WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2016 – 12:03 AM GMT

PDB ID : 9ICX
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA (NON GAPPED DNA ONLY)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-10-24
Resolution : 2.60 Å(reported)

The following versions of software and data (see references (i)) 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)
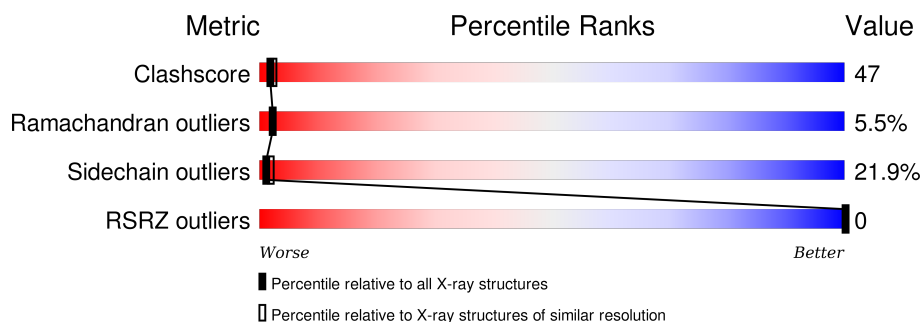Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
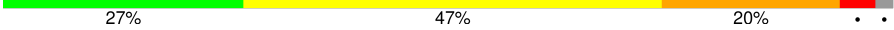*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Clashscore		47
Ramachandran outliers		5.5%
Sidechain outliers		21.9%
RSRZ outliers		0

Worse　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 >=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 <=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	6	50% · 50%
2	P	6	50% · 50%
3	A	335	27% · 47% · 20% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2985 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*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	6	Total 118	C 58	N 20	O 35	P 5	0	0	0

- 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 126	C 59	N 25	O 36	P 6	0	0	0

- 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 2623	C 1657	N 458	O 499	S 9	26	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total 91	O 91	0	0
5	P	14	Total 14	O 14	0	0
5	T	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
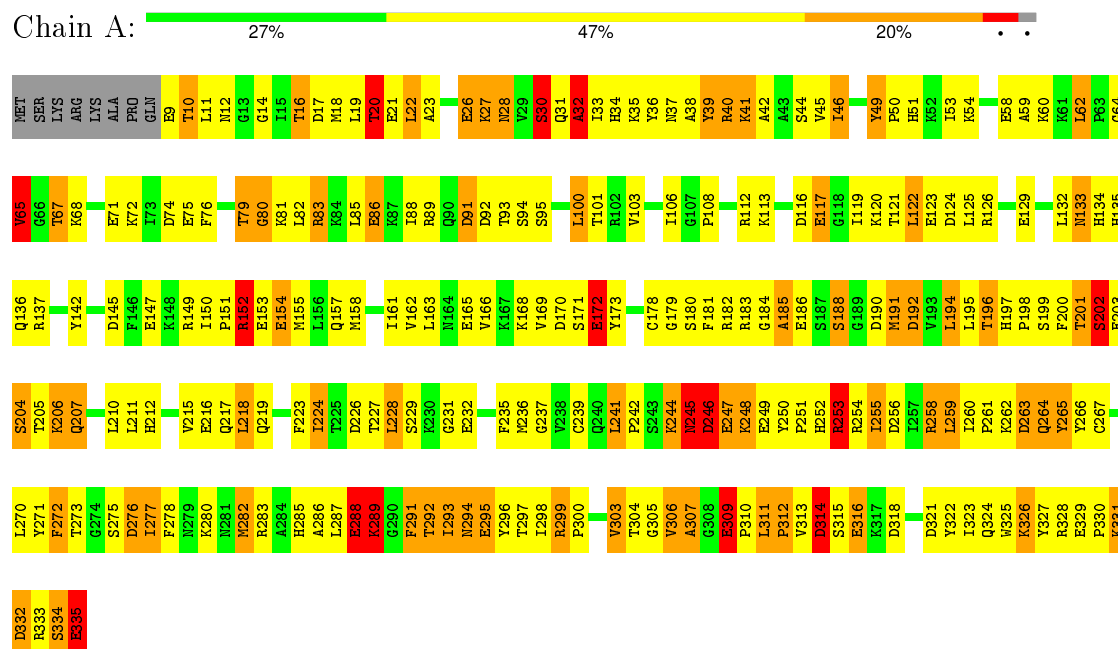
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*G)-3')

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 (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	179.01Å 57.73Å 48.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 9.99 – 2.58	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.60) 88.6 (9.99-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	1.29 (at 2.56Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.178 , (Not available) 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 100.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.46, <L^2> = 0.28$	Xtriage
Outliers	0 of 14481 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2985	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	1.93	3/131 (2.3%)	2.50	9/200 (4.5%)
2	P	2.40	5/141 (3.5%)	2.38	9/214 (4.2%)
3	A	1.30	27/2672 (1.0%)	1.73	50/3590 (1.4%)
All	All	1.40	35/2944 (1.2%)	1.81	68/4004 (1.7%)

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	1	0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DT	C1'-N1	13.10	1.66	1.49
3	A	154	GLU	CD-OE2	8.24	1.34	1.25
3	A	86	GLU	CD-OE1	7.55	1.33	1.25
3	A	203	GLU	CD-OE1	7.31	1.33	1.25
3	A	58	GLU	CD-OE1	7.21	1.33	1.25
3	A	147	GLU	CD-OE2	6.82	1.33	1.25
1	T	4	DT	C3'-O3'	-6.81	1.35	1.44
