



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 09:47 AM UTC

PDB ID : 7ICT / pdb_00007ict
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX, SOAKED IN THE PRESENCE OF ZNCL2 AND MGCL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
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

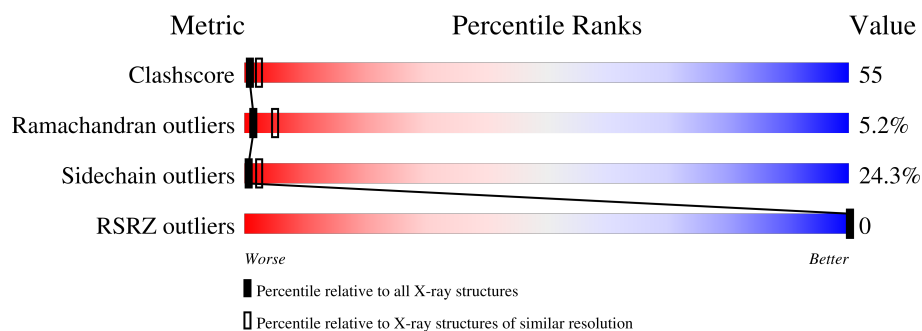
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

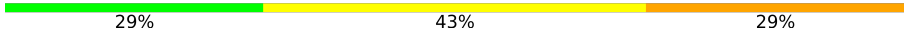
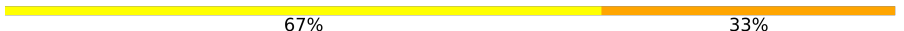
The reported resolution of this entry is 2.80 Å.

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	 29% 43% 29%
2	P	6	 67% 33%
3	A	335	 23% 41% 26% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3022 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 ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	22	Total 22	O 22	0	0
6	A	113	Total 113	O 113	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.

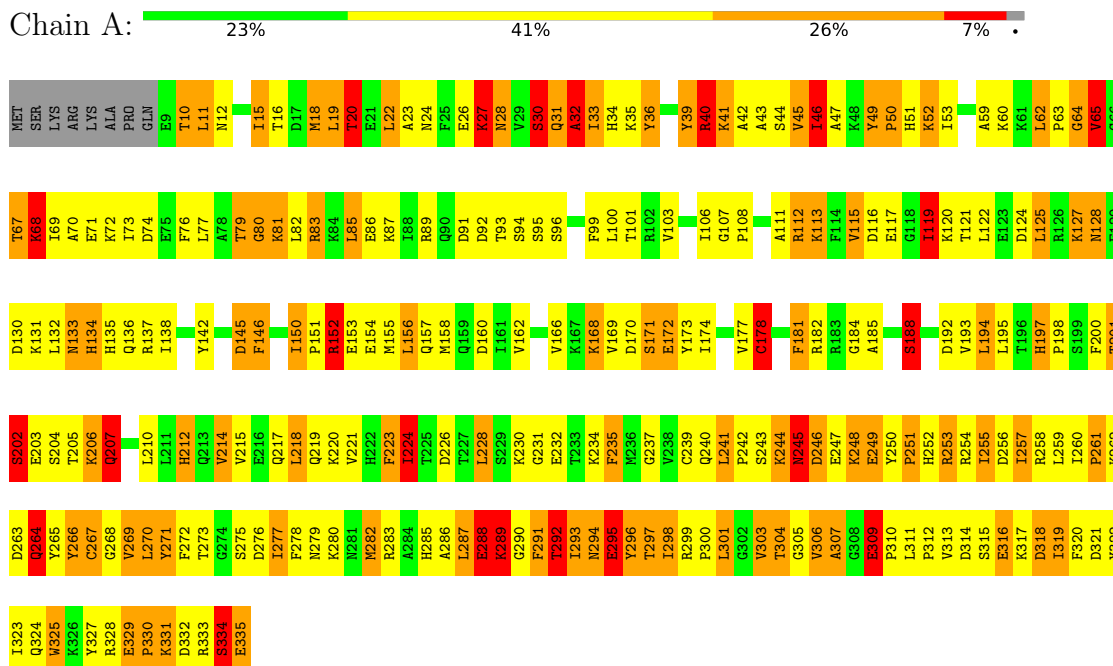
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- 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	178.78Å 57.74Å 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)	92.0 (20.00-2.80) 91.3 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	4.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.168 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 202.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3022	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 5.40% 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: ZN, 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	0.97	0/135	3.25	9/207 (4.3%)
2	P	1.35	2/141 (1.4%)	2.52	9/214 (4.2%)
3	A	1.67	24/2672 (0.9%)	2.17	120/3590 (3.3%)
All	All	1.63	26/2948 (0.9%)	2.26	138/4011 (3.4%)

