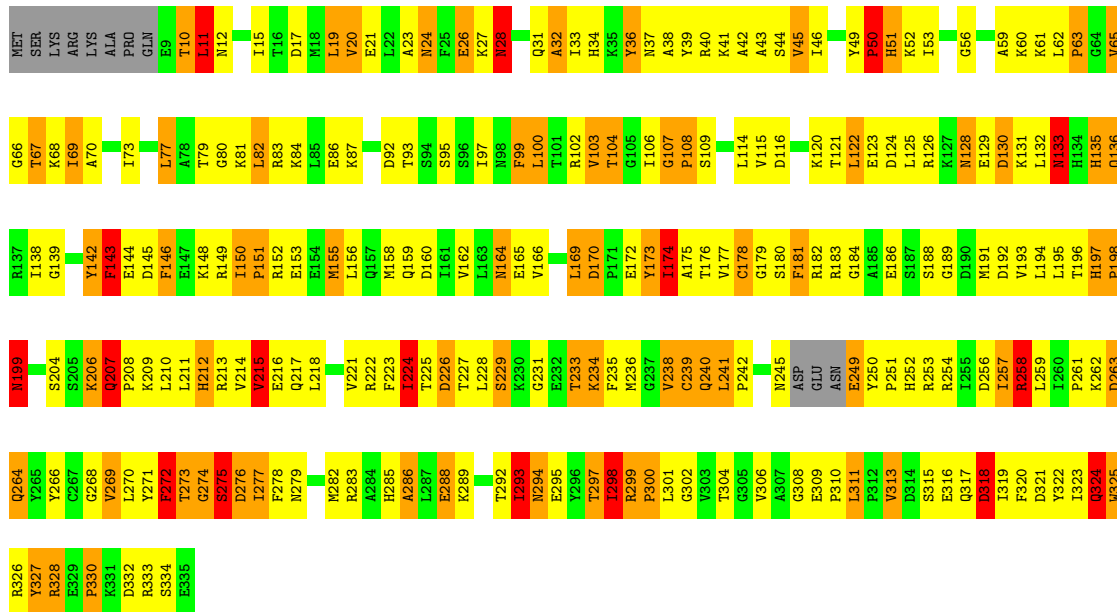
- Molecule 3: DNA POLYMERASE BETA

Chain A: 





• Molecule 3: DNA POLYMERASE BETA



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.30Å 56.80Å 86.70Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5754	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: MG, 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	C	0.70	0/187	1.75	4/287 (1.4%)
1	T	0.91	0/187	1.75	7/287 (2.4%)
2	D	0.87	0/155	2.13	10/237 (4.2%)
2	P	0.62	0/155	1.54	2/237 (0.8%)
3	A	1.47	11/2588 (0.4%)	2.12	109/3491 (3.1%)
3	B	1.49	11/2587 (0.4%)	2.10	94/3490 (2.7%)
All	All	1.42	22/5859 (0.4%)	2.07	226/8029 (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
1	C	0	6
1	T	0	5
2	D	0	3
2	P	0	1
All	All	0	15

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	299	ARG	N-CA	-7.71	1.38	1.45
3	B	224	ILE	N-CA	-6.79	1.38	1.46
3	B	300	PRO	N-CA	-6.70	1.39	1.47
3	B	114	LEU	C-N	-5.71	1.27	1.33
3	B	269	VAL	CA-CB	-5.65	1.48	1.54
3	B	36	TYR	CA-C	-5.58	1.45	1.52
3	A	133	ASN	N-CA	-5.49	1.39	1.45
3	A	224	ILE	N-CA	-5.45	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	294	ASN	N-CA	-5.43	1.39	1.46
3	B	298	ILE	CA-CB	-5.33	1.48	1.54
3	A	254	ARG	CA-C	-5.23	1.46	1.52
3	A	75	GLU	CA-CB	5.21	1.61	1.53
3	A	53	ILE	CA-C	-5.18	1.48	1.53
3	A	15	ILE	CA-CB	-5.17	1.48	1.54
3	A	256	ASP	N-CA	-5.16	1.39	1.46
3	B	298	ILE	N-CA	-5.14	1.40	1.46
3	B	104	THR	N-CA	-5.11	1.39	1.46
3	B	257	ILE	CA-CB	-5.09	1.47	1.54
3	A	255	ILE	C-N	-5.08	1.27	1.33
3	A	59	ALA	CA-C	-5.05	1.46	1.52
3	B	299	ARG	CA-C	-5.04	1.46	1.52
3	A	30	SER	CA-C	-5.00	1.46	1.52

