



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:53 PM EDT

PDB ID : 8ICQ / pdb_00008icq
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF OF DATP (0.1 MILLIMOLAR) AND MNCL2 (0.5 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-01-04
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

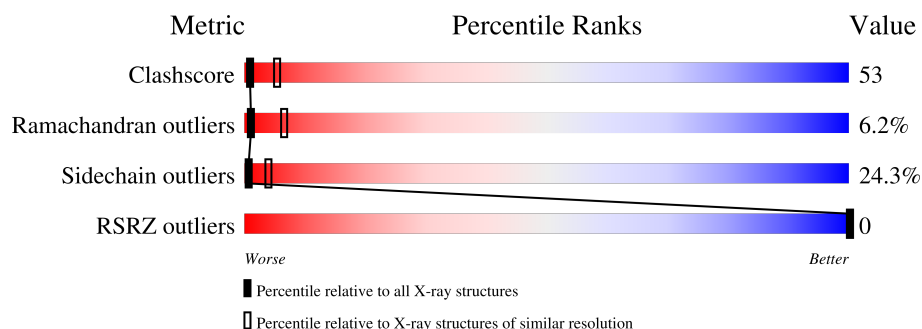
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	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		

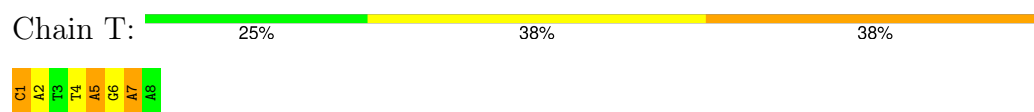
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	15	Total	O	0	0
			15	15		
5	P	16	Total	O	0	0
			16	16		
5	A	108	Total	O	0	0
			108	108		

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.

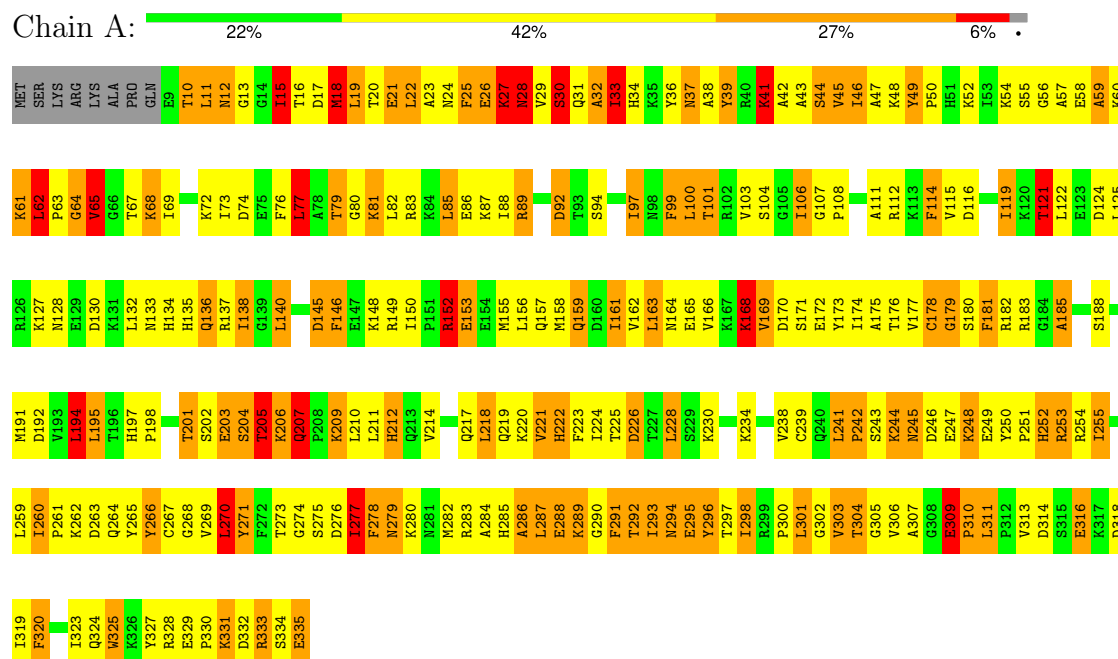
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.68Å 57.69Å 48.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.00) 90.5 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.159 , (Not available) 0.154 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 227.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3053	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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	1.05	0/162	3.43	9/249 (3.6%)
2	P	1.16	1/160 (0.6%)	3.49	14/243 (5.8%)
3	A	1.60	21/2672 (0.8%)	2.18	116/3590 (3.2%)
All	All	1.56	22/2994 (0.7%)	2.37	139/4082 (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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	15	ILE	CA-C	-8.57	1.42	1.52
3	A	224	ILE	CA-CB	-7.72	1.44	1.54
2	P	1	DT	OP3-P	7.23	1.62	1.48
3	A	195	LEU	CA-C	-6.31	1.45	1.52
3	A	138	ILE	CA-CB	-6.25	1.46	1.54
3	A	225	THR	CA-C	-6.03	1.44	1.52
3	A	242	PRO	N-CA	-5.94	1.39	1.47
3	A	55	SER	C-O	5.90	1.30	1.23
3	A	194	LEU	CA-C	-5.80	1.45	1.52
3	A	30	SER	C-N	-5.78	1.25	1.33
3	A	242	PRO	CA-C	-5.77	1.44	1.52
3	A	224	ILE	CA-C	-5.59	1.45	1.52
3	A	69	ILE	CA-CB	-5.50	1.46	1.54
3	A	94	SER	N-CA	-5.34	1.39	1.46
3	A	104	SER	CA-C	-5.34	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	26	GLU	C-N	-5.33	1.27	1.33
3	A	114	PHE	C-N	-5.19	1.27	1.33
3	A	270	LEU	C-N	-5.17	1.27	1.33
3	A	106	ILE	CA-C	-5.17	1.46	1.52
3	A	271	TYR	N-CA	-5.11	1.40	1.46
3	A	226	ASP	CA-C	-5.09	1.46	1.52
3	A	86	GLU	CD-OE1	5.02	1.34	1.25

