



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BPY
Title : HUMAN DNA POLYMERASE BETA COMPLEXED WITH GAPPED DNA AND DDCTP
Authors : Sawaya, H.Pelletier M.R.; Prasad, R.; Wilson, S.H.; Kraut, J.
Deposited on : 1997-04-15
Resolution : 2.20 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

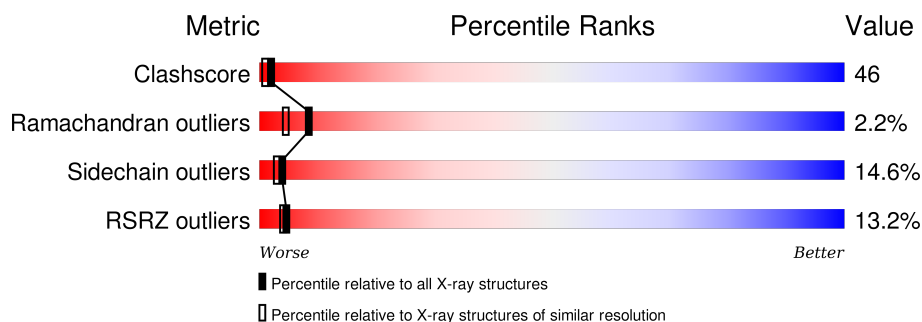
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 $\leq 5\%$. 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	16	<div> <div>6%</div> <div>56%</div> <div>44%</div> </div>
2	P	10	<div> <div>10%</div> <div>10%</div> <div>20%</div> <div>70%</div> </div>
3	D	5	<div> <div>20%</div> <div>40%</div> <div>40%</div> </div>
4	A	335	<div> <div>13%</div> <div>31%</div> <div>47%</div> <div>15%</div> <div>• •</div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3597 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*CP*GP*AP*CP*GP*GP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	16	Total	C	N	O	P	0	0	0
			323	153	63	92	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 4 is a protein called PROTEIN (DNA POLYMERASE BETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	326	Total	C	N	O	S	0	0	0
			2614	1652	457	496	9			

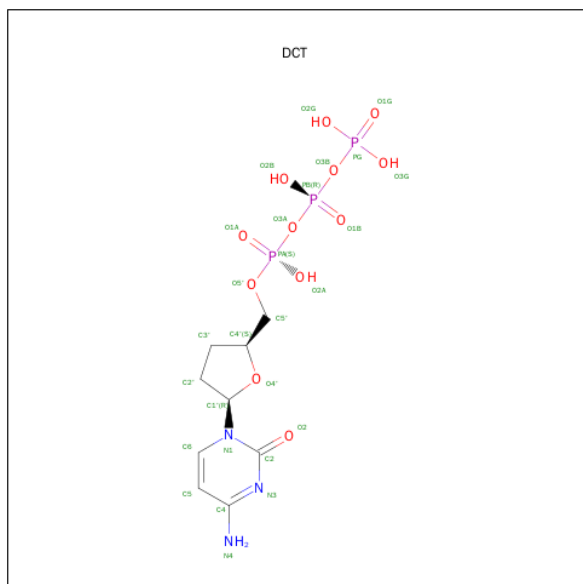
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 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
7	A	1	Total C N O P 27 9 3 12 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	223	Total O 223 223	0	0
8	D	27	Total O 27 27	0	0
8	P	21	Total O 21 21	0	0
8	T	50	Total O 50 50	0	0

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.

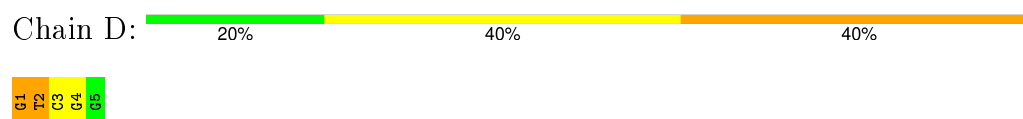
- Molecule 1: DNA (5'-D(*CP*CP*GP*AP*CP*GP*GP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3')



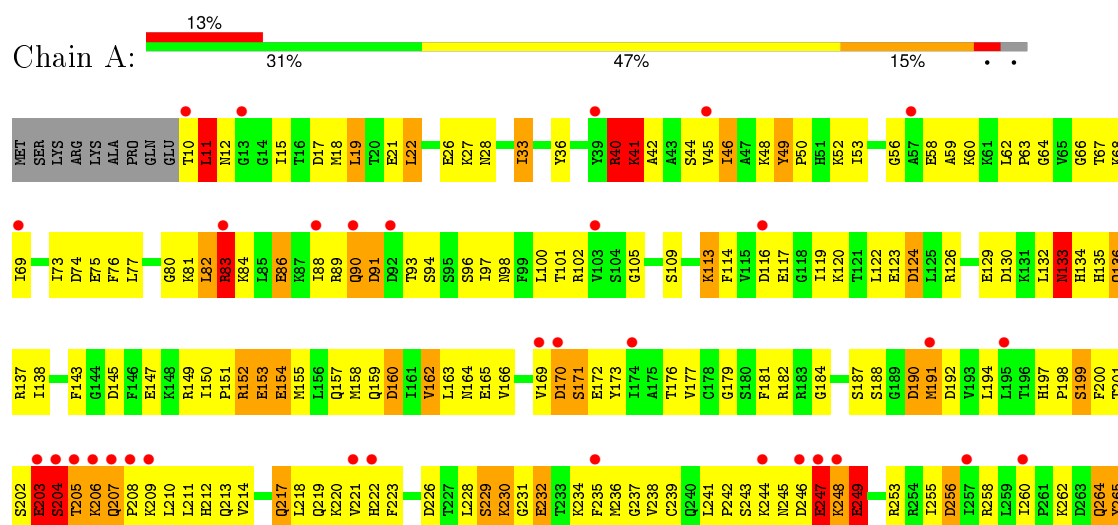
- Molecule 2: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*DOC)-3')