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	7	DC	C2-N1-C1'	-11.52	102.42	119.70
3	B	313	VAL	N-CA-C	11.05	118.03	106.21
3	A	128	ASN	CA-CB-CG	-10.65	101.95	112.60
3	B	251	PRO	CA-C-N	-10.22	108.82	122.42
3	B	251	PRO	C-N-CA	-10.22	108.82	122.42
2	D	4	DC	C2-N1-C1'	-10.10	104.55	119.70
3	A	197	HIS	CA-C-N	9.88	132.18	119.84
3	A	197	HIS	C-N-CA	9.88	132.18	119.84
3	A	193	VAL	N-CA-C	9.51	121.87	107.99
3	B	128	ASN	N-CA-C	9.45	124.36	113.02
2	D	4	DC	C6-N1-C1'	9.32	133.68	119.70
1	T	7	DC	P-O5'-C5'	-9.31	106.03	120.00
3	B	20	VAL	N-CA-C	9.31	119.35	110.42
3	B	293	ILE	CB-CA-C	-9.15	98.56	111.38
3	B	150	ILE	CA-C-N	-9.10	108.47	119.84
3	B	150	ILE	C-N-CA	-9.10	108.47	119.84
3	B	197	HIS	CA-C-N	9.06	131.16	119.84
3	B	197	HIS	C-N-CA	9.06	131.16	119.84
2	D	1	DC	C6-N1-C1'	-8.94	106.29	119.70
2	D	2	DG	C5'-C4'-C3'	-8.84	101.64	114.90
3	B	51	HIS	CA-CB-CG	8.81	122.61	113.80
1	T	7	DC	C2-N1-C1'	8.66	132.69	119.70
3	B	238	VAL	CB-CA-C	-8.64	97.71	110.33
1	C	7	DC	C6-N1-C1'	-8.55	106.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	31	GLN	N-CA-C	-8.48	101.61	111.03
3	B	146	PHE	CA-CB-CG	-8.43	105.37	113.80
3	A	120	LYS	N-CA-C	8.27	120.16	110.41
3	B	193	VAL	N-CA-C	8.21	119.92	107.77
3	B	318	ASP	CA-CB-CG	8.21	120.81	112.60
3	B	251	PRO	N-CA-CB	8.16	110.45	103.35
3	B	197	HIS	CA-CB-CG	8.11	121.91	113.80
3	A	122	LEU	N-CA-C	-8.07	102.57	111.36
3	B	227	THR	N-CA-C	7.79	121.22	108.52
3	A	99	PHE	CA-CB-CG	-7.71	106.09	113.80
3	B	298	ILE	N-CA-C	-7.69	97.41	108.17
3	B	301	LEU	N-CA-C	-7.68	96.74	108.96
3	B	269	VAL	N-CA-C	7.67	118.41	110.36
3	A	142	TYR	N-CA-C	7.60	122.65	113.23
3	A	320	PHE	CB-CA-C	-7.59	97.77	110.68
2	D	1	DC	C2-N1-C1'	7.54	131.01	119.70
3	A	199	ASN	CA-C-N	7.50	131.44	120.95
3	A	199	ASN	C-N-CA	7.50	131.44	120.95
1	T	7	DC	C6-N1-C1'	-7.49	108.47	119.70
3	B	11	LEU	N-CA-C	7.37	126.49	110.80
3	B	297	THR	N-CA-C	7.32	120.49	108.99
3	A	69	ILE	CB-CA-C	-7.21	102.27	112.22
3	A	211	LEU	N-CA-C	-7.15	103.18	110.97
3	B	45	VAL	N-CA-C	7.15	117.25	110.53
1	C	5	DG	C4-N9-C1'	-7.15	116.28	127.00
3	A	275	SER	N-CA-CB	7.05	122.41	110.49
3	B	133	ASN	N-CA-C	-7.04	100.77	110.35
3	B	142	TYR	O-C-N	7.04	130.29	121.64
3	A	107	GLY	C-N-CD	-7.02	96.22	125.00
3	A	243	SER	N-CA-C	7.01	117.75	108.07
3	A	310	PRO	N-CA-CB	6.97	110.57	103.25
3	A	121	THR	N-CA-CB	6.89	122.08	111.46
3	B	28	ASN	N-CA-C	6.87	121.83	113.38
3	B	65	VAL	N-CA-C	-6.86	99.89	109.21
3	A	333	ARG	N-CA-C	6.85	125.40	110.80
3	B	174	ILE	N-CA-CB	6.76	120.34	112.15
3	B	36	TYR	CB-CA-C	-6.75	100.29	110.88
3	A	251	PRO	N-CA-CB	6.68	109.63	103.15
3	B	63	PRO	CB-CA-C	-6.68	104.28	111.56
2	P	7	DC	C6-N1-C1'	6.63	129.65	119.70
3	B	302	GLY	N-CA-C	-6.62	102.49	113.02
3	A	20	VAL	N-CA-C	6.62	116.77	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	117	GLU	N-CA-C	-6.62	103.30	112.30
3	A	69	ILE	O-C-N	6.61	128.64	121.83
3	B	264	GLN	N-CA-CB	6.54	120.48	110.79
3	B	207	GLN	N-CA-C	6.53	124.24	109.81
3	B	164	ASN	CA-CB-CG	-6.52	106.08	112.60
3	A	266	TYR	CB-CA-C	6.52	121.24	110.81
3	A	195	LEU	N-CA-C	6.50	119.20	108.99
3	A	84	LYS	N-CA-C	-6.49	103.33	111.11
3	B	181	PHE	N-CA-C	-6.48	104.14	111.07
1	C	7	DC	C2-N1-C1'	6.48	129.41	119.70
3	A	133	ASN	N-CA-C	-6.45	99.79	110.17
1	T	5	DG	C4'-C3'-O3'	-6.45	100.33	110.00
3	A	24	ASN	CA-CB-CG	-6.43	106.17	112.60
3	A	34	HIS	CA-CB-CG	6.39	120.19	113.80
3	A	19	LEU	N-CA-C	6.38	118.77	111.11
3	B	288	GLU	N-CA-C	-6.36	104.34	111.28
3	A	11	LEU	N-CA-C	6.36	124.35	110.80
2	D	6	DC	C2-N1-C1'	-6.34	110.19	119.70
3	A	313	VAL	N-CA-C	6.34	122.52	109.34
3	A	69	ILE	N-CA-C	-6.32	104.33	110.72
3	B	108	PRO	N-CA-C	6.32	125.49	112.47
2	D	3	DG	C5'-C4'-C3'	6.25	124.27	114.90
2	D	3	DG	O5'-C5'-C4'	6.24	120.16	110.80
3	A	30	SER	CA-C-N	-6.21	112.19	120.63
3	A	30	SER	C-N-CA	-6.21	112.19	120.63
3	B	93	THR	N-CA-C	6.20	117.70	111.07
3	B	297	THR	CB-CA-C	-6.20	96.74	109.94
3	B	286	ALA	N-CA-C	6.19	118.58	111.02
3	B	254	ARG	N-CA-CB	6.18	119.28	110.44
3	B	82	LEU	N-CA-C	-6.17	98.93	109.24
3	B	272	PHE	CA-CB-CG	-6.16	107.64	113.80
3	A	82	LEU	N-CA-C	-6.13	97.83	108.69
3	A	75	GLU	CB-CG-CD	6.13	123.03	112.60
3	B	229	SER	CB-CA-C	6.11	120.34	109.65
3	B	239	CYS	CB-CA-C	-6.09	101.40	113.45
3	A	236	MET	CA-C-N	-6.06	110.24	121.15
3	A	236	MET	C-N-CA	-6.06	110.24	121.15
3	B	107	GLY	N-CA-C	-6.03	100.04	112.34
3	A	261	PRO	N-CA-C	-6.03	100.06	112.47
3	A	224	ILE	N-CA-C	-6.00	100.97	108.89
3	A	62	LEU	CA-C-N	5.99	125.93	119.76
3	A	62	LEU	C-N-CA	5.99	125.93	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	294	ASN	N-CA-CB	5.98	120.69	111.24
3	B	50	PRO	CB-CA-C	-5.96	101.73	111.56
3	B	263	ASP	CA-CB-CG	-5.95	106.65	112.60
3	A	210	LEU	N-CA-C	-5.93	103.99	111.11
3	A	330	PRO	N-CA-CB	5.89	109.43	103.25
3	A	298	ILE	N-CA-CB	5.88	119.52	111.41
3	A	160	ASP	CA-CB-CG	-5.88	106.72	112.60
3	A	30	SER	CA-C-O	-5.87	114.93	121.51
3	B	51	HIS	N-CA-C	-5.87	98.30	110.80
3	B	152	ARG	CB-CA-C	5.86	120.17	110.90
3	B	212	HIS	CA-CB-CG	-5.85	107.95	113.80
3	B	152	ARG	N-CA-C	5.84	117.45	111.14
3	A	216	GLU	N-CA-CB	5.84	118.64	109.94
3	A	174	ILE	N-CA-CB	5.83	116.89	110.53
3	B	176	THR	CB-CA-C	5.81	119.82	109.65
3	B	261	PRO	N-CA-CB	5.79	109.32	103.25
3	B	69	ILE	CA-CB-CG1	-5.78	100.57	110.40
3	A	309	GLU	O-C-N	5.76	126.21	121.31
3	A	311	LEU	CA-C-N	5.75	127.03	119.84
3	A	311	LEU	C-N-CA	5.75	127.03	119.84
3	B	234	LYS	N-CA-C	5.75	119.62	109.96
2	D	3	DG	C5'-C4'-O4'	5.75	118.02	109.40
3	B	298	ILE	N-CA-CB	5.74	119.06	111.25
3	A	227	THR	N-CA-C	5.72	118.20	108.02
3	A	198	PRO	N-CA-C	5.71	124.23	112.47
3	A	305	GLY	CA-C-N	5.70	132.24	121.97
3	A	305	GLY	C-N-CA	5.70	132.24	121.97
3	A	58	GLU	N-CA-C	-5.69	104.28	111.11
3	A	75	GLU	N-CA-CB	5.69	118.42	109.94
3	B	143	PHE	CA-CB-CG	-5.68	108.12	113.80
3	B	10	THR	CA-C-N	5.68	132.39	121.54
3	B	10	THR	C-N-CA	5.68	132.39	121.54
3	A	234	LYS	N-CA-CB	-5.68	102.17	111.66
3	A	62	LEU	CA-C-O	5.67	125.08	119.75
3	A	196	THR	N-CA-C	5.66	117.45	108.79
3	B	83	ARG	N-CA-CB	5.66	118.43	110.12
3	A	119	ILE	CB-CA-C	5.65	117.69	111.08
3	B	99	PHE	N-CA-C	5.65	117.13	110.97
3	B	300	PRO	CB-CA-C	-5.64	103.59	110.98
3	A	207	GLN	N-CA-C	5.60	122.19	109.81
3	A	216	GLU	CA-C-N	-5.58	111.82	120.31
3	A	216	GLU	C-N-CA	-5.58	111.82	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	316	GLU	CB-CG-CD	5.57	122.07	112.60
3	A	92	ASP	N-CA-CB	5.57	118.29	109.82
3	A	114	LEU	CA-C-N	-5.57	111.64	120.55
3	A	114	LEU	C-N-CA	-5.57	111.64	120.55
3	A	31	GLN	N-CA-CB	5.56	118.05	109.98
3	A	215	VAL	O-C-N	5.55	127.55	121.83
3	A	50	PRO	N-CA-C	5.54	123.88	112.47
3	B	299	ARG	O-C-N	5.53	125.69	121.65
3	A	254	ARG	N-CA-CB	5.51	118.11	110.17
3	B	269	VAL	O-C-N	5.51	127.45	121.94
3	A	309	GLU	CA-C-N	5.51	126.73	119.84
3	A	309	GLU	C-N-CA	5.51	126.73	119.84
3	B	298	ILE	CA-C-N	-5.50	112.86	122.38
3	B	298	ILE	C-N-CA	-5.50	112.86	122.38
3	B	199	ASN	N-CA-C	-5.49	106.08	112.89
3	A	75	GLU	N-CA-C	-5.49	104.52	111.11
3	A	213	ARG	N-CA-C	5.49	116.95	110.97
3	B	61	LYS	O-C-N	5.47	127.71	122.07
3	A	300	PRO	CB-CA-C	-5.46	103.94	111.21
1	T	10	DC	P-O5'-C5'	-5.45	111.82	120.00
3	A	304	THR	CA-CB-OG1	5.44	117.76	109.60
1	T	11	DG	C8-N9-C1'	-5.44	118.85	127.00
3	B	136	GLN	O-C-N	5.43	128.36	122.11
3	B	151	PRO	N-CA-C	-5.40	101.34	112.47
3	A	223	PHE	CA-C-N	-5.40	114.21	121.66
3	A	223	PHE	C-N-CA	-5.40	114.21	121.66
3	B	277	ILE	N-CA-CB	-5.40	104.16	110.64
3	B	313	VAL	N-CA-CB	5.40	117.68	112.28
3	A	260	ILE	CB-CA-C	-5.39	101.55	111.36
3	B	266	TYR	CB-CA-C	5.38	119.24	110.96
3	B	135	HIS	O-C-N	5.35	127.60	122.03
3	A	276	ASP	N-CA-CB	5.35	119.53	110.49
3	B	300	PRO	O-C-N	5.34	129.63	123.06
3	B	144	GLU	N-CA-CB	5.33	118.56	110.14
3	A	274	GLY	CA-C-N	5.32	131.71	121.54
3	A	274	GLY	C-N-CA	5.32	131.71	121.54
3	A	151	PRO	N-CA-CB	5.32	108.25	103.19
3	A	235	PHE	CA-C-N	-5.31	115.67	123.00
3	A	235	PHE	C-N-CA	-5.31	115.67	123.00
3	A	291	PHE	CB-CA-C	-5.30	99.05	110.45
3	B	269	VAL	CB-CA-C	-5.29	105.11	111.88
3	B	325	TRP	N-CA-CB	5.27	119.58	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	69	ILE	O-C-N	5.26	127.75	121.80
3	A	197	HIS	C-N-CD	-5.26	103.43	125.00
3	A	92	ASP	O-C-N	5.25	127.70	122.08
3	B	132	LEU	N-CA-C	5.25	118.10	109.76
3	A	232	GLU	N-CA-C	5.23	117.89	111.82
3	A	86	GLU	N-CA-CB	5.23	118.38	110.28
1	C	5	DG	P-O5'-C5'	-5.22	112.17	120.00
3	A	276	ASP	CA-CB-CG	5.22	117.82	112.60
3	A	286	ALA	N-CA-C	5.21	117.36	111.11
3	B	258	ARG	CA-C-N	5.21	130.51	123.11
3	B	258	ARG	C-N-CA	5.21	130.51	123.11
3	A	124	ASP	CA-CB-CG	5.20	117.80	112.60
3	A	108	PRO	CB-CA-C	-5.18	103.01	111.56
3	B	224	ILE	N-CA-C	-5.17	100.95	109.12
3	A	23	ALA	N-CA-C	5.17	116.60	111.07
2	D	6	DC	C6-N1-C1'	5.17	127.45	119.70
3	A	252	HIS	CA-C-N	-5.16	114.71	122.81
3	A	252	HIS	C-N-CA	-5.16	114.71	122.81
3	A	176	THR	CB-CA-C	-5.16	104.34	110.94
3	B	241	LEU	N-CA-CB	5.15	116.97	110.23
3	A	177	VAL	N-CA-CB	5.14	116.13	110.53
3	A	63	PRO	CB-CA-C	-5.12	104.86	111.46
3	A	307	ALA	N-CA-C	-5.10	102.14	110.20
3	B	107	GLY	CA-C-N	5.09	126.21	119.84
3	B	107	GLY	C-N-CA	5.09	126.21	119.84
3	B	325	TRP	CB-CA-C	-5.04	101.28	111.17
3	B	215	VAL	N-CA-C	-5.03	105.80	110.53
1	T	5	DG	C5'-C4'-O4'	5.03	116.94	109.40
3	B	166	VAL	N-CA-C	5.03	115.25	110.42
3	B	92	ASP	N-CA-C	5.02	116.75	111.28
3	A	25	PHE	N-CA-C	-5.02	105.70	111.07
3	A	209	LYS	N-CA-CB	5.01	118.06	110.14
3	A	107	GLY	CA-C-N	5.01	126.10	119.84
3	A	107	GLY	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	DG	Sidechain
1	C	4	DG	Sidechain
1	C	5	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	7	DC	Sidechain
1	C	8	DG	Sidechain
1	C	9	DC	Sidechain
2	D	1	DC	Sidechain
2	D	2	DG	Sidechain
2	D	7	DC	Sidechain
2	P	7	DC	Sidechain
1	T	10	DC	Sidechain
1	T	11	DG	Sidechain
1	T	4	DG	Sidechain
1	T	5	DG	Sidechain
1	T	8	DG	Sidechain

5.2 Too-close contacts [i](#)

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	C	167	0	89	13	0
1	T	167	0	89	9	0
2	D	139	0	79	13	0
2	P	139	0	79	18	2
3	A	2542	0	2488	332	2
3	B	2541	0	2486	290	0
4	A	1	0	0	0	0
5	A	27	0	12	8	0
5	B	27	0	12	1	0
6	A	1	0	0	2	0
6	B	3	0	0	0	0
All	All	5754	0	5334	658	2

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 60.

