



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:51 PM UTC

PDB ID : 9ICE / pdb_00009ice
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DATP (1 MILLIMOLAR) AND CUCL2 (0.1 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
Resolution : 3.30 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

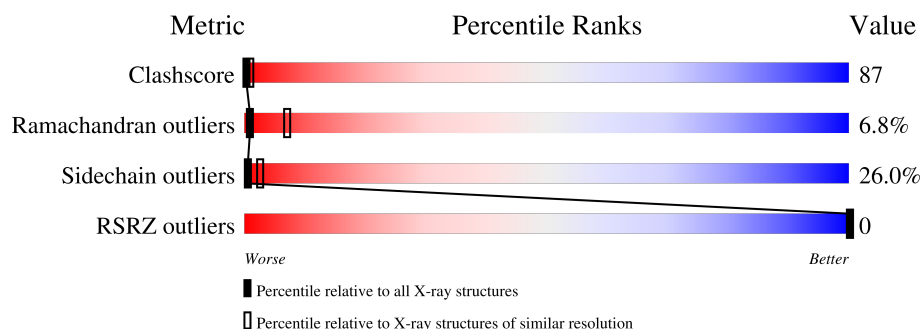
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	25% 25% 50%
2	P	7	14% 14% 71%
3	A	335	12% 47% 33% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3051 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		

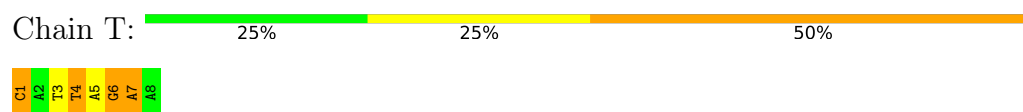
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	13	Total	O	0	0
			13	13		
5	P	17	Total	O	0	0
			17	17		
5	A	107	Total	O	0	0
			107	107		

3 Residue-property plots

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

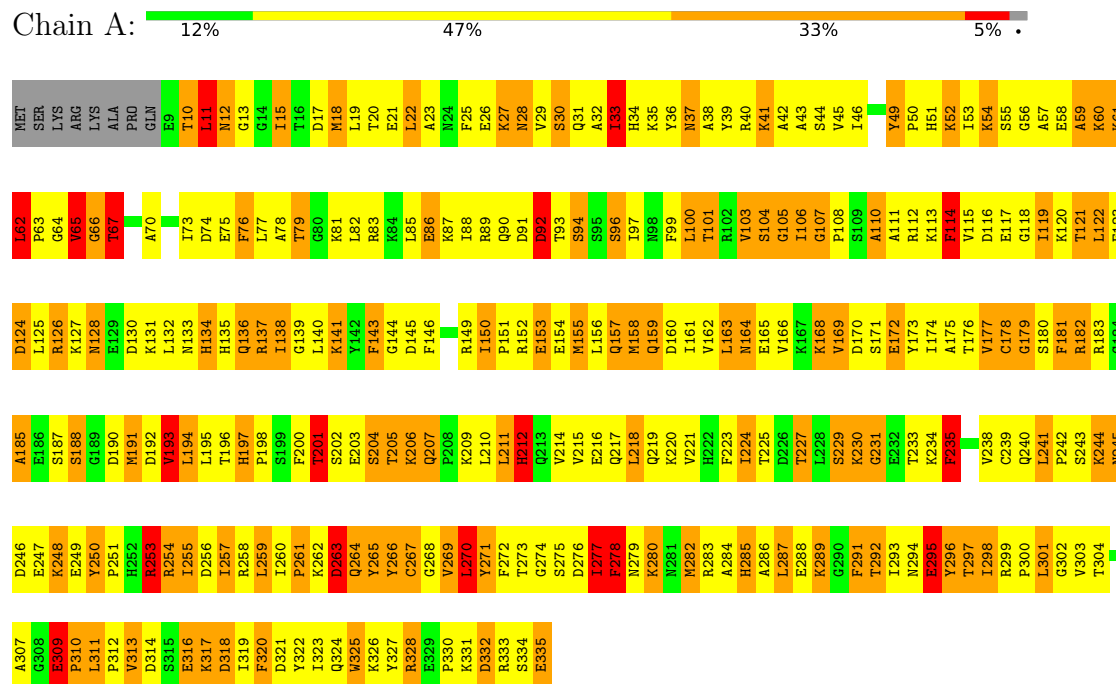
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.84Å 57.87Å 48.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-3.30) 93.0 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.186 , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.06 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3051	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.79	0/162	3.35	11/249 (4.4%)
2	P	1.07	1/160 (0.6%)	3.13	12/243 (4.9%)
3	A	1.46	14/2672 (0.5%)	2.20	131/3590 (3.6%)
All	All	1.41	15/2994 (0.5%)	2.35	154/4082 (3.8%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	65	VAL	CA-CB	-6.91	1.45	1.54
3	A	193	VAL	N-CA	-6.89	1.38	1.46
2	P	1	DT	OP3-P	6.69	1.61	1.48
3	A	192	ASP	C-N	-6.35	1.25	1.33
3	A	106	ILE	CA-C	-6.32	1.45	1.52
3	A	67	THR	N-CA	-6.26	1.39	1.46
3	A	116	ASP	CA-C	-5.54	1.45	1.52
3	A	178	CYS	N-CA	-5.48	1.40	1.46
3	A	124	ASP	C-N	-5.42	1.27	1.33
3	A	163	LEU	CA-C	-5.35	1.45	1.52
3	A	159	GLN	C-O	-5.29	1.17	1.24
3	A	59	ALA	CA-C	-5.27	1.46	1.52
3	A	250	TYR	C-N	-5.27	1.27	1.33
3	A	224	ILE	CA-CB	-5.22	1.48	1.54
3	A	66	GLY	C-N	-5.10	1.27	1.33