3	A	309	GLU	CD-OE2	6.78	1.33	1.25
3	A	117	GLU	CD-OE2	6.71	1.33	1.25
3	A	249	GLU	CD-OE2	6.71	1.33	1.25
3	A	21	GLU	CD-OE1	6.51	1.32	1.25
3	A	26	GLU	CD-OE1	6.51	1.32	1.25
3	A	316	GLU	CD-OE2	6.49	1.32	1.25
3	A	71	GLU	CD-OE1	6.39	1.32	1.25
2	P	1	DC	N1-C6	-6.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	172	GLU	CD-OE2	6.24	1.32	1.25
3	A	186	GLU	CD-OE1	6.21	1.32	1.25
3	A	123	GLU	CD-OE1	6.20	1.32	1.25
2	P	3	DG	C6-N1	-6.13	1.35	1.39
3	A	295	GLU	CD-OE1	6.05	1.32	1.25
3	A	329	GLU	CD-OE2	6.00	1.32	1.25
3	A	165	GLU	CD-OE2	5.97	1.32	1.25
3	A	335	GLU	CD-OE2	5.91	1.32	1.25
3	A	288	GLU	CD-OE2	5.82	1.32	1.25
1	T	2	DC	C3'-O3'	-5.70	1.36	1.44
1	T	3	DA	C3'-O3'	-5.67	1.36	1.44
3	A	232	GLU	CD-OE2	5.64	1.31	1.25
3	A	129	GLU	CD-OE1	5.58	1.31	1.25
3	A	326	LYS	CE-NZ	-5.55	1.35	1.49
3	A	153	GLU	CD-OE2	5.38	1.31	1.25
2	P	5	DT	C3'-O3'	-5.36	1.36	1.44
3	A	247	GLU	CD-OE1	5.31	1.31	1.25
2	P	6	DG	N9-C4	-5.29	1.33	1.38
3	A	9	GLU	CD-OE2	5.20	1.31	1.25
3	A	216	GLU	CD-OE2	5.15	1.31	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	253	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	T	5	DC	C2-N1-C1'	14.69	134.96	118.80
1	T	5	DC	C6-N1-C1'	-14.07	103.91	120.80
2	P	3	DG	P-O3'-C3'	12.00	134.10	119.70
3	A	253	ARG	NE-CZ-NH2	-11.19	114.71	120.30
3	A	192	ASP	CB-CG-OD2	-10.22	109.10	118.30
3	A	314	ASP	CB-CG-OD1	-8.92	110.27	118.30
3	A	263	ASP	CB-CG-OD2	-8.84	110.34	118.30
3	A	253	ARG	CD-NE-CZ	8.47	135.46	123.60
2	P	5	DT	O4'-C1'-N1	8.14	113.70	108.00
3	A	116	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	T	3	DA	O4'-C1'-N9	-7.20	102.96	108.00
3	A	190	ASP	CB-CG-OD2	-7.11	111.90	118.30
3	A	332	ASP	CB-CG-OD1	-7.07	111.94	118.30
3	A	190	ASP	CB-CG-OD1	6.94	124.55	118.30
2	P	4	DA	P-O3'-C3'	6.83	127.90	119.70
2	P	5	DT	C2-N1-C1'	6.67	128.87	118.20
3	A	83	ARG	NE-CZ-NH1	6.59	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	152	ARG	N-CA-CB	6.50	122.31	110.60
3	A	30	SER	C-N-CA	-6.45	105.57	121.70
3	A	32	ALA	N-CA-C	6.37	128.20	111.00
1	T	6	DT	P-O5'-C5'	-6.37	110.71	120.90
3	A	192	ASP	CB-CG-OD1	6.36	124.03	118.30
3	A	314	ASP	CB-CG-OD2	6.32	123.99	118.30
3	A	92	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	T	4	DT	C1'-O4'-C4'	-6.25	103.85	110.10
3	A	332	ASP	CB-CG-OD2	6.21	123.89	118.30
2	P	2	DA	O5'-P-OP1	-6.13	100.18	105.70
3	A	263	ASP	CB-CG-OD1	5.91	123.62	118.30
3	A	91	ASP	CB-CG-OD1	-5.89	113.00	118.30
3	A	226	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	T	7	DG	C8-N9-C1'	-5.84	119.40	127.00
3	A	304	THR	CA-CB-CG2	-5.83	104.23	112.40
3	A	170	ASP	CB-CG-OD1	5.82	123.54	118.30
3	A	245	ASN	CB-CA-C	5.76	121.93	110.40
3	A	92	ASP	CB-CG-OD1	5.71	123.44	118.30
3	A	334	SER	CB-CA-C	5.68	120.89	110.10
3	A	241	LEU	C-N-CD	-5.64	108.19	120.60
1	T	3	DA	C8-N9-C1'	5.63	137.84	127.70