All (658) 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:330:PRO:HD3	3:A:333:ARG:HH21	1.16	1.05
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.42	1.00
2:D:5:DG:H5''	3:B:107:GLY:H	1.29	0.97
2:D:1:DC:H2''	2:D:2:DG:N7	1.81	0.95
3:A:320:PHE:CD2	3:A:327:TYR:HA	2.03	0.94
1:C:8:DG:H5'	3:B:234:LYS:HB3	1.49	0.93
3:A:218:LEU:HD22	3:A:223:PHE:CD2	2.04	0.92
3:B:183:ARG:HH21	3:B:275:SER:HA	1.31	0.92
3:A:191:MET:HG2	3:A:193:VAL:HG12	1.52	0.91
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.53	0.90
3:A:299:ARG:HG3	3:A:307:ALA:HB1	1.54	0.90
3:A:330:PRO:HD3	3:A:333:ARG:NH2	1.86	0.89
3:B:271:TYR:HA	3:B:279:ASN:HD21	1.35	0.89
3:B:278:PHE:CZ	3:B:333:ARG:HD3	2.08	0.89
2:D:5:DG:H5''	3:B:107:GLY:N	1.86	0.89
3:B:271:TYR:HA	3:B:279:ASN:ND2	1.86	0.89
3:B:235:PHE:HD2	3:B:257:ILE:HG12	1.33	0.88
3:A:214:VAL:HG22	3:A:218:LEU:HD12	1.55	0.88
1:T:8:DG:H5''	3:A:231:GLY:HA3	1.56	0.87
3:B:67:THR:HG23	3:B:68:LYS:H	1.39	0.87
3:B:169:LEU:HD13	3:B:213:ARG:HH21	1.40	0.84
3:B:300:PRO:HG2	3:B:308:GLY:HA3	1.59	0.84
3:B:169:LEU:HB3	3:B:213:ARG:NH2	1.93	0.84
2:D:1:DC:H2''	2:D:2:DG:C8	2.13	0.83
3:A:167:LYS:HG2	3:A:171:PRO:HA	1.59	0.83
3:A:194:LEU:HD13	3:A:195:LEU:N	1.93	0.83
3:A:62:LEU:HD12	3:A:63:PRO:CD	2.07	0.83
3:A:201:THR:HA	3:A:261:PRO:HB3	1.60	0.82
3:A:11:LEU:HD23	3:A:12:ASN:CG	2.05	0.82
3:B:121:THR:H	3:B:124:ASP:HB2	1.44	0.81
3:A:240:GLN:HG2	3:A:241:LEU:N	1.95	0.81
3:A:329:GLU:HB3	3:A:331:LYS:NZ	1.95	0.81
3:A:193:VAL:HG22	3:A:257:ILE:HG23	1.61	0.81
3:B:182:ARG:HH22	3:B:269:VAL:HG11	1.45	0.80
3:B:41:LYS:HD2	3:B:42:ALA:N	1.96	0.80
3:B:62:LEU:HD12	3:B:63:PRO:CD	2.11	0.80
3:B:241:LEU:HD23	3:B:250:TYR:CE2	2.17	0.80
3:B:62:LEU:HD12	3:B:63:PRO:HD2	1.64	0.79
3:A:158:MET:O	3:A:162:VAL:HG23	1.83	0.79
3:B:199:ASN:HB2	3:B:207:GLN:OE1	1.83	0.79
3:A:24:ASN:HA	3:A:27:LYS:HB3	1.65	0.78
3:B:256:ASP:O	3:B:257:ILE:HD13	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:197:HIS:CD2	3:B:198:PRO:HD2	2.18	0.78
3:A:291:PHE:HA	3:A:301:LEU:HD13	1.66	0.78
3:A:240:GLN:HB2	3:A:252:HIS:HA	1.63	0.77
3:B:159:GLN:N	3:B:191:MET:HE1	2.00	0.77
3:B:217:GLN:O	3:B:221:VAL:HG22	1.85	0.77
3:B:158:MET:O	3:B:162:VAL:HG23	1.85	0.77
2:D:3:DG:H2''	2:D:4:DC:H6	1.50	0.76
3:B:206:LYS:C	3:B:208:PRO:HD3	2.10	0.76
3:A:11:LEU:CD2	3:A:12:ASN:H	1.98	0.76
3:A:300:PRO:HD2	3:A:308:GLY:HA3	1.69	0.75
3:B:100:LEU:O	3:B:103:VAL:HG23	1.87	0.75
3:A:298:ILE:HG23	3:A:311:LEU:HB2	1.69	0.74
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.23	0.74
3:B:320:PHE:HD1	3:B:323:ILE:HD11	1.52	0.74
3:B:211:LEU:O	3:B:214:VAL:HG12	1.88	0.74
3:A:66:GLY:H	3:A:69:ILE:HG13	1.53	0.74
3:A:11:LEU:HD23	3:A:12:ASN:H	1.52	0.73
3:B:299:ARG:HB2	3:B:300:PRO:HD2	1.70	0.73
2:D:3:DG:H2''	2:D:4:DC:C6	2.22	0.73
3:A:156:LEU:O	3:A:159:GLN:HB3	1.87	0.73
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.24	0.73
3:B:175:ALA:HB2	3:B:195:LEU:HD13	1.70	0.73
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.69	0.72
3:B:324:GLN:HE21	3:B:324:GLN:HA	1.53	0.72
3:A:74:ASP:HA	3:A:77:LEU:HB2	1.71	0.72
3:A:69:ILE:O	3:A:73:ILE:HG13	1.89	0.72
3:A:59:ALA:O	3:A:62:LEU:HB3	1.88	0.72
3:A:323:ILE:HG13	3:A:325:TRP:HB2	1.70	0.72
3:A:110:ALA:O	3:A:114:LEU:HG	1.90	0.72
3:B:313:VAL:HG11	3:B:319:ILE:HG12	1.70	0.72
3:B:174:ILE:O	3:B:195:LEU:HD12	1.90	0.72
3:A:209:LYS:HG2	3:A:212:HIS:HB2	1.73	0.71
3:A:206:LYS:C	3:A:208:PRO:HD3	2.15	0.71
3:A:320:PHE:HB3	3:A:325:TRP:O	1.91	0.71
3:A:15:ILE:HG12	3:A:46:ILE:CD1	2.21	0.71
1:T:8:DG:H4'	3:A:229:SER:OG	1.91	0.71
2:P:2:DG:H2'	2:P:3:DG:H8	1.55	0.71
3:A:218:LEU:HD22	3:A:223:PHE:HD2	1.53	0.71
3:B:172:GLU:HB3	3:B:197:HIS:CD2	2.26	0.70
3:A:156:LEU:HD13	3:A:159:GLN:NE2	2.05	0.70
2:P:2:DG:H2'	2:P:3:DG:C8	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:197:HIS:CG	3:B:198:PRO:HD2	2.26	0.69
3:B:153:GLU:O	3:B:156:LEU:HB3	1.92	0.69
3:A:26:GLU:OE2	3:A:35:LYS:HD2	1.92	0.69
3:A:258:ARG:HH21	3:A:295:GLU:HG3	1.55	0.69
3:A:300:PRO:HD2	3:A:308:GLY:CA	2.23	0.68
3:B:103:VAL:HB	3:B:106:ILE:HD12	1.74	0.68
2:P:1:DC:H2'	2:P:2:DG:C8	2.29	0.68
3:B:150:ILE:HG21	3:B:155:MET:HG2	1.74	0.68
3:A:264:GLN:HB3	3:A:296:TYR:O	1.92	0.68
3:A:320:PHE:HA	3:A:323:ILE:HG12	1.74	0.68
3:A:172:GLU:HB3	3:A:198:PRO:CG	2.24	0.68
3:A:240:GLN:HG2	3:A:241:LEU:H	1.58	0.67
5:A:338:DCT:C5'	5:A:338:DCT:H6	2.24	0.67
3:B:24:ASN:O	3:B:27:LYS:HB3	1.94	0.67
3:A:70:ALA:O	3:A:73:ILE:HB	1.94	0.67
2:P:7:DC:C6	5:A:338:DCT:H5	2.29	0.67
3:A:233:THR:O	3:A:258:ARG:HG3	1.94	0.67
3:A:18:MET:O	3:A:22:LEU:HD13	1.95	0.66
3:A:302:GLY:O	3:A:304:THR:N	2.29	0.66
3:A:260:ILE:HG22	3:A:261:PRO:N	2.10	0.66
3:B:258:ARG:NH2	3:B:295:GLU:HG3	2.10	0.66
3:A:214:VAL:CG2	3:A:218:LEU:HD12	2.24	0.66
3:A:329:GLU:HB3	3:A:331:LYS:HZ1	1.59	0.66
3:B:212:HIS:O	3:B:215:VAL:HG22	1.96	0.66
3:A:285:HIS:CE1	3:A:325:TRP:HE1	2.15	0.65
3:A:237:GLY:O	3:A:255:ILE:N	2.30	0.65
3:B:67:THR:O	3:B:70:ALA:HB3	1.97	0.65
3:B:150:ILE:CG2	3:B:155:MET:HG2	2.26	0.65
3:B:182:ARG:NH2	3:B:269:VAL:HG11	2.10	0.65
3:A:25:PHE:O	3:A:29:VAL:N	2.29	0.65
3:B:180:SER:HB2	3:B:188:SER:OG	1.95	0.65
3:A:183:ARG:HH11	3:A:273:THR:HG22	1.61	0.65
3:A:330:PRO:CD	3:A:333:ARG:HE	2.10	0.65
3:A:138:ILE:O	3:A:141:LYS:HB3	1.97	0.65
3:B:199:ASN:OD1	3:B:199:ASN:N	2.29	0.65
3:A:195:LEU:HD23	3:A:259:LEU:HB2	1.79	0.64
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.78	0.64
3:A:239:CYS:O	3:A:253:ARG:N	2.31	0.64
3:B:165:GLU:HB3	3:B:217:GLN:HG2	1.78	0.64
3:A:294:ASN:ND2	3:A:297:THR:O	2.30	0.64
3:A:15:ILE:O	3:A:19:LEU:HD13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:65:VAL:HG23	3:A:69:ILE:HB	1.80	0.64
2:D:4:DC:H5''	3:B:109:SER:CB	2.28	0.64
3:B:67:THR:HG23	3:B:68:LYS:N	2.11	0.64
3:A:70:ALA:HA	3:A:73:ILE:HD12	1.78	0.64
3:A:174:ILE:N	3:A:174:ILE:HD12	2.13	0.64
3:B:174:ILE:N	3:B:196:THR:O	2.28	0.64
3:B:62:LEU:HD12	3:B:63:PRO:HD3	1.80	0.63
3:A:266:TYR:CE1	3:A:315:SER:HA	2.34	0.63
3:B:210:LEU:O	3:B:213:ARG:HB2	1.98	0.63
2:P:6:DC:H2''	2:P:7:DC:C5'	2.28	0.63
3:A:294:ASN:OD1	3:A:296:TYR:HB2	1.99	0.63
3:B:206:LYS:HE2	3:B:207:GLN:HG3	1.81	0.63
3:A:207:GLN:O	3:A:210:LEU:HG	1.98	0.63
3:A:83:ARG:O	3:A:86:GLU:N	2.32	0.63
3:A:174:ILE:O	3:A:195:LEU:HD12	1.99	0.63
3:A:217:GLN:O	3:A:221:VAL:HG23	1.99	0.63
3:B:182:ARG:NH1	3:B:273:THR:OG1	2.31	0.63
3:B:135:HIS:CE1	3:B:228:LEU:HD22	2.33	0.63
3:B:174:ILE:O	3:B:195:LEU:HA	1.99	0.63
3:A:99:PHE:O	3:A:102:ARG:N	2.32	0.63
3:B:17:ASP:OD1	3:B:17:ASP:N	2.30	0.63
2:P:5:DG:H5''	3:A:107:GLY:H	1.64	0.63
3:A:191:MET:CG	3:A:193:VAL:HG12	2.28	0.63
3:A:201:THR:CA	3:A:261:PRO:HB3	2.27	0.62
3:A:258:ARG:NH2	3:A:295:GLU:HG3	2.14	0.62
3:B:37:ASN:HA	3:B:40:ARG:HG2	1.81	0.62
3:B:174:ILE:C	3:B:195:LEU:HD12	2.24	0.62
3:A:115:VAL:HG22	3:A:120:LYS:HD3	1.81	0.62
3:B:182:ARG:HB3	3:B:273:THR:HG23	1.80	0.62
3:B:194:LEU:HD13	3:B:195:LEU:N	2.15	0.62
1:C:8:DG:OP1	3:B:233:THR:N	2.28	0.62
3:A:293:ILE:HG22	3:A:294:ASN:N	2.14	0.62
3:A:115:VAL:O	3:A:118:GLY:N	2.31	0.62
3:B:103:VAL:HG12	3:B:139:GLY:HA3	1.82	0.62
3:A:42:ALA:O	3:A:46:ILE:HG23	2.00	0.61
3:A:174:ILE:HB	3:A:196:THR:HG22	1.81	0.61
1:T:8:DG:C5'	3:A:231:GLY:HA3	2.29	0.61
3:B:11:LEU:HD13	3:B:11:LEU:N	2.15	0.61