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-25.63	88.61	127.05
1	T	7	DA	C8-N9-C1'	23.67	162.56	127.05
1	T	4	DT	C6-N1-C1'	-20.78	88.19	119.35
1	T	4	DT	C2-N1-C1'	20.39	149.94	119.35
2	P	1	DT	C6-N1-C1'	-19.93	89.46	119.35
2	P	1	DT	C2-N1-C1'	18.84	147.61	119.35
2	P	6	DT	C6-N1-C1'	-17.75	92.72	119.35
2	P	6	DT	C2-N1-C1'	17.52	145.64	119.35
2	P	5	DA	C4-N9-C1'	15.36	150.09	127.05
2	P	5	DA	C8-N9-C1'	-14.37	105.49	127.05
3	A	192	ASP	CB-CA-C	-11.11	91.97	110.19
2	P	3	DT	C2-N1-C1'	10.54	135.17	119.35
2	P	2	DC	C2-N1-C1'	10.50	135.45	119.70
2	P	3	DT	C6-N1-C1'	-10.25	103.98	119.35
3	A	49	TYR	CA-C-N	9.71	130.90	120.12
3	A	49	TYR	C-N-CA	9.71	130.90	120.12
2	P	7	DG	C4-N9-C1'	-9.58	112.62	127.00
3	A	288	GLU	N-CA-C	-9.55	100.43	111.03
3	A	28	ASN	CA-CB-CG	-9.53	103.07	112.60
2	P	7	DG	C8-N9-C1'	8.88	140.31	127.00
2	P	2	DC	C6-N1-C1'	-8.76	106.56	119.70
3	A	260	ILE	O-C-N	8.49	127.04	121.69
3	A	168	LYS	N-CA-CB	8.45	122.53	109.94
3	A	192	ASP	N-CA-CB	8.34	123.65	110.55
3	A	303	VAL	N-CA-C	8.30	119.11	110.72
3	A	99	PHE	CA-CB-CG	-8.30	105.50	113.80
3	A	157	GLN	N-CA-CB	8.20	121.89	110.01
3	A	157	GLN	CB-CA-C	8.10	123.59	110.88
3	A	83	ARG	N-CA-CB	8.06	121.76	110.07
3	A	266	TYR	CA-CB-CG	-8.06	99.39	113.90
3	A	260	ILE	CB-CA-C	-8.02	101.48	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	333	ARG	N-CA-C	-7.94	103.67	112.72
3	A	219	GLN	CB-CA-C	-7.77	97.64	110.85
3	A	15	ILE	N-CA-CB	7.76	119.08	110.62
3	A	159	GLN	CB-CA-C	-7.68	98.04	110.79
3	A	146	PHE	CA-CB-CG	-7.47	106.33	113.80
3	A	68	LYS	N-CA-CB	7.46	120.80	109.91
3	A	318	ASP	CA-CB-CG	-7.27	105.33	112.60
3	A	212	HIS	CA-CB-CG	-7.26	106.54	113.80
3	A	30	SER	CA-C-N	-7.25	111.98	122.06
3	A	30	SER	C-N-CA	-7.25	111.98	122.06
3	A	176	THR	CA-C-N	-7.21	113.34	122.43
3	A	176	THR	C-N-CA	-7.21	113.34	122.43
3	A	164	ASN	CA-CB-CG	-7.18	105.42	112.60
3	A	33	ILE	N-CA-CB	-7.17	102.55	110.51
3	A	12	ASN	CB-CA-C	7.08	121.92	110.09
3	A	222	HIS	CA-CB-CG	-7.08	106.72	113.80
3	A	68	LYS	CB-CA-C	7.02	121.77	110.96
3	A	49	TYR	O-C-N	6.96	126.90	121.47
3	A	39	TYR	CA-CB-CG	-6.96	101.37	113.90
1	T	1	DC	P-O3'-C3'	6.90	130.55	120.20
3	A	20	THR	N-CA-CB	6.83	120.38	110.20
3	A	224	ILE	CA-CB-CG1	-6.71	99.00	110.40
3	A	32	ALA	N-CA-C	6.61	117.86	108.54
3	A	64	GLY	CA-C-N	-6.61	114.61	122.93
3	A	64	GLY	C-N-CA	-6.61	114.61	122.93
3	A	106	ILE	CB-CA-C	-6.57	101.98	110.98
3	A	161	ILE	N-CA-C	6.53	116.69	110.42
3	A	309	GLU	N-CA-C	6.51	124.20	109.81
3	A	87	LYS	CA-C-N	6.50	128.75	120.56
3	A	87	LYS	C-N-CA	6.50	128.75	120.56
1	T	5	DA	C4-N9-C1'	-6.46	117.37	127.05
3	A	27	LYS	N-CA-CB	-6.45	100.33	109.94
3	A	309	GLU	CA-C-N	6.43	127.88	119.84
3	A	309	GLU	C-N-CA	6.43	127.88	119.84
3	A	130	ASP	N-CA-C	6.39	119.06	111.71
3	A	149	ARG	CA-C-N	-6.38	117.17	123.04
3	A	149	ARG	C-N-CA	-6.38	117.17	123.04
3	A	92	ASP	N-CA-CB	6.36	119.24	110.01
3	A	134	HIS	CA-CB-CG	6.28	120.08	113.80
3	A	74	ASP	N-CA-CB	6.25	119.04	109.91
3	A	313	VAL	N-CA-C	6.24	116.85	107.80
3	A	116	ASP	CA-CB-CG	-6.22	106.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	291	PHE	N-CA-C	6.18	117.27	108.74
