Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BPF
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	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

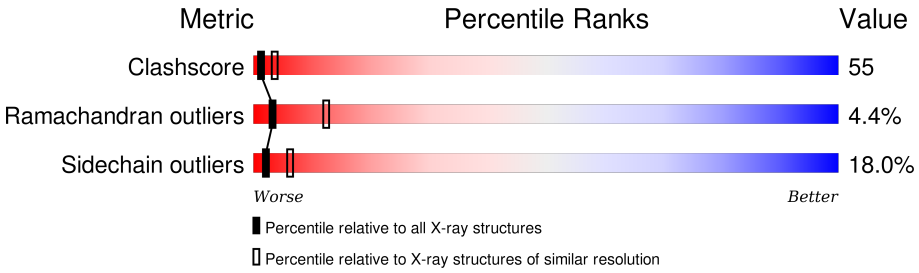
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	8	13% 63% 25%
2	P	7	29% 14% 57%
3	A	335	23% 48% 22% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2908 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
1	T	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
2	P	7	Total	C	N	O	P	0	0	0
			138	66	27	39	6			

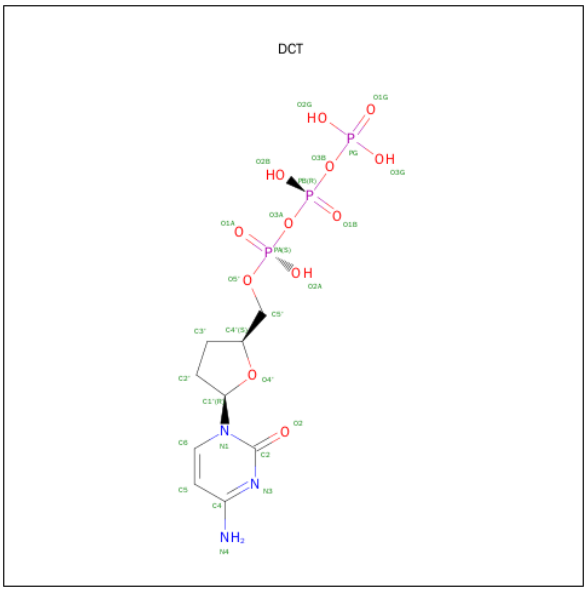
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	324	Total	C	N	O	S	0	0	0
			2543	1603	449	482	9			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	P	2	Total	O	0	0
			2	2		
6	T	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

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

Note EDS was not executed.

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

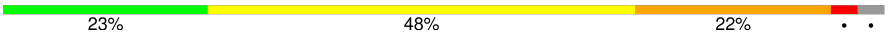
Chain T:

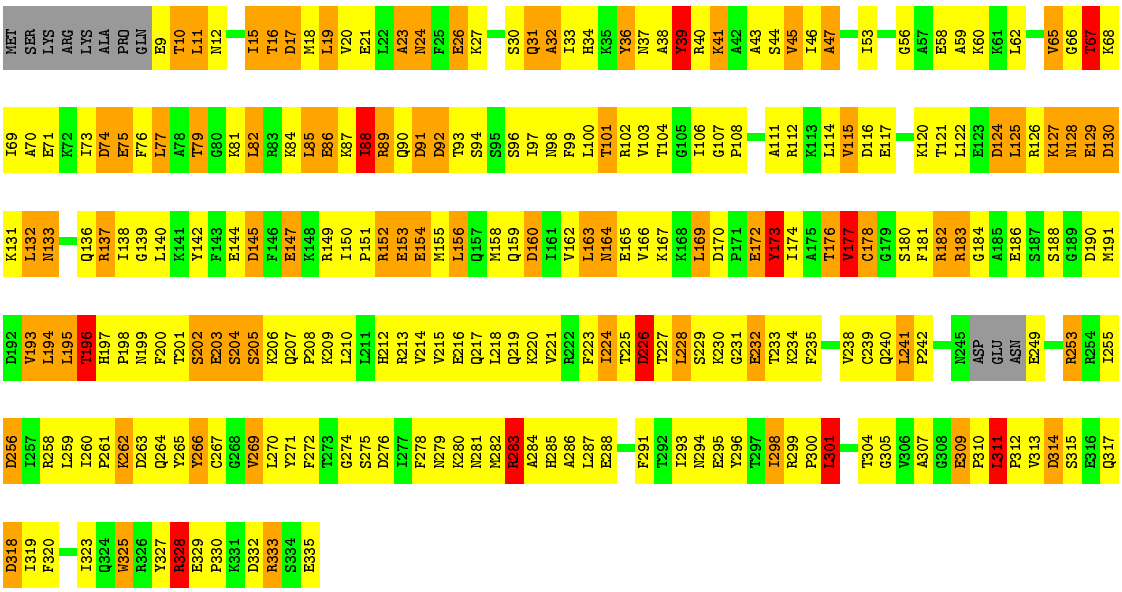
- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*GP*CP*C)-3')

Chain P:

- Molecule 3: PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7))

Chain A:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	94.90Å 94.90Å 117.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2908	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	T	2.33	8/187 (4.3%)	3.67	31/287 (10.8%)
2	P	2.25	9/154 (5.8%)	3.26	17/235 (7.2%)
3	A	1.24	25/2589 (1.0%)	1.82	60/3493 (1.7%)
All	All	1.41	42/2930 (1.4%)	2.11	108/4015 (2.7%)