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.31	0.61
3:A:299:ARG:CG	3:A:307:ALA:HB1	2.28	0.61
3:B:50:PRO:O	3:B:51:HIS:ND1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:274:GLY:HA2	3:B:278:PHE:CD2	2.36	0.61
1:T:10:DC:H2''	1:T:11:DG:C8	2.36	0.61
3:A:112:ARG:O	3:A:115:VAL:N	2.33	0.61
3:A:195:LEU:HG	3:A:196:THR:N	2.16	0.61
3:A:183:ARG:HH11	3:A:273:THR:CG2	2.14	0.61
3:B:311:LEU:HB3	3:B:322:TYR:CE1	2.36	0.61
3:A:31:GLN:HG3	3:A:32:ALA:H	1.66	0.61
1:T:4:DG:H1	5:A:338:DCT:HN41	1.47	0.61
3:A:287:LEU:HD23	3:A:301:LEU:HD21	1.83	0.61
3:B:297:THR:O	3:B:299:ARG:NH1	2.34	0.61
3:A:164:ASN:OD1	3:A:164:ASN:N	2.32	0.60
3:B:297:THR:HG21	3:B:310:PRO:HB3	1.83	0.60
3:A:67:THR:O	3:A:70:ALA:HB3	2.02	0.60
3:A:164:ASN:O	3:A:168:LYS:HG3	2.00	0.60
3:B:172:GLU:O	3:B:198:PRO:HD3	2.01	0.60
3:A:26:GLU:HG2	3:A:35:LYS:HB2	1.84	0.60
3:A:79:THR:O	3:A:81:LYS:N	2.31	0.60
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.17	0.60
3:A:281:ASN:O	3:A:284:ALA:HB3	2.01	0.60
3:B:155:MET:HE1	3:B:191:MET:HA	1.84	0.60
3:B:174:ILE:O	3:B:196:THR:N	2.29	0.60
3:B:326:ARG:HH12	3:B:328:ARG:HA	1.66	0.60
3:A:275:SER:O	3:A:278:PHE:N	2.34	0.60
3:A:330:PRO:HA	3:A:333:ARG:CG	2.29	0.60
3:B:315:SER:O	3:B:318:ASP:HB2	2.02	0.60
3:A:293:ILE:HG22	3:A:294:ASN:H	1.67	0.60
3:B:17:ASP:HA	3:B:20:VAL:HG12	1.84	0.60
3:B:38:ALA:HA	3:B:41:LYS:HE3	1.83	0.59
3:A:17:ASP:O	3:A:20:VAL:HG12	2.02	0.59
3:A:330:PRO:HD3	3:A:333:ARG:HE	1.66	0.59
3:B:309:GLU:OE1	3:B:310:PRO:HD2	2.01	0.59
2:P:6:DC:H2''	2:P:7:DC:O5'	2.01	0.59
3:B:258:ARG:NH2	3:B:295:GLU:OE2	2.32	0.59
3:B:294:ASN:ND2	3:B:299:ARG:HH22	2.00	0.59
3:A:191:MET:HG2	3:A:193:VAL:CG1	2.30	0.59
3:A:31:GLN:HG3	3:A:32:ALA:N	2.18	0.58
3:A:154:GLU:O	3:A:157:GLN:N	2.36	0.58
3:B:148:LYS:HB3	3:B:253:ARG:HH12	1.67	0.58
3:B:235:PHE:CD2	3:B:257:ILE:HG12	2.26	0.58
3:A:320:PHE:CE2	3:A:327:TYR:HA	2.37	0.58
3:B:99:PHE:O	3:B:102:ARG:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:257:ILE:HG22	3:B:258:ARG:N	2.18	0.58
3:B:330:PRO:O	3:B:333:ARG:N	2.31	0.58
3:B:172:GLU:HG3	3:B:198:PRO:HG3	1.84	0.58
3:B:240:GLN:O	3:B:242:PRO:HD3	2.03	0.58
3:B:70:ALA:O	3:B:73:ILE:HB	2.03	0.58
3:B:228:LEU:HB2	3:B:236:MET:HB2	1.85	0.58
3:A:320:PHE:CA	3:A:323:ILE:HG12	2.33	0.58
3:A:20:VAL:O	3:A:23:ALA:N	2.36	0.58
3:B:326:ARG:NH2	3:B:327:TYR:O	2.37	0.57
3:A:16:THR:HG23	3:A:46:ILE:HG13	1.86	0.57
3:A:19:LEU:O	3:A:22:LEU:HB2	2.04	0.57
3:B:103:VAL:HB	3:B:106:ILE:CD1	2.33	0.57
3:A:25:PHE:O	3:A:29:VAL:HB	2.05	0.57
3:A:207:GLN:N	3:A:208:PRO:HD3	2.19	0.57
3:B:268:GLY:O	3:B:271:TYR:HB3	2.04	0.57
1:C:6:DG:H4'	3:B:295:GLU:CD	2.29	0.57
3:B:235:PHE:C	3:B:236:MET:HG3	2.29	0.57
3:B:313:VAL:HG12	3:B:318:ASP:HB3	1.86	0.57
3:B:42:ALA:HA	3:B:45:VAL:HG12	1.86	0.57
3:B:169:LEU:CD1	3:B:213:ARG:HH21	2.16	0.57
3:B:235:PHE:HD2	3:B:257:ILE:CG1	2.11	0.57
3:B:172:GLU:HG3	3:B:198:PRO:CG	2.34	0.57
3:A:139:GLY:O	3:A:143:PHE:N	2.36	0.57
3:A:234:LYS:HE2	3:A:236:MET:CG	2.34	0.57
3:A:280:LYS:O	3:A:284:ALA:N	2.35	0.57
3:B:133:ASN:CG	3:B:136:GLN:HE21	2.10	0.57
3:B:213:ARG:O	3:B:216:GLU:HB2	2.05	0.57
3:B:223:PHE:CZ	3:B:239:CYS:HB2	2.40	0.57
3:A:297:THR:O	3:A:299:ARG:NH1	2.36	0.57
3:B:274:GLY:HA3	3:B:279:ASN:OD1	2.05	0.57
3:A:209:LYS:O	3:A:213:ARG:N	2.37	0.56
3:B:49:TYR:HE1	3:B:51:HIS:HB2	1.70	0.56
3:B:160:ASP:O	3:B:164:ASN:HB2	2.05	0.56
3:B:180:SER:HA	3:B:183:ARG:NH1	2.20	0.56
3:B:271:TYR:CE2	3:B:272:PHE:HD1	2.23	0.56
3:B:323:ILE:HG13	3:B:324:GLN:N	2.19	0.56
1:T:4:DG:N2	5:A:338:DCT:N3	2.48	0.56
1:C:10:DC:H2''	1:C:11:DG:O5'	2.05	0.56
3:A:84:LYS:NZ	6:A:401:HOH:O	2.38	0.56
3:A:156:LEU:HD13	3:A:159:GLN:HE22	1.69	0.56
3:B:317:GLN:CD	3:B:317:GLN:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:55:SER:O	3:A:58:GLU:HB3	2.05	0.56
3:A:174:ILE:N	3:A:196:THR:O	2.35	0.56
3:A:241:LEU:HD22	3:A:250:TYR:CD2	2.40	0.56
3:B:121:THR:OG1	3:B:124:ASP:N	2.37	0.56
3:B:139:GLY:O	3:B:143:PHE:N	2.33	0.56
3:B:206:LYS:HG3	3:B:207:GLN:N	2.21	0.56
3:B:324:GLN:O	3:B:325:TRP:HD1	1.89	0.56
3:A:133:ASN:OD1	3:A:134:HIS:N	2.39	0.56
3:B:169:LEU:HB3	3:B:213:ARG:HH21	1.67	0.56
3:A:22:LEU:N	3:A:22:LEU:HD12	2.21	0.56
3:A:157:GLN:O	3:A:160:ASP:HB2	2.05	0.56
3:A:217:GLN:HG2	3:A:221:VAL:HG23	1.87	0.56
3:A:218:LEU:O	3:A:223:PHE:HB3	2.06	0.56
3:B:299:ARG:HB2	3:B:300:PRO:CD	2.34	0.56
3:A:200:PHE:HE2	3:A:259:LEU:HG	1.70	0.56
3:A:291:PHE:CA	3:A:301:LEU:HD13	2.36	0.56
3:A:158:MET:O	3:A:161:ILE:HB	2.06	0.55
3:B:121:THR:O	3:B:124:ASP:N	2.39	0.55
1:C:8:DG:OP1	3:B:234:LYS:N	2.33	0.55
3:A:330:PRO:N	3:A:333:ARG:HE	2.04	0.55
3:A:45:VAL:HG13	3:A:62:LEU:HD21	1.89	0.55
3:A:24:ASN:O	3:A:27:LYS:HB3	2.07	0.55
3:B:79:THR:C	3:B:81:LYS:H	2.14	0.55
3:B:332:ASP:C	3:B:334:SER:H	2.14	0.55
2:P:6:DC:H2''	2:P:7:DC:H5'	1.89	0.55
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.87	0.55
3:A:283:ARG:NE	3:A:293:ILE:HB	2.21	0.55
3:B:182:ARG:CB	3:B:273:THR:HG23	2.36	0.55
3:A:162:VAL:O	3:A:166:VAL:HG23	2.07	0.55
3:B:325:TRP:CZ3	3:B:328:ARG:HD2	2.41	0.55
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.41	0.55
3:A:238:VAL:HG12	3:A:239:CYS:N	2.21	0.55
3:B:121:THR:N	3:B:124:ASP:HB2	2.19	0.55
3:B:195:LEU:O	3:B:259:LEU:HA	2.07	0.55
3:A:267:CYS:HB3	3:A:294:ASN:O	2.07	0.54
3:A:283:ARG:HE	3:A:293:ILE:HB	1.72	0.54
3:A:330:PRO:HD3	3:A:333:ARG:NE	2.23	0.54
3:B:142:TYR:CE1	3:B:252:HIS:CG	2.95	0.54
3:B:129:GLU:C	3:B:131:LYS:H	2.16	0.54
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.37	0.54
3:A:329:GLU:HB3	3:A:331:LYS:HZ2	1.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:99:PHE:HE2	3:B:122:LEU:HD23	1.72	0.54
3:B:225:THR:OG1	3:B:226:ASP:N	2.40	0.54
3:A:316:GLU:OE1	3:A:333:ARG:NH1	2.38	0.54
3:A:266:TYR:O	3:A:269:VAL:HG23	2.07	0.54
3:A:215:VAL:HG23	3:A:216:GLU:N	2.22	0.54
3:A:330:PRO:HD3	3:A:333:ARG:CZ	2.37	0.54
3:B:62:LEU:CD1	3:B:63:PRO:HD2	2.36	0.54
3:B:245:ASN:O	3:B:249:GLU:N	2.41	0.54
3:A:302:GLY:O	3:A:304:THR:HG22	2.08	0.54
3:B:26:GLU:O	3:B:32:ALA:HB3	2.08	0.54
3:B:294:ASN:ND2	3:B:299:ARG:HH12	2.06	0.54
3:A:294:ASN:HD22	3:A:299:ARG:NH2	2.06	0.53
3:A:132:LEU:HD22	3:A:136:GLN:HB3	1.89	0.53
3:B:271:TYR:CD2	3:B:272:PHE:N	2.77	0.53
1:C:10:DC:H2'	1:C:11:DG:C8	2.44	0.53
3:A:234:LYS:HG2	3:A:235:PHE:N	2.22	0.53
3:A:115:VAL:HG23	3:A:120:LYS:HB3	1.91	0.53
3:B:56:GLY:O	3:B:60:LYS:N	2.33	0.53
3:A:164:ASN:C	3:A:168:LYS:HG3	2.33	0.53
3:B:28:ASN:HB3	3:B:108:PRO:HG3	1.90	0.53
3:A:258:ARG:NH1	3:A:296:TYR:OH	2.35	0.53
3:A:330:PRO:O	3:A:333:ARG:HG3	2.09	0.53
3:B:211:LEU:O	3:B:215:VAL:HG13	2.09	0.53
3:A:193:VAL:HG22	3:A:257:ILE:CG2	2.37	0.53
1:C:10:DC:N3	1:C:11:DG:C6	2.77	0.52
3:A:133:ASN:O	3:A:137:ARG:HG3	2.10	0.52
3:A:226:ASP:N	3:A:226:ASP:OD1	2.42	0.52
3:B:194:LEU:HA	3:B:258:ARG:O	2.09	0.52
3:B:328:ARG:HH11	3:B:328:ARG:CG	2.22	0.52
3:B:183:ARG:HE	3:B:275:SER:HB2	1.73	0.52
3:A:130:ASP:OD1	3:A:131:LYS:HG3	2.08	0.52
3:B:195:LEU:N	3:B:258:ARG:O	2.39	0.52
3:B:263:ASP:OD1	3:B:263:ASP:N	2.41	0.52
3:B:169:LEU:O	3:B:170:ASP:HB2	2.08	0.52
3:B:223:PHE:CE2	3:B:239:CYS:HB2	2.44	0.52
1:C:4:DG:C2	1:C:5:DG:C6	2.97	0.52
3:A:115:VAL:CG2	3:A:120:LYS:HB3	2.39	0.52
3:A:194:LEU:HD13	3:A:195:LEU:H	1.74	0.52
3:B:258:ARG:HG3	3:B:259:LEU:N	2.24	0.52