3	A	271	TYR	CA-CB-CG	-6.18	102.78	113.90
3	A	278	PHE	CA-CB-CG	-6.13	107.67	113.80
1	T	5	DA	C8-N9-C1'	6.10	136.20	127.05
1	T	7	DA	N9-C1'-C2'	-6.10	104.36	113.50
3	A	252	HIS	CA-CB-CG	-6.05	107.75	113.80
3	A	17	ASP	CB-CA-C	5.99	121.03	110.85
3	A	286	ALA	CA-C-N	5.96	128.27	120.28
3	A	286	ALA	C-N-CA	5.96	128.27	120.28
3	A	145	ASP	CB-CA-C	-5.93	98.62	110.42
3	A	11	LEU	N-CA-C	-5.90	104.79	112.23
2	P	3	DT	N1-C1'-C2'	5.90	122.35	113.50
3	A	163	LEU	O-C-N	5.87	128.34	122.12
3	A	335	GLU	N-CA-CB	5.84	120.42	110.50
3	A	177	VAL	N-CA-CB	5.82	118.46	111.31
3	A	20	THR	CB-CA-C	5.81	121.34	110.70
2	P	3	DT	P-O5'-C5'	5.77	128.65	120.00
3	A	59	ALA	O-C-N	5.75	128.31	122.09
3	A	205	THR	N-CA-CB	5.74	120.19	110.49
3	A	24	ASN	N-CA-CB	5.71	119.16	110.14
3	A	292	THR	CB-CA-C	5.70	119.63	109.65
3	A	207	GLN	CA-C-N	5.68	125.53	119.28
3	A	207	GLN	C-N-CA	5.68	125.53	119.28
3	A	103	VAL	N-CA-CB	-5.65	104.55	110.82
3	A	77	LEU	N-CA-CB	5.64	118.51	110.16
3	A	320	PHE	CA-CB-CG	-5.59	108.21	113.80
3	A	153	GLU	N-CA-CB	5.57	118.24	109.94
3	A	303	VAL	N-CA-CB	5.56	118.92	110.58
3	A	334	SER	N-CA-C	5.53	118.83	111.75
3	A	277	ILE	N-CA-CB	5.53	117.64	110.57
3	A	270	LEU	CA-C-N	5.49	129.05	120.82
3	A	270	LEU	C-N-CA	5.49	129.05	120.82
3	A	114	PHE	CA-C-O	5.47	126.53	120.63
3	A	209	LYS	O-C-N	5.46	128.60	122.22
3	A	179	GLY	CA-C-N	5.45	128.13	120.28
3	A	179	GLY	C-N-CA	5.45	128.13	120.28
3	A	296	TYR	CB-CA-C	-5.43	100.67	109.13
3	A	316	GLU	CA-C-N	5.42	127.82	120.44
3	A	316	GLU	C-N-CA	5.42	127.82	120.44
3	A	271	TYR	N-CA-CB	-5.38	101.00	109.78
3	A	121	THR	N-CA-C	5.37	117.46	110.53
3	A	251	PRO	CA-C-O	-5.37	115.31	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	1	DC	C6-N1-C1'	-5.37	111.65	119.70
3	A	205	THR	N-CA-C	5.34	122.18	110.80
3	A	181	PHE	N-CA-C	-5.34	105.63	111.82
3	A	266	TYR	CA-C-O	-5.27	115.02	120.92
3	A	241	LEU	O-C-N	5.26	127.00	121.42
3	A	86	GLU	N-CA-CB	5.26	117.85	110.12
3	A	12	ASN	N-CA-C	5.25	119.79	113.17
3	A	152	ARG	CD-NE-CZ	-5.25	117.06	124.40
3	A	45	VAL	N-CA-CB	5.23	117.27	110.57
3	A	169	VAL	N-CA-CB	5.23	116.32	110.62
3	A	72	LYS	CB-CA-C	5.22	119.15	110.90
3	A	18	MET	CA-C-N	5.22	127.27	120.28
3	A	18	MET	C-N-CA	5.22	127.27	120.28
3	A	114	PHE	CA-CB-CG	-5.14	108.66	113.80
3	A	211	LEU	CA-C-N	5.13	127.47	120.54
3	A	211	LEU	C-N-CA	5.13	127.47	120.54
3	A	228	LEU	N-CA-C	-5.12	105.33	112.45
3	A	21	GLU	CA-C-N	5.12	127.45	120.54
3	A	21	GLU	C-N-CA	5.12	127.45	120.54
3	A	267	CYS	CB-CA-C	-5.10	102.88	110.88
3	A	62	LEU	CA-C-O	5.03	126.41	120.87
3	A	41	LYS	N-CA-C	-5.00	105.91	111.36
3	A	65	VAL	CA-C-O	5.00	125.92	120.57
3	A	178	CYS	CA-CB-SG	-5.00	102.90	114.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	68	LYS	CA
3	A	157	GLN	CA
3	A	309	GLU	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	145	0	80	7	0
2	P	144	0	81	13	0
3	A	2623	0	2641	284	0
4	A	2	0	0	0	0
5	A	108	0	0	14	0
5	P	16	0	0	0	0
5	T	15	0	0	1	0
All	All	3053	0	2802	301	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 53.

