



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 1ZQM / pdb_00001zqm
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF MNCL2 (15 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-12
Resolution : 3.20 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

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

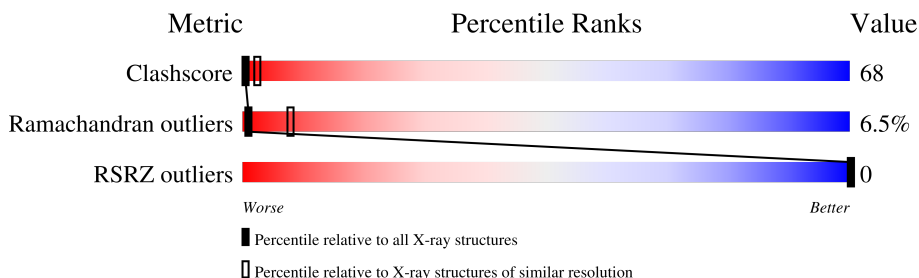
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	8	
2	P	7	
3	A	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3058 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			144	69	24	44	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	18	0	0
			2623	1657	458	499	9			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mn	0	0
			3	3		

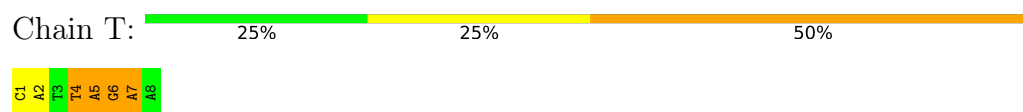
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	15	Total	O	0	0
			15	15		
5	P	21	Total	O	0	0
			21	21		
5	A	107	Total	O	0	0
			107	107		

3 Residue-property plots

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

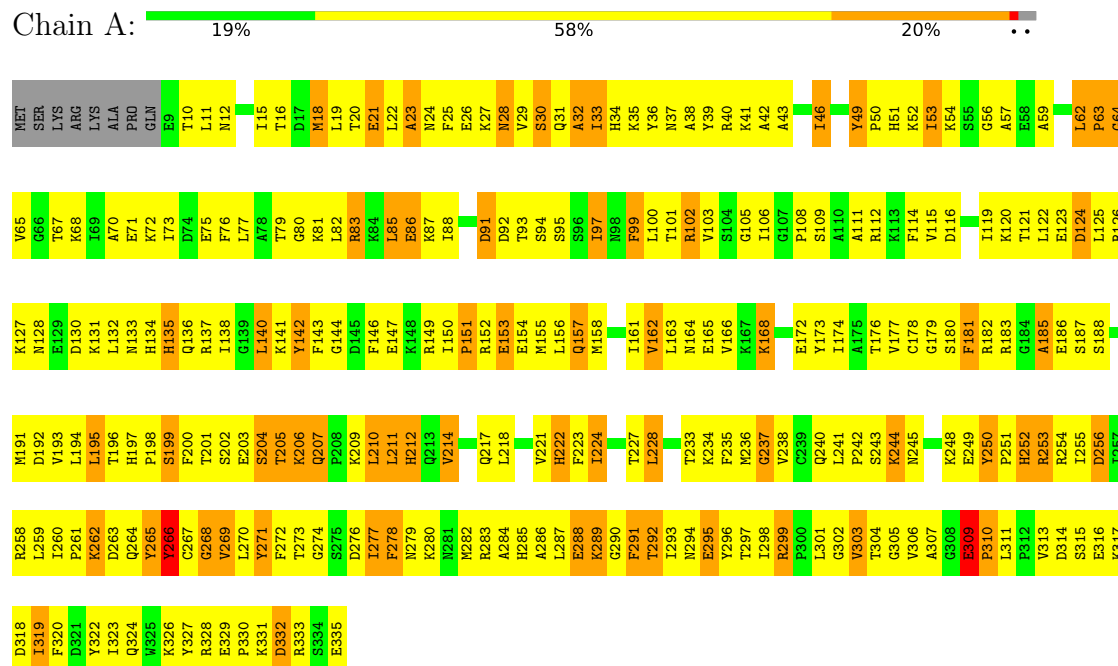
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.88Å 57.63Å 48.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	70.0 (20.00-3.20) 70.2 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.63Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.149 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 401.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.16	0/162	2.79	8/249 (3.2%)
2	P	1.33	1/160 (0.6%)	3.12	10/243 (4.1%)
3	A	1.46	13/2672 (0.5%)	2.25	113/3590 (3.1%)
All	All	1.44	14/2994 (0.5%)	2.35	131/4082 (3.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	DT	OP3-P	6.57	1.61	1.48
3	A	140	LEU	C-N	-6.05	1.26	1.33
3	A	234	LYS	N-CA	-6.01	1.39	1.46
3	A	162	VAL	CA-C	-5.80	1.45	1.52
3	A	222	HIS	CA-C	-5.79	1.45	1.52
3	A	28	ASN	CA-C	-5.68	1.47	1.53
3	A	162	VAL	CA-CB	-5.59	1.47	1.54
3	A	63	PRO	N-CA	-5.57	1.40	1.47
3	A	71	GLU	CA-C	-5.54	1.45	1.52
3	A	65	VAL	N-CA	-5.27	1.39	1.46
3	A	144	GLY	C-O	-5.24	1.16	1.23
3	A	97	ILE	N-CA	-5.23	1.40	1.46
3	A	70	ALA	N-CA	-5.12	1.40	1.46
3	A	269	VAL	N-CA	-5.07	1.40	1.46

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-21.64	86.89	119.35
2	P	1	DT	C2-N1-C1'	21.23	151.19	119.35
1	T	7	DA	C4-N9-C1'	-19.27	98.14	127.05
1	T	7	DA	C8-N9-C1'	19.23	155.89	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	7	DG	C4-N9-C1'	-17.83	100.25	127.00
2	P	7	DG	C8-N9-C1'	17.76	153.65	127.00
1	T	6	DG	C8-N9-C1'	16.75	152.12	127.00
1	T	6	DG	C4-N9-C1'	-16.52	102.22	127.00
2	P	5	DA	C4-N9-C1'	15.34	150.07	127.05
2	P	5	DA	C8-N9-C1'	-15.28	104.13	127.05
