



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:21 PM EDT

PDB ID : 1BPZ / pdb_00001bpz
Title : HUMAN DNA POLYMERASE BETA COMPLEXED WITH NICKED DNA
Authors : Sawaya, M.R.; Prasad, R.; Wilson, S.H.; Kraut, J.; Pelletier, H.
Deposited on : 1997-04-14
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

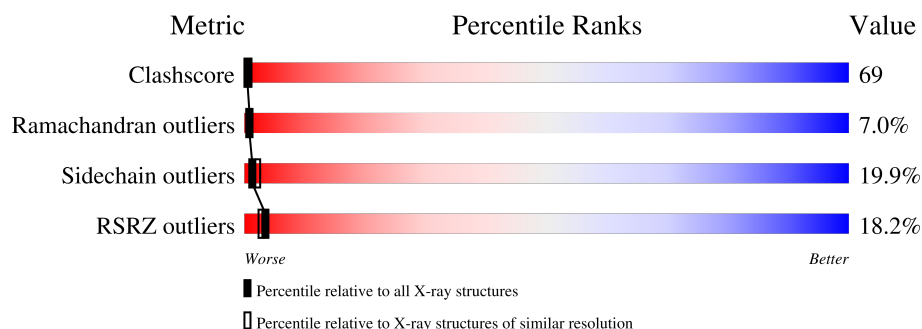
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	16	
2	P	11	
3	D	5	
4	A	335	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3333 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*CP*AP*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
			319	152	61	91	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			226	108	42	66	10			

- 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	331	Total	C	N	O	S	0	0	0
			2653	1676	464	504	9			

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

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

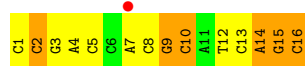
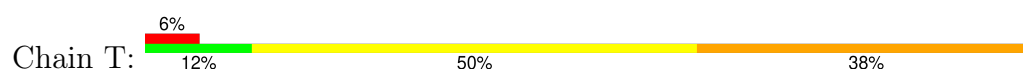
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	6	Total 6	O 6	0	0
6	P	6	Total 6	O 6	0	0
6	D	1	Total 1	O 1	0	0
6	A	14	Total 14	O 14	0	0

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*CP*GP*AP*CP*CP*AP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3')



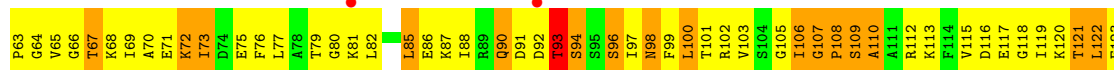
- Molecule 2: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*TP*G)-3')

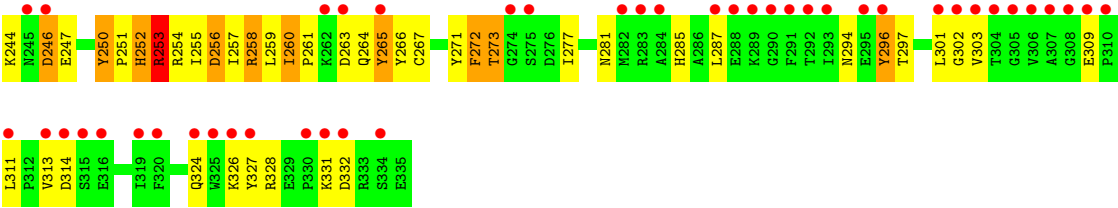


- Molecule 3: DNA (5'-D(*GP*TP*CP*GP*G)-3')



- 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	53.53Å 78.66Å 54.62Å 90.00° 107.54° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.60) 93.7 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.45Å)	Xtriage
Refinement program	TNT 5D	Depositor
R, R_{free}	0.243 , (Not available) 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.796	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 113.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3333	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: NA

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	1.17	0/357	2.01	17/547 (3.1%)
2	P	1.16	0/253	2.11	11/390 (2.8%)
3	D	1.35	0/118	2.10	6/179 (3.4%)
4	A	1.42	10/2703 (0.4%)	2.08	105/3632 (2.9%)
All	All	1.37	10/3431 (0.3%)	2.08	139/4748 (2.9%)

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
4	A	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8	GLN	C-N	8.45	1.45	1.33
4	A	29	VAL	CA-CB	-8.32	1.45	1.54
4	A	148	LYS	CA-C	-6.75	1.44	1.52
4	A	58	GLU	CD-OE1	6.04	1.36	1.25
4	A	213	GLN	N-CA	-5.82	1.39	1.46
4	A	121	THR	CA-C	-5.79	1.45	1.53
4	A	51	HIS	CA-C	-5.53	1.46	1.52
4	A	52	LYS	N-CA	-5.31	1.39	1.46
4	A	195	LEU	N-CA	-5.27	1.39	1.46
4	A	191	MET	CA-C	-5.24	1.46	1.52