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	3	0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DT	C1'-N1	7.73	1.72	1.49
3	A	160	ASP	C-N	-6.77	1.25	1.33
3	A	15	ILE	CA-C	-6.49	1.44	1.52
3	A	120	LYS	CA-C	-6.45	1.44	1.52
3	A	24	ASN	C-N	-6.40	1.25	1.33
3	A	224	ILE	CA-C	-6.39	1.45	1.52
3	A	15	ILE	CA-CB	-6.37	1.47	1.54
2	P	1	DC	OP3-P	6.31	1.61	1.48
3	A	160	ASP	C-O	-6.29	1.16	1.24
3	A	119	ILE	CA-C	-6.21	1.45	1.52
3	A	257	ILE	CA-CB	-5.96	1.47	1.54
3	A	330	PRO	N-CA	-5.78	1.40	1.47
3	A	125	LEU	CA-C	-5.76	1.45	1.52
3	A	269	VAL	N-CA	-5.58	1.39	1.46
3	A	36	TYR	N-CA	-5.49	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	94	SER	N-CA	-5.44	1.40	1.46
3	A	119	ILE	CA-CB	-5.33	1.47	1.54
3	A	115	VAL	CA-CB	-5.31	1.47	1.54
3	A	107	GLY	C-N	-5.26	1.26	1.34
3	A	27	LYS	N-CA	-5.24	1.40	1.46
3	A	220	LYS	C-O	-5.12	1.18	1.24
3	A	251	PRO	N-CA	-5.12	1.41	1.47
3	A	145	ASP	CG-OD2	5.05	1.34	1.25
3	A	212	HIS	C-N	-5.04	1.27	1.33
3	A	171	SER	CA-C	-5.04	1.45	1.52
3	A	271	TYR	CA-CB	-5.02	1.45	1.53