3:B:196:THR:OG1	3:B:262:LYS:HB2	2.10	0.52
3:B:297:THR:CG2	3:B:310:PRO:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:134:HIS:O	3:A:137:ARG:HB2	2.10	0.52
3:B:330:PRO:HA	3:B:333:ARG:HG3	1.92	0.52
3:B:178:CYS:SG	3:B:272:PHE:HB3	2.50	0.52
3:A:146:PHE:N	3:A:146:PHE:HD1	2.08	0.52
3:B:69:ILE:O	3:B:73:ILE:HG13	2.09	0.52
3:B:278:PHE:CE1	3:B:333:ARG:HD3	2.44	0.52
3:B:239:CYS:SG	3:B:253:ARG:HB2	2.49	0.51
3:B:285:HIS:CE1	3:B:325:TRP:HE1	2.28	0.51
3:A:75:GLU:HG2	3:A:81:LYS:O	2.10	0.51
3:A:125:LEU:HD23	3:A:140:LEU:HD13	1.91	0.51
3:B:79:THR:O	3:B:81:LYS:N	2.43	0.51
3:A:115:VAL:C	3:A:117:GLU:H	2.19	0.51
3:B:12:ASN:OD1	3:B:53:ILE:HG13	2.10	0.51
1:C:6:DG:H4'	3:B:295:GLU:OE1	2.10	0.51
3:A:132:LEU:HD22	3:A:136:GLN:CB	2.40	0.51
3:A:146:PHE:N	3:A:146:PHE:CD1	2.77	0.51
3:A:227:THR:HG23	3:A:235:PHE:HE1	1.76	0.51
3:B:82:LEU:O	3:B:86:GLU:HG2	2.11	0.51
3:A:290:GLY:O	3:A:301:LEU:N	2.32	0.51
3:B:121:THR:O	3:B:124:ASP:HB2	2.11	0.51
5:A:338:DCT:H6	5:A:338:DCT:H5''	1.93	0.51
3:B:179:GLY:O	3:B:182:ARG:HB2	2.11	0.51
3:B:212:HIS:N	3:B:212:HIS:CD2	2.78	0.51
1:C:8:DG:H5''	3:B:231:GLY:HA3	1.93	0.51
3:A:233:THR:O	3:A:233:THR:HG22	2.10	0.51
3:A:266:TYR:CD1	3:A:315:SER:HA	2.46	0.51
3:B:20:VAL:O	3:B:23:ALA:N	2.44	0.51
3:B:66:GLY:O	3:B:69:ILE:N	2.43	0.51
3:B:159:GLN:HG3	3:B:177:VAL:HG11	1.92	0.51
2:P:5:DG:OP1	3:A:107:GLY:O	2.29	0.50
3:A:87:LYS:O	3:A:91:ASP:N	2.44	0.50
3:A:316:GLU:O	3:A:319:ILE:HB	2.11	0.50
3:B:318:ASP:O	3:B:321:ASP:HB2	2.10	0.50
3:A:35:LYS:NZ	6:A:401:HOH:O	2.44	0.50
3:B:40:ARG:O	3:B:43:ALA:HB3	2.10	0.50
3:B:207:GLN:OE1	3:B:210:LEU:HD11	2.10	0.50
3:A:209:LYS:HG2	3:A:212:HIS:CB	2.41	0.50
3:B:20:VAL:O	3:B:23:ALA:HB3	2.12	0.50
3:B:26:GLU:HG3	3:B:32:ALA:CB	2.41	0.50
3:B:46:ILE:HG22	3:B:62:LEU:HD23	1.92	0.50
3:B:279:ASN:O	3:B:283:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:324:GLN:HE21	3:B:324:GLN:CA	2.17	0.50
2:D:5:DG:H5''	3:B:107:GLY:CA	2.41	0.50
3:A:98:ASN:O	3:A:101:THR:OG1	2.29	0.50
3:A:319:ILE:O	3:A:322:TYR:HB2	2.12	0.50
3:A:40:ARG:HG3	3:A:41:LYS:N	2.26	0.50
3:B:121:THR:OG1	3:B:124:ASP:OD1	2.30	0.50
3:A:62:LEU:HG	3:A:65:VAL:HG12	1.93	0.50
3:A:266:TYR:CZ	3:A:315:SER:HA	2.46	0.50
3:A:294:ASN:ND2	3:A:299:ARG:NH2	2.60	0.50
3:B:173:TYR:CD1	3:B:197:HIS:HB2	2.47	0.50
3:B:271:TYR:CE2	3:B:272:PHE:CD1	3.00	0.50
3:A:295:GLU:HG2	3:A:296:TYR:CD1	2.47	0.50
3:B:178:CYS:O	3:B:181:PHE:HB3	2.11	0.50
3:A:127:LYS:HD2	3:A:128:ASN:HD22	1.76	0.49
3:A:183:ARG:NH1	3:A:273:THR:O	2.45	0.49
3:B:40:ARG:HG3	3:B:41:LYS:N	2.27	0.49
3:B:53:ILE:HG21	3:B:59:ALA:HB2	1.94	0.49
3:B:177:VAL:HA	3:B:192:ASP:O	2.12	0.49
2:P:5:DG:O5'	3:A:107:GLY:HA3	2.12	0.49
3:B:17:ASP:O	3:B:20:VAL:HG12	2.12	0.49
3:B:182:ARG:C	3:B:184:GLY:H	2.19	0.49
3:B:300:PRO:O	3:B:308:GLY:N	2.45	0.49
3:A:11:LEU:HD23	3:A:12:ASN:OD1	2.12	0.49
3:B:37:ASN:HD22	3:B:40:ARG:HD3	1.77	0.49
3:B:292:THR:O	3:B:298:ILE:HA	2.12	0.49
3:A:239:CYS:O	3:A:252:HIS:HA	2.12	0.49
3:B:320:PHE:CD2	3:B:327:TYR:HA	2.48	0.49
3:A:316:GLU:OE1	3:A:333:ARG:NH2	2.46	0.49
3:A:294:ASN:HD22	3:A:299:ARG:NH1	2.11	0.49
2:D:6:DC:C2	2:D:7:DC:C5	3.00	0.49
3:A:129:GLU:O	3:A:131:LYS:N	2.46	0.49
3:A:320:PHE:CE1	3:A:327:TYR:CD2	3.00	0.49
3:B:84:LYS:O	3:B:87:LYS:HB3	2.13	0.49
2:P:2:DG:H2''	2:P:3:DG:O4'	2.13	0.48
3:A:323:ILE:O	3:A:324:GLN:HB2	2.11	0.48
3:B:146:PHE:HE1	3:B:252:HIS:O	1.95	0.48
3:A:328:ARG:HG2	3:A:328:ARG:HH11	1.78	0.48
3:A:183:ARG:NH1	3:A:273:THR:HG22	2.28	0.48
3:A:261:PRO:HB2	3:A:264:GLN:NE2	2.29	0.48
3:A:292:THR:HG23	3:A:292:THR:O	2.13	0.48
1:T:10:DC:H2''	1:T:11:DG:N7	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:106:ILE:HG12	3:A:136:GLN:HG2	1.96	0.48
3:A:142:TYR:HB3	3:A:146:PHE:CE1	2.49	0.48
3:B:285:HIS:CD2	3:B:325:TRP:NE1	2.81	0.48
3:B:292:THR:O	3:B:292:THR:HG22	2.13	0.48
3:B:313:VAL:C	3:B:315:SER:H	2.21	0.48
3:B:122:LEU:HD22	3:B:122:LEU:HA	1.58	0.48
2:P:5:DG:H5''	3:A:107:GLY:N	2.29	0.48
1:C:6:DG:H4'	3:B:295:GLU:OE2	2.14	0.48
3:A:133:ASN:C	3:A:137:ARG:HG3	2.39	0.48
3:A:127:LYS:HD2	3:A:128:ASN:ND2	2.28	0.48
3:B:27:LYS:HG3	3:B:28:ASN:N	2.29	0.48
3:B:156:LEU:O	3:B:159:GLN:HB3	2.14	0.48
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.41	0.47
3:B:298:ILE:HG23	3:B:298:ILE:O	2.14	0.47
3:B:299:ARG:HA	3:B:311:LEU:HD22	1.96	0.47
3:A:67:THR:HG23	3:A:68:LYS:N	2.29	0.47
3:A:215:VAL:CG2	3:A:216:GLU:N	2.77	0.47
3:B:39:TYR:O	3:B:43:ALA:HB2	2.15	0.47
2:D:3:DG:C2'	2:D:4:DC:C6	2.96	0.47
3:A:90:GLN:HA	3:A:90:GLN:HE21	1.80	0.47
3:A:93:THR:O	3:A:96:SER:HB2	2.15	0.47
3:B:49:TYR:HE1	3:B:51:HIS:O	1.97	0.47
1:T:9:DC:H2''	1:T:10:DC:C5'	2.44	0.47
3:A:159:GLN:O	3:A:162:VAL:HB	2.15	0.47
3:A:160:ASP:O	3:A:164:ASN:OD1	2.32	0.47
3:A:215:VAL:HA	3:A:218:LEU:HB2	1.96	0.47
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.21	0.47
3:B:12:ASN:HD21	3:B:53:ILE:H	1.61	0.47
3:B:19:LEU:HA	3:B:19:LEU:HD12	1.30	0.47
3:B:20:VAL:C	3:B:23:ALA:H	2.23	0.47
3:B:41:LYS:O	3:B:44:SER:HB3	2.15	0.47
3:B:221:VAL:O	3:B:222:ARG:HB2	2.14	0.47
3:A:62:LEU:CD1	3:A:63:PRO:HD2	2.29	0.47
3:A:150:ILE:CD1	3:A:190:ASP:HA	2.44	0.47
3:A:267:CYS:HB2	3:A:295:GLU:C	2.40	0.47
3:B:11:LEU:HD13	3:B:11:LEU:H	1.79	0.47
3:B:128:ASN:HB3	3:B:131:LYS:HD2	1.95	0.47
3:B:223:PHE:O	3:B:239:CYS:HA	2.14	0.47
3:B:262:LYS:O	3:B:262:LYS:HG2	2.15	0.47
3:B:328:ARG:HH11	3:B:328:ARG:HG2	1.80	0.47
2:D:5:DG:H2'	2:D:6:DC:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ILE:CG2	3:A:261:PRO:N	2.77	0.47
3:B:311:LEU:HB3	3:B:322:TYR:CZ	2.50	0.46
3:B:320:PHE:HA	3:B:323:ILE:HG12	1.95	0.46
3:A:33:ILE:CG2	3:A:34:HIS:N	2.77	0.46
3:A:240:GLN:NE2	3:A:241:LEU:O	2.44	0.46
3:A:255:ILE:CG1	3:A:256:ASP:N	2.79	0.46
3:A:294:ASN:C	3:A:296:TYR:H	2.22	0.46
3:B:37:ASN:O	3:B:40:ARG:HG2	2.16	0.46
3:B:196:THR:HG21	3:B:262:LYS:HG3	1.97	0.46
3:A:66:GLY:H	3:A:69:ILE:CG1	2.27	0.46
3:A:294:ASN:ND2	3:A:299:ARG:CZ	2.79	0.46
3:B:225:THR:OG1	3:B:238:VAL:HB	2.14	0.46
3:B:315:SER:N	3:B:318:ASP:OD1	2.49	0.46
3:A:20:VAL:HG13	3:A:21:GLU:N	2.31	0.46
3:A:258:ARG:NH2	3:A:295:GLU:CG	2.79	0.46
3:A:320:PHE:HA	3:A:323:ILE:CG1	2.42	0.46
3:A:323:ILE:CG1	3:A:325:TRP:HB2	2.43	0.46
3:A:300:PRO:CD	3:A:308:GLY:HA3	2.43	0.46
3:B:278:PHE:CE2	3:B:333:ARG:HD3	2.51	0.46
2:P:5:DG:H5"	3:A:105:GLY:O	2.15	0.46
3:A:132:LEU:CD2	3:A:136:GLN:HE21	2.29	0.46
3:B:11:LEU:H	3:B:11:LEU:CD1	2.29	0.46
3:A:271:TYR:O	5:A:338:DCT:H2"	2.15	0.46
3:A:77:LEU:HA	3:A:77:LEU:HD12	1.40	0.45
3:B:142:TYR:O	3:B:145:ASP:N	2.38	0.45
3:B:234:LYS:CG	3:B:235:PHE:N	2.78	0.45
3:A:256:ASP:OD1	3:A:257:ILE:N	2.49	0.45
3:B:123:GLU:O	3:B:126:ARG:HB2	2.15	0.45
3:B:174:ILE:HB	3:B:196:THR:HG22	1.97	0.45
3:B:240:GLN:HG2	3:B:241:LEU:N	2.30	0.45
3:A:16:THR:HA	3:A:46:ILE:HD11	1.97	0.45
3:A:167:LYS:HA	3:A:170:ASP:O	2.16	0.45
3:B:197:HIS:HA	3:B:198:PRO:HD3	1.47	0.45
3:A:170:ASP:OD1	3:A:171:PRO:HD2	2.16	0.45
3:A:173:TYR:HA	3:A:196:THR:O	2.16	0.45
3:A:200:PHE:O	3:A:201:THR:HG23	2.17	0.45
3:A:214:VAL:CG2	3:A:218:LEU:CD1	2.95	0.45
3:B:34:HIS:O	3:B:37:ASN:HB2	2.16	0.45
3:B:49:TYR:CE1	3:B:51:HIS:HB2	2.50	0.45
3:A:18:MET:SD	3:A:19:LEU:HD12	2.56	0.45
3:A:197:HIS:HA	3:A:198:PRO:HD3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:291:PHE:HA	3:A:299:ARG:O	2.16	0.45
