



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:01 AM GMT

PDB ID : 8ICQ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

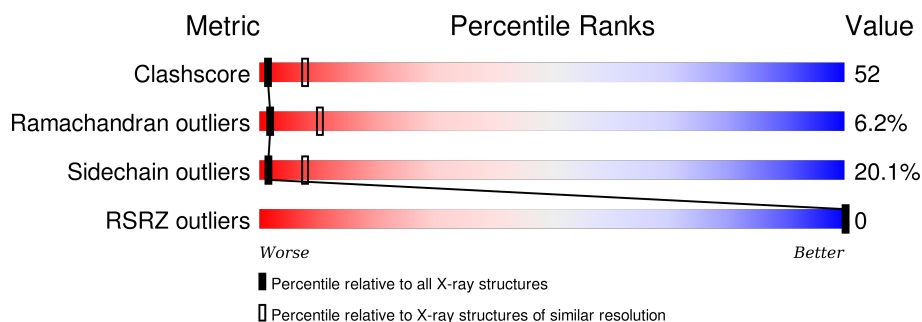
# 1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	A	342	-	-	-	X

## 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 (three-letter code: 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	A	108	Total	O	0	0
			108	108		
5	P	16	Total	O	0	0
			16	16		
5	T	15	Total	O	0	0
			15	15		



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.68 Å 57.69 Å 48.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 11.86 – 2.71	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.00) 87.6 (11.86-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.70 Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, $R_{free}$	0.159 , (Not available) 0.154 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , 108.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 12384 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	2.16	5/162 (3.1%)	3.70	22/249 (8.8%)
2	P	2.17	6/160 (3.8%)	3.89	23/243 (9.5%)
3	A	1.29	27/2672 (1.0%)	1.79	71/3590 (2.0%)
All	All	1.41	38/2994 (1.3%)	2.14	116/4082 (2.8%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	3	DT	N1-C2	9.28	1.45	1.38
1	T	6	DG	C3'-O3'	-8.89	1.32	1.44
3	A	86	GLU	CD-OE1	8.39	1.34	1.25
3	A	75	GLU	CD-OE1	8.30	1.34	1.25
2	P	2	DC	C1'-N1	8.25	1.59	1.49
3	A	165	GLU	CD-OE2	8.05	1.34	1.25
3	A	203	GLU	CD-OE1	8.04	1.34	1.25
3	A	249	GLU	CD-OE2	7.80	1.34	1.25
3	A	329	GLU	CD-OE2	7.59	1.34	1.25
1	T	1	DC	C3'-O3'	7.38	1.53	1.44
3	A	71	GLU	CD-OE1	7.15	1.33	1.25
3	A	216	GLU	CD-OE2	7.11	1.33	1.25
3	A	117	GLU	CD-OE2	7.08	1.33	1.25
2	P	3	DT	N1-C6	-7.07	1.33	1.38
3	A	147	GLU	CD-OE2	7.07	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DA	N9-C4	6.95	1.42	1.37
3	A	309	GLU	CD-OE2	6.90	1.33	1.25
3	A	288	GLU	CD-OE2	6.79	1.33	1.25
3	A	58	GLU	CD-OE1	6.62	1.32	1.25
3	A	154	GLU	CD-OE2	6.57	1.32	1.25
3	A	26	GLU	CD-OE1	6.40	1.32	1.25
1	T	5	DA	C5-C6	-6.39	1.35	1.41
3	A	123	GLU	CD-OE1	6.33	1.32	1.25
3	A	335	GLU	CD-OE2	6.31	1.32	1.25
3	A	186	GLU	CD-OE1	6.09	1.32	1.25
1	T	5	DA	C4'-O4'	-5.91	1.39	1.45
3	A	295	GLU	CD-OE2	5.90	1.32	1.25
3	A	153	GLU	CD-OE2	5.75	1.31	1.25
3	A	232	GLU	CD-OE2	5.71	1.31	1.25
3	A	172	GLU	CD-OE2	5.62	1.31	1.25
3	A	9	GLU	CD-OE2	5.43	1.31	1.25
1	T	3	DT	C4-C5	5.37	1.49	1.45
3	A	271	TYR	CB-CG	-5.35	1.43	1.51
2	P	3	DT	C2-N3	-5.33	1.33	1.37
3	A	247	GLU	CD-OE1	5.25	1.31	1.25
3	A	326	LYS	CE-NZ	-5.10	1.36	1.49
3	A	129	GLU	CD-OE1	5.06	1.31	1.25
2	P	3	DT	N3-C4	-5.01	1.34	1.38