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	4	DT	C6-N1-C1'	-29.18	75.57	119.35
1	T	4	DT	C2-N1-C1'	27.72	160.93	119.35
2	P	1	DT	C2-N1-C1'	25.09	156.98	119.35
2	P	1	DT	C6-N1-C1'	-24.03	83.31	119.35
2	P	5	DA	C8-N9-C1'	-13.62	106.61	127.05
2	P	5	DA	C4-N9-C1'	13.39	147.14	127.05
3	A	28	ASN	CA-CB-CG	-11.84	100.77	112.60
3	A	150	ILE	N-CA-C	11.46	117.99	107.56
1	T	7	DA	C8-N9-C1'	11.34	144.07	127.05
1	T	7	DA	C4-N9-C1'	-11.29	110.12	127.05
3	A	49	TYR	CA-C-N	11.09	130.84	119.64
3	A	49	TYR	C-N-CA	11.09	130.84	119.64
3	A	297	THR	N-CA-C	9.80	122.67	108.86
1	T	6	DG	C4-N9-C1'	-9.12	113.32	127.00
3	A	192	ASP	CB-CA-C	-9.10	96.88	110.62
1	T	6	DG	C8-N9-C1'	8.91	140.36	127.00
3	A	296	TYR	CB-CA-C	-8.72	97.91	109.16
3	A	311	LEU	CA-C-N	8.66	130.66	119.84
3	A	311	LEU	C-N-CA	8.66	130.66	119.84
3	A	59	ALA	O-C-N	8.57	131.28	122.03
2	P	4	DA	P-O3'-C3'	8.47	132.91	120.20
3	A	49	TYR	O-C-N	8.46	128.32	121.38
3	A	313	VAL	N-CA-C	8.43	120.41	108.36
1	T	4	DT	C1'-O4'-C4'	-8.41	97.09	109.70
3	A	241	LEU	O-C-N	8.30	128.90	121.18
3	A	116	ASP	CA-CB-CG	-8.29	104.31	112.60
3	A	179	GLY	CA-C-N	8.24	131.32	120.28
3	A	179	GLY	C-N-CA	8.24	131.32	120.28
3	A	231	GLY	CA-C-N	-8.19	109.54	122.73
3	A	231	GLY	C-N-CA	-8.19	109.54	122.73
3	A	168	LYS	N-CA-CB	8.13	123.03	109.78
3	A	253	ARG	N-CA-C	7.96	122.99	110.17
3	A	177	VAL	CB-CA-C	-7.82	102.79	111.23
1	T	6	DG	P-O5'-C5'	-7.74	108.39	120.00
3	A	271	TYR	N-CA-C	7.72	120.44	111.02
3	A	157	GLN	N-CA-CB	7.66	121.12	110.01
3	A	117	GLU	N-CA-C	-7.63	103.95	113.18
3	A	105	GLY	N-CA-C	-7.59	105.05	114.92
3	A	193	VAL	N-CA-CB	-7.59	101.92	111.41
3	A	17	ASP	N-CA-CB	7.52	120.91	110.01
3	A	105	GLY	CA-C-N	-7.38	113.63	122.93
3	A	105	GLY	C-N-CA	-7.38	113.63	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	65	VAL	CA-CB-CG1	-7.27	98.04	110.40
3	A	181	PHE	N-CA-C	-7.24	103.39	111.28
3	A	291	PHE	N-CA-C	7.22	117.80	108.34
3	A	317	LYS	N-CA-C	7.18	118.79	110.97
3	A	107	GLY	CA-C-N	7.12	126.64	119.24
3	A	107	GLY	C-N-CA	7.12	126.64	119.24
3	A	114	PHE	CA-CB-CG	-7.11	106.69	113.80
3	A	134	HIS	CA-CB-CG	7.09	120.89	113.80
3	A	110	ALA	N-CA-CB	7.06	120.60	110.16
3	A	282	MET	N-CA-CB	7.04	120.75	110.26
3	A	285	HIS	CA-CB-CG	-6.99	106.81	113.80
2	P	1	DT	C5'-C4'-O4'	6.88	119.72	109.40
3	A	271	TYR	CA-CB-CG	-6.86	101.55	113.90
3	A	253	ARG	CA-C-O	6.83	129.34	121.28
2	P	1	DT	O5'-C5'-C4'	6.80	121.00	110.80
3	A	17	ASP	CB-CA-C	6.67	121.34	110.88
3	A	136	GLN	CB-CG-CD	-6.62	101.35	112.60
3	A	320	PHE	N-CA-C	-6.57	104.05	111.14
3	A	11	LEU	N-CA-C	-6.55	104.14	111.28
3	A	235	PHE	N-CA-C	-6.49	99.17	109.23
3	A	276	ASP	N-CA-CB	6.49	120.21	110.22
3	A	106	ILE	N-CA-CB	6.46	118.75	110.99
3	A	107	GLY	O-C-N	6.43	128.20	121.77
3	A	291	PHE	CA-CB-CG	-6.42	107.38	113.80
3	A	316	GLU	CA-C-N	6.41	129.11	120.65
3	A	316	GLU	C-N-CA	6.41	129.11	120.65
3	A	313	VAL	N-CA-CB	-6.39	103.32	110.99
3	A	298	ILE	N-CA-CB	6.38	121.43	111.99
3	A	164	ASN	CB-CA-C	6.34	121.31	110.79
3	A	62	LEU	N-CA-C	6.30	118.65	110.40
3	A	124	ASP	CA-CB-CG	-6.30	106.30	112.60
3	A	116	ASP	N-CA-CB	6.29	119.91	110.22
3	A	254	ARG	CA-C-N	-6.26	112.78	122.68
3	A	254	ARG	C-N-CA	-6.26	112.78	122.68
3	A	63	PRO	N-CA-C	-6.26	101.34	110.80
3	A	303	VAL	N-CA-C	6.23	120.86	111.89
3	A	137	ARG	N-CA-C	-6.21	104.44	111.14
3	A	136	GLN	N-CA-CB	-6.17	100.38	110.14
3	A	11	LEU	CA-C-N	-6.17	111.94	122.56
3	A	11	LEU	C-N-CA	-6.17	111.94	122.56
3	A	309	GLU	CA-C-N	6.17	127.55	119.84
3	A	309	GLU	C-N-CA	6.17	127.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	270	LEU	O-C-N	6.16	128.42	122.07
3	A	63	PRO	N-CA-CB	6.16	108.78	103.36
3	A	197	HIS	CA-CB-CG	6.15	119.95	113.80
3	A	282	MET	N-CA-C	-6.11	103.96	112.45
3	A	241	LEU	CB-CA-C	-6.06	99.82	109.82
3	A	278	PHE	CA-C-N	6.05	128.85	120.63
3	A	278	PHE	C-N-CA	6.05	128.85	120.63
3	A	181	PHE	CA-CB-CG	-6.04	107.76	113.80
3	A	263	ASP	CA-CB-CG	6.04	118.64	112.60
3	A	34	HIS	CA-CB-CG	-6.03	107.77	113.80
3	A	332	ASP	CB-CA-C	6.03	118.64	111.22
3	A	92	ASP	CA-CB-CG	5.98	118.58	112.60
3	A	12	ASN	CB-CA-C	5.98	121.01	110.37
3	A	280	LYS	N-CA-C	-5.97	104.68	111.07
3	A	261	PRO	CB-CA-C	-5.97	105.05	111.56
3	A	32	ALA	N-CA-C	5.95	119.92	110.70
3	A	318	ASP	CA-C-N	5.95	128.06	120.56
3	A	318	ASP	C-N-CA	5.95	128.06	120.56
1	T	1	DC	P-O3'-C3'	5.92	129.07	120.20
3	A	309	GLU	N-CA-C	5.91	122.87	109.81
3	A	52	LYS	N-CA-CB	5.85	119.30	109.94
3	A	311	LEU	N-CA-C	5.82	117.86	109.48
3	A	103	VAL	N-CA-C	5.81	116.56	108.89
3	A	231	GLY	N-CA-C	-5.80	99.44	113.18
3	A	277	ILE	N-CA-C	5.77	115.99	110.74
3	A	17	ASP	N-CA-C	5.75	117.22	111.07
3	A	86	GLU	N-CA-CB	5.75	118.34	110.01
3	A	40	ARG	N-CA-CB	5.72	118.31	110.01
2	P	1	DT	P-O5'-C5'	5.72	128.58	120.00
3	A	122	LEU	CA-C-O	5.71	126.59	120.20
3	A	31	GLN	N-CA-C	-5.67	106.96	112.97
3	A	320	PHE	CA-C-N	5.67	128.14	120.38
3	A	320	PHE	C-N-CA	5.67	128.14	120.38
3	A	110	ALA	CB-CA-C	5.65	120.46	110.85
2	P	6	DT	N1-C1'-C2'	-5.62	105.07	113.50
3	A	269	VAL	CB-CA-C	5.59	119.93	112.22
3	A	138	ILE	N-CA-CB	5.57	118.12	110.54
3	A	285	HIS	N-CA-C	5.55	117.41	111.36
3	A	76	PHE	N-CA-C	-5.54	105.25	112.23
3	A	334	SER	N-CA-C	5.53	122.58	110.80
3	A	332	ASP	N-CA-CB	5.50	119.19	110.22
1	T	1	DC	C2-N1-C1'	5.47	127.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	TYR	CA-CB-CG	-5.46	104.06	113.90
3	A	332	ASP	N-CA-C	5.46	120.15	112.72
3	A	168	LYS	CB-CA-C	5.46	119.80	110.74
3	A	59	ALA	CB-CA-C	-5.45	102.51	110.95
3	A	12	ASN	N-CA-C	5.41	119.52	113.02
3	A	162	VAL	N-CA-CB	5.41	116.88	110.55
3	A	104	SER	N-CA-CB	5.40	117.96	109.69
1	T	1	DC	C6-N1-C1'	-5.36	111.66	119.70
3	A	158	MET	O-C-N	5.34	127.58	122.03
3	A	295	GLU	N-CA-C	5.28	122.05	110.80
3	A	101	THR	OG1-CB-CG2	5.28	119.85	109.30
3	A	101	THR	N-CA-CB	-5.27	100.69	110.18
3	A	134	HIS	CB-CA-C	5.25	120.87	110.42
3	A	86	GLU	CB-CA-C	5.18	119.02	110.88
3	A	201	THR	N-CA-C	5.18	115.37	108.38
3	A	212	HIS	CA-CB-CG	-5.17	108.63	113.80
3	A	312	PRO	CA-C-N	5.16	129.43	122.93
3	A	312	PRO	C-N-CA	5.16	129.43	122.93
3	A	138	ILE	O-C-N	5.16	126.87	121.87
2	P	6	DT	C2-N1-C1'	-5.15	111.62	119.35
3	A	292	THR	N-CA-CB	5.15	119.27	110.57
2	P	7	DG	C8-N9-C1'	5.14	134.71	127.00
3	A	164	ASN	N-CA-CB	5.12	117.64	110.12
2	P	5	DA	C5'-C4'-C3'	5.11	122.57	114.90
3	A	33	ILE	CA-CB-CG1	5.11	119.09	110.40
3	A	92	ASP	N-CA-CB	5.10	117.40	110.01
3	A	116	ASP	CA-C-N	-5.03	111.78	121.58
3	A	116	ASP	C-N-CA	-5.03	111.78	121.58