3:A:292:THR:O	3:A:299:ARG:NH1	2.49	0.45
3:A:294:ASN:HD22	3:A:299:ARG:CZ	2.29	0.45
2:P:1:DC:C2'	2:P:2:DG:C8	2.98	0.45
3:A:133:ASN:H	3:A:136:GLN:NE2	2.15	0.45
3:B:148:LYS:CB	3:B:253:ARG:HH12	2.29	0.45
3:B:325:TRP:CE3	3:B:328:ARG:HD2	2.52	0.45
3:B:269:VAL:O	3:B:273:THR:N	2.48	0.45
3:B:328:ARG:HH11	3:B:328:ARG:CB	2.30	0.45
3:A:27:LYS:HG3	3:A:28:ASN:N	2.24	0.45
3:A:67:THR:CG2	3:A:68:LYS:N	2.79	0.45
3:A:83:ARG:C	3:A:86:GLU:H	2.25	0.45
3:B:170:ASP:O	3:B:173:TYR:HB2	2.17	0.45
3:B:175:ALA:CB	3:B:195:LEU:HD13	2.45	0.45
3:B:279:ASN:HA	3:B:282:MET:HE2	1.99	0.45
3:B:33:ILE:HG23	3:B:34:HIS:N	2.32	0.44
3:B:79:THR:C	3:B:81:LYS:N	2.76	0.44
3:A:145:ASP:CG	3:A:251:PRO:HB3	2.42	0.44
3:A:225:THR:HB	3:A:226:ASP:OD1	2.16	0.44
3:A:234:LYS:HE2	3:A:236:MET:HG3	1.99	0.44
1:C:10:DC:C4	1:C:11:DG:C6	3.04	0.44
3:B:79:THR:HG23	3:B:81:LYS:O	2.17	0.44
3:B:325:TRP:CZ3	3:B:328:ARG:CD	3.00	0.44
3:A:62:LEU:HD12	3:A:63:PRO:N	2.31	0.44
3:A:132:LEU:HD22	3:A:136:GLN:HE21	1.81	0.44
3:A:183:ARG:NH1	3:A:273:THR:CG2	2.79	0.44
3:A:330:PRO:CA	3:A:333:ARG:HG3	2.36	0.44
3:B:11:LEU:N	3:B:11:LEU:CD1	2.80	0.44
3:B:286:ALA:O	3:B:289:LYS:N	2.51	0.44
3:B:20:VAL:HG13	3:B:21:GLU:N	2.33	0.44
3:A:150:ILE:HD11	3:A:190:ASP:HA	1.99	0.44
3:B:17:ASP:O	3:B:21:GLU:HG3	2.17	0.44
3:B:146:PHE:HD1	3:B:146:PHE:HA	1.47	0.44
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.76	0.44
3:A:213:ARG:O	3:A:216:GLU:N	2.51	0.44
3:A:277:ILE:H	3:A:277:ILE:HG12	1.45	0.44
3:A:283:ARG:HD3	3:A:293:ILE:HB	1.99	0.44
3:A:321:ASP:O	3:A:324:GLN:N	2.37	0.44
3:A:330:PRO:CD	3:A:333:ARG:HH21	2.06	0.44
3:A:11:LEU:HD22	3:A:12:ASN:H	1.80	0.44
3:A:174:ILE:N	3:A:174:ILE:CD1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:LEU:CD2	3:A:250:TYR:CD2	3.00	0.44
3:B:304:THR:HG23	3:B:306:VAL:HB	1.99	0.44
3:A:62:LEU:O	3:A:65:VAL:HG13	2.18	0.43
3:A:320:PHE:CE1	3:A:327:TYR:HD2	2.36	0.43
3:A:194:LEU:HD22	3:A:194:LEU:HA	1.78	0.43
3:A:201:THR:HA	3:A:261:PRO:CB	2.39	0.43
2:P:7:DC:C4	5:A:338:DCT:N4	2.86	0.43
3:A:177:VAL:O	3:A:177:VAL:HG13	2.18	0.43
3:B:53:ILE:HG13	3:B:53:ILE:H	1.62	0.43
3:A:126:ARG:HA	3:A:140:LEU:HD21	2.01	0.43
3:A:213:ARG:O	3:A:217:GLN:N	2.43	0.43
3:B:194:LEU:HA	3:B:194:LEU:HD22	1.81	0.43
3:A:217:GLN:HG2	3:A:221:VAL:CG2	2.48	0.43
3:B:33:ILE:O	3:B:36:TYR:HB3	2.18	0.43
3:B:103:VAL:CB	3:B:106:ILE:HD12	2.47	0.43
2:P:2:DG:C2'	2:P:3:DG:C8	3.01	0.43
3:A:212:HIS:O	3:A:216:GLU:HG3	2.19	0.43
3:B:332:ASP:C	3:B:334:SER:N	2.77	0.43
3:B:23:ALA:HB1	3:B:36:TYR:HD1	1.83	0.43
3:B:207:GLN:HB3	3:B:210:LEU:HD12	2.01	0.43
3:A:166:VAL:HG12	3:A:167:LYS:N	2.34	0.43
3:A:174:ILE:O	3:A:195:LEU:HA	2.18	0.43
3:A:283:ARG:CD	3:A:293:ILE:HB	2.49	0.43
3:B:77:LEU:HD13	3:B:77:LEU:HA	1.68	0.43
3:B:270:LEU:HD12	3:B:333:ARG:HH12	1.84	0.43
3:A:138:ILE:HG23	3:A:138:ILE:HD12	1.63	0.43
3:A:279:ASN:OD1	3:A:279:ASN:N	2.41	0.43
3:B:228:LEU:HD23	3:B:228:LEU:HA	1.72	0.43
3:B:294:ASN:HD22	3:B:299:ARG:HH22	1.67	0.43
3:A:24:ASN:C	3:A:27:LYS:HB3	2.44	0.42
3:A:172:GLU:HB3	3:A:198:PRO:CD	2.49	0.42
3:A:294:ASN:ND2	3:A:297:THR:H	2.17	0.42
3:B:257:ILE:HG22	3:B:258:ARG:H	1.83	0.42
3:A:274:GLY:HA3	3:A:279:ASN:HD21	1.84	0.42
3:A:294:ASN:HD22	3:A:299:ARG:HH22	1.67	0.42
3:A:299:ARG:HB2	3:A:300:PRO:HD2	2.01	0.42
3:B:328:ARG:HH11	3:B:328:ARG:HB3	1.84	0.42
2:P:7:DC:C5	5:A:338:DCT:H5	2.54	0.42
3:A:238:VAL:CG1	3:A:239:CYS:N	2.81	0.42
3:A:264:GLN:HE21	3:A:264:GLN:HB2	1.65	0.42
3:B:133:ASN:OD1	3:B:133:ASN:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:338:DCT:O1G	5:B:338:DCT:O1A	2.37	0.42
3:A:206:LYS:HG3	3:A:207:GLN:H	1.83	0.42
3:B:128:ASN:O	3:B:131:LYS:N	2.52	0.42
3:B:324:GLN:HA	3:B:324:GLN:NE2	2.28	0.42
3:A:99:PHE:HD2	3:A:100:LEU:CD1	2.32	0.42
3:A:172:GLU:HB3	3:A:198:PRO:HG3	2.01	0.42
3:A:301:LEU:O	3:A:303:VAL:N	2.52	0.42
3:A:316:GLU:O	3:A:320:PHE:HD1	2.02	0.42
2:D:5:DG:O5'	3:B:107:GLY:HA3	2.20	0.42
3:A:66:GLY:O	3:A:69:ILE:HG12	2.19	0.42
3:A:330:PRO:HA	3:A:333:ARG:CD	2.50	0.42
3:A:200:PHE:CE2	3:A:259:LEU:HG	2.51	0.42
3:A:316:GLU:HB3	3:A:320:PHE:HE1	1.85	0.42
3:B:62:LEU:HA	3:B:63:PRO:HD3	1.74	0.42
3:B:317:GLN:HG3	3:B:327:TYR:CD1	2.55	0.42
3:B:320:PHE:CZ	3:B:328:ARG:HB2	2.53	0.42
3:B:330:PRO:HA	3:B:333:ARG:NE	2.35	0.42
3:B:69:ILE:O	3:B:69:ILE:HG22	2.19	0.42
1:T:9:DC:H2''	1:T:10:DC:H5'	2.02	0.42
2:D:5:DG:H2'	2:D:6:DC:C6	2.55	0.42
3:A:33:ILE:O	3:A:37:ASN:N	2.47	0.42
3:A:146:PHE:HD1	3:A:146:PHE:H	1.67	0.42
3:A:237:GLY:N	3:A:255:ILE:O	2.33	0.42
3:B:207:GLN:N	3:B:208:PRO:HD3	2.35	0.42
3:B:283:ARG:CZ	3:B:294:ASN:HA	2.49	0.42
3:A:20:VAL:O	3:A:23:ALA:HB3	2.20	0.41
3:A:24:ASN:CA	3:A:27:LYS:HB3	2.40	0.41
3:A:294:ASN:ND2	3:A:299:ARG:NH1	2.68	0.41
3:A:183:ARG:NH1	3:A:273:THR:C	2.78	0.41
3:B:129:GLU:C	3:B:131:LYS:N	2.76	0.41
3:B:194:LEU:HD13	3:B:194:LEU:C	2.45	0.41
3:B:294:ASN:ND2	3:B:299:ARG:NH2	2.68	0.41
2:P:4:DC:H2'	2:P:5:DG:C8	2.55	0.41
3:A:180:SER:OG	3:A:188:SER:HB3	2.20	0.41
3:A:291:PHE:N	3:A:301:LEU:HD22	2.35	0.41
3:A:285:HIS:O	3:A:288:GLU:HB3	2.20	0.41
3:B:133:ASN:CB	3:B:136:GLN:HE21	2.33	0.41
3:A:11:LEU:C	3:A:13:GLY:H	2.28	0.41
3:B:23:ALA:HA	3:B:39:TYR:HD2	1.86	0.41
3:B:133:ASN:OD1	3:B:136:GLN:NE2	2.44	0.41
3:A:15:ILE:HG23	3:A:16:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:319:ILE:HG21	3:A:319:ILE:HD13	1.73	0.41
3:B:173:TYR:CE1	3:B:197:HIS:HB2	2.55	0.41
3:B:235:PHE:CD2	3:B:257:ILE:CG1	2.97	0.41
3:A:22:LEU:N	3:A:22:LEU:CD1	2.82	0.41
3:A:192:ASP:C	3:A:272:PHE:HE2	2.29	0.41
3:A:201:THR:C	3:A:261:PRO:HB3	2.46	0.41
3:B:150:ILE:HG13	3:B:189:GLY:O	2.21	0.41
3:B:172:GLU:HB3	3:B:197:HIS:NE2	2.36	0.41
3:B:172:GLU:OE1	3:B:172:GLU:HA	2.21	0.41
3:A:11:LEU:HD23	3:A:12:ASN:N	2.27	0.41
3:A:238:VAL:CG1	3:A:252:HIS:HB3	2.51	0.41
3:A:320:PHE:O	3:A:325:TRP:N	2.50	0.41
3:B:37:ASN:CA	3:B:40:ARG:HG2	2.49	0.41
3:B:149:ARG:O	3:B:151:PRO:HD3	2.20	0.41
3:B:234:LYS:HG3	3:B:235:PHE:N	2.35	0.41
3:B:270:LEU:HD12	3:B:333:ARG:NH1	2.36	0.41
3:B:275:SER:C	3:B:277:ILE:N	2.78	0.41
3:A:9:GLU:HB3	3:A:10:THR:H	1.73	0.41
3:A:125:LEU:CD2	3:A:140:LEU:HD13	2.51	0.41
3:A:295:GLU:C	3:A:296:TYR:CD1	2.99	0.41
3:B:136:GLN:O	3:B:139:GLY:N	2.54	0.41
3:B:182:ARG:NH2	3:B:269:VAL:CG1	2.80	0.41
3:B:313:VAL:C	3:B:315:SER:N	2.75	0.41
3:A:294:ASN:C	3:A:296:TYR:N	2.79	0.40
3:B:128:ASN:C	3:B:130:ASP:N	2.79	0.40
3:B:218:LEU:HB3	3:B:224:ILE:HG13	2.03	0.40
3:B:239:CYS:SG	3:B:253:ARG:O	2.78	0.40
3:A:134:HIS:HA	3:A:137:ARG:HD2	2.03	0.40
3:A:271:TYR:C	3:A:273:THR:N	2.79	0.40
3:A:331:LYS:H	3:A:331:LYS:HG3	1.21	0.40
3:B:182:ARG:C	3:B:184:GLY:N	2.78	0.40
3:A:23:ALA:O	3:A:36:TYR:HB2	2.20	0.40
3:A:292:THR:HG22	3:A:301:LEU:HD11	2.04	0.40
1:C:7:DC:H2'	1:C:7:DC:O5'	2.22	0.40
3:A:152:ARG:NH2	3:A:184:GLY:HA2	2.36	0.40
3:B:149:ARG:HH21	3:B:188:SER:HA	1.85	0.40
3:B:197:HIS:CD2	3:B:198:PRO:CD	2.99	0.40
3:B:285:HIS:O	3:B:288:GLU:HB3	2.22	0.40
3:B:293:ILE:HG22	3:B:294:ASN:N	2.37	0.40
3:A:115:VAL:C	3:A:117:GLU:N	2.80	0.40
3:A:134:HIS:O	3:A:137:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:211:LEU:O	3:A:214:VAL:HG12	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:DG:C5'	3:A:66:GLY:CA[2_655]	2.09	0.11
2:P:2:DG:O5'	3:A:66:GLY:CA[2_655]	2.15	0.05