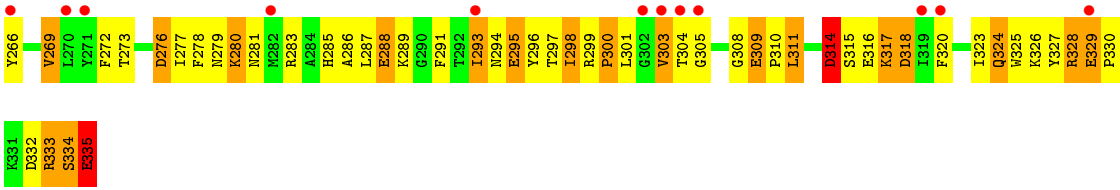


- Molecule 3: DNA (5'-D(*GP*TP*CP*GP*G)-3')



- Molecule 4: PROTEIN (DNA POLYMERASE BETA)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.54Å 79.82Å 54.94Å 90.00° 107.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-2.20) 91.8 (19.84-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.19Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.232 , 0.330 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 85.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 21104 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, DCT, DOC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	2.01	11/362 (3.0%)	2.28	21/556 (3.8%)
2	P	2.09	6/206 (2.9%)	2.47	14/317 (4.4%)
3	D	2.14	3/118 (2.5%)	2.36	6/179 (3.4%)
4	A	1.22	21/2663 (0.8%)	1.75	63/3578 (1.8%)
All	All	1.43	41/3349 (1.2%)	1.90	104/4630 (2.2%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DA	N9-C4	-10.09	1.31	1.37
3	D	1	DG	OP3-P	-8.54	1.50	1.61
4	A	232	GLU	CD-OE2	7.89	1.34	1.25
4	A	26	GLU	CD-OE1	7.70	1.34	1.25
4	A	117	GLU	CD-OE2	7.58	1.33	1.25
2	P	9	DG	C3'-O3'	-7.54	1.34	1.44
4	A	154	GLU	CD-OE2	7.51	1.33	1.25
4	A	21	GLU	CD-OE2	7.16	1.33	1.25
4	A	123	GLU	CD-OE1	7.09	1.33	1.25
4	A	153	GLU	CD-OE2	7.05	1.33	1.25
4	A	295	GLU	CD-OE2	7.05	1.33	1.25
4	A	147	GLU	CD-OE2	7.00	1.33	1.25
4	A	288	GLU	CD-OE2	6.98	1.33	1.25
1	T	3	DG	N9-C4	6.60	1.43	1.38
2	P	6	DT	C1'-N1	-6.42	1.38	1.47
1	T	8	DC	P-O5'	6.41	1.66	1.59
1	T	9	DG	C3'-O3'	-6.40	1.35	1.44
1	T	14	DA	N3-C4	-6.36	1.31	1.34
4	A	247	GLU	CD-OE2	6.32	1.32	1.25
2	P	2	DC	N3-C4	6.28	1.38	1.33
4	A	335	GLU	CD-OE2	6.26	1.32	1.25
4	A	75	GLU	CD-OE1	6.23	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	1	DC	N1-C6	-6.16	1.33	1.37
1	T	15	DG	N1-C2	-5.91	1.33	1.37
4	A	58	GLU	CD-OE1	5.90	1.32	1.25
4	A	249	GLU	CD-OE2	5.89	1.32	1.25
4	A	329	GLU	CD-OE2	5.72	1.31	1.25
4	A	129	GLU	CD-OE2	5.67	1.31	1.25
4	A	86	GLU	CD-OE1	5.67	1.31	1.25
1	T	15	DG	C6-N1	-5.63	1.35	1.39
2	P	4	DG	N3-C4	-5.57	1.31	1.35
4	A	203	GLU	CD-OE1	5.55	1.31	1.25
4	A	165	GLU	CD-OE2	5.52	1.31	1.25
3	D	1	DG	N9-C8	-5.33	1.34	1.37
3	D	4	DG	N3-C4	-5.29	1.31	1.35
1	T	9	DG	P-O5'	5.29	1.65	1.59
2	P	3	DT	C3'-O3'	-5.22	1.37	1.44
1	T	2	DC	O5'-C5'	-5.14	1.29	1.42
1	T	2	DC	P-O5'	-5.07	1.54	1.59
1	T	1	DC	C4-C5	-5.06	1.39	1.43
4	A	309	GLU	CD-OE2	5.01	1.31	1.25