All (301) 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:6:DT:H2''	2:P:7:DG:H5''	1.36	1.06
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.33	1.05
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.26	0.99
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.46	0.98
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.41	0.97
3:A:245:ASN:H	3:A:245:ASN:HD22	1.00	0.97
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.48	0.96
1:T:6:DG:H2''	1:T:7:DA:C8	2.03	0.93
3:A:245:ASN:HD22	3:A:245:ASN:N	1.63	0.91
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.55	0.89
3:A:11:LEU:HD23	3:A:11:LEU:H	1.40	0.85
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.42	0.84
3:A:18:MET:CE	3:A:76:PHE:HB2	2.09	0.83
3:A:16:THR:HG21	3:A:47:ALA:HB2	1.59	0.83
3:A:330:PRO:HA	3:A:333:ARG:CG	2.09	0.82
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.19	0.82
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.26	0.82
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.60	0.81
3:A:27:LYS:HG3	3:A:28:ASN:ND2	1.95	0.81
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.11	0.80
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.13	0.79
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.66	0.78
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.66	0.77
3:A:155:MET:HE2	3:A:188:SER:CB	2.15	0.77
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.15	0.77
3:A:150:ILE:CG2	3:A:158:MET:HE1	2.14	0.77
3:A:108:PRO:O	3:A:112:ARG:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.85	0.75
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.01	0.75
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.70	0.73
2:P:1:DT:H2''	2:P:2:DC:H5'	1.71	0.73
3:A:155:MET:HE2	3:A:188:SER:HB2	1.71	0.72
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.19	0.72
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.88	0.72
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.19	0.72
3:A:245:ASN:H	3:A:245:ASN:ND2	1.80	0.72
3:A:271:TYR:HB2	5:A:592:HOH:O	1.90	0.72
3:A:306:VAL:HG22	5:A:650:HOH:O	1.89	0.72
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.70	0.71
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.72	0.71
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.25	0.71
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.72	0.70
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.70
3:A:155:MET:HA	3:A:158:MET:HE3	1.72	0.70
3:A:327:TYR:HD1	3:A:328:ARG:N	1.89	0.70
3:A:289:LYS:HD3	3:A:289:LYS:N	2.07	0.70
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.74	0.70
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.74	0.70
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.74	0.69
2:P:5:DA:H2''	2:P:6:DT:C5'	2.22	0.69
3:A:18:MET:CE	3:A:82:LEU:HD13	2.23	0.69
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.73	0.69
3:A:119:ILE:N	3:A:119:ILE:HD13	2.08	0.68
3:A:207:GLN:O	3:A:210:LEU:HB2	1.93	0.68
2:P:5:DA:H2''	2:P:6:DT:H5'	1.75	0.68
3:A:295:GLU:CD	3:A:295:GLU:H	2.01	0.68
3:A:254:ARG:HB3	3:A:254:ARG:NH1	2.08	0.68
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.75	0.68
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.77	0.67
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.29	0.67
3:A:270:LEU:HD13	3:A:316:GLU:OE2	1.95	0.67
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.43	0.67
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.28	0.67
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.31	0.66
3:A:294:ASN:ND2	3:A:297:THR:H	1.94	0.66
3:A:309:GLU:N	3:A:309:GLU:OE1	2.29	0.66
3:A:245:ASN:N	3:A:245:ASN:ND2	2.39	0.66
3:A:294:ASN:HB2	3:A:295:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.60	0.65
3:A:140:LEU:HD12	3:A:140:LEU:O	1.97	0.65
