



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:05 PM UTC

PDB ID : 9ICK / pdb_00009ick
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX, SOAKED IN THE PRESENCE OF ARTIFICIAL MOTHER LIQUOR
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-16
Resolution : 2.70 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

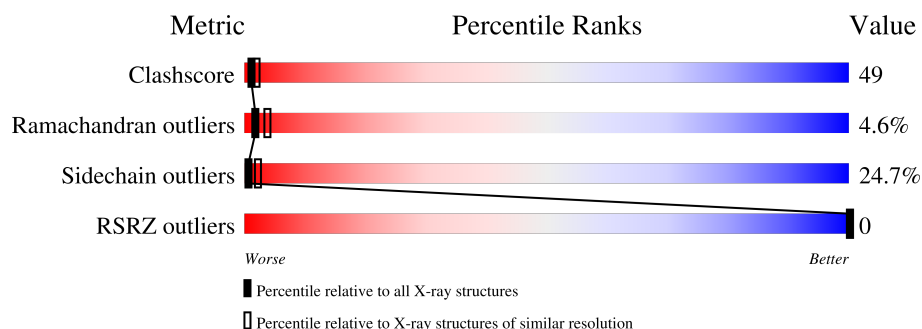
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	T	7	
2	P	6	
3	A	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3026 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3').

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

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

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

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

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

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

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

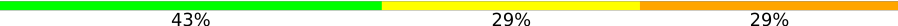
- Molecule 5 is water.

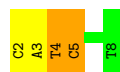
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	12	Total	O	0	0
			12	12		
5	P	21	Total	O	0	0
			21	21		
5	A	120	Total	O	0	0
			120	120		

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')

Chain T: 



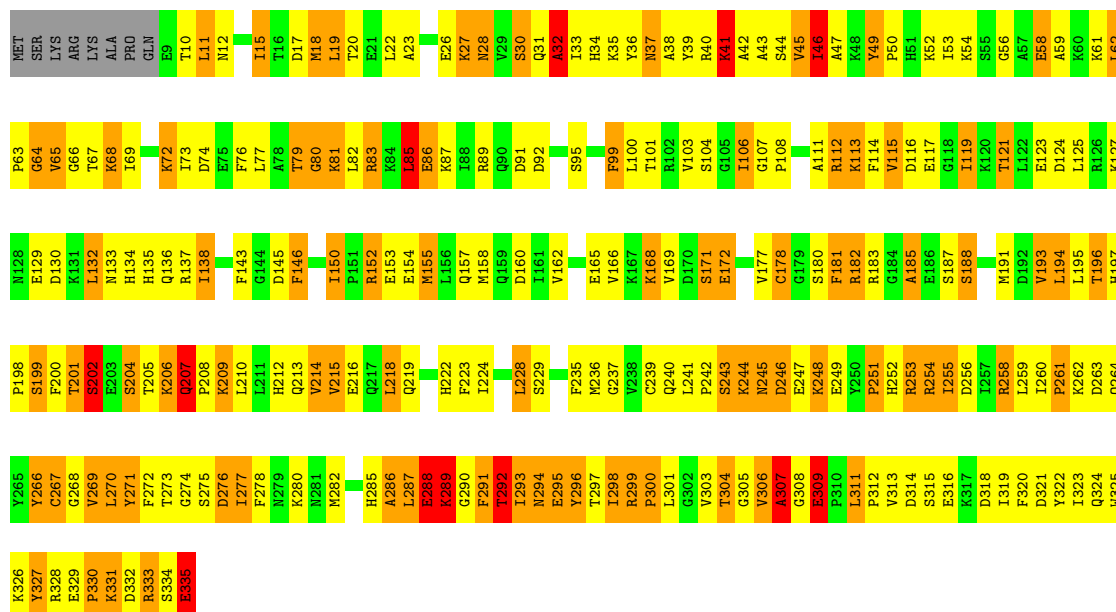
- Molecule 2: DNA (5'-D(*CP*AP*GP*AP*TP*G)-3')

