



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:05 AM UTC

PDB ID : 7ICV / pdb_00007icv
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF MNCL2 (0.1 MILLIMOLAR) AND IN THE ABSENCE OF NACL
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-10-24
Resolution : 2.80 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

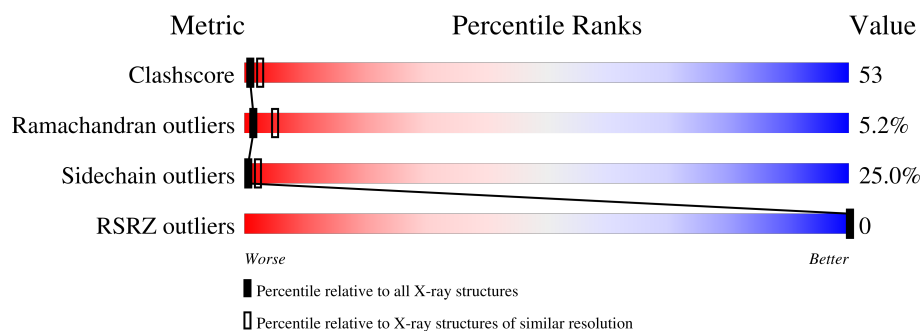
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	7	
2	P	6	
3	A	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3024 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*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	P	0	0	0
			126	59	25	36	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	26	0	0
			2623	1657	458	499	9			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

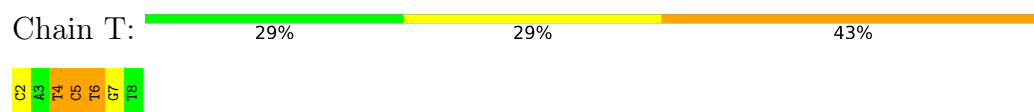
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	14	Total	O	0	0
			14	14		
5	P	20	Total	O	0	0
			20	20		
5	A	117	Total	O	0	0
			117	117		

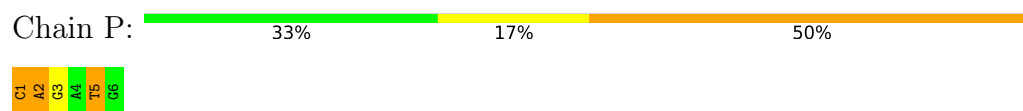
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

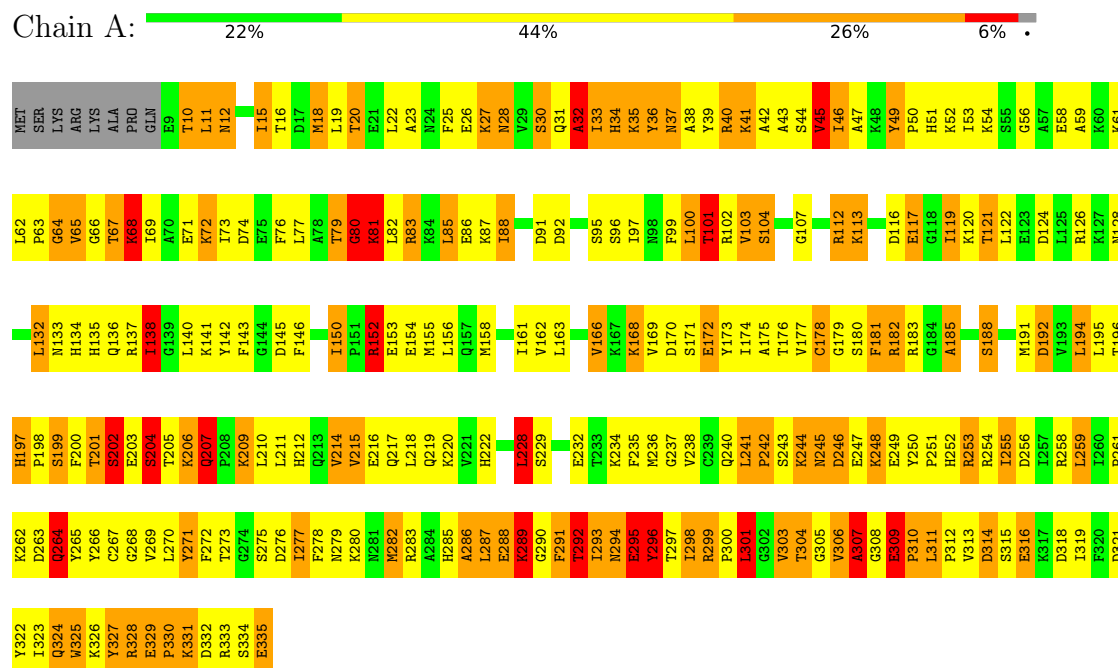
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- Molecule 2: DNA (5'-D(*CP*AP*GP*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	178.42Å 57.70Å 48.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.0 (20.00-2.80) 85.1 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	(Not available) , (Not available) 0.152 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 177.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3024	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	0.94	0/135	2.36	9/207 (4.3%)
2	P	1.25	2/141 (1.4%)	2.32	8/214 (3.7%)
3	A	1.55	11/2672 (0.4%)	2.15	116/3590 (3.2%)
All	All	1.51	13/2948 (0.4%)	2.17	133/4011 (3.3%)