3	A	299	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	A	192	ASP	CB-CA-C	-5.54	99.32	110.40
3	A	142	TYR	CB-CG-CD1	-5.52	117.69	121.00
3	A	86	GLU	N-CA-CB	5.51	120.52	110.60
3	A	291	PHE	N-CA-C	5.49	125.83	111.00
3	A	326	LYS	CD-CE-NZ	5.49	124.34	111.70
2	P	5	DT	C6-N1-C1'	-5.49	112.17	120.40
3	A	196	THR	N-CA-CB	5.46	120.68	110.30
3	A	74	ASP	CB-CG-OD1	5.44	123.20	118.30
3	A	86	GLU	CB-CA-C	5.42	121.25	110.40
2	P	1	DC	C2-N1-C1'	5.42	124.76	118.80
3	A	276	ASP	CB-CG-OD2	-5.38	113.46	118.30
3	A	16	THR	CA-CB-CG2	-5.33	104.93	112.40
3	A	116	ASP	CB-CG-OD1	5.30	123.07	118.30
1	T	7	DG	C4-N9-C1'	5.25	133.33	126.50
3	A	83	ARG	N-CA-CB	5.24	120.02	110.60
3	A	91	ASP	CB-CG-OD2	5.24	123.01	118.30
1	T	7	DG	O4'-C1'-N9	5.20	111.64	108.00
3	A	34	HIS	CA-CB-CG	-5.19	104.78	113.60
2	P	1	DC	C6-N1-C1'	-5.18	114.59	120.80
3	A	272	PHE	CB-CG-CD1	-5.16	117.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	39	TYR	CB-CG-CD1	-5.14	117.92	121.00
3	A	246	ASP	CB-CG-OD1	-5.10	113.71	118.30
3	A	266	TYR	CA-CB-CG	-5.09	103.73	113.40
3	A	304	THR	N-CA-CB	-5.07	100.66	110.30
3	A	49	TYR	C-N-CD	-5.05	109.49	120.60
2	P	2	DA	O4'-C4'-C3'	-5.05	102.48	104.50
3	A	20	THR	N-CA-CB	5.04	119.87	110.30
3	A	65	VAL	N-CA-CB	5.04	122.58	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	65	VAL	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	118	0	70	4	0
2	P	126	0	68	7	0
3	A	2623	0	2641	256	1
4	A	2	0	0	0	0
5	A	91	0	0	12	0
5	P	14	0	0	1	0
5	T	11	0	0	0	0
All	All	2985	0	2779	264	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 47.

All (264) 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)
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.25	1.10
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.29	1.07
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.54	1.04
3:A:12:ASN:HD21	3:A:53:ILE:H	1.03	0.99
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.61	0.97
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.48	0.93
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.04	0.93
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.51	0.93
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.51	0.92
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.52	0.92
2:P:1:DC:H2"	2:P:2:DA:H5"	1.56	0.88
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.93	0.87
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.05	0.86
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.06	0.85
3:A:11:LEU:HD23	3:A:11:LEU:H	1.41	0.85
3:A:155:MET:HA	3:A:158:MET:HE3	1.55	0.85
3:A:12:ASN:ND2	3:A:53:ILE:H	1.74	0.85
3:A:245:ASN:N	3:A:245:ASN:HD22	1.75	0.84
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.60	0.84
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.07	0.84