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	4	DT	C6-N1-C1'	-21.48	88.19	120.40
1	T	7	DA	C4-N9-C1'	-20.94	88.61	126.30
2	P	1	DT	C6-N1-C1'	-20.63	89.46	120.40
1	T	4	DT	C2-N1-C1'	19.84	149.94	118.20
1	T	7	DA	C8-N9-C1'	19.37	162.56	127.70
2	P	6	DT	C6-N1-C1'	-18.45	92.72	120.40
2	P	1	DT	C2-N1-C1'	18.38	147.61	118.20
2	P	6	DT	C2-N1-C1'	17.15	145.64	118.20
2	P	2	DC	C2-N1-C1'	15.13	135.45	118.80
2	P	5	DA	C4-N9-C1'	13.22	150.09	126.30
2	P	5	DA	C8-N9-C1'	-12.34	105.49	127.70
2	P	2	DC	C6-N1-C1'	-11.87	106.56	120.80
2	P	3	DT	C6-N1-C1'	-10.95	103.98	120.40
2	P	7	DG	C4-N9-C1'	-10.67	112.62	126.50
2	P	3	DT	C2-N1-C1'	10.61	135.17	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	DT	N3-C2-O2	-10.48	116.01	122.30
2	P	7	DG	C8-N9-C1'	10.24	140.31	127.00
3	A	39	TYR	CB-CG-CD1	-9.97	115.02	121.00
3	A	124	ASP	CB-CG-OD2	-9.71	109.56	118.30
3	A	130	ASP	CB-CG-OD2	-9.38	109.86	118.30
3	A	192	ASP	CB-CA-C	-9.21	91.97	110.40
1	T	5	DA	N1-C6-N6	9.07	124.04	118.60
1	T	1	DC	P-O3'-C3'	9.04	130.55	119.70
3	A	190	ASP	CB-CG-OD2	-8.81	110.37	118.30
3	A	145	ASP	CB-CG-OD2	-8.72	110.45	118.30
2	P	3	DT	O4'-C1'-N1	8.69	114.08	108.00
1	T	7	DA	O4'-C1'-N9	8.38	113.87	108.00
3	A	253	ARG	NE-CZ-NH1	8.24	124.42	120.30
3	A	253	ARG	NE-CZ-NH2	-8.24	116.18	120.30
3	A	258	ARG	NE-CZ-NH1	8.05	124.32	120.30
3	A	258	ARG	NE-CZ-NH2	-7.94	116.33	120.30
3	A	332	ASP	CB-CG-OD1	-7.87	111.22	118.30
3	A	192	ASP	CB-CG-OD2	-7.75	111.33	118.30
3	A	299	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	T	1	DC	C6-N1-C1'	-7.63	111.65	120.80
3	A	190	ASP	CB-CG-OD1	7.59	125.13	118.30
3	A	314	ASP	CB-CG-OD1	-7.51	111.54	118.30
3	A	256	ASP	CB-CG-OD1	7.41	124.97	118.30
3	A	266	TYR	CA-CB-CG	-7.37	99.39	113.40
3	A	192	ASP	N-CA-CB	7.25	123.65	110.60
3	A	256	ASP	CB-CG-OD2	-7.25	111.78	118.30
3	A	266	TYR	CB-CG-CD1	-7.24	116.66	121.00
3	A	116	ASP	CB-CG-OD2	-7.24	111.79	118.30
3	A	91	ASP	CB-CG-OD1	-7.10	111.91	118.30
2	P	2	DC	O4'-C1'-N1	7.05	112.94	108.00
1	T	5	DA	O4'-C1'-N9	-7.02	103.08	108.00
3	A	92	ASP	CB-CG-OD2	-6.97	112.03	118.30
3	A	333	ARG	NE-CZ-NH2	-6.91	116.85	120.30
3	A	124	ASP	CB-CG-OD1	6.80	124.42	118.30
3	A	168	LYS	N-CA-CB	6.63	122.53	110.60
3	A	263	ASP	CB-CG-OD2	-6.61	112.35	118.30
3	A	157	GLN	CB-CA-C	6.60	123.59	110.40
1	T	7	DA	O4'-C1'-C2'	6.59	111.17	105.90
3	A	130	ASP	CB-CG-OD1	6.58	124.22	118.30
3	A	246	ASP	CB-CG-OD1	-6.52	112.43	118.30
3	A	246	ASP	CB-CG-OD2	6.51	124.16	118.30
3	A	326	LYS	CD-CE-NZ	6.51	126.67	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	1	DC	C2-N1-C1'	6.50	125.95	118.80
