



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:50 am BST

PDB ID : 9ICK
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

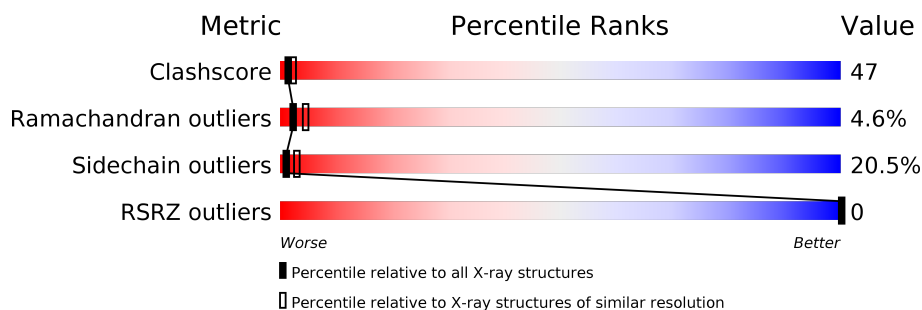
1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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 (three-letter code: NA) (formula: Na).

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

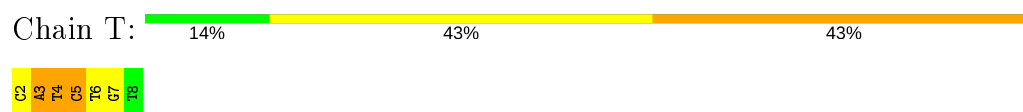
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	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 and DNA 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.

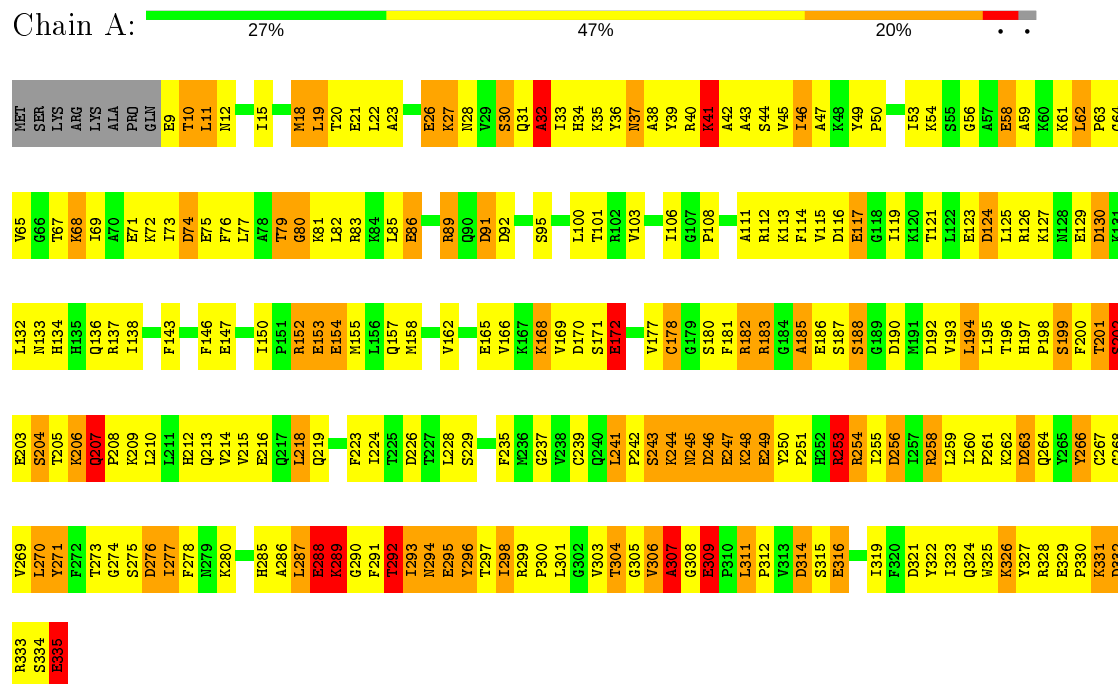
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.54 Å 57.73 Å 48.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 11.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.70) 90.7 (11.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	3.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.70 Å)	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)	0.16 , 104.9	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	2.22	5/135 (3.7%)	2.75	13/207 (6.3%)
2	P	2.57	9/141 (6.4%)	2.81	14/214 (6.5%)
3	A	1.29	27/2672 (1.0%)	1.63	56/3590 (1.6%)
All	All	1.43	41/2948 (1.4%)	1.79	83/4011 (2.1%)