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8	GLN	N-CA-C	11.33	134.93	110.80
4	A	29	VAL	N-CA-CB	-11.12	99.97	112.21
2	P	6	DT	N1-C1'-C2'	10.52	129.28	113.50
3	D	2	DT	P-O5'-C5'	-10.22	104.67	120.00
4	A	212	HIS	CA-CB-CG	-9.52	104.28	113.80
4	A	214	VAL	N-CA-C	9.44	120.26	110.72
4	A	154	GLU	N-CA-C	-9.25	101.20	111.28
4	A	140	LEU	N-CA-C	-9.14	101.21	111.82
4	A	101	THR	CA-CB-OG1	-9.12	95.92	109.60
1	T	13	DC	N1-C1'-C2'	8.76	126.64	113.50
4	A	109	SER	N-CA-CB	8.46	122.25	109.98
1	T	2	DC	P-O3'-C3'	8.41	132.82	120.20
4	A	27	LYS	CA-C-N	8.30	131.75	120.54
4	A	27	LYS	C-N-CA	8.30	131.75	120.54
4	A	40	ARG	N-CA-CB	8.27	122.00	110.01
4	A	246	ASP	CA-CB-CG	8.21	120.81	112.60
2	P	10	DT	P-O5'-C5'	-8.16	107.77	120.00
2	P	10	DT	C4-C5-C7	-8.07	110.30	122.40
4	A	164	ASN	N-CA-CB	8.04	121.72	110.07
4	A	7	PRO	CA-C-N	7.72	136.29	121.54
4	A	7	PRO	C-N-CA	7.72	136.29	121.54
4	A	6	ALA	CA-C-N	7.38	129.07	119.84
4	A	6	ALA	C-N-CA	7.38	129.07	119.84
4	A	149	ARG	CA-C-N	-7.32	116.30	123.04
4	A	149	ARG	C-N-CA	-7.32	116.30	123.04
1	T	5	DC	N1-C1'-C2'	7.24	124.36	113.50
4	A	164	ASN	CB-CA-C	7.21	122.29	110.90
2	P	5	DA	N9-C1'-C2'	7.20	124.29	113.50
4	A	132	LEU	CB-CA-C	-7.18	97.08	109.65
4	A	253	ARG	N-CA-C	6.93	120.24	109.07
4	A	140	LEU	CA-C-O	6.90	127.91	119.97
1	T	2	DC	O3'-P-O5'	6.85	114.27	104.00
4	A	260	ILE	N-CA-CB	-6.84	101.63	111.21
4	A	108	PRO	CA-C-N	-6.83	111.34	120.63
4	A	108	PRO	C-N-CA	-6.83	111.34	120.63
2	P	5	DA	P-O5'-C5'	-6.80	109.80	120.00
4	A	145	ASP	O-C-N	6.73	129.26	122.12
4	A	146	PHE	N-CA-C	6.70	118.58	111.28
2	P	7	DG	C4'-C3'-O3'	-6.68	99.98	110.00
4	A	252	HIS	CA-CB-CG	6.54	120.34	113.80
4	A	86	GLU	N-CA-CB	6.54	119.84	110.16
1	T	2	DC	C4'-C3'-O3'	6.50	119.75	110.00
1	T	12	DT	C4'-C3'-O3'	-6.47	100.30	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	157	GLN	N-CA-C	-6.44	103.38	111.11
4	A	72	LYS	CB-CA-C	6.43	120.86	110.96
4	A	51	HIS	CA-CB-CG	-6.41	107.39	113.80
4	A	148	LYS	CB-CA-C	-6.38	97.90	109.38
4	A	160	ASP	N-CA-C	6.38	117.92	110.97
4	A	272	PHE	CA-CB-CG	-6.36	107.44	113.80
4	A	223	PHE	CA-CB-CG	-6.32	107.48	113.80
2	P	5	DA	C4'-C3'-O3'	-6.32	100.53	110.00
4	A	134	HIS	O-C-N	6.29	128.57	122.03
4	A	40	ARG	CA-C-O	-6.26	114.25	120.82
3	D	3	DC	C4'-C3'-O3'	-6.23	100.65	110.00
4	A	190	ASP	CA-CB-CG	-6.22	106.38	112.60
4	A	86	GLU	CB-CA-C	6.12	121.26	110.85
4	A	222	HIS	CA-CB-CG	-6.12	107.68	113.80
2	P	8	DC	O3'-P-O5'	-6.07	94.90	104.00
4	A	41	LYS	N-CA-CB	6.05	118.96	109.94
4	A	70	ALA	N-CA-C	-6.05	104.60	111.07
1	T	16	DC	P-O5'-C5'	-6.02	110.97	120.00
1	T	14	DA	C4'-C3'-O3'	-6.02	100.97	110.00
4	A	21	GLU	N-CA-C	-6.01	104.64	111.14
4	A	267	CYS	N-CA-C	-5.98	104.67	111.07
1	T	4	DA	P-O5'-C5'	5.94	128.91	120.00
4	A	151	PRO	CB-CA-C	-5.90	106.91	111.87
4	A	145	ASP	N-CA-CB	5.90	118.80	110.12
1	T	14	DA	N9-C1'-C2'	5.89	122.33	113.50
4	A	170	ASP	CA-CB-CG	5.88	118.48	112.60
4	A	256	ASP	CA-CB-CG	-5.88	106.72	112.60
4	A	61	LYS	CB-CG-CD	5.88	124.81	111.30
4	A	193	VAL	N-CA-C	5.87	116.45	107.77
4	A	106	ILE	N-CA-CB	5.86	120.24	110.86
4	A	53	ILE	CA-CB-CG1	-5.85	100.45	110.40
4	A	195	LEU	N-CA-CB	-5.83	102.53	111.56
4	A	230	LYS	CB-CA-C	5.81	120.79	110.16
4	A	160	ASP	CA-CB-CG	-5.76	106.84	112.60
4	A	215	VAL	N-CA-C	-5.75	104.76	110.62
4	A	151	PRO	O-C-N	5.72	126.79	122.73
4	A	62	LEU	CA-C-O	5.71	125.74	120.60
1	T	14	DA	O4'-C1'-N9	-5.69	99.86	108.40
3	D	3	DC	P-O5'-C5'	5.68	128.53	120.00
4	A	127	LYS	N-CA-C	5.68	118.99	112.97
4	A	243	SER	N-CA-CB	5.67	118.37	109.69
4	A	233	THR	CA-C-N	-5.66	112.64	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	233	THR	C-N-CA	-5.66	112.64	122.37
4	A	51	HIS	CA-C-N	-5.64	115.26	122.77
4	A	51	HIS	C-N-CA	-5.64	115.26	122.77
4	A	227	THR	CA-CB-OG1	5.63	118.05	109.60
4	A	110	ALA	N-CA-CB	-5.61	101.30	109.82
4	A	223	PHE	N-CA-C	5.60	117.47	111.36
4	A	9	GLU	N-CA-CB	5.60	119.95	110.49
4	A	107	GLY	N-CA-C	-5.60	100.92	112.34
4	A	258	ARG	CD-NE-CZ	5.58	132.21	124.40
1	T	15	DG	C5'-C4'-C3'	5.55	123.22	114.90
2	P	7	DG	O3'-P-O5'	-5.55	95.68	104.00
4	A	35	LYS	CA-C-O	5.53	126.35	120.10
4	A	56	GLY	N-CA-C	-5.52	106.10	112.50
4	A	169	VAL	N-CA-CB	5.49	116.61	110.51
2	P	4	DG	C4'-C3'-O3'	-5.46	101.80	110.00
4	A	21	GLU	O-C-N	5.46	127.98	122.09
1	T	10	DC	C5'-C4'-C3'	5.43	123.05	114.90
4	A	314	ASP	CA-CB-CG	-5.43	107.17	112.60
4	A	182	ARG	N-CA-C	-5.42	105.54	111.82
4	A	193	VAL	CB-CA-C	-5.40	103.12	110.42
4	A	156	LEU	O-C-N	5.39	127.70	122.09
3	D	4	DG	C4-N9-C1'	-5.36	118.96	127.00
4	A	92	ASP	O-C-N	5.36	127.81	122.08
3	D	2	DT	N1-C1'-C2'	5.33	121.50	113.50
4	A	159	GLN	CA-C-N	-5.33	113.61	120.65
4	A	159	GLN	C-N-CA	-5.33	113.61	120.65
4	A	107	GLY	O-C-N	5.33	127.10	121.77
1	T	2	DC	C2'-C3'-O3'	5.32	119.48	111.50
4	A	222	HIS	N-CA-C	5.26	122.01	110.80
4	A	313	VAL	N-CA-C	5.23	115.63	107.99
1	T	12	DT	N1-C1'-C2'	5.22	121.34	113.50
4	A	93	THR	O-C-N	5.21	127.66	122.08
4	A	25	PHE	N-CA-C	5.20	117.63	111.33
4	A	85	LEU	CA-C-N	-5.20	112.91	120.29
4	A	85	LEU	C-N-CA	-5.20	112.91	120.29
4	A	285	HIS	CA-CB-CG	-5.18	108.61	113.80
4	A	281	ASN	N-CA-C	5.18	117.01	111.36
4	A	8	GLN	CA-C-N	-5.18	111.65	121.54
4	A	8	GLN	C-N-CA	-5.18	111.65	121.54
4	A	12	ASN	N-CA-C	5.18	120.45	113.72
4	A	62	LEU	CB-CA-C	5.17	116.30	108.86
4	A	22	LEU	CA-C-N	5.16	127.46	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	22	LEU	C-N-CA	5.16	127.46	120.65
4	A	213	GLN	CB-CA-C	5.15	119.04	110.81
1	T	9	DG	C4'-C3'-O3'	-5.14	102.29	110.00
2	P	7	DG	O4'-C1'-N9	-5.14	100.69	108.40
1	T	9	DG	O4'-C1'-N9	-5.09	100.77	108.40
4	A	297	THR	N-CA-C	5.08	114.85	108.45
4	A	272	PHE	N-CA-C	5.06	117.18	111.11
3	D	3	DC	N1-C1'-C2'	5.05	121.08	113.50
4	A	109	SER	CB-CA-C	5.05	118.78	110.95
4	A	134	HIS	CA-C-O	-5.05	115.70	121.00
4	A	134	HIS	CB-CA-C	-5.05	103.19	110.96
4	A	105	GLY	N-CA-C	-5.01	107.63	114.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	164	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	319	0	179	14	0
2	P	226	0	126	18	0
3	D	106	0	57	8	0
4	A	2653	0	2674	408	0
5	A	2	0	0	0	0
6	A	14	0	0	0	0
6	D	1	0	0	0	0
6	P	6	0	0	1	0
6	T	6	0	0	1	0
All	All	3333	0	3036	435	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 69.