Chain P: 



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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.54Å 57.73Å 48.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.70) 89.3 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	3.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.164 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 189.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3026	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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	1.04	0/135	2.12	7/207 (3.4%)
2	P	1.31	1/141 (0.7%)	2.11	7/214 (3.3%)
3	A	1.62	19/2672 (0.7%)	2.02	87/3590 (2.4%)
All	All	1.59	20/2948 (0.7%)	2.03	101/4011 (2.5%)

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	2	0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	215	VAL	C-N	-6.58	1.25	1.33
3	A	165	GLU	C-O	-6.49	1.16	1.24
3	A	65	VAL	C-N	-6.32	1.26	1.33
2	P	1	DC	OP3-P	6.17	1.60	1.48
3	A	330	PRO	N-CA	-6.17	1.39	1.47
3	A	58	GLU	CA-C	-5.86	1.45	1.52
3	A	15	ILE	CA-C	-5.83	1.45	1.52
3	A	236	MET	C-O	-5.66	1.17	1.24
3	A	251	PRO	N-CA	-5.60	1.40	1.47
3	A	115	VAL	CA-CB	-5.55	1.47	1.54
3	A	254	ARG	C-O	-5.54	1.17	1.23
3	A	160	ASP	CG-OD2	5.32	1.35	1.25
3	A	66	GLY	N-CA	-5.14	1.40	1.44
3	A	146	PHE	CA-C	-5.13	1.45	1.52
3	A	116	ASP	N-CA	-5.12	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	17	ASP	CG-OD1	5.04	1.34	1.25
3	A	106	ILE	C-O	-5.03	1.18	1.24
3	A	129	GLU	CD-OE1	5.01	1.34	1.25
3	A	145	ASP	CG-OD2	5.00	1.34	1.25
3	A	171	SER	CA-C	-5.00	1.45	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	49	TYR	CA-C-N	14.08	133.62	119.82
3	A	49	TYR	C-N-CA	14.08	133.62	119.82
2	P	5	DT	C2-N1-C1'	12.62	138.28	119.35
2	P	5	DT	C6-N1-C1'	-12.41	100.73	119.35
3	A	34	HIS	CA-CB-CG	-11.16	102.64	113.80
3	A	99	PHE	CA-CB-CG	-10.45	103.35	113.80
1	T	4	DT	C6-N1-C1'	-10.33	103.86	119.35
1	T	4	DT	C2-N1-C1'	10.17	134.60	119.35
1	T	5	DC	C6-N1-C1'	-9.39	105.62	119.70
1	T	5	DC	C2-N1-C1'	9.28	133.63	119.70
3	A	291	PHE	N-CA-C	8.57	122.09	109.07
3	A	64	GLY	N-CA-C	-8.20	105.32	115.08
3	A	49	TYR	O-C-N	8.06	128.33	121.31
3	A	116	ASP	CA-CB-CG	-8.05	104.55	112.60
3	A	40	ARG	N-CA-C	7.94	120.02	111.36
3	A	152	ARG	N-CA-CB	7.74	122.36	110.14
3	A	168	LYS	N-CA-CB	7.70	121.44	110.12
3	A	30	SER	CA-C-N	-7.63	109.07	122.26
3	A	30	SER	C-N-CA	-7.63	109.07	122.26
3	A	28	ASN	N-CA-C	7.52	119.56	111.36
3	A	32	ALA	N-CA-C	7.46	126.68	110.80
3	A	92	ASP	N-CA-CB	6.84	120.17	110.12
3	A	20	THR	N-CA-CB	6.80	119.94	110.07
1	T	2	DC	C2-N1-C1'	6.72	129.78	119.70
3	A	292	THR	N-CA-CB	6.71	121.49	110.69
2	P	4	DA	P-O3'-C3'	6.69	130.24	120.20
3	A	87	LYS	CA-C-N	6.65	129.57	120.46
3	A	87	LYS	C-N-CA	6.65	129.57	120.46
3	A	272	PHE	CA-CB-CG	-6.53	107.28	113.80
3	A	86	GLU	N-CA-CB	6.49	119.42	110.01
1	T	2	DC	C6-N1-C1'	-6.44	110.04	119.70
3	A	286	ALA	CA-C-N	6.35	128.78	120.28
3	A	286	ALA	C-N-CA	6.35	128.78	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	296	TYR	N-CA-C	6.32	121.28	113.50
3	A	335	GLU	N-CA-CB	6.31	121.23	110.50