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	333	ARG	NE-CZ-NH1	11.27	125.94	120.30
2	P	5	DA	C8-N9-C4	11.02	110.21	105.80
4	A	137	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	T	3	DG	O4'-C1'-N9	-10.51	100.64	108.00
4	A	204	SER	N-CA-C	9.91	137.75	111.00
2	P	8	DC	O4'-C1'-N1	9.25	114.48	108.00
1	T	8	DC	O4'-C1'-N1	9.08	114.35	108.00
4	A	74	ASP	CB-CG-OD2	-8.59	110.57	118.30
4	A	248	LYS	N-CA-CB	8.43	125.77	110.60
2	P	3	DT	O4'-C1'-N1	8.40	113.88	108.00
2	P	1	DG	C8-N9-C4	8.37	109.75	106.40
4	A	258	ARG	NE-CZ-NH1	8.33	124.47	120.30
4	A	258	ARG	NE-CZ-NH2	-8.30	116.15	120.30
4	A	160	ASP	CB-CG-OD2	-8.29	110.84	118.30
4	A	333	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	T	16	DC	O4'-C1'-N1	8.18	113.72	108.00
4	A	332	ASP	CB-CG-OD2	-8.06	111.05	118.30
4	A	145	ASP	CB-CG-OD2	-8.04	111.06	118.30
4	A	190	ASP	CB-CG-OD1	8.04	125.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	229	SER	N-CA-CB	8.02	122.53	110.50
4	A	91	ASP	CB-CG-OD1	7.88	125.40	118.30
1	T	1	DC	P-O3'-C3'	-7.88	110.24	119.70
4	A	205	THR	N-CA-CB	7.88	125.26	110.30
4	A	190	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	T	11	DA	C8-N9-C4	7.77	108.91	105.80
2	P	9	DG	O4'-C1'-N9	7.64	113.35	108.00
4	A	192	ASP	CB-CG-OD1	-7.64	111.43	118.30
4	A	74	ASP	CB-CG-OD1	7.54	125.08	118.30
1	T	4	DA	C8-N9-C4	7.50	108.80	105.80
4	A	314	ASP	CB-CG-OD1	-7.50	111.56	118.30
4	A	91	ASP	CB-CG-OD2	-7.40	111.64	118.30
4	A	256	ASP	CB-CG-OD1	7.36	124.92	118.30
4	A	276	ASP	CB-CG-OD1	7.33	124.90	118.30
4	A	116	ASP	CB-CG-OD2	-7.28	111.75	118.30
4	A	192	ASP	CB-CG-OD2	7.28	124.85	118.30
4	A	83	ARG	NE-CZ-NH1	7.24	123.92	120.30
4	A	297	THR	CB-CA-C	-7.12	92.37	111.60
4	A	152	ARG	NE-CZ-NH1	7.12	123.86	120.30
4	A	152	ARG	NE-CZ-NH2	-7.09	116.76	120.30
3	D	1	DG	C8-N9-C4	7.02	109.21	106.40
4	A	246	ASP	CB-CG-OD2	7.00	124.60	118.30
1	T	3	DG	N3-C4-N9	6.97	130.18	126.00
4	A	199	SER	N-CA-CB	-6.95	100.07	110.50
4	A	246	ASP	CB-CG-OD1	-6.95	112.04	118.30
2	P	2	DC	O4'-C1'-N1	6.93	112.85	108.00
4	A	17	ASP	CB-CG-OD1	-6.92	112.07	118.30
2	P	5	DA	N7-C8-N9	-6.91	110.34	113.80
4	A	137	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	D	4	DG	P-O3'-C3'	6.87	127.94	119.70
1	T	14	DA	C8-N9-C4	6.86	108.55	105.80
2	P	7	DG	O4'-C4'-C3'	6.81	110.08	106.00
1	T	2	DC	O4'-C1'-N1	-6.79	103.25	108.00
4	A	130	ASP	CB-CG-OD2	-6.76	112.22	118.30
3	D	2	DT	C5'-C4'-C3'	-6.75	101.95	114.10
4	A	204	SER	N-CA-CB	-6.71	100.43	110.50
4	A	41	LYS	N-CA-CB	6.66	122.58	110.60
3	D	1	DG	N3-C4-N9	6.56	129.93	126.00
1	T	5	DC	O4'-C1'-C2'	-6.44	100.75	105.90
1	T	15	DG	N1-C6-O6	-6.33	116.10	119.90
4	A	205	THR	N-CA-C	-6.31	93.97	111.00
4	A	120	LYS	CB-CA-C	-6.28	97.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	276	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	T	12	DT	O4'-C1'-N1	6.24	112.37	108.00
1	T	2	DC	P-O5'-C5'	-6.23	110.94	120.90
4	A	124	ASP	CB-CG-OD2	-6.20	112.72	118.30
4	A	332	ASP	CB-CG-OD1	6.11	123.80	118.30
4	A	17	ASP	CB-CG-OD2	6.09	123.78	118.30
4	A	213	GLN	CB-CA-C	-6.05	98.29	110.40
2	P	5	DA	O4'-C1'-C2'	6.05	110.74	105.90
4	A	152	ARG	N-CA-CB	6.03	121.46	110.60
4	A	49	TYR	CB-CG-CD2	-6.01	117.39	121.00
4	A	265	TYR	CB-CG-CD1	-5.98	117.41	121.00
3	D	1	DG	N9-C4-C5	-5.87	103.05	105.40
2	P	6	DT	C6-C5-C7	-5.86	119.38	122.90
2	P	2	DC	N1-C2-O2	-5.74	115.46	118.90
4	A	293	ILE	CB-CA-C	-5.68	100.25	111.60
4	A	298	ILE	N-CA-CB	5.67	123.83	110.80
1	T	3	DG	N9-C1'-C2'	5.65	123.33	112.60
4	A	171	SER	N-CA-CB	-5.61	102.09	110.50
2	P	6	DT	C4-C5-C7	5.59	122.36	119.00
4	A	334	SER	CB-CA-C	-5.55	99.55	110.10
4	A	133	ASN	N-CA-CB	5.51	120.53	110.60
4	A	130	ASP	CB-CG-OD1	5.44	123.20	118.30
4	A	226	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	T	11	DA	N7-C8-N9	-5.33	111.14	113.80
1	T	3	DG	N3-C4-C5	-5.32	125.94	128.60
1	T	1	DC	O4'-C1'-N1	5.32	111.72	108.00
3	D	4	DG	O4'-C1'-N9	5.31	111.72	108.00
4	A	256	ASP	CB-CG-OD2	-5.31	113.52	118.30
4	A	170	ASP	CB-CG-OD2	-5.27	113.56	118.30
4	A	44	SER	N-CA-CB	5.25	118.37	110.50
4	A	170	ASP	CB-CG-OD1	5.25	123.02	118.30
4	A	226	ASP	CB-CG-OD1	5.22	123.00	118.30
1	T	12	DT	O4'-C4'-C3'	5.21	109.13	106.00
4	A	40	ARG	N-CA-CB	5.21	119.97	110.60
4	A	318	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	P	2	DC	C6-N1-C2	5.19	122.38	120.30
1	T	2	DC	O4'-C4'-C3'	5.18	109.11	106.00
4	A	314	ASP	CB-CG-OD2	5.18	122.96	118.30
1	T	14	DA	P-O3'-C3'	5.13	125.86	119.70
4	A	207	GLN	N-CA-C	5.12	124.82	111.00
2	P	4	DG	O4'-C1'-N9	5.07	111.55	108.00
1	T	10	DC	N1-C1'-C2'	5.06	122.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	300	PRO	CB-CA-C	-5.02	99.45	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	323	0	179	13	0
2	P	202	0	114	5	0
3	D	106	0	57	9	0
4	A	2614	0	2635	269	0
5	A	2	0	0	0	0
6	A	2	0	0	0	0
7	A	27	0	12	0	0
8	A	223	0	0	20	0
8	D	27	0	0	2	0
8	P	21	0	0	2	0
8	T	50	0	0	3	0
All	All	3597	0	2997	286	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 46.