All (435) 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:155:MET:HE3	4:A:188:SER:HB2	1.29	1.13
4:A:18:MET:HE1	4:A:82:LEU:HD13	1.23	1.11
4:A:133:ASN:ND2	4:A:136:GLN:H	1.48	1.10
4:A:194:LEU:HD12	4:A:265:TYR:HE1	1.23	1.01
4:A:182:ARG:HE	4:A:273:THR:HG21	1.25	1.00
4:A:152:ARG:HA	4:A:155:MET:HB2	1.41	0.98
4:A:194:LEU:HD11	4:A:260:ILE:HD12	1.42	0.98
4:A:158:MET:HE1	4:A:253:ARG:HD2	1.46	0.97
4:A:133:ASN:HD21	4:A:136:GLN:H	1.13	0.96
4:A:169:VAL:HG11	4:A:214:VAL:HG12	1.48	0.94
4:A:134:HIS:CE1	4:A:138:ILE:HD11	2.03	0.93
4:A:18:MET:HE2	4:A:82:LEU:HD22	1.53	0.91
4:A:251:PRO:HG2	4:A:253:ARG:NH2	1.85	0.91
4:A:251:PRO:HG2	4:A:253:ARG:HH21	1.36	0.89
4:A:194:LEU:HD11	4:A:260:ILE:CD1	2.01	0.89
4:A:27:LYS:HE3	4:A:28:ASN:HD21	1.36	0.89
4:A:36:TYR:CE2	4:A:40:ARG:HD2	2.09	0.87
1:T:2:DC:H2"	1:T:3:DG:C8	2.11	0.86
4:A:138:ILE:HD12	4:A:138:ILE:H	1.41	0.85
4:A:135:HIS:CD2	4:A:228:LEU:HB3	2.12	0.85
4:A:150:ILE:CD1	4:A:253:ARG:HD3	2.05	0.85
4:A:195:LEU:HG	4:A:196:THR:N	1.91	0.85
4:A:207:GLN:HB2	4:A:209:LYS:HD3	1.57	0.84
4:A:133:ASN:ND2	4:A:136:GLN:HG3	1.93	0.83
4:A:122:LEU:HD21	4:A:140:LEU:HD11	1.58	0.83
4:A:194:LEU:HD12	4:A:265:TYR:CE1	2.13	0.82
4:A:158:MET:HE1	4:A:253:ARG:CD	2.08	0.82
4:A:133:ASN:CG	4:A:136:GLN:HG3	2.05	0.82
4:A:150:ILE:HD13	4:A:253:ARG:HD3	1.60	0.81
4:A:207:GLN:HB2	4:A:209:LYS:CD	2.10	0.81
3:D:4:DG:H2"	3:D:5:DG:C8	2.15	0.81
4:A:161:ILE:HG22	4:A:165:GLU:HG2	1.62	0.81
4:A:174:ILE:C	4:A:195:LEU:HD12	2.05	0.81
4:A:125:LEU:HB3	4:A:140:LEU:HD22	1.63	0.80
4:A:236:MET:HE3	4:A:254:ARG:NH2	1.97	0.80
4:A:33:ILE:HD12	4:A:33:ILE:H	1.46	0.79
4:A:133:ASN:ND2	4:A:136:GLN:N	2.30	0.79
4:A:150:ILE:HD11	4:A:253:ARG:HB3	1.65	0.79
1:T:8:DC:H5"	4:A:296:TYR:OH	1.83	0.78
4:A:37:ASN:HA	4:A:40:ARG:HG3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:18:MET:CE	4:A:82:LEU:HD22	2.14	0.78
4:A:27:LYS:HE3	4:A:28:ASN:ND2	1.98	0.78
4:A:41:LYS:O	4:A:45:VAL:HG13	1.83	0.77
4:A:90:GLN:NE2	4:A:91:ASP:N	2.32	0.77
4:A:208:PRO:HD2	4:A:209:LYS:HD2	1.65	0.77
4:A:122:LEU:CD2	4:A:140:LEU:HD11	2.14	0.77
4:A:169:VAL:HG22	4:A:173:TYR:HE2	1.49	0.76
4:A:146:PHE:CE1	4:A:254:ARG:HG2	2.21	0.76
4:A:155:MET:CE	4:A:188:SER:HB2	2.14	0.76
4:A:67:THR:O	4:A:71:GLU:HG3	1.86	0.75
4:A:241:LEU:HD22	4:A:242:PRO:HD2	1.69	0.75
4:A:230:LYS:NZ	4:A:230:LYS:HB3	2.02	0.75
4:A:200:PHE:CE2	4:A:259:LEU:HG	2.22	0.74
4:A:196:THR:HG23	4:A:265:TYR:CE1	2.23	0.74
4:A:169:VAL:CG2	4:A:213:GLN:HE21	2.00	0.74
4:A:162:VAL:O	4:A:166:VAL:HG13	1.88	0.73
4:A:182:ARG:HE	4:A:273:THR:CG2	1.99	0.73
4:A:38:ALA:O	4:A:41:LYS:HE2	1.88	0.73
4:A:211:LEU:O	4:A:215:VAL:HG23	1.88	0.73
4:A:196:THR:CG2	4:A:260:ILE:HB	2.18	0.73
4:A:218:LEU:HD22	4:A:223:PHE:CD2	2.24	0.73
4:A:241:LEU:CD2	4:A:242:PRO:HD2	2.19	0.73
4:A:18:MET:HE1	4:A:82:LEU:CD1	2.14	0.72
4:A:207:GLN:HB2	4:A:209:LYS:NZ	2.04	0.72
4:A:22:LEU:CD1	4:A:85:LEU:HD13	2.20	0.72
4:A:174:ILE:O	4:A:195:LEU:HD12	1.90	0.72
4:A:197:HIS:CG	4:A:198:PRO:HD2	2.26	0.71
4:A:26:GLU:OE1	4:A:35:LYS:HD2	1.89	0.71
4:A:138:ILE:HD12	4:A:138:ILE:N	2.02	0.71
4:A:156:LEU:O	4:A:159:GLN:HG2	1.91	0.71
2:P:2:DC:H2''	2:P:3:DT:O5'	1.90	0.71
4:A:169:VAL:HG23	4:A:213:GLN:HE21	1.56	0.71
4:A:201:THR:HG22	4:A:204:SER:HB3	1.74	0.70
2:P:11:DG:H4'	4:A:258:ARG:NH1	2.06	0.70
4:A:18:MET:CE	4:A:82:LEU:HD13	2.13	0.70
4:A:210:LEU:O	4:A:214:VAL:HG22	1.91	0.70
4:A:201:THR:C	4:A:261:PRO:HB3	2.17	0.70
4:A:236:MET:HA	4:A:256:ASP:OD1	1.91	0.69
4:A:19:LEU:HD12	4:A:43:ALA:CA	2.22	0.69
4:A:154:GLU:O	4:A:158:MET:HG3	1.92	0.69
4:A:123:GLU:O	4:A:126:ARG:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:228:LEU:CD2	4:A:237:GLY:HA2	2.23	0.69
4:A:152:ARG:O	4:A:156:LEU:HG	1.93	0.69
4:A:196:THR:HG22	4:A:260:ILE:HB	1.75	0.69
4:A:207:GLN:HB2	4:A:209:LYS:CE	2.22	0.69
4:A:236:MET:HG2	4:A:256:ASP:OD1	1.93	0.68