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 (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DT	C1'-N1	11.40	1.64	1.49
2	P	5	DT	N1-C2	10.05	1.46	1.38
1	T	3	DA	N9-C4	8.45	1.43	1.37
3	A	129	GLU	CD-OE1	8.38	1.34	1.25
3	A	249	GLU	CD-OE2	8.07	1.34	1.25
3	A	203	GLU	CD-OE1	7.74	1.34	1.25
3	A	329	GLU	CD-OE2	7.64	1.34	1.25
3	A	154	GLU	CD-OE2	7.59	1.33	1.25
3	A	86	GLU	CD-OE1	7.31	1.33	1.25
3	A	71	GLU	CD-OE1	6.99	1.33	1.25
3	A	309	GLU	CD-OE2	6.97	1.33	1.25
2	P	6	DG	N7-C5	-6.89	1.35	1.39
3	A	75	GLU	CD-OE1	6.87	1.33	1.25
3	A	26	GLU	CD-OE1	6.85	1.33	1.25
2	P	4	DA	N9-C4	-6.63	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	186	GLU	CD-OE1	6.56	1.32	1.25
3	A	58	GLU	CD-OE1	6.56	1.32	1.25
3	A	288	GLU	CD-OE2	6.39	1.32	1.25
2	P	6	DG	C5-C6	-6.35	1.36	1.42
3	A	165	GLU	CD-OE2	6.17	1.32	1.25
3	A	295	GLU	CD-OE1	6.16	1.32	1.25
3	A	216	GLU	CD-OE1	6.15	1.32	1.25
3	A	117	GLU	CD-OE2	6.14	1.32	1.25
3	A	21	GLU	CD-OE1	6.09	1.32	1.25
2	P	3	DG	C5-C6	-6.04	1.36	1.42
3	A	123	GLU	CD-OE1	6.02	1.32	1.25
1	T	7	DG	C1'-N9	-5.98	1.38	1.47
3	A	172	GLU	CD-OE2	5.96	1.32	1.25
3	A	335	GLU	CD-OE2	5.88	1.32	1.25
3	A	326	LYS	CE-NZ	-5.54	1.35	1.49
3	A	316	GLU	CD-OE1	5.47	1.31	1.25
1	T	5	DC	N3-C4	5.40	1.37	1.33
3	A	9	GLU	CD-OE2	5.35	1.31	1.25
2	P	3	DG	C6-N1	-5.34	1.35	1.39
2	P	5	DT	C3'-O3'	-5.26	1.37	1.44
3	A	153	GLU	CD-OE2	5.20	1.31	1.25
3	A	247	GLU	CD-OE1	5.15	1.31	1.25
1	T	5	DC	C2-N3	5.14	1.39	1.35
3	A	147	GLU	CD-OE2	5.10	1.31	1.25
1	T	5	DC	C3'-O3'	-5.06	1.37	1.44
2	P	6	DG	N9-C4	-5.04	1.33	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	5	DC	C2-N1-C1'	13.48	133.63	118.80
2	P	5	DT	C6-N1-C1'	-13.11	100.73	120.40
1	T	5	DC	C6-N1-C1'	-12.65	105.62	120.80
2	P	5	DT	C2-N1-C1'	12.55	138.28	118.20
2	P	2	DA	O4'-C4'-C3'	-11.71	98.97	106.00
1	T	4	DT	C6-N1-C1'	-11.03	103.86	120.40
1	T	4	DT	C2-N1-C1'	10.25	134.60	118.20
1	T	2	DC	C2-N1-C1'	9.98	129.78	118.80
1	T	2	DC	C6-N1-C1'	-8.97	110.04	120.80
3	A	253	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	P	4	DA	P-O3'-C3'	8.78	130.24	119.70
3	A	192	ASP	CB-CG-OD2	-8.63	110.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	N3-C2-O2	-8.36	117.28	122.30
2	P	1	DC	C2-N1-C1'	7.96	127.55	118.80
2	P	2	DA	C4'-C3'-C2'	-7.88	96.01	103.10
3	A	256	ASP	CB-CG-OD1	7.83	125.35	118.30
3	A	314	ASP	CB-CG-OD1	-7.81	111.27	118.30
3	A	126	ARG	NE-CZ-NH2	-7.75	116.42	120.30
3	A	126	ARG	NE-CZ-NH1	7.73	124.17	120.30
3	A	92	ASP	CB-CG-OD2	-7.70	111.37	118.30
3	A	190	ASP	CB-CG-OD2	-7.55	111.50	118.30
2	P	1	DC	C6-N1-C1'	-7.39	111.94	120.80
3	A	190	ASP	CB-CG-OD1	7.20	124.78	118.30