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	17	ASP	CA
3	A	168	LYS	CA
3	A	334	SER	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	18	0
2	P	144	0	81	26	0
3	A	2623	0	2641	450	0
4	A	2	0	0	0	0
5	A	107	0	0	24	0
5	P	17	0	0	1	0
5	T	13	0	0	5	0
All	All	3051	0	2802	485	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 87.

All (485) 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''	1.30	1.10
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.31	1.08
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.16	1.08
2:P:4:DA:H2''	2:P:5:DA:H5'	1.34	1.07
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.21	1.05
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.39	1.02
2:P:1:DT:H2''	2:P:2:DC:H5'	1.43	1.01
3:A:193:VAL:HB	3:A:257:ILE:HG23	1.43	1.01
3:A:195:LEU:HD23	3:A:259:LEU:HD13	1.42	1.01
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.23	1.00
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.43	1.00
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.50	0.94
3:A:277:ILE:HD13	3:A:277:ILE:H	1.33	0.94
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.04	0.92
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.51	0.92
3:A:245:ASN:H	3:A:245:ASN:HD22	0.99	0.91
3:A:155:MET:HA	3:A:158:MET:HE3	1.52	0.89
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.07	0.89
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.54	0.88
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.10	0.87
2:P:6:DT:H6	2:P:6:DT:H5'	1.41	0.86
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.10	0.86
3:A:11:LEU:HD23	3:A:11:LEU:H	1.40	0.85
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:HB	3:A:106:ILE:CD1	2.06	0.85
2:P:4:DA:H2''	2:P:5:DA:C5'	2.06	0.84
3:A:180:SER:HB3	3:A:183:ARG:NH2	1.93	0.83
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.59	0.83
3:A:218:LEU:HB2	3:A:224:ILE:CD1	2.09	0.81
2:P:6:DT:H2''	2:P:7:DG:C5'	2.09	0.81
3:A:182:ARG:HG2	3:A:273:THR:HG21	1.62	0.80
2:P:6:DT:C2'	2:P:7:DG:H5''	2.09	0.80
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.64	0.80
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.62	0.80
3:A:152:ARG:HA	3:A:155:MET:HB2	1.65	0.79
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.16	0.79
3:A:270:LEU:HA	3:A:316:GLU:OE2	1.82	0.79
3:A:82:LEU:O	3:A:86:GLU:HG2	1.83	0.79
3:A:182:ARG:NH1	3:A:273:THR:HG21	1.97	0.79
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.64	0.79
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.45	0.79
2:P:6:DT:H5'	2:P:6:DT:C6	2.17	0.78
3:A:245:ASN:H	3:A:245:ASN:ND2	1.79	0.78
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.14	0.78
3:A:223:PHE:CE1	3:A:239:CYS:HB2	2.18	0.78
2:P:5:DA:H1'	2:P:6:DT:H5''	1.66	0.77
3:A:277:ILE:HG12	3:A:335:GLU:CA	2.12	0.77
3:A:108:PRO:O	3:A:112:ARG:HG3	1.84	0.77
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.19	0.77
3:A:195:LEU:HG	3:A:196:THR:H	1.50	0.77
3:A:227:THR:HG23	3:A:235:PHE:CE2	2.19	0.77
3:A:323:ILE:O	3:A:324:GLN:HG2	1.85	0.77
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.20	0.76
3:A:180:SER:HA	3:A:183:ARG:HE	1.51	0.76
3:A:140:LEU:HD12	3:A:140:LEU:O	1.86	0.75
3:A:195:LEU:HD23	3:A:259:LEU:CD1	2.16	0.75
3:A:243:SER:HB3	3:A:249:GLU:HA	1.69	0.75
3:A:251:PRO:HG2	3:A:253:ARG:NE	2.02	0.75
3:A:37:ASN:HB3	5:A:556:HOH:O	1.85	0.75
3:A:121:THR:HG23	3:A:124:ASP:CG	2.12	0.74
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.22	0.74
3:A:188:SER:HB3	5:A:522:HOH:O	1.86	0.74
1:T:4:DT:H5'	5:T:617:HOH:O	1.87	0.73
1:T:4:DT:O5'	3:A:231:GLY:HA3	1.88	0.73
3:A:155:MET:HE2	3:A:188:SER:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:PRO:HA	3:A:333:ARG:CG	2.19	0.72
3:A:254:ARG:HH22	3:A:256:ASP:CG	1.96	0.72
3:A:218:LEU:N	3:A:218:LEU:HD13	2.03	0.72
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.71	0.72
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.72	0.72
1:T:3:DT:C6	1:T:4:DT:H72	2.25	0.72
3:A:194:LEU:HD23	3:A:269:VAL:CG2	2.19	0.72
3:A:233:THR:HB	5:A:538:HOH:O	1.88	0.72
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.19	0.71
3:A:270:LEU:CD2	3:A:319:ILE:HG21	2.20	0.71
3:A:255:ILE:HG12	3:A:256:ASP:H	1.53	0.71
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.72	0.71
3:A:179:GLY:O	3:A:182:ARG:HB3	1.91	0.70
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.71	0.70
3:A:175:ALA:HB2	3:A:195:LEU:CD1	2.21	0.70
3:A:27:LYS:HG3	3:A:28:ASN:N	2.04	0.70
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.72	0.70
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.21	0.70
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.06	0.69