3	A	49	TYR	CA-C-N	12.66	133.03	119.87
3	A	49	TYR	C-N-CA	12.66	133.03	119.87
1	T	4	DT	C6-N1-C1'	-12.33	100.85	119.35
3	A	222	HIS	CA-CB-CG	-11.90	101.90	113.80
1	T	4	DT	C2-N1-C1'	11.72	136.93	119.35
3	A	256	ASP	CA-CB-CG	10.59	123.19	112.60
3	A	99	PHE	CA-CB-CG	-10.55	103.25	113.80
1	T	5	DA	C4-N9-C1'	-9.77	112.39	127.05
3	A	18	MET	CA-C-N	9.75	133.34	120.28
3	A	18	MET	C-N-CA	9.75	133.34	120.28
1	T	5	DA	C8-N9-C1'	9.30	141.00	127.05
3	A	49	TYR	O-C-N	9.24	129.34	121.31
3	A	164	ASN	CA-CB-CG	-9.21	103.39	112.60
3	A	28	ASN	CA-CB-CG	-9.02	103.58	112.60
3	A	253	ARG	N-CA-C	8.94	123.81	109.24
3	A	181	PHE	CA-CB-CG	-8.46	105.34	113.80
3	A	21	GLU	N-CA-C	-8.42	101.69	111.03
2	P	6	DT	C6-N1-C1'	-8.07	107.25	119.35
2	P	2	DC	C2-N1-C1'	8.04	131.76	119.70
2	P	6	DT	C2-N1-C1'	7.87	131.15	119.35
3	A	214	VAL	N-CA-C	7.82	118.62	110.72
3	A	266	TYR	CA-CB-CG	-7.73	99.98	113.90
3	A	105	GLY	CA-C-N	7.68	131.97	122.37
3	A	105	GLY	C-N-CA	7.68	131.97	122.37
2	P	2	DC	C6-N1-C1'	-7.66	108.20	119.70
3	A	40	ARG	N-CA-C	7.35	119.08	111.14
3	A	18	MET	O-C-N	7.32	129.61	122.07
3	A	309	GLU	CA-C-N	7.29	128.95	119.84
3	A	309	GLU	C-N-CA	7.29	128.95	119.84
3	A	40	ARG	N-CA-CB	7.24	120.57	110.07
3	A	224	ILE	CA-CB-CG1	-7.18	98.19	110.40
3	A	53	ILE	CB-CA-C	7.16	122.00	111.33
3	A	146	PHE	CA-CB-CG	-7.03	106.77	113.80
3	A	224	ILE	CB-CA-C	7.01	119.60	110.91
3	A	168	LYS	N-CA-CB	6.92	120.25	109.94
3	A	164	ASN	N-CA-C	6.84	118.39	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	211	LEU	CA-C-N	6.83	131.06	120.82
3	A	211	LEU	C-N-CA	6.83	131.06	120.82
3	A	93	THR	CB-CA-C	-6.82	100.13	110.90
3	A	195	LEU	N-CA-C	6.81	120.61	109.24
3	A	228	LEU	N-CA-C	-6.79	103.01	112.45
3	A	292	THR	CB-CA-C	6.75	121.46	109.65
3	A	212	HIS	CA-CB-CG	-6.70	107.10	113.80
3	A	64	GLY	CA-C-N	-6.66	114.69	122.95
3	A	64	GLY	C-N-CA	-6.66	114.69	122.95
3	A	157	GLN	N-CA-CB	6.66	120.02	110.16
3	A	253	ARG	CD-NE-CZ	6.66	133.72	124.40
3	A	116	ASP	CA-CB-CG	-6.61	105.99	112.60
3	A	67	THR	CA-CB-OG1	6.54	119.42	109.60
3	A	233	THR	CA-CB-OG1	-6.44	99.94	109.60
3	A	68	LYS	N-CA-C	6.44	118.83	111.11
3	A	134	HIS	CA-CB-CG	6.32	120.12	113.80
3	A	299	ARG	CB-CA-C	6.27	117.35	108.76
3	A	237	GLY	CA-C-N	6.14	131.55	122.71
3	A	237	GLY	C-N-CA	6.14	131.55	122.71
3	A	250	TYR	N-CA-C	6.05	119.46	110.32
3	A	234	LYS	CA-C-O	6.03	127.04	119.98
3	A	303	VAL	N-CA-C	6.02	119.47	111.17
3	A	95	SER	O-C-N	6.01	128.34	122.09
3	A	288	GLU	N-CA-C	-5.98	104.39	111.03
3	A	157	GLN	CB-CA-C	5.94	120.95	110.85
3	A	151	PRO	N-CA-CB	5.91	108.56	103.36
3	A	291	PHE	N-CA-C	5.84	117.84	109.14
3	A	72	LYS	CB-CA-C	5.81	120.44	110.79