3	A	124	ASP	CB-CG-OD2	-7.09	111.92	118.30
3	A	307	ALA	N-CA-CB	7.03	119.94	110.10
3	A	307	ALA	CB-CA-C	6.98	120.58	110.10
3	A	170	ASP	CB-CG-OD1	6.78	124.40	118.30
3	A	254	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	A	152	ARG	N-CA-CB	6.54	122.36	110.60
1	T	3	DA	C2-N3-C4	6.50	113.85	110.60
3	A	91	ASP	CB-CG-OD1	-6.50	112.45	118.30
3	A	34	HIS	CA-CB-CG	-6.45	102.64	113.60
3	A	226	ASP	CB-CG-OD1	6.43	124.09	118.30
3	A	256	ASP	CB-CG-OD2	-6.29	112.64	118.30
3	A	130	ASP	CB-CG-OD2	-6.12	112.80	118.30
3	A	74	ASP	CB-CG-OD2	-6.11	112.81	118.30
3	A	168	LYS	N-CA-CB	6.02	121.44	110.60
3	A	271	TYR	CB-CG-CD1	-6.02	117.39	121.00
3	A	74	ASP	CB-CG-OD1	5.93	123.64	118.30
3	A	335	GLU	N-CA-CB	5.91	121.23	110.60
3	A	292	THR	N-CA-CB	5.89	121.49	110.30
2	P	4	DA	O4'-C1'-N9	-5.88	103.88	108.00
2	P	6	DG	C4-N9-C1'	-5.88	118.86	126.50
3	A	170	ASP	CB-CG-OD2	-5.87	113.02	118.30
3	A	32	ALA	N-CA-C	5.81	126.68	111.00
1	T	4	DT	P-O3'-C3'	5.78	126.63	119.70
1	T	6	DT	C6-N1-C2	5.76	124.18	121.30
3	A	253	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	A	250	TYR	CB-CG-CD1	-5.71	117.57	121.00
3	A	116	ASP	CB-CG-OD2	-5.71	113.16	118.30
3	A	241	LEU	C-N-CD	-5.68	108.11	120.60
3	A	332	ASP	CB-CG-OD1	-5.65	113.21	118.30
3	A	246	ASP	CB-CG-OD1	-5.58	113.28	118.30
3	A	334	SER	CB-CA-C	5.57	120.69	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	130	ASP	CB-CG-OD1	5.55	123.29	118.30
2	P	6	DG	N1-C6-O6	5.50	123.20	119.90
2	P	6	DG	C8-N9-C1'	5.48	134.12	127.00
2	P	5	DT	C5-C6-N1	-5.48	120.41	123.70
3	A	271	TYR	CA-CB-CG	-5.48	102.99	113.40
3	A	304	THR	N-CA-CB	-5.45	99.94	110.30
3	A	266	TYR	CA-CB-CG	-5.44	103.06	113.40
3	A	263	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	T	5	DC	P-O3'-C3'	5.38	126.16	119.70
3	A	263	ASP	CB-CG-OD1	5.36	123.12	118.30
3	A	89	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	A	92	ASP	N-CA-CB	5.32	120.17	110.60
3	A	183	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	A	332	ASP	CB-CG-OD2	5.26	123.04	118.30
3	A	253	ARG	CD-NE-CZ	5.18	130.85	123.60
2	P	6	DG	C6-C5-N7	-5.18	127.29	130.40
1	T	5	DC	N3-C4-C5	-5.14	119.85	121.90
3	A	226	ASP	CB-CG-OD2	-5.13	113.69	118.30
3	A	41	LYS	N-CA-CB	5.12	119.81	110.60
3	A	178	CYS	CA-CB-SG	-5.10	104.82	114.00
1	T	4	DT	N3-C2-O2	-5.09	119.24	122.30
1	T	6	DT	C6-N1-C1'	-5.09	112.76	120.40
3	A	124	ASP	CB-CG-OD1	5.07	122.87	118.30
3	A	20	THR	N-CA-CB	5.07	119.94	110.30
3	A	246	ASP	CB-CG-OD2	5.07	122.86	118.30
3	A	314	ASP	CB-CG-OD2	5.07	122.86	118.30
3	A	178	CYS	CB-CA-C	5.06	120.52	110.40
3	A	30	SER	C-N-CA	-5.05	109.07	121.70
3	A	326	LYS	CD-CE-NZ	5.04	123.30	111.70