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	4	DT	C6-N1-C1'	-24.17	83.09	119.35
1	T	4	DT	C2-N1-C1'	22.97	153.81	119.35
2	P	5	DT	C2-N1-C1'	15.80	143.05	119.35
2	P	5	DT	C6-N1-C1'	-13.92	98.47	119.35
3	A	49	TYR	CA-C-N	12.12	134.99	119.84
3	A	49	TYR	C-N-CA	12.12	134.99	119.84
1	T	5	DC	C2-N1-C1'	11.76	137.34	119.70
1	T	5	DC	C6-N1-C1'	-11.57	102.34	119.70
1	T	6	DT	C6-N1-C1'	-11.21	102.54	119.35
3	A	49	TYR	O-C-N	10.71	129.82	121.47
3	A	34	HIS	CA-CB-CG	-10.51	103.29	113.80
3	A	116	ASP	CA-CB-CG	-10.28	102.33	112.60
2	P	1	DC	C6-N1-C1'	-9.60	105.31	119.70
1	T	6	DT	C2-N1-C1'	9.50	133.60	119.35
3	A	40	ARG	N-CA-C	9.42	121.54	111.28
2	P	1	DC	C2-N1-C1'	9.10	133.35	119.70
3	A	192	ASP	CB-CA-C	-9.07	96.27	110.78
3	A	86	GLU	N-CA-CB	8.49	122.33	110.01
3	A	64	GLY	N-CA-C	-8.38	103.36	114.25
3	A	30	SER	CA-C-N	-8.27	109.11	122.26
3	A	30	SER	C-N-CA	-8.27	109.11	122.26
3	A	39	TYR	N-CA-CB	8.22	122.40	110.06
3	A	99	PHE	CA-CB-CG	-8.11	105.69	113.80
3	A	261	PRO	CB-CA-C	-8.09	101.44	111.64
3	A	168	LYS	N-CA-CB	7.84	121.81	110.06
3	A	272	PHE	CA-CB-CG	-7.75	106.05	113.80
3	A	318	ASP	CA-CB-CG	-7.71	104.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	6	DG	C8-N9-C1'	7.67	138.50	127.00
2	P	6	DG	C4-N9-C1'	-7.57	115.64	127.00
3	A	32	ALA	N-CA-C	7.52	126.81	110.80
3	A	181	PHE	CA-C-N	7.48	130.62	120.44
3	A	181	PHE	C-N-CA	7.48	130.62	120.44
1	T	4	DT	O4'-C1'-N1	7.38	119.48	108.40
3	A	67	THR	N-CA-C	7.25	118.83	111.07
3	A	291	PHE	N-CA-C	7.13	119.77	109.14
3	A	304	THR	N-CA-CB	-7.11	98.47	110.49
3	A	28	ASN	N-CA-C	7.01	119.00	111.36
3	A	329	GLU	N-CA-C	-7.00	101.55	109.60
1	T	4	DT	N1-C1'-C2'	6.97	123.95	113.50
3	A	156	LEU	N-CA-CB	6.97	120.36	110.12
3	A	107	GLY	N-CA-C	-6.91	98.24	112.34
3	A	330	PRO	N-CA-CB	6.91	110.93	103.33
3	A	65	VAL	N-CA-CB	6.89	119.79	111.31
3	A	67	THR	CB-CA-C	6.87	121.67	110.88
3	A	20	THR	CB-CA-C	6.78	122.05	110.79
3	A	296	TYR	N-CA-C	6.69	121.61	113.38
3	A	96	SER	O-C-N	6.63	129.15	122.12
3	A	50	PRO	CB-CA-C	-6.63	100.61	111.56
3	A	192	ASP	CA-CB-CG	6.63	119.23	112.60
3	A	152	ARG	N-CA-CB	6.53	120.46	110.14
3	A	319	ILE	N-CA-CB	6.43	117.63	110.62
2	P	3	DG	P-O3'-C3'	6.42	129.82	120.20
3	A	303	VAL	N-CA-C	6.32	120.88	112.04
3	A	86	GLU	CB-CA-C	6.26	120.72	110.88
3	A	292	THR	CB-CA-C	6.26	121.03	109.70
3	A	235	PHE	CA-CB-CG	-6.23	107.57	113.80
3	A	65	VAL	N-CA-C	6.19	117.38	107.73
3	A	297	THR	CB-CA-C	-6.12	99.66	111.78
3	A	288	GLU	N-CA-C	-6.09	104.27	111.03
3	A	83	ARG	N-CA-CB	6.05	118.78	110.01
3	A	319	ILE	N-CA-C	6.03	116.15	110.30
3	A	246	ASP	N-CA-C	6.01	123.61	110.80
3	A	228	LEU	N-CA-C	-5.95	102.46	111.56
3	A	309	GLU	CA-C-N	5.91	127.23	119.84
3	A	309	GLU	C-N-CA	5.91	127.23	119.84
3	A	188	SER	CA-C-N	5.91	126.38	119.94
3	A	188	SER	C-N-CA	5.91	126.38	119.94
3	A	296	TYR	CB-CA-C	-5.88	99.42	109.65