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
3	A	1	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	DC	OP3-P	7.24	1.62	1.48
3	A	192	ASP	CA-C	-6.40	1.45	1.52
2	P	5	DT	C1'-N1	6.05	1.67	1.49
3	A	242	PRO	N-CA	-6.05	1.40	1.47
3	A	215	VAL	C-N	-5.94	1.26	1.33
3	A	35	LYS	CA-C	-5.87	1.45	1.52
3	A	191	MET	C-N	5.75	1.41	1.33
3	A	116	ASP	N-CA	-5.71	1.38	1.46
3	A	66	GLY	N-CA	-5.68	1.40	1.44
3	A	104	SER	CA-C	-5.43	1.45	1.52
3	A	220	LYS	C-N	-5.21	1.28	1.34
3	A	138	ILE	CA-CB	-5.18	1.48	1.54
3	A	65	VAL	CA-CB	-5.13	1.48	1.54

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	C2-N1-C1'	16.48	144.07	119.35
2	P	5	DT	C6-N1-C1'	-14.63	97.41	119.35
3	A	192	ASP	N-CA-CB	13.92	132.37	110.65
1	T	4	DT	C6-N1-C1'	-13.39	99.26	119.35
3	A	49	TYR	CA-C-N	12.98	136.07	119.84
3	A	49	TYR	C-N-CA	12.98	136.07	119.84
1	T	4	DT	C2-N1-C1'	12.75	138.47	119.35
3	A	192	ASP	CB-CA-C	-11.23	91.51	110.16
3	A	192	ASP	CA-CB-CG	11.13	123.73	112.60
3	A	34	HIS	CA-CB-CG	-10.45	103.35	113.80
1	T	2	DC	C2-N1-C1'	8.90	133.04	119.70
3	A	49	TYR	O-C-N	8.70	128.25	121.47
3	A	99	PHE	CA-CB-CG	-8.61	105.19	113.80
3	A	40	ARG	N-CA-C	8.55	120.60	111.28
1	T	2	DC	C6-N1-C1'	-8.15	107.47	119.70
3	A	30	SER	CA-C-N	-7.96	110.17	122.60
3	A	30	SER	C-N-CA	-7.96	110.17	122.60
3	A	286	ALA	CA-C-N	7.49	130.31	120.28
3	A	286	ALA	C-N-CA	7.49	130.31	120.28
3	A	152	ARG	N-CA-CB	7.42	121.86	110.14
3	A	32	ALA	N-CA-C	7.40	126.56	110.80
3	A	33	ILE	N-CA-CB	-7.39	101.24	110.47
3	A	296	TYR	CB-CA-C	-7.34	97.21	109.55
3	A	266	TYR	N-CA-C	7.33	120.20	111.33
3	A	64	GLY	N-CA-C	-7.17	106.31	115.42
3	A	291	PHE	N-CA-C	7.13	120.01	109.24
3	A	92	ASP	N-CA-CB	7.00	120.16	110.01
3	A	178	CYS	CB-CA-C	6.88	124.11	110.42
3	A	146	PHE	CA-CB-CG	-6.82	106.98	113.80
3	A	49	TYR	CA-C-O	6.68	125.40	119.59
3	A	181	PHE	CA-C-N	6.53	129.56	120.29
3	A	181	PHE	C-N-CA	6.53	129.56	120.29
2	P	1	DC	C6-N1-C1'	-6.52	109.92	119.70
3	A	272	PHE	CA-CB-CG	-6.52	107.28	113.80
1	T	5	DC	C6-N1-C1'	-6.47	110.00	119.70
3	A	80	GLY	CA-C-N	-6.42	111.91	122.11
3	A	80	GLY	C-N-CA	-6.42	111.91	122.11
1	T	5	DC	C2-N1-C1'	6.33	129.20	119.70
3	A	102	ARG	CD-NE-CZ	-6.33	115.55	124.40
3	A	156	LEU	N-CA-CB	6.25	119.30	110.12
3	A	168	LYS	N-CA-CB	6.19	119.17	109.94
3	A	86	GLU	CB-CA-C	6.18	121.05	110.79
3	A	197	HIS	CA-C-N	6.17	126.36	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	197	HIS	C-N-CA	6.17	126.36	119.32
2	P	1	DC	C2-N1-C1'	6.15	128.93	119.70
3	A	204	SER	CA-C-N	-6.15	112.82	121.99
3	A	204	SER	C-N-CA	-6.15	112.82	121.99
3	A	292	THR	N-CA-CB	6.15	121.53	110.83
3	A	313	VAL	N-CA-C	6.15	116.78	108.17
3	A	296	TYR	N-CA-C	6.14	121.70	113.72
3	A	117	GLU	N-CA-C	-6.14	105.83	113.38
3	A	107	GLY	N-CA-C	-6.13	99.83	112.34
3	A	282	MET	N-CA-C	-6.06	104.75	111.71
3	A	86	GLU	N-CA-CB	6.03	118.99	110.12
3	A	266	TYR	CA-CB-CG	-6.00	103.10	113.90
3	A	304	THR	N-CA-CB	-5.95	100.43	110.49
3	A	28	ASN	N-CA-C	5.95	117.84	111.36
3	A	88	ILE	CA-CB-CG2	5.93	120.59	110.50
3	A	267	CYS	N-CA-C	-5.93	104.82	111.28
1	T	4	DT	P-O3'-C3'	5.92	129.09	120.20
3	A	292	THR	CB-CA-C	5.92	120.68	109.37
3	A	83	ARG	N-CA-CB	5.91	118.59	110.01
3	A	286	ALA	O-C-N	5.90	128.90	122.11