All (286) 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)
4:A:150:ILE:HD12	4:A:155:MET:HE1	1.28	1.12
4:A:285:HIS:HD2	4:A:323:ILE:HD12	1.17	1.07
4:A:230:LYS:HG3	4:A:235:PHE:HD1	1.13	1.06
4:A:316:GLU:H	4:A:317:LYS:NZ	1.53	1.06
4:A:207:GLN:HB3	4:A:209:LYS:HG2	1.41	1.03
4:A:83:ARG:HH11	4:A:83:ARG:HG2	1.24	1.02
4:A:316:GLU:N	4:A:317:LYS:HZ3	1.65	0.94
4:A:230:LYS:HG3	4:A:235:PHE:CD1	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:228:LEU:HD22	4:A:237:GLY:HA2	1.51	0.92
4:A:285:HIS:CD2	4:A:323:ILE:HD12	2.04	0.90
4:A:33:ILE:H	4:A:33:ILE:HD12	1.37	0.90
4:A:155:MET:HE3	4:A:188:SER:HB2	1.51	0.90
4:A:12:ASN:HD21	4:A:53:ILE:H	1.09	0.89
4:A:155:MET:CE	4:A:188:SER:HB2	2.04	0.88
4:A:113:LYS:HG2	4:A:114:PHE:N	1.91	0.86
4:A:315:SER:HB2	4:A:317:LYS:HE2	1.58	0.86
1:T:2:DC:H2''	1:T:3:DG:C8	2.13	0.84
4:A:11:LEU:HD11	4:A:52:LYS:HB2	1.60	0.83
4:A:133:ASN:ND2	4:A:136:GLN:HG3	1.92	0.83
4:A:316:GLU:H	4:A:317:LYS:HZ3	0.83	0.82
4:A:194:LEU:HD11	4:A:260:ILE:HG13	1.61	0.81
3:D:2:DT:H5'	4:A:66:GLY:HA3	1.62	0.81
4:A:207:GLN:HB3	4:A:209:LYS:CG	2.10	0.81
2:P:5:DA:H2'	2:P:6:DT:H71	1.63	0.80
4:A:243:SER:OG	4:A:249:GLU:HA	1.82	0.80
4:A:248:LYS:HG2	4:A:249:GLU:N	1.95	0.79
4:A:197:HIS:ND1	4:A:199:SER:HB3	1.96	0.79
4:A:18:MET:CE	4:A:82:LEU:HB2	2.13	0.79
4:A:328:ARG:HB3	4:A:328:ARG:HH11	1.46	0.78
4:A:191:MET:HG2	4:A:255:ILE:HG13	1.65	0.78
4:A:150:ILE:HD12	4:A:155:MET:CE	2.13	0.78
4:A:234:LYS:HE3	8:A:755:HOH:O	1.84	0.77
4:A:200:PHE:CD1	4:A:206:LYS:HB2	2.20	0.77
4:A:236:MET:HG3	4:A:256:ASP:OD1	1.85	0.77
3:D:2:DT:C5'	4:A:66:GLY:HA3	2.14	0.76
4:A:18:MET:HE2	4:A:82:LEU:HB2	1.66	0.75
4:A:69:ILE:O	4:A:73:ILE:HG13	1.85	0.75
4:A:41:LYS:HE2	4:A:64:GLY:CA	2.17	0.75
4:A:265:TYR:O	4:A:269:VAL:HG22	1.85	0.75
4:A:41:LYS:HE2	4:A:64:GLY:HA2	1.69	0.74
4:A:41:LYS:HD3	4:A:42:ALA:N	2.02	0.74
4:A:194:LEU:HD11	4:A:260:ILE:CG1	2.17	0.74
4:A:315:SER:CB	4:A:317:LYS:HE2	2.19	0.73
4:A:287:LEU:HD12	4:A:291:PHE:O	1.88	0.72
4:A:170:ASP:HB3	4:A:173:TYR:CD2	2.24	0.72
4:A:122:LEU:O	4:A:126:ARG:HG3	1.90	0.72
4:A:12:ASN:ND2	4:A:53:ILE:H	1.87	0.72
4:A:150:ILE:HB	4:A:155:MET:HE2	1.72	0.71
4:A:315:SER:HB2	4:A:317:LYS:CE	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:300:PRO:HD3	4:A:311:LEU:CD1	2.21	0.70
4:A:316:GLU:N	4:A:317:LYS:NZ	2.32	0.70
4:A:300:PRO:HD3	4:A:311:LEU:HD11	1.72	0.70
4:A:154:GLU:O	4:A:158:MET:HG3	1.90	0.69
4:A:18:MET:HE1	4:A:76:PHE:HB2	1.73	0.69
4:A:12:ASN:HD21	4:A:53:ILE:N	1.86	0.69
4:A:207:GLN:CB	4:A:209:LYS:HG2	2.22	0.69
4:A:33:ILE:H	4:A:33:ILE:CD1	1.94	0.69
4:A:200:PHE:HA	4:A:204:SER:OG	1.94	0.68
4:A:228:LEU:HD22	4:A:237:GLY:CA	2.24	0.68
4:A:209:LYS:HG3	4:A:210:LEU:N	2.10	0.67
4:A:138:ILE:N	4:A:138:ILE:HD13	2.08	0.67
4:A:328:ARG:HH11	4:A:328:ARG:CB	2.07	0.66
4:A:301:LEU:HD23	8:A:520:HOH:O	1.95	0.66
4:A:158:MET:O	4:A:162:VAL:HG22	1.96	0.66
4:A:42:ALA:O	4:A:46:ILE:HG23	1.96	0.66
4:A:289:LYS:HZ3	4:A:324:GLN:HG3	1.60	0.66
4:A:113:LYS:HE3	4:A:114:PHE:CD1	2.31	0.66
4:A:162:VAL:HG23	4:A:163:LEU:H	1.61	0.66
4:A:328:ARG:HD2	8:A:578:HOH:O	1.95	0.66
4:A:160:ASP:OD1	4:A:164:ASN:ND2	2.30	0.65
3:D:3:DC:H5'	8:D:649:HOH:O	1.96	0.65
4:A:133:ASN:H	4:A:136:GLN:HE21	1.43	0.65
4:A:303:VAL:HG23	4:A:304:THR:N	2.12	0.65
4:A:279:ASN:O	4:A:283:ARG:HG3	1.97	0.64
4:A:207:GLN:OE1	4:A:208:PRO:HD2	1.98	0.64
4:A:11:LEU:N	8:A:712:HOH:O	2.30	0.64
1:T:8:DC:H4'	4:A:295:GLU:OE2	1.98	0.64
4:A:289:LYS:NZ	4:A:324:GLN:HG3	2.12	0.64
4:A:328:ARG:O	4:A:333:ARG:NH1	2.29	0.64
4:A:133:ASN:HD21	4:A:135:HIS:HB3	1.62	0.64
3:D:1:DG:H5''	8:D:590:HOH:O	1.98	0.64
4:A:113:LYS:HA	8:A:661:HOH:O	1.98	0.63
1:T:13:DC:H2''	1:T:14:DA:C8	2.34	0.63
4:A:285:HIS:O	4:A:288:GLU:HB2	1.97	0.63
4:A:328:ARG:HH11	4:A:328:ARG:CG	2.10	0.63
4:A:41:LYS:HD3	4:A:42:ALA:H	1.63	0.63
4:A:278:PHE:CZ	4:A:333:ARG:HD2	2.33	0.63
4:A:40:ARG:NH1	4:A:276:ASP:OD2	2.31	0.63
4:A:109:SER:HB3	8:A:533:HOH:O	1.99	0.63
4:A:36:TYR:CZ	4:A:40:ARG:HD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:113:LYS:HE3	4:A:114:PHE:CE1	2.34	0.62
4:A:303:VAL:HG23	4:A:304:THR:H	1.63	0.62
4:A:212:HIS:N	8:A:752:HOH:O	2.30	0.62
4:A:162:VAL:O	4:A:166:VAL:HG23	2.00	0.62
1:T:1:DC:H2''	1:T:2:DC:O5'	2.00	0.62
4:A:244:LYS:H	4:A:247:GLU:HG2	1.64	0.62
3:D:2:DT:H5'	4:A:66:GLY:CA	2.29	0.62