3	A	268	GLY	N-CA-C	-5.80	105.77	112.73
3	A	314	ASP	N-CA-CB	5.73	118.62	111.00
3	A	24	ASN	CA-CB-CG	-5.71	106.89	112.60
3	A	86	GLU	N-CA-CB	5.69	118.26	110.01
3	A	135	HIS	N-CA-C	-5.67	104.79	110.97
3	A	23	ALA	N-CA-C	5.65	117.13	110.97
3	A	192	ASP	CA-C-N	-5.63	115.69	122.90
3	A	192	ASP	C-N-CA	-5.63	115.69	122.90
3	A	21	GLU	O-C-N	5.62	128.10	122.03
3	A	142	TYR	N-CA-C	5.62	118.92	112.57
3	A	332	ASP	N-CA-C	5.59	119.19	112.93
3	A	62	LEU	N-CA-C	5.57	118.22	110.20
3	A	105	GLY	O-C-N	5.55	129.92	122.70
3	A	28	ASN	N-CA-C	5.53	119.61	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	147	GLU	CB-CG-CD	-5.50	103.26	112.60
3	A	124	ASP	CA-CB-CG	-5.49	107.11	112.60
3	A	33	ILE	CA-C-N	5.48	127.88	120.65
3	A	33	ILE	C-N-CA	5.48	127.88	120.65
3	A	277	ILE	N-CA-CB	5.46	118.78	110.58
3	A	253	ARG	CA-C-O	5.44	126.36	120.43
3	A	186	GLU	N-CA-CB	5.44	119.56	110.32
3	A	224	ILE	N-CA-CB	5.44	116.64	110.72
3	A	153	GLU	CA-C-N	5.41	129.83	120.58
3	A	153	GLU	C-N-CA	5.41	129.83	120.58
3	A	181	PHE	O-C-N	5.41	127.86	122.08
3	A	222	HIS	N-CA-CB	5.41	119.62	110.49
3	A	318	ASP	CA-CB-CG	-5.40	107.20	112.60
3	A	21	GLU	CB-CA-C	-5.39	102.59	110.95
3	A	227	THR	N-CA-CB	5.39	119.05	110.65
3	A	210	LEU	N-CA-C	-5.36	104.68	111.11
3	A	85	LEU	N-CA-C	-5.36	105.35	111.14
3	A	143	PHE	CB-CA-C	5.34	119.42	110.92
3	A	252	HIS	CA-CB-CG	-5.34	108.46	113.80
3	A	46	ILE	CB-CA-C	5.28	120.33	112.16
3	A	193	VAL	N-CA-C	5.26	115.66	107.99
3	A	91	ASP	N-CA-CB	5.25	119.37	110.49
3	A	30	SER	CA-C-N	-5.20	114.43	122.49
3	A	30	SER	C-N-CA	-5.20	114.43	122.49
3	A	186	GLU	CB-CG-CD	5.20	121.44	112.60
3	A	83	ARG	N-CA-CB	5.17	117.57	110.07
3	A	102	ARG	CD-NE-CZ	-5.16	117.18	124.40
3	A	227	THR	CB-CA-C	5.16	118.72	110.16
3	A	57	ALA	N-CA-CB	-5.15	101.79	110.49
3	A	91	ASP	N-CA-C	5.14	121.76	110.80
3	A	176	THR	CA-C-N	-5.14	116.58	122.95
3	A	176	THR	C-N-CA	-5.14	116.58	122.95
3	A	253	ARG	NE-CZ-NH1	5.13	126.63	121.50
3	A	52	LYS	CA-C-N	-5.13	114.01	120.98
3	A	52	LYS	C-N-CA	-5.13	114.01	120.98
3	A	319	ILE	CB-CA-C	-5.12	105.33	112.04
3	A	130	ASP	CA-CB-CG	5.07	117.67	112.60
3	A	278	PHE	CA-CB-CG	-5.07	108.73	113.80
3	A	64	GLY	N-CA-C	-5.06	108.63	115.36
3	A	309	GLU	O-C-N	5.04	127.12	121.32
3	A	267	CYS	O-C-N	5.04	127.53	122.09
3	A	271	TYR	CA-CB-CG	-5.03	104.85	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	161	ILE	CB-CA-C	-5.01	105.48	112.04

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	145	0	80	6	0
2	P	144	0	81	18	0
3	A	2623	0	2641	364	0
4	A	3	0	0	0	0
5	A	107	0	0	18	0
5	P	21	0	0	2	0
5	T	15	0	0	2	0
All	All	3058	0	2802	385	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 68.