3	A	87	LYS	CB-CA-C	5.89	120.03	110.96
3	A	40	ARG	N-CA-CB	5.88	118.77	110.12
3	A	271	TYR	CA-CB-CG	-5.86	103.36	113.90
1	T	5	DC	P-O3'-C3'	5.86	128.98	120.20
3	A	103	VAL	N-CA-CB	5.83	116.89	110.53
3	A	328	ARG	N-CA-C	5.82	118.15	108.20
3	A	295	GLU	CB-CG-CD	5.80	122.46	112.60
3	A	246	ASP	N-CA-C	5.80	123.15	110.80
3	A	81	LYS	N-CA-CB	-5.79	101.53	111.21
3	A	101	THR	N-CA-CB	-5.79	101.00	110.14
3	A	203	GLU	O-C-N	5.78	128.81	122.11
3	A	116	ASP	CA-CB-CG	-5.77	106.83	112.60
3	A	312	PRO	CA-C-N	5.75	130.32	123.19
3	A	312	PRO	C-N-CA	5.75	130.32	123.19
3	A	191	MET	CA-C-O	-5.75	114.12	120.38
3	A	207	GLN	CA-C-N	5.74	125.27	119.19
3	A	207	GLN	C-N-CA	5.74	125.27	119.19
2	P	2	DA	C4'-C3'-C2'	-5.68	93.88	102.40
3	A	178	CYS	CA-CB-SG	-5.64	101.43	114.40
3	A	299	ARG	N-CA-C	5.62	118.81	110.32
3	A	92	ASP	N-CA-C	5.62	117.08	111.07
3	A	209	LYS	O-C-N	5.62	128.07	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	45	VAL	N-CA-C	5.60	115.79	110.53
2	P	1	DC	P-O3'-C3'	5.60	128.59	120.20
3	A	228	LEU	N-CA-C	-5.58	103.02	111.56
3	A	67	THR	CB-CA-C	5.56	119.61	110.88
3	A	309	GLU	CA-C-N	5.51	126.73	119.84
3	A	309	GLU	C-N-CA	5.51	126.73	119.84
3	A	96	SER	N-CA-C	5.50	117.36	111.36
3	A	307	ALA	CB-CA-C	5.50	121.36	110.42
3	A	161	ILE	N-CA-C	5.48	115.68	110.53
3	A	166	VAL	CB-CA-C	-5.48	104.74	112.14
3	A	20	THR	N-CA-CB	5.47	118.26	110.16
2	P	1	DC	P-O5'-C5'	-5.45	111.82	120.00
3	A	116	ASP	N-CA-C	-5.44	106.61	113.20
3	A	329	GLU	N-CA-C	-5.43	102.29	109.84
3	A	316	GLU	N-CA-C	-5.42	105.93	112.54
3	A	240	GLN	N-CA-C	5.41	117.31	108.55
3	A	327	TYR	N-CA-CB	5.39	118.03	109.51
3	A	241	LEU	O-C-N	5.37	125.88	121.31
1	T	6	DT	C6-N1-C1'	-5.37	111.30	119.35
3	A	232	GLU	N-CA-C	5.37	119.68	113.18
3	A	36	TYR	CA-CB-CG	-5.35	104.27	113.90
3	A	177	VAL	CB-CA-C	5.34	118.79	111.31
3	A	335	GLU	N-CA-CB	5.33	119.56	110.50
3	A	229	SER	N-CA-CB	5.33	119.56	110.71
3	A	307	ALA	N-CA-CB	5.33	119.50	110.49
3	A	12	ASN	CA-C-N	5.33	126.01	119.99
3	A	12	ASN	C-N-CA	5.33	126.01	119.99
3	A	12	ASN	CA-CB-CG	5.32	117.92	112.60
3	A	138	ILE	CB-CA-C	-5.32	104.96	112.14
3	A	216	GLU	CB-CG-CD	-5.31	103.57	112.60
2	P	5	DT	N1-C1'-C2'	5.29	121.44	113.50
3	A	92	ASP	CB-CA-C	5.28	119.17	110.88
3	A	214	VAL	N-CA-CB	5.25	118.45	110.58
3	A	303	VAL	CB-CA-C	5.25	116.60	110.88
3	A	181	PHE	O-C-N	5.24	127.67	122.12
3	A	88	ILE	CA-CB-CG1	5.23	119.30	110.40
3	A	220	LYS	N-CA-C	-5.14	105.57	111.07
3	A	310	PRO	N-CA-C	5.11	123.00	112.47
3	A	241	LEU	CA-C-N	5.10	125.38	119.93
3	A	241	LEU	C-N-CA	5.10	125.38	119.93
3	A	68	LYS	N-CA-C	5.09	116.91	111.36
3	A	264	GLN	N-CA-CB	5.09	119.08	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	30	SER	N-CA-C	-5.07	101.89	109.79
3	A	222	HIS	CA-CB-CG	-5.04	108.76	113.80
3	A	301	LEU	N-CA-C	5.03	116.95	109.25
3	A	51	HIS	CA-CB-CG	5.03	118.83	113.80
3	A	246	ASP	N-CA-CB	5.03	118.98	110.49
3	A	330	PRO	N-CA-CB	5.01	108.84	103.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	246	ASP	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	122	0	69	2	0
2	P	126	0	68	11	0
3	A	2623	0	2641	283	1
4	A	2	0	0	0	0
5	A	117	0	0	7	0
5	P	20	0	0	2	0
5	T	14	0	0	1	0
All	All	3024	0	2778	296	1