4:A:200:PHE:HD1	4:A:206:LYS:HB2	1.65	0.62
4:A:172:GLU:OE1	4:A:198:PRO:HG2	2.00	0.62
4:A:299:ARG:HB3	4:A:308:GLY:O	2.00	0.61
1:T:13:DC:H2''	1:T:14:DA:H8	1.66	0.61
4:A:248:LYS:HG2	4:A:249:GLU:H	1.64	0.60
4:A:244:LYS:N	4:A:247:GLU:HG2	2.16	0.60
4:A:11:LEU:HD11	4:A:52:LYS:CB	2.31	0.60
4:A:264:GLN:HB3	4:A:296:TYR:O	2.02	0.60
4:A:317:LYS:N	4:A:317:LYS:HD3	2.16	0.60
4:A:328:ARG:HB3	4:A:328:ARG:NH1	2.16	0.60
4:A:317:LYS:H	4:A:317:LYS:HD3	1.67	0.59
4:A:133:ASN:ND2	4:A:136:GLN:H	2.00	0.59
4:A:317:LYS:H	4:A:317:LYS:CD	2.15	0.59
4:A:154:GLU:O	4:A:158:MET:HE2	2.03	0.59
4:A:133:ASN:ND2	4:A:135:HIS:HB3	2.18	0.58
4:A:228:LEU:N	4:A:236:MET:O	2.33	0.58
4:A:18:MET:HE2	4:A:82:LEU:CB	2.33	0.58
4:A:18:MET:HE1	4:A:82:LEU:HB2	1.86	0.58
4:A:303:VAL:HG23	4:A:304:THR:HG23	1.86	0.58
4:A:18:MET:HE3	4:A:76:PHE:CD1	2.39	0.58
4:A:150:ILE:CD1	4:A:155:MET:HE1	2.18	0.57
3:D:1:DG:OP1	4:A:68:LYS:NZ	2.33	0.57
4:A:133:ASN:N	4:A:136:GLN:HE21	2.02	0.57
3:D:1:DG:OP2	4:A:68:LYS:HD3	2.04	0.57
4:A:162:VAL:HG23	4:A:163:LEU:N	2.18	0.57
1:T:10:DC:OP1	4:A:231:GLY:HA3	2.05	0.57
4:A:301:LEU:HD11	4:A:305:GLY:C	2.25	0.57
4:A:132:LEU:HA	4:A:136:GLN:NE2	2.20	0.56
4:A:201:THR:H	4:A:204:SER:HB2	1.68	0.56
4:A:159:GLN:O	4:A:162:VAL:HG23	2.04	0.56
4:A:326:LYS:O	4:A:326:LYS:HG3	2.06	0.56
4:A:219:GLN:O	4:A:222:HIS:N	2.29	0.56
4:A:318:ASP:OD1	4:A:318:ASP:N	2.36	0.56
4:A:201:THR:H	4:A:204:SER:CB	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:155:MET:HE3	4:A:188:SER:CB	2.33	0.55
4:A:113:LYS:NZ	8:A:696:HOH:O	2.38	0.55
4:A:133:ASN:HD22	4:A:135:HIS:N	2.05	0.55
4:A:201:THR:O	4:A:204:SER:HB2	2.07	0.54
4:A:80:GLY:O	4:A:81:LYS:HD3	2.07	0.54
4:A:15:ILE:HG22	4:A:19:LEU:HD22	1.89	0.54
4:A:244:LYS:CB	4:A:247:GLU:HG2	2.38	0.53
4:A:197:HIS:HA	8:A:774:HOH:O	2.07	0.53
4:A:207:GLN:CG	4:A:209:LYS:HD3	2.37	0.53
4:A:217:GLN:O	4:A:217:GLN:HG3	2.06	0.53
4:A:205:THR:O	4:A:205:THR:HG22	2.07	0.53
4:A:83:ARG:HG2	4:A:83:ARG:NH1	2.01	0.53
4:A:228:LEU:HB2	4:A:236:MET:O	2.09	0.53
4:A:18:MET:O	4:A:22:LEU:HD22	2.09	0.53
4:A:134:HIS:CE1	4:A:138:ILE:HG12	2.44	0.52
4:A:84:LYS:O	4:A:88:ILE:HG13	2.08	0.52
4:A:153:GLU:O	4:A:157:GLN:HG3	2.09	0.52
4:A:291:PHE:CB	4:A:298:ILE:HD11	2.39	0.52
4:A:320:PHE:HB3	4:A:325:TRP:O	2.09	0.52
4:A:207:GLN:HB3	4:A:209:LYS:HE2	1.91	0.52
4:A:83:ARG:HH11	4:A:83:ARG:CG	2.12	0.52
4:A:243:SER:N	8:A:558:HOH:O	2.43	0.52
4:A:203:GLU:OE1	4:A:203:GLU:O	2.28	0.52
4:A:197:HIS:CE1	4:A:199:SER:HB3	2.45	0.51
4:A:48:LYS:HE3	4:A:334:SER:HB2	1.92	0.51
4:A:291:PHE:CG	4:A:298:ILE:HD11	2.45	0.51
4:A:155:MET:HE2	4:A:188:SER:HB2	1.89	0.51
4:A:287:LEU:HA	4:A:291:PHE:O	2.09	0.51
4:A:133:ASN:H	4:A:136:GLN:NE2	2.09	0.51
4:A:199:SER:O	4:A:204:SER:OG	2.28	0.51
4:A:329:GLU:HB3	4:A:330:PRO:HD2	1.92	0.50
4:A:11:LEU:HD12	4:A:52:LYS:HA	1.93	0.50
4:A:135:HIS:HE1	4:A:236:MET:HE1	1.75	0.50
4:A:166:VAL:CG1	4:A:173:TYR:HB3	2.41	0.50
4:A:207:GLN:CD	4:A:209:LYS:HD3	2.32	0.50
4:A:219:GLN:NE2	8:A:631:HOH:O	2.41	0.50
4:A:208:PRO:HA	8:A:577:HOH:O	2.11	0.50
4:A:207:GLN:HG3	4:A:209:LYS:NZ	2.26	0.49
4:A:278:PHE:CE1	4:A:333:ARG:HD2	2.47	0.49
2:P:2:DC:H4'	2:P:3:DT:OP1	2.12	0.49
4:A:201:THR:O	4:A:203:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:11:DA:H5'	4:A:229:SER:HB3	1.95	0.49
4:A:209:LYS:HG3	4:A:210:LEU:H	1.78	0.49
4:A:98:ASN:O	4:A:102:ARG:HG3	2.11	0.49
4:A:154:GLU:C	4:A:158:MET:HE2	2.32	0.49
4:A:266:TYR:HA	4:A:269:VAL:CG2	2.43	0.49
4:A:291:PHE:HB3	4:A:298:ILE:HD11	1.94	0.49
3:D:2:DT:H5''	4:A:66:GLY:HA3	1.92	0.48
4:A:90:GLN:HG2	4:A:90:GLN:O	2.01	0.48
4:A:200:PHE:HD1	4:A:206:LYS:CB	2.25	0.48
4:A:300:PRO:HD3	4:A:311:LEU:HD13	1.94	0.48
4:A:323:ILE:C	4:A:324:GLN:HG2	2.33	0.48
4:A:323:ILE:O	4:A:324:GLN:HG2	2.13	0.48
1:T:2:DC:H2''	1:T:3:DG:H8	1.73	0.48
4:A:238:VAL:HA	4:A:253:ARG:O	2.13	0.48
4:A:301:LEU:HD11	4:A:305:GLY:O	2.14	0.47
4:A:56:GLY:O	4:A:59:ALA:N	2.46	0.47
4:A:150:ILE:CG2	4:A:158:MET:HE1	2.43	0.47
1:T:6:DG:C6	1:T:7:DG:C6	3.03	0.47
4:A:303:VAL:CG2	4:A:304:THR:H	2.28	0.47
4:A:45:VAL:HG23	4:A:46:ILE:N	2.30	0.47
4:A:158:MET:HE1	8:A:557:HOH:O	2.14	0.47
4:A:207:GLN:HG3	4:A:209:LYS:HD3	1.95	0.47
4:A:300:PRO:HD2	4:A:309:GLU:O	2.14	0.47
4:A:86:GLU:OE1	4:A:89:ARG:NH1	2.47	0.47
4:A:328:ARG:HH11	4:A:328:ARG:HG2	1.79	0.47