3	A	304	THR	N-CA-CB	-6.24	99.94	110.49
3	A	327	TYR	N-CA-CB	6.21	119.32	109.51
3	A	313	VAL	N-CA-C	6.16	116.74	107.75
3	A	41	LYS	N-CA-CB	6.15	119.81	110.28
3	A	228	LEU	N-CA-C	-6.12	103.23	112.04
3	A	138	ILE	CB-CA-C	-6.12	104.14	111.97
3	A	246	ASP	N-CA-C	6.07	123.72	110.80
3	A	271	TYR	CA-CB-CG	-6.06	102.99	113.90
3	A	266	TYR	CA-CB-CG	-6.02	103.06	113.90
3	A	214	VAL	N-CA-CB	5.96	118.64	110.54
3	A	83	ARG	N-CA-CB	5.95	118.64	110.01
3	A	261	PRO	CB-CA-C	-5.84	103.92	111.46
3	A	87	LYS	CB-CA-C	5.76	120.03	110.81
3	A	204	SER	CA-C-N	-5.75	113.38	121.72
3	A	204	SER	C-N-CA	-5.75	113.38	121.72
3	A	20	THR	CB-CA-C	5.75	119.98	110.90
3	A	292	THR	CB-CA-C	5.74	119.70	109.38
3	A	193	VAL	N-CA-C	5.72	116.53	108.36
3	A	333	ARG	N-CA-C	-5.71	106.17	113.02
3	A	123	GLU	CB-CA-C	5.68	119.80	110.88
3	A	286	ALA	O-C-N	5.68	128.00	122.09
3	A	240	GLN	N-CA-C	5.66	117.60	108.32
3	A	318	ASP	CA-CB-CG	-5.64	106.96	112.60
3	A	181	PHE	CB-CA-C	-5.64	101.09	110.68
3	A	307	ALA	N-CA-CB	5.59	119.94	110.49
3	A	222	HIS	CA-CB-CG	-5.58	108.22	113.80
3	A	288	GLU	N-CA-C	-5.54	104.93	110.97
3	A	86	GLU	CB-CA-C	5.54	119.58	110.88
3	A	209	LYS	O-C-N	5.51	127.96	122.12
3	A	160	ASP	CA-CB-CG	-5.50	107.10	112.60
3	A	146	PHE	N-CA-CB	5.50	118.69	110.22
2	P	3	DG	P-O5'-C5'	5.49	128.24	120.00
3	A	292	THR	N-CA-C	5.46	118.38	109.59
3	A	46	ILE	N-CA-CB	5.46	119.98	110.65
3	A	181	PHE	CA-C-N	5.45	128.59	120.31
3	A	181	PHE	C-N-CA	5.45	128.59	120.31
2	P	6	DG	C4-N9-C1'	-5.43	118.86	127.00
3	A	28	ASN	CB-CA-C	-5.39	101.69	110.85
3	A	85	LEU	N-CA-C	-5.28	105.52	111.28
3	A	269	VAL	CB-CA-C	-5.28	105.12	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	49	TYR	CA-C-O	5.25	124.66	119.51
3	A	267	CYS	N-CA-C	-5.25	105.64	111.36
2	P	1	DC	C2-N1-C1'	5.23	127.55	119.70
3	A	92	ASP	CB-CA-C	5.20	119.43	110.79
2	P	1	DC	C6-N1-C1'	-5.17	111.94	119.70
3	A	334	SER	CB-CA-C	5.16	120.69	110.42
3	A	246	ASP	N-CA-CB	5.15	119.20	110.49
3	A	196	THR	N-CA-CB	5.13	119.67	111.56
3	A	216	GLU	N-CA-CB	-5.13	102.58	110.12
3	A	207	GLN	CA-C-N	5.12	124.73	119.05
3	A	207	GLN	C-N-CA	5.12	124.73	119.05
3	A	40	ARG	N-CA-CB	5.11	117.73	110.16
3	A	307	ALA	CB-CA-C	5.10	120.58	110.42
3	A	320	PHE	O-C-N	5.10	127.39	122.09
1	T	5	DC	O3'-P-O5'	-5.09	96.36	104.00
3	A	222	HIS	CB-CA-C	-5.09	101.74	111.06
3	A	178	CYS	CB-CA-C	5.07	120.52	110.42
3	A	299	ARG	CA-C-N	5.07	126.46	120.23
3	A	299	ARG	C-N-CA	5.07	126.46	120.23
3	A	107	GLY	N-CA-C	-5.06	102.01	112.34
3	A	300	PRO	CB-CA-C	-5.06	106.05	111.56
3	A	155	MET	CA-C-N	5.02	127.01	120.28
3	A	155	MET	C-N-CA	5.02	127.01	120.28
3	A	104	SER	CA-C-N	-5.00	116.32	123.08
3	A	104	SER	C-N-CA	-5.00	116.32	123.08
3	A	252	HIS	CA-CB-CG	-5.00	108.80	113.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	246	ASP	CA
3	A	292	THR	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	3	0
2	P	126	0	68	13	0
3	A	2623	0	2641	255	1
4	A	2	0	0	0	0
5	A	120	0	0	8	0
5	P	21	0	0	4	0
5	T	12	0	0	1	0
All	All	3026	0	2778	270	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 49.