All (385) 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:31:GLN:NE2	3:A:112:ARG:HH12	1.48	1.11
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.35	1.09
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.30	1.08
2:P:6:DT:H2''	2:P:7:DG:H5''	1.10	1.06
3:A:245:ASN:HD22	3:A:245:ASN:N	1.54	1.04
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.45	0.99
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.98	0.96
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.45	0.96
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.47	0.96
2:P:5:DA:H2''	2:P:6:DT:H5''	1.49	0.95
3:A:243:SER:HB3	3:A:249:GLU:HA	1.48	0.95
3:A:245:ASN:H	3:A:245:ASN:ND2	1.57	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:6:DG:H2''	1:T:7:DA:C8	2.04	0.92
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.12	0.90
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.54	0.90
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.03	0.89
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.36	0.88
3:A:152:ARG:HA	3:A:155:MET:HB2	1.56	0.87
2:P:6:DT:C2'	2:P:7:DG:H5''	2.02	0.87
2:P:5:DA:H2''	2:P:6:DT:C5'	2.05	0.86
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.57	0.86
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.10	0.85
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.08	0.84
3:A:218:LEU:HD23	3:A:224:ILE:HD11	1.59	0.83
3:A:201:THR:HA	3:A:261:PRO:HB3	1.60	0.83
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.44	0.83
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.60	0.82
3:A:201:THR:HA	3:A:261:PRO:CB	2.08	0.82
3:A:128:ASN:N	3:A:128:ASN:HD22	1.75	0.82
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.63	0.81
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.15	0.80
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.17	0.80
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.64	0.80
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.17	0.79
3:A:330:PRO:HA	3:A:333:ARG:CG	2.12	0.79
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.12	0.79
3:A:18:MET:O	3:A:21:GLU:HB2	1.84	0.78
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.77	0.78
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.66	0.78
3:A:217:GLN:HE21	3:A:217:GLN:HA	1.46	0.77
3:A:243:SER:CB	3:A:249:GLU:HA	2.16	0.75
3:A:165:GLU:CB	3:A:217:GLN:HG3	2.15	0.75
3:A:138:ILE:HD12	3:A:228:LEU:CD1	2.17	0.74
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.21	0.74
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.68	0.74
3:A:92:ASP:HB3	5:A:629:HOH:O	1.87	0.74
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.69	0.73
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.03	0.73
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.70	0.72
3:A:162:VAL:O	3:A:166:VAL:HG23	1.90	0.72
2:P:4:DA:H5'	5:P:563:HOH:O	1.89	0.71
3:A:26:GLU:HA	3:A:30:SER:OG	1.89	0.71
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.06	0.70
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.88	0.70
3:A:270:LEU:HD22	3:A:319:ILE:HD13	1.73	0.70
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.72	0.70
3:A:289:LYS:HD3	3:A:289:LYS:N	2.05	0.70
3:A:121:THR:HG23	3:A:124:ASP:CG	2.15	0.70
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.72	0.69
3:A:138:ILE:HD12	3:A:228:LEU:HD12	1.74	0.69
3:A:294:ASN:O	3:A:296:TYR:N	2.26	0.69
3:A:165:GLU:HA	3:A:168:LYS:CG	2.22	0.69
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.69
3:A:76:PHE:HD1	3:A:77:LEU:HD12	1.58	0.69
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.75	0.68
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.08	0.68
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.74	0.68
3:A:103:VAL:HB	3:A:106:ILE:CD1	2.18	0.67
3:A:128:ASN:N	3:A:128:ASN:ND2	2.39	0.67
3:A:331:LYS:HG2	3:A:332:ASP:N	2.05	0.67
3:A:82:LEU:HD23	3:A:85:LEU:CB	2.22	0.67
3:A:22:LEU:HD22	3:A:85:LEU:HD13	1.77	0.67
3:A:214:VAL:O	3:A:218:LEU:HD13	1.95	0.67