4:A:160:ASP:O	4:A:164:ASN:ND2	2.44	0.47
4:A:244:LYS:H	4:A:247:GLU:CG	2.28	0.47
4:A:91:ASP:OD1	4:A:94:SER:OG	2.31	0.46
4:A:262:LYS:NZ	8:A:775:HOH:O	2.48	0.46
4:A:326:LYS:HG2	8:A:578:HOH:O	2.14	0.46
8:T:517:HOH:O	4:A:232:GLU:HG2	2.15	0.46
4:A:211:LEU:HB3	8:A:752:HOH:O	2.15	0.46
4:A:149:ARG:NH2	4:A:187:SER:O	2.49	0.46
4:A:207:GLN:CB	4:A:209:LYS:HE2	2.46	0.46
4:A:155:MET:HE3	4:A:190:ASP:O	2.15	0.45
4:A:197:HIS:CE1	4:A:199:SER:CB	2.98	0.45
4:A:62:LEU:HB3	4:A:63:PRO:HD2	1.97	0.45
4:A:314:ASP:O	4:A:315:SER:HB3	2.16	0.45
4:A:105:GLY:CA	4:A:135:HIS:CD2	2.99	0.45
4:A:330:PRO:HA	4:A:333:ARG:HG3	1.97	0.45
1:T:13:DC:C2'	1:T:14:DA:C8	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:105:GLY:HA3	4:A:135:HIS:CD2	2.52	0.45
1:T:11:DA:N3	8:T:805:HOH:O	2.36	0.45
4:A:133:ASN:HD21	4:A:136:GLN:HG3	1.79	0.45
4:A:40:ARG:HB2	4:A:277:ILE:HD11	1.97	0.45
4:A:12:ASN:HB3	4:A:46:ILE:HD11	1.99	0.45
2:P:7:DG:H2''	2:P:8:DC:O5'	2.17	0.45
4:A:289:LYS:NZ	4:A:324:GLN:CG	2.79	0.45
4:A:60:LYS:HE3	4:A:67:THR:HB	1.99	0.45
4:A:93:THR:O	4:A:97:ILE:HG13	2.17	0.45
4:A:207:GLN:HB3	4:A:209:LYS:CD	2.46	0.44
4:A:18:MET:CE	4:A:76:PHE:CD1	3.00	0.44
4:A:303:VAL:CG2	4:A:304:THR:N	2.79	0.44
4:A:177:VAL:CG1	4:A:181:PHE:CD2	3.00	0.44
4:A:265:TYR:OH	4:A:269:VAL:HG11	2.17	0.44
4:A:265:TYR:CE1	4:A:269:VAL:HG13	2.53	0.44
4:A:209:LYS:CG	4:A:210:LEU:N	2.79	0.44
4:A:91:ASP:HB3	4:A:94:SER:OG	2.16	0.44
4:A:289:LYS:HD3	4:A:289:LYS:HA	1.59	0.44
4:A:334:SER:O	4:A:335:GLU:HB2	2.18	0.44
4:A:86:GLU:O	4:A:89:ARG:HB2	2.17	0.44
4:A:132:LEU:CA	4:A:136:GLN:HE21	2.31	0.44
4:A:255:ILE:HG12	4:A:256:ASP:N	2.33	0.44
4:A:329:GLU:HB3	4:A:330:PRO:CD	2.48	0.44
4:A:177:VAL:HG12	4:A:181:PHE:CD2	2.53	0.44
4:A:119:ILE:HG23	4:A:124:ASP:HB3	2.00	0.44
4:A:328:ARG:NH1	4:A:328:ARG:CG	2.79	0.43
4:A:223:PHE:O	4:A:239:CYS:HA	2.18	0.43
4:A:157:GLN:NE2	8:A:516:HOH:O	2.29	0.43
4:A:122:LEU:HG	4:A:126:ARG:HD2	1.99	0.43
4:A:150:ILE:HG23	4:A:158:MET:HE1	2.00	0.43
4:A:244:LYS:CA	4:A:247:GLU:HG2	2.48	0.43
4:A:209:LYS:HE2	4:A:210:LEU:HG	2.00	0.43
1:T:7:DG:OP1	4:A:287:LEU:HD11	2.17	0.43
4:A:28:ASN:HB3	4:A:101:THR:HG21	2.00	0.43
4:A:40:ARG:HH12	4:A:276:ASP:CG	2.21	0.43
2:P:4:DG:H5'	8:P:677:HOH:O	2.18	0.43
4:A:207:GLN:HB3	4:A:209:LYS:CE	2.49	0.43
8:T:598:HOH:O	4:A:280:LYS:HD2	2.18	0.43
4:A:289:LYS:HZ2	4:A:324:GLN:CG	2.32	0.42
4:A:309:GLU:HA	4:A:310:PRO:HD2	1.76	0.42
4:A:133:ASN:N	4:A:136:GLN:NE2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:113:LYS:CE	4:A:114:PHE:CD1	3.02	0.42
4:A:49:TYR:HA	4:A:50:PRO:HD3	1.71	0.42
4:A:311:LEU:N	4:A:311:LEU:HD13	2.34	0.42
4:A:320:PHE:CD1	4:A:327:TYR:HD1	2.38	0.42
2:P:5:DA:H1'	8:P:731:HOH:O	2.19	0.42
4:A:283:ARG:O	4:A:286:ALA:HB3	2.19	0.42
4:A:159:GLN:O	4:A:163:LEU:HD23	2.20	0.42
4:A:40:ARG:HG3	8:A:683:HOH:O	2.19	0.42
1:T:2:DC:H2''	1:T:3:DG:N7	2.33	0.42
4:A:245:ASN:HD22	4:A:245:ASN:HA	1.75	0.42
4:A:194:LEU:HD11	4:A:260:ILE:HG12	2.00	0.41
4:A:293:ILE:CG2	4:A:294:ASN:N	2.79	0.41
4:A:11:LEU:CD1	4:A:52:LYS:HB2	2.41	0.41
3:D:1:DG:H2''	3:D:2:DT:O5'	2.20	0.41
4:A:150:ILE:CB	4:A:155:MET:HE2	2.47	0.41
4:A:150:ILE:CG2	4:A:158:MET:CE	2.98	0.41
4:A:151:PRO:HD2	4:A:154:GLU:HB2	2.02	0.41
4:A:311:LEU:CD1	4:A:311:LEU:N	2.84	0.41
4:A:182:ARG:C	4:A:184:GLY:H	2.23	0.41
4:A:113:LYS:CE	4:A:114:PHE:CE1	3.03	0.41
4:A:241:LEU:HA	4:A:242:PRO:HD3	1.91	0.41
4:A:83:ARG:O	4:A:86:GLU:HB2	2.21	0.41
4:A:219:GLN:O	4:A:221:VAL:N	2.54	0.41
4:A:41:LYS:N	8:A:683:HOH:O	2.52	0.41
4:A:273:THR:HB	8:A:622:HOH:O	2.21	0.41
4:A:281:ASN:HA	4:A:281:ASN:HD22	1.66	0.40
4:A:150:ILE:HG12	4:A:253:ARG:HD2	2.02	0.40
4:A:173:TYR:OH	4:A:210:LEU:HA	2.21	0.40
4:A:22:LEU:HA	4:A:22:LEU:HD13	1.60	0.40
4:A:150:ILE:HG22	4:A:155:MET:HG2	2.03	0.40
4:A:207:GLN:CG	4:A:209:LYS:CD	3.00	0.40
4:A:207:GLN:CB	4:A:209:LYS:CE	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	324/335 (97%)	285 (88%)	32 (10%)	7 (2%)	8 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	11	LEU
4	A	179	GLY
4	A	202	SER
4	A	220	LYS
4	A	143	PHE
4	A	249	GLU
4	A	303	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	287/295 (97%)	245 (85%)	42 (15%)	4 3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	THR
4	A	11	LEU
4	A	19	LEU
4	A	22	LEU
4	A	27	LYS
4	A	33	ILE
4	A	40	ARG
4	A	41	LYS
4	A	46	ILE
4	A	77	LEU