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	T	0	4
2	P	0	5
All	All	0	9

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	4	DG	C3'-O3'	-12.50	1.27	1.44
2	P	6	DC	N1-C6	-9.53	1.31	1.37
3	A	153	GLU	CD-OE2	7.86	1.34	1.25
1	T	9	DC	N1-C6	-7.79	1.32	1.37
3	A	172	GLU	CD-OE1	7.61	1.34	1.25
3	A	154	GLU	CD-OE1	7.46	1.33	1.25
3	A	147	GLU	CD-OE1	7.39	1.33	1.25
3	A	232	GLU	CD-OE2	7.37	1.33	1.25
3	A	309	GLU	CD-OE1	7.02	1.33	1.25
3	A	165	GLU	CD-OE1	6.89	1.33	1.25
3	A	58	GLU	CD-OE1	6.83	1.33	1.25
3	A	295	GLU	CD-OE2	6.72	1.33	1.25
3	A	9	GLU	CD-OE1	6.70	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	LEU	N-CA	-6.59	1.33	1.46
3	A	249	GLU	CD-OE2	6.50	1.32	1.25
3	A	144	GLU	CD-OE2	6.47	1.32	1.25
3	A	216	GLU	CD-OE1	6.33	1.32	1.25
3	A	75	GLU	CD-OE1	6.30	1.32	1.25
3	A	186	GLU	CD-OE1	6.24	1.32	1.25
2	P	7	DC	N3-C4	-6.17	1.29	1.33
3	A	21	GLU	CD-OE1	6.16	1.32	1.25
3	A	329	GLU	CD-OE1	6.13	1.32	1.25
3	A	86	GLU	CD-OE1	6.05	1.32	1.25
2	P	5	DG	N9-C4	5.95	1.42	1.38
1	T	7	DC	C3'-O3'	-5.86	1.36	1.44
2	P	6	DC	C4-C5	-5.86	1.38	1.43
1	T	4	DG	O3'-P	-5.82	1.54	1.61
3	A	129	GLU	CD-OE2	5.80	1.32	1.25
1	T	6	DG	C6-N1	-5.71	1.35	1.39
2	P	4	DC	C1'-N1	5.69	1.56	1.49
1	T	10	DC	C1'-N1	-5.53	1.39	1.47
1	T	9	DC	N3-C4	-5.48	1.30	1.33
3	A	271	TYR	CB-CG	-5.45	1.43	1.51
3	A	203	GLU	CD-OE2	5.40	1.31	1.25
3	A	288	GLU	CD-OE1	5.29	1.31	1.25
1	T	8	DG	C4'-C3'	-5.23	1.47	1.52
2	P	2	DG	C3'-O3'	-5.18	1.37	1.44
3	A	24	ASN	CA-CB	5.12	1.66	1.53
3	A	335	GLU	CD-OE1	5.12	1.31	1.25
2	P	4	DC	C3'-O3'	-5.11	1.37	1.44
2	P	7	DC	N1-C6	-5.10	1.34	1.37
2	P	2	DG	C2-N3	5.07	1.36	1.32