2	P	1	DC	P-O3'-C3'	5.86	128.99	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	240	GLN	CB-CA-C	-5.86	98.76	110.42
3	A	249	GLU	CA-C-N	-5.83	113.04	122.48
3	A	249	GLU	C-N-CA	-5.83	113.04	122.48
3	A	68	LYS	N-CA-C	5.75	117.55	111.28
3	A	131	LYS	N-CA-C	5.70	119.97	113.19
3	A	15	ILE	N-CA-CB	5.69	116.82	110.51
3	A	87	LYS	CB-CA-C	5.67	120.20	110.79
3	A	241	LEU	C-N-CD	-5.63	101.91	125.00
3	A	292	THR	N-CA-CB	5.61	120.51	110.80
3	A	40	ARG	CA-C-N	-5.60	112.34	120.29
3	A	40	ARG	C-N-CA	-5.60	112.34	120.29
3	A	46	ILE	N-CA-CB	5.59	120.22	110.65
3	A	31	GLN	CB-CA-C	5.59	118.94	109.55
3	A	92	ASP	N-CA-CB	5.59	118.43	110.16
3	A	28	ASN	CA-CB-CG	-5.58	107.02	112.60
3	A	68	LYS	CA-CB-CG	-5.58	102.95	114.10
3	A	267	CYS	N-CA-C	-5.57	104.83	111.69
3	A	330	PRO	CB-CA-C	5.57	121.81	112.62
3	A	92	ASP	CB-CA-C	5.56	120.31	110.85
3	A	146	PHE	CA-CB-CG	-5.56	108.24	113.80
1	T	3	DA	P-O5'-C5'	5.54	128.31	120.00
3	A	301	LEU	N-CA-C	5.53	117.74	108.96
3	A	329	GLU	N-CA-CB	5.53	117.87	109.75
3	A	178	CYS	CB-CA-C	5.51	121.38	110.42
3	A	270	LEU	O-C-N	5.50	127.97	122.03
3	A	316	GLU	CA-C-N	5.50	127.92	120.44
3	A	316	GLU	C-N-CA	5.50	127.92	120.44
3	A	40	ARG	N-CA-CB	5.49	118.18	110.12
3	A	197	HIS	CA-C-N	5.48	124.94	119.24
3	A	197	HIS	C-N-CA	5.48	124.94	119.24
3	A	266	TYR	CA-CB-CG	-5.48	104.04	113.90
3	A	20	THR	N-CA-CB	5.47	118.16	110.12
3	A	116	ASP	CA-C-N	-5.47	111.88	122.06
3	A	116	ASP	C-N-CA	-5.47	111.88	122.06
2	P	5	DT	C4'-C3'-O3'	-5.47	101.80	110.00
3	A	31	GLN	CA-C-N	5.40	131.86	121.54
3	A	31	GLN	C-N-CA	5.40	131.86	121.54
3	A	232	GLU	N-CA-CB	5.39	118.69	110.44
3	A	264	GLN	CB-CG-CD	-5.36	103.49	112.60
3	A	184	GLY	N-CA-C	5.35	121.05	114.69
3	A	127	LYS	CA-C-N	-5.34	115.22	123.17
3	A	127	LYS	C-N-CA	-5.34	115.22	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	181	PHE	CB-CA-C	-5.33	101.62	110.68
3	A	171	SER	O-C-N	5.32	128.27	122.20
3	A	214	VAL	N-CA-CB	5.29	118.51	110.58
3	A	181	PHE	O-C-N	5.27	127.70	122.12
3	A	295	GLU	CB-CA-C	5.26	119.13	110.88
3	A	334	SER	CB-CA-C	5.24	120.84	110.42
3	A	74	ASP	N-CA-CB	5.23	117.55	109.91
3	A	245	ASN	CB-CA-C	5.23	119.45	111.76
3	A	70	ALA	N-CA-C	-5.23	105.50	111.14
3	A	309	GLU	N-CA-C	5.21	121.32	109.81
3	A	134	HIS	N-CA-C	5.20	117.36	111.02
3	A	203	GLU	O-C-N	5.19	128.99	122.19
3	A	269	VAL	CA-C-N	-5.18	113.58	120.63
3	A	269	VAL	C-N-CA	-5.18	113.58	120.63
3	A	96	SER	N-CA-C	5.15	116.90	111.28
3	A	87	LYS	CA-C-N	5.14	127.14	120.56
3	A	87	LYS	C-N-CA	5.14	127.14	120.56
3	A	85	LEU	N-CA-C	-5.11	105.79	111.36
3	A	297	THR	N-CA-C	5.10	115.08	107.88
3	A	46	ILE	CA-CB-CG2	5.08	119.13	110.50
3	A	246	ASP	N-CA-CB	5.07	119.06	110.49
3	A	223	PHE	CA-CB-CG	-5.06	108.74	113.80
3	A	207	GLN	CA-C-N	5.04	124.53	119.19
3	A	207	GLN	C-N-CA	5.04	124.53	119.19
3	A	241	LEU	O-C-N	5.03	125.86	121.18
3	A	49	TYR	CA-C-O	5.03	123.96	119.59
3	A	269	VAL	CB-CA-C	-5.02	104.38	112.16