3:A:188:SER:HB3	5:A:522:HOH:O	1.97	0.65
3:A:15:ILE:CD1	3:A:77:LEU:HD11	2.22	0.65
3:A:234:LYS:HD3	5:A:617:HOH:O	1.95	0.65
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.79	0.65
3:A:152:ARG:HA	3:A:155:MET:HB2	1.79	0.64
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.26	0.64
3:A:328:ARG:O	3:A:333:ARG:NE	2.27	0.64
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.62	0.64
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.80	0.64
3:A:180:SER:CB	3:A:183:ARG:HH21	2.08	0.64
3:A:121:THR:HG23	3:A:124:ASP:CG	2.22	0.63
3:A:254:ARG:HB3	3:A:254:ARG:CZ	2.28	0.63
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.80	0.63
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.14	0.62
3:A:41:LYS:NZ	3:A:64:GLY:O	2.33	0.61
3:A:41:LYS:O	3:A:44:SER:HB3	2.01	0.60
3:A:97:ILE:O	3:A:101:THR:HB	2.01	0.60
3:A:248:LYS:O	3:A:248:LYS:HG2	1.99	0.60
3:A:11:LEU:HD23	3:A:11:LEU:N	2.13	0.60
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.37	0.60
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.37	0.60
3:A:38:ALA:O	3:A:41:LYS:HD3	2.02	0.60
3:A:41:LYS:HD3	3:A:42:ALA:H	1.67	0.60
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.67	0.59
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.16	0.59
3:A:11:LEU:H	3:A:11:LEU:CD2	2.12	0.59
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.83	0.59
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.84	0.59
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.17	0.59
3:A:28:ASN:ND2	3:A:28:ASN:N	2.48	0.58
3:A:279:ASN:O	3:A:283:ARG:HG3	2.02	0.58
3:A:73:ILE:HG22	3:A:77:LEU:HD21	1.85	0.58
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.33	0.58
3:A:162:VAL:O	3:A:166:VAL:HG23	2.04	0.58
3:A:291:PHE:HD1	3:A:300:PRO:HA	1.67	0.58
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.39	0.58
3:A:58:GLU:O	3:A:61:LYS:HG3	2.04	0.58
3:A:60:LYS:HG3	3:A:60:LYS:O	2.03	0.57
3:A:79:THR:O	3:A:81:LYS:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:O	3:A:19:LEU:HB2	2.04	0.57
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.18	0.57
3:A:260:ILE:HG22	3:A:261:PRO:N	2.18	0.57
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.34	0.57
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.87	0.57
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.86	0.57
3:A:182:ARG:HB3	3:A:273:THR:HG23	1.87	0.56
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.34	0.56
3:A:159:GLN:O	3:A:163:LEU:HG	2.05	0.56
3:A:303:VAL:C	3:A:305:GLY:H	2.13	0.56
3:A:310:PRO:HB3	5:A:626:HOH:O	2.04	0.56
3:A:89:ARG:HD3	3:A:89:ARG:C	2.30	0.56
3:A:32:ALA:O	3:A:36:TYR:HB3	2.05	0.56
3:A:145:ASP:OD2	3:A:252:HIS:N	2.28	0.56
3:A:15:ILE:CD1	3:A:73:ILE:HG23	2.29	0.55
3:A:183:ARG:HH11	3:A:275:SER:CB	2.20	0.55
3:A:33:ILE:O	3:A:37:ASN:HB2	2.06	0.55
3:A:27:LYS:HG3	3:A:28:ASN:N	2.20	0.55
3:A:41:LYS:HD3	3:A:42:ALA:N	2.22	0.55
3:A:288:GLU:O	3:A:290:GLY:N	2.40	0.55
3:A:133:ASN:ND2	5:A:512:HOH:O	2.38	0.55
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.22	0.55
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.37	0.54
3:A:270:LEU:C	3:A:270:LEU:HD12	2.29	0.54
3:A:300:PRO:HD3	3:A:311:LEU:HD22	1.90	0.54
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.90	0.53
3:A:158:MET:CB	3:A:191:MET:HE1	2.39	0.53
3:A:28:ASN:N	3:A:28:ASN:HD22	2.03	0.53
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.89	0.53
2:P:1:DT:H2''	2:P:2:DC:C5'	2.36	0.53
3:A:170:ASP:OD2	3:A:197:HIS:NE2	2.42	0.53
3:A:288:GLU:C	3:A:290:GLY:H	2.17	0.53
1:T:5:DA:H2''	1:T:6:DG:O5'	2.09	0.53
3:A:303:VAL:O	3:A:305:GLY:N	2.41	0.53
3:A:132:LEU:HB3	3:A:136:GLN:HB2	1.91	0.52
3:A:158:MET:HB3	3:A:191:MET:HE1	1.91	0.52
3:A:331:LYS:HG2	3:A:332:ASP:N	2.16	0.52
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.40	0.52
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.91	0.52