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.60	0.82
3:A:245:ASN:H	3:A:245:ASN:HD22	1.27	0.81
3:A:16:THR:O	3:A:20:THR:HG23	1.80	0.81
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.18	0.79
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.65	0.79
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.48	0.79
3:A:277:ILE:HD13	3:A:277:ILE:H	1.47	0.79
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.64	0.78
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.83	0.78
3:A:326:LYS:HE2	3:A:328:ARG:HE	1.48	0.78
3:A:166:VAL:O	3:A:169:VAL:HG12	1.84	0.78
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.01	0.76
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.66	0.76
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.67	0.75
3:A:133:ASN:ND2	3:A:136:GLN:H	1.85	0.75
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.52	0.74
3:A:85:LEU:O	3:A:89:ARG:HG3	1.88	0.74
2:P:1:DC:H2"	2:P:2:DA:C5'	2.17	0.73
3:A:12:ASN:HD21	3:A:53:ILE:N	1.84	0.73
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.23	0.73
3:A:212:HIS:HB3	5:A:541:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.04	0.72
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.25	0.72
3:A:133:ASN:H	3:A:136:GLN:HE21	1.38	0.71
3:A:278:PHE:HB2	3:A:333:ARG:O	1.91	0.71
3:A:306:VAL:HG23	3:A:307:ALA:N	2.06	0.70
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.27	0.70
3:A:133:ASN:H	3:A:136:GLN:NE2	1.90	0.69
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.75	0.68
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.23	0.68
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.76	0.68
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.23	0.68
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.76	0.67
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.24	0.67
3:A:270:LEU:HD21	3:A:282:MET:CE	2.24	0.67
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.09	0.67
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.66
3:A:262:LYS:HG3	3:A:262:LYS:O	1.94	0.66
3:A:27:LYS:HG3	3:A:28:ASN:N	2.10	0.66
3:A:31:GLN:N	5:A:641:HOH:O	2.29	0.66
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.30	0.65
3:A:314:ASP:N	3:A:318:ASP:OD2	2.27	0.65
3:A:59:ALA:O	3:A:62:LEU:HB2	1.96	0.65
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.78	0.65
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.25	0.65
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.76	0.65
3:A:79:THR:O	3:A:81:LYS:N	2.29	0.65
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.09	0.65
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.44	0.65
3:A:120:LYS:N	3:A:124:ASP:OD2	2.28	0.64
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.27	0.64
3:A:80:GLY:O	3:A:81:LYS:HG2	1.98	0.64
2:P:4:DA:H5"	5:P:614:HOH:O	1.98	0.64