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 53.

All (296) 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)
2:P:5:DT:N1	2:P:5:DT:C1'	1.67	1.53
2:P:5:DT:C1'	2:P:5:DT:C6	2.30	1.13
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.52	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.31	1.07
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.37	1.04
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.43	0.99
2:P:1:DC:H2''	2:P:2:DA:H5''	1.40	0.98
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.31	0.94
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.04	0.93
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.68	0.92
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.07	0.92
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.52	0.91
3:A:245:ASN:N	3:A:245:ASN:HD22	1.71	0.88
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.54	0.88
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.55	0.87
3:A:11:LEU:HD23	3:A:11:LEU:H	1.41	0.85
2:P:1:DC:C2'	2:P:2:DA:H5''	2.05	0.85
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.59	0.83
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.08	0.83
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.09	0.82
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.60	0.82
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.63	0.81
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.21	0.80
3:A:207:GLN:O	3:A:210:LEU:HB2	1.82	0.80
3:A:155:MET:HE3	3:A:188:SER:OG	1.82	0.79
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.64	0.79
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.98	0.79
3:A:27:LYS:HG3	3:A:28:ASN:HD22	1.49	0.78
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.18	0.78
3:A:331:LYS:HD2	3:A:332:ASP:N	1.98	0.78
3:A:271:TYR:HB2	5:A:592:HOH:O	1.83	0.77
3:A:12:ASN:HD21	3:A:53:ILE:H	1.34	0.76
3:A:154:GLU:O	3:A:158:MET:HG3	1.87	0.74
3:A:155:MET:HA	3:A:158:MET:HE3	1.67	0.74
3:A:27:LYS:HG3	3:A:28:ASN:N	2.01	0.74
3:A:212:HIS:HB3	5:A:541:HOH:O	1.85	0.74
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.70	0.74
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.18	0.73
5:T:617:HOH:O	3:A:234:LYS:HD3	1.87	0.73
3:A:58:GLU:O	3:A:61:LYS:HB2	1.89	0.73
3:A:255:ILE:HG12	3:A:256:ASP:N	2.04	0.72
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.71	0.72
3:A:201:THR:HA	3:A:261:PRO:HB3	1.71	0.72
3:A:18:MET:HE1	3:A:76:PHE:CB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.19	0.72
3:A:262:LYS:O	3:A:262:LYS:HG3	1.90	0.72
3:A:278:PHE:HB2	3:A:333:ARG:O	1.89	0.71
3:A:155:MET:HA	3:A:158:MET:CE	2.19	0.71
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.73	0.71
1:T:4:DT:H2''	1:T:5:DC:O5'	1.91	0.71
3:A:245:ASN:HD22	3:A:245:ASN:H	1.37	0.70
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.21	0.70
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.20	0.70
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.23	0.69
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.23	0.69
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.92	0.69
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.58	0.68
3:A:28:ASN:HD22	3:A:28:ASN:N	1.91	0.68
3:A:68:LYS:O	3:A:72:LYS:HE3	1.93	0.68
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.75	0.68
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.08	0.67
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.10	0.67
3:A:155:MET:HE3	3:A:188:SER:CB	2.25	0.67
3:A:124:ASP:O	3:A:128:ASN:ND2	2.29	0.66
3:A:12:ASN:HA	5:A:642:HOH:O	1.95	0.66
3:A:201:THR:HA	3:A:261:PRO:CB	2.26	0.66
3:A:245:ASN:N	3:A:245:ASN:ND2	2.44	0.65