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	7	DC	C2-N1-C1'	-23.10	93.39	118.80
1	T	8	DG	C8-N9-C1'	22.07	155.69	127.00
1	T	8	DG	C4-N9-C1'	-21.16	98.99	126.50
1	T	10	DC	C2-N1-C1'	-18.22	98.76	118.80
1	T	9	DC	C2-N1-C1'	-15.33	101.94	118.80
2	P	7	DC	C6-N1-C1'	15.02	138.82	120.80
3	A	241	LEU	C-N-CD	-14.05	89.69	120.60
3	A	190	ASP	CB-CG-OD1	11.63	128.77	118.30
1	T	9	DC	C6-N1-C1'	11.40	134.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	170	ASP	CB-CG-OD1	-11.20	108.22	118.30
1	T	7	DC	C2-N1-C1'	-11.13	106.56	118.80
3	A	256	ASP	CB-CG-OD1	-11.04	108.36	118.30
3	A	190	ASP	CB-CG-OD2	-10.55	108.81	118.30
2	P	2	DG	C8-N9-C1'	-10.39	113.49	127.00
3	A	256	ASP	CB-CG-OD2	10.27	127.55	118.30
1	T	6	DG	C8-N9-C1'	10.11	140.14	127.00
3	A	196	THR	CA-CB-CG2	9.97	126.36	112.40
1	T	9	DC	O4'-C4'-C3'	-9.84	100.09	106.00
2	P	6	DC	C2-N1-C1'	-9.66	108.17	118.80
3	A	74	ASP	CB-CG-OD1	-9.63	109.63	118.30
1	T	6	DG	C4-N9-C1'	-9.58	114.04	126.50
3	A	328	ARG	NE-CZ-NH1	9.57	125.09	120.30
3	A	301	LEU	N-CA-CB	9.47	129.34	110.40
2	P	5	DG	O4'-C1'-C2'	-9.32	98.44	105.90
3	A	332	ASP	CB-CG-OD1	-9.21	110.01	118.30
3	A	39	TYR	CB-CG-CD1	-8.89	115.66	121.00
1	T	4	DG	C4-N9-C1'	-8.85	115.00	126.50
1	T	4	DG	C8-N9-C1'	8.70	138.31	127.00
1	T	7	DC	C6-N1-C1'	8.61	131.13	120.80
1	T	8	DG	P-O5'-C5'	-8.58	107.17	120.90
3	A	74	ASP	CB-CG-OD2	8.56	126.00	118.30
2	P	5	DG	C4-N9-C1'	8.46	137.50	126.50
3	A	328	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	P	3	DG	P-O5'-C5'	-8.29	107.63	120.90
2	P	7	DC	O4'-C4'-C3'	-8.14	101.12	106.00
2	P	5	DG	C8-N9-C1'	-8.10	116.47	127.00
2	P	6	DC	C6-N1-C1'	7.91	130.29	120.80
3	A	17	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	T	10	DC	C6-N1-C2	7.57	123.33	120.30
3	A	267	CYS	CA-CB-SG	-7.55	100.41	114.00
3	A	160	ASP	CB-CG-OD1	-7.34	111.69	118.30
3	A	152	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	T	10	DC	O4'-C1'-N1	-7.19	102.97	108.00
3	A	314	ASP	CB-CG-OD1	7.01	124.61	118.30
3	A	145	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	T	5	DG	C1'-O4'-C4'	-6.96	103.14	110.10
3	A	271	TYR	CB-CG-CD2	-6.76	116.94	121.00
3	A	23	ALA	C-N-CA	-6.60	105.19	121.70
3	A	170	ASP	CB-CG-OD2	6.60	124.24	118.30
1	T	10	DC	O4'-C4'-C3'	-6.60	101.86	104.50
3	A	176	THR	CA-CB-CG2	-6.56	103.22	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	196	THR	CA-CB-OG1	-6.50	95.36	109.00
3	A	152	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	T	10	DC	P-O3'-C3'	-6.45	111.96	119.70
3	A	314	ASP	CB-CG-OD2	-6.43	112.51	118.30
3	A	130	ASP	CB-CG-OD1	-6.41	112.53	118.30
3	A	173	TYR	CB-CA-C	-6.41	97.58	110.40
1	T	10	DC	C6-N1-C1'	6.39	128.47	120.80
3	A	234	LYS	N-CA-CB	6.38	122.08	110.60
3	A	178	CYS	CA-CB-SG	-6.34	102.59	114.00
3	A	283	ARG	NE-CZ-NH2	-6.31	117.14	120.30
3	A	333	ARG	CD-NE-CZ	-6.28	114.81	123.60
3	A	116	ASP	CB-CG-OD1	-6.21	112.71	118.30
3	A	92	ASP	CB-CG-OD1	-6.18	112.73	118.30
3	A	137	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	P	5	DG	P-O5'-C5'	-6.09	111.16	120.90
3	A	182	ARG	NE-CZ-NH1	6.09	123.34	120.30
3	A	276	ASP	CB-CG-OD2	-6.01	112.89	118.30
3	A	124	ASP	CB-CG-OD1	-5.97	112.92	118.30
3	A	301	LEU	CA-C-N	-5.97	104.26	116.20
2	P	7	DC	N1-C2-O2	5.90	122.44	118.90
1	T	9	DC	O4'-C1'-N1	-5.89	103.88	108.00
2	P	7	DC	C4'-C3'-C2'	-5.88	97.81	103.10
3	A	152	ARG	N-CA-CB	5.86	121.15	110.60
3	A	91	ASP	CB-CG-OD1	-5.84	113.04	118.30
3	A	39	TYR	CA-CB-CG	-5.83	102.32	113.40
3	A	36	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	T	5	DG	C8-N9-C1'	-5.73	119.55	127.00
3	A	311	LEU	CB-CA-C	-5.71	99.35	110.20
1	T	7	DC	O4'-C1'-N1	-5.69	104.02	108.00
2	P	2	DG	O4'-C1'-N9	5.68	111.98	108.00
1	T	4	DG	O4'-C1'-N9	-5.63	104.06	108.00
1	T	5	DG	C4-N9-C1'	5.60	133.78	126.50
3	A	91	ASP	CB-CG-OD2	5.58	123.33	118.30
3	A	145	ASP	CB-CG-OD2	5.55	123.30	118.30
1	T	10	DC	P-O5'-C5'	-5.55	112.03	120.90
3	A	253	ARG	NE-CZ-NH2	-5.49	117.55	120.30
3	A	177	VAL	CA-CB-CG1	-5.48	102.69	110.90
3	A	23	ALA	N-CA-CB	5.46	117.74	110.10
2	P	5	DG	O5'-P-OP1	-5.43	100.81	105.70
3	A	163	LEU	CA-CB-CG	-5.43	102.81	115.30
3	A	195	LEU	C-N-CA	-5.42	108.15	121.70
3	A	332	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	5	DG	C8-N9-C4	-5.39	104.24	106.40
3	A	160	ASP	CB-CG-OD2	5.36	123.13	118.30
1	T	5	DG	O4'-C1'-C2'	-5.33	101.64	105.90
1	T	9	DC	O4'-C1'-C2'	-5.30	101.66	105.90
2	P	1	DC	C2-N1-C1'	-5.29	112.98	118.80
3	A	226	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	T	9	DC	P-O3'-C3'	5.16	125.89	119.70
3	A	47	ALA	CB-CA-C	5.13	117.80	110.10
3	A	132	LEU	CA-CB-CG	-5.12	103.51	115.30
1	T	4	DG	C8-N9-C4	-5.12	104.35	106.40
1	T	7	DC	P-O5'-C5'	-5.11	112.73	120.90
3	A	224	ILE	N-CA-C	-5.10	97.22	111.00
3	A	318	ASP	CB-CG-OD2	5.09	122.88	118.30
3	A	40	ARG	O-C-N	5.06	130.80	122.70
1	T	5	DG	P-O3'-C3'	5.04	125.75	119.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	1	DC	Sidechain
2	P	2	DG	Sidechain
2	P	3	DG	Sidechain
2	P	5	DG	Sidechain
2	P	7	DC	Sidechain
1	T	10	DC	Sidechain
1	T	4	DG	Sidechain
1	T	6	DG	Sidechain
1	T	9	DC	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	167	0	89	12	0
2	P	138	0	77	9	0
3	A	2543	0	2491	289	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	27	0	12	7	0
6	A	27	0	0	4	0
6	P	2	0	0	0	0
6	T	2	0	0	0	0
All	All	2908	0	2669	302	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 55.