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.40	0.67
3:A:35:LYS:O	3:A:38:ALA:HB3	1.95	0.66
3:A:285:HIS:NE2	5:A:574:HOH:O	2.28	0.66
3:A:140:LEU:HD12	3:A:140:LEU:O	1.96	0.66
3:A:295:GLU:N	3:A:295:GLU:OE1	2.28	0.66
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.24	0.66
3:A:306:VAL:HG22	5:A:632:HOH:O	1.95	0.66
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.77	0.66
3:A:83:ARG:O	3:A:86:GLU:N	2.29	0.66
3:A:211:LEU:HB3	3:A:212:HIS:HD2	1.61	0.66
1:T:1:DC:H2"	1:T:2:DA:OP2	1.93	0.65
3:A:18:MET:CE	3:A:76:PHE:HB2	2.26	0.65
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.65
3:A:128:ASN:HB3	3:A:131:LYS:HG3	1.79	0.65
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.11	0.65
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.32	0.65
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.79	0.64
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.27	0.64
3:A:243:SER:OG	3:A:249:GLU:HG3	1.98	0.64
3:A:12:ASN:HD21	3:A:53:ILE:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:79:THR:O	3:A:81:LYS:N	2.30	0.64
3:A:15:ILE:CG2	3:A:46:ILE:HD11	2.28	0.63
3:A:56:GLY:O	3:A:59:ALA:N	2.32	0.63
3:A:141:LYS:HE2	3:A:142:TYR:OH	1.98	0.63
3:A:41:LYS:HD3	3:A:42:ALA:H	1.64	0.62
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.81	0.62
3:A:99:PHE:O	3:A:102:ARG:HG3	1.99	0.62
3:A:245:ASN:HD22	3:A:245:ASN:H	0.74	0.62
3:A:12:ASN:HA	5:A:549:HOH:O	2.00	0.62
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.34	0.62
3:A:111:ALA:O	3:A:115:VAL:HG23	1.99	0.62
3:A:150:ILE:N	3:A:188:SER:O	2.31	0.62
3:A:82:LEU:CD2	3:A:85:LEU:HB2	2.26	0.62
3:A:200:PHE:O	3:A:262:LYS:N	2.32	0.62
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.34	0.61
3:A:248:LYS:O	3:A:248:LYS:HG2	2.00	0.61
3:A:253:ARG:NH1	5:A:503:HOH:O	2.34	0.60
3:A:211:LEU:HB3	3:A:212:HIS:CD2	2.37	0.60
3:A:133:ASN:O	3:A:137:ARG:HG3	2.01	0.60
3:A:266:TYR:HA	3:A:269:VAL:HB	1.84	0.60
3:A:127:LYS:HE3	3:A:127:LYS:HA	1.83	0.60
2:P:6:DT:H5'	5:P:561:HOH:O	2.02	0.60
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.82	0.60
3:A:205:THR:HA	5:A:609:HOH:O	2.02	0.60
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.83	0.59
3:A:295:GLU:HA	5:A:580:HOH:O	2.01	0.59
3:A:316:GLU:O	3:A:320:PHE:HD1	1.85	0.59
3:A:22:LEU:HD22	3:A:85:LEU:CD1	2.31	0.59
3:A:120:LYS:N	3:A:124:ASP:OD2	2.29	0.59
3:A:211:LEU:HD12	3:A:211:LEU:O	2.02	0.59
3:A:201:THR:CA	3:A:261:PRO:HB3	2.32	0.59
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.83	0.59
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.85	0.58
3:A:323:ILE:O	3:A:324:GLN:HG2	2.03	0.58
3:A:152:ARG:CA	3:A:155:MET:HB2	2.31	0.58
3:A:286:ALA:O	3:A:291:PHE:N	2.35	0.58
1:T:4:DT:H71	5:T:645:HOH:O	2.02	0.58
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.39	0.58
3:A:181:PHE:HD1	5:A:530:HOH:O	1.86	0.58
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.34	0.58
3:A:75:GLU:O	3:A:79:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:LEU:HD22	3:A:85:LEU:HD22	1.86	0.57
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.38	0.57
3:A:309:GLU:N	3:A:309:GLU:OE1	2.37	0.57
2:P:5:DA:C2'	2:P:6:DT:H5''	2.27	0.57
3:A:73:ILE:O	3:A:77:LEU:HD13	2.04	0.57
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.05	0.57
3:A:34:HIS:O	3:A:38:ALA:N	2.34	0.57
3:A:201:THR:HA	3:A:261:PRO:CA	2.34	0.57
3:A:31:GLN:N	5:A:623:HOH:O	2.29	0.57
3:A:211:LEU:HD12	3:A:211:LEU:C	2.29	0.57
3:A:255:ILE:HG12	3:A:256:ASP:N	2.19	0.57
3:A:180:SER:CA	3:A:183:ARG:HH21	2.17	0.57
3:A:149:ARG:NH2	3:A:188:SER:HA	2.19	0.57
3:A:288:GLU:C	3:A:290:GLY:H	2.14	0.56
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.35	0.56
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.87	0.56
3:A:140:LEU:HD12	3:A:140:LEU:C	2.31	0.56
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.41	0.56
3:A:33:ILE:O	3:A:36:TYR:HD2	1.89	0.56
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.15	0.56
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.87	0.55