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	40	ARG	CA
3	A	86	GLU	CA
3	A	246	ASP	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	122	0	69	6	0
2	P	126	0	68	12	0
3	A	2623	0	2641	289	1
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	113	0	0	13	0
6	P	22	0	0	1	0
6	T	13	0	0	2	0
All	All	3022	0	2778	304	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 55.

All (304) 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'	1.72	1.51
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.26	1.14
2:P:5:DT:C1'	2:P:5:DT:C6	2.37	1.07
2:P:1:DC:H2''	2:P:2:DA:H5''	1.40	1.03
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.42	1.02
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.49	0.94
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.51	0.91
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.05	0.91
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.68	0.90
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.09	0.87
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.55	0.87
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.56	0.86
3:A:245:ASN:N	3:A:245:ASN:HD22	1.74	0.86
3:A:11:LEU:HD23	3:A:11:LEU:H	1.39	0.85
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.58	0.83
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.61	0.82
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.25	0.82
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.60	0.81
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.09	0.81
2:P:1:DC:H2''	2:P:2:DA:C5'	2.11	0.80
3:A:300:PRO:HD3	3:A:311:LEU:CD1	2.13	0.79
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.11	0.79
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.13	0.79
3:A:271:TYR:HB2	6:A:592:HOH:O	1.82	0.79
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.14	0.78
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.66	0.78
3:A:68:LYS:O	3:A:72:LYS:HE3	1.83	0.78
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.80	0.77
3:A:207:GLN:HB3	3:A:210:LEU:HD12	1.64	0.77
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.66	0.77
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.67	0.77
3:A:85:LEU:O	3:A:89:ARG:HG3	1.83	0.77
3:A:207:GLN:O	3:A:210:LEU:HB2	1.85	0.76
3:A:41:LYS:HD3	3:A:42:ALA:H	1.51	0.75
3:A:133:ASN:H	3:A:136:GLN:HE21	1.33	0.74
3:A:69:ILE:O	3:A:73:ILE:HG13	1.86	0.74
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.16	0.74
3:A:16:THR:O	3:A:20:THR:HG23	1.88	0.74
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.17	0.74
3:A:155:MET:HE3	3:A:188:SER:OG	1.88	0.73
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.89	0.73
3:A:59:ALA:O	3:A:62:LEU:HB2	1.89	0.72
3:A:202:SER:HB2	3:A:263:ASP:OD1	1.88	0.72
3:A:331:LYS:HD2	3:A:332:ASP:N	2.03	0.72
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.19	0.72
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.19	0.72
3:A:15:ILE:O	3:A:19:LEU:HD22	1.89	0.72
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.71	0.71
3:A:154:GLU:O	3:A:158:MET:HG3	1.89	0.71
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.20	0.71
3:A:41:LYS:HD3	3:A:42:ALA:N	2.06	0.71
3:A:215:VAL:O	3:A:219:GLN:HG3	1.92	0.70
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.40	0.69
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.73	0.69
3:A:255:ILE:HG12	3:A:256:ASP:N	2.05	0.69
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.06	0.69
3:A:113:LYS:O	3:A:117:GLU:HG3	1.92	0.69
3:A:267:CYS:SG	3:A:297:THR:HA	2.32	0.69
3:A:80:GLY:O	3:A:81:LYS:HG2	1.92	0.68
2:P:5:DT:C6	2:P:5:DT:C2'	2.76	0.68
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.75	0.68
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.74	0.68
3:A:306:VAL:HG23	3:A:307:ALA:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:202:SER:HB2	3:A:263:ASP:CG	2.19	0.68
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.29	0.67
3:A:262:LYS:O	3:A:262:LYS:HG3	1.94	0.67
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.10	0.67
3:A:121:THR:O	3:A:124:ASP:HB2	1.95	0.66
3:A:12:ASN:HD21	3:A:53:ILE:H	1.44	0.66
3:A:319:ILE:O	3:A:322:TYR:HB2	1.95	0.66
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.60	0.66
3:A:79:THR:O	3:A:81:LYS:N	2.26	0.65
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.30	0.65
3:A:31:GLN:N	6:A:641:HOH:O	2.30	0.65
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.79	0.65
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.78	0.64
1:T:7:DG:N3	6:T:634:HOH:O	2.30	0.64
3:A:44:SER:O	3:A:47:ALA:HB3	1.98	0.64
3:A:155:MET:SD	3:A:158:MET:HE3	2.38	0.64
3:A:245:ASN:N	3:A:245:ASN:ND2	2.46	0.64
3:A:150:ILE:HG21	3:A:158:MET:CE	2.28	0.64
3:A:253:ARG:NH1	6:A:503:HOH:O	2.29	0.63
3:A:166:VAL:O	3:A:169:VAL:HG12	1.98	0.63
3:A:267:CYS:N	6:A:508:HOH:O	2.29	0.63
2:P:5:DT:H6	2:P:5:DT:H2'	1.63	0.63
3:A:133:ASN:ND2	3:A:136:GLN:H	1.97	0.63
3:A:278:PHE:HB2	3:A:333:ARG:O	1.99	0.63
3:A:152:ARG:NH2	3:A:181:PHE:O	2.32	0.62
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.34	0.62
3:A:278:PHE:CE1	3:A:328:ARG:HD2	2.34	0.62