All (302) 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:16:THR:HG23	3:A:46:ILE:HD11	1.23	1.12
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.37	1.00
3:A:180:SER:HA	3:A:183:ARG:HH12	1.24	0.99
1:T:9:DC:N4	2:P:3:DG:H1	1.65	0.95
3:A:158:MET:HG2	3:A:241:LEU:HD11	1.54	0.89
3:A:180:SER:HA	3:A:183:ARG:NH1	1.88	0.88
3:A:233:THR:HG21	3:A:258:ARG:HH11	1.41	0.85
1:T:4:DG:N3	3:A:283:ARG:HD2	1.91	0.85
1:T:9:DC:H42	2:P:3:DG:H1	0.89	0.85
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.05	0.84
3:A:16:THR:HG23	3:A:46:ILE:CD1	2.07	0.84
3:A:233:THR:HG22	3:A:258:ARG:HD2	1.59	0.83
3:A:233:THR:HG21	3:A:258:ARG:NH1	1.96	0.81
3:A:41:LYS:HB3	3:A:41:LYS:HZ2	1.45	0.81
3:A:16:THR:CG2	3:A:46:ILE:HD11	2.10	0.81
5:A:338:DCT:H6	5:A:338:DCT:C5'	2.12	0.80
3:A:15:ILE:HG12	3:A:16:THR:N	1.97	0.80
1:T:4:DG:H21	3:A:283:ARG:CZ	1.93	0.79
1:T:8:DG:H5"	3:A:231:GLY:HA3	1.65	0.79
3:A:11:LEU:HD22	3:A:11:LEU:H	1.49	0.77
3:A:299:ARG:HH11	3:A:299:ARG:HG2	1.48	0.77
3:A:264:GLN:HE22	3:A:296:TYR:HB3	1.50	0.77
3:A:214:VAL:O	3:A:218:LEU:HD12	1.86	0.76
3:A:67:THR:HG23	3:A:68:LYS:H	1.50	0.75
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.02	0.75
3:A:174:ILE:O	3:A:195:LEU:HD12	1.87	0.75
3:A:198:PRO:HB3	3:A:262:LYS:HD3	1.69	0.75
3:A:154:GLU:O	3:A:158:MET:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ASN:ND2	3:A:53:ILE:H	1.86	0.73
3:A:82:LEU:CB	3:A:85:LEU:HB3	2.18	0.73
3:A:12:ASN:HD21	3:A:53:ILE:H	1.35	0.73
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.70	0.73
3:A:169:LEU:HB3	3:A:213:ARG:NH2	2.04	0.73
3:A:266:TYR:HA	3:A:269:VAL:CG2	2.19	0.72
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.05	0.72
3:A:204:SER:CB	3:A:206:LYS:HE2	2.20	0.71
3:A:108:PRO:HB2	3:A:112:ARG:NH2	2.05	0.71
3:A:41:LYS:O	3:A:44:SER:HB3	1.91	0.70
3:A:140:LEU:O	3:A:140:LEU:HD12	1.91	0.70
3:A:133:ASN:H	3:A:136:GLN:NE2	1.89	0.70
3:A:266:TYR:HA	3:A:269:VAL:HG23	1.74	0.70
3:A:228:LEU:HD23	3:A:228:LEU:N	2.06	0.70
1:T:8:DG:OP1	3:A:231:GLY:HA3	1.92	0.69
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.74	0.69
3:A:195:LEU:O	3:A:259:LEU:HD12	1.92	0.69
3:A:169:LEU:N	3:A:169:LEU:HD23	2.06	0.69
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.23	0.68
3:A:183:ARG:HB2	3:A:183:ARG:HH11	1.58	0.68
2:P:5:DG:OP2	3:A:108:PRO:HD2	1.93	0.68
3:A:233:THR:CG2	3:A:258:ARG:HH11	2.08	0.67
3:A:11:LEU:HD13	3:A:11:LEU:H	1.58	0.67
3:A:158:MET:HG2	3:A:241:LEU:CD1	2.24	0.67
3:A:11:LEU:HD13	3:A:11:LEU:N	2.10	0.67
3:A:180:SER:HB2	3:A:188:SER:OG	1.94	0.67
3:A:88:ILE:O	3:A:90:GLN:N	2.28	0.66
3:A:23:ALA:HB1	3:A:36:TYR:CD1	2.30	0.66
3:A:31:GLN:O	3:A:33:ILE:N	2.28	0.66
3:A:212:HIS:HD2	3:A:230:LYS:HE2	1.60	0.66
3:A:160:ASP:O	3:A:164:ASN:ND2	2.30	0.65
3:A:11:LEU:N	3:A:11:LEU:HD22	2.11	0.65
3:A:328:ARG:HH11	3:A:328:ARG:CG	2.10	0.65
3:A:97:ILE:HG22	3:A:98:ASN:N	2.12	0.65
3:A:149:ARG:O	3:A:151:PRO:HD3	1.97	0.64
3:A:115:VAL:CG2	3:A:120:LYS:HB3	2.27	0.64
3:A:299:ARG:NH1	3:A:299:ARG:HG2	2.12	0.64
3:A:125:LEU:O	3:A:128:ASN:N	2.30	0.64
3:A:36:TYR:O	3:A:39:TYR:HB2	1.97	0.64
3:A:279:ASN:O	3:A:283:ARG:HG3	1.97	0.64
3:A:196:THR:HG21	3:A:262:LYS:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:183:ARG:CG	3:A:183:ARG:HH11	2.11	0.64
3:A:208:PRO:CD	3:A:209:LYS:H	2.10	0.64
3:A:17:ASP:O	3:A:20:VAL:HG12	1.98	0.64
3:A:330:PRO:HA	3:A:333:ARG:HE	1.63	0.63
3:A:104:THR:HG22	3:A:139:GLY:CA	2.28	0.63
3:A:115:VAL:HG22	3:A:120:LYS:HB3	1.80	0.63