3:A:18:MET:HE3	3:A:82:LEU:HD13	1.75	0.69
3:A:194:LEU:HD23	3:A:269:VAL:HG23	1.74	0.69
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.21	0.69
3:A:255:ILE:HG12	3:A:256:ASP:N	2.07	0.68
3:A:11:LEU:HD23	3:A:11:LEU:N	2.07	0.68
3:A:60:LYS:HZ1	3:A:66:GLY:HA2	1.59	0.68
3:A:33:ILE:O	3:A:37:ASN:HB2	1.94	0.68
3:A:105:GLY:HA3	3:A:136:GLN:HG2	1.76	0.68
3:A:146:PHE:HB2	5:A:514:HOH:O	1.95	0.68
3:A:243:SER:OG	3:A:249:GLU:HG3	1.94	0.67
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.75	0.67
1:T:7:DA:H61	2:P:1:DT:H3	1.42	0.67
1:T:7:DA:N6	2:P:1:DT:H3	1.91	0.67
3:A:152:ARG:HD2	3:A:185:ALA:O	1.94	0.67
3:A:270:LEU:HD21	3:A:282:MET:CE	2.22	0.67
3:A:251:PRO:HG2	3:A:253:ARG:CZ	2.24	0.67
3:A:288:GLU:C	3:A:289:LYS:HD3	2.20	0.67
3:A:277:ILE:H	3:A:277:ILE:CD1	2.07	0.67
3:A:214:VAL:HG23	3:A:215:VAL:H	1.59	0.67
3:A:211:LEU:O	3:A:214:VAL:HG22	1.95	0.67
3:A:21:GLU:HB3	3:A:85:LEU:HD11	1.78	0.67
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.29	0.66
3:A:245:ASN:HD22	3:A:245:ASN:N	1.74	0.66
1:T:5:DA:H1'	5:T:564:HOH:O	1.96	0.66
3:A:164:ASN:O	3:A:168:LYS:HG2	1.94	0.66
3:A:253:ARG:NH1	5:A:503:HOH:O	2.29	0.66
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.24	0.66
3:A:328:ARG:O	3:A:333:ARG:NE	2.28	0.66
3:A:190:ASP:OD1	3:A:190:ASP:N	2.28	0.66
3:A:280:LYS:O	3:A:284:ALA:N	2.29	0.66
2:P:1:DT:C2'	2:P:2:DC:H5'	2.24	0.66
3:A:182:ARG:O	3:A:330:PRO:HB2	1.96	0.66
3:A:253:ARG:NE	5:A:521:HOH:O	2.29	0.65
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.26	0.65
3:A:214:VAL:HG23	3:A:215:VAL:N	2.11	0.65
3:A:169:VAL:HG22	3:A:170:ASP:N	2.11	0.65
3:A:254:ARG:NH1	3:A:255:ILE:O	2.29	0.65
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.11	0.65
3:A:240:GLN:NE2	3:A:250:TYR:O	2.30	0.65
3:A:295:GLU:N	3:A:295:GLU:OE1	2.29	0.65
3:A:103:VAL:HG22	3:A:143:PHE:HD2	1.62	0.65
3:A:200:PHE:HB2	5:A:625:HOH:O	1.97	0.65
3:A:309:GLU:N	3:A:309:GLU:OE1	2.30	0.65
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.78	0.64
3:A:59:ALA:O	3:A:65:VAL:HG21	1.96	0.64
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.61	0.64
3:A:327:TYR:HD1	3:A:328:ARG:N	1.95	0.64
3:A:165:GLU:OE1	3:A:168:LYS:HD3	1.98	0.64
3:A:155:MET:HE2	3:A:188:SER:CB	2.28	0.63
3:A:11:LEU:HA	3:A:52:LYS:NZ	2.14	0.63
3:A:294:ASN:O	3:A:296:TYR:N	2.26	0.63
3:A:128:ASN:N	3:A:128:ASN:HD22	1.97	0.63
3:A:137:ARG:NH1	5:A:515:HOH:O	2.32	0.63
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.13	0.63
3:A:195:LEU:O	3:A:260:ILE:HB	1.99	0.63
3:A:319:ILE:O	3:A:323:ILE:HG12	1.99	0.63
3:A:320:PHE:O	3:A:325:TRP:N	2.30	0.62
1:T:3:DT:C2'	1:T:4:DT:H72	2.30	0.62
3:A:124:ASP:O	3:A:128:ASN:ND2	2.31	0.62
3:A:182:ARG:HH11	3:A:182:ARG:HG2	1.65	0.62
3:A:282:MET:HB2	3:A:325:TRP:HZ3	1.62	0.62
3:A:286:ALA:O	3:A:291:PHE:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.82	0.61
3:A:45:VAL:HG23	3:A:46:ILE:H	1.64	0.61
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.35	0.61
3:A:172:GLU:HG3	3:A:198:PRO:CG	2.31	0.61
3:A:73:ILE:HG22	3:A:77:LEU:HD13	1.81	0.61
3:A:270:LEU:HD23	3:A:319:ILE:HG21	1.81	0.61
3:A:326:LYS:HE3	3:A:328:ARG:NH2	2.15	0.61
3:A:38:ALA:O	3:A:41:LYS:HD3	2.01	0.60
3:A:240:GLN:NE2	5:A:591:HOH:O	2.35	0.60
3:A:156:LEU:CD2	3:A:181:PHE:HE1	2.14	0.60
3:A:238:VAL:HA	3:A:253:ARG:O	1.99	0.60
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.25	0.60
3:A:291:PHE:O	3:A:301:LEU:HD22	2.01	0.60
3:A:294:ASN:ND2	5:A:580:HOH:O	2.33	0.60
3:A:144:GLY:N	5:A:590:HOH:O	2.34	0.60
3:A:166:VAL:O	3:A:169:VAL:HG13	2.00	0.60
3:A:74:ASP:O	3:A:77:LEU:N	2.34	0.60
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.31	0.60
3:A:165:GLU:HB2	3:A:218:LEU:CD1	2.31	0.60
3:A:38:ALA:O	3:A:41:LYS:NZ	2.29	0.60
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.84	0.60
3:A:57:ALA:O	3:A:60:LYS:HB3	2.02	0.59
3:A:11:LEU:H	3:A:11:LEU:CD2	2.11	0.59
3:A:313:VAL:HA	3:A:318:ASP:OD2	2.02	0.59
3:A:266:TYR:O	3:A:270:LEU:N	2.33	0.59
3:A:128:ASN:N	3:A:128:ASN:ND2	2.51	0.59
3:A:195:LEU:HG	3:A:196:THR:N	2.16	0.59
3:A:299:ARG:HD3	3:A:310:PRO:HG3	1.84	0.59
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.68	0.59
3:A:97:ILE:HG23	3:A:111:ALA:HB1	1.84	0.58
1:T:6:DG:H2"	1:T:7:DA:C8	2.37	0.58
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.37	0.58
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.10	0.58
3:A:169:VAL:HG13	3:A:170:ASP:H	1.69	0.58
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.39	0.58
3:A:203:GLU:O	3:A:205:THR:N	2.37	0.58
3:A:263:ASP:C	3:A:264:GLN:HG2	2.29	0.58
3:A:79:THR:C	3:A:81:LYS:H	2.12	0.58
3:A:253:ARG:NH2	5:A:620:HOH:O	2.30	0.58