All (270) 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:1:DC:H2''	2:P:2:DA:H5''	1.28	1.14
2:P:5:DT:H2''	2:P:6:DG:H5'	1.31	1.08
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.41	1.03
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.55	1.03
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.45	0.98
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.97	0.95
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.47	0.94
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.53	0.90
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.67	0.90
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.56	0.88
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.11	0.85
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.57	0.84
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.60	0.82
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.10	0.82
3:A:11:LEU:HD23	3:A:11:LEU:H	1.43	0.81
3:A:331:LYS:HD2	3:A:332:ASP:N	1.96	0.80
2:P:1:DC:C2'	2:P:2:DA:H5''	2.10	0.80
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.12	0.80
3:A:12:ASN:HD21	3:A:53:ILE:H	1.29	0.80
2:P:2:DA:C8	2:P:2:DA:H5'	2.17	0.79
3:A:212:HIS:HB3	5:A:541:HOH:O	1.83	0.78
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.66	0.78
3:A:271:TYR:HB2	5:A:592:HOH:O	1.83	0.77
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.00	0.76
3:A:166:VAL:O	3:A:169:VAL:HG12	1.86	0.75
3:A:68:LYS:O	3:A:72:LYS:HE3	1.87	0.75
3:A:259:LEU:O	3:A:260:ILE:HD13	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:HG21	3:A:158:MET:CE	2.18	0.74
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.52	0.74
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.68	0.74
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.03	0.73
3:A:27:LYS:HG3	3:A:28:ASN:N	2.04	0.73
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.18	0.72
3:A:18:MET:HE1	3:A:76:PHE:CB	2.20	0.72
3:A:245:ASN:HD22	3:A:245:ASN:N	1.88	0.72
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.89	0.72
3:A:41:LYS:HD3	3:A:42:ALA:N	2.05	0.72
3:A:278:PHE:HB2	3:A:333:ARG:O	1.90	0.71
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.71	0.71
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.36	0.71
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.05	0.71
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.70
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.72	0.70
3:A:41:LYS:O	3:A:45:VAL:HG13	1.92	0.69
3:A:255:ILE:HG12	3:A:256:ASP:N	2.07	0.69
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.26	0.69
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.75	0.69
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.22	0.69
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.26	0.69
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.57	0.69
3:A:111:ALA:O	3:A:115:VAL:HG23	1.93	0.68
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.92	0.68
3:A:152:ARG:HA	3:A:155:MET:HB2	1.74	0.68
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.67
3:A:18:MET:CE	3:A:76:PHE:HB2	2.24	0.67
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.35	0.67
3:A:215:VAL:O	3:A:219:GLN:HG3	1.95	0.66
3:A:295:GLU:CD	3:A:295:GLU:H	2.03	0.66
3:A:31:GLN:N	5:A:641:HOH:O	2.27	0.66
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.77	0.66
3:A:286:ALA:O	3:A:291:PHE:HB2	1.96	0.65