3:A:133:ASN:ND2	3:A:136:GLN:H	1.96	0.63
2:P:5:DG:P	3:A:107:GLY:HA3	2.39	0.63
3:A:82:LEU:O	3:A:86:GLU:N	2.29	0.62
3:A:233:THR:CG2	3:A:258:ARG:HD2	2.28	0.62
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.33	0.62
3:A:270:LEU:HD21	3:A:282:MET:CE	2.30	0.62
3:A:133:ASN:HD22	3:A:133:ASN:C	2.03	0.62
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.35	0.61
3:A:154:GLU:OE1	3:A:253:ARG:NH2	2.30	0.61
3:A:86:GLU:OE1	3:A:86:GLU:HA	1.99	0.61
3:A:301:LEU:HD23	3:A:301:LEU:O	2.00	0.61
3:A:333:ARG:HD2	6:A:405:HOH:O	2.02	0.60
3:A:41:LYS:HB3	3:A:41:LYS:NZ	2.05	0.60
3:A:317:GLN:HG3	3:A:327:TYR:CD2	2.36	0.60
3:A:328:ARG:HB3	3:A:328:ARG:HH11	1.66	0.59
3:A:238:VAL:HG12	3:A:239:CYS:N	2.16	0.59
3:A:328:ARG:HH11	3:A:328:ARG:CB	2.15	0.59
3:A:159:GLN:O	3:A:163:LEU:HG	2.01	0.59
3:A:100:LEU:HD11	3:A:125:LEU:CD2	2.33	0.59
2:P:2:DG:H2"	2:P:3:DG:H5'	1.85	0.58
3:A:299:ARG:HB2	3:A:300:PRO:HD2	1.85	0.58
3:A:104:THR:HG22	3:A:139:GLY:HA3	1.84	0.58
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.34	0.58
3:A:38:ALA:O	3:A:41:LYS:NZ	2.35	0.58
3:A:125:LEU:HB3	3:A:140:LEU:HD22	1.85	0.58
3:A:133:ASN:HD21	3:A:136:GLN:HG3	1.69	0.58
3:A:183:ARG:CB	3:A:183:ARG:HH11	2.17	0.57
3:A:278:PHE:HB2	3:A:333:ARG:O	2.02	0.57
3:A:281:ASN:O	3:A:284:ALA:HB3	2.04	0.57
3:A:153:GLU:O	3:A:156:LEU:HB2	2.04	0.57
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.86	0.57
3:A:129:GLU:HA	3:A:132:LEU:HD12	1.86	0.57
3:A:77:LEU:N	3:A:77:LEU:HD13	2.19	0.57
3:A:121:THR:HG1	3:A:124:ASP:H	1.49	0.57
2:P:2:DG:C2'	2:P:3:DG:H5'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:75:GLU:O	3:A:79:THR:HG23	2.05	0.56
3:A:265:TYR:O	3:A:269:VAL:HG22	2.05	0.56
3:A:224:ILE:HD13	3:A:235:PHE:CZ	2.40	0.56
3:A:98:ASN:O	3:A:101:THR:HB	2.04	0.56
3:A:62:LEU:O	3:A:65:VAL:HG13	2.05	0.56
3:A:31:GLN:HG3	3:A:32:ALA:N	2.19	0.56
3:A:100:LEU:O	3:A:103:VAL:HG23	2.06	0.56
3:A:210:LEU:O	3:A:214:VAL:HG12	2.07	0.55
1:T:8:DG:H5"	3:A:231:GLY:CA	2.34	0.55
3:A:204:SER:HB2	3:A:206:LYS:HG2	1.87	0.55
3:A:330:PRO:HD3	3:A:333:ARG:NH2	2.21	0.55
3:A:328:ARG:HH11	3:A:328:ARG:HG2	1.72	0.55
3:A:293:ILE:HG12	3:A:298:ILE:HB	1.88	0.55
3:A:133:ASN:H	3:A:136:GLN:HE21	1.53	0.55
3:A:300:PRO:HD3	3:A:309:GLU:O	2.07	0.55
3:A:198:PRO:HD2	3:A:199:ASN:H	1.71	0.54
3:A:279:ASN:HA	6:A:426:HOH:O	2.08	0.54
3:A:194:LEU:HD13	3:A:195:LEU:N	2.22	0.54
3:A:59:ALA:O	3:A:62:LEU:HB2	2.07	0.54
3:A:164:ASN:O	3:A:167:LYS:N	2.41	0.54
3:A:102:ARG:NH2	3:A:147:GLU:OE2	2.41	0.54
3:A:100:LEU:HD11	3:A:125:LEU:HD21	1.88	0.54
3:A:223:PHE:O	3:A:239:CYS:HA	2.08	0.54
3:A:16:THR:HG22	3:A:43:ALA:HB1	1.90	0.53
3:A:283:ARG:O	3:A:287:LEU:HD13	2.08	0.53
3:A:274:GLY:CA	5:A:338:DCT:H2"	2.39	0.53
3:A:108:PRO:HB2	3:A:112:ARG:HH22	1.73	0.53
3:A:240:GLN:O	3:A:242:PRO:HD3	2.09	0.53
3:A:88:ILE:C	3:A:90:GLN:H	2.11	0.53
3:A:227:THR:C	3:A:228:LEU:HD23	2.29	0.53
3:A:104:THR:HG22	3:A:139:GLY:HA2	1.90	0.53
3:A:202:SER:N	3:A:263:ASP:OD1	2.37	0.53
3:A:149:ARG:NH2	5:A:338:DCT:O2G	2.42	0.52
3:A:301:LEU:HD23	3:A:301:LEU:C	2.30	0.52
3:A:71:GLU:O	3:A:74:ASP:N	2.42	0.52
3:A:287:LEU:HD12	3:A:291:PHE:O	2.08	0.52
5:A:338:DCT:H5'	5:A:338:DCT:H6	1.89	0.52
3:A:285:HIS:CD2	3:A:325:TRP:NE1	2.78	0.52
3:A:46:ILE:HD12	3:A:47:ALA:HA	1.91	0.52
3:A:128:ASN:N	3:A:128:ASN:ND2	2.57	0.52
3:A:84:LYS:O	3:A:87:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:56:GLY:O	3:A:59:ALA:HB3	2.10	0.52
3:A:70:ALA:O	3:A:73:ILE:HB	2.09	0.51