3:A:28:ASN:HD22	3:A:28:ASN:N	1.95	0.62
3:A:254:ARG:HH11	3:A:255:ILE:H	1.45	0.62
3:A:212:HIS:HB3	6:A:541:HOH:O	1.98	0.62
3:A:11:LEU:H	3:A:11:LEU:CD2	2.11	0.62
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.81	0.62
3:A:259:LEU:O	3:A:260:ILE:HD13	2.01	0.61
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.82	0.61
3:A:124:ASP:O	3:A:128:ASN:ND2	2.29	0.61
3:A:207:GLN:HB3	3:A:210:LEU:CD1	2.30	0.61
3:A:333:ARG:NH1	6:A:584:HOH:O	2.29	0.61
3:A:41:LYS:NZ	3:A:64:GLY:O	2.30	0.60
3:A:201:THR:HA	3:A:261:PRO:CB	2.31	0.60
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.32	0.60
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.32	0.60
3:A:254:ARG:NH1	3:A:255:ILE:H	2.00	0.59
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.65	0.59
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.37	0.59
3:A:150:ILE:HD13	3:A:253:ARG:CG	2.31	0.59
1:T:4:DT:H2''	1:T:5:DC:O5'	2.01	0.59
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.38	0.59
3:A:254:ARG:NH1	3:A:255:ILE:N	2.51	0.59
3:A:68:LYS:O	3:A:71:GLU:HB3	2.03	0.59
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.15	0.58
3:A:288:GLU:C	3:A:290:GLY:H	2.11	0.58
3:A:133:ASN:O	3:A:137:ARG:HG3	2.04	0.58
3:A:26:GLU:HA	3:A:30:SER:OG	2.04	0.58
3:A:18:MET:HE1	3:A:76:PHE:CB	2.33	0.58
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.03	0.58
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.34	0.58
2:P:2:DA:C8	2:P:2:DA:H5'	2.39	0.57
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.86	0.57
3:A:278:PHE:CZ	3:A:333:ARG:HD3	2.39	0.57
3:A:157:GLN:NE2	3:A:244:LYS:HZ1	2.01	0.57
3:A:217:GLN:HA	3:A:217:GLN:HE21	1.69	0.57
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.42	0.57
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.92	0.57
6:T:617:HOH:O	3:A:234:LYS:HD3	2.05	0.56
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.35	0.56
3:A:49:TYR:CZ	3:A:51:HIS:HB2	2.40	0.56
3:A:157:GLN:NE2	3:A:244:LYS:HZ3	2.04	0.56
3:A:254:ARG:HH11	3:A:255:ILE:N	2.03	0.56
3:A:287:LEU:HD12	3:A:287:LEU:O	2.06	0.56
3:A:133:ASN:H	3:A:136:GLN:NE2	2.00	0.55
3:A:155:MET:O	3:A:158:MET:HB2	2.05	0.55
3:A:157:GLN:HE21	3:A:244:LYS:NZ	2.03	0.55
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.89	0.55
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.89	0.55
3:A:253:ARG:CG	3:A:253:ARG:HH11	2.20	0.55
3:A:133:ASN:C	3:A:133:ASN:HD22	2.15	0.54
3:A:18:MET:HE3	3:A:76:PHE:CD2	2.43	0.54
3:A:245:ASN:HD22	3:A:245:ASN:H	1.51	0.54
3:A:41:LYS:O	3:A:45:VAL:HG13	2.07	0.54
3:A:169:VAL:HG13	3:A:170:ASP:N	2.22	0.54
3:A:294:ASN:C	3:A:294:ASN:HD22	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:277:ILE:CG1	3:A:335:GLU:HA	2.38	0.54
3:A:150:ILE:N	3:A:188:SER:O	2.37	0.53
3:A:152:ARG:HA	3:A:155:MET:HB2	1.88	0.53
3:A:328:ARG:O	3:A:333:ARG:NE	2.32	0.53
3:A:300:PRO:HD3	3:A:311:LEU:HD11	1.89	0.53
3:A:313:VAL:HG13	3:A:318:ASP:HB2	1.91	0.53
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.74	0.53
3:A:200:PHE:HB2	6:A:625:HOH:O	2.07	0.53
3:A:162:VAL:O	3:A:166:VAL:HG23	2.09	0.52
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.90	0.52
3:A:325:TRP:HD1	6:A:583:HOH:O	1.92	0.52
3:A:289:LYS:HG3	3:A:324:GLN:HG3	1.92	0.52
3:A:155:MET:HA	3:A:158:MET:HE3	1.92	0.52
3:A:288:GLU:O	3:A:290:GLY:N	2.41	0.52
3:A:201:THR:HG23	3:A:204:SER:HB3	1.92	0.51
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.10	0.51
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.90	0.51
3:A:15:ILE:HG22	3:A:19:LEU:HD22	1.93	0.51
3:A:150:ILE:HG13	3:A:188:SER:O	2.10	0.51
1:T:4:DT:H2''	1:T:5:DC:C5'	2.41	0.51
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.51	0.51
3:A:292:THR:O	3:A:298:ILE:HA	2.10	0.51
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.51
3:A:33:ILE:HA	3:A:36:TYR:HB3	1.91	0.51
3:A:321:ASP:O	3:A:324:GLN:N	2.43	0.51
3:A:292:THR:HG23	6:A:580:HOH:O	2.11	0.51
3:A:108:PRO:O	3:A:112:ARG:HG3	2.10	0.50
2:P:5:DT:C2'	2:P:5:DT:H6	2.17	0.50
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.41	0.50
3:A:166:VAL:HG12	3:A:173:TYR:HB3	1.93	0.50
2:P:4:DA:H5''	6:P:614:HOH:O	2.10	0.50
3:A:217:GLN:O	3:A:221:VAL:HG22	2.12	0.50
3:A:295:GLU:CD	3:A:295:GLU:H	2.18	0.50
3:A:43:ALA:O	3:A:47:ALA:HB2	2.12	0.50
3:A:303:VAL:C	3:A:305:GLY:H	2.19	0.50
3:A:27:LYS:HG3	3:A:28:ASN:HD22	1.77	0.50
3:A:264:GLN:HA	6:A:536:HOH:O	2.12	0.49
3:A:323:ILE:O	3:A:324:GLN:HG3	2.12	0.49
1:T:4:DT:O5'	3:A:231:GLY:HA3	2.12	0.49
3:A:248:LYS:O	3:A:248:LYS:HG2	2.12	0.49
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:THR:HA	3:A:261:PRO:HB3	1.95	0.49
3:A:243:SER:HB3	3:A:249:GLU:HA	1.94	0.48
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.95	0.48
3:A:132:LEU:N	3:A:132:LEU:HD23	2.28	0.48
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.28	0.48
3:A:270:LEU:HD12	3:A:316:GLU:OE2	2.14	0.48
3:A:150:ILE:O	3:A:188:SER:N	2.42	0.48
3:A:259:LEU:HD12	3:A:260:ILE:H	1.77	0.48
3:A:133:ASN:HD22	3:A:135:HIS:N	2.11	0.48
3:A:255:ILE:HG23	3:A:255:ILE:O	2.14	0.48
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.43	0.48
3:A:298:ILE:HG22	6:A:578:HOH:O	2.13	0.48