3:A:265:TYR:O	3:A:269:VAL:N	2.29	0.58
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:326:LYS:HE3	3:A:328:ARG:HH21	1.69	0.58
3:A:165:GLU:OE2	3:A:221:VAL:HG11	2.03	0.58
3:A:200:PHE:HE2	3:A:261:PRO:HD3	1.69	0.58
3:A:300:PRO:HG3	3:A:311:LEU:HD13	1.84	0.58
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.85	0.58
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.03	0.57
3:A:152:ARG:CA	3:A:155:MET:HB2	2.34	0.57
3:A:60:LYS:NZ	3:A:67:THR:N	2.52	0.57
3:A:264:GLN:HB3	3:A:296:TYR:O	2.04	0.57
3:A:274:GLY:O	3:A:278:PHE:HD2	1.87	0.57
3:A:279:ASN:O	3:A:283:ARG:N	2.28	0.57
3:A:140:LEU:HD12	3:A:140:LEU:C	2.29	0.57
3:A:152:ARG:O	3:A:156:LEU:HG	2.04	0.57
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.86	0.57
3:A:151:PRO:HG2	3:A:154:GLU:CD	2.30	0.57
3:A:18:MET:O	3:A:22:LEU:HD23	2.04	0.57
3:A:176:THR:HG22	3:A:178:CYS:SG	2.44	0.57
3:A:267:CYS:SG	3:A:297:THR:HA	2.45	0.57
3:A:288:GLU:O	3:A:289:LYS:HD3	2.05	0.57
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.40	0.57
3:A:278:PHE:HB2	3:A:333:ARG:O	2.04	0.57
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.86	0.56
3:A:73:ILE:O	3:A:77:LEU:HD13	2.06	0.56
3:A:83:ARG:O	3:A:86:GLU:N	2.38	0.56
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.36	0.56
3:A:259:LEU:O	3:A:260:ILE:HG12	2.06	0.56
3:A:121:THR:O	3:A:124:ASP:N	2.39	0.56
3:A:180:SER:CB	3:A:183:ARG:HH21	2.04	0.56
3:A:223:PHE:CD1	3:A:239:CYS:HB2	2.41	0.56
3:A:87:LYS:O	3:A:90:GLN:N	2.39	0.56
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.40	0.55
3:A:60:LYS:HZ2	3:A:67:THR:N	2.03	0.55
3:A:92:ASP:O	3:A:96:SER:N	2.29	0.55
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.41	0.55
3:A:79:THR:O	3:A:81:LYS:N	2.37	0.55
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.06	0.55
3:A:157:GLN:HE22	3:A:244:LYS:NZ	2.04	0.55
3:A:155:MET:HA	3:A:158:MET:CE	2.32	0.55
3:A:114:PHE:HZ	3:A:132:LEU:HD23	1.71	0.55
3:A:200:PHE:HE2	3:A:261:PRO:CD	2.19	0.55
3:A:311:LEU:O	3:A:313:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:172:GLU:HB3	3:A:197:HIS:HE2	1.72	0.55
3:A:248:LYS:O	3:A:248:LYS:HG2	2.06	0.55
3:A:165:GLU:HB3	3:A:217:GLN:HG2	1.89	0.55
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.88	0.55
1:T:7:DA:H1'	5:T:634:HOH:O	2.05	0.54
3:A:56:GLY:N	3:A:74:ASP:OD2	2.40	0.54
3:A:165:GLU:CB	3:A:217:GLN:HG3	2.35	0.54
3:A:200:PHE:HE2	3:A:261:PRO:N	2.04	0.54
3:A:229:SER:O	3:A:235:PHE:HA	2.07	0.54
3:A:121:THR:OG1	3:A:123:GLU:N	2.40	0.54
3:A:156:LEU:HD21	3:A:181:PHE:HE1	1.73	0.54
3:A:206:LYS:HG2	5:A:624:HOH:O	2.07	0.54
3:A:212:HIS:H	3:A:212:HIS:CD2	2.26	0.54
3:A:230:LYS:HG3	3:A:235:PHE:HD2	1.72	0.54
3:A:250:TYR:CB	3:A:251:PRO:HD2	2.37	0.54
3:A:115:VAL:O	3:A:118:GLY:N	2.41	0.53
3:A:35:LYS:O	3:A:38:ALA:HB3	2.08	0.53
3:A:194:LEU:HD23	3:A:269:VAL:HG22	1.88	0.53
3:A:177:VAL:HB	3:A:181:PHE:CE2	2.43	0.53
3:A:45:VAL:HG23	3:A:46:ILE:N	2.23	0.53
3:A:200:PHE:CE2	3:A:261:PRO:N	2.77	0.53
3:A:282:MET:HB3	5:A:555:HOH:O	2.07	0.53
3:A:104:SER:O	3:A:136:GLN:HA	2.09	0.53
3:A:212:HIS:O	3:A:216:GLU:HB2	2.09	0.53
3:A:277:ILE:CG1	3:A:335:GLU:HA	2.23	0.53
3:A:58:GLU:O	3:A:61:LYS:HG3	2.08	0.53
3:A:214:VAL:O	3:A:217:GLN:N	2.42	0.53
3:A:118:GLY:O	3:A:120:LYS:HG3	2.09	0.53
3:A:207:GLN:O	3:A:210:LEU:N	2.29	0.52
3:A:309:GLU:N	3:A:310:PRO:HD3	2.24	0.52
3:A:183:ARG:HH11	3:A:275:SER:HA	1.74	0.52
3:A:318:ASP:O	3:A:322:TYR:N	2.41	0.52
3:A:121:THR:O	3:A:124:ASP:HB2	2.10	0.52
3:A:103:VAL:O	3:A:106:ILE:N	2.34	0.52
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.36	0.52
3:A:200:PHE:C	3:A:201:THR:HG22	2.34	0.52
1:T:1:DC:O2	2:P:7:DG:N1	2.43	0.52
3:A:122:LEU:HD21	3:A:126:ARG:NH2	2.24	0.52
1:T:4:DT:O2	2:P:4:DA:H2	1.94	0.51
3:A:25:PHE:CE1	3:A:88:ILE:HG12	2.46	0.51
3:A:74:ASP:O	3:A:78:ALA:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:243:SER:O	3:A:244:LYS:O	2.29	0.51
3:A:171:SER:N	5:A:552:HOH:O	2.43	0.51
3:A:15:ILE:CD1	3:A:73:ILE:HG23	2.39	0.51
3:A:18:MET:HG3	3:A:82:LEU:HD22	1.92	0.51
3:A:317:LYS:HG3	3:A:321:ASP:OD2	2.11	0.51
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.26	0.51
3:A:294:ASN:ND2	5:A:593:HOH:O	2.44	0.51
3:A:58:GLU:O	3:A:61:LYS:HD2	2.11	0.51
3:A:292:THR:O	3:A:298:ILE:HA	2.10	0.51
3:A:175:ALA:HB2	3:A:195:LEU:HD12	1.92	0.51
3:A:53:ILE:O	3:A:54:LYS:HD2	2.11	0.51
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.46	0.50
3:A:106:ILE:HG22	3:A:107:GLY:N	2.26	0.50
3:A:77:LEU:N	3:A:77:LEU:HD12	2.26	0.50
3:A:317:LYS:HD2	3:A:321:ASP:OD1	2.11	0.50
1:T:6:DG:N3	5:T:651:HOH:O	2.35	0.50
3:A:26:GLU:O	3:A:30:SER:O	2.29	0.50
1:T:5:DA:H2''	1:T:6:DG:O5'	2.12	0.50