3:A:82:LEU:O	3:A:85:LEU:N	2.44	0.51
3:A:102:ARG:HH21	3:A:147:GLU:CD	2.13	0.51
2:P:1:DC:O3'	2:P:2:DG:O4'	2.28	0.51
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.91	0.51
3:A:85:LEU:O	3:A:88:ILE:HG22	2.10	0.51
3:A:33:ILE:HG23	3:A:34:HIS:N	2.26	0.51
3:A:215:VAL:HG11	3:A:235:PHE:CD2	2.45	0.51
3:A:177:VAL:HG22	3:A:181:PHE:CD2	2.46	0.51
3:A:15:ILE:O	3:A:18:MET:N	2.43	0.51
3:A:221:VAL:HG12	3:A:221:VAL:O	2.11	0.50
3:A:106:ILE:CG2	3:A:111:ALA:HB2	2.41	0.50
3:A:238:VAL:CG1	3:A:239:CYS:N	2.74	0.50
3:A:274:GLY:HA3	5:A:338:DCT:H2"	1.94	0.50
5:A:338:DCT:O2B	5:A:338:DCT:O1A	2.30	0.50
3:A:198:PRO:CB	3:A:262:LYS:HD3	2.39	0.50
3:A:133:ASN:ND2	3:A:136:GLN:HG3	2.27	0.50
3:A:12:ASN:HD21	3:A:53:ILE:N	2.06	0.50
3:A:96:SER:O	3:A:99:PHE:HB3	2.12	0.50
3:A:311:LEU:HB3	3:A:312:PRO:HD2	1.92	0.49
3:A:117:GLU:OE1	3:A:131:LYS:NZ	2.42	0.49
3:A:122:LEU:HD13	3:A:122:LEU:C	2.32	0.49
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.46	0.49
1:T:9:DC:H5'	3:A:229:SER:HB3	1.93	0.49
3:A:152:ARG:O	3:A:156:LEU:HD22	2.13	0.49
3:A:204:SER:O	3:A:206:LYS:HD3	2.13	0.49
3:A:193:VAL:HG22	3:A:193:VAL:O	2.12	0.49
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.94	0.48
3:A:197:HIS:O	3:A:200:PHE:HB3	2.13	0.48
3:A:152:ARG:NH2	3:A:181:PHE:O	2.45	0.48
3:A:278:PHE:CE2	3:A:333:ARG:CD	2.96	0.48
3:A:299:ARG:CD	3:A:307:ALA:HB1	2.44	0.48
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.94	0.48
3:A:212:HIS:CD2	3:A:230:LYS:HE2	2.44	0.48
3:A:183:ARG:HE	3:A:275:SER:HB3	1.78	0.48
3:A:204:SER:HB3	3:A:206:LYS:HE2	1.93	0.48
3:A:162:VAL:HG12	3:A:163:LEU:HD23	1.95	0.48
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.44	0.48
3:A:140:LEU:HD12	3:A:140:LEU:C	2.31	0.48
3:A:180:SER:CA	3:A:183:ARG:HH12	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:LEU:HB3	3:A:65:VAL:HG11	1.96	0.48
3:A:194:LEU:HA	3:A:194:LEU:HD22	1.48	0.47
1:T:4:DG:H2"	1:T:5:DG:O5'	2.14	0.47
3:A:38:ALA:HB1	3:A:41:LYS:HZ1	1.78	0.47
3:A:133:ASN:O	3:A:137:ARG:HG3	2.15	0.47
3:A:138:ILE:CG2	3:A:142:TYR:HD2	2.27	0.47
3:A:197:HIS:CG	3:A:198:PRO:CD	2.97	0.47
3:A:330:PRO:HD3	3:A:333:ARG:HH21	1.80	0.47
3:A:217:GLN:O	3:A:221:VAL:HG23	2.14	0.47
3:A:46:ILE:CG1	3:A:47:ALA:N	2.78	0.47
3:A:299:ARG:HB2	3:A:300:PRO:CD	2.43	0.47
3:A:46:ILE:HG13	3:A:47:ALA:N	2.30	0.47
3:A:158:MET:HB2	3:A:191:MET:CE	2.45	0.46
3:A:224:ILE:HD13	3:A:235:PHE:CE1	2.50	0.46
3:A:172:GLU:HG2	3:A:198:PRO:HG3	1.97	0.46
3:A:41:LYS:O	3:A:45:VAL:HG12	2.14	0.46
3:A:304:THR:HG23	3:A:305:GLY:N	2.31	0.46
3:A:208:PRO:CG	3:A:209:LYS:H	2.28	0.46
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.28	0.46
3:A:77:LEU:HA	3:A:77:LEU:HD12	1.22	0.46
3:A:183:ARG:HG3	3:A:183:ARG:HH11	1.77	0.46
3:A:115:VAL:HG23	3:A:120:LYS:HB3	1.98	0.46
3:A:88:ILE:HG23	3:A:89:ARG:N	2.31	0.46
1:T:4:DG:H21	3:A:283:ARG:NE	2.11	0.46
3:A:182:ARG:C	3:A:184:GLY:H	2.19	0.46
3:A:294:ASN:OD1	3:A:296:TYR:HB2	2.16	0.46
3:A:255:ILE:CG1	3:A:256:ASP:N	2.79	0.45
3:A:127:LYS:HE2	3:A:127:LYS:HB3	1.76	0.45
3:A:19:LEU:HA	3:A:19:LEU:HD12	1.52	0.45
3:A:23:ALA:O	3:A:36:TYR:HD1	1.99	0.45
3:A:76:PHE:HD1	3:A:77:LEU:HD13	1.81	0.45
3:A:196:THR:CG2	3:A:262:LYS:HA	2.46	0.45
3:A:202:SER:HB3	3:A:264:GLN:OE1	2.17	0.45
3:A:158:MET:HB2	3:A:191:MET:HE3	1.98	0.45
3:A:75:GLU:OE2	3:A:82:LEU:HA	2.15	0.45
2:P:1:DC:H2"	2:P:2:DG:C8	2.51	0.45
3:A:282:MET:HE2	6:A:426:HOH:O	2.16	0.45
3:A:330:PRO:CD	3:A:333:ARG:HH21	2.30	0.45