1	T	4	DT	O4'-C1'-C2'	-6.40	100.78	105.90
3	A	74	ASP	CB-CG-OD1	6.40	124.06	118.30
3	A	219	GLN	CB-CA-C	-6.38	97.64	110.40
3	A	39	TYR	CA-CB-CG	-6.33	101.37	113.40
1	T	7	DA	C8-N9-C4	6.33	108.33	105.80
3	A	224	ILE	CA-CB-CG1	-6.32	99.00	111.00
3	A	39	TYR	CB-CG-CD2	6.30	124.78	121.00
3	A	157	GLN	N-CA-CB	6.27	121.89	110.60
3	A	314	ASP	CB-CG-OD2	6.22	123.90	118.30
3	A	83	ARG	N-CA-CB	6.20	121.76	110.60
1	T	5	DA	C6-C5-N7	-6.18	127.97	132.30
3	A	159	GLN	CB-CA-C	-6.18	98.04	110.40
3	A	178	CYS	CA-CB-SG	-6.17	102.90	114.00
3	A	145	ASP	CB-CG-OD1	6.14	123.83	118.30
1	T	5	DA	C4-C5-N7	6.11	113.75	110.70
3	A	160	ASP	CB-CG-OD2	-5.93	112.96	118.30
3	A	170	ASP	CB-CG-OD1	5.92	123.63	118.30
3	A	145	ASP	CB-CA-C	-5.89	98.62	110.40
3	A	333	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	A	79	THR	CA-CB-CG2	-5.83	104.24	112.40
3	A	116	ASP	CB-CG-OD1	5.80	123.52	118.30
2	P	2	DC	C6-N1-C2	-5.79	117.98	120.30
3	A	17	ASP	CB-CG-OD2	5.79	123.51	118.30
3	A	12	ASN	CB-CA-C	5.76	121.92	110.40
3	A	332	ASP	CB-CG-OD2	5.74	123.46	118.30
3	A	27	LYS	N-CA-CB	-5.71	100.33	110.60
3	A	68	LYS	CB-CA-C	5.69	121.77	110.40
3	A	170	ASP	CB-CG-OD2	-5.68	113.19	118.30
3	A	68	LYS	N-CA-CB	5.67	120.80	110.60
3	A	17	ASP	CB-CG-OD1	-5.64	113.22	118.30
3	A	92	ASP	CB-CG-OD1	5.61	123.35	118.30
3	A	271	TYR	CA-CB-CG	-5.59	102.78	113.40
3	A	91	ASP	CB-CG-OD2	5.59	123.33	118.30
1	T	1	DC	O4'-C1'-C2'	5.57	110.36	105.90
2	P	3	DT	N1-C2-O2	5.53	127.52	123.10
1	T	5	DA	C5-N7-C8	-5.52	101.14	103.90
3	A	335	GLU	N-CA-CB	5.46	120.42	110.60
3	A	250	TYR	CB-CG-CD1	-5.38	117.77	121.00
2	P	3	DT	O4'-C1'-C2'	-5.34	101.63	105.90
3	A	271	TYR	N-CA-CB	-5.33	101.00	110.60
2	P	5	DA	O4'-C1'-C2'	-5.32	101.64	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	17	ASP	CB-CA-C	5.31	121.03	110.40
3	A	20	THR	N-CA-CB	5.30	120.38	110.30
1	T	1	DC	C6-N1-C2	5.24	122.40	120.30
3	A	205	THR	N-CA-CB	5.21	120.19	110.30
3	A	276	ASP	CB-CG-OD1	5.17	122.95	118.30
2	P	3	DT	C1'-O4'-C4'	-5.14	104.96	110.10
3	A	18	MET	CG-SD-CE	-5.13	91.99	100.20
2	P	3	DT	N1-C1'-C2'	5.13	122.35	112.60
2	P	3	DT	C5-C6-N1	-5.11	120.64	123.70
2	P	5	DA	O4'-C1'-N9	5.08	111.56	108.00
3	A	276	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	T	4	DT	C6-C5-C7	-5.07	119.86	122.90
3	A	260	ILE	CB-CA-C	-5.06	101.48	111.60
1	T	5	DA	C5-C6-N6	-5.06	119.65	123.70
1	T	5	DA	P-O5'-C5'	-5.04	112.83	120.90
3	A	89	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	T	5	DA	N9-C4-C5	-5.01	103.80	105.80