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.23	0.64
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.27	0.64
3:A:113:LYS:O	3:A:117:GLU:HG3	1.97	0.64
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.30	0.64
3:A:207:GLN:O	3:A:210:LEU:HB2	1.98	0.64
3:A:201:THR:HA	3:A:261:PRO:CB	2.27	0.64
3:A:201:THR:HA	3:A:261:PRO:HB3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.78	0.64
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.80	0.64
3:A:326:LYS:HG3	3:A:326:LYS:O	1.99	0.63
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.80	0.63
3:A:80:GLY:O	3:A:81:LYS:HG2	1.98	0.63
3:A:306:VAL:HG23	3:A:307:ALA:N	2.13	0.62
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.29	0.62
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.00	0.61
3:A:330:PRO:HA	3:A:333:ARG:CG	2.25	0.61
2:P:5:DT:C2'	2:P:6:DG:H5'	2.19	0.61
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.00	0.61
3:A:202:SER:HB2	3:A:263:ASP:CG	2.26	0.61
3:A:27:LYS:HG3	3:A:28:ASN:HD22	1.66	0.61
3:A:182:ARG:NH2	3:A:316:GLU:OE2	2.29	0.60
2:P:5:DT:H1'	5:P:565:HOH:O	2.02	0.59
3:A:248:LYS:O	3:A:248:LYS:HG2	2.01	0.59
3:A:23:ALA:O	3:A:36:TYR:HD1	1.86	0.59
3:A:155:MET:HA	3:A:158:MET:HE3	1.83	0.59
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.84	0.59
3:A:41:LYS:HD3	3:A:42:ALA:H	1.68	0.58
2:P:3:DG:H1'	5:P:511:HOH:O	2.02	0.58
3:A:157:GLN:HE22	3:A:244:LYS:HZ3	1.51	0.58
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.16	0.58
3:A:28:ASN:N	3:A:28:ASN:HD22	2.02	0.57
2:P:2:DA:H5'	2:P:2:DA:H8	1.66	0.57
3:A:11:LEU:H	3:A:11:LEU:CD2	2.15	0.57
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.67	0.57
3:A:152:ARG:NH2	3:A:181:PHE:O	2.38	0.57
3:A:201:THR:HG23	3:A:204:SER:HB3	1.86	0.57
3:A:276:ASP:O	3:A:280:LYS:HG3	2.05	0.57
3:A:308:GLY:O	3:A:309:GLU:HB2	2.04	0.57
3:A:303:VAL:C	3:A:305:GLY:H	2.14	0.56
3:A:162:VAL:O	3:A:166:VAL:HG23	2.06	0.56
3:A:326:LYS:HE2	3:A:328:ARG:HE	1.69	0.56
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.36	0.56
2:P:3:DG:N3	5:P:511:HOH:O	2.32	0.56
3:A:85:LEU:O	3:A:89:ARG:HG3	2.06	0.56
3:A:243:SER:HB3	3:A:249:GLU:HA	1.88	0.55
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.22	0.55
3:A:268:GLY:O	3:A:271:TYR:HB3	2.06	0.55
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.42	0.55
3:A:155:MET:HE2	3:A:188:SER:HB2	1.88	0.55
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.22	0.55
3:A:298:ILE:HG22	5:A:578:HOH:O	2.07	0.54
3:A:327:TYR:CD1	3:A:328:ARG:N	2.76	0.54
3:A:262:LYS:O	3:A:262:LYS:HG3	2.07	0.54
3:A:245:ASN:N	3:A:245:ASN:ND2	2.55	0.54
3:A:200:PHE:HB2	5:A:625:HOH:O	2.07	0.54
3:A:264:GLN:HA	5:A:536:HOH:O	2.08	0.54
3:A:35:LYS:O	3:A:38:ALA:HB3	2.08	0.54
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.92	0.53
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.35	0.53
3:A:12:ASN:ND2	3:A:53:ILE:H	2.03	0.53
3:A:79:THR:C	3:A:81:LYS:H	2.15	0.53
3:A:69:ILE:O	3:A:73:ILE:HG13	2.08	0.53
3:A:154:GLU:O	3:A:158:MET:HG3	2.09	0.53
3:A:79:THR:O	3:A:81:LYS:N	2.41	0.53
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.45	0.52
3:A:327:TYR:HD1	3:A:328:ARG:N	2.06	0.52
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.45	0.52
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.39	0.52
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.24	0.52
3:A:81:LYS:NZ	3:A:86:GLU:OE1	2.35	0.52