3:A:330:PRO:HA	3:A:333:ARG:CG	2.26	0.65
3:A:201:THR:HG23	3:A:204:SER:HB3	1.78	0.65
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.20	0.65
2:P:2:DA:C8	2:P:2:DA:H5'	2.32	0.65
3:A:41:LYS:NZ	3:A:64:GLY:O	2.28	0.65
3:A:121:THR:N	3:A:124:ASP:OD2	2.30	0.64
3:A:31:GLN:N	5:A:641:HOH:O	2.26	0.64
3:A:41:LYS:O	3:A:45:VAL:HG13	1.96	0.64
3:A:133:ASN:H	3:A:136:GLN:NE2	1.96	0.64
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.80	0.64
3:A:194:LEU:HD12	3:A:258:ARG:HG3	1.78	0.64
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.79	0.63
3:A:16:THR:O	3:A:20:THR:HG23	1.98	0.63
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.64	0.63
3:A:18:MET:CE	3:A:76:PHE:HB2	2.27	0.63
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.79	0.63
3:A:12:ASN:ND2	3:A:53:ILE:H	1.98	0.62
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.14	0.62
3:A:33:ILE:O	3:A:37:ASN:HB2	1.99	0.62
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.12	0.62
3:A:306:VAL:HG23	3:A:307:ALA:N	2.13	0.62
3:A:183:ARG:HH11	3:A:275:SER:HA	1.65	0.62
3:A:41:LYS:HD3	3:A:42:ALA:N	2.14	0.62
3:A:319:ILE:O	3:A:322:TYR:HB2	1.99	0.62
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.80	0.62
3:A:150:ILE:HB	3:A:155:MET:HE2	1.83	0.61
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.00	0.61
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.83	0.61
3:A:326:LYS:HG3	3:A:326:LYS:O	1.99	0.61
3:A:162:VAL:O	3:A:166:VAL:HG23	2.01	0.60
3:A:132:LEU:HD23	3:A:132:LEU:N	2.15	0.60
3:A:121:THR:O	3:A:124:ASP:HB2	2.03	0.59
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.03	0.58
3:A:11:LEU:HD23	3:A:11:LEU:N	2.16	0.58
3:A:183:ARG:HD3	3:A:273:THR:O	2.04	0.58
3:A:254:ARG:HH11	3:A:255:ILE:H	1.51	0.58
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.34	0.57
3:A:295:GLU:CD	3:A:295:GLU:H	2.11	0.57
3:A:248:LYS:O	3:A:248:LYS:HG2	2.03	0.57
3:A:62:LEU:HB3	3:A:63:PRO:HD2	1.86	0.57
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.69	0.57
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.19	0.57
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.86	0.57
3:A:11:LEU:H	3:A:11:LEU:CD2	2.17	0.56
3:A:279:ASN:O	3:A:283:ARG:N	2.35	0.56
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.87	0.56
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.20	0.56
3:A:180:SER:HB2	3:A:185:ALA:CB	2.36	0.56
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.31	0.56
3:A:113:LYS:O	3:A:117:GLU:HG3	2.06	0.56
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.88	0.55
3:A:321:ASP:O	3:A:324:GLN:N	2.37	0.55
3:A:166:VAL:O	3:A:169:VAL:HG12	2.07	0.55
3:A:120:LYS:N	3:A:124:ASP:OD2	2.30	0.55
3:A:315:SER:OG	3:A:316:GLU:N	2.40	0.55
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.42	0.55
3:A:288:GLU:C	3:A:290:GLY:H	2.16	0.54
3:A:43:ALA:O	3:A:47:ALA:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:DG:H1'	5:P:511:HOH:O	2.07	0.54
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.88	0.54
1:T:6:DT:H2''	1:T:7:DG:C8	2.43	0.54
3:A:133:ASN:O	3:A:137:ARG:HG3	2.08	0.54
3:A:103:VAL:HG22	3:A:143:PHE:CD1	2.42	0.54
3:A:286:ALA:O	3:A:291:PHE:HB2	2.08	0.54
3:A:308:GLY:O	3:A:309:GLU:HB2	2.08	0.54
3:A:23:ALA:O	3:A:36:TYR:HD1	1.91	0.53
3:A:215:VAL:O	3:A:219:GLN:HG3	2.07	0.53
3:A:41:LYS:HD3	3:A:42:ALA:H	1.73	0.53
3:A:245:ASN:H	3:A:245:ASN:ND2	2.04	0.53
3:A:327:TYR:CD1	3:A:328:ARG:N	2.76	0.53
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.06	0.53
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.72	0.53
3:A:236:MET:HG2	3:A:254:ARG:HH22	1.74	0.53
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.43	0.53