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Mol	Chain	Res	Type
4	A	82	LEU
4	A	83	ARG
4	A	90	GLN
4	A	96	SER
4	A	100	LEU
4	A	113	LYS
4	A	133	ASN
4	A	136	GLN
4	A	152	ARG
4	A	162	VAL
4	A	169	VAL
4	A	171	SER
4	A	176	THR
4	A	191	MET
4	A	203	GLU
4	A	204	SER
4	A	206	LYS
4	A	214	VAL
4	A	217	GLN
4	A	218	LEU
4	A	230	LYS
4	A	247	GLU
4	A	264	GLN
4	A	269	VAL
4	A	272	PHE
4	A	280	LYS
4	A	311	LEU
4	A	314	ASP
4	A	317	LYS
4	A	324	GLN
4	A	328	ARG
4	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	12	ASN
4	A	28	ASN
4	A	90	GLN
4	A	133	ASN
4	A	136	GLN
4	A	157	GLN

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Mol	Chain	Res	Type
4	A	217	GLN
4	A	245	ASN
4	A	264	GLN
4	A	279	ASN
4	A	281	ASN
4	A	285	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DOC	P	10	1,2	11,19,20	0.93	0	14,26,29	2.02	4 (28%)

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
2	DOC	P	10	1,2	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	10	DOC	C2'-C3'-C4'	2.37	107.21	102.59
2	P	10	DOC	C2-N3-C4	3.62	120.71	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	10	DOC	C2'-C1'-N1	4.05	120.69	112.49
2	P	10	DOC	O4'-C1'-C2'	4.06	111.07	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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$
7	DCT	A	338	5	20,28,28	1.38	2 (10%)	29,43,43	1.26	4 (13%)