4:A:32:ALA:HB1	4:A:35:LYS:HB2	1.76	0.68
4:A:93:THR:O	4:A:97:ILE:HG13	1.93	0.68
2:P:11:DG:H4'	4:A:258:ARG:HH12	1.58	0.68
4:A:174:ILE:O	4:A:195:LEU:HA	1.94	0.68
2:P:11:DG:H5''	4:A:192:ASP:OD2	1.92	0.68
4:A:194:LEU:HD22	4:A:258:ARG:HB2	1.75	0.68
4:A:36:TYR:CZ	4:A:40:ARG:HD2	2.28	0.68
4:A:59:ALA:HA	4:A:62:LEU:HD23	1.75	0.68
4:A:194:LEU:HD13	4:A:195:LEU:H	1.58	0.68
4:A:218:LEU:HD22	4:A:223:PHE:HD2	1.58	0.68
1:T:1:DC:HO5'	1:T:1:DC:H6	1.42	0.67
4:A:152:ARG:NH2	4:A:184:GLY:HA2	2.09	0.67
4:A:122:LEU:HD21	4:A:140:LEU:CD1	2.24	0.67
4:A:138:ILE:O	4:A:141:LYS:HB3	1.94	0.67
4:A:15:ILE:CG2	4:A:46:ILE:HD13	2.24	0.67
4:A:226:ASP:N	4:A:226:ASP:OD1	2.28	0.67
4:A:69:ILE:O	4:A:73:ILE:HG13	1.95	0.66
4:A:122:LEU:HA	4:A:125:LEU:HD12	1.78	0.66
4:A:169:VAL:HG22	4:A:173:TYR:CE2	2.31	0.66
4:A:42:ALA:O	4:A:45:VAL:HG22	1.95	0.66
4:A:170:ASP:HB3	4:A:173:TYR:CD2	2.31	0.66
4:A:110:ALA:HA	4:A:113:LYS:HE2	1.79	0.65
4:A:159:GLN:O	4:A:163:LEU:HD23	1.95	0.65
4:A:152:ARG:CA	4:A:155:MET:HB2	2.20	0.65
2:P:7:DG:H2''	2:P:8:DC:O5'	1.95	0.65
4:A:224:ILE:HG23	4:A:238:VAL:O	1.96	0.65
4:A:125:LEU:HB3	4:A:140:LEU:CD2	2.26	0.65
4:A:150:ILE:CG2	4:A:155:MET:HG2	2.26	0.65
4:A:7:PRO:C	4:A:8:GLN:HG2	2.22	0.65
4:A:228:LEU:N	4:A:228:LEU:HD22	2.12	0.65
4:A:28:ASN:O	4:A:108:PRO:HB3	1.97	0.64
4:A:132:LEU:HD13	4:A:136:GLN:CB	2.27	0.64
4:A:158:MET:CE	4:A:253:ARG:HD2	2.24	0.64
4:A:244:LYS:HB3	4:A:247:GLU:HB2	1.79	0.64
4:A:196:THR:HA	4:A:259:LEU:CD1	2.27	0.64
4:A:201:THR:HG22	4:A:204:SER:CB	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:153:GLU:O	4:A:156:LEU:HB2	1.98	0.64
4:A:207:GLN:CB	4:A:209:LYS:HD3	2.28	0.63
4:A:216:GLU:HA	4:A:219:GLN:OE1	1.98	0.63
1:T:2:DC:H2''	1:T:3:DG:H8	1.63	0.63
4:A:173:TYR:OH	4:A:210:LEU:HA	1.97	0.63
4:A:132:LEU:HD13	4:A:136:GLN:HB2	1.79	0.63
4:A:154:GLU:OE1	4:A:253:ARG:NH1	2.32	0.63
4:A:255:ILE:HG12	4:A:256:ASP:N	2.14	0.63
4:A:133:ASN:HD21	4:A:136:GLN:N	1.91	0.62
4:A:87:LYS:O	4:A:90:GLN:NE2	2.30	0.62
1:T:14:DA:H2''	1:T:15:DG:O5'	1.99	0.62
4:A:59:ALA:O	4:A:62:LEU:N	2.29	0.62
4:A:169:VAL:CG2	4:A:173:TYR:HE2	2.13	0.61
4:A:238:VAL:HG12	4:A:239:CYS:N	2.15	0.61
4:A:7:PRO:O	4:A:8:GLN:HG2	1.99	0.61
4:A:87:LYS:HA	4:A:90:GLN:HG3	1.81	0.61
4:A:90:GLN:HE21	4:A:91:ASP:N	1.97	0.61
4:A:91:ASP:OD2	4:A:94:SER:HB3	2.00	0.61
4:A:190:ASP:N	4:A:190:ASP:OD1	2.29	0.61
2:P:1:DG:H2''	2:P:2:DC:O5'	2.00	0.61
4:A:152:ARG:O	4:A:156:LEU:N	2.29	0.61
4:A:172:GLU:HB3	4:A:198:PRO:CG	2.29	0.61
4:A:194:LEU:CD1	4:A:265:TYR:HE1	2.07	0.61
4:A:102:ARG:NH2	4:A:147:GLU:OE1	2.29	0.60
4:A:250:TYR:HB3	4:A:251:PRO:CD	2.31	0.60
4:A:172:GLU:HB3	4:A:198:PRO:HG2	1.82	0.60
4:A:186:GLU:N	4:A:186:GLU:OE1	2.29	0.60
4:A:177:VAL:HG12	4:A:178:CYS:N	2.17	0.60
4:A:192:ASP:HB3	4:A:258:ARG:NH2	2.17	0.60
4:A:155:MET:HE3	4:A:188:SER:CB	2.20	0.60
4:A:200:PHE:HE2	4:A:259:LEU:HG	1.63	0.60
4:A:122:LEU:HD22	4:A:126:ARG:CZ	2.32	0.59
4:A:161:ILE:CG2	4:A:165:GLU:HG2	2.29	0.59
4:A:180:SER:O	4:A:183:ARG:N	2.35	0.59
2:P:11:DG:N2	4:A:271:TYR:OH	2.29	0.59
4:A:15:ILE:O	4:A:18:MET:HG2	2.02	0.59
4:A:65:VAL:HG12	4:A:66:GLY:N	2.18	0.59
4:A:48:LYS:O	4:A:50:PRO:HD3	2.03	0.59
4:A:21:GLU:CG	4:A:85:LEU:HD21	2.32	0.59
4:A:150:ILE:HG22	4:A:155:MET:HG2	1.85	0.59
4:A:110:ALA:O	4:A:113:LYS:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:207:GLN:OE1	4:A:209:LYS:HE2	2.03	0.58
4:A:209:LYS:O	4:A:213:GLN:HB3	2.02	0.58
4:A:192:ASP:HB3	4:A:258:ARG:HH22	1.68	0.58
4:A:196:THR:HG22	4:A:260:ILE:H	1.68	0.58
4:A:135:HIS:HD2	4:A:228:LEU:HB3	1.66	0.58
4:A:150:ILE:HG23	4:A:253:ARG:HH11	1.69	0.58
4:A:228:LEU:HB2	4:A:236:MET:O	2.04	0.58
4:A:150:ILE:O	4:A:187:SER:HA	2.04	0.58
4:A:25:PHE:CD2	4:A:88:ILE:HG21	2.38	0.58
4:A:326:LYS:NZ	4:A:328:ARG:HA	2.19	0.57
4:A:102:ARG:HH21	4:A:147:GLU:CD	2.10	0.57
4:A:177:VAL:HG12	4:A:178:CYS:H	1.69	0.57