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	247	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	262	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 (262) 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:31:GLN:HE21	3:A:112:ARG:HH12	0.97	0.95
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:18:MET:HE1	3:A:76:PHE:HB2	1.62	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:245:ASN:N	3:A:245:ASN:HD22	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:255:ILE:HG12	3:A:256:ASP:N	2.07	0.69
3:A:41:LYS:O	3:A:45:VAL:HG13	1.92	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:178:CYS:SG	3:A:194:LEU:HD23	2.35	0.67
3:A:18:MET:CE	3:A:76:PHE:HB2	2.24	0.67
3:A:215:VAL:O	3:A:219:GLN:HG3	1.95	0.66
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.77	0.66
3:A:31:GLN:N	5:A:641:HOH:O	2.27	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

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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:150:ILE:HG21	3:A:158:MET:HE1	1.79	0.64
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.80	0.64
3:A:326:LYS:O	3:A:326:LYS:HG3	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:295:GLU:H	3:A:295:GLU:CD	2.03	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
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.00	0.61
2:P:5:DT:C2'	2:P:6:DG:H5'	2.19	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
3:A:248:LYS:HG2	3:A:248:LYS:O	2.01	0.59
2:P:5:DT:H1'	5:P:565:HOH:O	2.02	0.59
3:A:23:ALA:O	3:A:36:TYR:HD1	1.86	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:244:LYS:CB	3:A:245:ASN:HD22	2.16	0.58
3:A:28:ASN:HD22	3:A:28:ASN:N	2.02	0.57
3:A:11:LEU:CD2	3:A:11:LEU:H	2.15	0.57
2:P:2:DA:H8	2:P:2:DA:H5'	1.66	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:162:VAL:O	3:A:166:VAL:HG23	2.06	0.56
3:A:202:SER:HB2	3:A:263:ASP:CG	2.26	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:155:MET:HE2	3:A:188:SER:HB2	1.87	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:157:GLN:HE22	3:A:244:LYS:HZ3	1.54	0.55
3:A:150:ILE:HG21	3:A:158:MET:HE3	1.87	0.55
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:268:GLY:O	3:A:271:TYR:HB3	2.06	0.55
3:A:196:THR:OG1	3:A:197:HIS:N	2.40	0.55
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.88	0.55
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.42	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:HA	3:A:288:GLU:OE1	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: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:182:ARG:HG2	3:A:273:THR:HG23	1.90	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:18:MET:HE3	3:A:76:PHE:CD2	2.45	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:HD22	3:A:294:ASN:N	2.07	0.52
3:A:202:SER:HB2	3:A:263:ASP:OD1	2.10	0.52
3:A:303:VAL:C	3:A:305:GLY:H	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.93	0.50
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:79:THR:C	3:A:81:LYS:H	2.15	0.49
3:A:199:SER:OG	3:A:199:SER:O	2.29	0.49
3:A:18:MET:HE1	3:A:76:PHE:CB	2.40	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: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:HA	3:A:287:LEU:HD13	1.49	0.48
3:A:200:PHE:O	3:A:262:LYS:N	2.42	0.48
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.13	0.47
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: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:103:VAL:HG22	3:A:143:PHE:HD2	1.80	0.47
3:A:44:SER:O	3:A:47:ALA:HB3	2.15	0.47
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.97	0.47
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.36	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:150:ILE:CG2	3:A:158:MET:HE1	2.44	0.46
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.97	0.46