3:A:237:GLY:O	3:A:254:ARG:NH1	2.30	0.64
3:A:298:ILE:HG22	5:A:578:HOH:O	1.96	0.64
1:T:4:DT:H2"	1:T:5:DC:O5'	1.98	0.64
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.13	0.64
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.12	0.64
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.27	0.63
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.80	0.63
3:A:282:MET:HG2	5:A:555:HOH:O	1.98	0.63
3:A:18:MET:HE3	3:A:76:PHE:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:200:PHE:HB2	5:A:625:HOH:O	1.99	0.62
3:A:191:MET:HG2	3:A:255:ILE:CG1	2.16	0.61
3:A:202:SER:HB2	3:A:263:ASP:CG	2.21	0.61
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.14	0.61
3:A:44:SER:HB2	5:A:608:HOH:O	1.99	0.61
3:A:288:GLU:HA	3:A:288:GLU:OE1	1.92	0.61
3:A:41:LYS:O	3:A:45:VAL:HG13	2.00	0.61
3:A:207:GLN:HB2	5:A:625:HOH:O	2.01	0.60
3:A:313:VAL:HG13	3:A:318:ASP:HB2	1.82	0.60
3:A:150:ILE:O	3:A:188:SER:N	2.34	0.60
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.83	0.60
3:A:163:LEU:HD23	3:A:163:LEU:N	2.17	0.60
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.34	0.59
3:A:60:LYS:CA	3:A:65:VAL:HG22	2.28	0.59
2:P:2:DA:C8	2:P:2:DA:H5'	2.38	0.59
3:A:38:ALA:O	3:A:41:LYS:HD2	2.02	0.58
3:A:60:LYS:HE2	3:A:67:THR:HA	1.84	0.58
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.67	0.58
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.86	0.58
3:A:137:ARG:HB3	5:A:622:HOH:O	2.03	0.58
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.34	0.57
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.35	0.57
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.20	0.57
3:A:201:THR:HG23	3:A:204:SER:HB3	1.86	0.56
3:A:68:LYS:O	3:A:72:LYS:HE3	2.05	0.56
3:A:333:ARG:HD2	5:A:584:HOH:O	2.04	0.56
3:A:315:SER:OG	3:A:316:GLU:N	2.38	0.56
3:A:133:ASN:HD21	3:A:136:GLN:H	1.53	0.56
3:A:202:SER:N	3:A:263:ASP:OD1	2.35	0.56
3:A:326:LYS:O	3:A:326:LYS:HG3	2.05	0.56
3:A:278:PHE:CZ	3:A:333:ARG:HD3	2.40	0.56
3:A:228:LEU:HB2	3:A:236:MET:O	2.06	0.56
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.88	0.55
3:A:18:MET:CE	3:A:76:PHE:HB2	2.30	0.55
3:A:11:LEU:CD2	3:A:11:LEU:H	2.15	0.55
3:A:196:THR:OG1	3:A:197:HIS:N	2.39	0.55
3:A:207:GLN:O	3:A:210:LEU:HB2	2.07	0.54
3:A:229:SER:HB3	5:A:513:HOH:O	2.07	0.54
3:A:200:PHE:O	3:A:262:LYS:N	2.31	0.54
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.89	0.54
3:A:211:LEU:HB2	3:A:259:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:LYS:HD3	3:A:42:ALA:N	2.24	0.53
3:A:150:ILE:N	3:A:188:SER:O	2.38	0.53
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.44	0.53
3:A:28:ASN:HD22	3:A:28:ASN:N	2.04	0.53
3:A:121:THR:O	3:A:124:ASP:HB2	2.08	0.53
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.22	0.53
3:A:294:ASN:ND2	3:A:297:THR:H	2.06	0.53