3:A:287:LEU:HD12	3:A:287:LEU:O	2.11	0.50
3:A:316:GLU:OE1	3:A:333:ARG:NH2	2.39	0.50
5:P:568:HOH:O	3:A:110:ALA:HB2	2.12	0.50
3:A:183:ARG:HD3	3:A:273:THR:O	2.12	0.50
3:A:248:LYS:HD2	3:A:248:LYS:N	2.27	0.50
3:A:18:MET:HE3	3:A:82:LEU:CD1	2.41	0.49
3:A:150:ILE:CG2	3:A:158:MET:HE1	2.41	0.49
3:A:133:ASN:ND2	3:A:135:HIS:H	2.11	0.49
3:A:282:MET:HA	3:A:325:TRP:CH2	2.47	0.49
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.43	0.49
3:A:132:LEU:O	3:A:137:ARG:NE	2.42	0.49
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.47	0.49
3:A:18:MET:O	3:A:21:GLU:HB2	2.13	0.49
3:A:278:PHE:CD2	3:A:333:ARG:HB3	2.47	0.49
3:A:35:LYS:O	3:A:38:ALA:N	2.45	0.49
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.95	0.48
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.95	0.48
3:A:251:PRO:HG2	3:A:253:ARG:HE	1.75	0.48
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.81	0.48
3:A:65:VAL:H	3:A:65:VAL:HG13	1.10	0.48
3:A:214:VAL:CG2	3:A:215:VAL:H	2.26	0.48
1:T:7:DA:N6	2:P:1:DT:N3	2.55	0.48
3:A:114:PHE:CZ	3:A:132:LEU:CD2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:212:HIS:HB3	5:A:541:HOH:O	2.12	0.48
3:A:149:ARG:HD3	5:A:656:HOH:O	2.12	0.48
3:A:201:THR:O	3:A:203:GLU:N	2.47	0.48
3:A:238:VAL:HG12	3:A:239:CYS:N	2.27	0.48
3:A:295:GLU:HA	5:A:592:HOH:O	2.14	0.48
3:A:300:PRO:HG3	3:A:311:LEU:CD1	2.43	0.48
3:A:326:LYS:HG3	3:A:326:LYS:O	2.11	0.48
3:A:41:LYS:HZ1	3:A:42:ALA:HB2	1.79	0.48
3:A:62:LEU:N	3:A:62:LEU:CD1	2.77	0.48
3:A:318:ASP:O	3:A:321:ASP:HB2	2.13	0.48
3:A:330:PRO:C	3:A:333:ARG:HG2	2.39	0.48
2:P:5:DA:C1'	2:P:6:DT:H5''	2.41	0.48
3:A:91:ASP:CG	3:A:93:THR:HB	2.39	0.48
3:A:323:ILE:C	3:A:324:GLN:HG2	2.39	0.48
3:A:114:PHE:HD1	3:A:114:PHE:HA	1.41	0.47
3:A:278:PHE:O	3:A:282:MET:N	2.47	0.47
3:A:123:GLU:HA	3:A:126:ARG:HG3	1.97	0.47
3:A:268:GLY:HA2	3:A:295:GLU:O	2.14	0.47
3:A:62:LEU:N	3:A:62:LEU:HD13	2.29	0.47
3:A:270:LEU:HD13	3:A:316:GLU:OE2	2.14	0.47
3:A:275:SER:OG	3:A:277:ILE:HD13	2.15	0.47
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.47
3:A:59:ALA:C	3:A:65:VAL:HG21	2.40	0.47
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.52	0.47
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.79	0.47
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.45	0.47
3:A:97:ILE:HG23	3:A:111:ALA:CB	2.45	0.47
3:A:170:ASP:OD1	3:A:172:GLU:N	2.28	0.47
3:A:211:LEU:HD12	3:A:214:VAL:CG2	2.45	0.47
2:P:1:DT:H2'	2:P:2:DC:C6	2.50	0.47
3:A:205:THR:HA	5:A:624:HOH:O	2.14	0.47
3:A:150:ILE:HG22	3:A:155:MET:HG2	1.96	0.47
3:A:193:VAL:H	3:A:193:VAL:HG23	1.36	0.46
3:A:207:GLN:HB3	3:A:210:LEU:CD1	2.45	0.46
3:A:322:TYR:C	3:A:324:GLN:H	2.21	0.46
3:A:26:GLU:OE1	3:A:30:SER:OG	2.29	0.46
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.52	0.46
3:A:195:LEU:HD12	3:A:195:LEU:HA	1.63	0.46
3:A:195:LEU:CD2	3:A:259:LEU:HD13	2.29	0.46
3:A:49:TYR:HE2	3:A:51:HIS:HB2	1.79	0.46
3:A:135:HIS:O	3:A:139:GLY:N	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:156:LEU:N	3:A:156:LEU:HD23	2.29	0.46
3:A:327:TYR:HD1	3:A:328:ARG:H	1.62	0.46
3:A:41:LYS:NZ	3:A:42:ALA:HB2	2.30	0.46
3:A:217:GLN:HA	3:A:217:GLN:HE21	1.76	0.46
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.51	0.46
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.96	0.46
3:A:191:MET:CG	3:A:255:ILE:HG13	2.31	0.46
3:A:212:HIS:CD2	3:A:212:HIS:N	2.82	0.46
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.79	0.46
2:P:4:DA:C2'	2:P:5:DA:H5'	2.24	0.46
3:A:122:LEU:HD21	3:A:126:ARG:CZ	2.46	0.46
2:P:5:DA:P	3:A:107:GLY:HA3	2.57	0.45
3:A:176:THR:HB	3:A:265:TYR:OH	2.16	0.45
3:A:218:LEU:HD23	3:A:224:ILE:HD11	1.98	0.45
1:T:3:DT:N1	1:T:4:DT:H72	2.30	0.45
3:A:60:LYS:HZ1	3:A:66:GLY:CA	2.28	0.45
3:A:282:MET:CB	3:A:325:TRP:CZ3	3.00	0.45
3:A:165:GLU:HG3	3:A:221:VAL:HG21	1.97	0.45
3:A:180:SER:O	3:A:185:ALA:HB3	2.16	0.45
3:A:75:GLU:O	3:A:75:GLU:HG2	2.16	0.45
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.52	0.45
3:A:289:LYS:HD3	3:A:289:LYS:N	2.25	0.45
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.97	0.45
3:A:55:SER:HA	3:A:74:ASP:OD1	2.17	0.45
3:A:278:PHE:HE2	3:A:333:ARG:HD2	1.76	0.45
3:A:326:LYS:O	3:A:328:ARG:HG2	2.17	0.45
3:A:76:PHE:HD1	3:A:77:LEU:HD12	1.82	0.45
3:A:115:VAL:C	3:A:118:GLY:H	2.25	0.45
3:A:130:ASP:C	3:A:132:LEU:H	2.24	0.45
3:A:151:PRO:HD2	3:A:154:GLU:OE1	2.16	0.45
3:A:191:MET:HA	5:A:502:HOH:O	2.17	0.45
3:A:163:LEU:N	3:A:163:LEU:HD23	2.27	0.44
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.98	0.44
3:A:76:PHE:CD1	3:A:76:PHE:C	2.95	0.44
3:A:282:MET:SD	3:A:320:PHE:CE1	3.10	0.44
3:A:119:ILE:HG22	3:A:124:ASP:CB	2.47	0.44
