



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:52 PM UTC

PDB ID : 1BPX / pdb_00001bpx
Title : DNA POLYMERASE BETA/DNA COMPLEX
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Deposited on : 1997-04-11
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

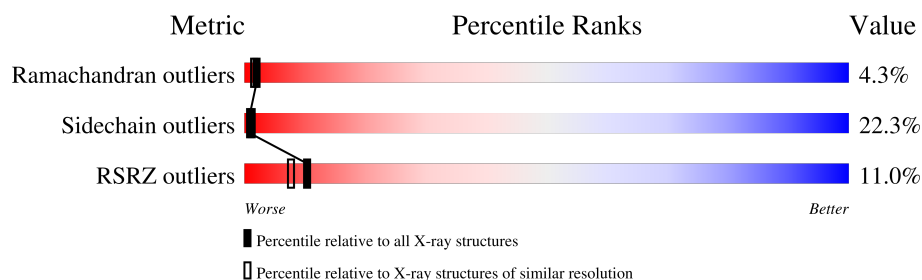
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

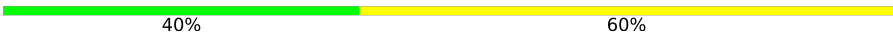
The reported resolution of this entry is 2.40 Å.

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))
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	T	16	
2	P	10	
3	D	5	
4	A	335	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3368 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*CP*GP*AP*CP*GP*GP*CP*GP*CP*AP*TP*CP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	16	Total	C	N	O	P	0	0	0
			323	153	63	92	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 4 is a protein called PROTEIN (DNA POLYMERASE BETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	331	Total	C	N	O	S	0	0	0
			2653	1676	464	504	9			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	21	Total 21	O 21	0	0
6	P	14	Total 14	O 14	0	0
6	D	6	Total 6	O 6	0	0
6	A	40	Total 40	O 40	0	0

3 Residue-property plots [i](#)

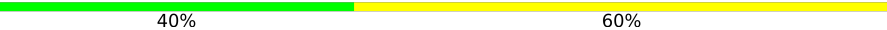
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

Chain T: 

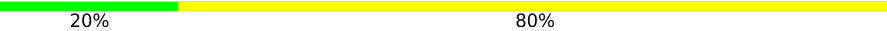


- Molecule 2: DNA (5'-D(*GP*CP*TP*GP*AP*TP*GP*CP*GP*C)-3')

Chain P: 



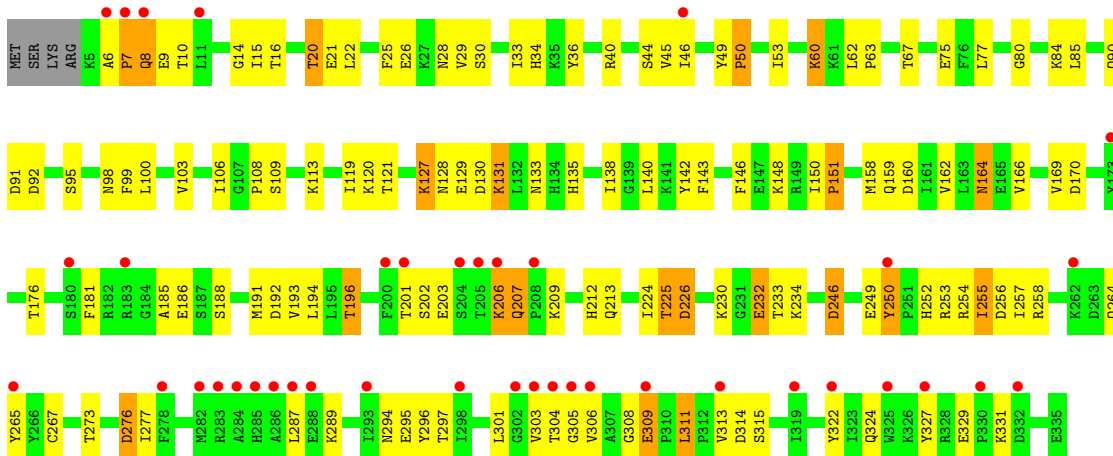
- Molecule 3: DNA (5'-D(*GP*TP*CP*GP*G)-3')