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.49	0.52
1:T:4:DT:OP1	3:A:231:GLY:HA3	2.09	0.52
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.91	0.52
3:A:202:SER:HB2	3:A:263:ASP:OD1	2.09	0.52
3:A:108:PRO:O	3:A:112:ARG:HG3	2.09	0.52
3:A:81:LYS:NZ	3:A:86:GLU:OE1	2.30	0.52
3:A:18:MET:HE3	3:A:76:PHE:CG	2.45	0.51
3:A:306:VAL:CG2	3:A:307:ALA:N	2.74	0.51
3:A:35:LYS:O	3:A:38:ALA:HB3	2.11	0.51
3:A:267:CYS:N	5:A:508:HOH:O	2.31	0.51
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.40	0.51
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.51
3:A:169:VAL:HG13	3:A:173:TYR:HE2	1.76	0.51
3:A:248:LYS:HG2	3:A:248:LYS:O	2.09	0.51
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.44	0.51
3:A:215:VAL:O	3:A:219:GLN:HG3	2.11	0.51
3:A:18:MET:HE1	3:A:76:PHE:CB	2.34	0.50
3:A:276:ASP:O	3:A:280:LYS:HG3	2.11	0.50
3:A:321:ASP:O	3:A:324:GLN:N	2.41	0.50
3:A:303:VAL:C	3:A:305:GLY:H	2.13	0.50
3:A:60:LYS:HE2	3:A:67:THR:CA	2.41	0.50
3:A:155:MET:HA	3:A:158:MET:CE	2.36	0.50
3:A:245:ASN:H	3:A:245:ASN:ND2	2.03	0.50
3:A:30:SER:HB2	3:A:32:ALA:H	1.76	0.50
3:A:169:VAL:HG13	3:A:173:TYR:CE2	2.46	0.49
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.12	0.49
3:A:133:ASN:HD22	3:A:135:HIS:N	2.10	0.49
3:A:245:ASN:N	3:A:245:ASN:ND2	2.48	0.49
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.48	0.49
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.26	0.48
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.13	0.48
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.81	0.48
3:A:250:TYR:HB3	3:A:251:PRO:CD	2.39	0.48
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:ALA:O	3:A:291:PHE:HB2	2.14	0.47
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.43	0.47
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.44	0.47
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.79	0.47
3:A:133:ASN:O	3:A:137:ARG:HG3	2.14	0.47
3:A:122:LEU:HD22	3:A:126:ARG:CZ	2.44	0.47
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.50	0.47
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.96	0.47
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.14	0.47
3:A:68:LYS:NZ	3:A:68:LYS:CB	2.78	0.47
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.58	0.47
3:A:149:ARG:NH2	3:A:188:SER:HA	2.30	0.46
3:A:75:GLU:O	3:A:79:THR:HG23	2.16	0.46
3:A:196:THR:HG22	3:A:265:TYR:CE1	2.50	0.46
3:A:217:GLN:HA	3:A:217:GLN:HE21	1.77	0.46
3:A:223:PHE:O	3:A:239:CYS:HA	2.16	0.46
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.15	0.46
3:A:331:LYS:HD2	3:A:332:ASP:N	2.30	0.46
3:A:326:LYS:HE2	3:A:328:ARG:NE	2.24	0.46
3:A:259:LEU:O	3:A:260:ILE:HD13	2.15	0.46
3:A:309:GLU:HA	3:A:309:GLU:OE1	2.16	0.46
3:A:154:GLU:O	3:A:158:MET:HG3	2.15	0.46
3:A:33:ILE:HA	3:A:36:TYR:HB3	1.97	0.46