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
7	DCT	A	338	5	-	0/18/31/31	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	338	DCT	O4'-C1'	-2.96	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	338	DCT	PA-O2A	-2.85	1.42	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	338	DCT	O3G-PG-O3B	-2.21	95.07	105.09
7	A	338	DCT	O2G-PG-O1G	2.20	117.65	110.58
7	A	338	DCT	O4'-C1'-N1	2.76	112.50	107.72
7	A	338	DCT	C2-N3-C4	2.82	119.59	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	16/16 (100%)	0.66	1 (6%) 23 23	41, 49, 68, 69	0
2	P	9/10 (90%)	1.08	1 (11%) 7 7	49, 53, 64, 66	0
3	D	5/5 (100%)	0.39	0 100 100	38, 41, 44, 47	0
4	A	326/335 (97%)	1.06	45 (13%) 4 3	32, 48, 70, 97	0
All	All	356/366 (97%)	1.04	47 (13%) 4 4	32, 49, 70, 97	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	205	THR	10.8
4	A	208	PRO	7.8
4	A	204	SER	5.5
4	A	303	VAL	4.7
4	A	247	GLU	4.2
4	A	10	THR	4.0
4	A	206	LYS	3.8
4	A	57	ALA	3.7
4	A	248	LYS	3.5
4	A	293	ILE	3.4
4	A	329	GLU	3.3
4	A	305	GLY	3.2
4	A	203	GLU	3.1
4	A	191	MET	3.1
4	A	221	VAL	3.0
4	A	266	TYR	3.0
4	A	304	THR	2.8
4	A	69	ILE	2.8
4	A	207	GLN	2.7
4	A	244	LYS	2.6
4	A	246	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	169	VAL	2.6
4	A	302	GLY	2.6
4	A	222	HIS	2.5
4	A	13	GLY	2.5
1	T	13	DC	2.5
4	A	320	PHE	2.5
4	A	195	LEU	2.4
4	A	270	LEU	2.4
4	A	282	MET	2.4
4	A	116	ASP	2.4
4	A	83	ARG	2.4
4	A	92	ASP	2.3
4	A	170	ASP	2.3
4	A	235	PHE	2.3
4	A	209	LYS	2.3
4	A	174	ILE	2.3
4	A	103	VAL	2.3
4	A	90	GLN	2.2
4	A	319	ILE	2.2
4	A	271	TYR	2.2
4	A	257	ILE	2.2
4	A	45	VAL	2.1
4	A	39	TYR	2.1
4	A	260	ILE	2.0
2	P	5	DA	2.0
4	A	88	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	DOC	P	10	18/19	0.93	0.14	-	32,47,56,56	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
7	DCT	A	338	27/27	0.93	0.15	-1.17	27,41,48,57	0
6	NA	A	341	1/1	0.99	0.12	-1.60	29,29,29,29	0
6	NA	A	342	1/1	0.96	0.11	-2.68	38,38,38,38	0
5	MG	A	340	1/1	0.87	0.20	-	49,49,49,49	0
5	MG	A	339	1/1	0.90	0.15	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.