Chain D: 



- Molecule 4: PROTEIN (DNA POLYMERASE BETA)

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.77Å 79.39Å 54.62Å 90.00° 106.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.40) 96.7 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.39Å)	Xtriage
Refinement program	TNT 5D	Depositor
R, R_{free}	0.253 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 132.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3368	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	1.14	0/362	1.81	8/556 (1.4%)
2	P	1.13	0/227	1.98	9/349 (2.6%)
3	D	1.37	0/118	1.99	5/179 (2.8%)
4	A	1.56	14/2703 (0.5%)	2.10	100/3632 (2.8%)
All	All	1.49	14/3410 (0.4%)	2.06	122/4716 (2.6%)

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
4	A	1	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8	GLN	C-N	8.45	1.45	1.33
4	A	256	ASP	CA-C	-8.23	1.42	1.52
4	A	257	ILE	CA-C	-7.09	1.43	1.52
4	A	120	LYS	CA-C	-6.75	1.45	1.53
4	A	29	VAL	CA-CB	-6.54	1.45	1.54
4	A	257	ILE	N-CA	-6.10	1.39	1.46
4	A	62	LEU	N-CA	-6.00	1.37	1.45
4	A	84	LYS	CA-C	-5.60	1.45	1.52
4	A	121	THR	CA-C	-5.55	1.45	1.52
4	A	63	PRO	N-CA	-5.20	1.40	1.47
4	A	26	GLU	CD-OE2	5.10	1.35	1.25
4	A	255	ILE	N-CA	-5.04	1.40	1.46
4	A	131	LYS	N-CA	-5.02	1.40	1.46
4	A	151	PRO	N-CA	-5.01	1.41	1.47