3:A:201:THR:HA	3:A:261:PRO:CB	2.40	0.51
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HD23	3:A:319:ILE:HG21	1.93	0.51
3:A:266:TYR:O	3:A:270:LEU:N	2.40	0.51
3:A:205:THR:HA	5:A:624:HOH:O	2.10	0.51
3:A:280:LYS:O	3:A:284:ALA:N	2.35	0.51
3:A:295:GLU:OE1	3:A:295:GLU:N	2.27	0.51
2:P:5:DA:H2"	2:P:6:DT:H5"	1.92	0.51
3:A:212:HIS:N	3:A:212:HIS:CD2	2.76	0.51
3:A:172:GLU:HB3	3:A:197:HIS:HE2	1.74	0.50
3:A:15:ILE:HD13	3:A:73:ILE:CG2	2.30	0.50
3:A:57:ALA:HA	3:A:60:LYS:HB3	1.92	0.50
1:T:2:DA:C2	2:P:7:DG:N2	2.79	0.50
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.90	0.50
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.34	0.50
1:T:1:DC:H2"	1:T:2:DA:OP2	2.12	0.50
3:A:31:GLN:HB2	3:A:112:ARG:HH12	1.76	0.50
3:A:217:GLN:O	3:A:220:LYS:HB3	2.11	0.50
3:A:254:ARG:NH1	3:A:255:ILE:N	2.60	0.50
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.93	0.50
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.93	0.50
3:A:175:ALA:HB2	3:A:195:LEU:CD1	2.42	0.50
3:A:12:ASN:HA	5:A:553:HOH:O	2.11	0.49
3:A:181:PHE:HA	5:A:530:HOH:O	2.12	0.49
3:A:292:THR:O	3:A:298:ILE:HA	2.12	0.49
3:A:243:SER:HB3	3:A:249:GLU:HA	1.92	0.49
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.80	0.49
3:A:302:GLY:N	3:A:307:ALA:HB3	2.26	0.49
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.25	0.49
3:A:226:ASP:HB2	3:A:238:VAL:HB	1.93	0.49
3:A:146:PHE:HZ	3:A:238:VAL:HG22	1.77	0.49
3:A:180:SER:HA	3:A:183:ARG:HE	1.78	0.49
3:A:323:ILE:C	3:A:324:GLN:HG2	2.38	0.49
3:A:150:ILE:N	3:A:188:SER:O	2.30	0.49
3:A:309:GLU:O	3:A:311:LEU:HD13	2.12	0.49
3:A:175:ALA:HB2	3:A:195:LEU:HD12	1.95	0.49
3:A:201:THR:HA	3:A:261:PRO:HB3	1.95	0.49
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.95	0.48
3:A:33:ILE:HG23	3:A:34:HIS:H	1.78	0.48
3:A:180:SER:HB2	3:A:185:ALA:CB	2.43	0.48
3:A:183:ARG:HD3	3:A:273:THR:O	2.13	0.48
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.28	0.48
2:P:5:DA:H2"	2:P:6:DT:H71	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:5:DA:C2'	2:P:6:DT:H5''	2.43	0.48
3:A:119:ILE:HG22	3:A:124:ASP:HB2	1.95	0.47
1:T:6:DG:H1'	5:T:651:HOH:O	2.14	0.47
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.96	0.47
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.80	0.47
3:A:119:ILE:HG21	3:A:125:LEU:HD23	1.96	0.47
3:A:204:SER:O	3:A:204:SER:OG	2.28	0.46
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.48	0.46
3:A:31:GLN:HE21	3:A:112:ARG:HH22	1.64	0.46
3:A:217:GLN:O	3:A:221:VAL:HG13	2.16	0.46
3:A:223:PHE:O	3:A:239:CYS:HA	2.15	0.46
3:A:31:GLN:HB2	3:A:112:ARG:NH1	2.31	0.46
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.44	0.46
3:A:79:THR:C	3:A:81:LYS:H	2.22	0.46
3:A:250:TYR:HB3	5:A:577:HOH:O	2.16	0.46
3:A:31:GLN:HE21	3:A:112:ARG:CZ	2.29	0.46
3:A:254:ARG:NH1	3:A:254:ARG:CB	2.79	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.79	0.45
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.45	0.45
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.52	0.45
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.16	0.45
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.99	0.45
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.80	0.45
3:A:26:GLU:O	3:A:30:SER:O	2.35	0.45
3:A:48:LYS:HE3	5:A:607:HOH:O	2.15	0.45
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.52	0.45
3:A:263:ASP:O	3:A:264:GLN:HG2	2.17	0.45
3:A:270:LEU:CD2	3:A:319:ILE:HG21	2.47	0.45
3:A:278:PHE:HE1	3:A:328:ARG:HD3	1.79	0.45
3:A:33:ILE:O	3:A:36:TYR:HD2	1.99	0.45
3:A:106:ILE:HG22	3:A:107:GLY:O	2.17	0.45
3:A:31:GLN:HE21	3:A:112:ARG:NH2	2.15	0.45
3:A:183:ARG:NH1	3:A:275:SER:CB	2.80	0.45
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.68	0.45
3:A:298:ILE:HG22	5:A:578:HOH:O	2.17	0.45
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.50	0.44