4:A:193:VAL:O	4:A:258:ARG:N	2.37	0.57
4:A:26:GLU:HA	4:A:30:SER:HB2	1.87	0.57
4:A:116:ASP:C	4:A:118:GLY:H	2.14	0.56
4:A:19:LEU:HD12	4:A:43:ALA:HA	1.87	0.56
4:A:25:PHE:CE2	4:A:88:ILE:HG12	2.40	0.56
4:A:200:PHE:CD2	4:A:259:LEU:HD21	2.41	0.56
4:A:228:LEU:HD22	4:A:237:GLY:HA2	1.87	0.56
4:A:228:LEU:HD23	4:A:237:GLY:HA2	1.87	0.56
2:P:1:DG:H8	2:P:1:DG:H5'	1.70	0.55
4:A:99:PHE:HD1	4:A:102:ARG:HD3	1.71	0.55
4:A:33:ILE:HD12	4:A:33:ILE:N	2.19	0.55
4:A:15:ILE:HG21	4:A:46:ILE:HD13	1.87	0.55
4:A:196:THR:HB	4:A:260:ILE:O	2.06	0.55
4:A:201:THR:HG22	4:A:204:SER:OG	2.07	0.54
4:A:206:LYS:O	4:A:208:PRO:HD3	2.07	0.54
4:A:259:LEU:HD12	4:A:260:ILE:N	2.23	0.54
4:A:169:VAL:HG23	4:A:213:GLN:NE2	2.21	0.54
3:D:1:DG:OP1	4:A:68:LYS:NZ	2.30	0.54
4:A:23:ALA:O	4:A:36:TYR:HD1	1.90	0.54
4:A:259:LEU:HD12	4:A:260:ILE:H	1.72	0.54
4:A:12:ASN:HB3	4:A:46:ILE:HD12	1.90	0.54
4:A:134:HIS:ND1	4:A:138:ILE:HD11	2.22	0.54
4:A:192:ASP:CB	4:A:258:ARG:HH22	2.20	0.54
4:A:326:LYS:HZ2	4:A:328:ARG:HA	1.71	0.54
4:A:12:ASN:HD21	4:A:53:ILE:H	1.55	0.54
4:A:123:GLU:O	4:A:127:LYS:HG3	2.08	0.54
4:A:169:VAL:CG1	4:A:214:VAL:HG12	2.30	0.53
1:T:7:DA:H2''	1:T:8:DC:O5'	2.07	0.53
4:A:18:MET:HG3	4:A:19:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:230:LYS:HB3	4:A:230:LYS:HZ1	1.71	0.53
4:A:21:GLU:HB3	4:A:85:LEU:HD21	1.90	0.53
4:A:164:ASN:O	4:A:167:LYS:HB3	2.08	0.53
4:A:240:GLN:HG2	4:A:241:LEU:N	2.24	0.53
4:A:38:ALA:O	4:A:41:LYS:N	2.41	0.53
4:A:241:LEU:HB2	4:A:250:TYR:CD2	2.42	0.53
4:A:115:VAL:HA	4:A:119:ILE:O	2.08	0.53
4:A:160:ASP:OD1	4:A:164:ASN:ND2	2.42	0.53
4:A:25:PHE:HE2	4:A:88:ILE:HG12	1.74	0.53
2:P:10:DT:H2"	2:P:11:DG:C8	2.44	0.53
4:A:196:THR:HA	4:A:259:LEU:HD12	1.91	0.53
4:A:21:GLU:CB	4:A:85:LEU:HD21	2.38	0.53
4:A:193:VAL:O	4:A:257:ILE:HA	2.09	0.53
4:A:140:LEU:HD12	4:A:140:LEU:O	2.08	0.52
4:A:196:THR:HG22	4:A:260:ILE:CB	2.38	0.52
4:A:197:HIS:ND1	4:A:198:PRO:N	2.58	0.52
4:A:216:GLU:HA	4:A:219:GLN:HB2	1.90	0.52
4:A:121:THR:O	4:A:125:LEU:HG	2.10	0.52
4:A:235:PHE:CZ	4:A:237:GLY:HA3	2.44	0.52
4:A:9:GLU:C	4:A:11:LEU:H	2.18	0.52
4:A:138:ILE:H	4:A:138:ILE:CD1	2.18	0.52
4:A:33:ILE:H	4:A:33:ILE:CD1	2.13	0.52
4:A:110:ALA:HA	4:A:113:LYS:CE	2.39	0.52
4:A:155:MET:HE1	4:A:190:ASP:C	2.34	0.52
4:A:209:LYS:O	4:A:213:GLN:N	2.29	0.52
4:A:122:LEU:HD22	4:A:126:ARG:NH1	2.25	0.52
4:A:133:ASN:C	4:A:133:ASN:HD22	2.18	0.52
4:A:221:VAL:O	4:A:221:VAL:HG22	2.09	0.51
4:A:22:LEU:HD11	4:A:85:LEU:HD13	1.91	0.51
4:A:94:SER:O	4:A:98:ASN:N	2.40	0.51
4:A:150:ILE:HG21	4:A:155:MET:HG2	1.92	0.51
4:A:126:ARG:O	4:A:129:GLU:OE1	2.28	0.51
4:A:150:ILE:HD12	4:A:155:MET:HE2	1.93	0.51
4:A:173:TYR:CE1	4:A:210:LEU:HD22	2.45	0.51
4:A:25:PHE:CE2	4:A:88:ILE:HD13	2.46	0.51
4:A:173:TYR:OH	4:A:210:LEU:HD23	2.10	0.51
4:A:194:LEU:HD13	4:A:195:LEU:N	2.23	0.51
4:A:76:PHE:O	4:A:80:GLY:N	2.41	0.51
4:A:15:ILE:HG22	4:A:46:ILE:HD13	1.92	0.50
4:A:32:ALA:CB	4:A:35:LYS:HB2	2.40	0.50
4:A:162:VAL:HA	4:A:218:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:110:ALA:O	4:A:113:LYS:N	2.44	0.50
1:T:15:DG:H2''	1:T:16:DC:C6	2.47	0.50
4:A:33:ILE:O	4:A:37:ASN:OD1	2.30	0.50
4:A:134:HIS:O	4:A:137:ARG:N	2.43	0.50
2:P:11:DG:O3'	4:A:272:PHE:O	2.29	0.50
4:A:151:PRO:O	4:A:154:GLU:N	2.44	0.50
4:A:196:THR:HG22	4:A:260:ILE:N	2.27	0.50
2:P:1:DG:H2'	2:P:2:DC:C6	2.47	0.49
4:A:87:LYS:O	4:A:90:GLN:HG3	2.12	0.49
4:A:150:ILE:HG22	4:A:155:MET:CG	2.42	0.49
4:A:96:SER:HB3	4:A:120:LYS:HB2	1.94	0.49
4:A:209:LYS:HD2	4:A:209:LYS:H	1.77	0.49
4:A:58:GLU:O	4:A:61:LYS:HB3	2.13	0.49
4:A:112:ARG:O	4:A:116:ASP:OD1	2.30	0.49
4:A:183:ARG:O	4:A:185:ALA:N	2.45	0.49
4:A:132:LEU:HA	4:A:136:GLN:HE21	1.78	0.49
4:A:165:GLU:CB	4:A:218:LEU:HG	2.43	0.49
4:A:155:MET:O	4:A:158:MET:HB2	2.12	0.48
4:A:28:ASN:OD1	4:A:98:ASN:ND2	2.46	0.48
4:A:241:LEU:HD23	4:A:242:PRO:HD2	1.94	0.48