3:A:88:ILE:HG23	3:A:89:ARG:H	1.82	0.45
3:A:208:PRO:CG	3:A:209:LYS:N	2.80	0.45
3:A:317:GLN:O	3:A:320:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:46:ILE:C	3:A:46:ILE:HD12	2.37	0.45
3:A:198:PRO:CD	3:A:199:ASN:H	2.30	0.44
3:A:255:ILE:HG13	3:A:256:ASP:N	2.32	0.44
3:A:225:THR:OG1	3:A:226:ASP:OD1	2.29	0.44
3:A:126:ARG:NH1	3:A:126:ARG:HG3	2.33	0.44
3:A:150:ILE:HG22	3:A:155:MET:HG2	2.00	0.44
1:T:7:DC:H2"	1:T:8:DG:O5'	2.17	0.44
3:A:323:ILE:HG13	3:A:325:TRP:HB2	2.00	0.44
3:A:93:THR:HG23	3:A:94:SER:N	2.32	0.44
3:A:299:ARG:HB3	3:A:310:PRO:HA	2.00	0.44
3:A:66:GLY:O	3:A:69:ILE:N	2.51	0.43
3:A:103:VAL:CG2	3:A:106:ILE:HD12	2.49	0.43
3:A:164:ASN:O	3:A:167:LYS:HB2	2.19	0.43
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.52	0.43
3:A:126:ARG:NE	3:A:140:LEU:HD11	2.32	0.43
3:A:208:PRO:CD	3:A:209:LYS:N	2.80	0.43
3:A:317:GLN:HA	3:A:327:TYR:HD2	1.83	0.43
3:A:266:TYR:O	3:A:269:VAL:HG23	2.19	0.43
3:A:255:ILE:HG13	3:A:256:ASP:H	1.83	0.43
3:A:214:VAL:CG2	3:A:218:LEU:HD11	2.48	0.43
3:A:260:ILE:HD13	3:A:260:ILE:HA	1.68	0.43
3:A:163:LEU:N	3:A:163:LEU:HD23	2.25	0.43
3:A:11:LEU:CD1	3:A:11:LEU:H	2.22	0.43
3:A:204:SER:HB2	3:A:206:LYS:CG	2.48	0.43
3:A:228:LEU:CD2	3:A:228:LEU:N	2.79	0.43
5:A:338:DCT:C4'	5:A:338:DCT:H6	2.28	0.43
3:A:328:ARG:NH1	3:A:328:ARG:CB	2.82	0.43
3:A:156:LEU:HD13	3:A:156:LEU:HA	1.44	0.42
3:A:114:LEU:HD23	3:A:114:LEU:HA	1.50	0.42
3:A:23:ALA:HB1	3:A:36:TYR:HD1	1.81	0.42
3:A:333:ARG:HD3	3:A:333:ARG:HH11	1.46	0.42
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.79	0.42
3:A:178:CYS:HA	3:A:182:ARG:HB3	2.01	0.42
3:A:204:SER:HB2	3:A:206:LYS:HE2	1.99	0.42
3:A:270:LEU:HD12	6:A:405:HOH:O	2.19	0.42
3:A:330:PRO:HG3	3:A:333:ARG:HH21	1.85	0.42
3:A:215:VAL:HG21	3:A:230:LYS:HE3	2.01	0.42
3:A:177:VAL:HG22	3:A:181:PHE:HD2	1.85	0.42
3:A:299:ARG:NE	3:A:307:ALA:HB1	2.34	0.42
3:A:169:LEU:H	3:A:169:LEU:HD23	1.81	0.42
3:A:112:ARG:O	3:A:115:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:314:ASP:O	3:A:315:SER:HB3	2.20	0.42
3:A:319:ILE:HG13	3:A:319:ILE:H	1.68	0.42
3:A:38:ALA:C	3:A:41:LYS:HZ2	2.23	0.41
2:P:2:DG:C2'	2:P:3:DG:C5'	2.98	0.41
3:A:198:PRO:CD	3:A:199:ASN:N	2.83	0.41
3:A:104:THR:HG23	3:A:104:THR:O	2.20	0.41
3:A:201:THR:O	3:A:203:GLU:N	2.54	0.41
3:A:126:ARG:HH11	3:A:126:ARG:HG3	1.86	0.41
3:A:286:ALA:HA	3:A:323:ILE:HG22	2.03	0.41
3:A:169:LEU:N	3:A:169:LEU:CD2	2.79	0.41
3:A:206:LYS:HB2	3:A:207:GLN:H	1.39	0.41
3:A:206:LYS:HG3	3:A:207:GLN:HG2	2.02	0.41
3:A:328:ARG:HB3	3:A:328:ARG:NH1	2.31	0.41
3:A:24:ASN:HA	3:A:27:LYS:HB3	2.03	0.41
3:A:159:GLN:N	3:A:191:MET:HE1	2.36	0.41
3:A:208:PRO:HB3	3:A:232:GLU:HB3	2.01	0.41
3:A:327:TYR:O	3:A:328:ARG:HG3	2.21	0.41
3:A:219:GLN:O	3:A:221:VAL:N	2.53	0.41
3:A:138:ILE:HG23	3:A:142:TYR:CD2	2.56	0.41
3:A:75:GLU:O	3:A:75:GLU:HG2	2.21	0.40
3:A:26:GLU:O	3:A:30:SER:HB2	2.22	0.40
3:A:26:GLU:HG3	3:A:32:ALA:CB	2.52	0.40
3:A:142:TYR:O	3:A:145:ASP:HB2	2.22	0.40
3:A:201:THR:HB	3:A:263:ASP:OD1	2.22	0.40
1:T:4:DG:C2	3:A:283:ARG:HD2	2.54	0.40
3:A:38:ALA:HA	3:A:41:LYS:NZ	2.36	0.40
3:A:11:LEU:CD2	3:A:11:LEU:H	2.16	0.40
3:A:280:LYS:O	3:A:284:ALA:HB2	2.21	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	320/335 (96%)	258 (81%)	48 (15%)	14 (4%)	3 12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	89	ARG
3	A	91	ASP
3	A	10	THR
3	A	67	THR
3	A	82	LEU
3	A	88	ILE
3	A	204	SER
3	A	205	SER
3	A	220	LYS
3	A	262	LYS
3	A	164	ASN
3	A	202	SER
3	A	81	LYS