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.97	0.47
3:A:28:ASN:N	3:A:28:ASN:ND2	2.60	0.47
3:A:172:GLU:O	3:A:198:PRO:HD3	2.14	0.47
3:A:11:LEU:O	3:A:12:ASN:ND2	2.48	0.47
3:A:60:LYS:CA	3:A:65:VAL:HG22	2.35	0.47
3:A:63:PRO:C	3:A:65:VAL:H	2.22	0.47
3:A:80:GLY:C	3:A:81:LYS:HG2	2.38	0.47
3:A:276:ASP:O	3:A:280:LYS:HG3	2.15	0.47
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.96	0.47
3:A:173:TYR:OH	3:A:210:LEU:O	2.30	0.47
3:A:223:PHE:CE2	3:A:239:CYS:HB2	2.50	0.47
3:A:261:PRO:HG2	3:A:264:GLN:HG2	1.97	0.47
3:A:26:GLU:HA	3:A:26:GLU:OE1	2.15	0.47
3:A:241:LEU:HB3	3:A:242:PRO:HD2	1.97	0.47
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.45	0.46
3:A:286:ALA:O	3:A:291:PHE:N	2.47	0.46
3:A:200:PHE:HB2	3:A:210:LEU:HD11	1.96	0.46
3:A:79:THR:C	3:A:81:LYS:H	2.20	0.46
3:A:269:VAL:HG12	3:A:269:VAL:O	2.15	0.46
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.45	0.46
3:A:127:LYS:HD2	3:A:127:LYS:HA	1.76	0.46
3:A:260:ILE:HG23	3:A:260:ILE:HD12	1.57	0.45
3:A:254:ARG:HD2	3:A:254:ARG:HA	1.76	0.45
3:A:133:ASN:ND2	3:A:133:ASN:C	2.74	0.45
3:A:275:SER:OG	3:A:334:SER:O	2.28	0.45
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.43	0.45
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.51	0.45
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.42	0.45
3:A:278:PHE:CE2	3:A:333:ARG:CD	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:MET:CE	3:A:76:PHE:HB2	2.41	0.45
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.68	0.45
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.52	0.45
3:A:257:ILE:HG22	3:A:258:ARG:N	2.29	0.45
3:A:32:ALA:O	3:A:36:TYR:N	2.30	0.45
3:A:331:LYS:CD	3:A:332:ASP:N	2.78	0.45
3:A:111:ALA:O	3:A:115:VAL:HG23	2.17	0.44
3:A:205:THR:O	3:A:206:LYS:O	2.35	0.44
3:A:207:GLN:HB2	6:A:625:HOH:O	2.17	0.44
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.60	0.44
3:A:11:LEU:CD2	3:A:11:LEU:N	2.77	0.44
3:A:194:LEU:HD12	3:A:258:ARG:HG2	2.00	0.44
3:A:138:ILE:HG22	3:A:142:TYR:HD2	1.82	0.44
3:A:253:ARG:HG2	3:A:253:ARG:HH11	1.82	0.44
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.52	0.44
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.76	0.44
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.44
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.94	0.44
3:A:52:LYS:HD3	6:A:554:HOH:O	2.18	0.44
1:T:4:DT:O2	2:P:4:DA:H2	2.01	0.43
3:A:244:LYS:CB	3:A:245:ASN:ND2	2.78	0.43
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.07	0.43
2:P:5:DT:N1	2:P:5:DT:H1'	2.09	0.43
3:A:195:LEU:O	3:A:260:ILE:N	2.50	0.43
3:A:142:TYR:CE1	3:A:252:HIS:CG	3.06	0.43
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.26	0.43
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.70	0.43
3:A:320:PHE:CD1	3:A:325:TRP:HE3	2.37	0.43
3:A:218:LEU:HD12	3:A:218:LEU:HA	1.83	0.43
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.70	0.42
3:A:174:ILE:HG21	3:A:174:ILE:HD13	1.72	0.42
3:A:169:VAL:CG1	3:A:170:ASP:N	2.82	0.42
3:A:282:MET:SD	3:A:320:PHE:CE1	3.12	0.42
3:A:177:VAL:HG22	3:A:193:VAL:HG22	2.00	0.42
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.54	0.42
3:A:146:PHE:HD1	3:A:146:PHE:HA	1.58	0.42
3:A:250:TYR:HB3	3:A:251:PRO:CD	2.50	0.42
3:A:265:TYR:O	3:A:268:GLY:N	2.51	0.42
3:A:327:TYR:HD1	3:A:328:ARG:H	1.68	0.42
3:A:145:ASP:CG	3:A:252:HIS:H	2.28	0.42
3:A:223:PHE:CE2	3:A:239:CYS:CB	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:42:ALA:O	3:A:46:ILE:HG23	2.20	0.42
3:A:156:LEU:HD23	3:A:181:PHE:CE1	2.55	0.42
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.96	0.42
3:A:245:ASN:ND2	3:A:245:ASN:H	2.16	0.42
3:A:265:TYR:HB3	3:A:266:TYR:H	1.76	0.42
3:A:68:LYS:NZ	3:A:68:LYS:CB	2.79	0.42
3:A:259:LEU:HD12	3:A:260:ILE:N	2.35	0.42
3:A:237:GLY:O	3:A:254:ARG:NH1	2.53	0.41
3:A:152:ARG:O	3:A:155:MET:HB2	2.20	0.41
3:A:291:PHE:HE1	3:A:311:LEU:HD21	1.85	0.41
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.20	0.41
3:A:288:GLU:C	3:A:290:GLY:N	2.78	0.41
3:A:315:SER:C	3:A:317:LYS:N	2.78	0.41
3:A:235:PHE:CD2	3:A:235:PHE:C	2.96	0.41
3:A:217:GLN:NE2	3:A:217:GLN:CA	2.79	0.41
3:A:221:VAL:HG22	3:A:221:VAL:H	1.46	0.41
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.36	0.41
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.58	0.41
2:P:2:DA:H5'	2:P:2:DA:H2'	1.63	0.41
3:A:151:PRO:HD2	3:A:154:GLU:HB2	2.02	0.41
3:A:306:VAL:O	3:A:307:ALA:HB2	2.21	0.41
3:A:217:GLN:HE21	3:A:217:GLN:CA	2.29	0.41
3:A:293:ILE:HD13	3:A:298:ILE:CD1	2.51	0.41
3:A:311:LEU:CD1	3:A:311:LEU:N	2.83	0.41
3:A:261:PRO:HG2	3:A:264:GLN:HG3	2.02	0.41
3:A:279:ASN:O	3:A:283:ARG:HG3	2.21	0.40
3:A:320:PHE:CE1	3:A:325:TRP:HE3	2.39	0.40
1:T:4:DT:P	3:A:231:GLY:HA3	2.61	0.40
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.95	0.40
3:A:138:ILE:HG22	3:A:142:TYR:CD2	2.55	0.40
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.36	0.40
3:A:18:MET:O	3:A:22:LEU:HD22	2.21	0.40
3:A:27:LYS:CG	3:A:28:ASN:ND2	2.84	0.40
3:A:134:HIS:O	3:A:138:ILE:HG12	2.22	0.40
3:A:119:ILE:HG21	3:A:125:LEU:HD23	2.03	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]	1.98	0.22