3:A:288:GLU:C	3:A:290:GLY:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.97	0.46
3:A:58:GLU:O	3:A:61:LYS:HB2	2.15	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
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.51	0.45
3:A:49:TYR:CE2	3:A:53:ILE:HG12	2.51	0.45
3:A:267:CYS:SG	3:A:297:THR:HA	2.55	0.45
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.63	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:206:LYS:O	3:A:207:GLN:HB2	2.18	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:285:HIS:NE2	3:A:289:LYS:CG	2.81	0.44
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.30	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:63:PRO:C	3:A:65:VAL:H	2.21	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:43:ALA:O	3:A:47:ALA:HB2	2.19	0.43
3:A:306:VAL:CG2	3:A:307:ALA:N	2.77	0.43
3:A:172:GLU:CG	3:A:198:PRO:CG	2.96	0.43
3:A:254:ARG:NH1	3:A:255:ILE:H	2.16	0.43
2:P:4:DA:H5''	5:P:614:HOH:O	2.17	0.43
3:A:10:THR:O	3:A:10:THR:HG23	2.19	0.43
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:59:ALA:O	3:A:62:LEU:N	2.31	0.42
2:P:2:DA:H2''	2:P:3:DG:OP2	2.19	0.42
3:A:26:GLU:HG3	3:A:35:LYS:HB3	2.01	0.42
3:A:11:LEU:N	3:A:11:LEU:CD2	2.79	0.42
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.55	0.42
3:A:294:ASN:ND2	3:A:294:ASN:N	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
3:A:138:ILE:HG23	3:A:138:ILE:HD13	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:204:SER:O	3:A:204:SER:OG	2.33	0.42
1:T:5:DC:H5'	3:A:229:SER:HB2	2.00	0.42
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:HA	3:A:311:LEU:HD12	1.82	0.42
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.66	0.42
3:A:177:VAL:HG22	3:A:193:VAL:HG22	2.02	0.42
3:A:146:PHE:HA	3:A:146:PHE:HD1	1.61	0.41
3:A:194:LEU:HA	3:A:194:LEU:HD12	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:311:LEU:HA	3:A:312:PRO:HD3	1.91	0.41
3:A:195:LEU:O	3:A:260:ILE:N	2.52	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:150:ILE:CG2	3:A:158:MET:CE	2.95	0.41
3:A:76:PHE:O	3:A:79:THR:O	2.38	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:264:GLN:HE21	3:A:264:GLN:HB3	1.44	0.40
2:P:5:DT:H2''	2:P:6:DG:C5'	2.23	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
3:A:259:LEU:HA	3:A:259:LEU:HD12	1.70	0.40
1:T:3:DA:H1'	5:T:617:HOH:O	2.21	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

5.3.1 Protein backbone

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

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%)	229 (80%)	59 (20%)	1 3

All (59) 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	40	ARG
3	A	41	LYS
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
3	A	79	THR
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	130	ASP
3	A	153	GLU
3	A	168	LYS
3	A	171	SER
3	A	172	GLU
3	A	182	ARG
3	A	188	SER
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	202	SER
3	A	204	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	258	ARG
3	A	270	LEU

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Mol	Chain	Res	Type
3	A	276	ASP
3	A	277	ILE
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	296	TYR
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	331	LYS
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	90	GLN
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	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 [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	7/7 (100%)	-1.13	0 100 100	23, 32, 63, 100	0
2	P	6/6 (100%)	-1.49	0 100 100	22, 30, 32, 38	0
3	A	324/335 (96%)	-1.07	0 100 100	12, 38, 84, 100	0
All	All	337/348 (96%)	-1.08	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 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. 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	0.97	0.08	34,34,34,34	0
4	NA	A	342	1/1	0.98	0.11	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.