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.90	0.52
3:A:196:THR:OG1	3:A:197:HIS:N	2.40	0.52
3:A:275:SER:OG	3:A:277:ILE:HG12	2.09	0.52
3:A:209:LYS:O	3:A:213:GLN:HG3	2.10	0.52
3:A:294:ASN:N	3:A:294:ASN:HD22	2.07	0.52
3:A:202:SER:HB2	3:A:263:ASP:OD1	2.10	0.52
3:A:208:PRO:O	3:A:212:HIS:HD2	1.92	0.52
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.92	0.51
3:A:133:ASN:O	3:A:137:ARG:HG3	2.11	0.51
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.93	0.51
3:A:180:SER:HB2	3:A:185:ALA:CB	2.41	0.51
3:A:150:ILE:N	3:A:188:SER:O	2.35	0.51
3:A:294:ASN:HD22	3:A:294:ASN:H	1.58	0.51
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.93	0.51
3:A:288:GLU:C	3:A:290:GLY:H	2.19	0.50
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.40	0.50
3:A:319:ILE:O	3:A:322:TYR:HB2	2.12	0.50
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.41	0.50
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.93	0.50
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.46	0.50
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.57	0.50
3:A:199:SER:O	3:A:199:SER:OG	2.29	0.49
3:A:287:LEU:HD12	3:A:287:LEU:O	2.13	0.49
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.43	0.49
3:A:205:THR:O	3:A:206:LYS:O	2.31	0.49
3:A:266:TYR:HA	3:A:269:VAL:HB	1.95	0.49
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.43	0.49
1:T:4:DT:H2''	1:T:5:DC:O5'	2.13	0.48
3:A:63:PRO:C	3:A:65:VAL:H	2.21	0.48
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.48	0.48
3:A:121:THR:O	3:A:124:ASP:HB2	2.13	0.48
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.26	0.48
3:A:56:GLY:HA3	3:A:74:ASP:OD2	2.14	0.48
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.96	0.48
3:A:241:LEU:HB3	3:A:242:PRO:HD2	1.96	0.48
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.49	0.48
3:A:200:PHE:O	3:A:262:LYS:N	2.42	0.48
3:A:292:THR:CG2	3:A:299:ARG:HH21	2.26	0.47
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.43	0.47
3:A:133:ASN:ND2	5:A:596:HOH:O	2.47	0.47
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.13	0.47
3:A:205:THR:O	3:A:205:THR:HG23	2.13	0.47
3:A:237:GLY:O	3:A:254:ARG:NH1	2.47	0.47
3:A:44:SER:O	3:A:47:ALA:HB3	2.15	0.47
3:A:103:VAL:HG22	3:A:143:PHE:HD2	1.80	0.47
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.36	0.47
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.97	0.47
3:A:288:GLU:O	3:A:290:GLY:N	2.49	0.46
3:A:315:SER:OG	3:A:316:GLU:N	2.48	0.46
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.30	0.46
3:A:321:ASP:O	3:A:324:GLN:N	2.46	0.46
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.38	0.46
3:A:183:ARG:HD3	3:A:273:THR:O	2.16	0.46
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.97	0.46
3:A:58:GLU:O	3:A:61:LYS:HB2	2.15	0.46
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.97	0.46
3:A:134:HIS:HD2	5:A:515:HOH:O	1.99	0.45
3:A:127:LYS:HD2	3:A:127:LYS:HA	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:TYR:CE2	3:A:53:ILE:HG12	2.51	0.45
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.51	0.45
3:A:267:CYS:SG	3:A:297:THR:HA	2.55	0.45
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.98	0.45
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.05	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.80	0.44
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.68	0.44
3:A:326:LYS:CE	3:A:328:ARG:HE	2.31	0.44