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	150	ILE	C-N-CD	-11.42	78.20	125.00
4	A	8	GLN	N-CA-C	11.31	134.89	110.80
2	P	10	DC	P-O5'-C5'	-10.17	104.75	120.00
4	A	226	ASP	N-CA-C	9.39	121.83	110.19
2	P	6	DT	N1-C1'-C2'	9.13	127.20	113.50
4	A	34	HIS	CA-CB-CG	-8.81	104.99	113.80
3	D	2	DT	N1-C1'-C2'	8.54	126.31	113.50
4	A	30	SER	N-CA-C	8.34	121.57	111.40
4	A	246	ASP	CA-CB-CG	8.24	120.84	112.60
4	A	233	THR	CA-C-N	-8.20	110.65	122.94
4	A	233	THR	C-N-CA	-8.20	110.65	122.94
4	A	181	PHE	CA-CB-CG	-8.01	105.79	113.80
4	A	206	LYS	N-CA-C	8.00	121.52	110.24
4	A	60	LYS	N-CA-CB	8.00	122.05	110.06
4	A	212	HIS	CA-CB-CG	-7.87	105.93	113.80
4	A	314	ASP	N-CA-CB	7.81	121.96	110.56
4	A	7	PRO	CA-C-N	7.76	136.36	121.54
4	A	7	PRO	C-N-CA	7.76	136.36	121.54
4	A	91	ASP	CA-CB-CG	-7.52	105.08	112.60
4	A	267	CYS	N-CA-C	-7.48	103.07	111.07
4	A	6	ALA	CA-C-N	7.39	129.08	119.84
4	A	6	ALA	C-N-CA	7.39	129.08	119.84
1	T	13	DC	N1-C1'-C2'	7.32	124.48	113.50
4	A	108	PRO	N-CA-CB	7.28	110.89	103.25
4	A	185	ALA	N-CA-C	7.20	120.75	109.96
1	T	14	DA	N9-C1'-C2'	7.18	124.28	113.50
4	A	160	ASP	N-CA-C	7.12	119.04	111.28
4	A	193	VAL	N-CA-C	7.04	118.00	107.51
4	A	49	TYR	CA-C-N	6.99	128.57	119.84
4	A	49	TYR	C-N-CA	6.99	128.57	119.84
4	A	257	ILE	O-C-N	6.95	130.76	123.05
4	A	84	LYS	N-CA-C	-6.92	103.67	111.07
4	A	36	TYR	N-CA-C	-6.92	103.67	111.14
4	A	297	THR	N-CA-C	6.89	117.36	108.34
4	A	67	THR	N-CA-C	6.87	119.40	111.02
4	A	14	GLY	CA-C-N	6.82	129.20	120.88
4	A	14	GLY	C-N-CA	6.82	129.20	120.88
4	A	50	PRO	N-CA-CB	6.82	110.41	103.25
4	A	44	SER	N-CA-C	6.82	118.40	110.97
4	A	143	PHE	CA-CB-CG	6.80	120.60	113.80
4	A	49	TYR	N-CA-C	6.77	123.20	109.60
2	P	5	DA	N9-C1'-C2'	6.74	123.61	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	253	ARG	N-CA-C	6.71	118.95	108.96
4	A	164	ASN	N-CA-C	6.69	118.36	111.14
4	A	50	PRO	CA-C-N	-6.62	111.48	122.21
4	A	50	PRO	C-N-CA	-6.62	111.48	122.21
4	A	130	ASP	N-CA-C	-6.60	105.23	113.28
4	A	113	LYS	N-CA-C	-6.57	103.81	110.97
4	A	135	HIS	CA-CB-CG	-6.45	107.35	113.80
2	P	7	DG	N9-C1'-C2'	6.40	123.10	113.50
4	A	207	GLN	N-CA-CB	6.39	120.41	110.12
4	A	196	THR	CA-CB-OG1	6.38	119.18	109.60
4	A	313	VAL	N-CA-C	6.32	116.93	107.51
4	A	119	ILE	N-CA-C	6.32	117.90	109.37
4	A	252	HIS	CA-C-N	-6.31	111.53	121.87
4	A	252	HIS	C-N-CA	-6.31	111.53	121.87
4	A	164	ASN	N-CA-CB	6.29	119.19	110.07
4	A	28	ASN	CA-CB-CG	-6.29	106.31	112.60
4	A	170	ASP	CA-C-O	-6.22	114.55	121.51
4	A	103	VAL	N-CA-C	6.20	116.43	108.12
4	A	15	ILE	CB-CA-C	-6.20	103.76	111.94