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	145	0	80	7	0
2	P	144	0	81	13	0
3	A	2623	0	2641	277	0
4	A	2	0	0	0	0
5	A	108	0	0	15	0
5	P	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	15	0	0	1	0
All	All	3053	0	2802	294	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 52.

All (294) 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:18:MET:HE1	3:A:76:PHE:HB2	1.50	0.93
1:T:6:DG:H2''	1:T:7:DA:C8	2.03	0.93
3:A:245:ASN:N	3:A:245:ASN:HD22	1.63	0.91
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.57	0.85
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: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:73:ILE:HG22	3:A:77:LEU:CD2	2.15	0.77
3:A:282:MET:HE2	5:A:555:HOH:O	1.84	0.77
3:A:245:ASN:H	3:A:245:ASN:ND2	1.80	0.77
3:A:108:PRO:O	3:A:112:ARG:HG3	1.85	0.76
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:TYR:HB2	5:A:592:HOH:O	1.90	0.72
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.19	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:291:PHE:CD2	3:A:323:ILE:HG22	2.25	0.71
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.72	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:327:TYR:HD1	3:A:328:ARG:N	1.89	0.70
3:A:289:LYS:N	3:A:289:LYS:HD3	2.07	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:HD13	3:A:119:ILE:N	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:254:ARG:NH1	3:A:254:ARG:HB3	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
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.60	0.65
3:A:140:LEU:O	3:A:140:LEU:HD12	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:330:PRO:HA	3:A:333:ARG:HG2	1.80	0.64
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:CB	3:A:183:ARG:HH21	2.08	0.64
3:A:254:ARG:HB3	3:A:254:ARG:CZ	2.28	0.63
3:A:295:GLU:H	3:A:295:GLU:CD	2.01	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: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:HG2	3:A:248:LYS:O	1.99	0.60
3:A:11:LEU:N	3:A:11:LEU:HD23	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:CD2	3:A:11:LEU:H	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:121:THR:HG23	3:A:124:ASP:CG	2.22	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:291:PHE:HD1	3:A:300:PRO:HA	1.67	0.58
3:A:162:VAL:O	3:A:166:VAL:HG23	2.04	0.58
3:A:58:GLU:O	3:A:61:LYS:HG3	2.04	0.58
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.39	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
3:A:15:ILE:O	3:A:19:LEU:HB2	2.04	0.57
3:A:150:ILE:HG21	3:A:158:MET:HE3	1.85	0.57
3:A:41:LYS:NZ	3:A:64:GLY:O	2.33	0.57
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.18	0.57
3:A:260:ILE:HG22	3:A:261:PRO:N	2.18	0.57
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.87	0.57
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:310:PRO:HB3	5:A:626:HOH:O	2.04	0.56
3:A:32:ALA:O	3:A:36:TYR:HB3	2.05	0.56
3:A:41:LYS:HZ3	3:A:42:ALA:HB2	1.70	0.56
3:A:145:ASP:OD2	3:A:252:HIS:N	2.28	0.56
3:A:183:ARG:HH11	3:A:275:SER:CB	2.20	0.55
3:A:15:ILE:CD1	3:A:73:ILE:HG23	2.29	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:154:GLU:O	3:A:158:MET:HE2	2.06	0.55
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.37	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:28:ASN:HD22	3:A:28:ASN:N	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
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: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:303:VAL:C	3:A:305:GLY:H	2.13	0.52
3:A:89:ARG:C	3:A:89:ARG:HD3	2.30	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
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:295:GLU:OE1	3:A:295:GLU:N	2.27	0.51
3:A:280:LYS:O	3:A:284:ALA:N	2.35	0.51
3:A:205:THR:HA	5:A:624:HOH:O	2.10	0.51
2:P:5:DA:H2''	2:P:6:DT:H5''	1.92	0.51
3:A:212:HIS:CD2	3:A:212:HIS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:LEU:HD23	3:A:85:LEU:HB2	1.93	0.50
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.93	0.50
3:A:175:ALA:HB2	3:A:195:LEU:CD1	2.42	0.50
3:A:292:THR:O	3:A:298:ILE:HA	2.12	0.49
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: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:180:SER:HA	3:A:183:ARG:HE	1.78	0.49
3:A:146:PHE:HZ	3:A:238:VAL:HG22	1.77	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:154:GLU:C	3:A:158:MET:HE2	2.33	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: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:33:ILE:HG23	3:A:34:HIS:H	1.78	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
3:A:270:LEU:C	3:A:270:LEU:HD12	2.29	0.48
3:A:288:GLU:C	3:A:290:GLY:H	2.17	0.48
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
3:A:150:ILE:HG21	3:A:158:MET:CE	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:18:MET:HE3	3:A:76:PHE:HB2	1.96	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.79	0.45