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.63	0.45
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.31	0.45
3:A:145:ASP:HB3	3:A:252:HIS:O	2.16	0.45
3:A:150:ILE:HG21	3:A:158:MET:CE	2.43	0.45
3:A:212:HIS:CD2	3:A:212:HIS:H	2.34	0.45
3:A:26:GLU:HA	3:A:30:SER:OG	2.16	0.45
3:A:18:MET:CE	3:A:76:PHE:CD2	3.00	0.45
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.98	0.45
3:A:272:PHE:HA	3:A:272:PHE:HD1	1.51	0.45
3:A:152:ARG:NH2	3:A:181:PHE:O	2.50	0.45
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.29	0.45
3:A:184:GLY:O	3:A:185:ALA:O	2.36	0.44
3:A:327:TYR:HD1	3:A:328:ARG:N	2.14	0.44
3:A:41:LYS:CD	3:A:42:ALA:N	2.79	0.44
3:A:11:LEU:N	3:A:11:LEU:HD23	2.13	0.44
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.21	0.44
3:A:14:GLY:O	3:A:17:ASP:N	2.50	0.44
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.99	0.44
3:A:79:THR:C	3:A:81:LYS:H	2.21	0.44
3:A:312:PRO:O	3:A:322:TYR:OH	2.26	0.44
3:A:241:LEU:HB3	3:A:242:PRO:HD2	2.00	0.44
3:A:151:PRO:HD2	3:A:154:GLU:OE1	2.17	0.44
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.67	0.44
3:A:212:HIS:CD2	3:A:212:HIS:N	2.84	0.44
3:A:311:LEU:HA	3:A:311:LEU:HD12	1.64	0.44
3:A:11:LEU:N	3:A:11:LEU:CD2	2.80	0.43
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.81	0.43
3:A:88:ILE:HG21	3:A:88:ILE:HD13	1.76	0.43
3:A:200:PHE:C	3:A:201:THR:HG22	2.35	0.43
3:A:158:MET:O	3:A:162:VAL:HG23	2.18	0.43
3:A:172:GLU:CG	3:A:198:PRO:CG	2.97	0.43
3:A:196:THR:HB	3:A:265:TYR:CD1	2.54	0.43
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.40	0.43
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.84	0.43
3:A:106:ILE:HG21	3:A:106:ILE:HD13	1.82	0.43
3:A:12:ASN:HB3	3:A:46:ILE:HD11	2.00	0.43
3:A:195:LEU:O	3:A:260:ILE:N	2.51	0.43
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.53	0.43
3:A:133:ASN:HD22	3:A:133:ASN:C	2.22	0.43
3:A:183:ARG:NH1	3:A:275:SER:HA	2.34	0.43
3:A:227:THR:HG23	3:A:235:PHE:CE2	2.53	0.42
1:T:7:DG:N2	2:P:2:DA:C2	2.88	0.42
3:A:172:GLU:HG3	3:A:198:PRO:HG3	2.02	0.42
3:A:267:CYS:SG	3:A:297:THR:HA	2.58	0.42
3:A:179:GLY:O	3:A:182:ARG:HB3	2.19	0.42
3:A:254:ARG:NH1	3:A:255:ILE:H	2.16	0.42
3:A:218:LEU:HB3	3:A:224:ILE:HD12	2.01	0.42
3:A:264:GLN:HA	5:A:536:HOH:O	2.19	0.42
3:A:122:LEU:O	3:A:126:ARG:HG3	2.19	0.42
3:A:22:LEU:HA	3:A:22:LEU:HD13	1.77	0.42
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.80	0.42
3:A:254:ARG:NH1	3:A:255:ILE:N	2.68	0.42
3:A:255:ILE:HG12	3:A:256:ASP:N	2.35	0.42
1:T:4:DT:H5"	3:A:231:GLY:HA3	2.01	0.42
3:A:134:HIS:HE1	3:A:227:THR:O	2.02	0.41
3:A:12:ASN:CB	3:A:46:ILE:HD12	2.47	0.41
2:P:1:DC:H2"	2:P:2:DA:H5'	2.01	0.41
3:A:155:MET:SD	3:A:158:MET:CE	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:322:TYR:C	3:A:324:GLN:H	2.23	0.41
3:A:100:LEU:HD13	3:A:100:LEU:N	2.34	0.41