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	320/335 (96%)	234 (73%)	55 (17%)	31 (10%)	0	6
3	B	320/335 (96%)	248 (78%)	48 (15%)	24 (8%)	1	9
All	All	640/670 (96%)	482 (75%)	103 (16%)	55 (9%)	0	7

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	127	LYS
3	A	130	ASP
3	A	143	PHE
3	A	198	PRO
3	A	206	LYS
3	A	207	GLN
3	A	222	ARG
3	A	275	SER
3	A	276	ASP
3	A	303	VAL

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Mol	Chain	Res	Type
3	A	333	ARG
3	A	334	SER
3	B	11	LEU
3	B	32	ALA
3	B	50	PRO
3	B	143	PHE
3	B	186	GLU
3	B	207	GLN
3	A	80	GLY
3	A	164	ASN
3	A	205	SER
3	A	265	TYR
3	A	306	VAL
3	A	330	PRO
3	B	10	THR
3	B	67	THR
3	B	80	GLY
3	B	204	SER
3	B	276	ASP
3	B	327	TYR
3	A	10	THR
3	A	116	ASP
3	A	262	LYS
3	A	274	GLY
3	A	302	GLY
3	A	310	PRO
3	B	206	LYS
3	B	240	GLN
3	B	273	THR
3	B	274	GLY
3	B	275	SER
3	A	32	ALA
3	A	93	THR
3	B	52	LYS
3	A	12	ASN
3	B	120	LYS
3	B	130	ASP
3	B	198	PRO
3	B	324	GLN
3	A	108	PRO
3	A	319	ILE
3	B	330	PRO