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%)	219 (82%)	48 (18%)	2 6

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	15	ILE
3	A	16	THR
3	A	19	LEU
3	A	26	GLU
3	A	31	GLN

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Mol	Chain	Res	Type
3	A	37	ASN
3	A	39	TYR
3	A	41	LYS
3	A	45	VAL
3	A	65	VAL
3	A	67	THR
3	A	77	LEU
3	A	79	THR
3	A	85	LEU
3	A	88	ILE
3	A	92	ASP
3	A	101	THR
3	A	115	VAL
3	A	125	LEU
3	A	127	LYS
3	A	128	ASN
3	A	130	ASP
3	A	133	ASN
3	A	156	LEU
3	A	169	LEU
3	A	173	TYR
3	A	176	THR
3	A	177	VAL
3	A	183	ARG
3	A	193	VAL
3	A	194	LEU
3	A	196	THR
3	A	205	SER
3	A	226	ASP
3	A	228	LEU
3	A	266	TYR
3	A	269	VAL
3	A	272	PHE
3	A	283	ARG
3	A	298	ILE
3	A	301	LEU
3	A	311	LEU
3	A	313	VAL
3	A	318	ASP
3	A	325	TRP
3	A	328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	31	GLN
3	A	51	HIS
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	164	ASN
3	A	199	ASN
3	A	252	HIS
3	A	264	GLN
3	A	281	ASN
3	A	285	HIS
3	A	324	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 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	$\#\|Z\|>2$
5	DCT	A	338	4	20,28,28	1.32	3 (15%)	29,43,43	1.77	9 (31%)

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	4	-	0/18/31/31	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	338	DCT	PG-O2G	-2.91	1.44	1.54
5	A	338	DCT	C6-C5	-2.76	1.32	1.38
5	A	338	DCT	O5'-C5'	-2.43	1.34	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	338	DCT	C3'-C2'-C1'	-4.36	97.84	102.71
5	A	338	DCT	O4'-C4'-C5'	-3.62	104.19	109.54
5	A	338	DCT	PB-O3A-PA	-3.02	124.26	132.73
5	A	338	DCT	O5'-PA-O1A	-2.31	100.65	109.62
5	A	338	DCT	O4'-C1'-N1	2.06	111.28	107.72
5	A	338	DCT	O2G-PG-O1G	2.25	117.81	110.58
5	A	338	DCT	O2A-PA-O1A	2.48	125.98	112.53
5	A	338	DCT	C2'-C1'-N1	2.80	118.15	112.49
5	A	338	DCT	C2-N3-C4	3.24	120.19	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	338	DCT	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.