4	A	138	ILE	N-CA-CB	6.17	117.36	110.51
3	D	1	DG	O3'-P-O5'	-6.17	94.75	104.00
4	A	314	ASP	CB-CA-C	6.13	120.93	110.56
4	A	67	THR	CB-CA-C	6.13	120.67	110.92
1	T	2	DC	P-O3'-C3'	6.12	129.37	120.20
2	P	7	DG	O4'-C1'-N9	-6.10	99.25	108.40
3	D	5	DG	C4-N9-C1'	-6.06	117.91	127.00
2	P	7	DG	C4'-C3'-O3'	-6.06	100.91	110.00
4	A	20	THR	CB-CA-C	6.04	120.82	110.79
4	A	196	THR	N-CA-CB	6.03	120.75	111.46
1	T	3	DG	P-O5'-C5'	-6.01	110.99	120.00
4	A	28	ASN	N-CA-C	5.95	117.45	110.97
1	T	9	DG	C4'-C3'-O3'	-5.93	101.11	110.00
4	A	170	ASP	N-CA-C	-5.91	100.34	109.14
4	A	30	SER	N-CA-CB	5.87	118.82	110.13
4	A	250	TYR	C-N-CD	-5.79	101.28	125.00
4	A	311	LEU	CA-C-N	5.73	127.01	119.84
4	A	311	LEU	C-N-CA	5.73	127.01	119.84
4	A	309	GLU	CA-C-N	5.70	125.63	119.76
4	A	309	GLU	C-N-CA	5.70	125.63	119.76
4	A	146	PHE	CA-CB-CG	-5.68	108.11	113.80
2	P	2	DC	N1-C1'-C2'	-5.67	105.00	113.50
4	A	62	LEU	CA-C-O	5.66	126.87	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	166	VAL	O-C-N	5.66	127.36	121.87
4	A	329	GLU	N-CA-C	-5.64	102.96	110.07
4	A	75	GLU	N-CA-C	-5.63	105.05	111.07
4	A	196	THR	CA-CB-CG2	5.63	120.06	110.50
4	A	9	GLU	N-CA-CB	5.60	119.95	110.49
4	A	63	PRO	CB-CA-C	-5.55	102.39	111.56
4	A	276	ASP	N-CA-CB	5.54	118.34	110.13
4	A	151	PRO	CB-CA-C	5.53	120.69	111.56
4	A	99	PHE	CA-CB-CG	-5.53	108.27	113.80
4	A	142	TYR	N-CA-C	5.48	119.67	113.15
4	A	60	LYS	O-C-N	5.47	127.92	122.12
4	A	140	LEU	N-CA-C	-5.45	105.23	111.07
4	A	253	ARG	CD-NE-CZ	-5.42	116.81	124.40
3	D	4	DG	C4-N9-C1'	-5.41	118.88	127.00
4	A	127	LYS	N-CA-CB	5.41	118.79	110.46
4	A	80	GLY	N-CA-C	-5.40	107.82	115.43
3	D	4	DG	O5'-C5'-C4'	-5.39	102.71	110.80
4	A	49	TYR	O-C-N	5.38	126.05	121.20
1	T	8	DC	C5'-C4'-C3'	-5.30	106.95	114.90
4	A	224	ILE	CA-C-N	-5.29	111.43	121.54
4	A	224	ILE	C-N-CA	-5.29	111.43	121.54
4	A	14	GLY	O-C-N	5.29	127.30	122.17
4	A	148	LYS	CA-C-N	-5.27	113.38	120.87
4	A	148	LYS	C-N-CA	-5.27	113.38	120.87
1	T	12	DT	N1-C1'-C2'	5.27	121.41	113.50
4	A	192	ASP	N-CA-CB	5.26	119.04	110.37
4	A	202	SER	N-CA-C	5.24	121.97	110.80
4	A	50	PRO	N-CA-C	5.18	123.14	112.47
4	A	296	TYR	N-CA-C	5.17	119.47	111.56
4	A	8	GLN	CA-C-N	-5.17	111.67	121.54
4	A	8	GLN	C-N-CA	-5.17	111.67	121.54
4	A	106	ILE	O-C-N	5.15	129.76	122.97
4	A	193	VAL	CB-CA-C	5.13	118.50	111.31
4	A	303	VAL	N-CA-C	-5.11	106.27	112.76
4	A	322	TYR	N-CA-C	5.11	117.24	111.11
1	T	14	DA	O4'-C1'-N9	-5.06	100.81	108.40
2	P	9	DG	O3'-P-O5'	-5.02	96.48	104.00
2	P	2	DC	C4'-C3'-O3'	5.01	117.51	110.00