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.30	0.44
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.81	0.44
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.98	0.44
3:A:197:HIS:CG	3:A:198:PRO:CD	3.00	0.44
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.30	0.44
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.47	0.44
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.47	0.44
3:A:150:ILE:O	3:A:187:SER:HA	2.17	0.44
3:A:270:LEU:HD13	3:A:316:GLU:OE1	2.18	0.44
2:P:2:DA:H5'	2:P:2:DA:H2'	1.52	0.43
3:A:322:TYR:C	3:A:324:GLN:H	2.25	0.43
3:A:43:ALA:O	3:A:47:ALA:HB2	2.19	0.43
3:A:235:PHE:CD2	3:A:235:PHE:C	2.95	0.43
3:A:172:GLU:CG	3:A:198:PRO:CG	2.96	0.43
3:A:206:LYS:O	3:A:207:GLN:HB2	2.18	0.43
2:P:4:DA:H5''	5:P:614:HOH:O	2.17	0.43
3:A:254:ARG:NH1	3:A:255:ILE:H	2.16	0.43
2:P:2:DA:H2''	2:P:3:DG:OP2	2.19	0.42
3:A:59:ALA:O	3:A:62:LEU:N	2.31	0.42
3:A:255:ILE:HG23	3:A:255:ILE:O	2.17	0.42
3:A:327:TYR:HE1	3:A:333:ARG:NH2	2.11	0.42
3:A:26:GLU:HG3	3:A:35:LYS:HB3	2.01	0.42
3:A:36:TYR:CD2	3:A:36:TYR:C	2.96	0.42
3:A:11:LEU:CD2	3:A:11:LEU:N	2.79	0.42
3:A:259:LEU:C	3:A:260:ILE:HD13	2.42	0.42
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.66	0.42
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.55	0.42
3:A:294:ASN:N	3:A:294:ASN:ND2	2.68	0.42
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.54	0.42
3:A:254:ARG:HH11	3:A:255:ILE:H	1.65	0.42
1:T:5:DC:H5'	3:A:229:SER:HB2	2.00	0.42
3:A:138:ILE:HD13	3:A:138:ILE:HG23	1.70	0.42
3:A:79:THR:C	3:A:81:LYS:N	2.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:108:PRO:O	3:A:112:ARG:HG3	2.20	0.42
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.66	0.42
3:A:223:PHE:O	3:A:239:CYS:HB2	2.19	0.42
3:A:267:CYS:O	3:A:271:TYR:HB2	2.20	0.42
3:A:311:LEU:HD12	3:A:311:LEU:HA	1.82	0.42
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.66	0.42
3:A:177:VAL:HG22	3:A:193:VAL:HG22	2.02	0.42
3:A:157:GLN:NE2	3:A:244:LYS:HZ3	2.15	0.41
3:A:146:PHE:HD1	3:A:146:PHE:HA	1.61	0.41
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.69	0.41
3:A:285:HIS:NE2	3:A:289:LYS:HG3	2.35	0.41
3:A:294:ASN:ND2	3:A:297:THR:H	2.18	0.41
3:A:327:TYR:HD1	3:A:328:ARG:H	1.69	0.41
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.41	0.41
3:A:135:HIS:C	3:A:135:HIS:CD2	2.98	0.41
3:A:182:ARG:HH22	3:A:316:GLU:CD	2.25	0.41
3:A:311:LEU:HA	3:A:312:PRO:HD3	1.91	0.41
3:A:18:MET:HG2	3:A:19:LEU:N	2.31	0.41
3:A:36:TYR:CD2	3:A:37:ASN:N	2.89	0.41
3:A:195:LEU:O	3:A:260:ILE:N	2.52	0.41
3:A:76:PHE:O	3:A:79:THR:O	2.38	0.41
3:A:150:ILE:CG2	3:A:158:MET:CE	2.95	0.41
3:A:18:MET:HE2	3:A:82:LEU:HD13	2.02	0.41
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.36	0.41
3:A:331:LYS:HD2	3:A:332:ASP:CB	2.51	0.41
3:A:266:TYR:O	3:A:270:LEU:HB2	2.21	0.40
3:A:274:GLY:HA3	3:A:275:SER:HA	1.91	0.40
3:A:294:ASN:HD22	3:A:294:ASN:C	2.29	0.40
2:P:5:DT:H2''	2:P:6:DG:C5'	2.23	0.40
3:A:99:PHE:CD2	3:A:99:PHE:C	3.00	0.40
3:A:264:GLN:HE21	3:A:264:GLN:HB3	1.44	0.40
3:A:132:LEU:HB3	3:A:136:GLN:HB3	2.04	0.40
3:A:132:LEU:HD23	3:A:132:LEU:N	2.35	0.40
3:A:210:LEU:HB3	3:A:259:LEU:HD21	2.03	0.40
3:A:276:ASP:OD1	3:A:276:ASP:N	2.54	0.40
1:T:3:DA:H1'	5:T:617:HOH:O	2.21	0.40
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.70	0.40
3:A:288:GLU:C	3:A:290:GLY:N	2.79	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]	1.84	0.36