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Mol	Chain	Res	Type
3	A	208	PRO
3	B	170	ASP

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	267/296 (90%)	215 (80%)	52 (20%)	1	9
3	B	267/296 (90%)	223 (84%)	44 (16%)	2	14
All	All	534/592 (90%)	438 (82%)	96 (18%)	2	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	16	THR
3	A	26	GLU
3	A	31	GLN
3	A	36	TYR
3	A	41	LYS
3	A	45	VAL
3	A	65	VAL
3	A	67	THR
3	A	69	ILE
3	A	74	ASP
3	A	77	LEU
3	A	85	LEU
3	A	90	GLN
3	A	93	THR
3	A	100	LEU
3	A	103	VAL
3	A	104	THR
3	A	115	VAL
3	A	122	LEU
3	A	128	ASN

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Mol	Chain	Res	Type
3	A	130	ASP
3	A	133	ASN
3	A	136	GLN
3	A	144	GLU
3	A	156	LEU
3	A	164	ASN
3	A	176	THR
3	A	180	SER
3	A	193	VAL
3	A	194	LEU
3	A	196	THR
3	A	205	SER
3	A	207	GLN
3	A	214	VAL
3	A	225	THR
3	A	226	ASP
3	A	241	LEU
3	A	249	GLU
3	A	255	ILE
3	A	257	ILE
3	A	264	GLN
3	A	269	VAL
3	A	272	PHE
3	A	295	GLU
3	A	299	ARG
3	A	301	LEU
3	A	304	THR
3	A	311	LEU
3	A	324	GLN
3	A	327	TYR
3	A	331	LYS
3	B	11	LEU
3	B	15	ILE
3	B	19	LEU
3	B	24	ASN
3	B	26	GLU
3	B	28	ASN
3	B	31	GLN
3	B	65	VAL
3	B	77	LEU
3	B	95	SER
3	B	97	ILE

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Mol	Chain	Res	Type
3	B	100	LEU
3	B	103	VAL
3	B	104	THR
3	B	115	VAL
3	B	116	ASP
3	B	122	LEU
3	B	125	LEU
3	B	133	ASN
3	B	138	ILE
3	B	155	MET
3	B	169	LEU
3	B	173	TYR
3	B	174	ILE
3	B	178	CYS
3	B	199	ASN
3	B	209	LYS
3	B	215	VAL
3	B	224	ILE
3	B	226	ASP
3	B	229	SER
3	B	233	THR
3	B	249	GLU
3	B	258	ARG
3	B	264	GLN
3	B	272	PHE
3	B	275	SER
3	B	276	ASP
3	B	293	ILE
3	B	298	ILE
3	B	311	LEU
3	B	318	ASP
3	B	324	GLN
3	B	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	34	HIS
3	A	90	GLN
3	A	128	ASN
3	A	133	ASN

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Mol	Chain	Res	Type
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	264	GLN
3	A	294	ASN
3	A	324	GLN
3	B	28	ASN
3	B	31	GLN
3	B	37	ASN
3	B	128	ASN
3	B	136	GLN
3	B	159	GLN
3	B	281	ASN
3	B	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
5	DCT	A	338	-	27,28,28	4.47	7 (25%)	37,43,43	1.52	6 (16%)
5	DCT	B	338	-	27,28,28	3.08	5 (18%)	37,43,43	1.15	2 (5%)

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
5	DCT	A	338	-	-	7/22/31/31	0/2/2/2
5	DCT	B	338	-	-	6/22/31/31	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	338	DCT	PA-O3A	-15.64	1.42	1.59
5	A	338	DCT	PB-O3A	-14.22	1.44	1.59
5	B	338	DCT	PA-O3A	-12.93	1.45	1.59
5	A	338	DCT	PB-O3B	-7.11	1.51	1.59
5	B	338	DCT	PB-O3A	-5.55	1.53	1.59
5	B	338	DCT	PB-O3B	-5.21	1.53	1.59
5	A	338	DCT	C1'-N1	-3.14	1.40	1.48
5	B	338	DCT	C1'-N1	3.00	1.55	1.48
5	A	338	DCT	C2-N1	-2.93	1.33	1.40
5	B	338	DCT	PG-O2G	-2.67	1.44	1.54
5	A	338	DCT	O5'-C5'	-2.48	1.35	1.44
5	A	338	DCT	PA-O2A	-2.06	1.45	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	338	DCT	C1'-N1-C6	-4.46	112.75	121.53
5	A	338	DCT	C5-C6-N1	-3.90	115.50	121.84
5	A	338	DCT	C6-N1-C2	2.83	125.23	120.46
5	B	338	DCT	C1'-N1-C2	-2.70	113.19	117.83
5	A	338	DCT	C4'-O4'-C1'	2.50	112.17	109.81
5	A	338	DCT	O2G-PG-O1G	2.45	120.39	110.83
5	A	338	DCT	O2B-PB-O1B	2.17	122.56	112.44
5	B	338	DCT	C5-C6-N1	-2.14	118.36	121.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

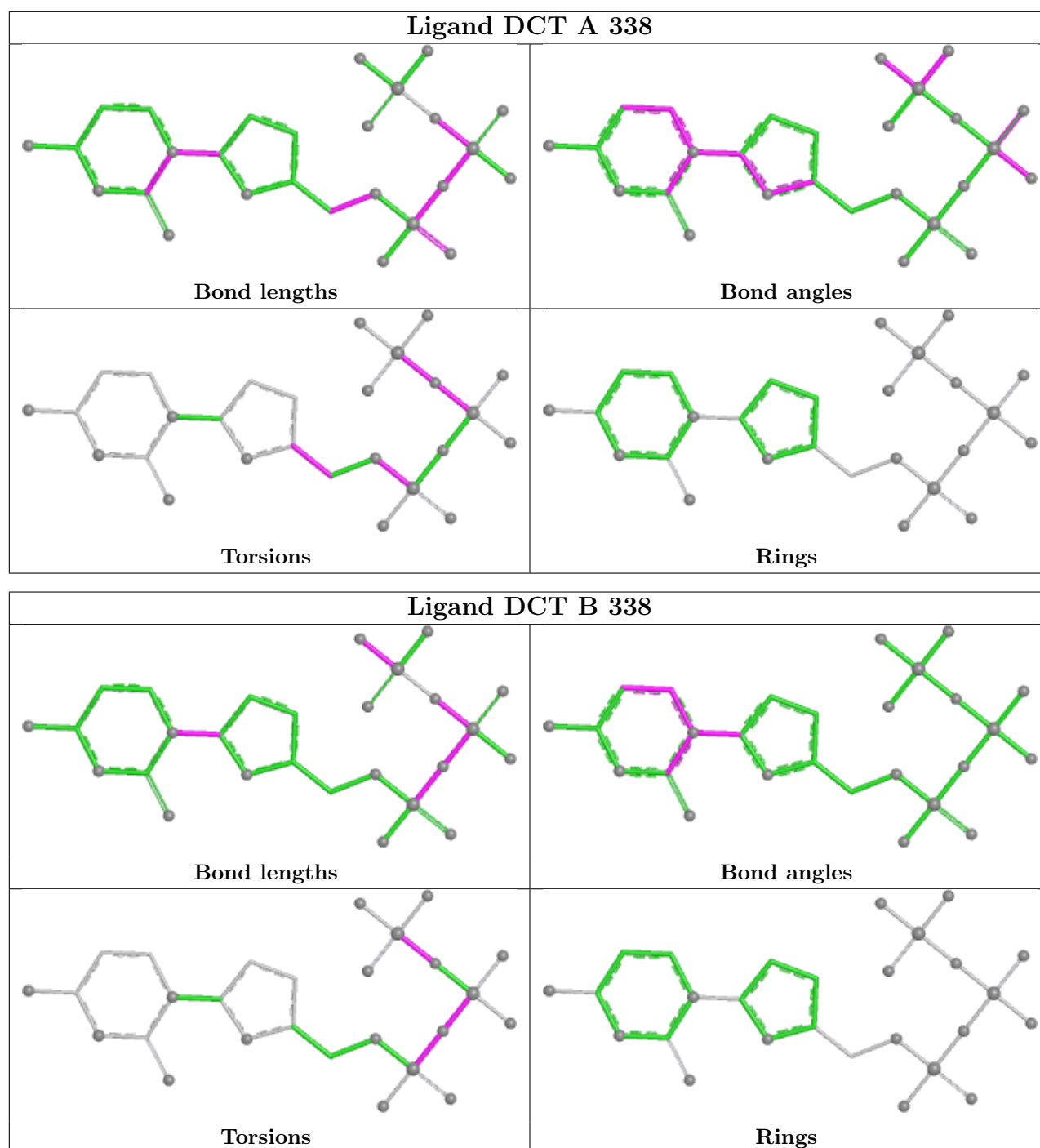
Mol	Chain	Res	Type	Atoms
5	A	338	DCT	C5'-O5'-PA-O2A
5	A	338	DCT	C5'-O5'-PA-O3A
5	B	338	DCT	PA-O3A-PB-O1B
5	B	338	DCT	PB-O3B-PG-O1G
5	A	338	DCT	PB-O3B-PG-O3G
5	A	338	DCT	C5'-O5'-PA-O1A
5	B	338	DCT	PA-O3A-PB-O2B
5	B	338	DCT	PB-O3B-PG-O2G
5	B	338	DCT	PB-O3B-PG-O3G
5	A	338	DCT	C3'-C4'-C5'-O5'
5	A	338	DCT	PG-O3B-PB-O1B
5	A	338	DCT	PG-O3B-PB-O2B
5	B	338	DCT	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	338	DCT	8	0
5	B	338	DCT	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.



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.