4:A:194:LEU:CD1	4:A:195:LEU:N	2.77	0.48
4:A:202:SER:N	4:A:261:PRO:HB3	2.27	0.48
4:A:202:SER:OG	4:A:264:GLN:NE2	2.46	0.48
2:P:11:DG:OP1	4:A:190:ASP:OD2	2.31	0.48
4:A:201:THR:HA	4:A:261:PRO:CB	2.44	0.48
4:A:240:GLN:CG	4:A:241:LEU:N	2.76	0.48
4:A:243:SER:OG	4:A:247:GLU:O	2.31	0.48
4:A:49:TYR:CD2	4:A:53:ILE:HD11	2.48	0.48
4:A:62:LEU:HB3	4:A:63:PRO:HD2	1.93	0.48
4:A:132:LEU:HD13	4:A:136:GLN:HB3	1.96	0.48
4:A:209:LYS:CD	4:A:209:LYS:H	2.27	0.48
4:A:195:LEU:O	4:A:259:LEU:HA	2.13	0.48
4:A:200:PHE:CZ	4:A:261:PRO:HD3	2.49	0.48
4:A:99:PHE:O	4:A:102:ARG:HG3	2.14	0.48
4:A:132:LEU:HA	4:A:136:GLN:NE2	2.29	0.48
4:A:123:GLU:CD	4:A:123:GLU:H	2.22	0.47
4:A:133:ASN:HD22	4:A:135:HIS:N	2.13	0.47
4:A:165:GLU:O	4:A:217:GLN:HG2	2.15	0.47
4:A:196:THR:HG22	4:A:260:ILE:CA	2.43	0.47
2:P:1:DG:H5'	2:P:1:DG:C8	2.48	0.47
2:P:1:DG:H2'	2:P:2:DC:C5	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:19:LEU:HD12	4:A:43:ALA:HB2	1.97	0.47
4:A:23:ALA:C	4:A:36:TYR:HD1	2.22	0.47
4:A:65:VAL:CG1	4:A:66:GLY:N	2.78	0.47
4:A:151:PRO:O	4:A:153:GLU:N	2.47	0.47
4:A:197:HIS:ND1	4:A:198:PRO:HD2	2.29	0.47
4:A:200:PHE:CD2	4:A:259:LEU:HG	2.50	0.47
4:A:240:GLN:CG	4:A:241:LEU:H	2.27	0.47
4:A:75:GLU:OE1	4:A:82:LEU:HD12	2.15	0.47
4:A:169:VAL:HG11	4:A:214:VAL:CG1	2.33	0.47
4:A:91:ASP:OD2	4:A:94:SER:N	2.37	0.47
4:A:186:GLU:O	4:A:187:SER:HB3	2.15	0.47
4:A:232:GLU:HG3	4:A:233:THR:HG23	1.97	0.47
4:A:19:LEU:HD12	4:A:43:ALA:CB	2.45	0.46
4:A:201:THR:CA	4:A:261:PRO:HB3	2.46	0.46
4:A:202:SER:OG	4:A:263:ASP:OD1	2.33	0.46
3:D:2:DT:H4'	4:A:41:LYS:NZ	2.31	0.46
2:P:1:DG:C2'	2:P:2:DC:C6	2.99	0.46
4:A:72:LYS:HD3	4:A:82:LEU:HD21	1.97	0.46
4:A:170:ASP:CB	4:A:173:TYR:CD2	2.99	0.46
4:A:196:THR:CG2	4:A:265:TYR:CD1	2.99	0.46
4:A:255:ILE:CG1	4:A:256:ASP:N	2.78	0.46
4:A:138:ILE:HG23	4:A:142:TYR:CE2	2.50	0.46
4:A:18:MET:CG	4:A:19:LEU:N	2.79	0.46
4:A:59:ALA:O	4:A:62:LEU:HB2	2.16	0.46
4:A:59:ALA:O	4:A:62:LEU:HD23	2.16	0.46
4:A:165:GLU:OE1	4:A:168:LYS:NZ	2.49	0.46
4:A:152:ARG:NH2	4:A:181:PHE:O	2.49	0.46
4:A:161:ILE:HG22	4:A:218:LEU:CD2	2.46	0.46
4:A:165:GLU:OE1	4:A:221:VAL:HG11	2.16	0.46
4:A:122:LEU:O	4:A:126:ARG:HG2	2.15	0.46
4:A:197:HIS:ND1	4:A:198:PRO:CD	2.79	0.46
4:A:238:VAL:CG1	4:A:239:CYS:N	2.79	0.46
4:A:212:HIS:NE2	4:A:216:GLU:OE2	2.49	0.45
4:A:6:ALA:HB2	4:A:48:LYS:HE2	1.98	0.45
3:D:4:DG:H2''	3:D:5:DG:H8	1.75	0.45
4:A:192:ASP:N	4:A:192:ASP:OD1	2.44	0.45
4:A:196:THR:HG21	4:A:265:TYR:CD1	2.52	0.45
4:A:228:LEU:HD23	4:A:237:GLY:CA	2.47	0.45
1:T:15:DG:C2'	1:T:16:DC:C6	2.99	0.45
4:A:241:LEU:CB	4:A:250:TYR:CD2	2.99	0.45
2:P:10:DT:C2'	2:P:11:DG:C8	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:163:LEU:N	4:A:163:LEU:CD2	2.80	0.45
4:A:254:ARG:NH1	4:A:255:ILE:O	2.40	0.45
4:A:99:PHE:CD1	4:A:102:ARG:HD3	2.50	0.45
4:A:106:ILE:HG23	4:A:110:ALA:HB3	1.99	0.45
4:A:207:GLN:HG3	4:A:210:LEU:HG	1.98	0.45
4:A:12:ASN:HB3	4:A:46:ILE:CD1	2.47	0.45
4:A:106:ILE:HG22	4:A:107:GLY:O	2.17	0.45
4:A:138:ILE:N	4:A:138:ILE:CD1	2.77	0.45
4:A:254:ARG:NH2	4:A:256:ASP:OD2	2.48	0.45
4:A:96:SER:CB	4:A:120:LYS:HB2	2.47	0.44
4:A:182:ARG:NE	4:A:273:THR:HG21	2.10	0.44
4:A:202:SER:N	4:A:261:PRO:CB	2.80	0.44
4:A:236:MET:HE2	4:A:236:MET:HB3	1.70	0.44
4:A:90:GLN:NE2	4:A:91:ASP:CA	2.79	0.44
4:A:103:VAL:HG22	4:A:143:PHE:CD1	2.52	0.44
4:A:194:LEU:HD13	4:A:258:ARG:O	2.16	0.44
4:A:241:LEU:HD23	4:A:241:LEU:HA	1.66	0.44
4:A:96:SER:O	4:A:100:LEU:HB2	2.18	0.44
4:A:25:PHE:CE2	4:A:88:ILE:CG2	3.00	0.44
4:A:152:ARG:NH2	4:A:184:GLY:CA	2.77	0.44
4:A:161:ILE:HG22	4:A:165:GLU:CG	2.40	0.44
4:A:22:LEU:HD12	4:A:22:LEU:HA	1.78	0.44
4:A:25:PHE:CE2	4:A:88:ILE:CG1	3.00	0.44
4:A:228:LEU:HD22	4:A:228:LEU:H	1.80	0.44
2:P:4:DG:N7	6:P:506:HOH:O	2.35	0.44
3:D:1:DG:P	4:A:68:LYS:HD3	2.58	0.44
4:A:19:LEU:O	4:A:22:LEU:HB2	2.17	0.44
4:A:150:ILE:HG12	4:A:253:ARG:CZ	2.47	0.44