3:A:148:LYS:HB3	5:A:620:HOH:O	2.18	0.44
3:A:276:ASP:O	3:A:280:LYS:HG3	2.17	0.44
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.56	0.44
3:A:254:ARG:NH1	3:A:255:ILE:H	2.15	0.44
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.61	0.44
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.53	0.43
3:A:124:ASP:O	3:A:128:ASN:ND2	2.47	0.43
2:P:5:DA:C2'	2:P:6:DT:H71	2.49	0.43
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.27	0.43
3:A:112:ARG:O	3:A:115:VAL:HB	2.18	0.43
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.46	0.43
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.49	0.43
3:A:111:ALA:O	3:A:115:VAL:HG23	2.19	0.43
3:A:119:ILE:HG23	3:A:124:ASP:HB3	2.01	0.43
3:A:195:LEU:O	3:A:260:ILE:N	2.51	0.43
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.66	0.43
2:P:1:DT:C2'	2:P:2:DC:H5'	2.44	0.43
3:A:327:TYR:HE1	3:A:333:ARG:NH2	2.12	0.43
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.48	0.43
1:T:7:DA:H61	2:P:1:DT:H3	1.65	0.43
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.59	0.43
3:A:278:PHE:CE1	3:A:325:TRP:HZ3	2.37	0.43
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.97	0.43
3:A:259:LEU:HD12	3:A:260:ILE:H	1.84	0.43
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.49	0.43
3:A:243:SER:O	3:A:244:LYS:O	2.37	0.43
3:A:266:TYR:HA	3:A:269:VAL:HB	2.00	0.43
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.54	0.43
3:A:25:PHE:CD1	3:A:25:PHE:C	2.97	0.42
3:A:179:GLY:O	3:A:182:ARG:HB3	2.19	0.42
3:A:203:GLU:O	3:A:205:THR:N	2.52	0.42
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.97	0.42
3:A:323:ILE:O	3:A:324:GLN:HG2	2.19	0.42
1:T:2:DA:C2	2:P:7:DG:C2	3.08	0.42
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.70	0.42
3:A:99:PHE:CD2	3:A:99:PHE:C	2.96	0.42
3:A:327:TYR:C	3:A:327:TYR:CD1	2.97	0.42
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.42
3:A:73:ILE:O	3:A:77:LEU:HD22	2.20	0.42
3:A:156:LEU:HD23	3:A:156:LEU:HA	1.84	0.42
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.40	0.42
3:A:274:GLY:HA3	3:A:275:SER:HA	1.88	0.42
3:A:36:TYR:CD2	3:A:36:TYR:C	2.95	0.42
3:A:241:LEU:HA	3:A:242:PRO:HD2	1.77	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.78	0.42
3:A:125:LEU:HD22	3:A:132:LEU:HD21	2.02	0.42
3:A:33:ILE:H	3:A:33:ILE:HG22	1.54	0.41
3:A:218:LEU:N	3:A:218:LEU:CD1	2.82	0.41
3:A:170:ASP:OD1	3:A:171:SER:N	2.54	0.41
3:A:330:PRO:O	3:A:333:ARG:HG2	2.20	0.41
3:A:25:PHE:CG	3:A:88:ILE:HD13	2.55	0.41
3:A:152:ARG:HD2	3:A:185:ALA:O	2.20	0.41
3:A:152:ARG:HH11	3:A:152:ARG:HD3	1.64	0.41
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.20	0.41
3:A:270:LEU:HD13	3:A:270:LEU:HA	1.64	0.41
3:A:320:PHE:HB3	5:A:657:HOH:O	2.21	0.41
3:A:19:LEU:HD23	3:A:43:ALA:HA	2.01	0.41
3:A:128:ASN:ND2	3:A:128:ASN:N	2.68	0.41
3:A:133:ASN:O	3:A:137:ARG:HG3	2.20	0.41
3:A:209:LYS:HA	3:A:212:HIS:HB2	2.02	0.41
3:A:76:PHE:HD2	3:A:77:LEU:CD1	2.33	0.41
3:A:201:THR:C	3:A:261:PRO:HB3	2.46	0.41
3:A:262:LYS:O	3:A:262:LYS:HG3	2.16	0.41
3:A:205:THR:O	3:A:206:LYS:HB2	2.21	0.41
3:A:221:VAL:HG13	3:A:221:VAL:H	1.65	0.41
3:A:286:ALA:HA	3:A:323:ILE:HG21	2.03	0.41
3:A:268:GLY:O	3:A:271:TYR:HB3	2.20	0.41
3:A:41:LYS:HZ3	3:A:42:ALA:HB2	1.86	0.40
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.66	0.40
3:A:325:TRP:HD1	3:A:325:TRP:HA	1.72	0.40
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.85	0.40
3:A:183:ARG:HH11	3:A:275:SER:HB3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	271 (83%)	34 (10%)	20 (6%)	1 6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	289	LYS
3	A	304	THR
3	A	13	GLY
3	A	28	ASN
3	A	185	ALA
3	A	207	GLN
3	A	265	TYR
3	A	309	GLU
3	A	310	PRO
3	A	10	THR
3	A	80	GLY
3	A	222	HIS
3	A	246	ASP
3	A	206	LYS
3	A	247	GLU
3	A	202	SER
3	A	56	GLY