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.21	0.55
3:A:196:THR:OG1	3:A:197:HIS:N	2.40	0.55
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.87	0.55
3:A:53:ILE:O	3:A:54:LYS:HD2	2.06	0.55
3:A:15:ILE:HG22	3:A:19:LEU:HD22	1.88	0.55
3:A:38:ALA:O	3:A:41:LYS:HD3	2.07	0.55
3:A:123:GLU:O	3:A:127:LYS:HG2	2.07	0.55
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.88	0.54
3:A:108:PRO:O	3:A:112:ARG:HG3	2.08	0.54
3:A:152:ARG:NH2	3:A:181:PHE:O	2.34	0.54
3:A:278:PHE:HB2	3:A:333:ARG:O	2.07	0.54
1:T:6:DG:O6	2:P:2:DC:N3	2.41	0.54
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.37	0.54
3:A:83:ARG:O	3:A:87:LYS:N	2.35	0.54
3:A:79:THR:C	3:A:81:LYS:H	2.16	0.54
3:A:122:LEU:HD22	3:A:126:ARG:NH1	2.22	0.54
3:A:245:ASN:N	3:A:245:ASN:ND2	2.30	0.54
3:A:271:TYR:HB2	5:A:580:HOH:O	2.07	0.54
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.75	0.54
3:A:328:ARG:O	3:A:333:ARG:NE	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:264:GLN:NE2	3:A:297:THR:HG23	2.23	0.53
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.73	0.53
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.89	0.53
3:A:327:TYR:HD1	3:A:328:ARG:N	2.07	0.53
3:A:180:SER:HA	3:A:183:ARG:HH21	1.73	0.53
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.39	0.53
3:A:276:ASP:O	3:A:280:LYS:HG3	2.09	0.53
3:A:328:ARG:HB2	3:A:333:ARG:CD	2.39	0.53
2:P:6:DT:H2'	2:P:7:DG:C8	2.44	0.53
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.44	0.53
3:A:323:ILE:C	3:A:324:GLN:HG2	2.33	0.53
3:A:124:ASP:O	3:A:128:ASN:ND2	2.41	0.53
3:A:101:THR:HA	3:A:106:ILE:HG22	1.91	0.52
3:A:103:VAL:O	3:A:106:ILE:HB	2.09	0.52
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.55	0.52
3:A:82:LEU:CD2	3:A:85:LEU:HD22	2.39	0.52
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.90	0.52
3:A:240:GLN:NE2	3:A:250:TYR:O	2.41	0.52
2:P:5:DA:H2''	2:P:6:DT:H5'	1.89	0.52
3:A:15:ILE:O	3:A:19:LEU:HB2	2.09	0.52
3:A:266:TYR:O	3:A:270:LEU:HB2	2.09	0.52
3:A:11:LEU:HD23	3:A:11:LEU:H	1.75	0.52
3:A:183:ARG:NH2	5:A:615:HOH:O	2.43	0.52
3:A:274:GLY:O	3:A:278:PHE:HD2	1.93	0.52
3:A:288:GLU:O	3:A:290:GLY:N	2.43	0.52
3:A:212:HIS:CD2	3:A:212:HIS:N	2.75	0.52
3:A:259:LEU:O	3:A:260:ILE:HD13	2.10	0.52
3:A:149:ARG:HH21	3:A:187:SER:C	2.18	0.51
3:A:195:LEU:O	3:A:260:ILE:N	2.44	0.51
3:A:218:LEU:HD23	3:A:224:ILE:CD1	2.37	0.51
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.26	0.51
3:A:158:MET:O	3:A:162:VAL:HG23	2.11	0.51
3:A:108:PRO:O	3:A:111:ALA:HB3	2.10	0.51
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.11	0.51
3:A:217:GLN:O	3:A:221:VAL:HG13	2.11	0.51
3:A:284:ALA:O	3:A:287:LEU:HB2	2.11	0.51
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.41	0.51
3:A:155:MET:HE2	3:A:188:SER:HB2	1.92	0.51
3:A:254:ARG:HB3	3:A:254:ARG:NH1	2.26	0.51
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.93	0.50
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.45	0.50
3:A:12:ASN:OD1	3:A:51:HIS:O	2.29	0.50
3:A:265:TYR:CE2	3:A:269:VAL:HG21	2.47	0.50
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.79	0.50
3:A:100:LEU:O	3:A:106:ILE:HG21	2.12	0.50
3:A:270:LEU:HD22	3:A:319:ILE:CD1	2.40	0.50
3:A:240:GLN:HA	5:A:568:HOH:O	2.11	0.50
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.42	0.50
2:P:6:DT:H5'	2:P:6:DT:H6	1.77	0.50
3:A:179:GLY:O	3:A:182:ARG:HB3	2.11	0.50
3:A:41:LYS:HD3	3:A:42:ALA:N	2.27	0.50
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.46	0.50
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.40	0.50
3:A:127:LYS:HD2	3:A:127:LYS:N	2.27	0.49
3:A:133:ASN:O	3:A:137:ARG:N	2.45	0.49
3:A:254:ARG:NH1	3:A:255:ILE:N	2.60	0.49
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.95	0.49
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.76	0.49
3:A:30:SER:HB3	5:A:555:HOH:O	2.13	0.49
3:A:204:SER:O	3:A:206:LYS:N	2.46	0.49
3:A:207:GLN:O	3:A:210:LEU:HB2	2.13	0.49
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.41	0.49