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.09	0.52
3:A:292:THR:CG2	3:A:299:ARG:HH21	2.23	0.52
3:A:155:MET:HE3	3:A:188:SER:HB2	1.92	0.52
3:A:254:ARG:HH11	3:A:255:ILE:N	2.07	0.52
3:A:179:GLY:O	3:A:182:ARG:HB3	2.09	0.52
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.75	0.52
3:A:292:THR:C	3:A:293:ILE:HG12	2.31	0.52
2:P:5:DT:C6	2:P:5:DT:C2'	2.91	0.51
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.45	0.51
3:A:134:HIS:NE2	3:A:138:ILE:HD11	2.26	0.51
3:A:152:ARG:NH2	3:A:181:PHE:O	2.42	0.51
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.76	0.51
3:A:69:ILE:O	3:A:73:ILE:HG13	2.10	0.51
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.92	0.51
3:A:276:ASP:O	3:A:280:LYS:HG3	2.11	0.50
3:A:44:SER:O	3:A:47:ALA:HB3	2.12	0.50
3:A:205:THR:O	3:A:206:LYS:O	2.29	0.50
3:A:293:ILE:HG23	3:A:298:ILE:HG13	1.93	0.50
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.25	0.50
3:A:183:ARG:HH11	3:A:275:SER:CA	2.25	0.50
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.19	0.50
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.47	0.50
3:A:155:MET:CE	3:A:188:SER:HB2	2.41	0.49
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.45	0.49
3:A:254:ARG:NH1	3:A:255:ILE:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.36	0.49
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.23	0.49
3:A:242:PRO:HG2	5:A:589:HOH:O	2.12	0.49
3:A:292:THR:O	3:A:298:ILE:HA	2.12	0.49
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.94	0.49
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.95	0.49
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.48	0.49
3:A:175:ALA:HB2	3:A:195:LEU:CD1	2.43	0.49
3:A:254:ARG:NH1	3:A:255:ILE:H	2.11	0.49
3:A:68:LYS:O	3:A:71:GLU:HB3	2.13	0.48
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.49	0.48
3:A:32:ALA:O	3:A:36:TYR:N	2.32	0.48
3:A:150:ILE:N	3:A:188:SER:O	2.41	0.48
3:A:183:ARG:NH1	3:A:275:SER:HA	2.28	0.48
3:A:41:LYS:H	3:A:41:LYS:HD2	1.79	0.48
3:A:145:ASP:CG	3:A:252:HIS:H	2.22	0.48
3:A:194:LEU:CD1	3:A:258:ARG:HG3	2.44	0.48
3:A:255:ILE:O	3:A:255:ILE:HG23	2.13	0.48
3:A:288:GLU:O	3:A:290:GLY:N	2.47	0.48
3:A:169:VAL:HG13	3:A:170:ASP:N	2.29	0.47
3:A:299:ARG:HB3	3:A:300:PRO:CD	2.40	0.47
3:A:200:PHE:HB2	5:A:625:HOH:O	2.14	0.47
3:A:325:TRP:HD1	5:A:583:HOH:O	1.97	0.47
3:A:155:MET:HA	3:A:158:MET:HE2	1.97	0.47
3:A:63:PRO:C	3:A:65:VAL:H	2.23	0.47
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.30	0.47
3:A:250:TYR:HB3	3:A:251:PRO:CD	2.45	0.47
3:A:145:ASP:HB3	3:A:252:HIS:O	2.14	0.46
3:A:199:SER:O	3:A:199:SER:OG	2.30	0.46
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.50	0.46
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.70	0.46
3:A:285:HIS:NE2	3:A:289:LYS:HG3	2.30	0.46
3:A:56:GLY:HA3	3:A:74:ASP:OD2	2.15	0.46
3:A:292:THR:HG21	3:A:299:ARG:HH21	1.81	0.46
3:A:155:MET:SD	3:A:158:MET:HE3	2.56	0.46
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.89	0.46
2:P:2:DA:H5'	2:P:2:DA:H8	1.76	0.46
3:A:62:LEU:HB3	3:A:63:PRO:CD	2.45	0.46
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.45	0.46
3:A:268:GLY:O	3:A:271:TYR:HB3	2.16	0.46
3:A:314:ASP:N	3:A:318:ASP:OD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:HG22	3:A:143:PHE:CE1	2.50	0.45
3:A:150:ILE:HG13	3:A:188:SER:O	2.16	0.45
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.52	0.45
3:A:138:ILE:H	3:A:138:ILE:HG12	1.48	0.45
3:A:200:PHE:O	3:A:262:LYS:N	2.36	0.45
3:A:211:LEU:HB2	3:A:259:LEU:HD22	1.99	0.45
3:A:80:GLY:O	3:A:81:LYS:HG2	2.17	0.45
3:A:176:THR:HG22	3:A:178:CYS:SG	2.56	0.45
3:A:32:ALA:O	3:A:36:TYR:HB3	2.16	0.45
3:A:201:THR:OG1	3:A:202:SER:N	2.50	0.45