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%)	280 (86%)	28 (9%)	17 (5%)	1 5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	80	GLY
3	A	202	SER
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU
3	A	289	LYS
3	A	309	GLU
3	A	334	SER
3	A	10	THR
3	A	246	ASP
3	A	91	ASP
3	A	207	GLN
3	A	307	ALA
3	A	185	ALA
3	A	178	CYS
3	A	312	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	218 (76%)	70 (24%)	1 2

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	18	MET
3	A	19	LEU
3	A	20	THR
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	40	ARG
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	79	THR
3	A	81	LYS
3	A	93	THR
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	122	LEU
3	A	128	ASN
3	A	130	ASP
3	A	133	ASN
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	188	SER

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Mol	Chain	Res	Type
3	A	194	LEU
3	A	201	THR
3	A	202	SER
3	A	214	VAL
3	A	218	LEU
3	A	224	ILE
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	264	GLN
3	A	277	ILE
3	A	282	MET
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
3	A	298	ILE
3	A	304	THR
3	A	306	VAL
3	A	309	GLU
3	A	314	ASP
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	133	ASN
3	A	136	GLN

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Mol	Chain	Res	Type
3	A	157	GLN
3	A	159	GLN
3	A	207	GLN
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 [i](#)

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 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 [i](#)

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	7/7 (100%)	-1.19	0 100 100	22, 32, 67, 100	0
2	P	6/6 (100%)	-1.44	0 100 100	23, 30, 39, 40	0
3	A	324/335 (96%)	-0.88	0 100 100	10, 36, 85, 100	0
All	All	337/348 (96%)	-0.89	0 100 100	10, 36, 85, 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	0.94	0.06	46,46,46,46	0
4	NA	A	341	1/1	0.95	0.06	31,31,31,31	0
5	ZN	A	343	1/1	0.95	0.07	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.