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.45	0.45
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.52	0.45
3:A:270:LEU:HD23	3:A:319:ILE:HD13	1.99	0.45
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.16	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: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:263:ASP:O	3:A:264:GLN:HG2	2.17	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: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:298:ILE:HG22	5:A:578:HOH:O	2.17	0.45
3:A:183:ARG:NH1	3:A:275:SER:CB	2.80	0.45
3:A:31:GLN:HE21	3:A:112:ARG:NH2	2.15	0.45
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.68	0.45
3:A:323:ILE:C	3:A:324:GLN:HG2	2.38	0.44
3:A:276:ASP:O	3:A:280:LYS:HG3	2.17	0.44
3:A:148:LYS:HB3	5:A:620:HOH:O	2.18	0.44
3:A:22:LEU:HA	3:A:22:LEU:HD13	1.50	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:159:GLN:HG2	3:A:159:GLN:O	2.17	0.44
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.86	0.44
3:A:287:LEU:HA	3:A:287:LEU:HD13	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:112:ARG:O	3:A:115:VAL:HB	2.18	0.43
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	3:A:259:LEU:HD12	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
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.59	0.43
1:T:7:DA:H61	2:P:1:DT:H3	1.65	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:285:HIS:CE1	3:A:289:LYS:HG2	2.54	0.43
3:A:266:TYR:HA	3:A:269:VAL:HB	2.00	0.43
3:A:243:SER:O	3:A:244:LYS:O	2.37	0.43
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.49	0.43
3:A:323:ILE:O	3:A:324:GLN:HG2	2.19	0.42
3:A:179:GLY:O	3:A:182:ARG:HB3	2.19	0.42
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.97	0.42
3:A:203:GLU:O	3:A:205:THR:N	2.52	0.42
1:T:2:DA:C2	2:P:7:DG:C2	3.08	0.42
3:A:62:LEU:HA	3:A:62:LEU:HD12	1.70	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:HA	3:A:156:LEU:HD23	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:241:LEU:HA	3:A:242:PRO:HD2	1.77	0.42
3:A:125:LEU:HD22	3:A:132:LEU:HD21	2.02	0.42
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.78	0.42
3:A:33:ILE:H	3:A:33:ILE:HG22	1.54	0.41
3:A:218:LEU:CD1	3:A:218:LEU:N	2.82	0.41
3:A:330:PRO:O	3:A:333:ARG:HG2	2.20	0.41
3:A:170:ASP:OD1	3:A:171:SER:N	2.54	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:25:PHE:CG	3:A:88:ILE:HD13	2.55	0.41
3:A:270:LEU:HD13	3:A:270:LEU:HA	1.64	0.41
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.20	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:N	3:A:128:ASN:ND2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:THR:C	3:A:81:LYS:H	2.22	0.41
3:A:18:MET:HE2	3:A:82:LEU:CD1	2.38	0.41
3:A:205:THR:O	3:A:206:LYS:HB2	2.21	0.41
3:A:262:LYS:O	3:A:262:LYS:HG3	2.16	0.41
3:A:286:ALA:HA	3:A:323:ILE:HG21	2.03	0.41
3:A:221:VAL:HG13	3:A:221:VAL:H	1.65	0.41
3:A:268:GLY:O	3:A:271:TYR:HB3	2.20	0.41
3:A:171:SER:O	3:A:171:SER:OG	2.35	0.41
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.66	0.40
3:A:325:TRP:HA	3:A:325:TRP:HD1	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
3:A:204:SER:OG	3:A:204:SER:O	2.28	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%)	2	10

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

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Mol	Chain	Res	Type
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 [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%)	230 (80%)	58 (20%)	<b>1</b> <b>8</b>

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	15	ILE
3	A	18	MET
3	A	22	LEU
3	A	25	PHE
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS

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Mol	Chain	Res	Type
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	54	LYS
3	A	61	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
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	100	LEU
3	A	101	THR
3	A	121	THR
3	A	136	GLN
3	A	152	ARG
3	A	168	LYS
3	A	169	VAL
3	A	194	LEU
3	A	201	THR
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	258	ARG
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	301	LEU
3	A	309	GLU

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Mol	Chain	Res	Type
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	327	TYR
3	A	331	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	128	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	T	8/8 (100%)	-0.72	0 100 100	18, 38, 96, 99	0
2	P	7/7 (100%)	-1.19	0 100 100	16, 28, 47, 82	0
3	A	324/335 (96%)	-1.18	0 100 100	3, 31, 83, 99	0
All	All	339/350 (96%)	-1.17	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	A	342	1/1	0.84	0.14	3.03	44,44,44,44	0
4	NA	A	341	1/1	0.95	0.07	-0.63	10,10,10,10	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.