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.67	0.45
3:A:56:GLY:O	3:A:59:ALA:N	2.50	0.45
3:A:80:GLY:C	3:A:81:LYS:HG2	2.42	0.45
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.76	0.45
3:A:97:ILE:O	3:A:101:THR:HB	2.17	0.44
3:A:210:LEU:HD23	3:A:210:LEU:HA	1.81	0.44
3:A:228:LEU:HB2	3:A:236:MET:O	2.17	0.44
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.47	0.44
3:A:209:LYS:HD3	3:A:209:LYS:HA	1.54	0.44
3:A:88:ILE:HD13	3:A:88:ILE:HG21	1.74	0.44
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.63	0.44
2:P:5:DT:N1	2:P:5:DT:H1'	2.07	0.44
3:A:15:ILE:HD11	3:A:77:LEU:CD1	2.47	0.44
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.48	0.44
2:P:2:DA:H5'	2:P:2:DA:H2'	1.33	0.44
3:A:27:LYS:CG	3:A:28:ASN:ND2	2.80	0.44
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.44
3:A:294:ASN:C	3:A:294:ASN:HD22	2.24	0.44
3:A:303:VAL:C	3:A:305:GLY:H	2.25	0.44
3:A:202:SER:HB2	3:A:263:ASP:CG	2.42	0.44
3:A:244:LYS:CB	3:A:245:ASN:ND2	2.78	0.44
3:A:311:LEU:HD12	3:A:311:LEU:HA	1.69	0.44
3:A:330:PRO:HA	3:A:333:ARG:HG2	2.00	0.44
3:A:11:LEU:N	3:A:11:LEU:CD2	2.79	0.43
3:A:49:TYR:CE2	3:A:53:ILE:HG12	2.53	0.43
3:A:119:ILE:HA	3:A:124:ASP:HB3	1.99	0.43
3:A:201:THR:HG1	3:A:263:ASP:CG	2.20	0.43
3:A:76:PHE:O	3:A:79:THR:O	2.36	0.43
3:A:103:VAL:HG12	3:A:104:SER:N	2.33	0.43
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.18	0.43
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.09	0.43
3:A:236:MET:HG2	3:A:254:ARG:NH2	2.33	0.43
3:A:138:ILE:HG22	3:A:142:TYR:CD2	2.53	0.43
3:A:196:THR:OG1	3:A:197:HIS:N	2.51	0.43
3:A:174:ILE:HD13	3:A:174:ILE:HG21	1.67	0.43
3:A:35:LYS:O	3:A:38:ALA:HB3	2.19	0.43
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.83	0.43
3:A:135:HIS:C	3:A:135:HIS:CD2	2.97	0.43
3:A:12:ASN:CB	3:A:46:ILE:HD12	2.49	0.43
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.65	0.43
3:A:194:LEU:CD1	3:A:258:ARG:CG	2.97	0.42
3:A:15:ILE:HG12	3:A:73:ILE:HG23	2.01	0.42
3:A:322:TYR:HD1	3:A:322:TYR:HA	1.62	0.42
3:A:122:LEU:O	3:A:126:ARG:HG3	2.19	0.42
3:A:36:TYR:CD2	3:A:37:ASN:N	2.87	0.42
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.54	0.42
3:A:152:ARG:O	3:A:155:MET:HB2	2.20	0.42
3:A:299:ARG:HE	3:A:299:ARG:HB2	1.61	0.42
3:A:237:GLY:C	3:A:238:VAL:HG23	2.43	0.42
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.71	0.42
3:A:322:TYR:C	3:A:324:GLN:H	2.28	0.42
2:P:3:DG:N3	5:P:511:HOH:O	2.37	0.42
3:A:241:LEU:HA	3:A:242:PRO:HD3	1.83	0.42
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.35	0.42
3:A:42:ALA:O	3:A:46:ILE:HG23	2.20	0.41
3:A:243:SER:HB3	3:A:249:GLU:HA	2.02	0.41
3:A:150:ILE:O	3:A:188:SER:N	2.45	0.41
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.46	0.41
3:A:33:ILE:HG23	3:A:34:HIS:N	2.36	0.41
3:A:287:LEU:HD12	3:A:287:LEU:O	2.20	0.41
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.56	0.41
3:A:155:MET:SD	3:A:158:MET:CE	3.09	0.41
3:A:194:LEU:HD13	3:A:258:ARG:HD3	2.03	0.41
3:A:243:SER:OG	3:A:249:GLU:HG3	2.21	0.41
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.93	0.41
3:A:62:LEU:CB	3:A:63:PRO:HD2	2.47	0.41
3:A:265:TYR:O	3:A:269:VAL:HG23	2.21	0.41
3:A:289:LYS:HG3	3:A:323:ILE:O	2.21	0.41
3:A:327:TYR:HD1	3:A:328:ARG:N	2.18	0.41
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.51	0.41
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.40
3:A:163:LEU:HA	3:A:163:LEU:HD23	1.85	0.40
3:A:264:GLN:HE21	3:A:264:GLN:HB3	1.33	0.40
3:A:59:ALA:C	3:A:61:LYS:N	2.78	0.40
3:A:10:THR:O	3:A:10:THR:HG23	2.20	0.40
3:A:172:GLU:CG	3:A:198:PRO:CG	2.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:ARG:NH1	3:A:117:GLU:CB[3_558]	1.80	0.40