3:A:163:LEU:N	3:A:163:LEU:HD23	2.23	0.49
3:A:302:GLY:N	3:A:307:ALA:HB2	2.26	0.49
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.60	0.48
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.28	0.48
3:A:121:THR:O	3:A:124:ASP:HB2	2.12	0.48
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.79	0.48
3:A:154:GLU:O	3:A:158:MET:HE2	2.13	0.48
3:A:203:GLU:O	3:A:205:THR:N	2.46	0.48
3:A:319:ILE:O	3:A:322:TYR:HB2	2.13	0.48
2:P:6:DT:C2'	2:P:7:DG:C8	2.97	0.48
3:A:19:LEU:O	3:A:22:LEU:HB2	2.14	0.48
3:A:25:PHE:CD2	3:A:88:ILE:HD11	2.49	0.48
3:A:73:ILE:CG2	3:A:77:LEU:HD22	2.42	0.48
3:A:77:LEU:N	3:A:77:LEU:CD1	2.77	0.48
3:A:56:GLY:O	3:A:59:ALA:HB3	2.13	0.47
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.48	0.47
2:P:1:DT:C2'	2:P:2:DC:C6	2.97	0.47
3:A:158:MET:HB2	3:A:158:MET:HE3	1.49	0.47
3:A:180:SER:HB2	3:A:185:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:212:HIS:CD2	3:A:212:HIS:H	2.31	0.47
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.96	0.47
3:A:41:LYS:CE	3:A:64:GLY:HA3	2.38	0.47
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.42	0.47
3:A:29:VAL:HG21	3:A:94:SER:CB	2.45	0.47
3:A:154:GLU:C	3:A:158:MET:HE2	2.40	0.47
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.80	0.47
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.78	0.46
3:A:237:GLY:O	3:A:254:ARG:NH1	2.48	0.46
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.41	0.46
3:A:158:MET:HG2	3:A:223:PHE:CZ	2.51	0.46
3:A:173:TYR:O	3:A:174:ILE:HG12	2.15	0.46
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.42	0.46
3:A:133:ASN:H	3:A:136:GLN:HE21	1.64	0.46
3:A:158:MET:HG3	3:A:241:LEU:HD21	1.97	0.46
3:A:254:ARG:CA	3:A:254:ARG:HH11	2.28	0.46
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.98	0.46
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.25	0.46
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.81	0.46
3:A:198:PRO:C	3:A:200:PHE:H	2.24	0.46
3:A:265:TYR:HD2	3:A:266:TYR:CE1	2.33	0.46
3:A:326:LYS:HG3	3:A:326:LYS:O	2.15	0.46
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.26	0.45
3:A:133:ASN:ND2	3:A:135:HIS:H	2.15	0.45
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.97	0.45
3:A:18:MET:HG2	3:A:19:LEU:N	2.27	0.45
3:A:249:GLU:HG3	3:A:250:TYR:H	1.81	0.45
3:A:282:MET:HE3	5:A:550:HOH:O	2.15	0.45
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.99	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.79	0.45
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.49	0.45
3:A:200:PHE:CE2	3:A:261:PRO:N	2.85	0.45
3:A:15:ILE:HG21	3:A:46:ILE:CD1	2.46	0.45
3:A:127:LYS:HB2	3:A:128:ASN:HD22	1.82	0.45
3:A:36:TYR:CD2	3:A:37:ASN:N	2.85	0.45
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.99	0.45
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.29	0.45
3:A:320:PHE:CE2	3:A:328:ARG:HG3	2.51	0.45
1:T:4:DT:H2"	1:T:5:DA:C8	2.52	0.45
5:T:545:HOH:O	3:A:133:ASN:HB2	2.17	0.45
3:A:302:GLY:N	3:A:307:ALA:CB	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:1:DT:H2''	2:P:2:DC:O4'	2.17	0.45
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.99	0.45
3:A:156:LEU:HA	3:A:156:LEU:HD23	1.54	0.44
3:A:243:SER:HB3	3:A:249:GLU:CA	2.34	0.44
3:A:133:ASN:C	3:A:137:ARG:HG3	2.41	0.44
3:A:249:GLU:CG	3:A:250:TYR:N	2.80	0.44
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.98	0.44
3:A:15:ILE:HG22	3:A:15:ILE:O	2.16	0.44
3:A:258:ARG:NH2	3:A:272:PHE:CZ	2.86	0.44
3:A:127:LYS:C	3:A:128:ASN:HD22	2.25	0.44
3:A:79:THR:HG23	3:A:79:THR:H	1.44	0.44
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.41	0.44
3:A:200:PHE:C	3:A:201:THR:HG22	2.42	0.44
3:A:250:TYR:HA	3:A:251:PRO:HD3	1.88	0.44
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.45	0.44
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.96	0.44
3:A:97:ILE:HG23	3:A:111:ALA:HB1	2.00	0.44
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.70	0.44
3:A:149:ARG:NH2	3:A:188:SER:CA	2.80	0.44
3:A:303:VAL:C	3:A:305:GLY:H	2.26	0.44