4:A:177:VAL:HG13	4:A:192:ASP:O	2.17	0.44
4:A:197:HIS:CG	4:A:198:PRO:CD	2.99	0.44
4:A:75:GLU:O	4:A:79:THR:OG1	2.28	0.43
4:A:27:LYS:HB3	4:A:28:ASN:H	1.53	0.43
4:A:76:PHE:HA	4:A:81:LYS:O	2.18	0.43
4:A:218:LEU:CD2	4:A:223:PHE:CD2	2.99	0.43
4:A:241:LEU:HB3	4:A:250:TYR:CE2	2.54	0.43
1:T:1:DC:H6	1:T:1:DC:O5'	1.97	0.43
4:A:150:ILE:HA	4:A:151:PRO:HD2	1.90	0.43
4:A:161:ILE:O	4:A:165:GLU:HG2	2.18	0.43
4:A:179:GLY:O	4:A:183:ARG:HG3	2.18	0.43
4:A:195:LEU:HA	4:A:265:TYR:OH	2.18	0.43
3:D:2:DT:H4'	4:A:41:LYS:HZ1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:61:LYS:O	4:A:61:LYS:HG2	2.05	0.43
4:A:87:LYS:CA	4:A:90:GLN:HG3	2.47	0.43
4:A:85:LEU:HD12	4:A:85:LEU:HA	1.58	0.43
4:A:141:LYS:HB3	4:A:142:TYR:H	1.52	0.43
4:A:11:LEU:HD23	4:A:11:LEU:HA	1.78	0.43
4:A:60:LYS:C	4:A:62:LEU:N	2.74	0.43
4:A:196:THR:HA	4:A:259:LEU:HD11	2.01	0.43
4:A:254:ARG:HH22	4:A:256:ASP:CG	2.27	0.43
4:A:10:THR:H	4:A:10:THR:HG22	1.56	0.43
4:A:122:LEU:HD23	4:A:140:LEU:HD11	1.99	0.43
4:A:213:GLN:O	4:A:216:GLU:HB2	2.18	0.43
1:T:9:DG:H2''	1:T:10:DC:H6	1.84	0.43
4:A:224:ILE:HA	4:A:239:CYS:HA	2.00	0.43
4:A:259:LEU:HD12	4:A:259:LEU:HA	1.72	0.43
4:A:25:PHE:CE2	4:A:88:ILE:CD1	3.01	0.43
4:A:33:ILE:N	4:A:33:ILE:CD1	2.82	0.43
4:A:165:GLU:HB3	4:A:218:LEU:HG	2.01	0.43
4:A:165:GLU:CG	4:A:218:LEU:CD2	2.97	0.42
4:A:37:ASN:HA	4:A:40:ARG:CG	2.45	0.42
4:A:25:PHE:CD1	4:A:25:PHE:C	2.97	0.42
4:A:122:LEU:CD2	4:A:126:ARG:CZ	2.97	0.42
4:A:228:LEU:O	4:A:229:SER:HB3	2.18	0.42
3:D:2:DT:H5''	4:A:64:GLY:O	2.20	0.42
4:A:29:VAL:HG12	4:A:29:VAL:O	2.19	0.42
4:A:38:ALA:C	4:A:41:LYS:HE2	2.44	0.42
4:A:133:ASN:ND2	4:A:133:ASN:C	2.78	0.42
1:T:15:DG:H2''	1:T:16:DC:O5'	2.20	0.42
4:A:97:ILE:HG21	4:A:97:ILE:HD13	1.47	0.42
4:A:116:ASP:C	4:A:118:GLY:N	2.76	0.42
4:A:142:TYR:CE1	4:A:252:HIS:ND1	2.87	0.42
4:A:191:MET:HG3	4:A:192:ASP:N	2.34	0.42
4:A:150:ILE:CG1	4:A:253:ARG:HD3	2.47	0.42
4:A:156:LEU:HA	4:A:156:LEU:HD23	1.74	0.42
4:A:196:THR:CG2	4:A:265:TYR:CE1	2.99	0.42
1:T:9:DG:C4	1:T:10:DC:C5	3.08	0.42
1:T:14:DA:H2''	1:T:15:DG:C5'	2.50	0.42
3:D:1:DG:OP2	4:A:68:LYS:HD3	2.19	0.42
4:A:152:ARG:C	4:A:155:MET:HB2	2.44	0.42
4:A:195:LEU:N	4:A:258:ARG:O	2.47	0.42
4:A:60:LYS:HA	4:A:65:VAL:HB	2.01	0.41
4:A:132:LEU:CA	4:A:136:GLN:HE21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:197:HIS:CD2	4:A:198:PRO:HD2	2.55	0.41
4:A:200:PHE:HD2	4:A:259:LEU:HD11	1.85	0.41
4:A:128:ASN:O	4:A:130:ASP:N	2.53	0.41
4:A:150:ILE:N	4:A:188:SER:O	2.32	0.41
4:A:207:GLN:HB2	4:A:209:LYS:HZ2	1.82	0.41
4:A:37:ASN:CA	4:A:40:ARG:HG3	2.43	0.41
4:A:149:ARG:NH2	4:A:187:SER:O	2.32	0.41
1:T:3:DG:N2	6:T:509:HOH:O	2.46	0.41
4:A:181:PHE:CD1	4:A:181:PHE:C	2.98	0.41
4:A:240:GLN:HG2	4:A:241:LEU:H	1.86	0.41
2:P:8:DC:H2''	2:P:9:DG:O5'	2.20	0.41
4:A:62:LEU:HA	4:A:63:PRO:HD3	1.72	0.41
4:A:133:ASN:HD21	4:A:135:HIS:HB3	1.86	0.41
4:A:207:GLN:CB	4:A:209:LYS:NZ	2.79	0.41
4:A:222:HIS:ND1	4:A:222:HIS:N	2.68	0.41
4:A:67:THR:H	4:A:67:THR:HG22	1.31	0.41
4:A:151:PRO:C	4:A:153:GLU:N	2.79	0.41
4:A:201:THR:HA	4:A:261:PRO:HB3	2.03	0.41
4:A:128:ASN:O	4:A:131:LYS:HG2	2.21	0.40
4:A:90:GLN:NE2	4:A:90:GLN:C	2.79	0.40
4:A:122:LEU:O	4:A:125:LEU:HB2	2.21	0.40
4:A:169:VAL:HG21	4:A:213:GLN:HG3	2.03	0.40
4:A:235:PHE:CE1	4:A:237:GLY:HA3	2.56	0.40
4:A:6:ALA:HA	4:A:7:PRO:HD3	1.60	0.40
4:A:100:LEU:HD22	4:A:115:VAL:CG2	2.51	0.40
4:A:130:ASP:OD1	4:A:131:LYS: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
4	A	329/335 (98%)	248 (75%)	58 (18%)	23 (7%)	1 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	7	PRO
4	A	8	GLN
4	A	141	LYS
4	A	152	ARG
4	A	302	GLY
4	A	129	GLU
4	A	142	TYR
4	A	184	GLY
4	A	202	SER
4	A	265	TYR
4	A	327	TYR
4	A	27	LYS
4	A	42	ALA
4	A	117	GLU
4	A	222	HIS
4	A	187	SER
4	A	143	PHE
4	A	221	VAL
4	A	250	TYR
4	A	266	TYR
4	A	309	GLU
4	A	50	PRO
4	A	242	PRO