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
4	A	314	ASP	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
4	A	329/335 (98%)	268 (82%)	47 (14%)	14 (4%)	2 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	7	PRO
4	A	8	GLN
4	A	129	GLU
4	A	250	TYR
4	A	92	ASP
4	A	232	GLU
4	A	308	GLY
4	A	50	PRO
4	A	265	TYR
4	A	305	GLY
4	A	225	THR
4	A	309	GLU
4	A	306	VAL
4	A	53	ILE

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
4	A	291/295 (99%)	226 (78%)	65 (22%)	1 1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	THR
4	A	16	THR
4	A	20	THR
4	A	21	GLU
4	A	22	LEU
4	A	25	PHE
4	A	33	ILE
4	A	40	ARG
4	A	45	VAL
4	A	46	ILE
4	A	60	LYS
4	A	77	LEU
4	A	85	LEU
4	A	90	GLN
4	A	95	SER
4	A	98	ASN
4	A	100	LEU
4	A	109	SER
4	A	127	LYS
4	A	128	ASN
4	A	131	LYS
4	A	133	ASN
4	A	151	PRO
4	A	158	MET
4	A	159	GLN
4	A	162	VAL
4	A	164	ASN
4	A	169	VAL
4	A	176	THR
4	A	186	GLU

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Mol	Chain	Res	Type
4	A	188	SER
4	A	191	MET
4	A	194	LEU
4	A	196	THR
4	A	201	THR
4	A	203	GLU
4	A	206	LYS
4	A	207	GLN
4	A	209	LYS
4	A	213	GLN
4	A	225	THR
4	A	226	ASP
4	A	230	LYS
4	A	232	GLU
4	A	234	LYS
4	A	246	ASP
4	A	249	GLU
4	A	254	ARG
4	A	255	ILE
4	A	258	ARG
4	A	264	GLN
4	A	273	THR
4	A	276	ASP
4	A	277	ILE
4	A	287	LEU
4	A	289	LYS
4	A	294	ASN
4	A	295	GLU
4	A	301	LEU
4	A	304	THR
4	A	311	LEU
4	A	315	SER
4	A	324	GLN
4	A	327	TYR
4	A	331	LYS

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

Mol	Chain	Res	Type
4	A	8	GLN
4	A	12	ASN
4	A	28	ASN

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Mol	Chain	Res	Type
4	A	90	GLN
4	A	98	ASN
4	A	133	ASN
4	A	135	HIS
4	A	136	GLN
4	A	159	GLN
4	A	164	ASN
4	A	212	HIS
4	A	213	GLN
4	A	217	GLN
4	A	245	ASN
4	A	281	ASN
4	A	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	16/16 (100%)	0.00	0 100 100	42, 56, 69, 71	0
2	P	10/10 (100%)	0.02	0 100 100	45, 54, 72, 73	0
3	D	5/5 (100%)	-0.66	0 100 100	32, 40, 48, 49	0
4	A	331/335 (98%)	0.84	40 (12%) 8 6	12, 53, 99, 100	75 (22%)
All	All	362/366 (98%)	0.76	40 (11%) 10 8	12, 53, 99, 100	75 (20%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	293	ILE	5.7
4	A	8	GLN	4.0
4	A	303	VAL	3.7
4	A	11	LEU	3.5
4	A	322	TYR	3.5
4	A	6	ALA	3.3
4	A	183	ARG	3.3
4	A	208	PRO	3.3
4	A	330	PRO	3.2
4	A	306	VAL	3.2
4	A	313	VAL	3.1
4	A	319	ILE	3.1
4	A	265	TYR	3.1
4	A	332	ASP	3.0
4	A	250	TYR	2.9
4	A	327	TYR	2.9
4	A	284	ALA	2.8
4	A	180	SER	2.8
4	A	298	ILE	2.8
4	A	205	THR	2.8
4	A	304	THR	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	305	GLY	2.7
4	A	204	SER	2.7
4	A	7	PRO	2.5
4	A	325	TRP	2.5
4	A	285	HIS	2.5
4	A	46	ILE	2.4
4	A	302	GLY	2.4
4	A	278	PHE	2.4
4	A	287	LEU	2.3
4	A	200	PHE	2.3
4	A	206	LYS	2.3
4	A	173	TYR	2.3
4	A	286	ALA	2.2
4	A	309	GLU	2.1
4	A	262	LYS	2.1
4	A	288	GLU	2.1
4	A	283	ARG	2.1
4	A	201	THR	2.1
4	A	282	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	D	342	1/1	0.93	0.08	54,54,54,54	0
5	NA	A	341	1/1	0.96	0.05	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.