3:A:180:SER:HB2	3:A:185:ALA:CB	2.47	0.44
3:A:206:LYS:N	5:A:624:HOH:O	2.50	0.44
2:P:5:DA:H1'	2:P:6:DT:C5'	2.42	0.44
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.99	0.44
3:A:106:ILE:CG2	3:A:107:GLY:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:300:PRO:HD2	3:A:309:GLU:O	2.17	0.44
3:A:261:PRO:C	3:A:263:ASP:N	2.74	0.44
3:A:271:TYR:CD2	3:A:272:PHE:N	2.86	0.44
3:A:249:GLU:HG3	3:A:250:TYR:H	1.82	0.44
2:P:5:DA:H2''	2:P:6:DT:H5'	1.99	0.44
3:A:19:LEU:HB3	3:A:43:ALA:HB2	2.00	0.44
3:A:79:THR:C	3:A:81:LYS:N	2.76	0.44
3:A:204:SER:O	3:A:204:SER:OG	2.32	0.44
3:A:15:ILE:HD13	3:A:73:ILE:CG2	2.46	0.44
3:A:70:ALA:O	3:A:73:ILE:HB	2.18	0.44
3:A:133:ASN:C	3:A:137:ARG:HG3	2.43	0.44
1:T:4:DT:N3	2:P:4:DA:C2	2.82	0.43
3:A:302:GLY:HA3	3:A:307:ALA:HB2	2.00	0.43
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.70	0.43
3:A:128:ASN:O	3:A:131:LYS:N	2.52	0.43
3:A:10:THR:CG2	3:A:11:LEU:N	2.79	0.43
3:A:57:ALA:HA	3:A:60:LYS:HB2	1.99	0.43
3:A:165:GLU:O	3:A:169:VAL:HG12	2.18	0.43
3:A:57:ALA:HA	3:A:60:LYS:CB	2.49	0.43
3:A:65:VAL:O	3:A:65:VAL:HG23	2.18	0.43
3:A:156:LEU:CD2	3:A:181:PHE:CE1	2.99	0.43
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.53	0.43
3:A:292:THR:C	3:A:293:ILE:HD13	2.43	0.43
3:A:27:LYS:CG	3:A:28:ASN:N	2.79	0.43
3:A:127:LYS:C	3:A:128:ASN:ND2	2.76	0.43
3:A:316:GLU:O	3:A:320:PHE:HD2	2.02	0.43
1:T:1:DC:H6	1:T:1:DC:H2'	1.46	0.43
5:T:617:HOH:O	3:A:234:LYS:HD3	2.18	0.43
3:A:27:LYS:CB	3:A:36:TYR:CD1	3.01	0.43
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.84	0.43
3:A:218:LEU:N	3:A:218:LEU:CD1	2.76	0.43
3:A:261:PRO:C	3:A:263:ASP:H	2.27	0.43
3:A:259:LEU:C	3:A:260:ILE:HG12	2.44	0.43
3:A:112:ARG:O	3:A:115:VAL:HB	2.19	0.42
3:A:296:TYR:C	3:A:297:THR:HG23	2.44	0.42
3:A:11:LEU:HA	3:A:52:LYS:HZ2	1.84	0.42
3:A:200:PHE:CE2	3:A:261:PRO:CA	3.03	0.42
3:A:265:TYR:HB3	3:A:266:TYR:H	1.56	0.42
2:P:5:DA:H2''	2:P:6:DT:C5'	2.49	0.42
3:A:20:THR:O	3:A:23:ALA:HB3	2.19	0.42
3:A:22:LEU:HD22	3:A:85:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:30:SER:HA	5:A:641:HOH:O	2.18	0.42
3:A:143:PHE:CD1	3:A:143:PHE:C	2.97	0.42
3:A:91:ASP:OD2	3:A:93:THR:HB	2.19	0.42
3:A:197:HIS:CD2	3:A:198:PRO:CD	2.98	0.42
3:A:158:MET:HG2	3:A:223:PHE:CZ	2.55	0.42
3:A:11:LEU:C	3:A:12:ASN:ND2	2.78	0.42
3:A:56:GLY:H	3:A:74:ASP:CG	2.28	0.42
3:A:133:ASN:HD22	3:A:135:HIS:H	1.67	0.42
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.55	0.42
3:A:322:TYR:C	3:A:324:GLN:N	2.78	0.42
3:A:235:PHE:CD1	3:A:235:PHE:C	2.97	0.42
3:A:12:ASN:ND2	5:A:642:HOH:O	2.43	0.41
3:A:119:ILE:HG22	3:A:124:ASP:HB2	2.02	0.41
3:A:193:VAL:HB	3:A:257:ILE:CG2	2.31	0.41
3:A:298:ILE:HG21	3:A:322:TYR:CD2	2.55	0.41
3:A:149:ARG:NH2	3:A:187:SER:O	2.53	0.41
3:A:177:VAL:HB	3:A:181:PHE:HE2	1.82	0.41
3:A:198:PRO:C	3:A:200:PHE:H	2.28	0.41
3:A:260:ILE:HG23	3:A:261:PRO:HD2	2.01	0.41
3:A:298:ILE:HD13	3:A:322:TYR:HD2	1.85	0.41
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.98	0.41
3:A:211:LEU:HD12	3:A:214:VAL:HG22	2.03	0.41
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.47	0.41
3:A:121:THR:OG1	3:A:124:ASP:N	2.52	0.41
3:A:151:PRO:HB2	3:A:153:GLU:HG2	2.03	0.41
3:A:175:ALA:CB	3:A:195:LEU:HD12	2.51	0.41
3:A:214:VAL:CG2	3:A:215:VAL:N	2.77	0.41
3:A:133:ASN:O	3:A:137:ARG:HG3	2.19	0.41
3:A:157:GLN:O	3:A:160:ASP:HB3	2.21	0.41
3:A:254:ARG:HH11	3:A:254:ARG:HD2	1.69	0.41
2:P:5:DA:H2''	2:P:6:DT:H71	2.02	0.41
3:A:111:ALA:O	3:A:115:VAL:HG23	2.21	0.41
3:A:119:ILE:H	3:A:119:ILE:HG12	1.40	0.41
2:P:5:DA:H8	2:P:5:DA:H2'	1.55	0.41
3:A:15:ILE:CD1	3:A:73:ILE:CG2	2.99	0.41
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.48	0.41
3:A:60:LYS:HD2	3:A:60:LYS:HA	1.81	0.41
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.40	0.41
3:A:122:LEU:HA	3:A:125:LEU:HD12	2.03	0.41
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.99	0.41
3:A:61:LYS:C	3:A:62:LEU:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:ASP:OD1	3:A:93:THR:HB	2.20	0.41
3:A:250:TYR:CB	3:A:251:PRO:CD	2.99	0.41
3:A:285:HIS:HD2	3:A:323:ILE:CD1	2.09	0.41
3:A:77:LEU:N	3:A:77:LEU:CD1	2.83	0.40
3:A:277:ILE:C	3:A:279:ASN:N	2.78	0.40
1:T:7:DA:N1	2:P:1:DT:C2	2.89	0.40
3:A:327:TYR:CD1	3:A:327:TYR:C	2.99	0.40
3:A:15:ILE:HG22	3:A:46:ILE:CD1	2.52	0.40
3:A:62:LEU:HA	3:A:62:LEU:HD12	1.77	0.40
3:A:291:PHE:HB3	3:A:292:THR:H	1.59	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%)	244 (75%)	59 (18%)	22 (7%)	1 7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	202	SER
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	246	ASP
3	A	295	GLU
3	A	13	GLY
3	A	141	LYS
3	A	185	ALA
3	A	206	LYS
3	A	229	SER