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	291/295 (99%)	233 (80%)	58 (20%)	1 2

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	THR
4	A	16	THR
4	A	19	LEU
4	A	22	LEU
4	A	40	ARG
4	A	41	LYS
4	A	46	ILE
4	A	61	LYS
4	A	67	THR
4	A	73	ILE
4	A	77	LEU
4	A	90	GLN
4	A	93	THR
4	A	94	SER
4	A	96	SER
4	A	98	ASN
4	A	100	LEU
4	A	109	SER
4	A	122	LEU
4	A	124	ASP
4	A	127	LYS
4	A	131	LYS
4	A	132	LEU
4	A	133	ASN
4	A	140	LEU
4	A	151	PRO
4	A	162	VAL
4	A	164	ASN
4	A	166	VAL
4	A	169	VAL
4	A	176	THR
4	A	180	SER
4	A	187	SER
4	A	192	ASP
4	A	194	LEU
4	A	195	LEU
4	A	201	THR
4	A	203	GLU
4	A	206	LYS
4	A	213	GLN
4	A	225	THR
4	A	226	ASP
4	A	230	LYS

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Mol	Chain	Res	Type
4	A	232	GLU
4	A	236	MET
4	A	246	ASP
4	A	253	ARG
4	A	273	THR
4	A	277	ILE
4	A	287	LEU
4	A	294	ASN
4	A	296	TYR
4	A	301	LEU
4	A	303	VAL
4	A	311	LEU
4	A	324	GLN
4	A	331	LYS
4	A	332	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	12	ASN
4	A	28	ASN
4	A	90	GLN
4	A	98	ASN
4	A	133	ASN
4	A	136	GLN
4	A	164	ASN
4	A	213	GLN
4	A	245	ASN
4	A	264	GLN
4	A	279	ASN
4	A	281	ASN
4	A	285	HIS
4	A	294	ASN
4	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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%)	0.10	1 (6%) 26 20	27, 45, 91, 92	0
2	P	11/11 (100%)	0.04	0 100 100	30, 38, 66, 92	0
3	D	5/5 (100%)	-0.45	0 100 100	18, 26, 37, 38	0
4	A	331/335 (98%)	0.97	65 (19%) 3 2	16, 48, 99, 100	75 (22%)
All	All	363/367 (98%)	0.89	66 (18%) 3 3	16, 47, 99, 100	75 (20%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	274	GLY	7.0
4	A	10	THR	6.8
4	A	303	VAL	4.8
4	A	9	GLU	4.7
4	A	324	GLN	4.6
4	A	290	GLY	4.4
4	A	314	ASP	4.2
4	A	313	VAL	4.1
4	A	292	THR	3.9
4	A	291	PHE	3.9
4	A	316	GLU	3.9
4	A	319	ILE	3.8
4	A	8	GLN	3.6
4	A	301	LEU	3.5
4	A	306	VAL	3.5
4	A	304	THR	3.4
4	A	200	PHE	3.4
4	A	11	LEU	3.3
4	A	246	ASP	3.3
4	A	173	TYR	3.2
4	A	330	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
4	A	288	GLU	3.2
4	A	334	SER	3.1
4	A	293	ILE	3.1
4	A	81	LYS	3.1
4	A	320	PHE	3.1
4	A	265	TYR	3.0
4	A	183	ARG	3.0
4	A	282	MET	3.0
4	A	245	ASN	2.9
1	T	7	DA	2.9
4	A	204	SER	2.8
4	A	309	GLU	2.8
4	A	310	PRO	2.7
4	A	308	GLY	2.7
4	A	325	TRP	2.7
4	A	327	TYR	2.7
4	A	275	SER	2.7
4	A	289	LYS	2.7
4	A	302	GLY	2.6
4	A	205	THR	2.6
4	A	315	SER	2.6
4	A	331	LYS	2.6
4	A	7	PRO	2.5
4	A	160	ASP	2.5
4	A	326	LYS	2.5
4	A	175	ALA	2.5
4	A	201	THR	2.5
4	A	262	LYS	2.5
4	A	332	ASP	2.4
4	A	92	ASP	2.4
4	A	307	ALA	2.4
4	A	194	LEU	2.3
4	A	211	LEU	2.3
4	A	184	GLY	2.3
4	A	263	ASP	2.3
4	A	311	LEU	2.3
4	A	283	ARG	2.2
4	A	206	LYS	2.1
4	A	6	ALA	2.1
4	A	287	LEU	2.1
4	A	5	LYS	2.1
4	A	305	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	284	ALA	2.1
4	A	296	TYR	2.0
4	A	295	GLU	2.0

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($\text{\AA}^2$)	Q<0.9
5	NA	A	341	1/1	0.97	0.08	22,22,22,22	0
5	NA	A	342	1/1	0.99	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.