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%)	218 (76%)	70 (24%)	1 4

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

Mol	Chain	Res	Type
3	A	10	THR

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Mol	Chain	Res	Type
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	25	PHE
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	41	LYS
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	61	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	89	ARG
3	A	92	ASP
3	A	97	ILE
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR
3	A	122	LEU
3	A	136	GLN
3	A	138	ILE
3	A	140	LEU
3	A	152	ARG
3	A	153	GLU
3	A	161	ILE
3	A	168	LYS
3	A	169	VAL
3	A	174	ILE
3	A	194	LEU

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Mol	Chain	Res	Type
3	A	201	THR
3	A	203	GLU
3	A	214	VAL
3	A	218	LEU
3	A	221	VAL
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	270	LEU
3	A	277	ILE
3	A	279	ASN
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
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	98	ASN
3	A	128	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	212	HIS

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Mol	Chain	Res	Type
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN
3	A	324	GLN

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 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	8/8 (100%)	-0.62	0 100 100	18, 38, 96, 99	0
2	P	7/7 (100%)	-0.95	0 100 100	16, 28, 47, 82	0
3	A	324/335 (96%)	-1.00	0 100 100	3, 31, 83, 99	0
All	All	339/350 (96%)	-0.99	0 100 100	3, 32, 84, 99	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	0.88	0.06	44,44,44,44	0
4	NA	A	341	1/1	0.99	0.02	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.