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Mol	Chain	Res	Type
3	A	265	TYR
3	A	60	LYS
3	A	278	PHE
3	A	134	HIS
3	A	247	GLU
3	A	212	HIS
3	A	262	LYS
3	A	207	GLN
3	A	220	LYS
3	A	242	PRO
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%)	213 (74%)	75 (26%)	0 2

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	15	ILE
3	A	18	MET
3	A	22	LEU
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	54	LYS
3	A	61	LYS
3	A	62	LEU
3	A	65	VAL

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Mol	Chain	Res	Type
3	A	67	THR
3	A	79	THR
3	A	89	ARG
3	A	92	ASP
3	A	94	SER
3	A	96	SER
3	A	100	LEU
3	A	101	THR
3	A	113	LYS
3	A	114	PHE
3	A	119	ILE
3	A	121	THR
3	A	126	ARG
3	A	128	ASN
3	A	138	ILE
3	A	141	LYS
3	A	143	PHE
3	A	145	ASP
3	A	153	GLU
3	A	155	MET
3	A	159	GLN
3	A	161	ILE
3	A	169	VAL
3	A	172	GLU
3	A	174	ILE
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	193	VAL
3	A	194	LEU
3	A	201	THR
3	A	211	LEU
3	A	218	LEU
3	A	219	GLN
3	A	225	THR
3	A	227	THR
3	A	230	LYS
3	A	235	PHE
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE

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Mol	Chain	Res	Type
3	A	257	ILE
3	A	259	LEU
3	A	263	ASP
3	A	264	GLN
3	A	267	CYS
3	A	270	LEU
3	A	277	ILE
3	A	287	LEU
3	A	289	LYS
3	A	301	LEU
3	A	304	THR
3	A	309	GLU
3	A	314	ASP
3	A	325	TRP
3	A	328	ARG
3	A	331	LYS
3	A	332	ASP
3	A	335	GLU

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	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	197	HIS
3	A	212	HIS
3	A	217	GLN
3	A	245	ASN
3	A	252	HIS
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%)	-0.64	0 100 100	18, 44, 99, 100	0
2	P	7/7 (100%)	-0.55	0 100 100	20, 41, 54, 83	0
3	A	324/335 (96%)	-0.58	0 100 100	4, 38, 96, 100	0
All	All	339/350 (96%)	-0.58	0 100 100	4, 39, 96, 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	341	1/1	0.98	0.09	1,1,1,1	0
4	NA	A	342	1/1	0.98	0.05	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.