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%)	287 (88%)	23 (7%)	15 (5%)	2 4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	206	LYS
3	A	244	LYS
3	A	246	ASP
3	A	247	GLU
3	A	309	GLU
3	A	202	SER
3	A	289	LYS
3	A	10	THR
3	A	80	GLY
3	A	91	ASP
3	A	207	GLN
3	A	307	ALA
3	A	304	THR

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%)	217 (75%)	71 (25%)	1 2

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	18	MET
3	A	19	LEU
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	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	112	ARG
3	A	113	LYS
3	A	119	ILE
3	A	121	THR
3	A	130	ASP
3	A	132	LEU
3	A	150	ILE
3	A	153	GLU
3	A	168	LYS
3	A	171	SER
3	A	172	GLU
3	A	182	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	188	SER
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	202	SER
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	228	LEU
3	A	243	SER
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	270	LEU
3	A	276	ASP
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	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	90	GLN
3	A	98	ASN
3	A	134	HIS
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN

5.3.3 RNA [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	7/7 (100%)	-1.20	0 100 100	23, 32, 63, 100	0
2	P	6/6 (100%)	-1.50	0 100 100	22, 30, 32, 38	0
3	A	324/335 (96%)	-0.93	0 100 100	12, 38, 84, 100	0
All	All	337/348 (96%)	-0.95	0 100 100	12, 37, 84, 100	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	A	341	1/1	0.89	0.07	34,34,34,34	0
4	NA	A	342	1/1	0.98	0.06	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.