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.42	0.43
3:A:112:ARG:O	3:A:115:VAL:HB	2.17	0.43
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.77	0.43
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.43	0.43
3:A:31:GLN:O	3:A:33:ILE:N	2.49	0.43
3:A:102:ARG:HH11	3:A:102:ARG:HD3	1.59	0.43
3:A:152:ARG:O	3:A:155:MET:HB2	2.18	0.43
3:A:315:SER:C	3:A:317:LYS:N	2.76	0.43
3:A:294:ASN:C	3:A:296:TYR:H	2.24	0.43
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.71	0.43
3:A:265:TYR:O	3:A:268:GLY:N	2.51	0.43
3:A:201:THR:C	3:A:261:PRO:HB3	2.44	0.43
3:A:277:ILE:HG13	3:A:335:GLU:HB2	2.00	0.43
3:A:22:LEU:O	3:A:25:PHE:HB3	2.18	0.43
3:A:262:LYS:O	3:A:262:LYS:HG3	2.18	0.43
3:A:243:SER:O	3:A:244:LYS:O	2.37	0.42
3:A:271:TYR:CD2	3:A:271:TYR:C	2.95	0.42
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.40	0.42
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.60	0.42
3:A:16:THR:O	3:A:20:THR:HG23	2.19	0.42
3:A:293:ILE:HA	5:A:581:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.34	0.42
2:P:1:DT:H2'	2:P:2:DC:C6	2.53	0.42
3:A:54:LYS:HD2	3:A:54:LYS:HA	1.59	0.42
3:A:165:GLU:CA	3:A:168:LYS:HG2	2.33	0.42
3:A:271:TYR:CD2	3:A:272:PHE:N	2.87	0.42
3:A:180:SER:HA	3:A:183:ARG:NH2	2.33	0.42
3:A:286:ALA:HB1	3:A:291:PHE:HB2	2.02	0.42
3:A:266:TYR:HB2	3:A:313:VAL:HG11	2.01	0.42
3:A:331:LYS:CG	3:A:332:ASP:N	2.80	0.42
3:A:25:PHE:CE2	3:A:88:ILE:HD11	2.55	0.41
3:A:29:VAL:HG21	3:A:94:SER:HA	2.01	0.41
3:A:81:LYS:HZ2	3:A:86:GLU:CB	2.33	0.41
3:A:261:PRO:O	3:A:263:ASP:N	2.52	0.41
1:T:7:DA:H61	2:P:1:DT:H3	1.68	0.41
2:P:1:DT:H2''	2:P:2:DC:C6	2.55	0.41
3:A:22:LEU:HD21	3:A:82:LEU:HD21	2.00	0.41
3:A:195:LEU:HG	3:A:196:THR:N	2.35	0.41
3:A:12:ASN:ND2	5:A:624:HOH:O	2.53	0.41
3:A:270:LEU:CG	3:A:282:MET:HE1	2.50	0.41
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.50	0.41
3:A:200:PHE:CD2	3:A:260:ILE:C	2.98	0.41
3:A:278:PHE:HZ	3:A:320:PHE:HZ	1.69	0.41
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.41
3:A:29:VAL:CG2	3:A:94:SER:HA	2.50	0.41
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.20	0.41
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.50	0.41
3:A:62:LEU:HD12	3:A:63:PRO:CD	2.43	0.41
3:A:22:LEU:CD2	3:A:85:LEU:HD13	2.48	0.41
3:A:242:PRO:HB2	5:A:577:HOH:O	2.19	0.41
2:P:5:DA:P	3:A:109:SER:HB3	2.61	0.41
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.74	0.41
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.64	0.41
3:A:205:THR:HG23	3:A:205:THR:O	2.22	0.40
3:A:283:ARG:HG3	5:A:550:HOH:O	2.21	0.40
3:A:302:GLY:H	3:A:307:ALA:HB2	1.86	0.40
3:A:22:LEU:HD21	3:A:82:LEU:CD2	2.52	0.40
3:A:127:LYS:C	3:A:128:ASN:ND2	2.79	0.40
3:A:301:LEU:HA	3:A:307:ALA:HB3	2.03	0.40
3:A:326:LYS:O	3:A:328:ARG:HG2	2.20	0.40
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.57	0.40
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:303:VAL:O	3:A:303:VAL:HG22	2.22	0.40
3:A:180:SER:HA	3:A:183:ARG:HE	1.86	0.40
3:A:244:LYS:H	3:A:244:LYS:HG2	1.72	0.40
3:A:329:GLU:O	3:A:333:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	269 (83%)	35 (11%)	21 (6%)	1 8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	202	SER
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	265	TYR
3	A	266	TYR
3	A	289	LYS
3	A	295	GLU
3	A	10	THR
3	A	80	GLY
3	A	91	ASP
3	A	262	LYS
3	A	185	ALA
3	A	199	SER
3	A	206	LYS
3	A	222	HIS

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Mol	Chain	Res	Type
3	A	207	GLN
3	A	304	THR
3	A	310	PRO
3	A	309	GLU

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	8/8 (100%)	-0.69	0 100 100	23, 44, 87, 97	0
2	P	7/7 (100%)	-0.97	0 100 100	18, 21, 46, 74	0
3	A	325/335 (97%)	-0.99	0 100 100	2, 33, 82, 100	0
All	All	340/350 (97%)	-0.98	0 100 100	2, 33, 84, 100	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MN	A	341	1/1	0.94	0.09	26,26,26,26	0
4	MN	A	340	1/1	0.95	0.03	89,89,89,89	0
4	MN	A	342	1/1	0.97	0.08	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.