3:A:205:THR:O	3:A:206:LYS:O	2.38	0.41
3:A:50:PRO:HG2	3:A:51:HIS:CD2	2.56	0.41
3:A:278:PHE:CE2	3:A:333:ARG:CD	3.00	0.41
3:A:196:THR:CG2	3:A:265:TYR:CD1	3.04	0.41
3:A:40:ARG:HB2	3:A:40:ARG:HE	1.51	0.41
3:A:331:LYS:O	3:A:331:LYS:HG2	2.09	0.41
3:A:299:ARG:HB3	3:A:300:PRO:HD2	2.03	0.41
3:A:251:PRO:HG2	3:A:253:ARG:CZ	2.51	0.40
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.48	0.40
3:A:122:LEU:HD22	3:A:126:ARG:NH2	2.36	0.40
2:P:1:DC:C2'	2:P:2:DA:H5"	2.38	0.40
3:A:161:ILE:HD13	3:A:161:ILE:HG21	1.80	0.40
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.10	0.40
3:A:218:LEU:HD12	3:A:218:LEU:HA	1.89	0.40
3:A:264:GLN:HE21	3:A:264:GLN:HB3	1.38	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]	1.79	0.41

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%)	278 (86%)	29 (9%)	18 (6%)	2	2

All (18) Ramachandran outliers are listed below:

Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	244	LYS
3	A	307	ALA
3	A	10	THR
3	A	80	GLY
3	A	246	ASP
3	A	247	GLU
3	A	289	LYS
3	A	309	GLU
3	A	91	ASP
3	A	334	SER
3	A	310	PRO
3	A	207	GLN
3	A	265	TYR
3	A	312	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	225 (78%)	63 (22%)	1 2

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	19	LEU
3	A	20	THR
3	A	22	LEU
3	A	27	LYS
3	A	28	ASN
3	A	30	SER
3	A	37	ASN
3	A	40	ARG

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Mol	Chain	Res	Type
3	A	41	LYS
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	79	THR
3	A	93	THR
3	A	94	SER
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	113	LYS
3	A	122	LEU
3	A	133	ASN
3	A	152	ARG
3	A	168	LYS
3	A	171	SER
3	A	172	GLU
3	A	188	SER
3	A	191	MET
3	A	192	ASP
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	202	SER
3	A	204	SER
3	A	218	LEU
3	A	224	ILE
3	A	228	LEU
3	A	245	ASN
3	A	246	ASP
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	259	LEU
3	A	264	GLN
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	288	GLU

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Mol	Chain	Res	Type
3	A	289	LYS
3	A	292	THR
3	A	293	ILE
3	A	294	ASN
3	A	303	VAL
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	90	GLN
3	A	98	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	252	HIS
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 carbohydrates 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	6/6 (100%)	-1.42	0	100	100	25, 29, 48, 61	0
2	P	6/6 (100%)	-1.58	0	100	100	27, 30, 32, 34	0
3	A	324/335 (96%)	-1.01	0	100	100	9, 37, 81, 100	0
All	All	336/347 (96%)	-1.03	0	100	100	9, 36, 81, 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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	NA	A	342	1/1	0.97	0.09	-0.58	45,45,45,45	0
4	NA	A	341	1/1	0.99	0.04	-2.59	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.