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%)	284 (87%)	24 (7%)	17 (5%)	1 5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU
3	A	289	LYS
3	A	309	GLU
3	A	10	THR
3	A	202	SER
3	A	246	ASP

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Mol	Chain	Res	Type
3	A	334	SER
3	A	264	GLN
3	A	91	ASP
3	A	324	GLN
3	A	307	ALA
3	A	80	GLY
3	A	310	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
3	A	288/295 (98%)	216 (75%)	72 (25%)	0 2

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	79	THR
3	A	81	LYS

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Mol	Chain	Res	Type
3	A	85	LEU
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	112	ARG
3	A	113	LYS
3	A	119	ILE
3	A	121	THR
3	A	132	LEU
3	A	138	ILE
3	A	140	LEU
3	A	150	ILE
3	A	152	ARG
3	A	153	GLU
3	A	168	LYS
3	A	171	SER
3	A	172	GLU
3	A	182	ARG
3	A	188	SER
3	A	192	ASP
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	202	SER
3	A	204	SER
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	228	LEU
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	259	LEU
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
3	A	289	LYS
3	A	292	THR
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU

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Mol	Chain	Res	Type
3	A	296	TYR
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	51	HIS
3	A	90	GLN
3	A	98	ASN
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN

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 [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 [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	7/7 (100%)	-1.33	0 100 100	22, 33, 64, 100	0
2	P	6/6 (100%)	-1.50	0 100 100	24, 28, 33, 37	0
3	A	324/335 (96%)	-1.03	0 100 100	9, 36, 83, 99	0
All	All	337/348 (96%)	-1.04	0 100 100	9, 35, 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	NA	A	342	1/1	0.99	0.06	54,54,54,54	0
4	NA	A	341	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.